



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 10:20 pm GMT

PDB ID : 8BEL  
EMDB ID : EMD-16007  
Title : Cryo-EM structure of the Arabidopsis thaliana I+III<sub>2</sub> supercomplex (CIII membrane domain)  
Authors : Klusch, N.; Kuehlbrandt, W.  
Deposited on : 2022-10-21  
Resolution : 2.25 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](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 : 1.8.4, CSD as541be (2020)  
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

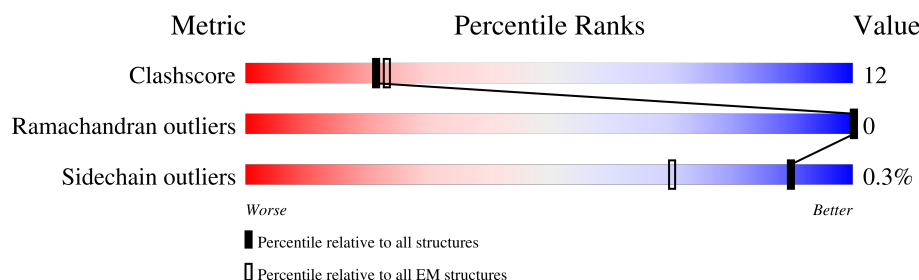
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.25 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	C	393	
1	M	393	
2	D	272	
2	N	272	
3	E	307	
3	O	307	
4	G	72	
4	Q	72	

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Mol	Chain	Length	Quality of chain
5	H	69	
5	R	69	
6	I	72	
6	S	72	
7	J	57	
7	T	57	

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 18929 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		
1	M	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	40	SER	PRO	variant	UNP P42792
M	40	SER	PRO	variant	UNP P42792

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	179	Total	C	N	O	S	0	0
			1404	899	244	256	5		
2	N	179	Total	C	N	O	S	0	0
			1404	899	244	256	5		

- Molecule 3 is a protein called Cytochrome c1 2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		
3	O	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 8-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	69	Total	C	N	O	S	0	0
			581	387	95	98	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	68	Total	C	N	O	S	0	0
			572	382	93	96	1		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	64	Total	C	N	O	S	0	0
			518	334	87	91	6		
5	R	63	Total	C	N	O	S	0	0
			511	329	86	90	6		

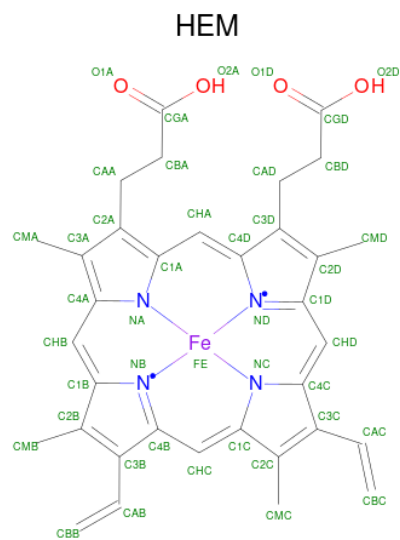
- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	57	Total	C	N	O	S	0	0
			476	310	85	80	1		
6	S	57	Total	C	N	O	S	0	0
			476	310	85	80	1		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

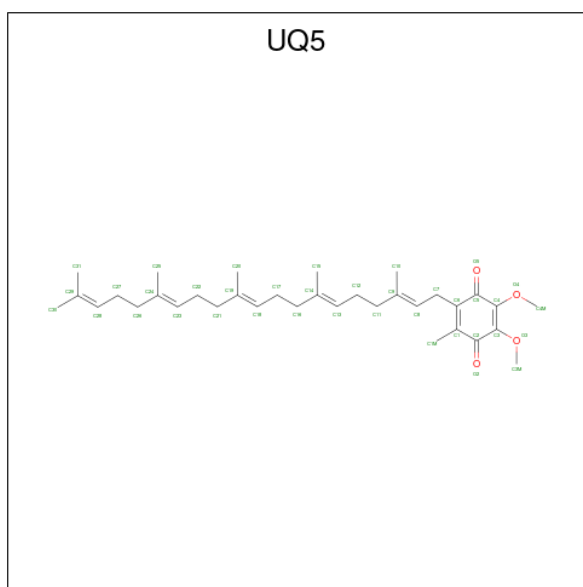
Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	28	Total	C	N	O	0	0
			203	137	33	33		
7	T	28	Total	C	N	O	0	0
			205	139	34	32		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



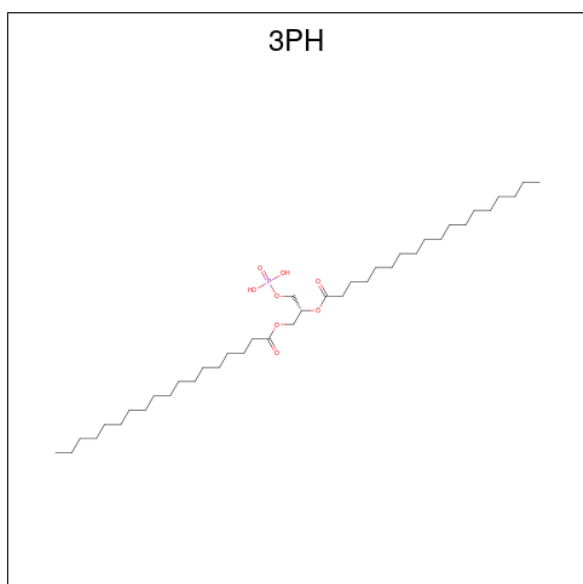
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	M	1	Total 43	C 34	Fe 1	N 4	O 4	0
8	O	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 9 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula: C<sub>34</sub>H<sub>50</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



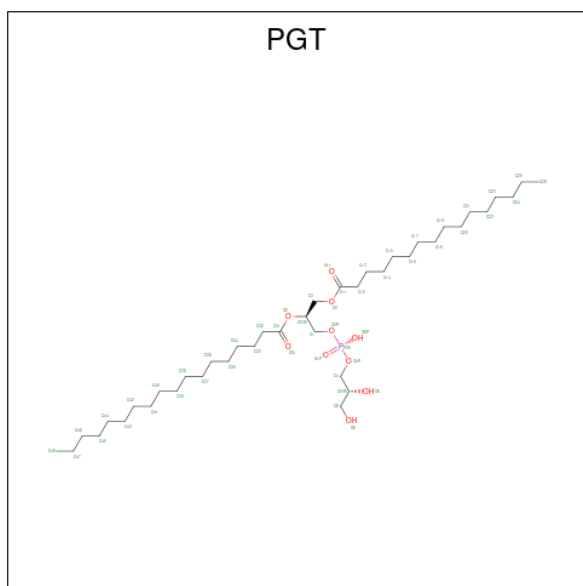
Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			38	34	4	
9	C	1	Total	C	O	0
			38	34	4	
9	M	1	Total	C	O	0
			38	34	4	

- Molecule 10 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	O	P	0
			33	24	8	1	
10	G	1	Total	C	O	P	0
			33	24	8	1	
10	I	1	Total	C	O	P	0
			32	23	8	1	
10	M	1	Total	C	O	P	0
			44	35	8	1	
10	T	1	Total	C	O	P	0
			41	32	8	1	
10	T	1	Total	C	O	P	0
			48	39	8	1	

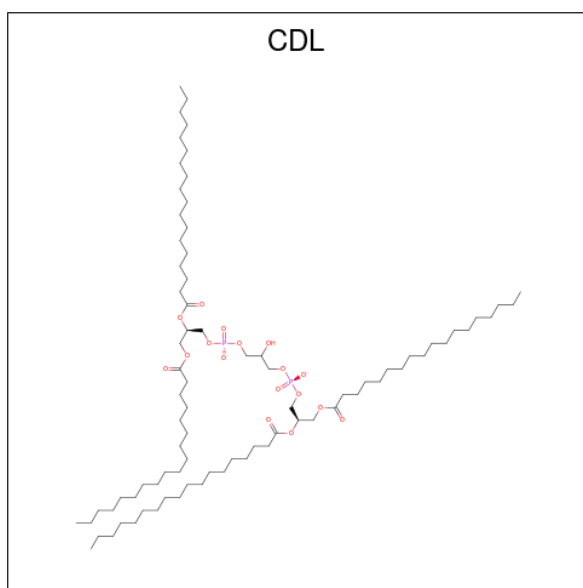
- Molecule 11 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	O	P	0
			41	30	10	1	
11	C	1	Total	C	O	P	0
			51	40	10	1	
11	G	1	Total	C	O	P	0
			51	40	10	1	
11	M	1	Total	C	O	P	0
			37	26	10	1	

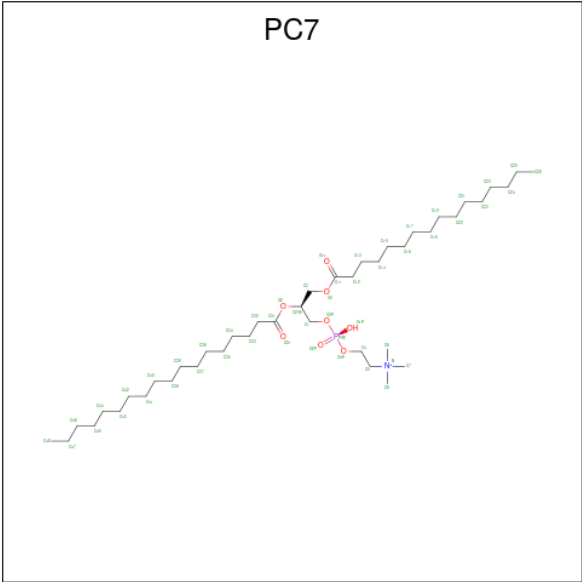
- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled

as "Ligand of Interest" by depositor).



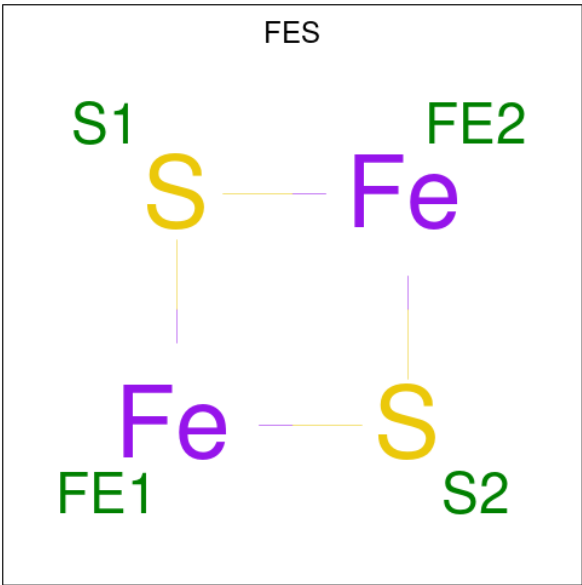
Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total	C	O	P	0
			81	62	17	2	
12	C	1	Total	C	O	P	0
			85	66	17	2	
12	G	1	Total	C	O	P	0
			85	66	17	2	
12	M	1	Total	C	O	P	0
			77	58	17	2	
12	N	1	Total	C	O	P	0
			81	62	17	2	
12	O	1	Total	C	O	P	0
			88	69	17	2	
12	Q	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 13 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



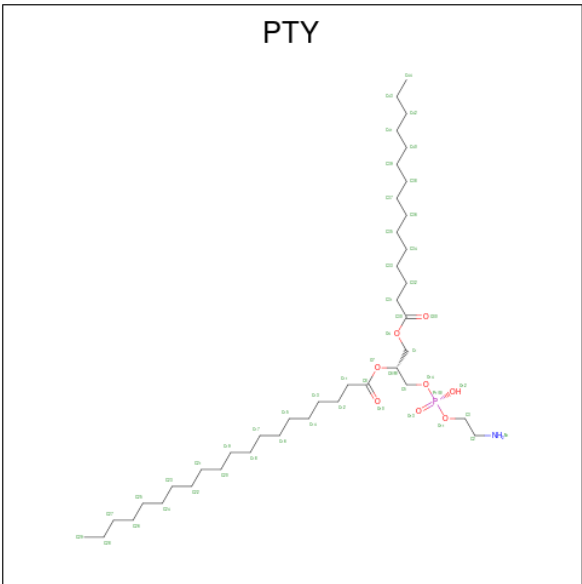
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
13	D	1	Total	C	N	O	P	0
			34	24	1	8	1	
13	G	1	Total	C	N	O	P	0
			52	42	1	8	1	
13	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
13	N	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
14	D	1	Total	Fe	S	0
			4	2	2	
14	N	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



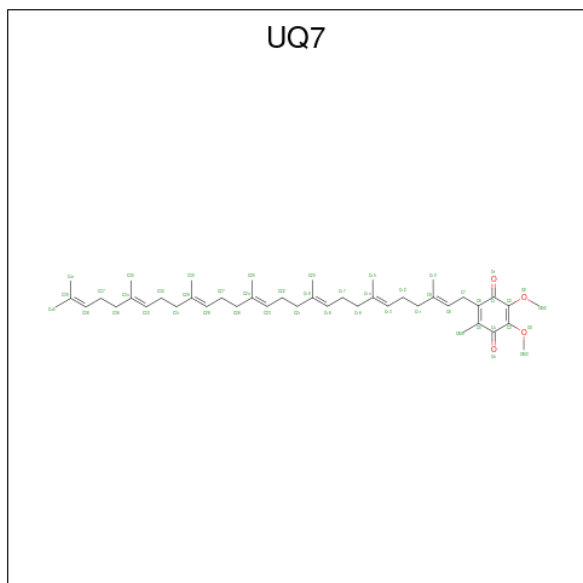
Mol	Chain	Residues	Atoms					AltConf
15	J	1	Total	C	N	O	P	0
			41	31	1	8	1	

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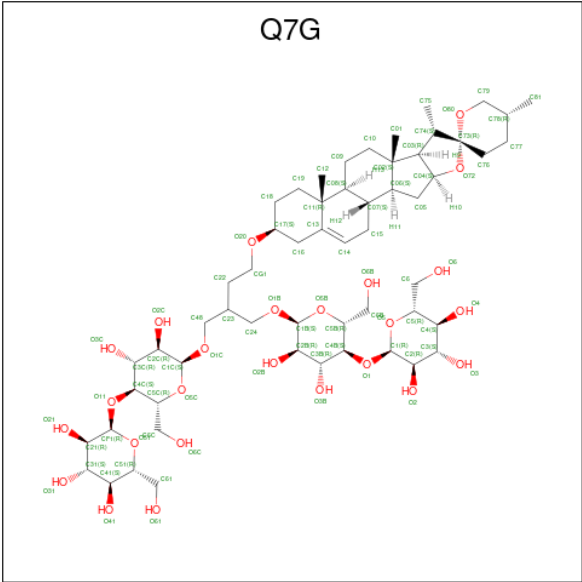
Mol	Chain	Residues	Atoms					AltConf
15	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	T	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 16 is UBIQUINONE-7 (three-letter code: UQ7) (formula:  $C_{44}H_{66}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			48	44	4	

- Molecule 17 is 2-([(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl)-4-([(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy)butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (three-letter code: Q7G) (formula:  $C_{56}H_{92}O_{25}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	M	1	Total	C	O	0
			39	34	5	
17	M	1	Total	C	O	0
			39	34	5	

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	C	179	Total	O	0
			179	179	
18	D	32	Total	O	0
			32	32	
18	E	159	Total	O	0
			159	159	
18	G	30	Total	O	0
			30	30	
18	H	13	Total	O	0
			13	13	
18	I	20	Total	O	0
			20	20	
18	M	138	Total	O	0
			138	138	
18	N	33	Total	O	0
			33	33	
18	O	111	Total	O	0
			111	111	
18	Q	13	Total	O	0
			13	13	

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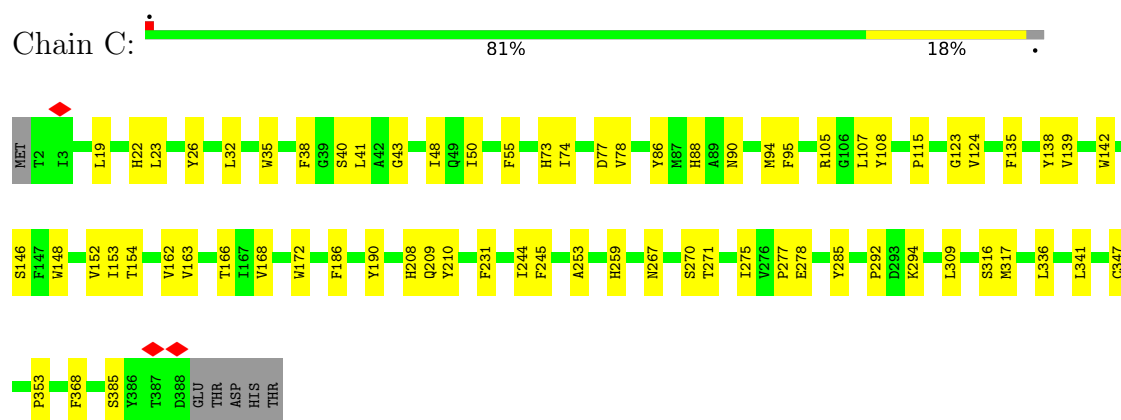
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Mol	Chain	Residues	Atoms		AltConf
18	R	2	Total 2	O 2	0
18	S	13	Total 13	O 13	0
18	T	1	Total 1	O 1	0

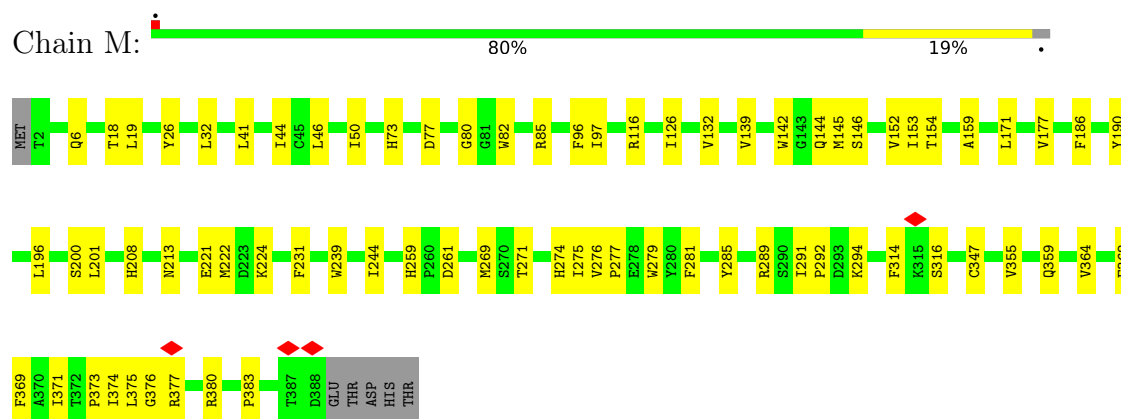
### 3 Residue-property plots

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

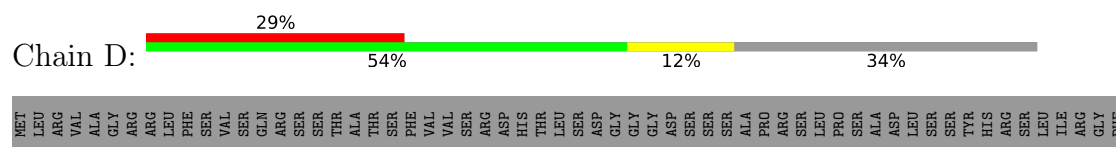
- Molecule 1: Cytochrome b

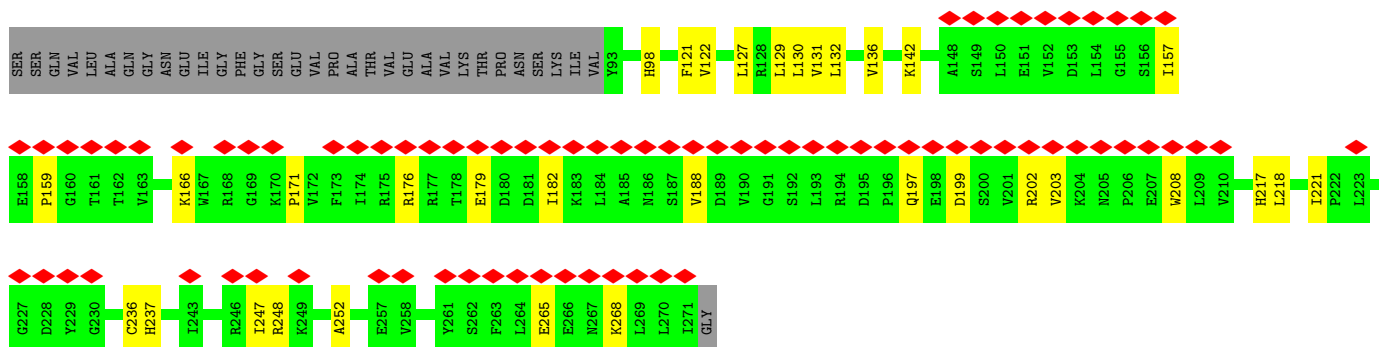


- Molecule 1: Cytochrome b

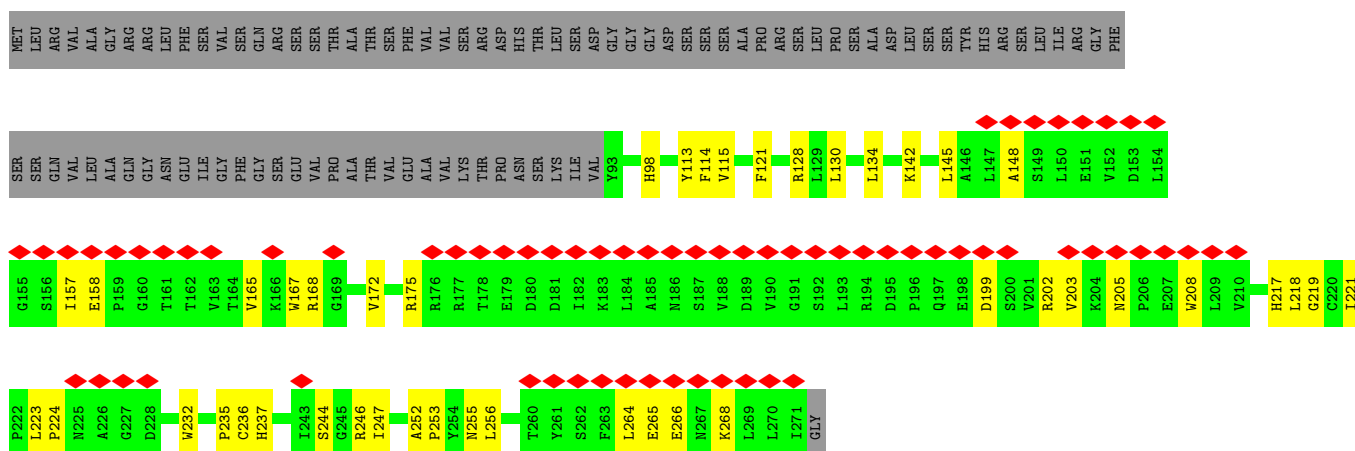


- Molecule 2: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

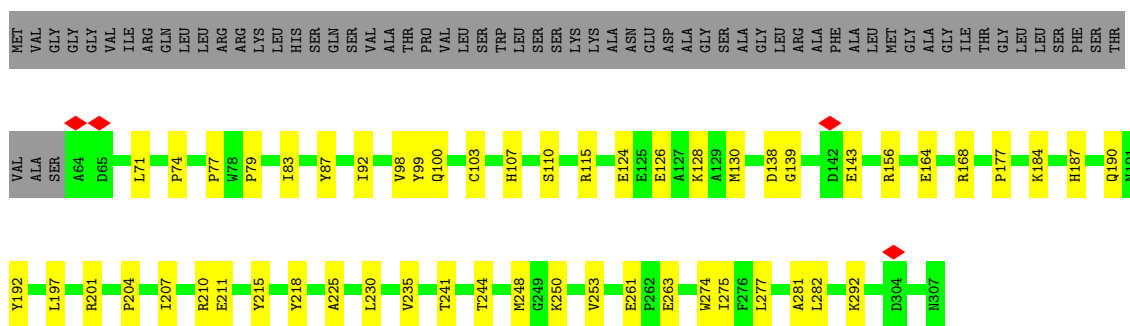




• Molecule 2: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

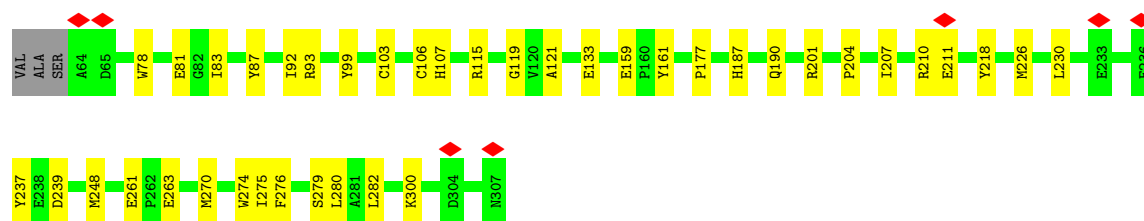


• Molecule 3: Cytochrome c1 2, heme protein, mitochondrial



• Molecule 3: Cytochrome c1 2, heme protein, mitochondrial

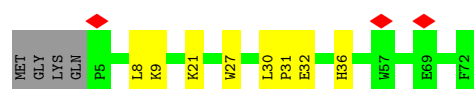
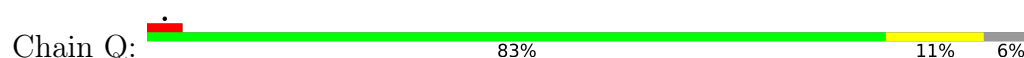




- Molecule 4: Cytochrome b-c1 complex subunit 8-1, mitochondrial



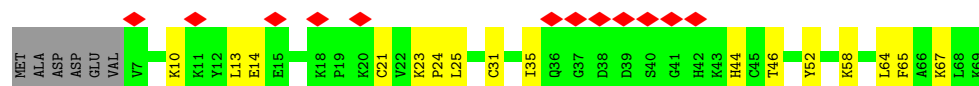
- Molecule 4: Cytochrome b-c1 complex subunit 8-1, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 6-1, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit 6-1, mitochondrial

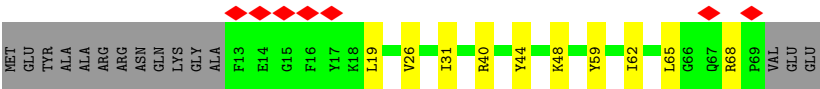


- Molecule 6: Cytochrome b-c1 complex subunit 9, mitochondrial

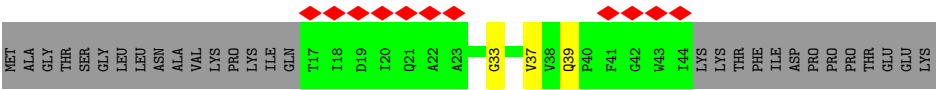
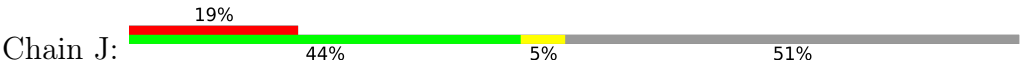


- Molecule 6: Cytochrome b-c1 complex subunit 9, mitochondrial

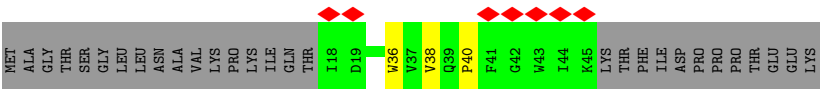
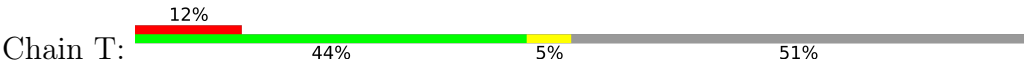




• Molecule 7: Cytochrome b-c1 complex subunit 10, mitochondrial



• Molecule 7: Cytochrome b-c1 complex subunit 10, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	10.977	Depositor
Minimum map value	-3.645	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.288	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	145.542, 163.30501, 142.677	wwPDB
Map dimensions	249, 285, 254	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	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: 3PH, PC7, HEM, CDL, UQ5, UQ7, PTY, Q7G, PGT, FES

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	C	0.47	1/3208 (0.0%)	0.60	1/4395 (0.0%)
1	M	0.45	0/3208	0.64	2/4395 (0.0%)
2	D	0.31	0/1441	0.52	0/1961
2	N	0.38	0/1441	0.63	2/1961 (0.1%)
3	E	0.36	0/1968	0.56	0/2672
3	O	0.37	0/1968	0.55	0/2672
4	G	0.39	0/600	0.50	0/815
4	Q	0.34	0/591	0.60	0/802
5	H	0.29	0/531	0.47	0/713
5	R	0.43	0/524	0.69	1/703 (0.1%)
6	I	0.68	1/488 (0.2%)	0.77	0/655
6	S	0.39	0/488	0.69	0/655
7	J	0.44	0/210	0.78	1/290 (0.3%)
7	T	0.24	0/212	0.39	0/291
All	All	0.41	2/16878 (0.0%)	0.60	7/22980 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	63	SER	CA-CB	-6.47	1.43	1.52
1	C	88	HIS	C-O	-5.41	1.13	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	96	PHE	CB-CA-C	6.31	123.02	110.40
5	R	65	PHE	CB-CA-C	5.73	121.87	110.40
2	N	175	ARG	CB-CA-C	-5.73	98.94	110.40
2	N	114	PHE	CB-CA-C	5.38	121.16	110.40
1	C	86	TYR	CB-CA-C	5.36	121.12	110.40

There are no chirality outliers.

There are no planarity outliers.

## 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	C	3093	0	3074	75	0
1	M	3093	0	3074	94	0
2	D	1404	0	1395	31	0
2	N	1404	0	1395	38	0
3	E	1917	0	1844	47	0
3	O	1917	0	1844	36	0
4	G	581	0	589	17	0
4	Q	572	0	582	8	0
5	H	518	0	518	14	0
5	R	511	0	511	14	0
6	I	476	0	469	10	0
6	S	476	0	469	14	0
7	J	203	0	197	1	0
7	T	205	0	203	4	0
8	C	86	0	60	2	0
8	E	43	0	30	5	0
8	M	86	0	60	1	0
8	O	43	0	30	5	0
9	C	76	0	100	17	0
9	M	38	0	50	8	0
10	C	33	0	38	1	0
10	G	33	0	39	1	0
10	I	32	0	37	3	0
10	M	44	0	64	6	0
10	T	89	0	133	2	0
11	C	92	0	133	10	0
11	G	51	0	78	2	0
11	M	37	0	47	4	0
12	C	166	0	232	19	0
12	G	85	0	120	6	0
12	M	77	0	98	8	0
12	N	81	0	112	3	0
12	O	88	0	123	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Q	70	0	87	6	0
13	C	51	0	79	9	0
13	D	34	0	42	1	0
13	G	52	0	84	5	0
13	M	45	0	60	2	0
13	N	39	0	52	6	0
14	D	4	0	0	0	0
14	N	4	0	0	1	0
15	J	41	0	58	0	0
15	M	40	0	56	2	0
15	T	29	0	31	1	0
16	M	48	0	66	12	0
17	M	78	0	0	0	0
18	C	179	0	0	17	0
18	D	32	0	0	1	0
18	E	159	0	0	14	0
18	G	30	0	0	3	0
18	H	13	0	0	1	0
18	I	20	0	0	1	0
18	M	138	0	0	21	0
18	N	33	0	0	4	0
18	O	111	0	0	8	0
18	Q	13	0	0	1	0
18	R	2	0	0	3	0
18	S	13	0	0	5	0
18	T	1	0	0	0	0
All	All	18929	0	18363	421	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 12.

The worst 5 of 421 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)
1:M:316:SER:HB2	18:M:565:HOH:O	1.38	1.18
1:M:154:THR:HG22	1:M:171:LEU:HD21	1.18	1.13
1:M:154:THR:CG2	1:M:171:LEU:HD21	1.86	1.05
1:C:292:PRO:HA	18:N:425:HOH:O	1.57	1.01
1:M:154:THR:HG22	1:M:171:LEU:CD2	1.91	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	385/393 (98%)	376 (98%)	9 (2%)	0	100	100
1	M	385/393 (98%)	374 (97%)	11 (3%)	0	100	100
2	D	177/272 (65%)	168 (95%)	9 (5%)	0	100	100
2	N	177/272 (65%)	166 (94%)	11 (6%)	0	100	100
3	E	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
3	O	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
4	G	67/72 (93%)	67 (100%)	0	0	100	100
4	Q	66/72 (92%)	65 (98%)	1 (2%)	0	100	100
5	H	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
5	R	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
6	I	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
6	S	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
7	J	26/57 (46%)	25 (96%)	1 (4%)	0	100	100
7	T	26/57 (46%)	23 (88%)	3 (12%)	0	100	100
All	All	2026/2484 (82%)	1966 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	330/336 (98%)	328 (99%)	2 (1%)	84	89
1	M	330/336 (98%)	328 (99%)	2 (1%)	84	89
2	D	155/232 (67%)	155 (100%)	0	100	100
2	N	155/232 (67%)	155 (100%)	0	100	100
3	E	200/247 (81%)	199 (100%)	1 (0%)	86	91
3	O	200/247 (81%)	200 (100%)	0	100	100
4	G	63/65 (97%)	63 (100%)	0	100	100
4	Q	62/65 (95%)	62 (100%)	0	100	100
5	H	58/62 (94%)	58 (100%)	0	100	100
5	R	57/62 (92%)	57 (100%)	0	100	100
6	I	48/59 (81%)	48 (100%)	0	100	100
6	S	48/59 (81%)	48 (100%)	0	100	100
7	J	16/41 (39%)	16 (100%)	0	100	100
7	T	16/41 (39%)	16 (100%)	0	100	100
All	All	1738/2084 (83%)	1733 (100%)	5 (0%)	90	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	95	PHE
1	C	190	TYR
3	E	292	LYS
1	M	85	ARG
1	M	190	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	274	HIS
2	N	96	HIS

### 5.3.3 RNA ⓘ

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](#)

39 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
15	PTY	T	103	-	28,28,49	1.12	4 (14%)	31,33,54	1.18	2 (6%)
13	PC7	D	302	-	33,33,51	1.17	4 (12%)	39,41,59	1.07	2 (5%)
8	HEM	C	402	1	41,50,50	1.60	8 (19%)	45,82,82	1.88	10 (22%)
8	HEM	M	402	1	41,50,50	1.78	8 (19%)	45,82,82	2.05	15 (33%)
11	PGT	M	406	-	36,36,50	1.20	3 (8%)	39,42,56	1.11	2 (5%)
12	CDL	Q	101	-	69,69,99	1.04	8 (11%)	75,81,111	1.16	5 (6%)
10	3PH	G	101	-	32,32,47	0.75	1 (3%)	36,37,52	0.67	1 (2%)
11	PGT	G	102	-	50,50,50	1.07	3 (6%)	53,56,56	1.06	2 (3%)
16	UQ7	M	404	-	48,48,48	0.66	2 (4%)	58,61,61	0.77	3 (5%)
8	HEM	E	400	3	41,50,50	1.44	3 (7%)	45,82,82	1.43	9 (20%)
11	PGT	C	407	-	50,50,50	1.09	3 (6%)	53,56,56	1.04	2 (3%)
10	3PH	T	101	-	40,40,47	0.68	1 (2%)	44,45,52	0.65	1 (2%)
14	FES	N	301	2	0,4,4	-	-	-	-	-
14	FES	D	301	2	0,4,4	-	-	-	-	-
13	PC7	M	409	-	43,43,51	1.03	4 (9%)	48,50,59	1.13	2 (4%)
15	PTY	J	101	-	40,40,49	0.33	0	43,45,54	0.38	0
9	UQ5	M	403	-	38,38,38	0.48	0	46,49,49	0.62	1 (2%)
10	3PH	I	101	-	31,31,47	0.76	1 (3%)	35,36,52	0.76	2 (5%)
13	PC7	C	410	-	50,50,51	0.97	4 (8%)	56,58,59	1.07	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	PTY	M	407	-	39,39,49	0.97	4 (10%)	42,44,54	1.06	2 (4%)
12	CDL	C	408	-	80,80,99	0.37	0	86,92,111	0.56	2 (2%)
10	3PH	T	102	-	47,47,47	0.64	1 (2%)	51,52,52	0.59	1 (1%)
10	3PH	C	405	12	32,32,47	0.74	1 (3%)	36,37,52	0.77	1 (2%)
12	CDL	O	402	-	87,87,99	0.93	8 (9%)	93,99,111	1.11	4 (4%)
11	PGT	C	406	-	40,40,50	0.38	0	43,46,56	0.43	0
8	HEM	O	401	3	41,50,50	1.78	10 (24%)	45,82,82	2.41	14 (31%)
8	HEM	M	401	1	41,50,50	1.65	9 (21%)	45,82,82	1.92	14 (31%)
17	Q7G	M	411	-	44,44,90	0.76	1 (2%)	66,68,138	1.40	10 (15%)
12	CDL	C	409	10	84,84,99	0.94	7 (8%)	90,96,111	1.10	4 (4%)
17	Q7G	M	410	-	44,44,90	0.72	1 (2%)	66,68,138	1.36	11 (16%)
9	UQ5	C	403	-	38,38,38	0.94	2 (5%)	46,49,49	0.83	0
13	PC7	G	104	-	51,51,51	0.97	4 (7%)	57,59,59	1.02	2 (3%)
9	UQ5	C	404	-	38,38,38	0.46	0	46,49,49	0.82	1 (2%)
12	CDL	N	302	-	80,80,99	0.96	8 (10%)	86,92,111	1.16	4 (4%)
12	CDL	G	103	-	84,84,99	0.96	8 (9%)	90,96,111	1.11	4 (4%)
10	3PH	M	405	-	43,43,47	0.66	1 (2%)	47,48,52	0.62	1 (2%)
12	CDL	M	408	-	76,76,99	0.99	8 (10%)	82,88,111	1.11	4 (4%)
13	PC7	N	303	-	38,38,51	0.39	0	44,46,59	0.64	1 (2%)
8	HEM	C	401	1	41,50,50	1.49	6 (14%)	45,82,82	1.45	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PTY	T	103	-	-	18/32/32/53	-
13	PC7	D	302	-	-	14/37/37/55	-
8	HEM	C	402	1	-	6/12/54/54	-
8	HEM	M	402	1	-	2/12/54/54	-
11	PGT	M	406	-	-	21/41/41/55	-
12	CDL	Q	101	-	-	38/80/80/110	-
10	3PH	G	101	-	-	16/34/34/49	-
11	PGT	G	102	-	-	37/55/55/55	-
16	UQ7	M	404	-	-	19/45/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	E	400	3	-	2/12/54/54	-
11	PGT	C	407	-	-	22/55/55/55	-
10	3PH	T	101	-	-	14/42/42/49	-
14	FES	N	301	2	-	-	0/1/1/1
14	FES	D	301	2	-	-	0/1/1/1
13	PC7	M	409	-	-	20/45/45/55	-
15	PTY	J	101	-	-	5/44/44/53	-
9	UQ5	M	403	-	-	9/33/57/57	0/1/1/1
10	3PH	I	101	-	-	15/33/33/49	-
13	PC7	C	410	-	-	19/54/54/55	-
15	PTY	M	407	-	-	18/43/43/53	-
12	CDL	C	408	-	-	48/91/91/110	-
10	3PH	T	102	-	-	13/49/49/49	-
10	3PH	C	405	12	-	17/34/34/49	-
12	CDL	O	402	-	-	35/98/98/110	-
11	PGT	C	406	-	-	14/45/45/55	-
8	HEM	O	401	3	-	4/12/54/54	-
8	HEM	M	401	1	-	2/12/54/54	-
17	Q7G	M	411	-	-	0/12/100/200	0/6/6/10
12	CDL	C	409	10	-	43/95/95/110	-
17	Q7G	M	410	-	-	3/12/100/200	0/6/6/10
9	UQ5	C	403	-	-	10/33/57/57	0/1/1/1
13	PC7	G	104	-	-	20/55/55/55	-
9	UQ5	C	404	-	-	13/33/57/57	0/1/1/1
12	CDL	N	302	-	-	35/91/91/110	-
12	CDL	G	103	-	-	31/95/95/110	-
10	3PH	M	405	-	-	20/45/45/49	-
12	CDL	M	408	-	-	42/87/87/110	-
13	PC7	N	303	-	-	11/42/42/55	-
8	HEM	C	401	1	-	2/12/54/54	-

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	402	HEM	C1B-NB	-6.39	1.29	1.40
8	O	401	HEM	C1B-NB	-5.57	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	401	HEM	C1B-NB	-4.83	1.32	1.40
8	C	402	HEM	C1B-NB	-4.13	1.33	1.40
8	M	402	HEM	FE-NB	4.07	2.17	1.96

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	401	HEM	CHC-C4B-NB	7.94	133.06	124.43
8	M	402	HEM	C1B-NB-C4B	6.16	111.44	105.07
8	C	402	HEM	C1B-NB-C4B	6.11	111.38	105.07
8	O	401	HEM	C1B-NB-C4B	5.65	110.91	105.07
8	O	401	HEM	CHD-C1D-ND	5.16	130.04	124.43

There are no chirality outliers.

5 of 658 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	403	UQ5	C17-C18-C19-C20
9	C	403	UQ5	C17-C18-C19-C21
9	M	403	UQ5	C9-C11-C12-C13
10	C	405	3PH	C1-O11-P-O13
10	C	405	3PH	C1-O11-P-O14

There are no ring outliers.

34 monomers are involved in 141 short contacts:

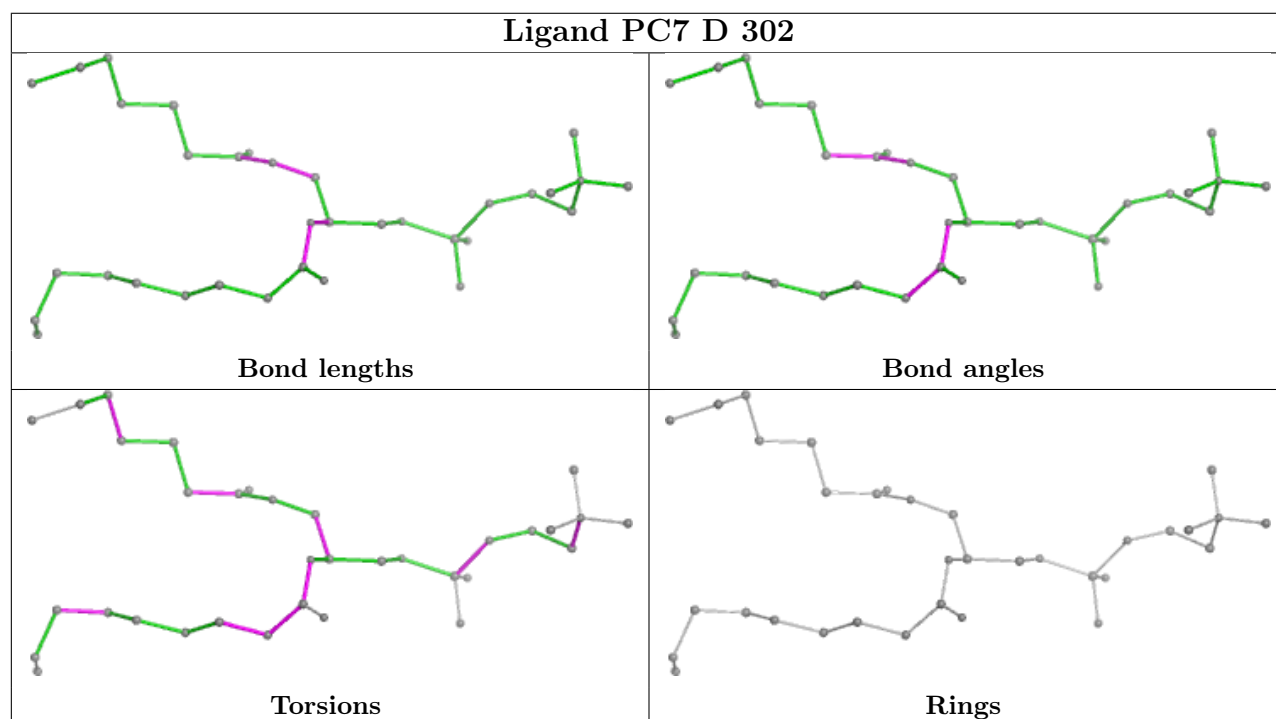
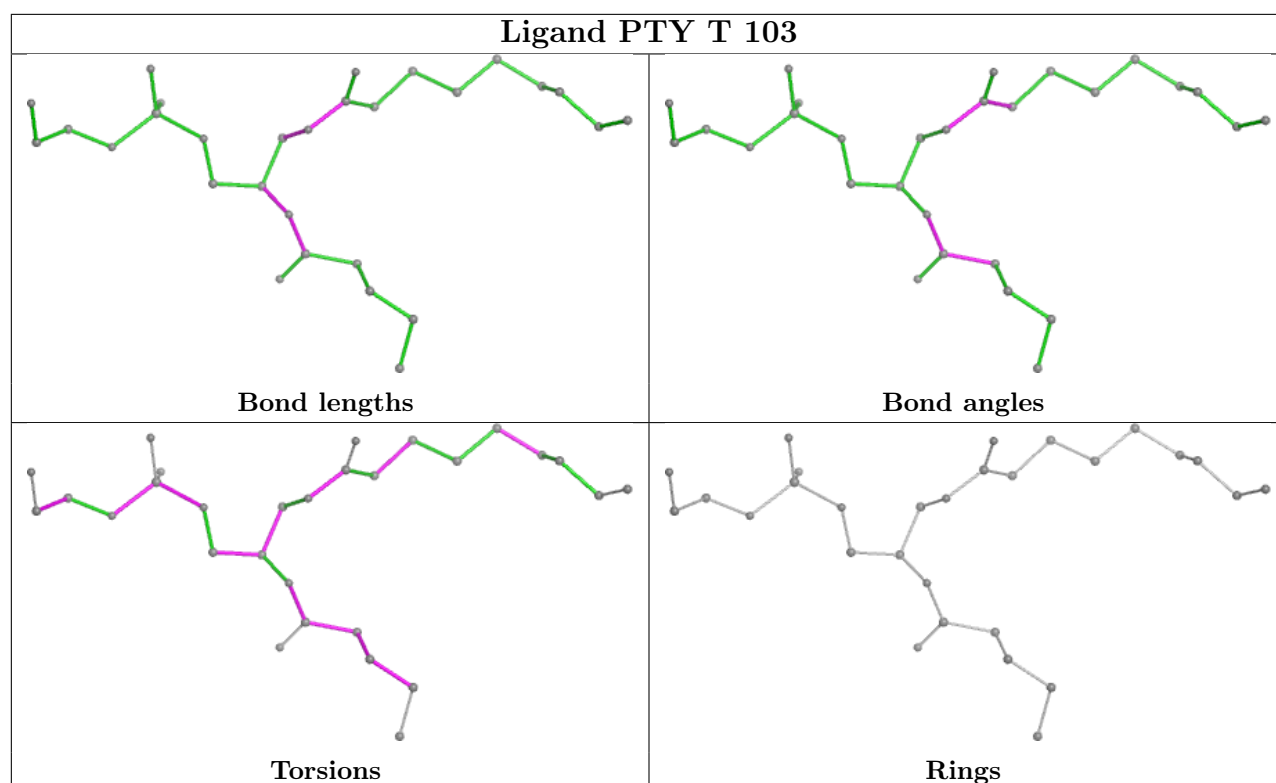
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	103	PTY	1	0
13	D	302	PC7	1	0
8	C	402	HEM	1	0
8	M	402	HEM	1	0
11	M	406	PGT	4	0
12	Q	101	CDL	6	0
10	G	101	3PH	1	0
11	G	102	PGT	2	0
16	M	404	UQ7	12	0
8	E	400	HEM	5	0
11	C	407	PGT	4	0
10	T	101	3PH	2	0
14	N	301	FES	1	0
13	M	409	PC7	2	0

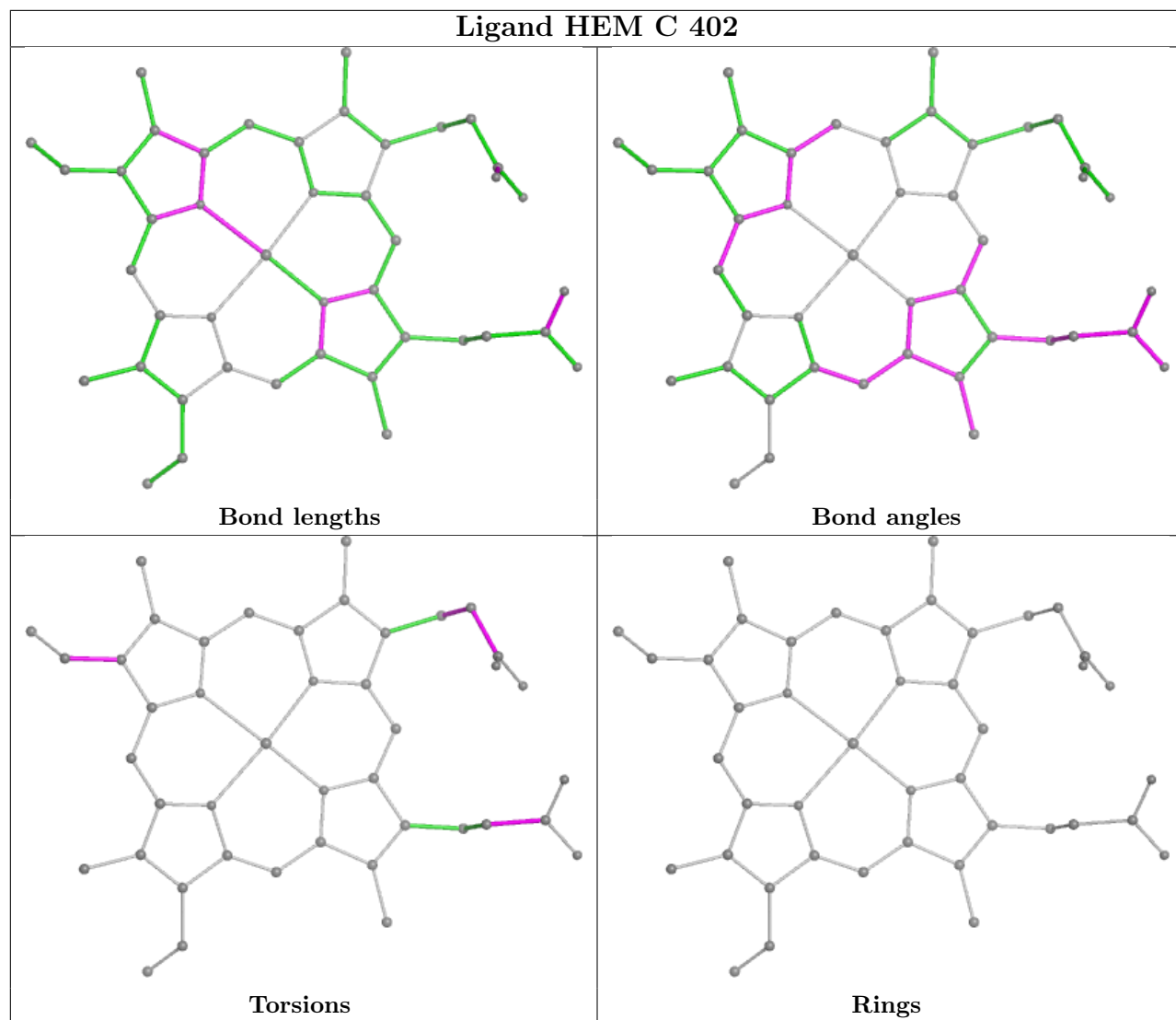
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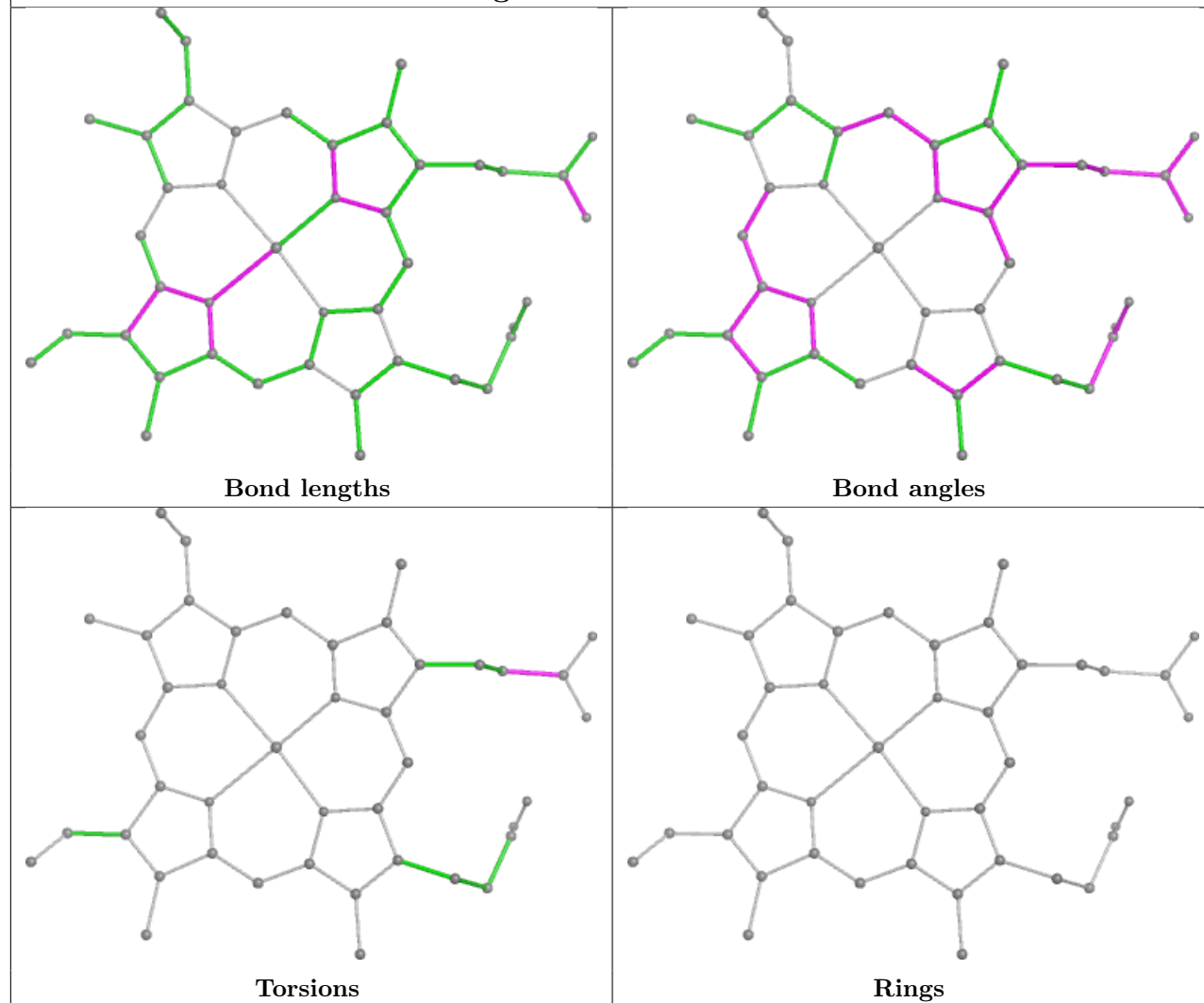
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	403	UQ5	8	0
10	I	101	3PH	3	0
13	C	410	PC7	9	0
15	M	407	PTY	2	0
12	C	408	CDL	9	0
10	T	102	3PH	1	0
10	C	405	3PH	1	0
12	O	402	CDL	7	0
11	C	406	PGT	6	0
8	O	401	HEM	5	0
12	C	409	CDL	10	0
9	C	403	UQ5	11	0
13	G	104	PC7	5	0
9	C	404	UQ5	6	0
12	N	302	CDL	3	0
12	G	103	CDL	6	0
10	M	405	3PH	6	0
12	M	408	CDL	8	0
13	N	303	PC7	6	0
8	C	401	HEM	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.

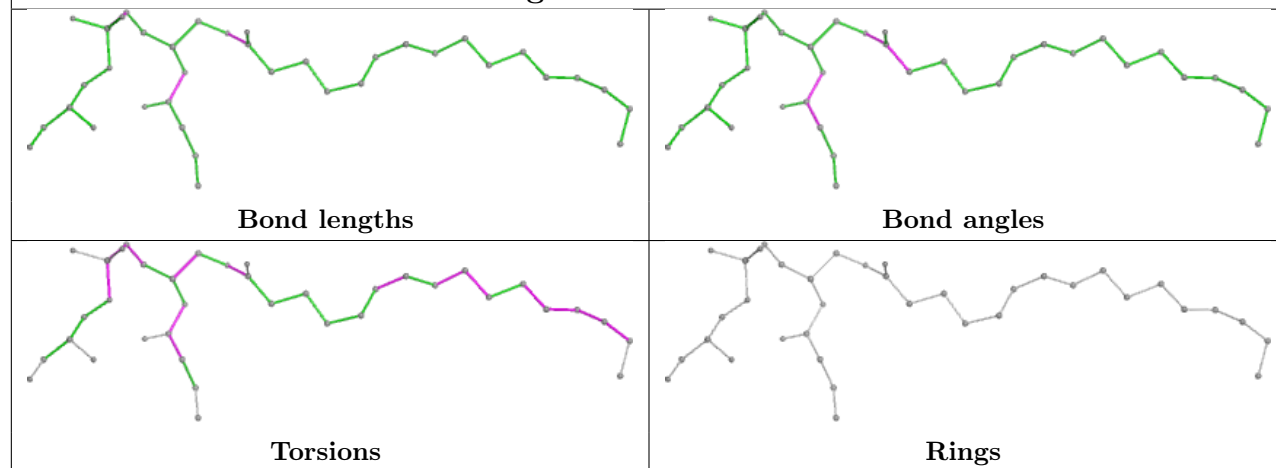


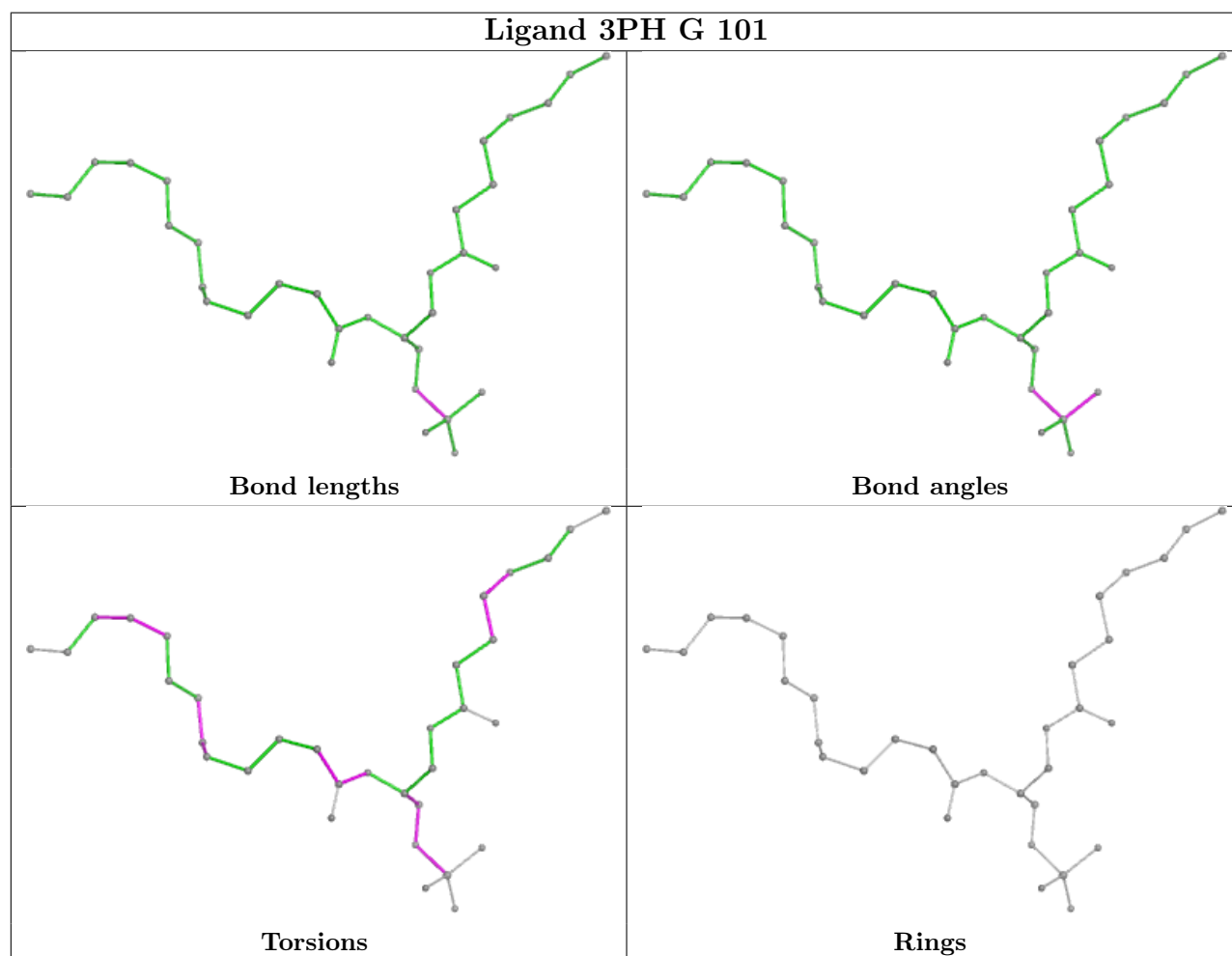
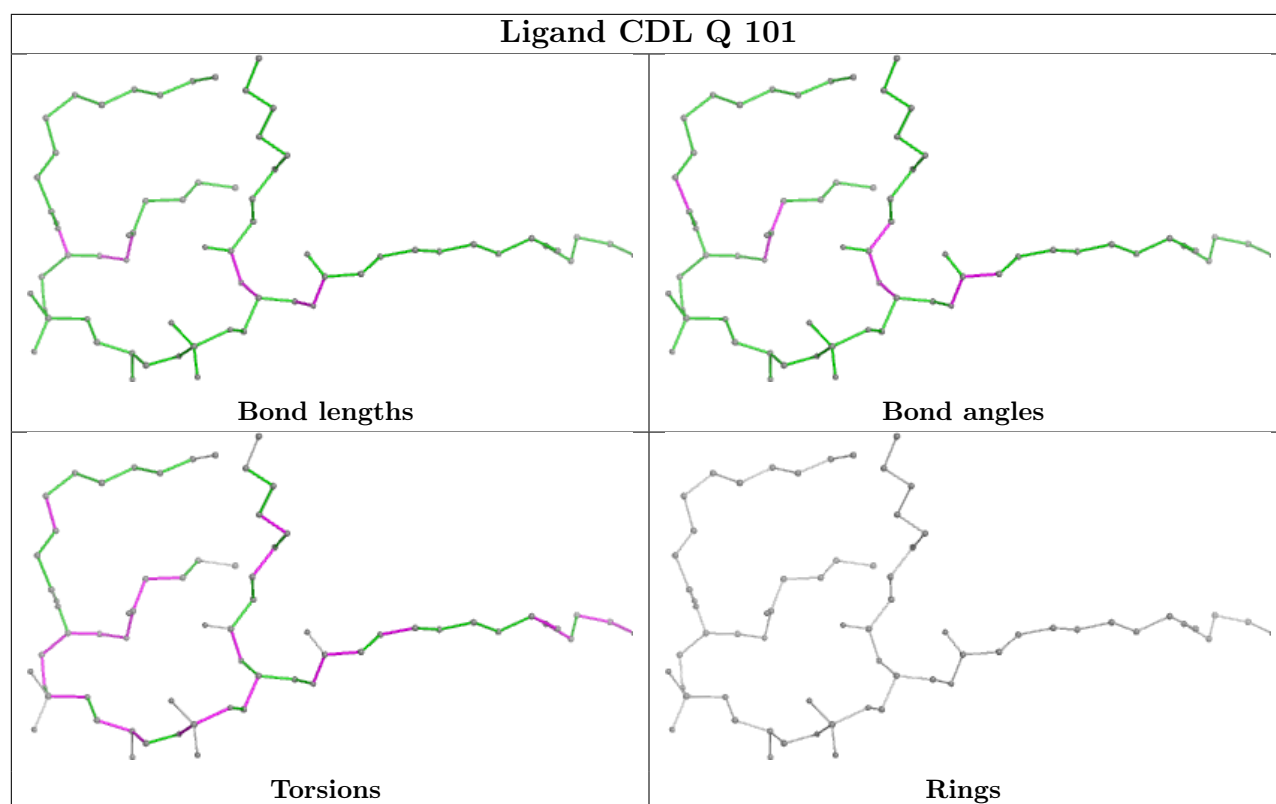


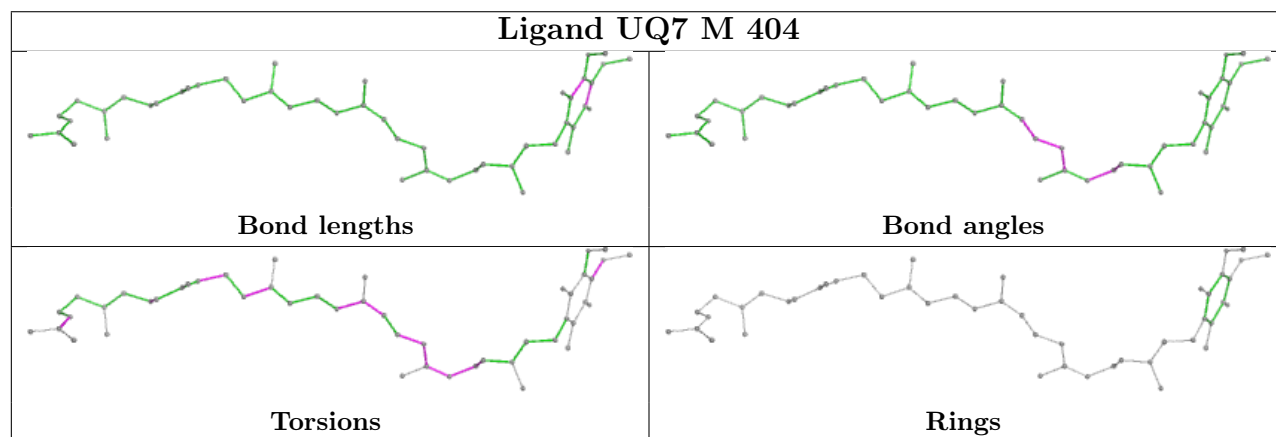
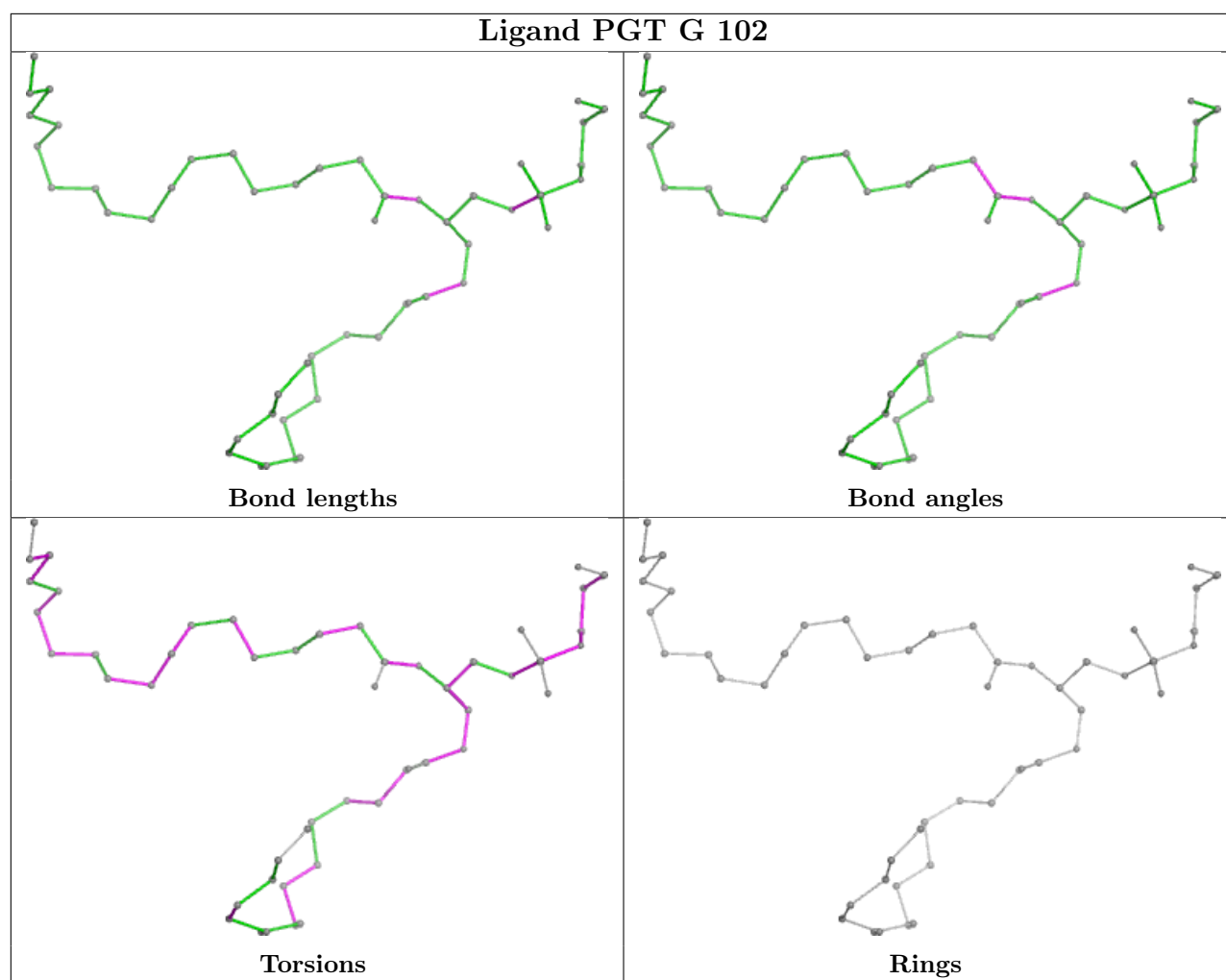
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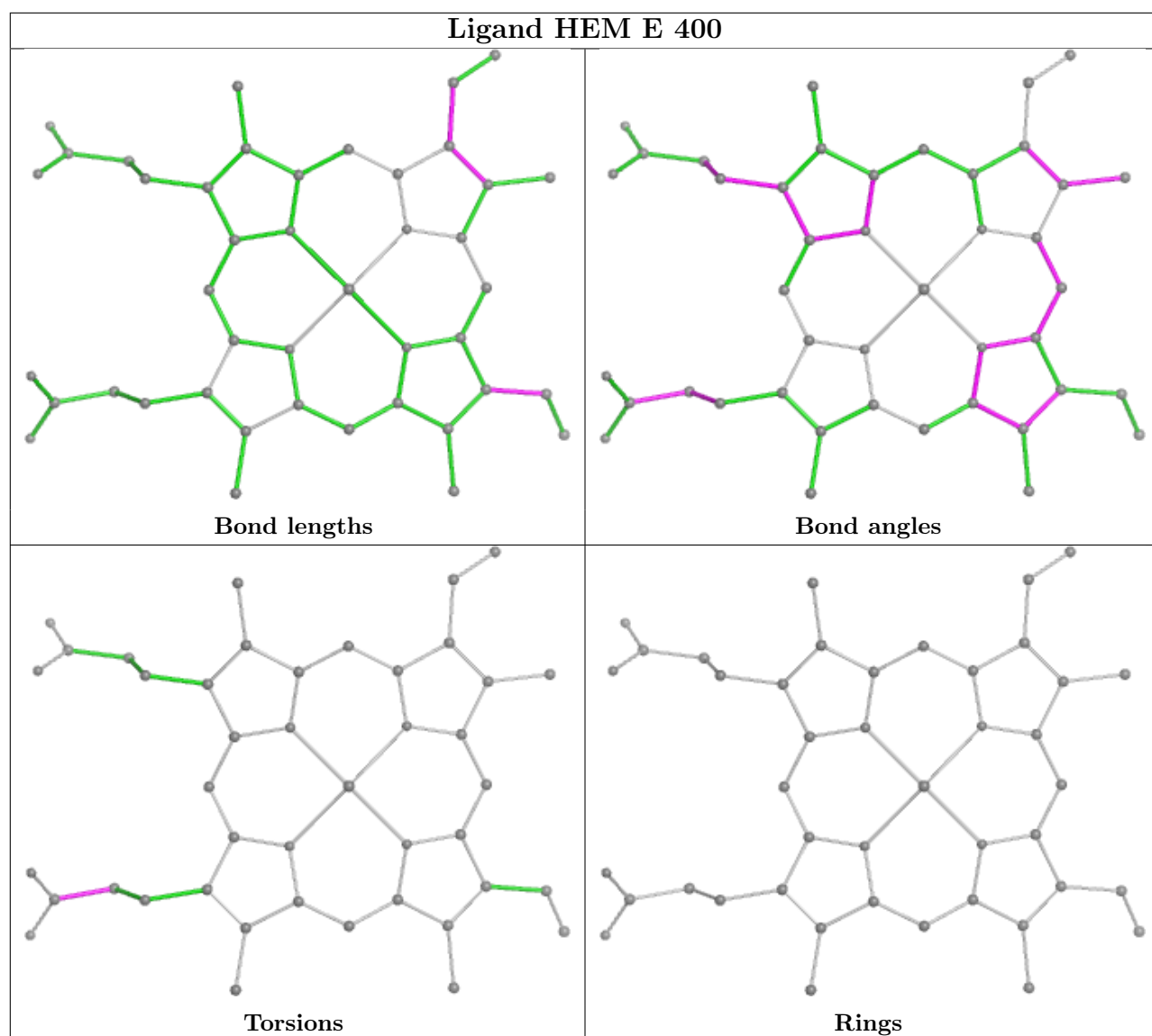


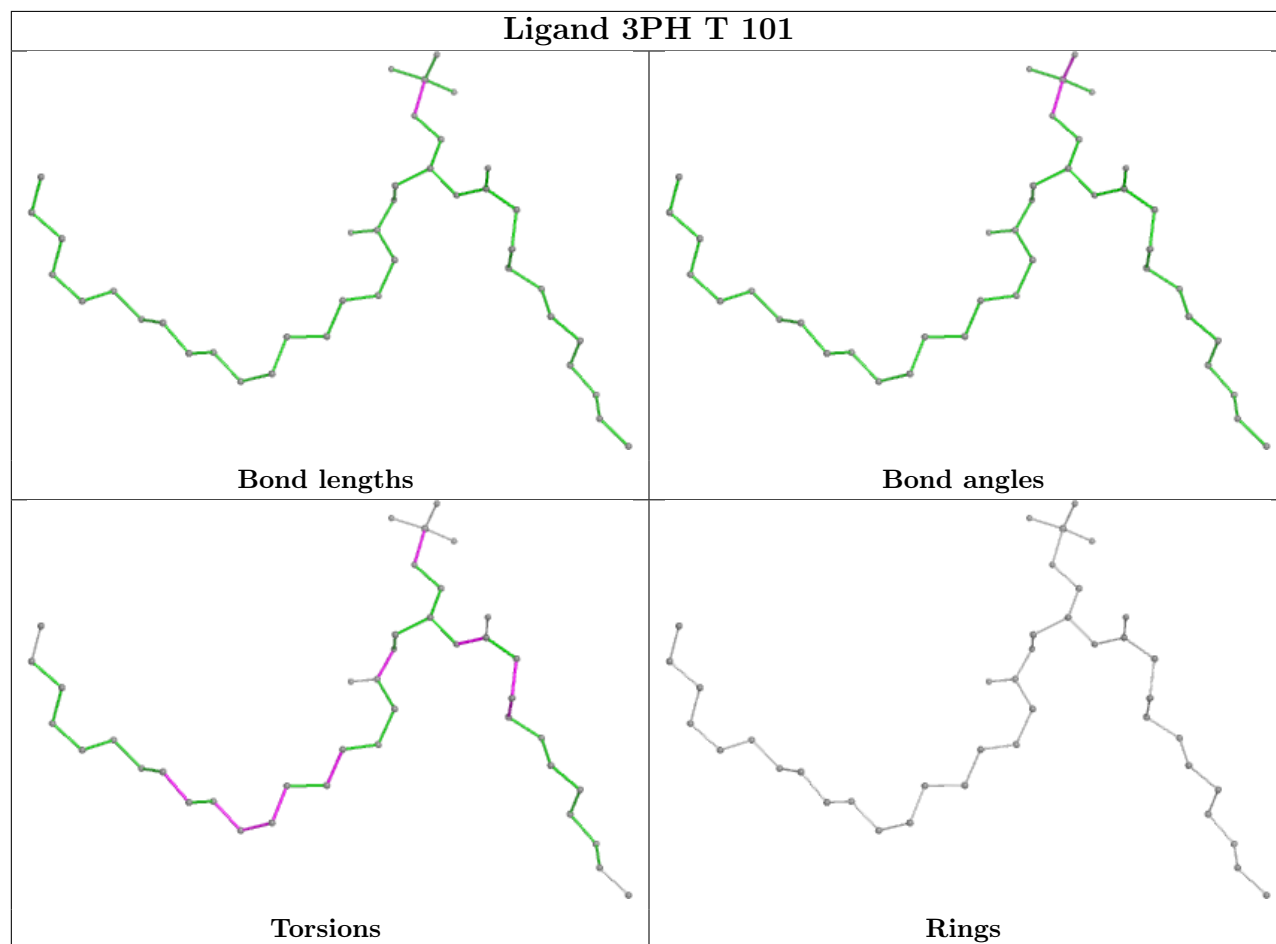
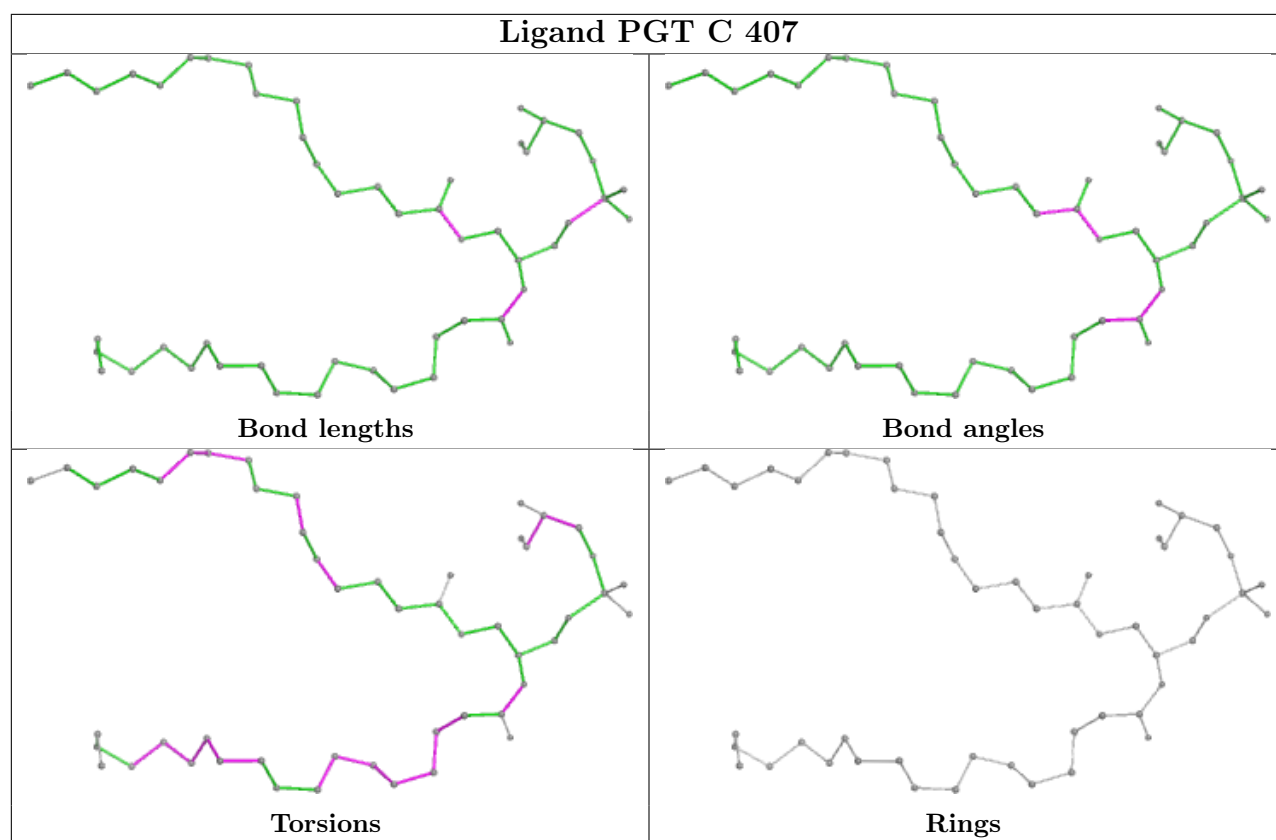
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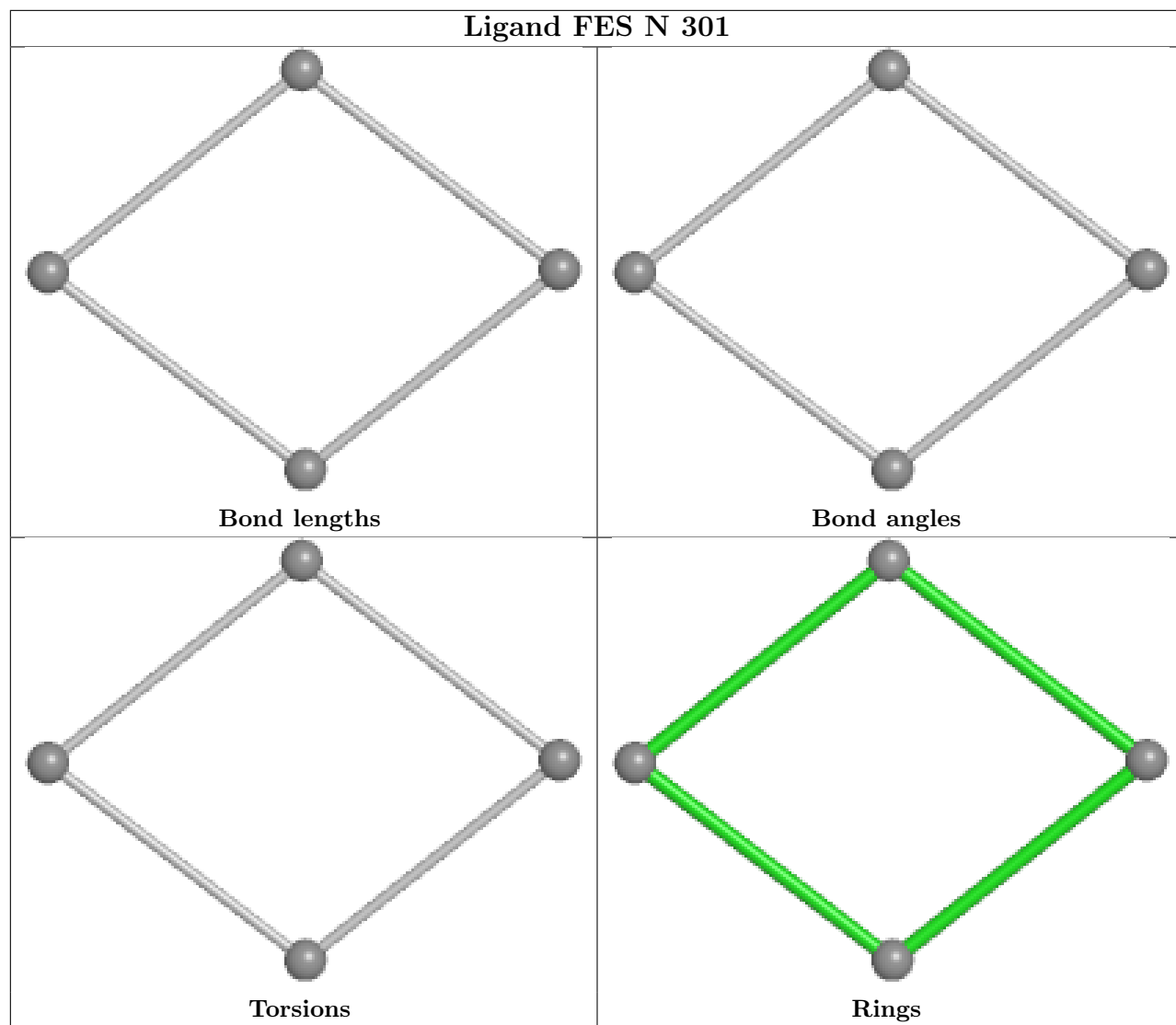


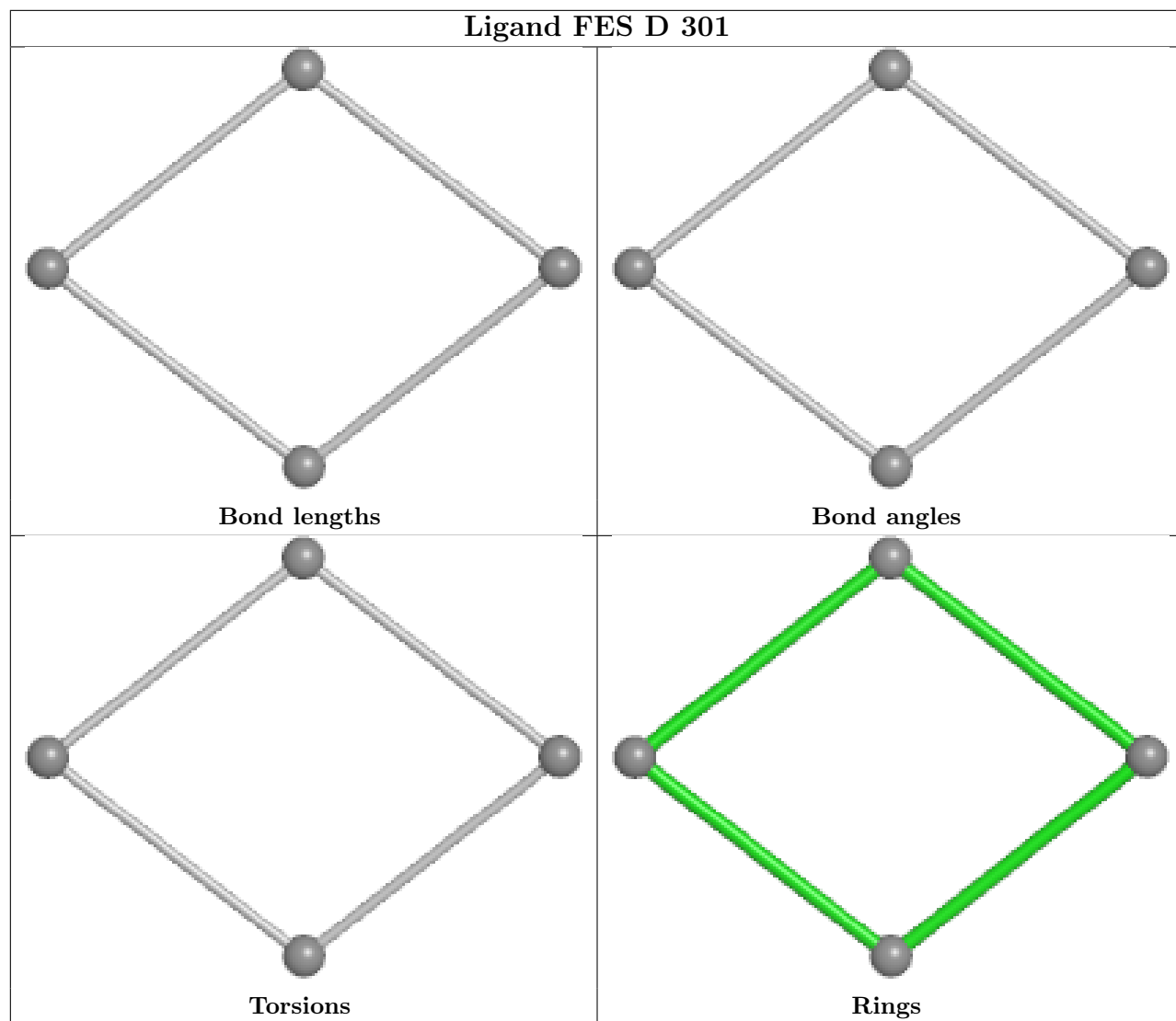


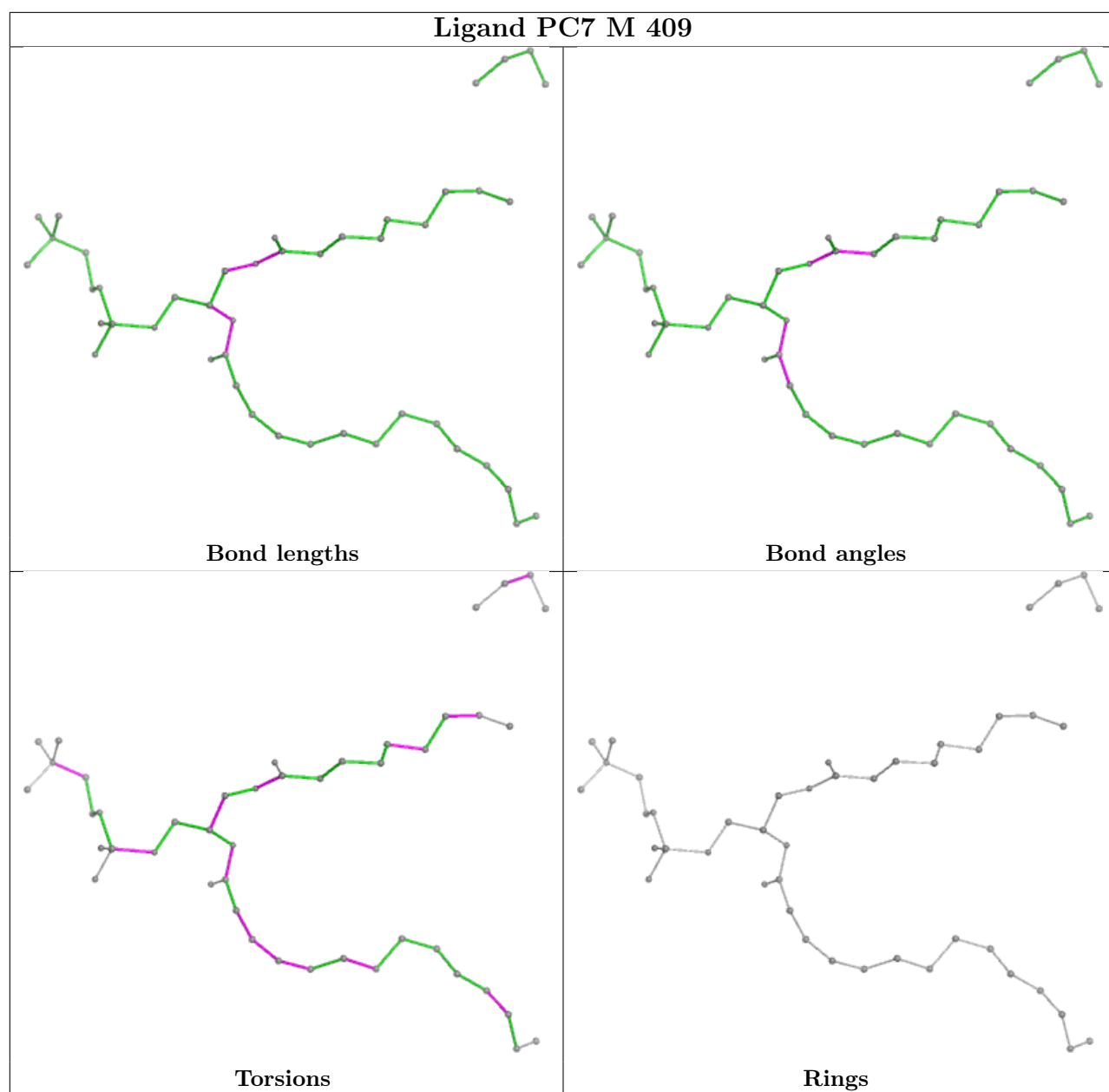


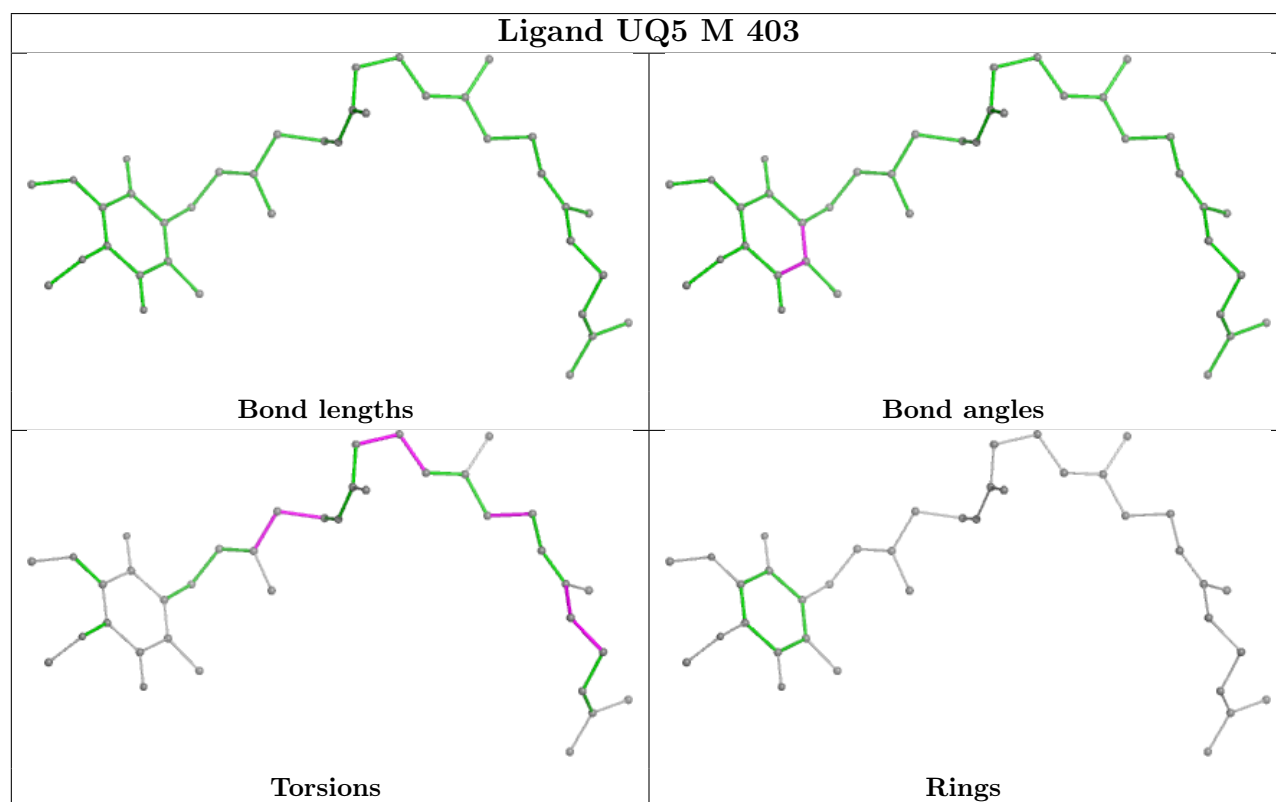
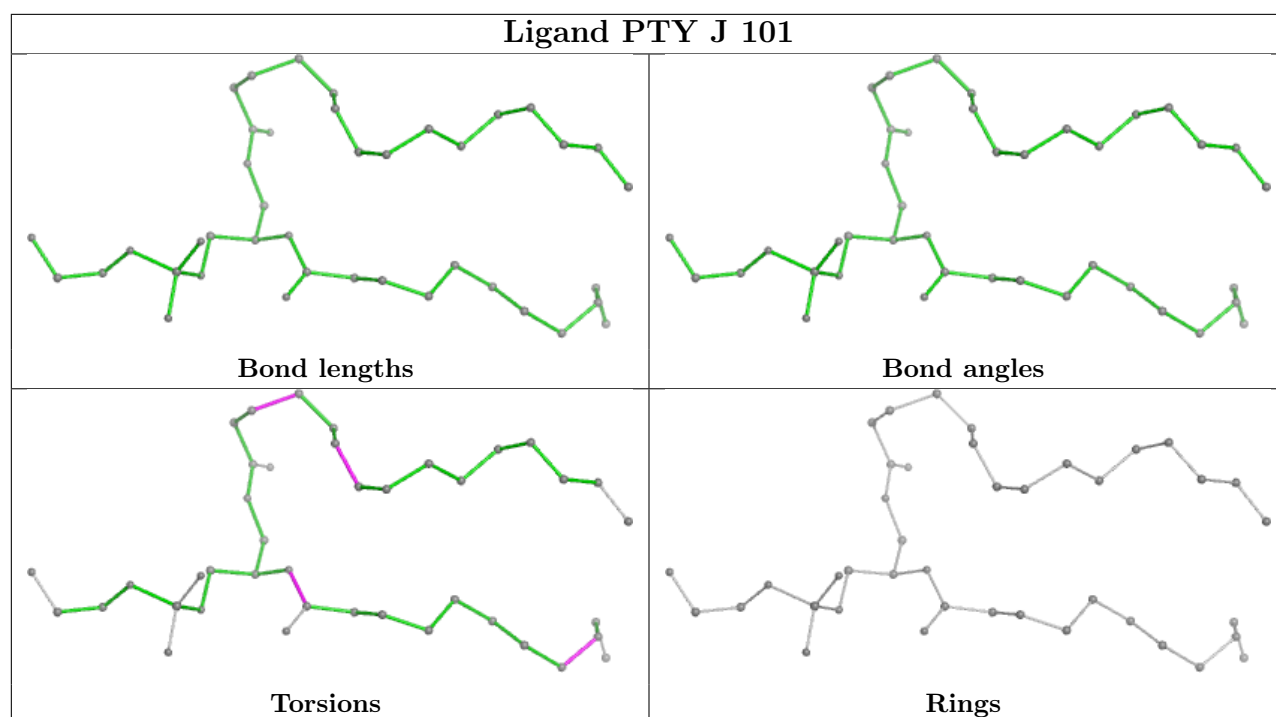


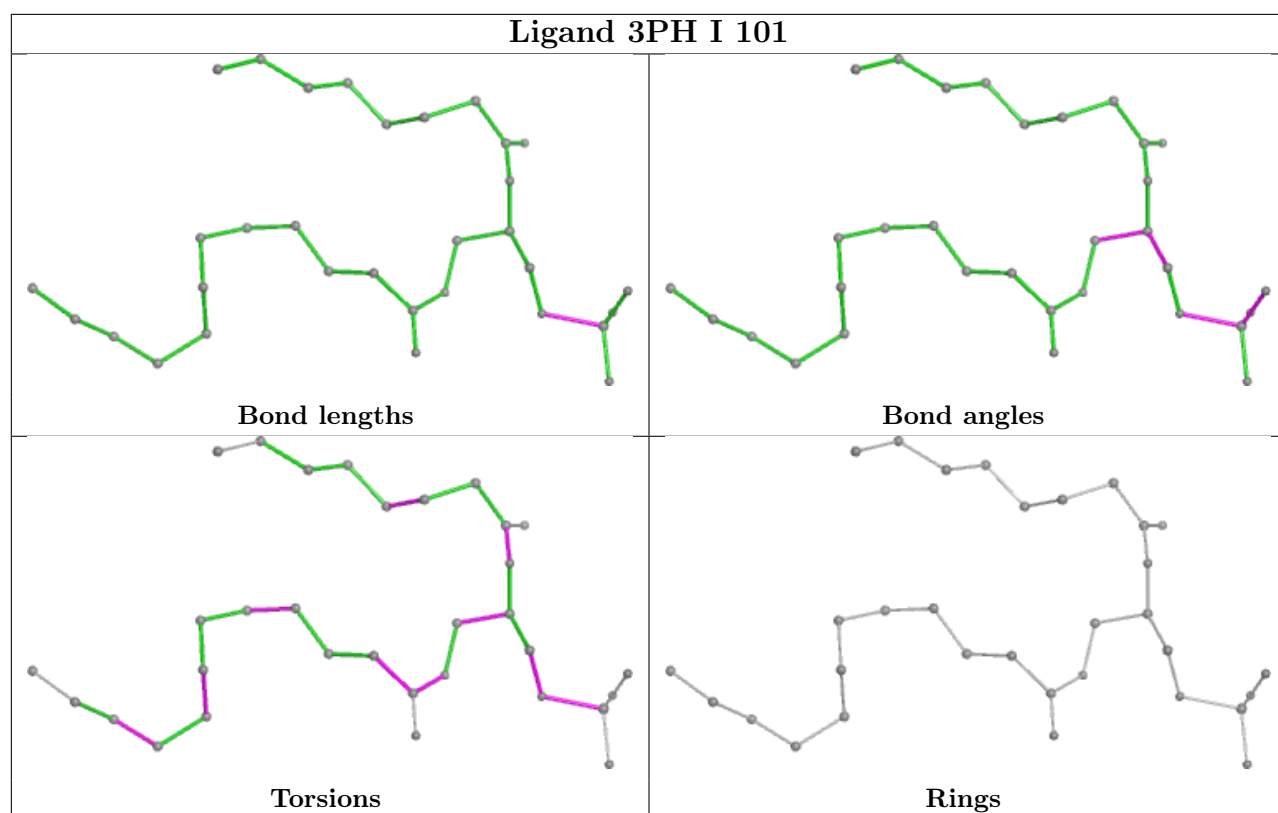


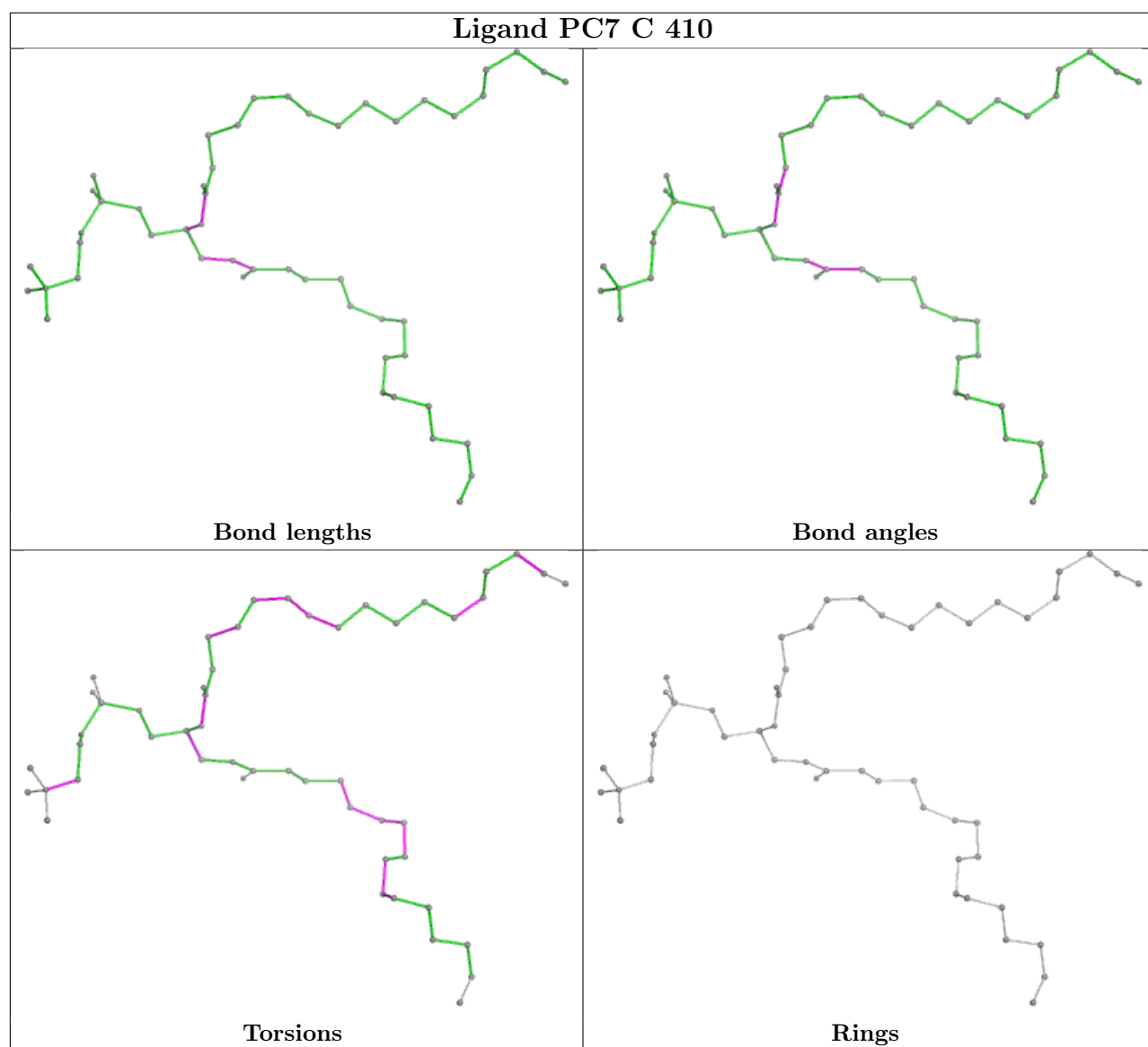


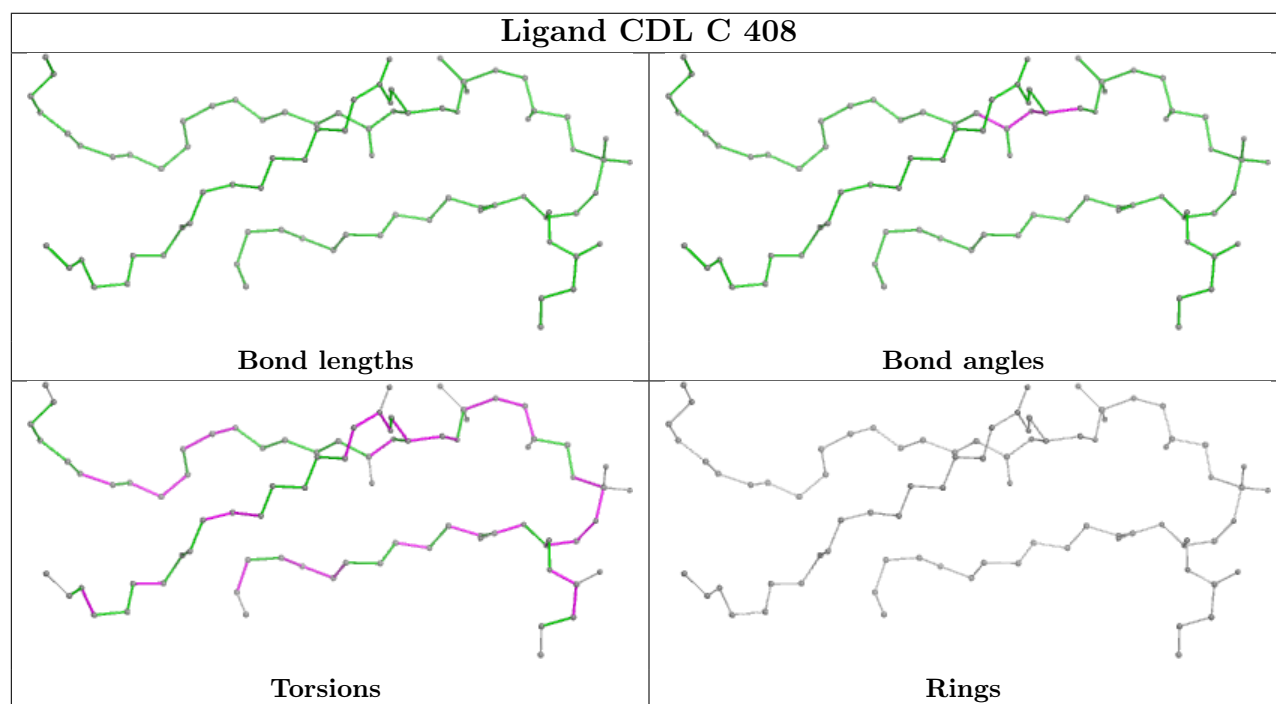
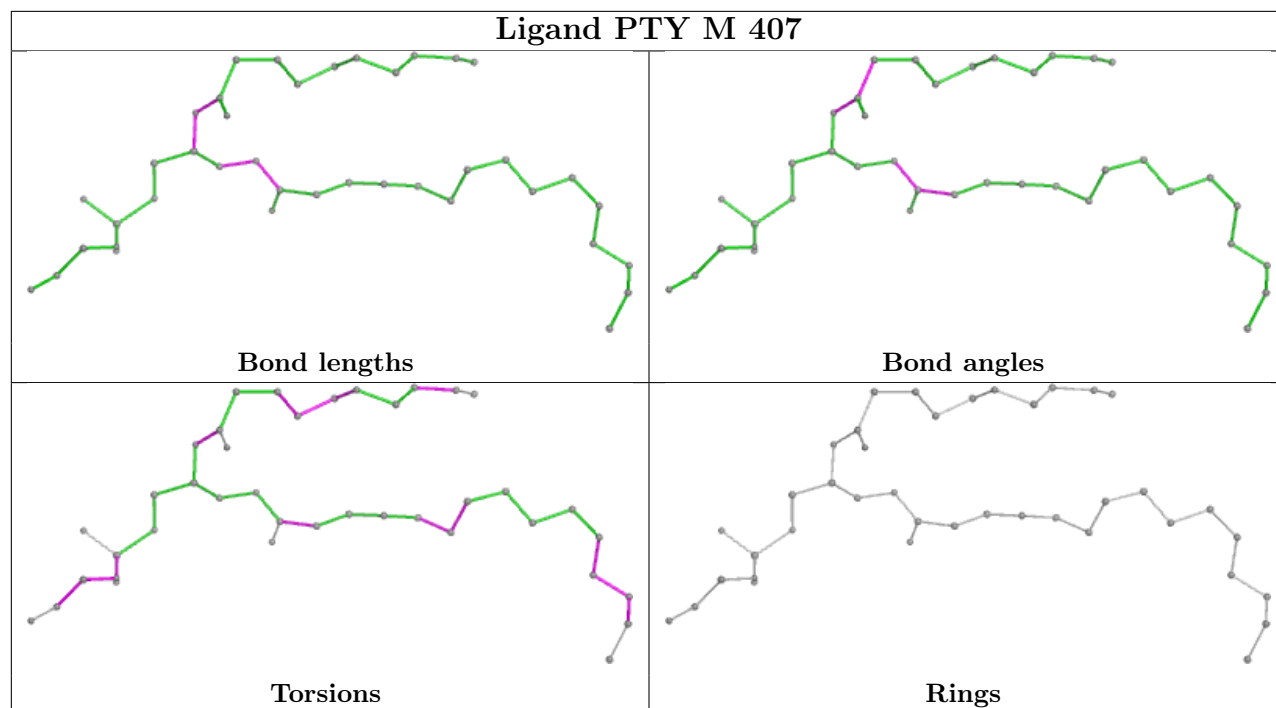


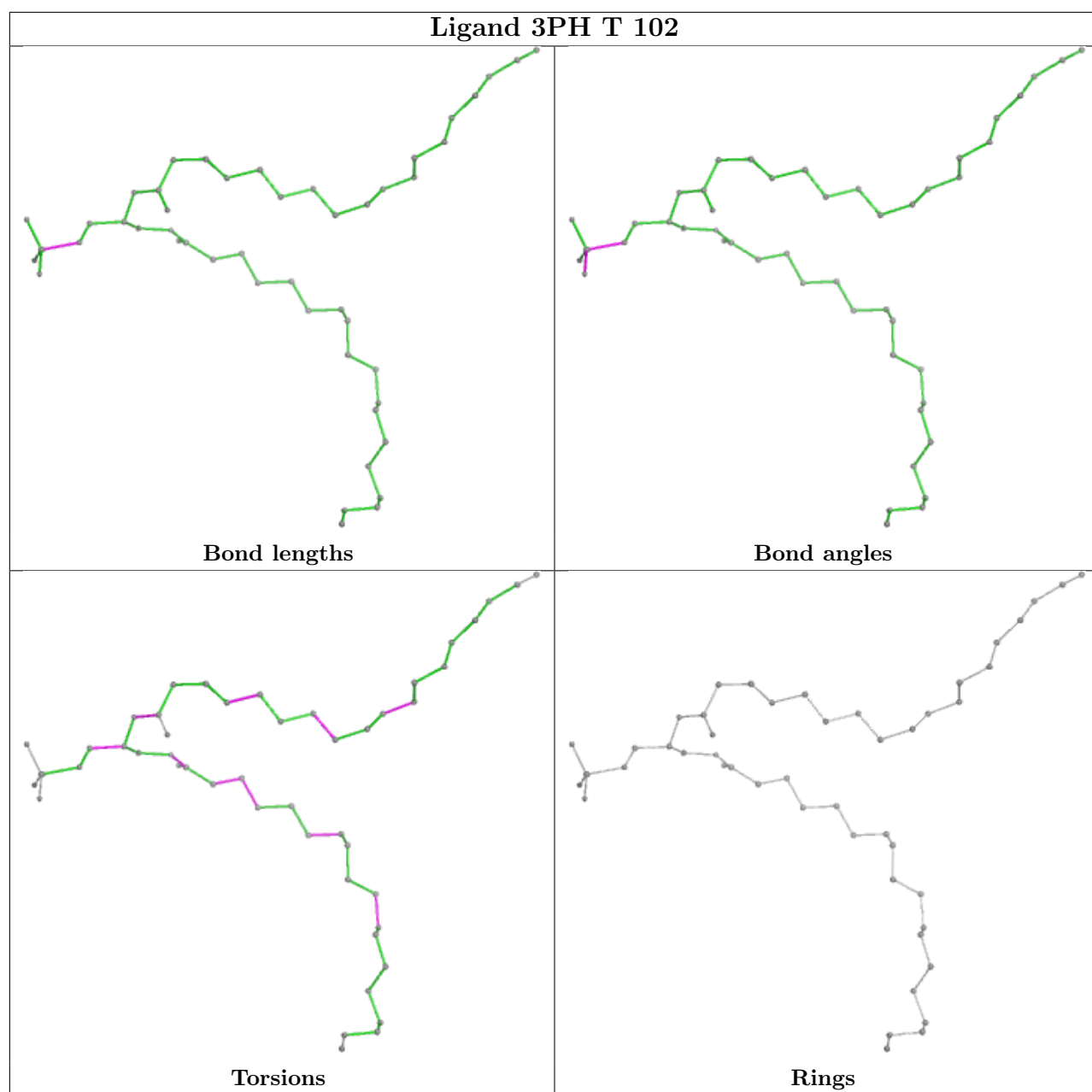


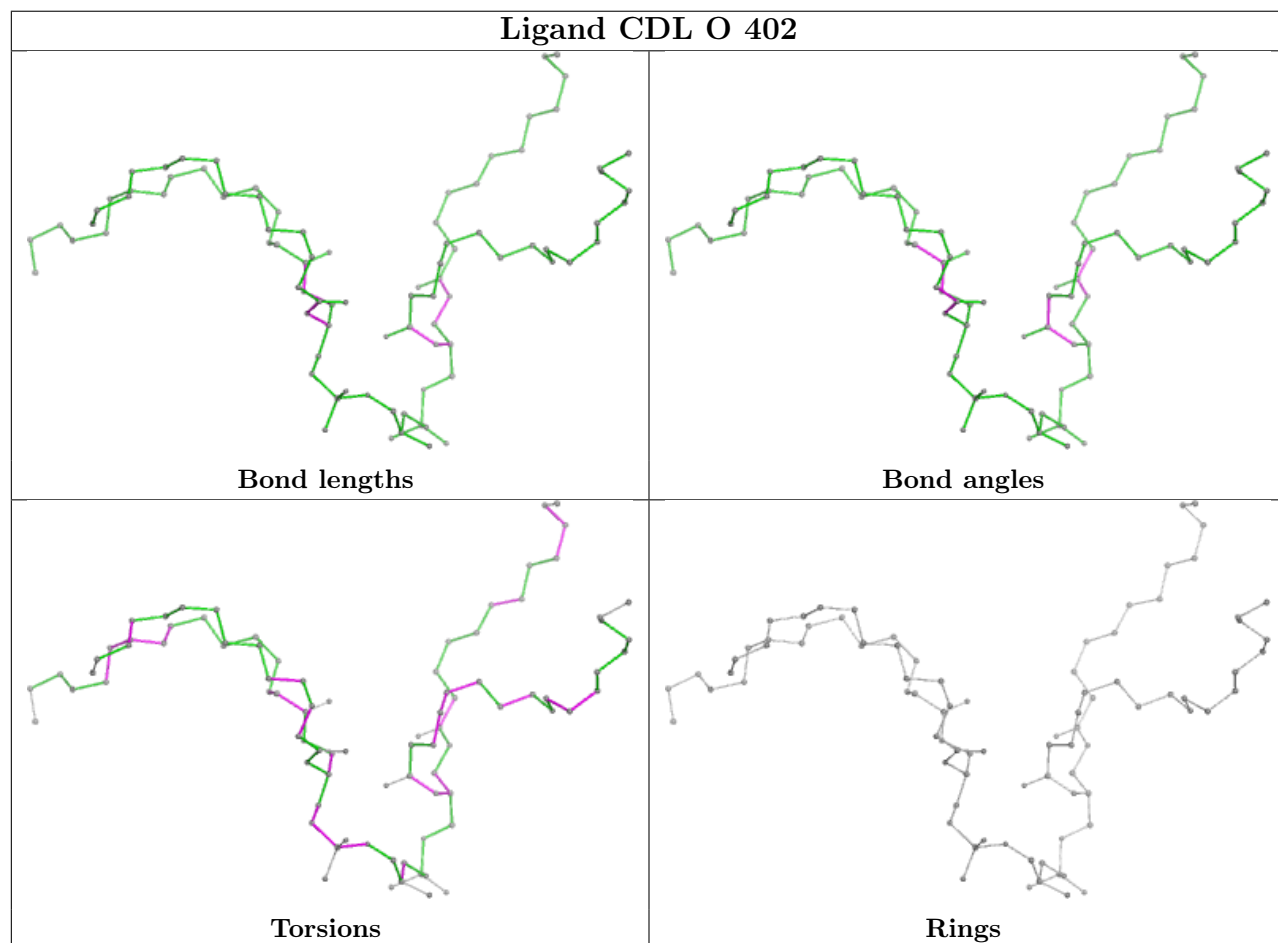
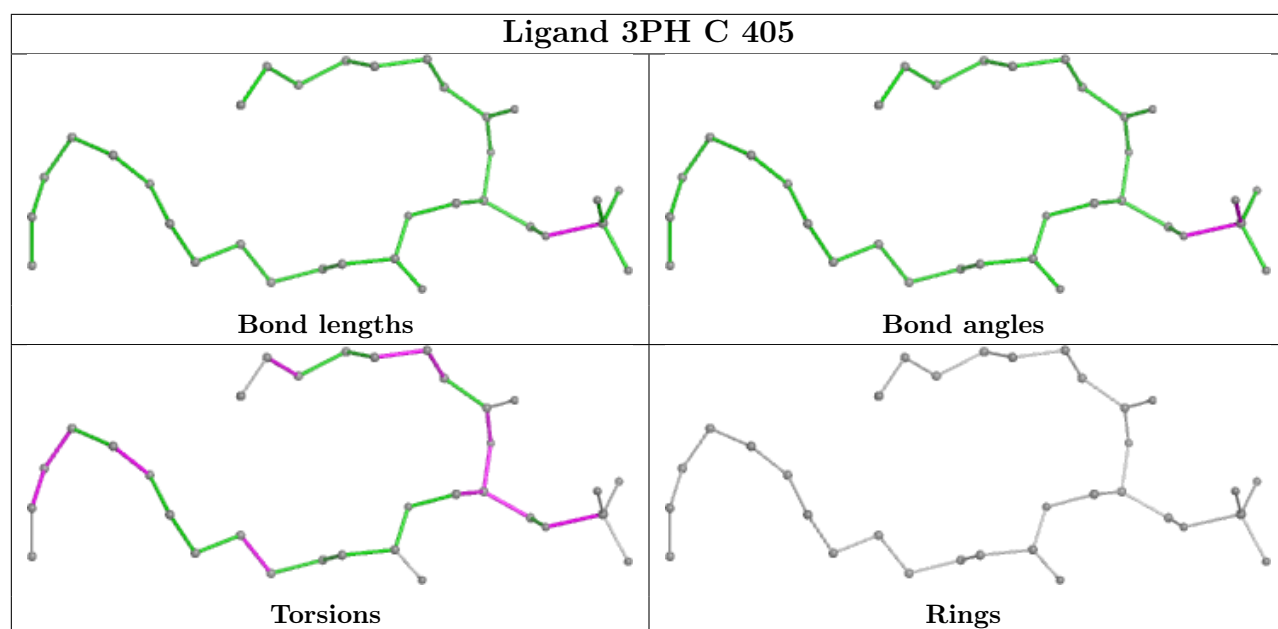


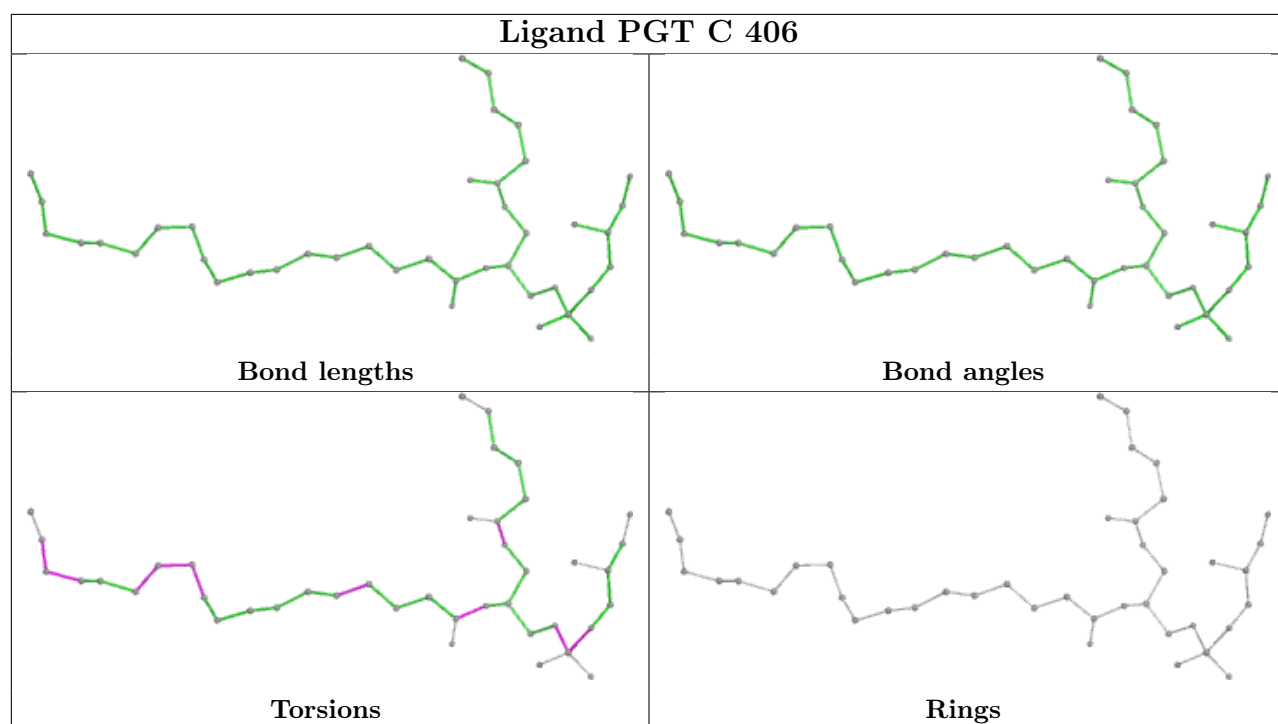


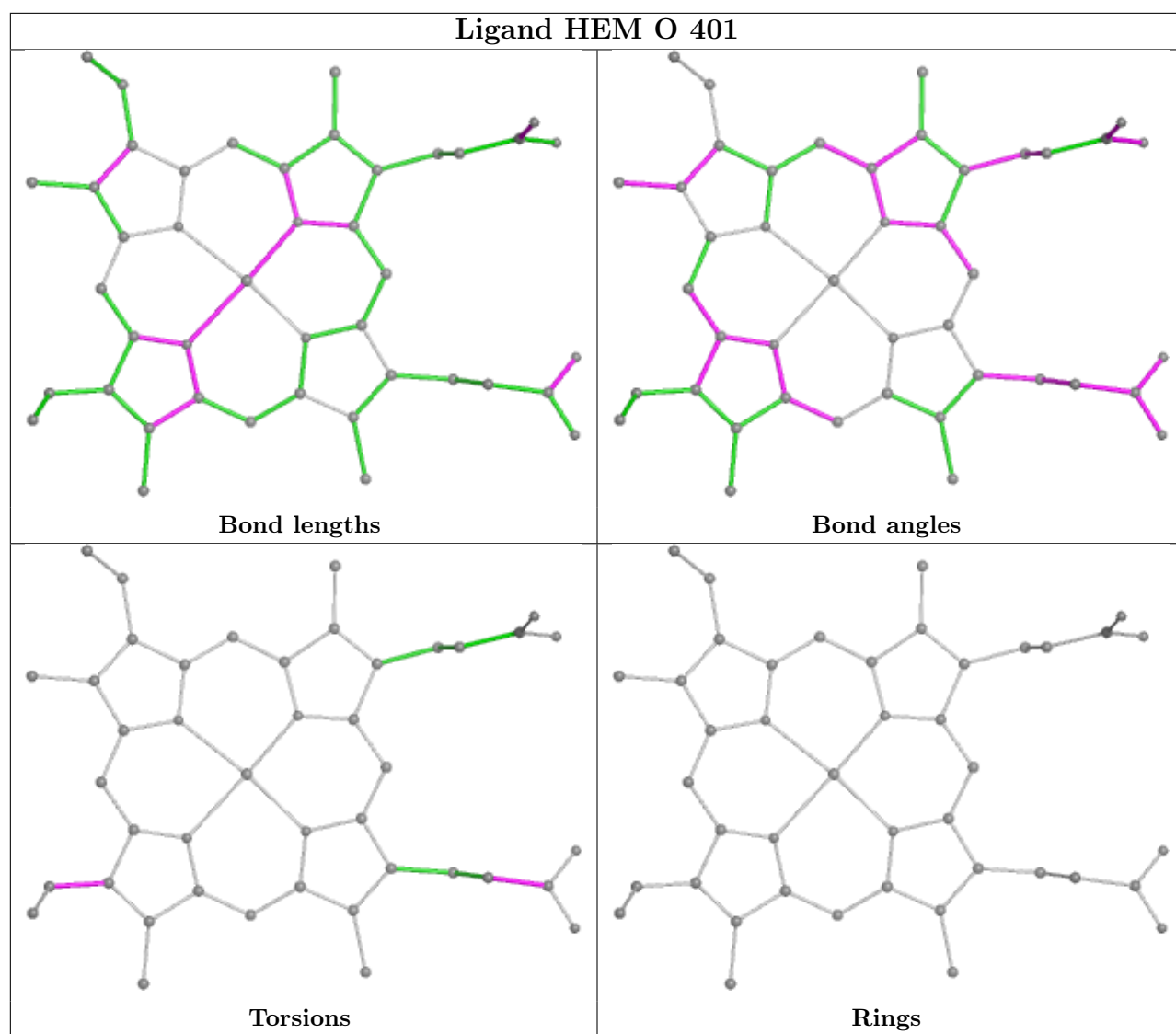




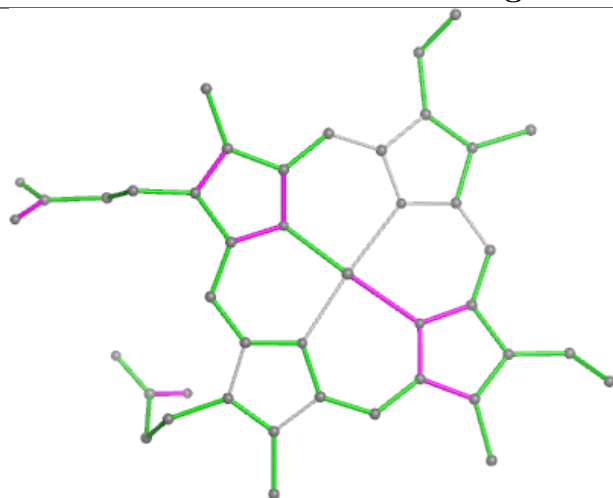




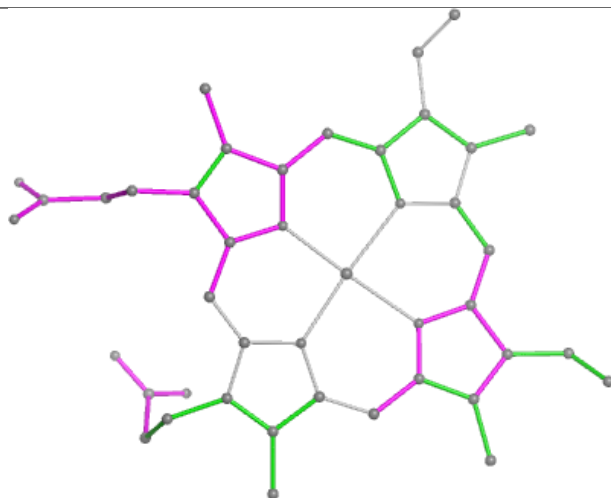




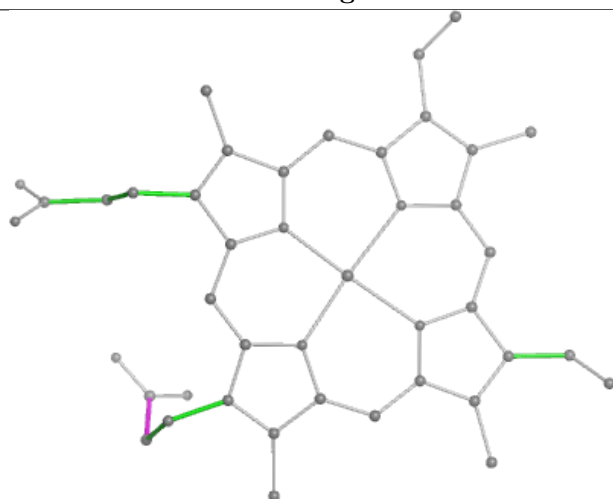
## Ligand HEM M 401



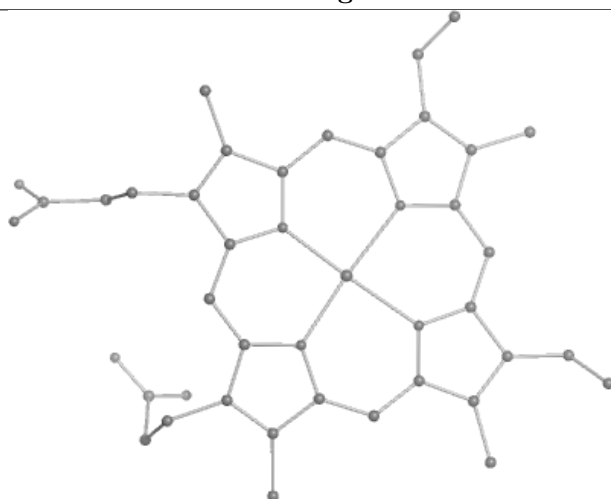
Bond lengths



Bond angles

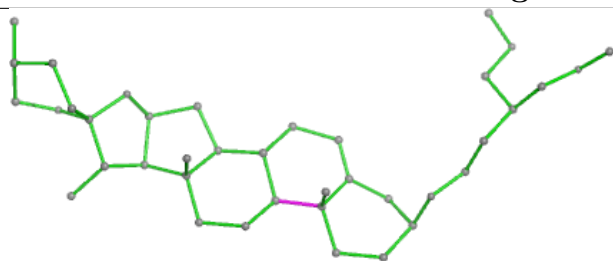


Torsions

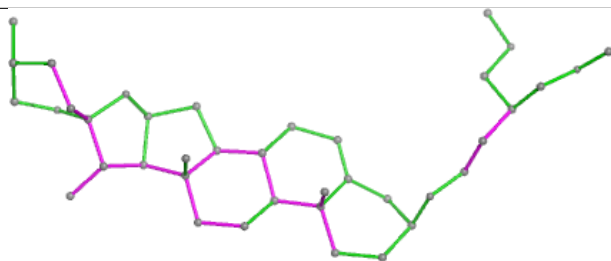


Rings

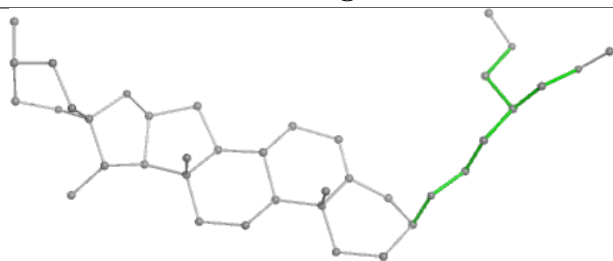
## Ligand Q7G M 411



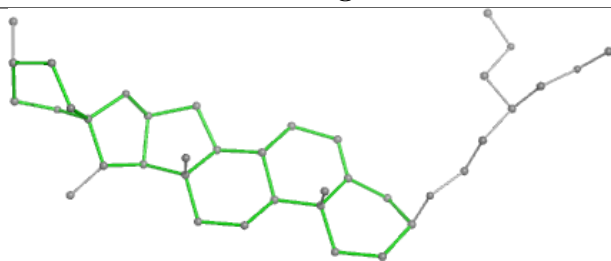
Bond lengths



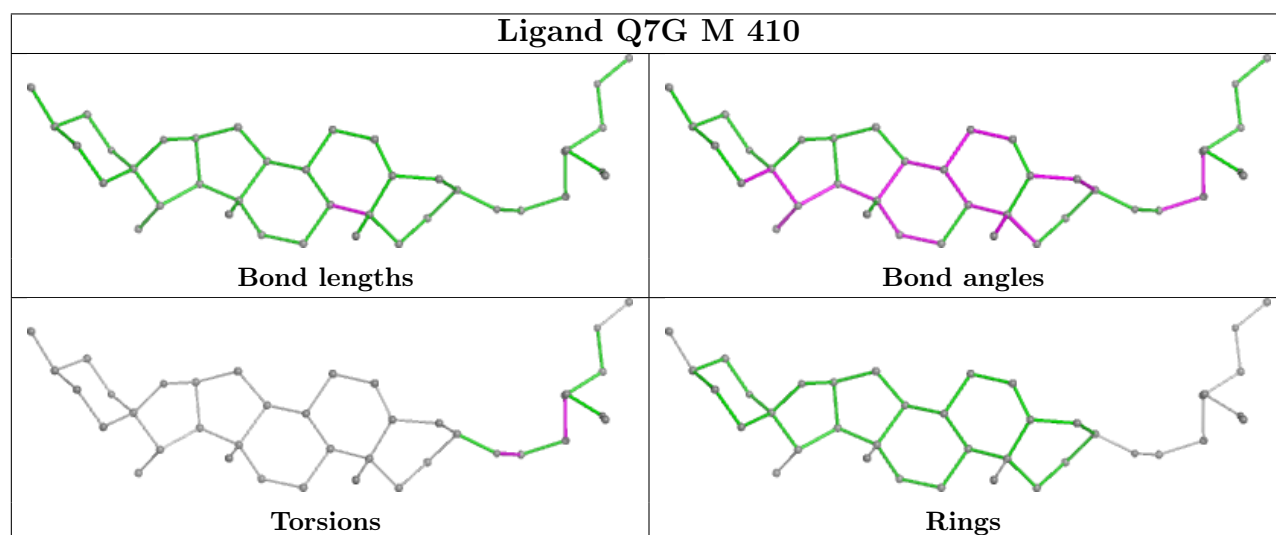
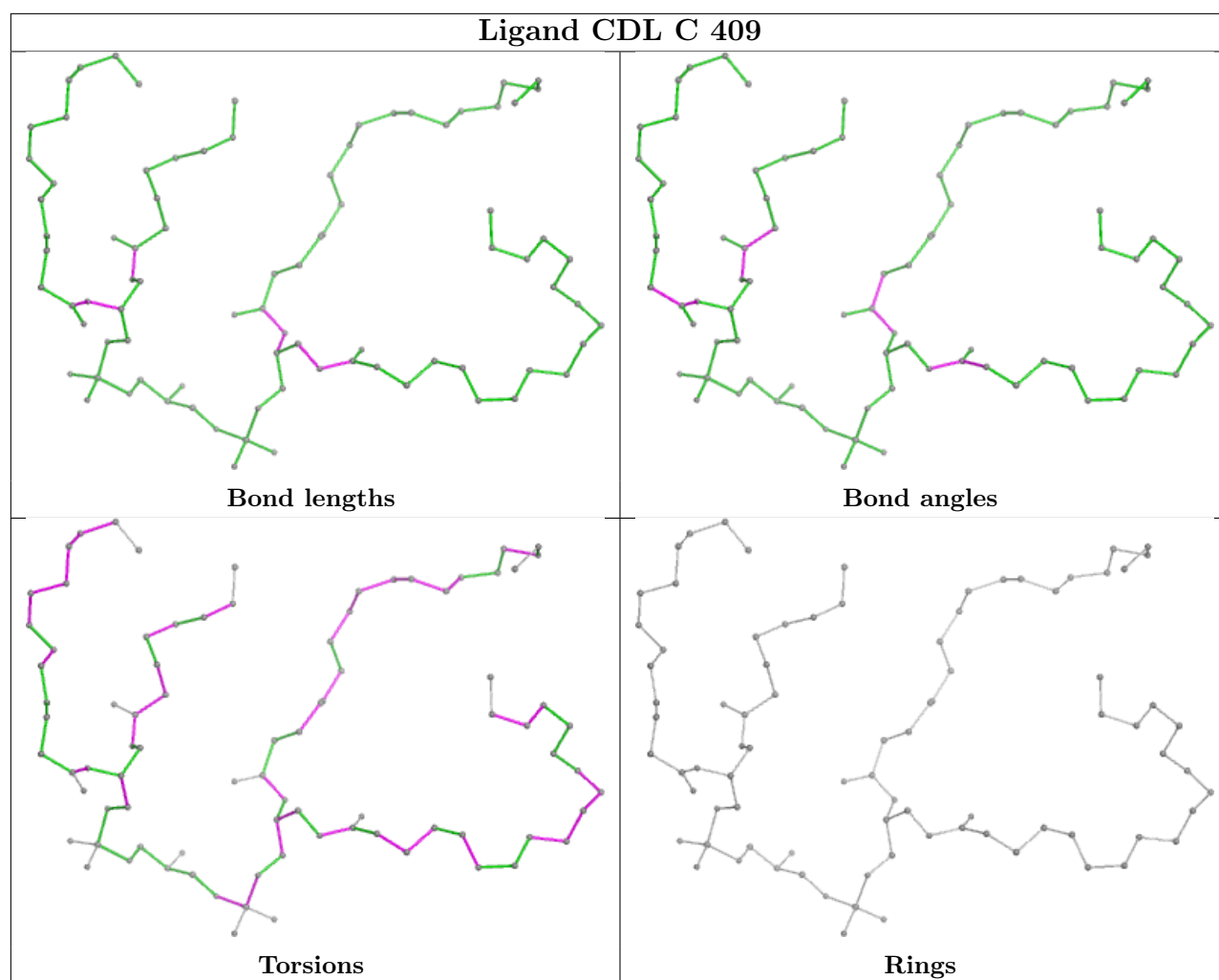
Bond angles

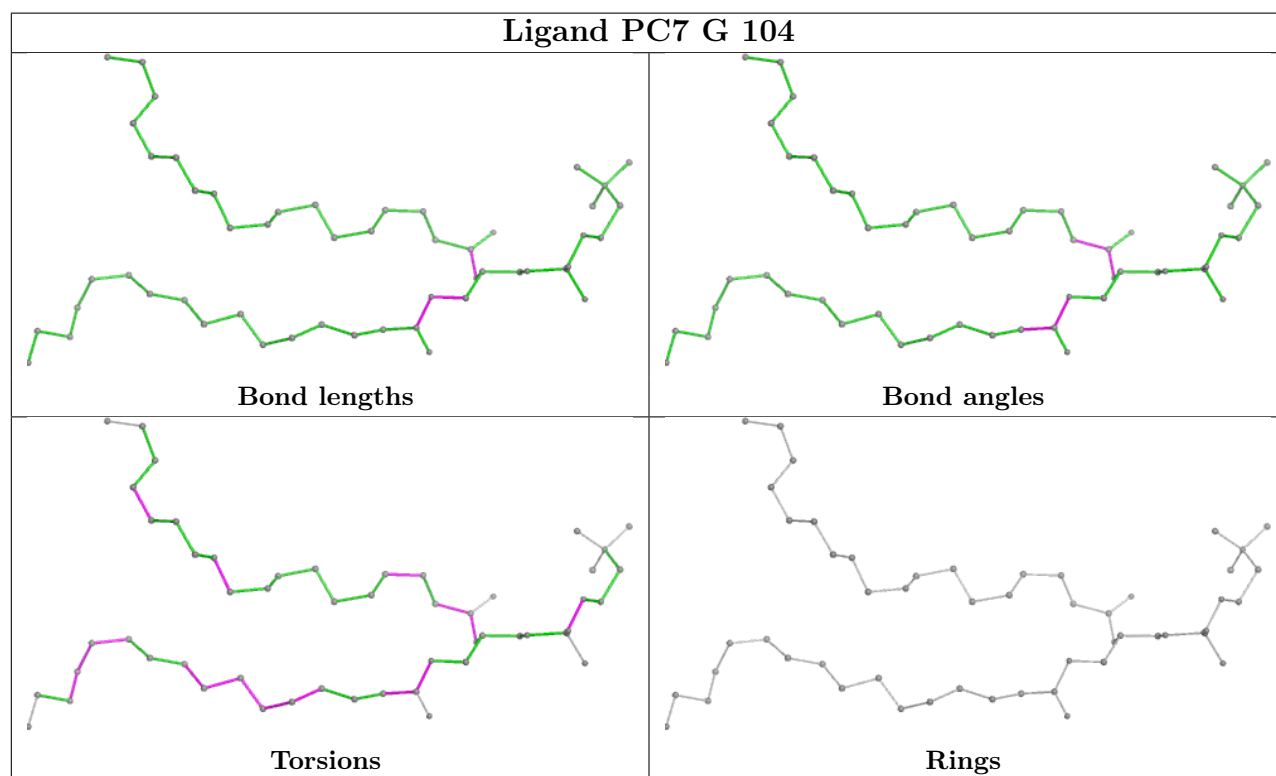
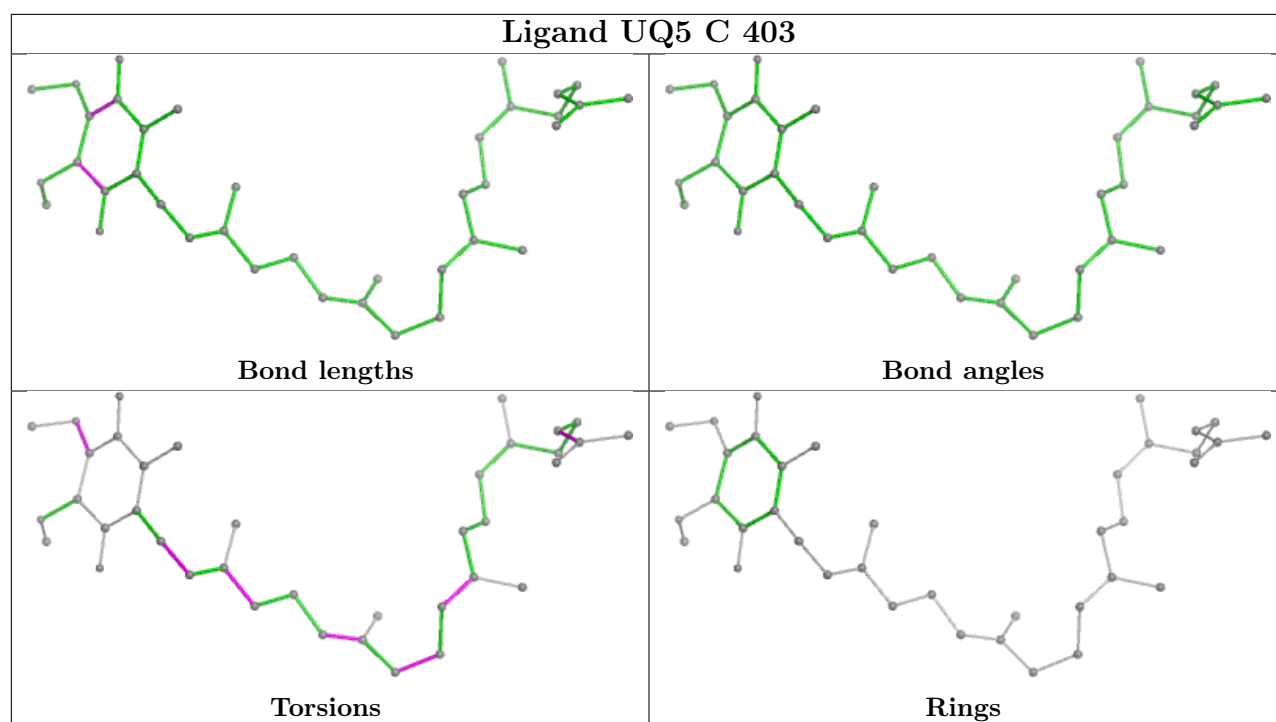


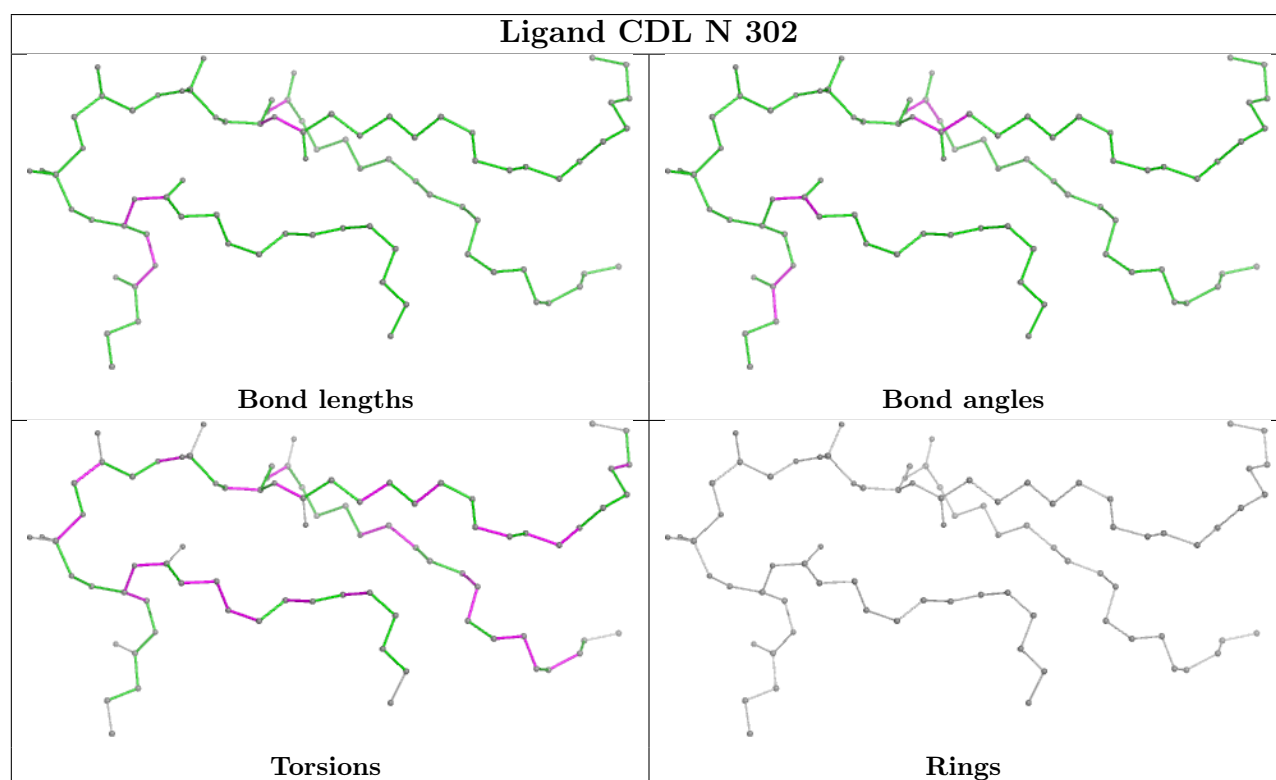
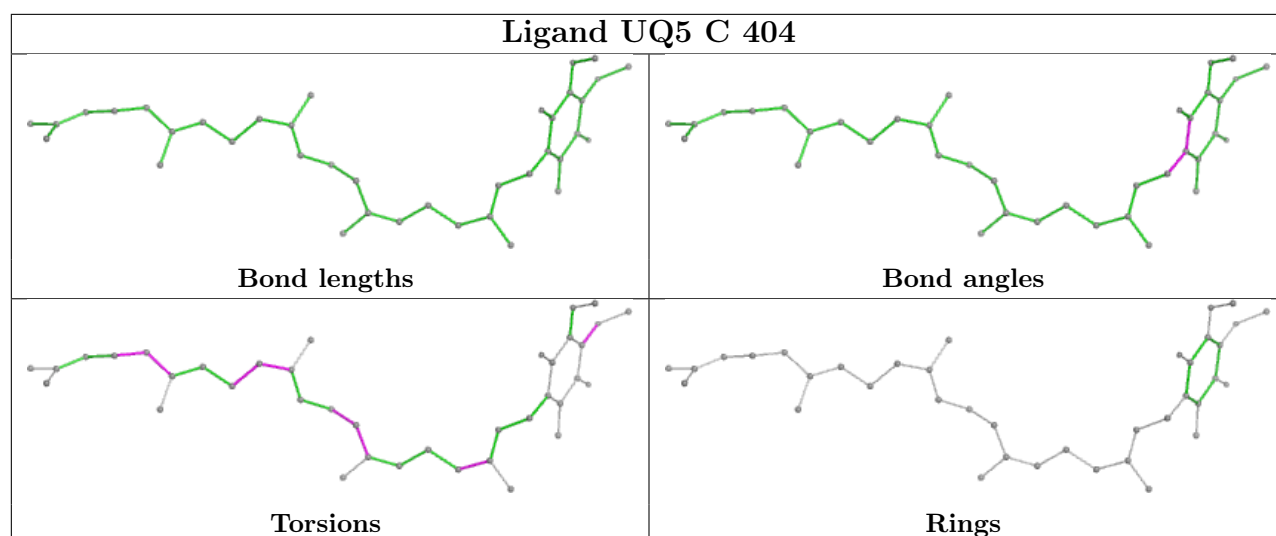
Torsions

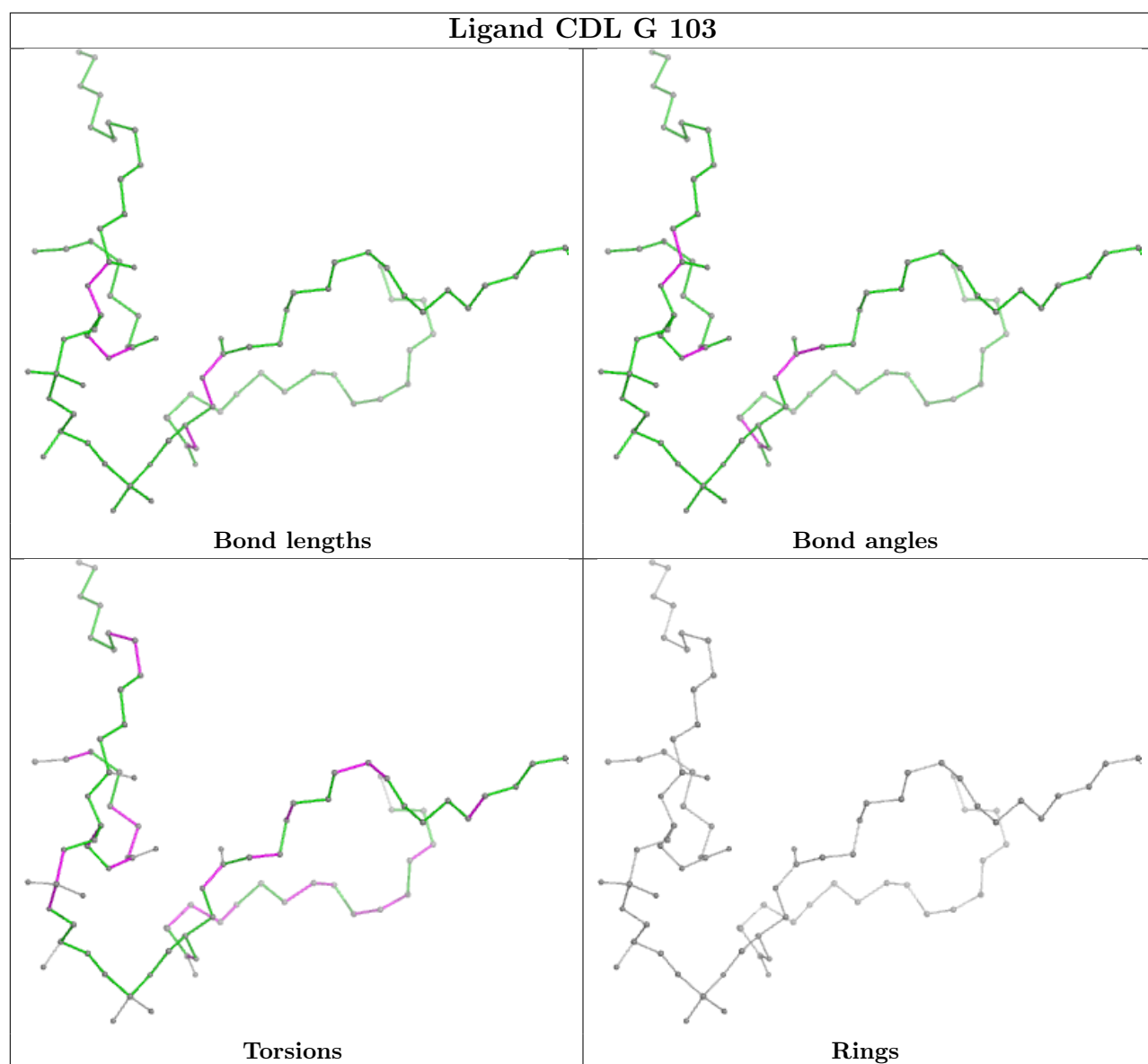


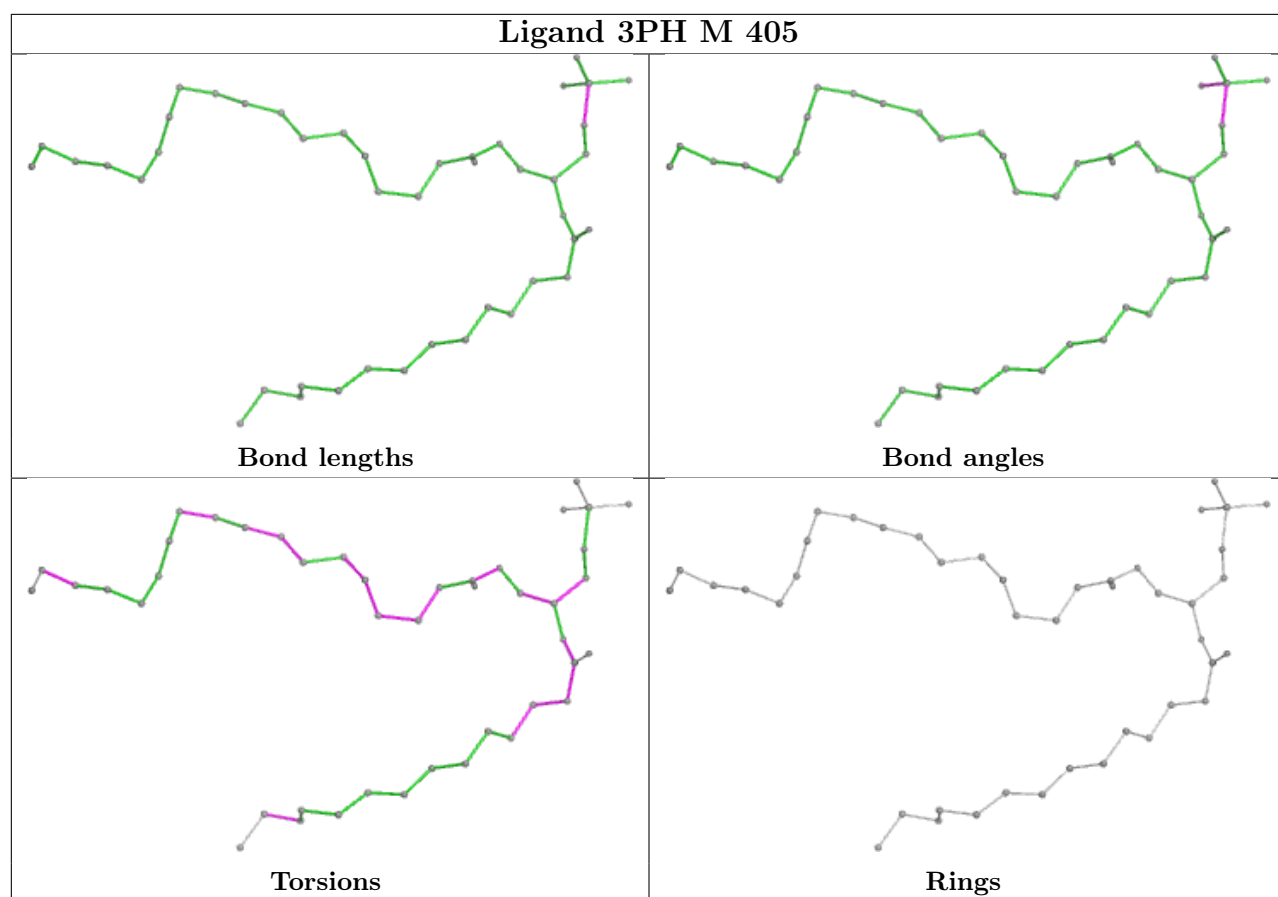
Rings

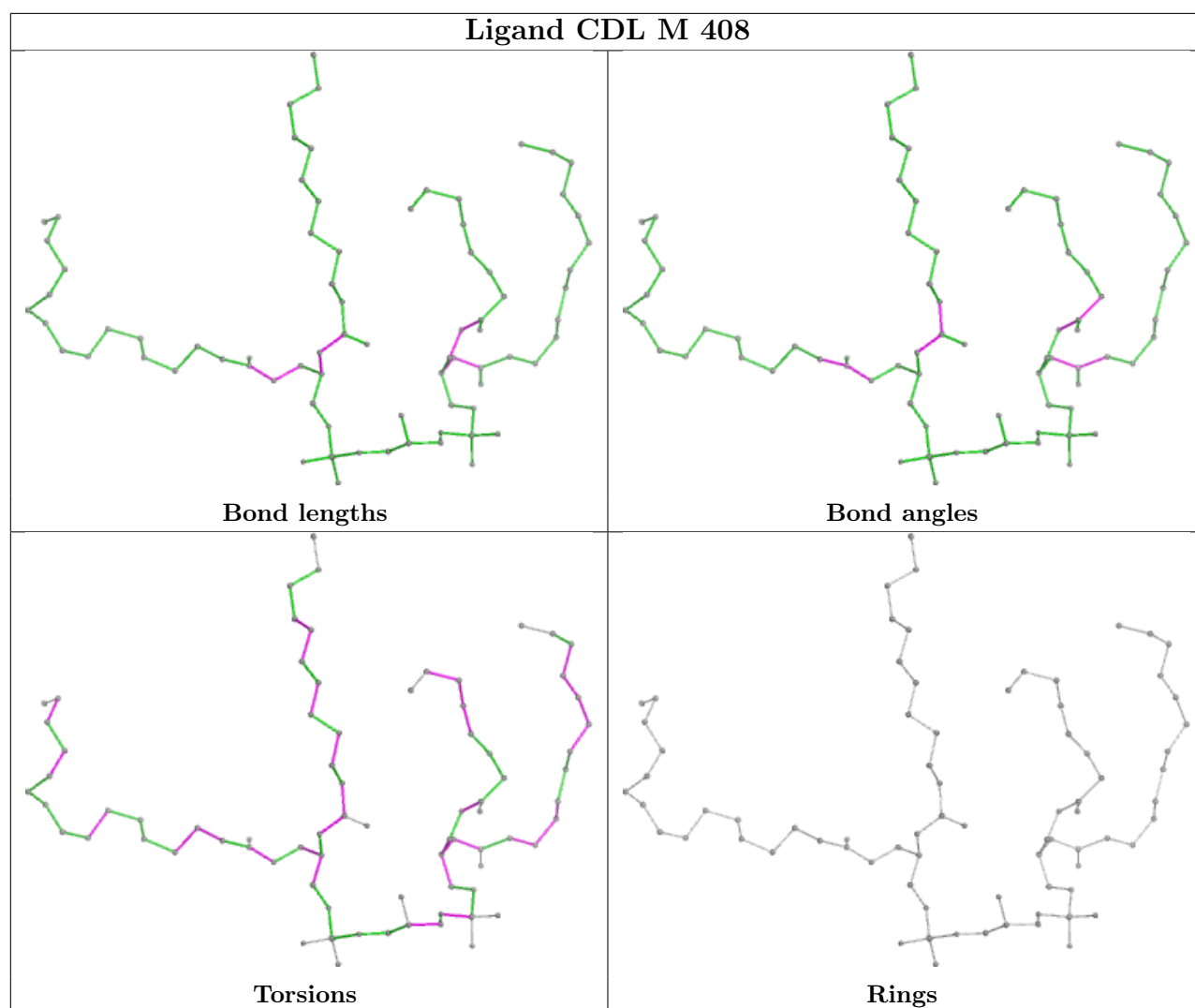


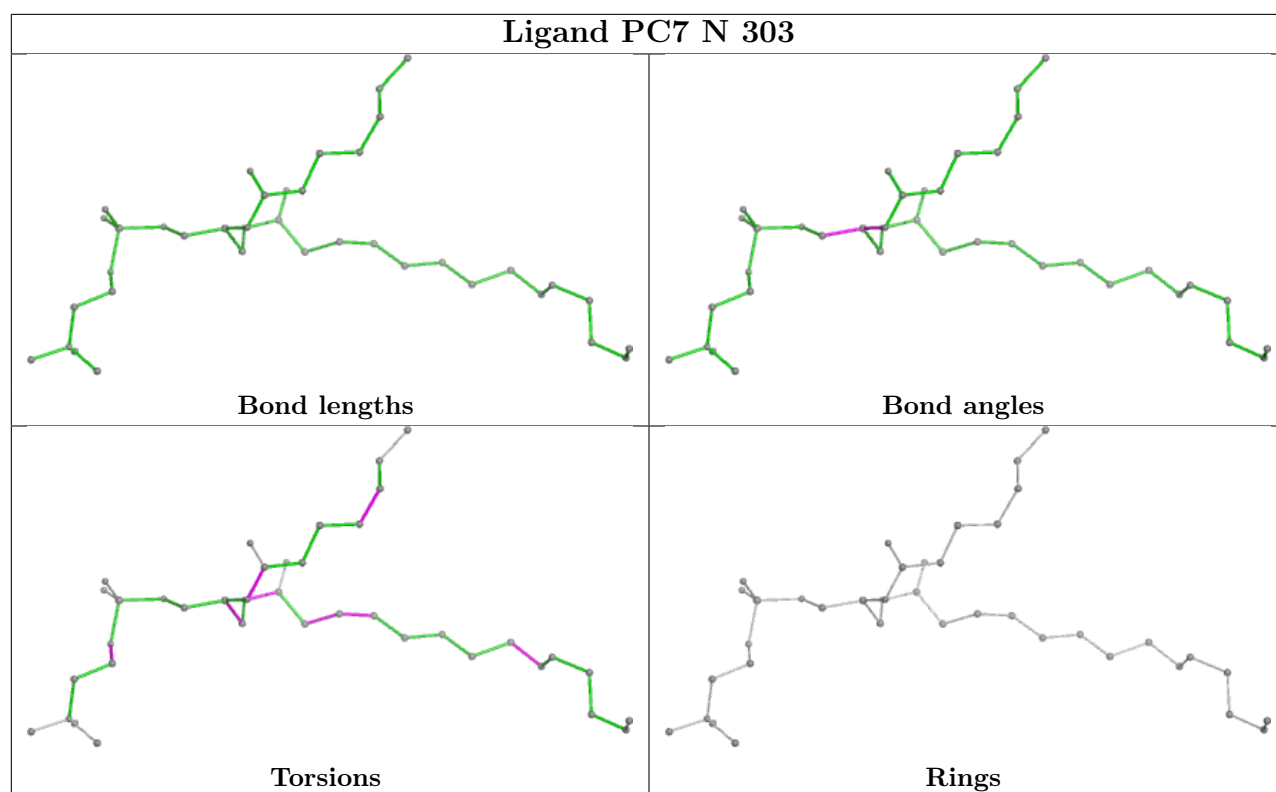


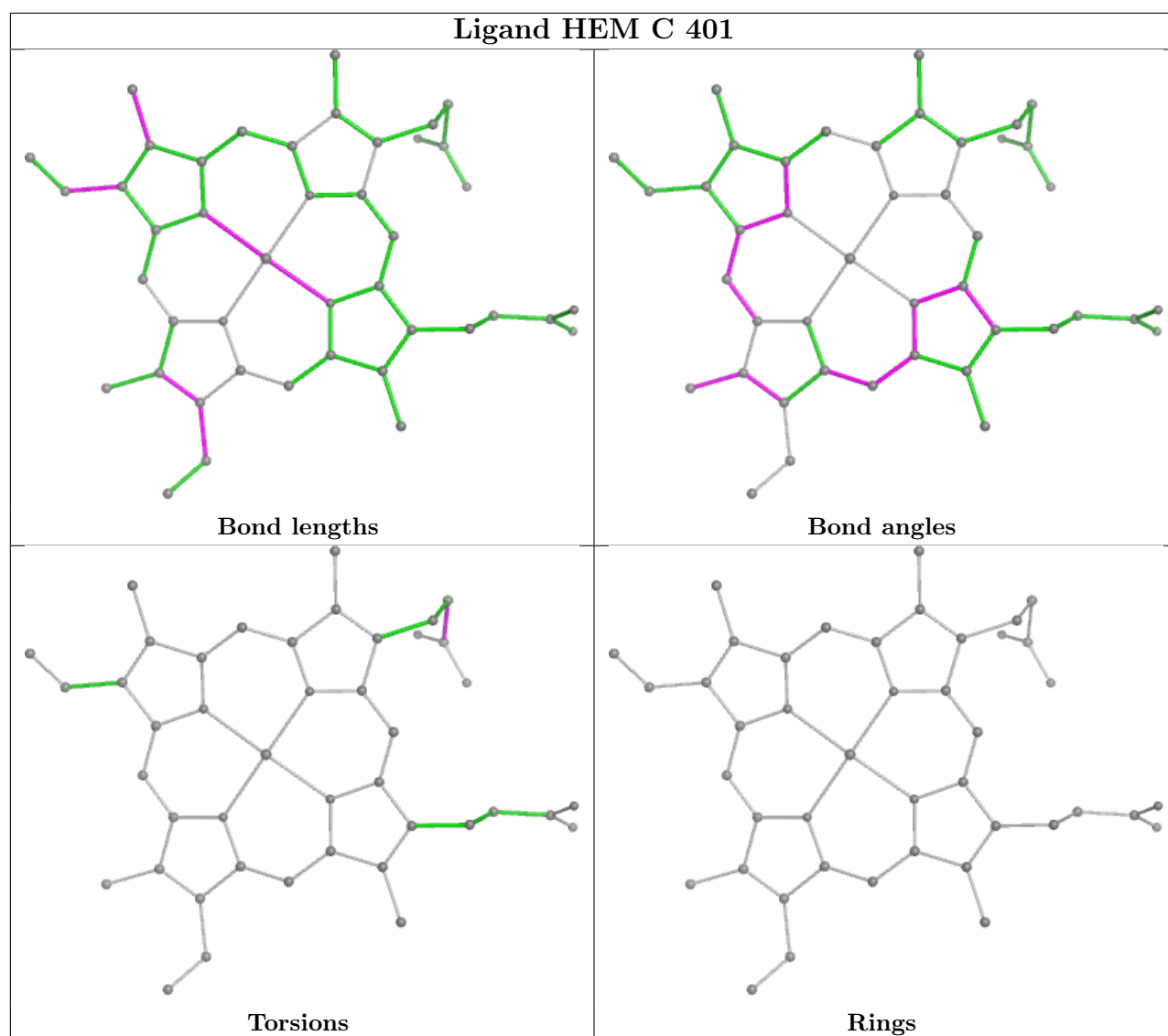












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

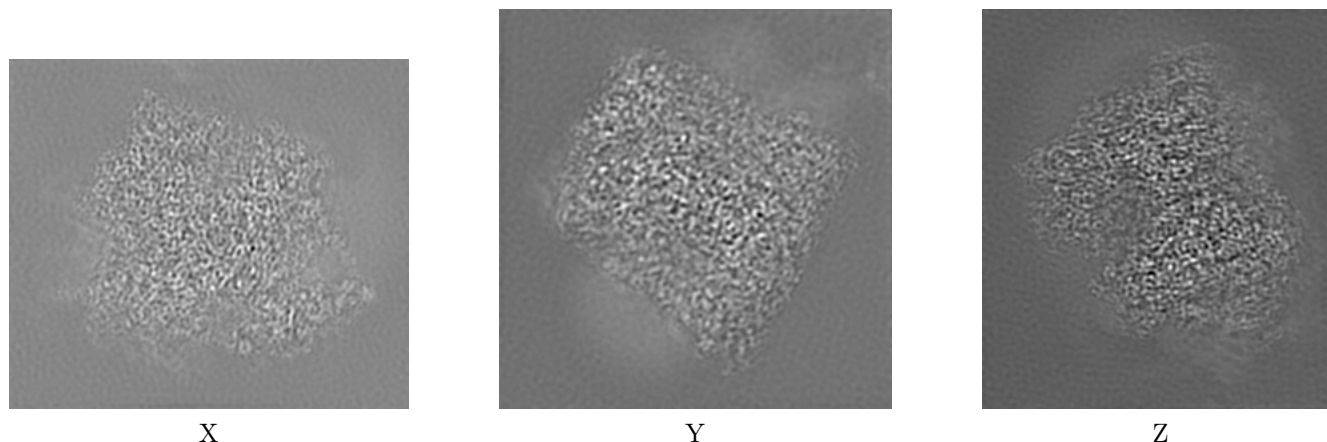
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16007. These allow visual inspection of the internal detail of the map and identification of artifacts.

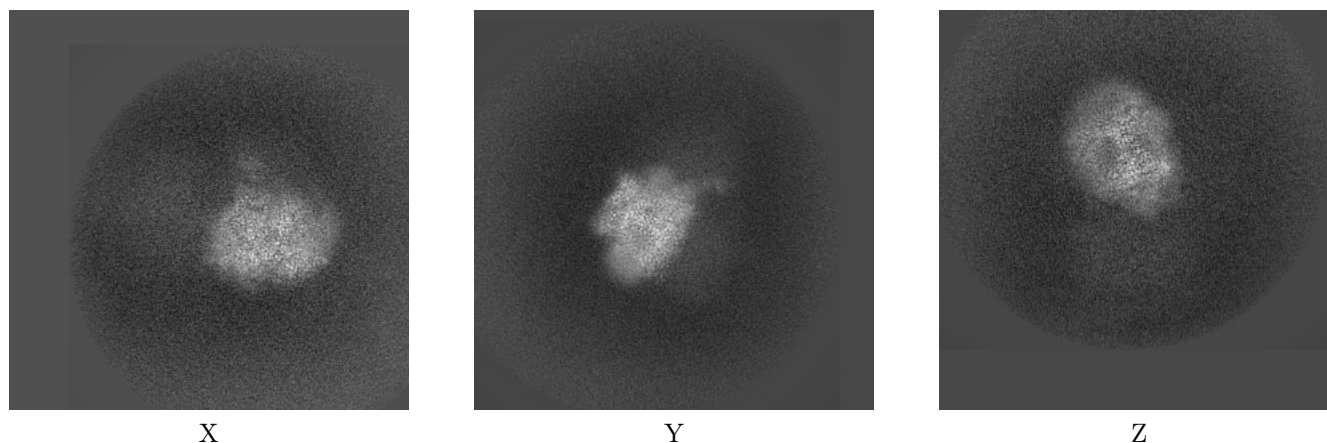
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



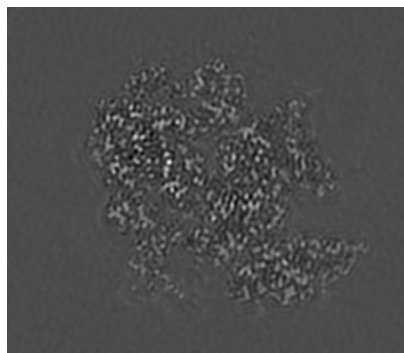
#### 6.1.2 Raw map



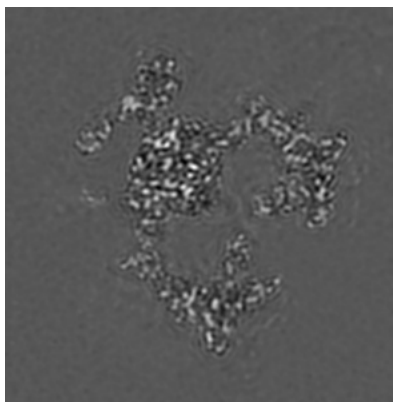
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

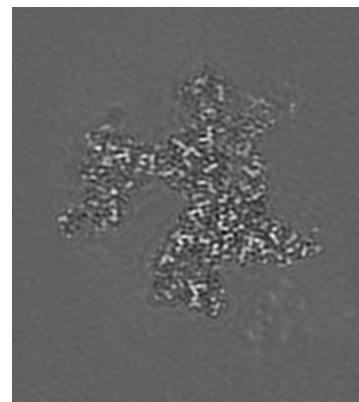
### 6.2.1 Primary map



X Index: 127

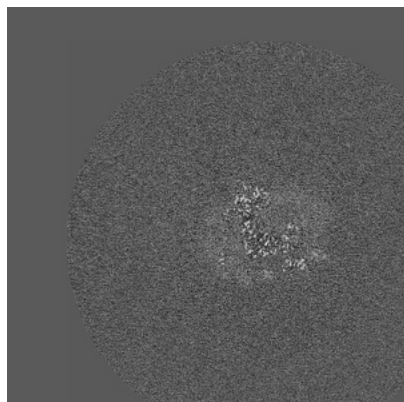


Y Index: 142

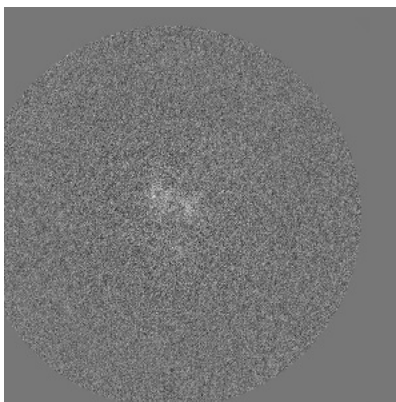


Z Index: 124

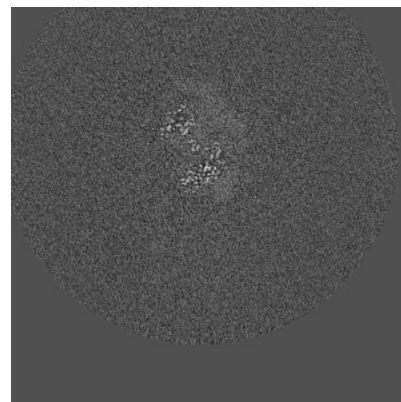
### 6.2.2 Raw map



X Index: 375



Y Index: 375

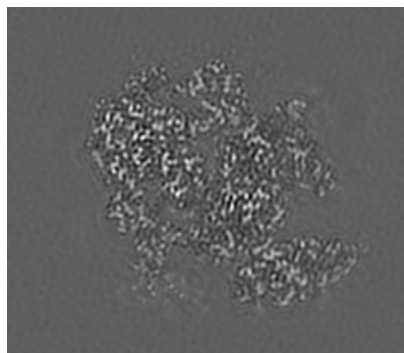


Z Index: 375

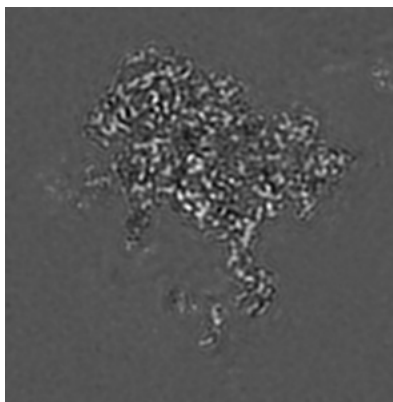
The images above show central slices of the map in three orthogonal directions.

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

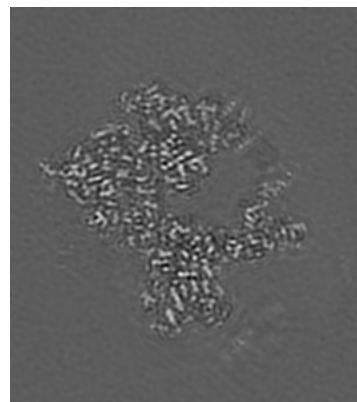
### 6.3.1 Primary map



X Index: 126

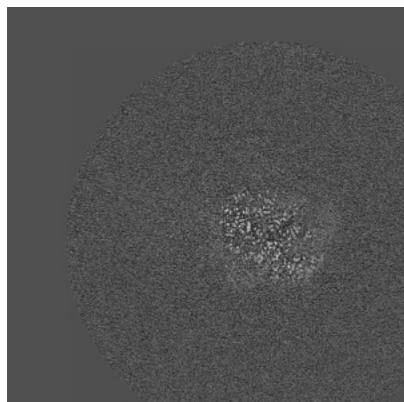


Y Index: 121

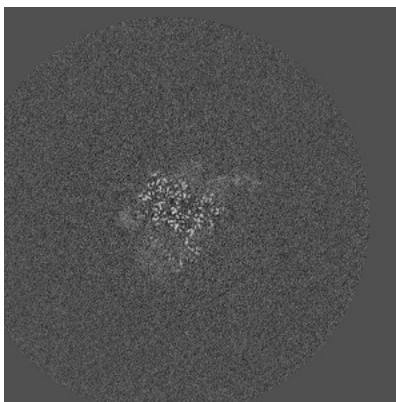


Z Index: 146

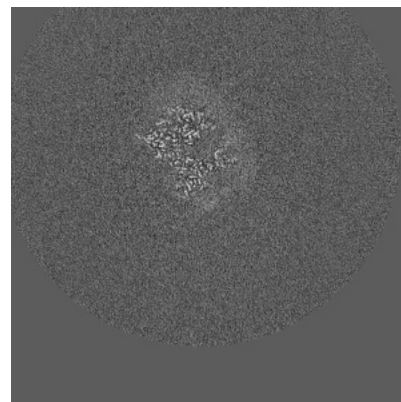
### 6.3.2 Raw map



X Index: 343



Y Index: 458

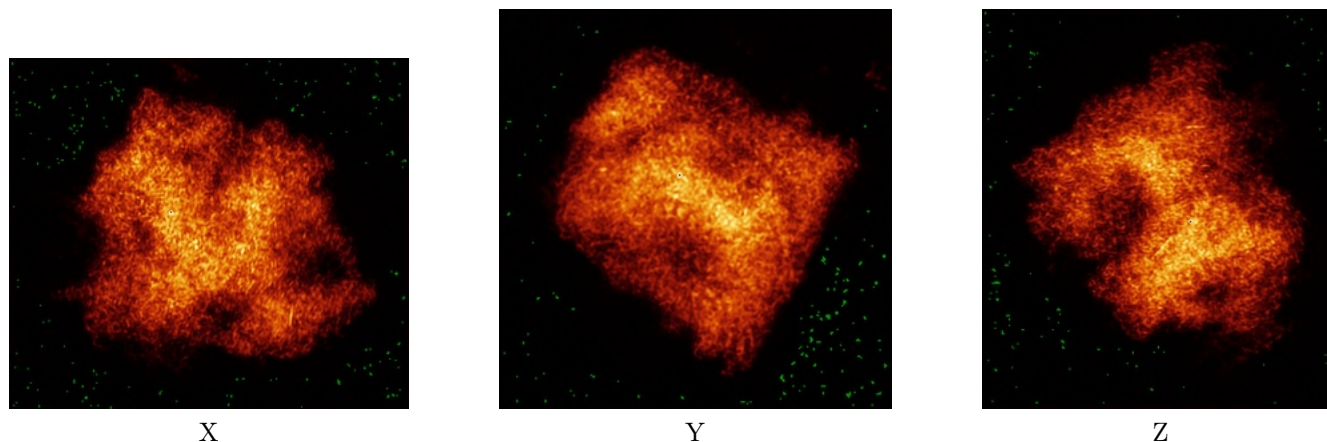


Z Index: 344

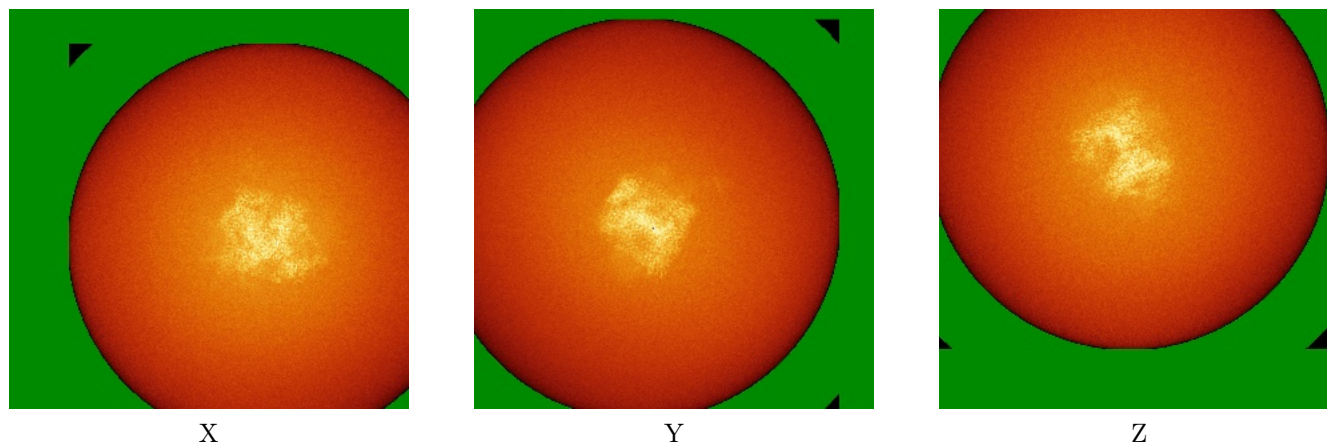
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



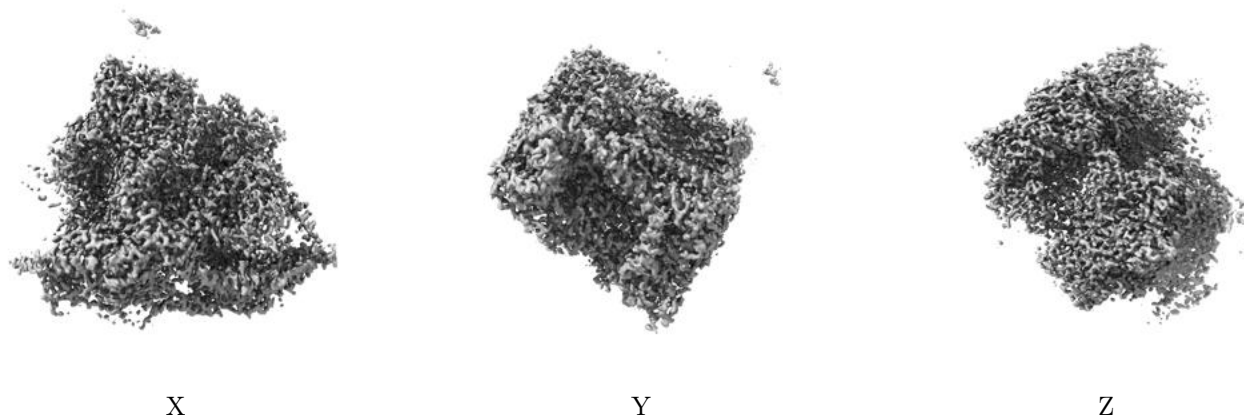
### 6.4.2 Raw map



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

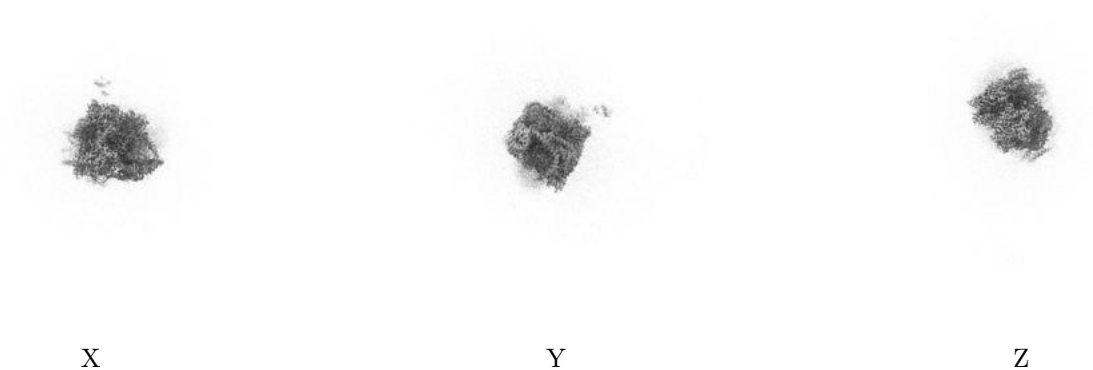
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

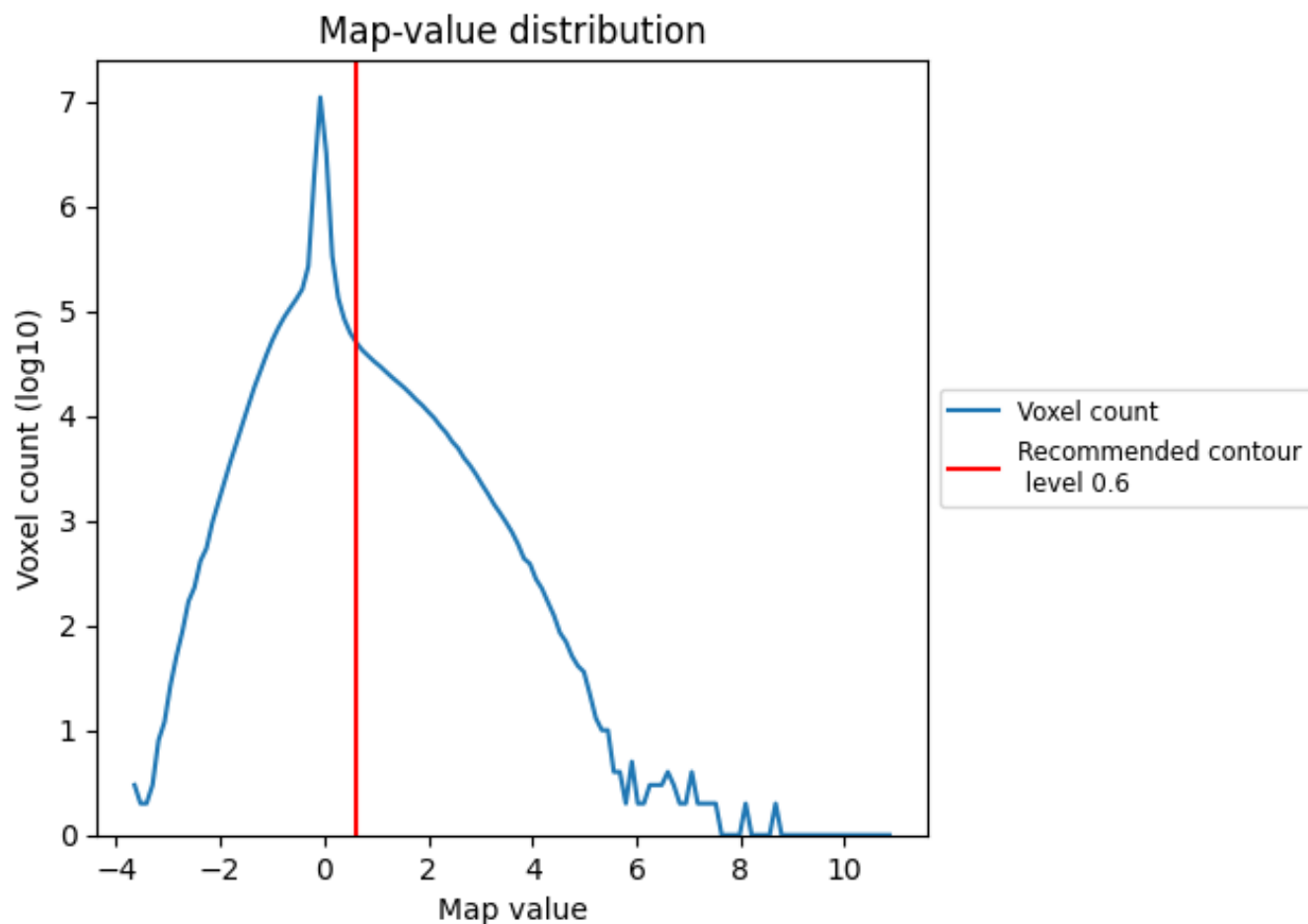
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

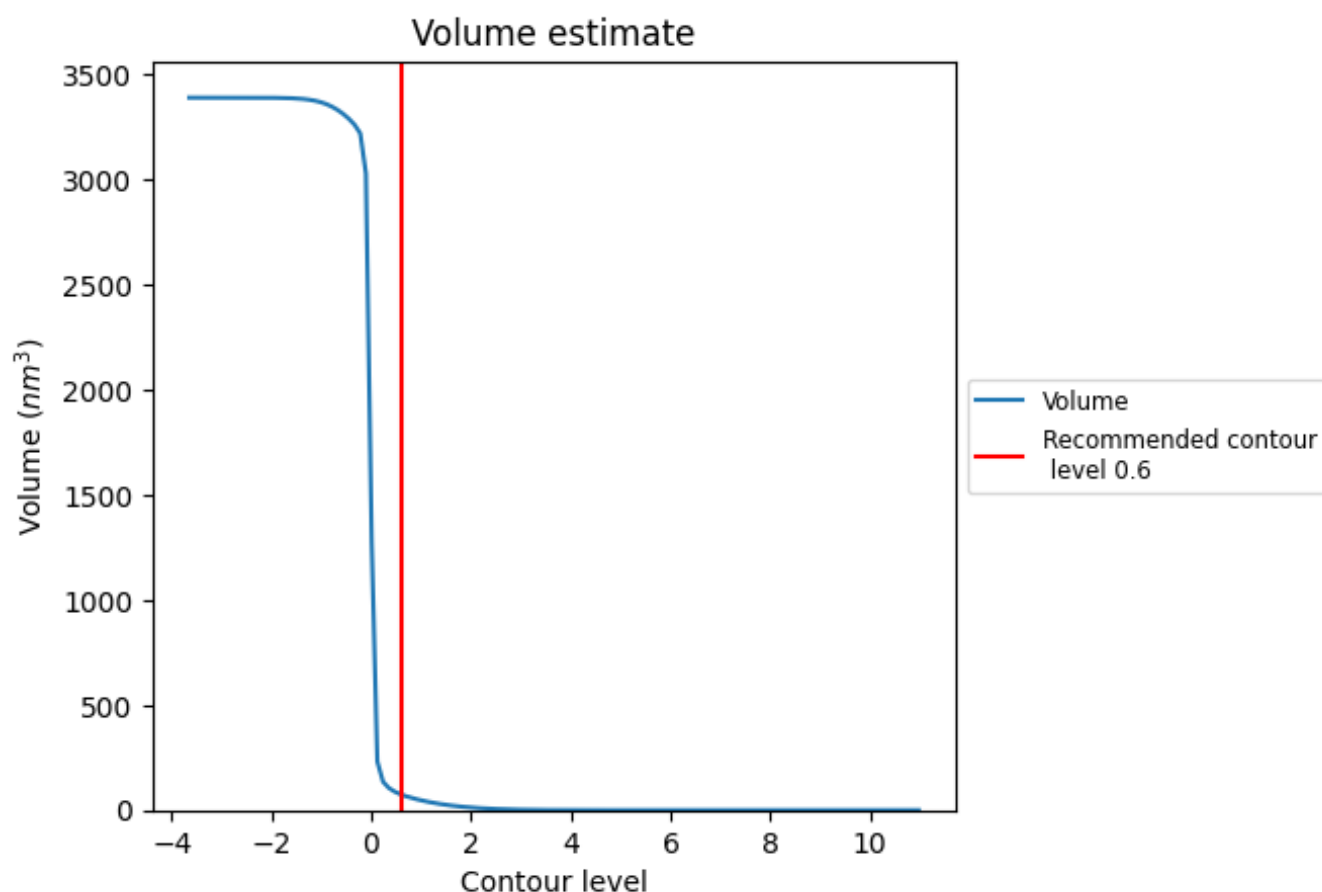
This section contains the results of statistical analysis of the map.

### 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 75 nm<sup>3</sup>; this corresponds to an approximate mass of 68 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

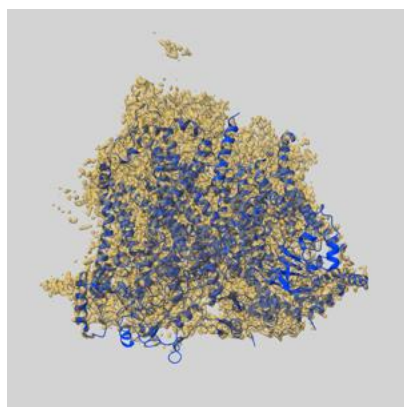
## 8 Fourier-Shell correlation

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

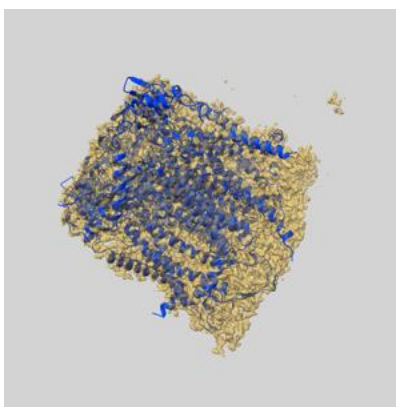
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16007 and PDB model 8BEL. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

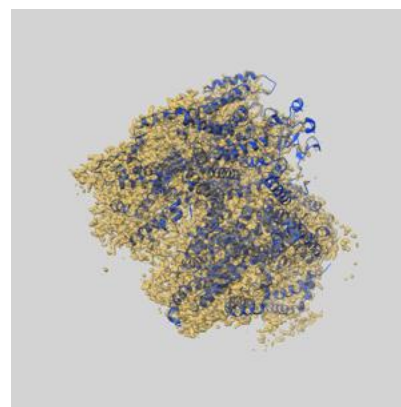
### 9.1 Map-model overlay [i](#)



X



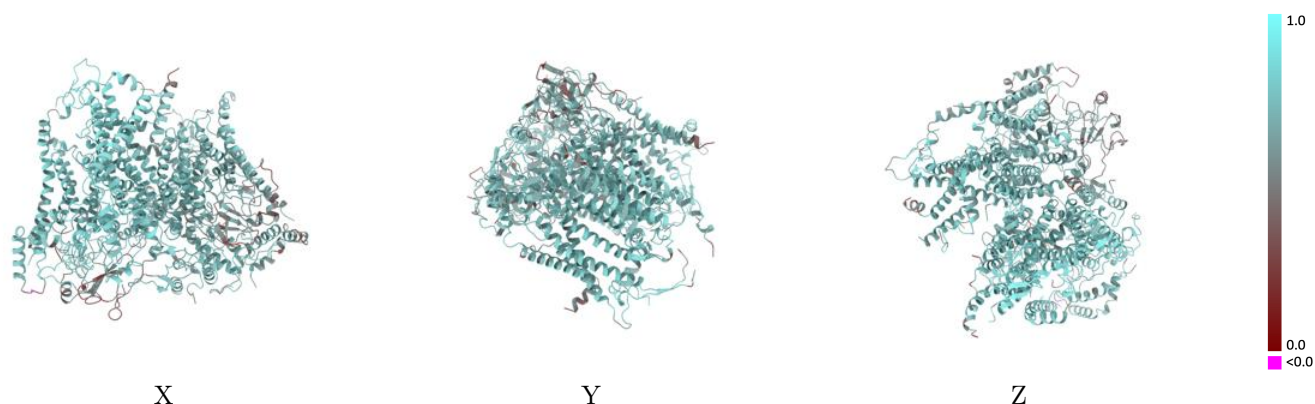
Y



Z

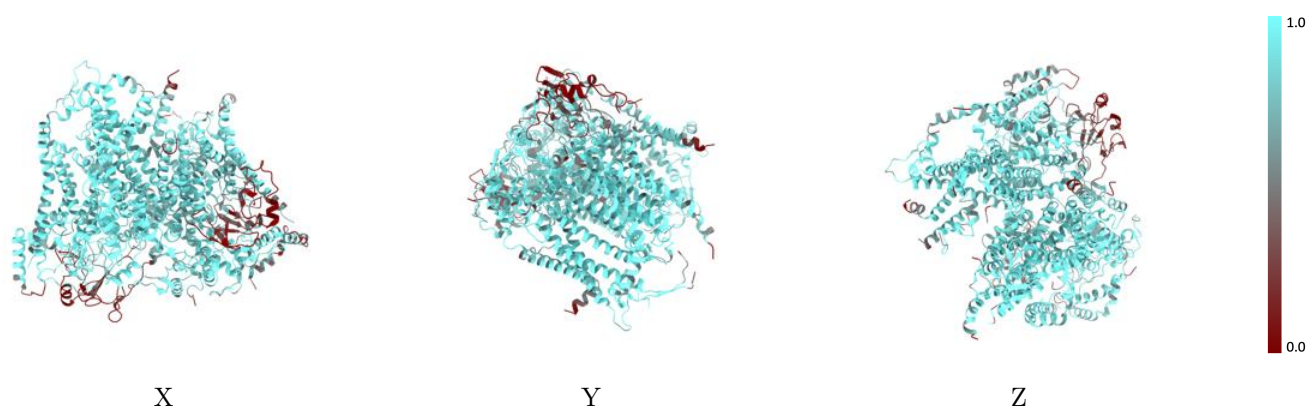
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



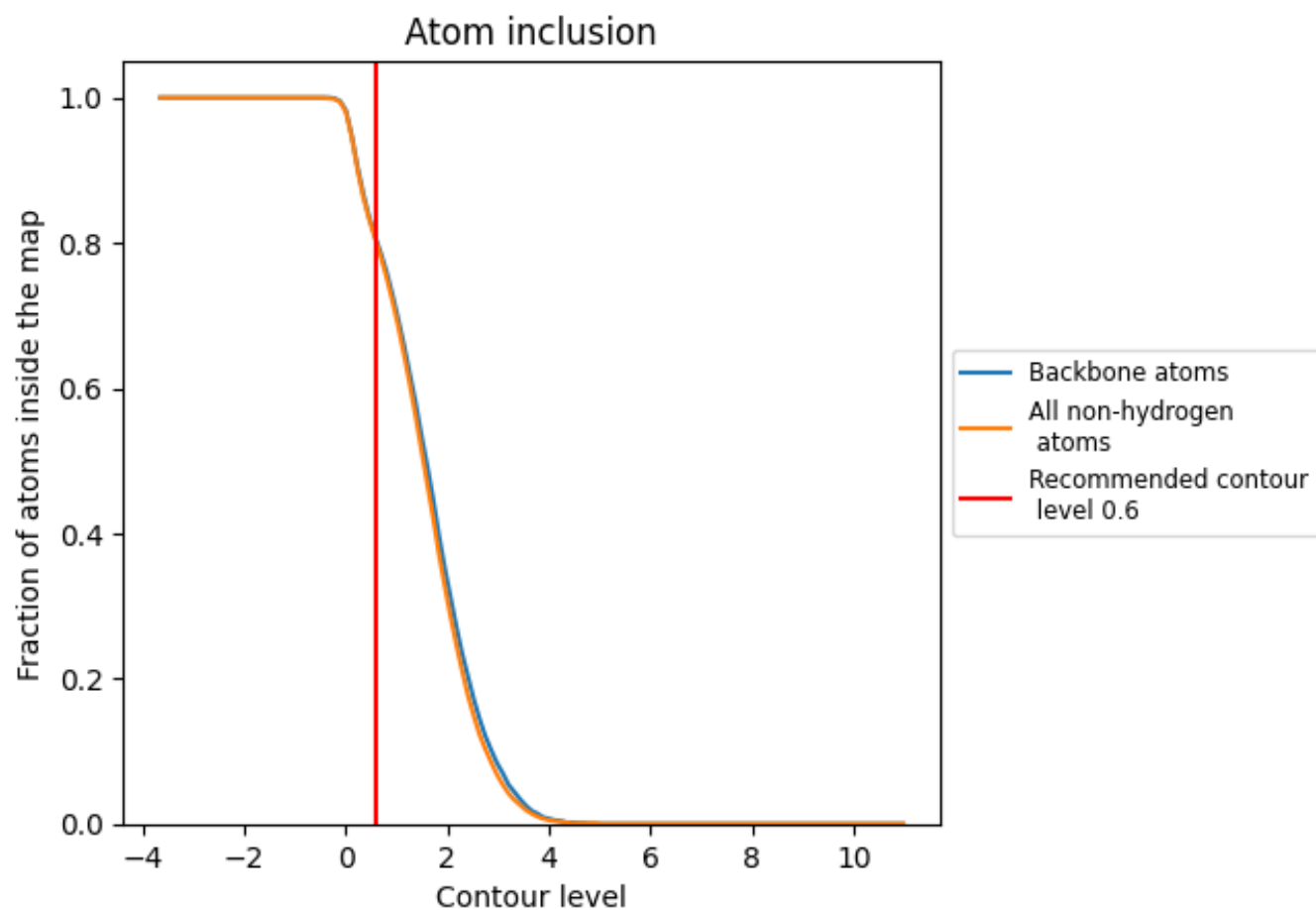
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8020	<div></div> 0.6820
C	<div></div> 0.9050	<div></div> 0.7310
D	<div></div> 0.5210	<div></div> 0.5940
E	<div></div> 0.9330	<div></div> 0.7410
G	<div></div> 0.7630	<div></div> 0.6610
H	<div></div> 0.7980	<div></div> 0.6640
I	<div></div> 0.8270	<div></div> 0.7040
J	<div></div> 0.4560	<div></div> 0.5700
M	<div></div> 0.8830	<div></div> 0.7050
N	<div></div> 0.5570	<div></div> 0.5950
O	<div></div> 0.8840	<div></div> 0.7010
Q	<div></div> 0.7650	<div></div> 0.6440
R	<div></div> 0.6490	<div></div> 0.5850
S	<div></div> 0.7690	<div></div> 0.6440
T	<div></div> 0.5490	<div></div> 0.6090

