



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 09:32 PM EST

PDB ID : 7JRG
EMDB ID : EMD-22445
Title : Plant Mitochondrial complex III2 from *Vigna radiata*
Authors : Maldonado, M.; Letts, J.A.
Deposited on : 2020-08-12
Resolution : 3.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

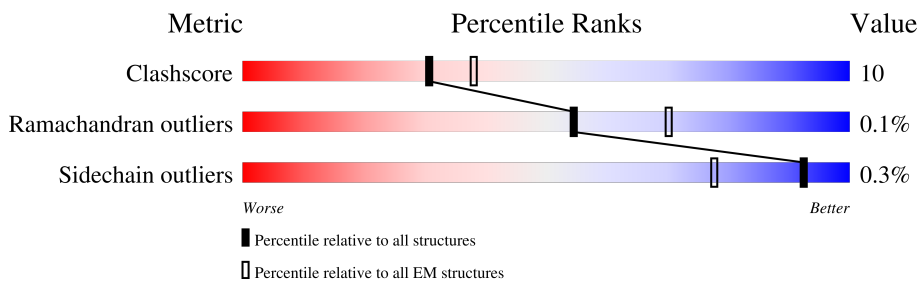
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	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	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 32930 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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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	77	Total	C	N	O	S	0	0
			597	392	100	104	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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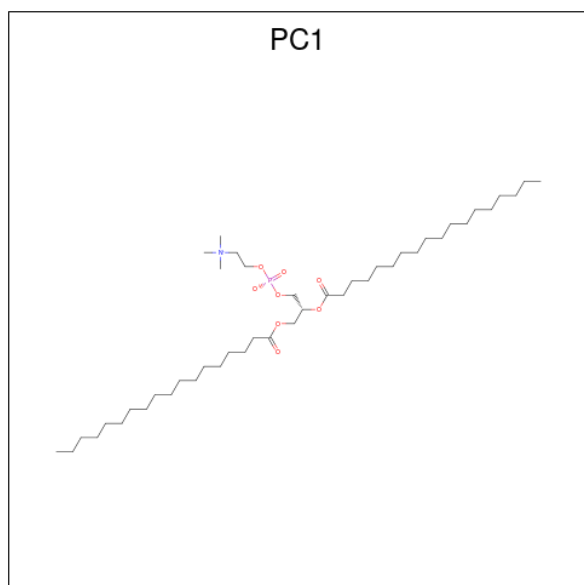
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	W	32	226	150	36	39	1	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

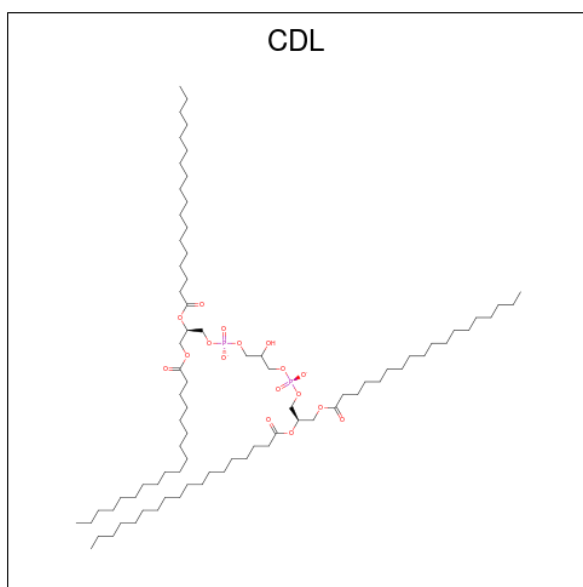
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
11	A	1	1	1	0
11	M	1	1	1	0

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	38	28	1	8	1	0
12	M	1	40	30	1	8	1	0
12	S	1	38	28	1	8	1	0

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	A	1	Total 69	C 50	O 17	P 2	0
13	C	1	Total 123	C 85	O 34	P 4	0
13	C	1	Total 123	C 85	O 34	P 4	0
13	D	1	Total 68	C 49	O 17	P 2	0
13	M	1	Total 70	C 51	O 17	P 2	0
13	O	1	Total 145	C 107	O 34	P 4	0
13	O	1	Total 145	C 107	O 34	P 4	0
13	P	1	Total 63	C 44	O 17	P 2	0
13	S	1	Total 55	C 36	O 17	P 2	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

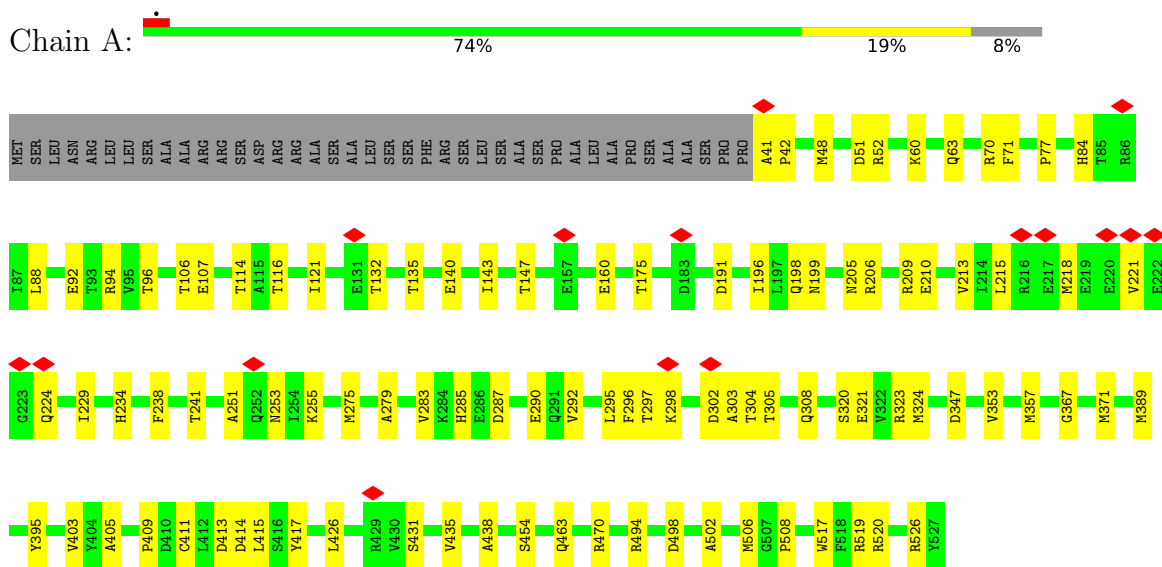
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	N	O	P	0
			206	146	6	48	6	
15	C	1	Total	C	N	O	P	0
			206	146	6	48	6	
15	C	1	Total	C	N	O	P	0
			206	146	6	48	6	
15	C	1	Total	C	N	O	P	0
			206	146	6	48	6	
15	C	1	Total	C	N	O	P	0
			206	146	6	48	6	
15	F	1	Total	C	N	O	P	0
			83	63	2	16	2	
15	F	1	Total	C	N	O	P	0
			83	63	2	16	2	
15	G	1	Total	C	N	O	P	0
			37	27	1	8	1	
15	M	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	O	1	Total	C	N	O	P	0
			189	139	5	40	5	
15	O	1	Total	C	N	O	P	0
			189	139	5	40	5	
15	O	1	Total	C	N	O	P	0
			189	139	5	40	5	
15	O	1	Total	C	N	O	P	0
			189	139	5	40	5	
15	O	1	Total	C	N	O	P	0
			189	139	5	40	5	
15	W	1	Total	C	N	O	P	0
			56	36	2	16	2	
15	W	1	Total	C	N	O	P	0
			56	36	2	16	2	

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

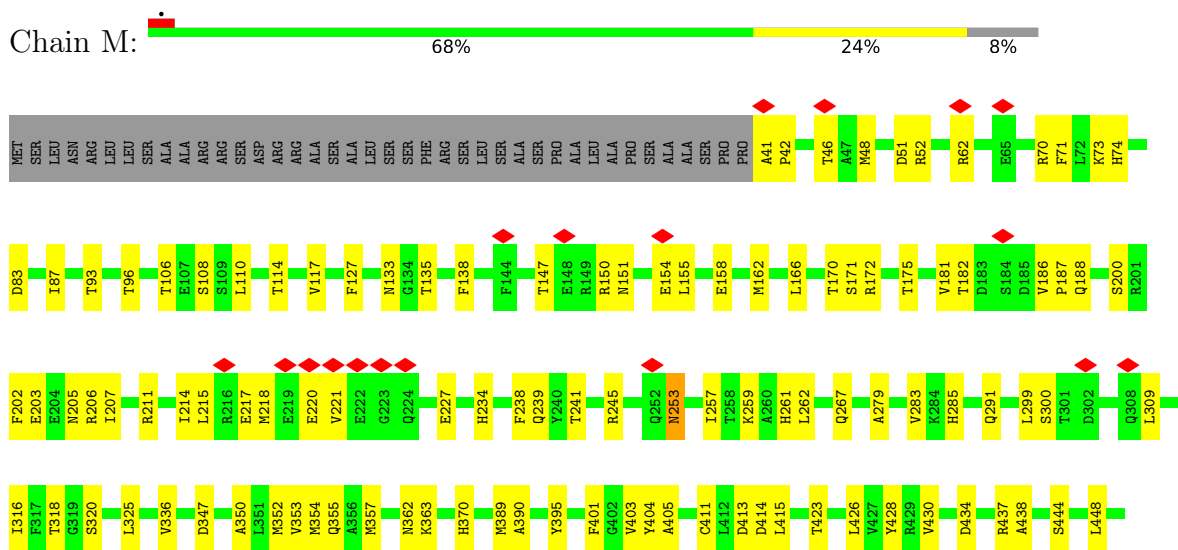
3 Residue-property plots

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

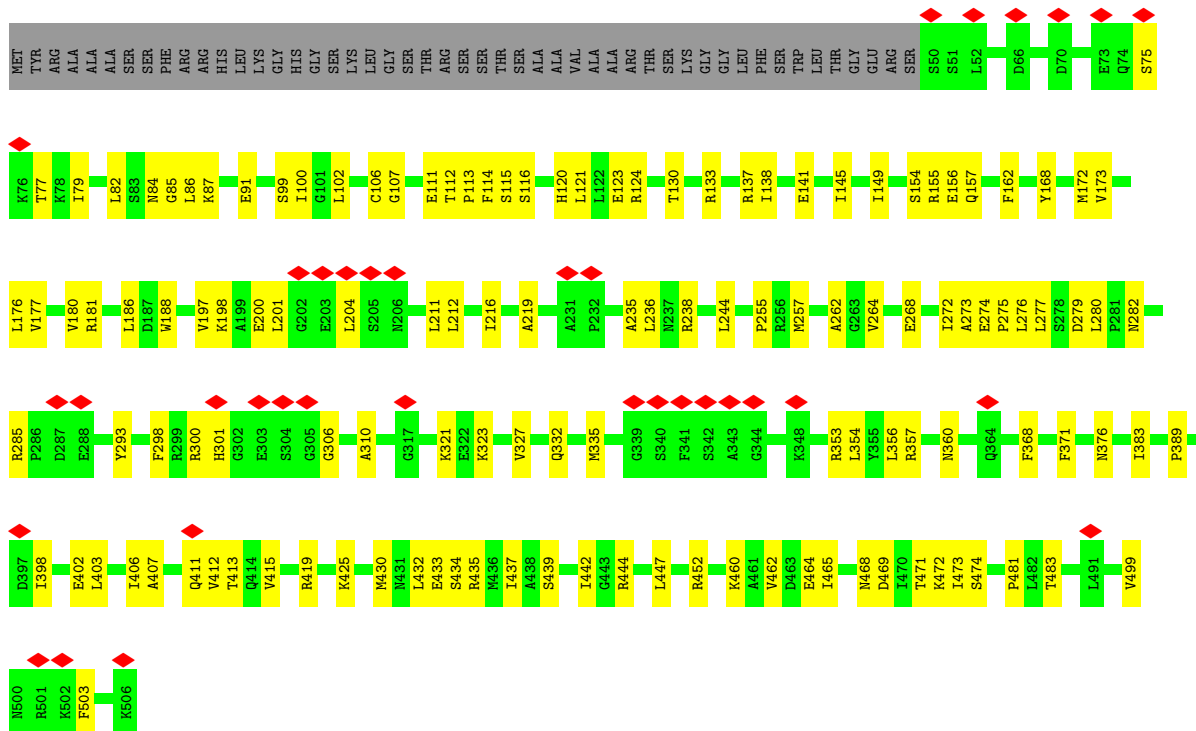


- Molecule 1: Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1

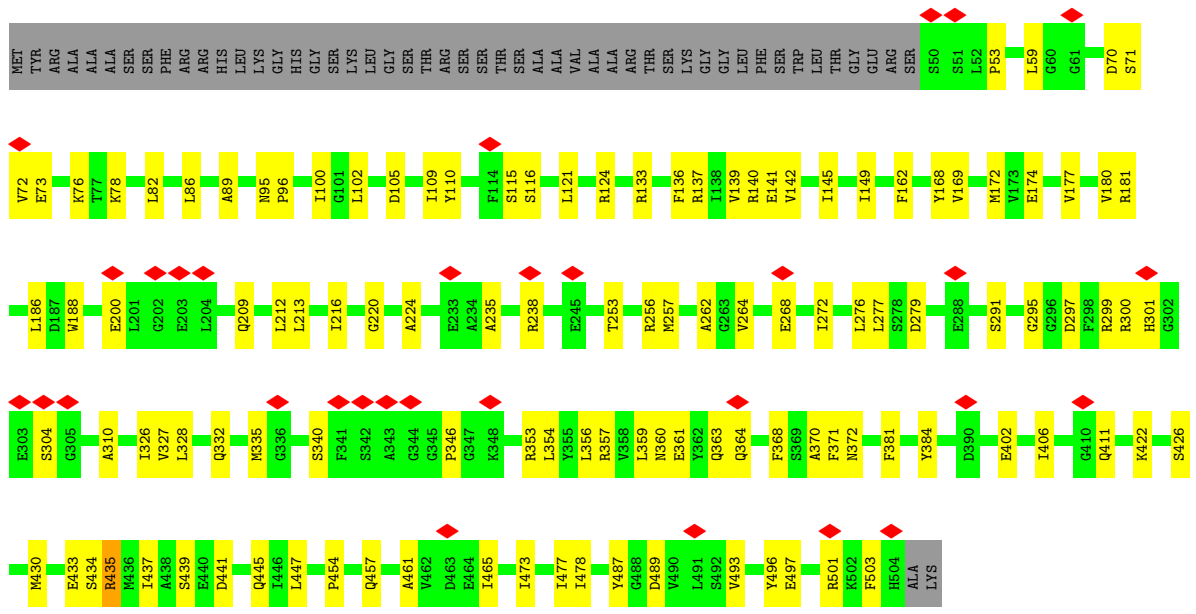




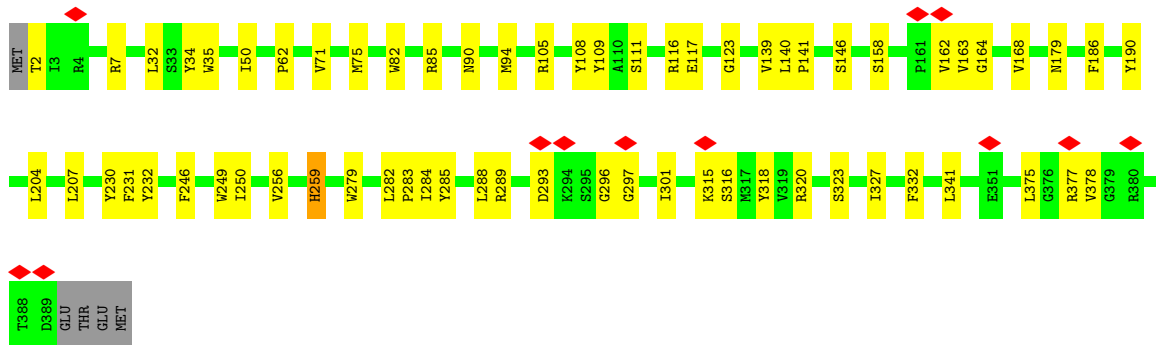
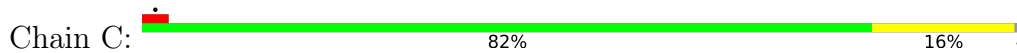
• Molecule 2: Alpha-MPP



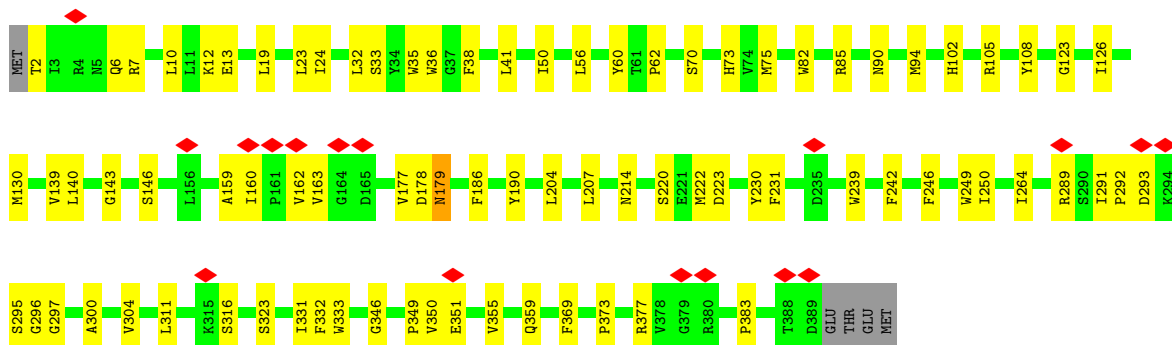
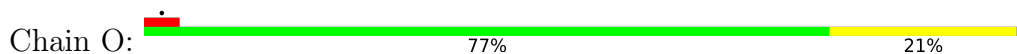
• Molecule 2: Alpha-MPP



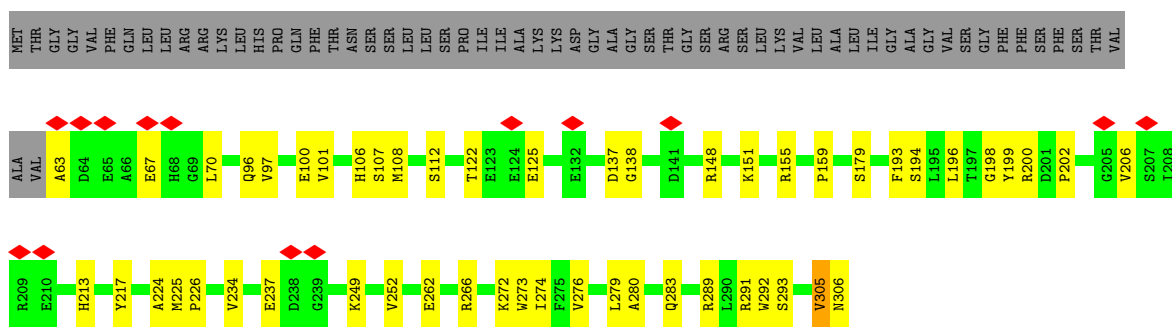
• Molecule 3: COB



• Molecule 3: COB

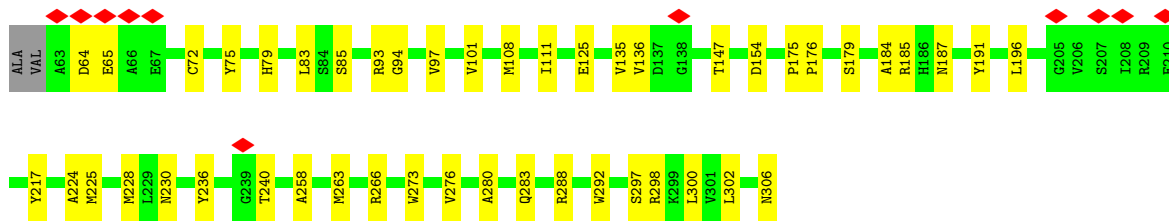


• Molecule 4: cytochrome c1-2, heme protein, mitochondrial

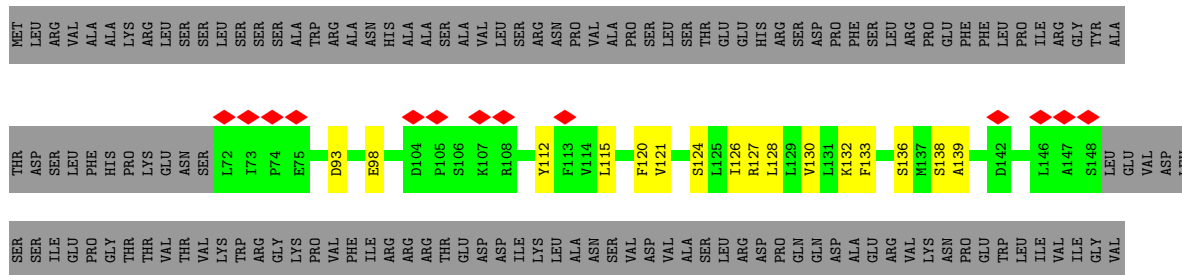


• Molecule 4: cytochrome c1-2, heme protein, mitochondrial

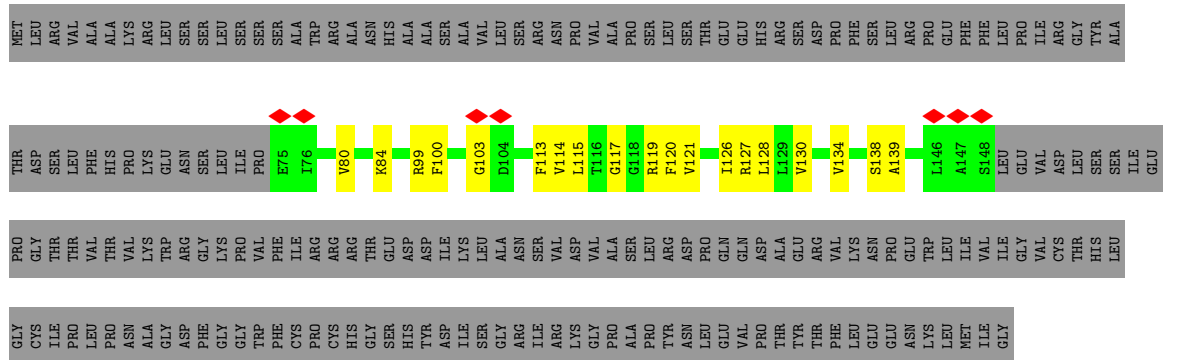




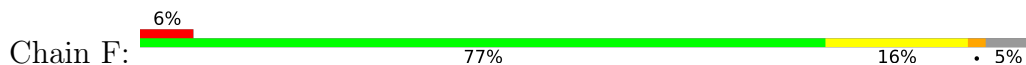
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



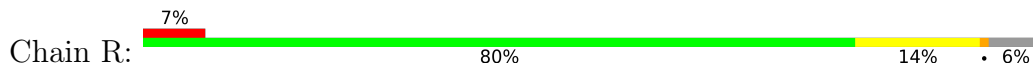
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 6: Cytochrome b-c1 complex subunit 7

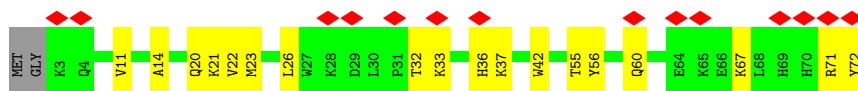


• Molecule 6: Cytochrome b-c1 complex subunit 7

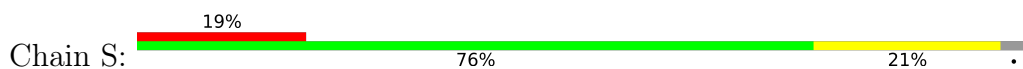




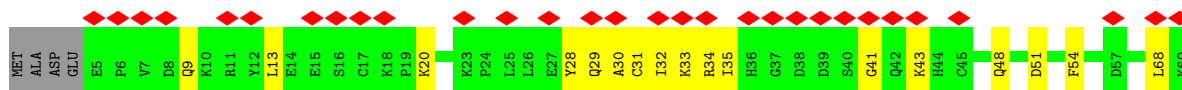
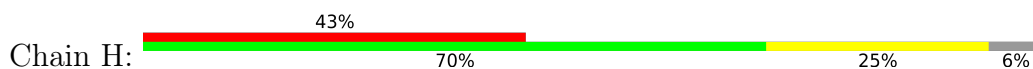
- Molecule 7: cytochrome b-c1 complex subunit 8



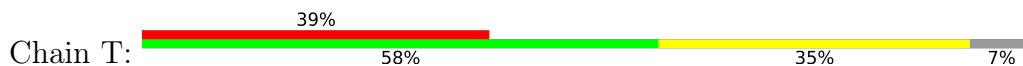
- Molecule 7: cytochrome b-c1 complex subunit 8



- Molecule 8: Cytochrome b-c1 complex subunit 6



- Molecule 8: Cytochrome b-c1 complex subunit 6



- Molecule 9: cytochrome b-c1 complex subunit 9

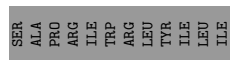
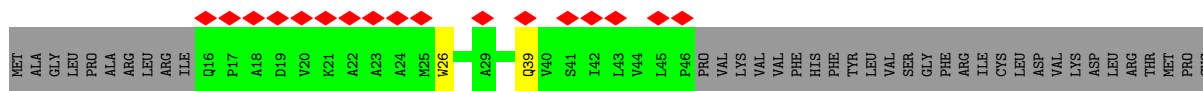


- Molecule 9: cytochrome b-c1 complex subunit 9

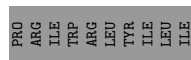
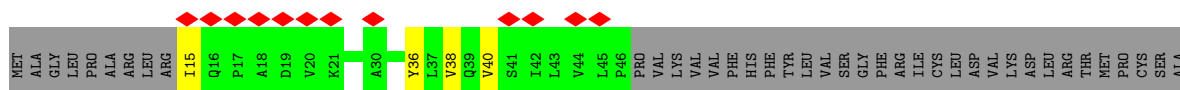
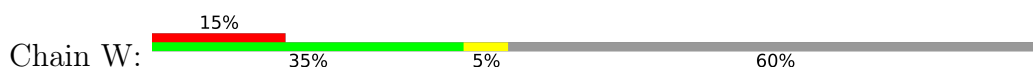




• Molecule 10: QCR10



• Molecule 10: QCR10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48111	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	1.820	Depositor
Minimum map value	-0.839	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.5	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 i

5.1 Standard geometry i

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

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	0.45	0/2663
4	P	0.34	0/1962	0.45	0/2663
5	E	0.33	0/612	0.45	0/831
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	0.29	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	0.30	0/490	0.43	0/660
9	V	0.30	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
All	All	0.33	0/32134	0.47	2/43641 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	111	LEU	CA-CB-CG	5.48	127.91	115.30
6	R	111	LEU	CA-CB-CG	5.23	127.33	115.30

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	67	0
1	M	3838	0	3797	95	0
2	B	3471	0	3471	97	0
2	N	3456	0	3453	90	0
3	C	3104	0	3070	57	0
3	O	3104	0	3070	67	0
4	D	1910	0	1843	43	0
4	P	1910	0	1843	36	0
5	E	597	0	620	16	0
5	Q	574	0	591	17	0
6	F	965	0	982	21	0
6	R	959	0	977	15	0
7	G	578	0	599	18	0
7	S	578	0	599	13	0
8	H	536	0	528	15	0
8	T	527	0	521	19	0
9	J	480	0	486	8	0
9	V	476	0	483	11	0
10	K	218	0	230	2	0
10	W	226	0	241	3	0
11	A	1	0	0	0	0
11	M	1	0	0	0	0
12	A	38	0	50	3	0
12	M	40	0	54	6	0
12	S	38	0	50	2	0
13	A	69	0	85	1	0
13	C	123	0	134	5	0
13	D	68	0	83	2	0
13	M	70	0	87	6	0
13	O	145	0	184	10	0
13	P	63	0	70	2	0
13	S	55	0	54	2	0
14	C	86	0	60	8	0
14	O	86	0	60	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	206	0	259	13	0
15	F	83	0	120	3	0
15	G	37	0	48	1	0
15	M	45	0	67	2	0
15	O	189	0	254	5	0
15	W	56	0	60	0	0
16	D	43	0	30	6	0
16	P	43	0	30	4	0
All	All	32930	0	33040	645	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 10.

The worst 5 of 645 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:187:PRO:HB3	1:M:291:GLN:HE22	1.40	0.86
3:C:75:MET:HE1	3:C:82:TRP:HA	1.60	0.84
6:F:16:LEU:HD12	15:F:201:3PE:H352	1.65	0.79
3:C:315:LYS:HE3	3:C:377:ARG:HH21	1.47	0.79
3:O:162:VAL:HG13	3:O:163:VAL:HG13	1.64	0.79

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%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	233 (96%)	9 (4%)	0	100	100
4	P	242/306 (79%)	229 (95%)	13 (5%)	0	100	100
5	E	75/271 (28%)	68 (91%)	7 (9%)	0	100	100
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
All	All	3943/4838 (82%)	3671 (93%)	270 (7%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	435	ARG
2	B	113	PRO

5.3.2 Protein sidechains [i](#)

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%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	407/438 (93%)	405 (100%)	2 (0%)	88	95
2	B	378/414 (91%)	378 (100%)	0	100	100
2	N	377/414 (91%)	376 (100%)	1 (0%)	92	96
3	C	333/338 (98%)	331 (99%)	2 (1%)	86	94
3	O	333/338 (98%)	332 (100%)	1 (0%)	92	96
4	D	198/247 (80%)	196 (99%)	2 (1%)	76	90
4	P	198/247 (80%)	198 (100%)	0	100	100
5	E	65/233 (28%)	65 (100%)	0	100	100
5	Q	62/233 (27%)	62 (100%)	0	100	100
6	F	102/107 (95%)	101 (99%)	1 (1%)	76	90
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
All	All	3349/4060 (82%)	3338 (100%)	11 (0%)	92	96

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

Mol	Chain	Res	Type
1	M	253	ASN
1	M	520	ARG
3	O	179	ASN
2	N	435	ARG
4	D	305	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	95	HIS

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Mol	Chain	Res	Type
4	D	96	GLN
8	T	48	GLN
7	S	20	GLN
2	B	332	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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	$\# Z > 2$
13	CDL	P	502	-	62,62,99	0.37	0	68,74,111	0.44	0
15	3PE	W	101	-	27,27,50	0.40	0	30,32,55	0.40	0
12	PC1	M	604	-	39,39,53	0.34	0	45,47,61	0.37	0
13	CDL	A	603	-	68,68,99	0.35	0	74,80,111	0.32	0
13	CDL	C	401	-	63,63,99	0.37	0	69,75,111	0.34	0
15	3PE	C	407	-	32,32,50	0.37	0	35,37,55	0.32	0
13	CDL	M	603	-	69,69,99	0.36	0	75,81,111	0.38	0
15	3PE	O	407	-	38,38,50	0.34	0	41,43,55	0.35	0
14	HEM	C	403	3	41,50,50	1.30	4 (9%)	45,82,82	1.76	9 (20%)
15	3PE	O	401	-	35,35,50	0.36	0	38,40,55	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	3PE	C	405	-	28,28,50	0.40	0	31,33,55	0.41	0
15	3PE	F	202	-	50,50,50	0.31	0	53,55,55	0.31	0
15	3PE	O	405	-	29,29,50	0.38	0	32,34,55	0.34	0
14	HEM	C	402	3	41,50,50	1.29	4 (9%)	45,82,82	1.82	11 (24%)
15	3PE	C	408	-	26,26,50	0.40	0	29,31,55	0.34	0
15	3PE	M	602	-	44,44,50	0.32	0	47,49,55	0.33	0
13	CDL	O	406	-	63,63,99	0.37	0	69,75,111	0.41	0
15	3PE	O	408	-	32,32,50	0.37	0	35,37,55	0.34	0
15	3PE	G	101	-	36,36,50	0.35	0	39,41,55	0.31	0
15	3PE	C	406	-	44,44,50	0.32	0	47,49,55	0.37	0
13	CDL	S	102	-	54,54,99	0.39	0	60,66,111	0.38	0
15	3PE	O	409	-	50,50,50	0.30	0	53,55,55	0.32	0
16	HEC	P	501	4	32,50,50	2.08	4 (12%)	24,82,82	2.31	14 (58%)
15	3PE	F	201	-	31,31,50	0.39	0	34,36,55	0.54	0
13	CDL	C	410	-	58,58,99	0.38	0	64,70,111	0.33	0
12	PC1	A	602	-	37,37,53	0.35	0	43,45,61	0.28	0
15	3PE	C	409	-	33,33,50	0.37	0	36,38,55	0.33	0
13	CDL	D	502	-	67,67,99	0.36	0	73,79,111	0.36	0
13	CDL	O	402	-	80,80,99	0.34	0	86,92,111	0.38	0
14	HEM	O	403	3	41,50,50	1.33	4 (9%)	45,82,82	1.84	11 (24%)
14	HEM	O	404	3	41,50,50	1.33	4 (9%)	45,82,82	1.74	8 (17%)
15	3PE	W	102	-	27,27,50	0.40	0	30,32,55	0.36	0
16	HEC	D	501	4	32,50,50	2.13	4 (12%)	24,82,82	2.32	14 (58%)
12	PC1	S	101	-	37,37,53	0.34	0	43,45,61	0.34	0
15	3PE	C	404	-	37,37,50	0.35	0	40,42,55	0.37	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
13	CDL	P	502	-	-	16/73/73/110	-
15	3PE	W	101	-	-	7/31/31/54	-
12	PC1	M	604	-	-	6/43/43/57	-
13	CDL	A	603	-	-	17/79/79/110	-
13	CDL	C	401	-	-	11/74/74/110	-
15	3PE	C	407	-	-	8/36/36/54	-
13	CDL	M	603	-	-	10/80/80/110	-
15	3PE	O	407	-	-	10/42/42/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEM	C	403	3	-	6/12/54/54	-
15	3PE	O	401	-	-	13/39/39/54	-
15	3PE	C	405	-	-	8/32/32/54	-
15	3PE	F	202	-	-	13/54/54/54	-
15	3PE	O	405	-	-	5/33/33/54	-
14	HEM	C	402	3	-	3/12/54/54	-
15	3PE	C	408	-	-	11/30/30/54	-
15	3PE	M	602	-	-	16/48/48/54	-
13	CDL	O	406	-	-	17/74/74/110	-
15	3PE	O	408	-	-	7/36/36/54	-
15	3PE	G	101	-	-	6/40/40/54	-
15	3PE	C	406	-	-	15/48/48/54	-
13	CDL	S	102	-	-	17/65/65/110	-
15	3PE	O	409	-	-	6/54/54/54	-
16	HEC	P	501	4	-	2/10/54/54	-
15	3PE	F	201	-	-	9/35/35/54	-
13	CDL	C	410	-	-	8/69/69/110	-
12	PC1	A	602	-	-	6/41/41/57	-
15	3PE	C	409	-	-	5/37/37/54	-
13	CDL	D	502	-	-	19/78/78/110	-
13	CDL	O	402	-	-	16/91/91/110	-
14	HEM	O	403	3	-	8/12/54/54	-
14	HEM	O	404	3	-	7/12/54/54	-
15	3PE	W	102	-	-	9/31/31/54	-
16	HEC	D	501	4	-	2/10/54/54	-
12	PC1	S	101	-	-	7/41/41/57	-
15	3PE	C	404	-	-	10/41/41/54	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	C3C-C2C	-6.87	1.33	1.40
16	P	501	HEC	C3C-C2C	-6.77	1.33	1.40
16	D	501	HEC	C2B-C3B	-6.75	1.33	1.40
16	P	501	HEC	C2B-C3B	-6.58	1.33	1.40
14	O	403	HEM	C4D-ND	-3.96	1.33	1.40

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	403	HEM	CHC-C4B-NB	4.83	129.68	124.43
14	C	402	HEM	CHC-C4B-NB	4.76	129.60	124.43
14	C	402	HEM	CHB-C1B-NB	4.42	129.85	124.38
16	D	501	HEC	CMD-C2D-C1D	-4.38	121.72	128.46
14	O	404	HEM	CHB-C1B-NB	4.34	129.74	124.38

There are no chirality outliers.

5 of 336 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	602	PC1	C11-O13-P-O12
12	S	101	PC1	C1-O11-P-O12
12	S	101	PC1	C1-O11-P-O14
12	S	101	PC1	C1-O11-P-O13
13	A	603	CDL	CB2-OB2-PB2-OB3

There are no ring outliers.

29 monomers are involved in 79 short contacts:

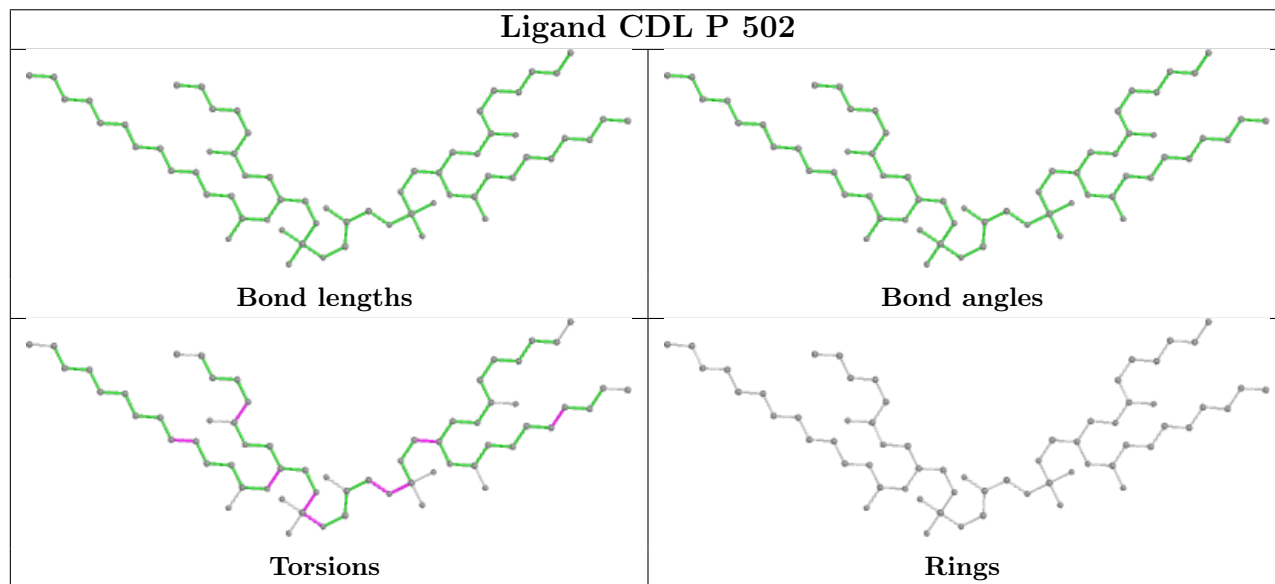
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	502	CDL	2	0
12	M	604	PC1	6	0
13	A	603	CDL	1	0
13	C	401	CDL	3	0
15	C	407	3PE	2	0
13	M	603	CDL	6	0
15	O	407	3PE	1	0
14	C	403	HEM	5	0
15	O	401	3PE	1	0
15	C	405	3PE	4	0
14	C	402	HEM	3	0
15	C	408	3PE	3	0
15	M	602	3PE	2	0
13	O	406	CDL	1	0
15	G	101	3PE	1	0
15	C	406	3PE	4	0
13	S	102	CDL	2	0
15	O	409	3PE	3	0
16	P	501	HEC	4	0
15	F	201	3PE	3	0
13	C	410	CDL	2	0

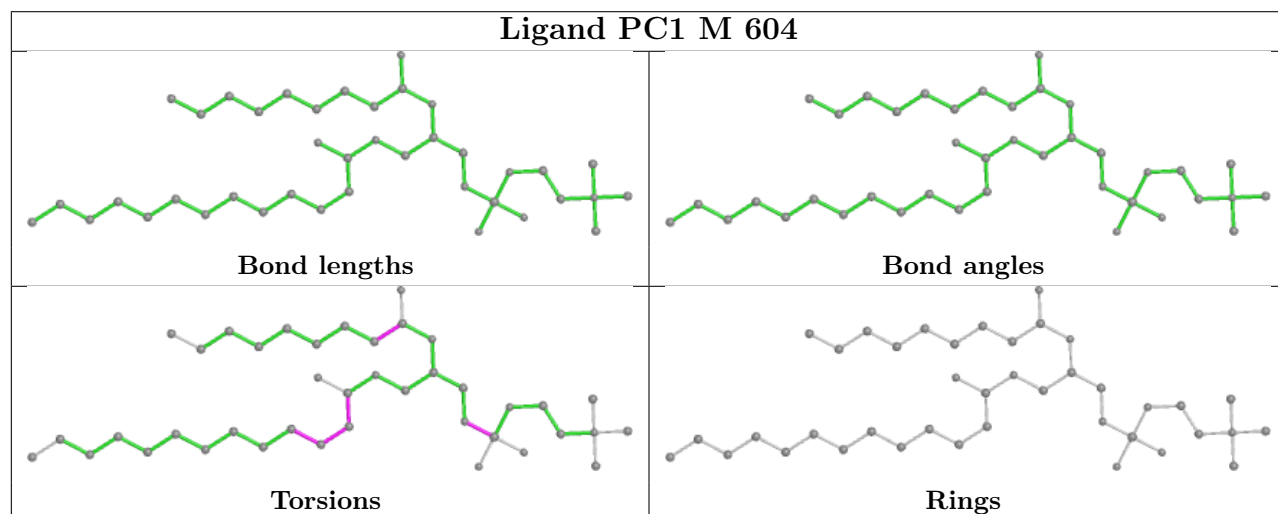
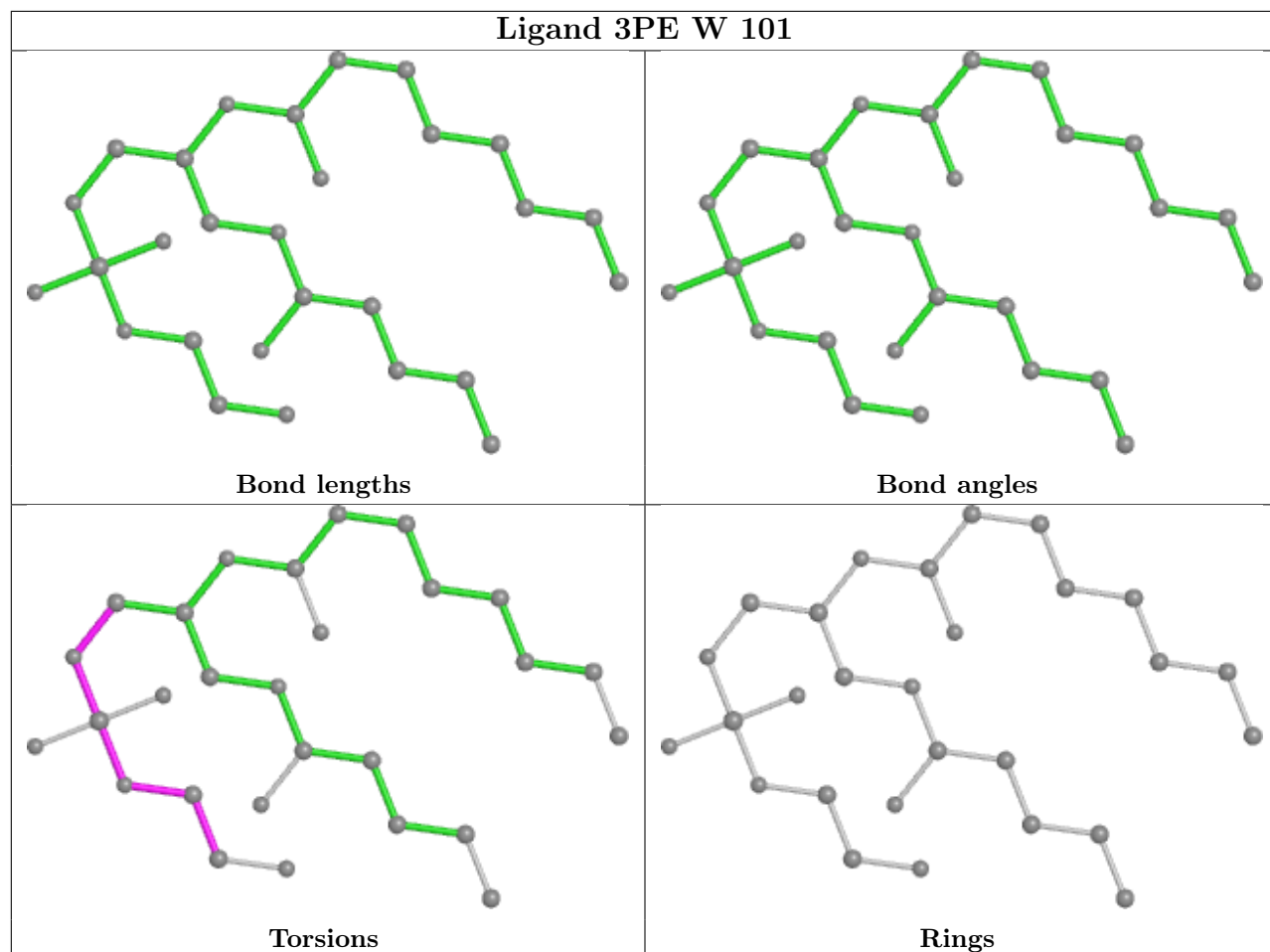
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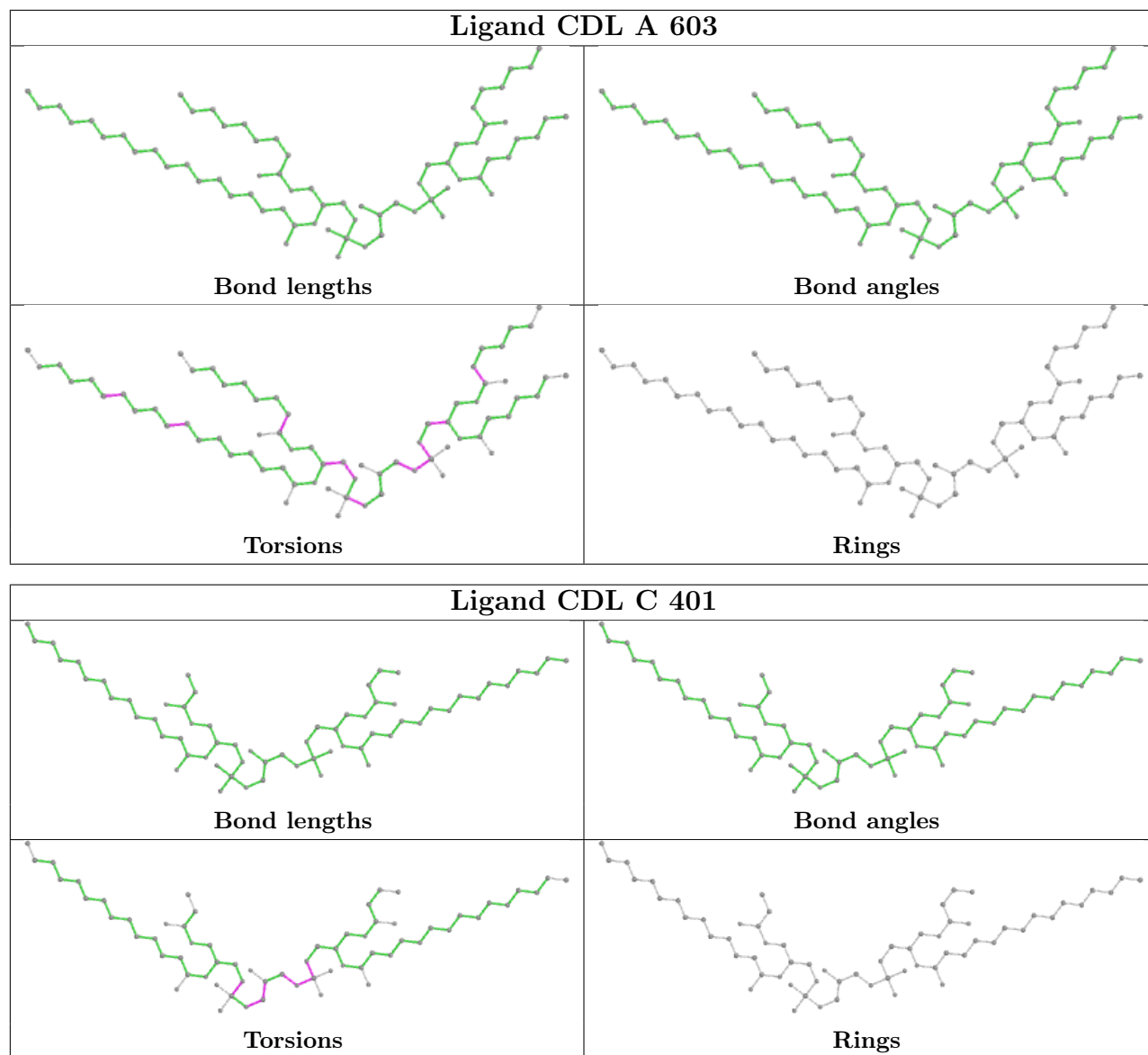
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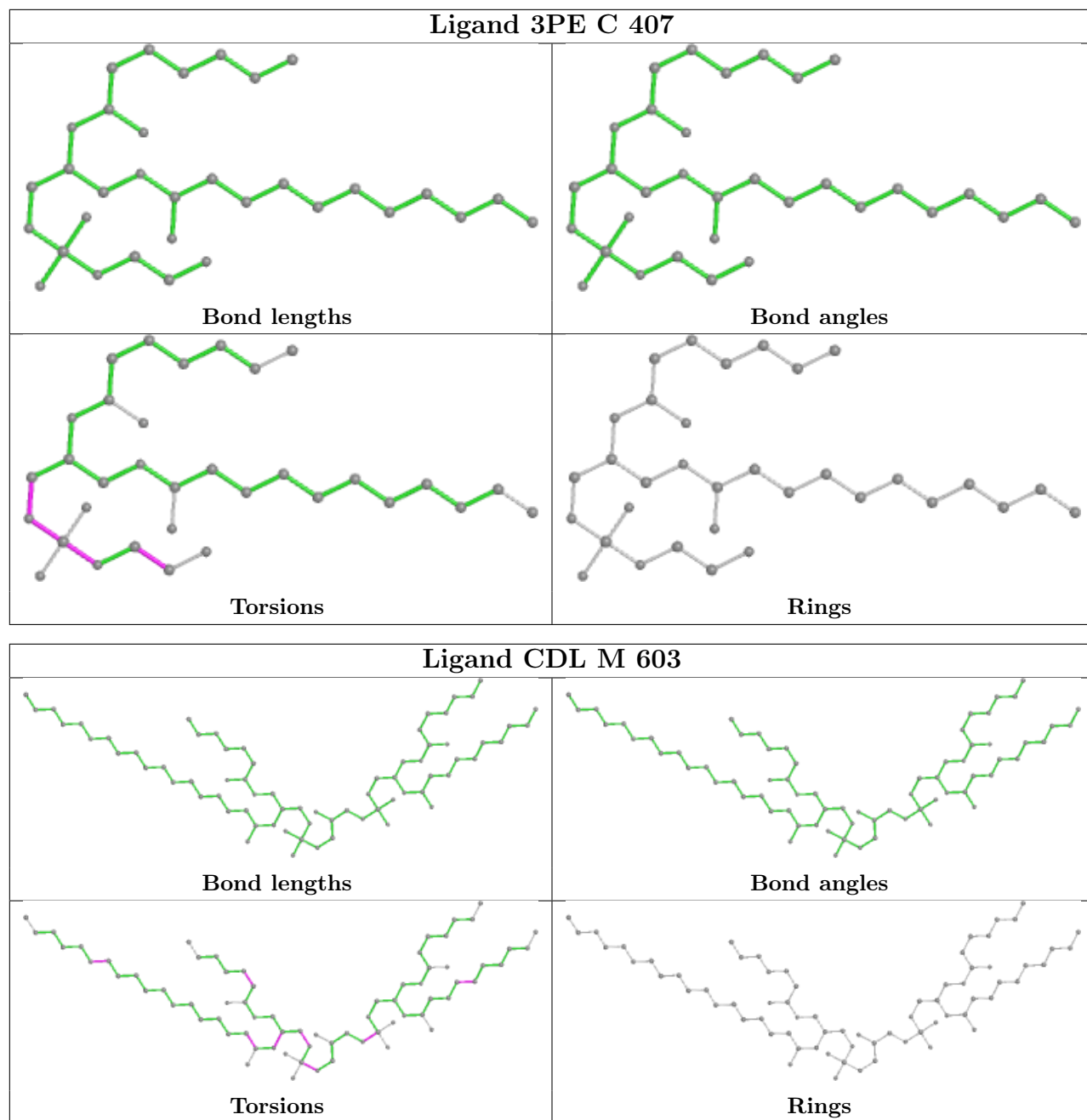
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	602	PC1	3	0
15	C	409	3PE	1	0
13	D	502	CDL	2	0
13	O	402	CDL	9	0
14	O	403	HEM	3	0
14	O	404	HEM	6	0
16	D	501	HEC	6	0
12	S	101	PC1	2	0

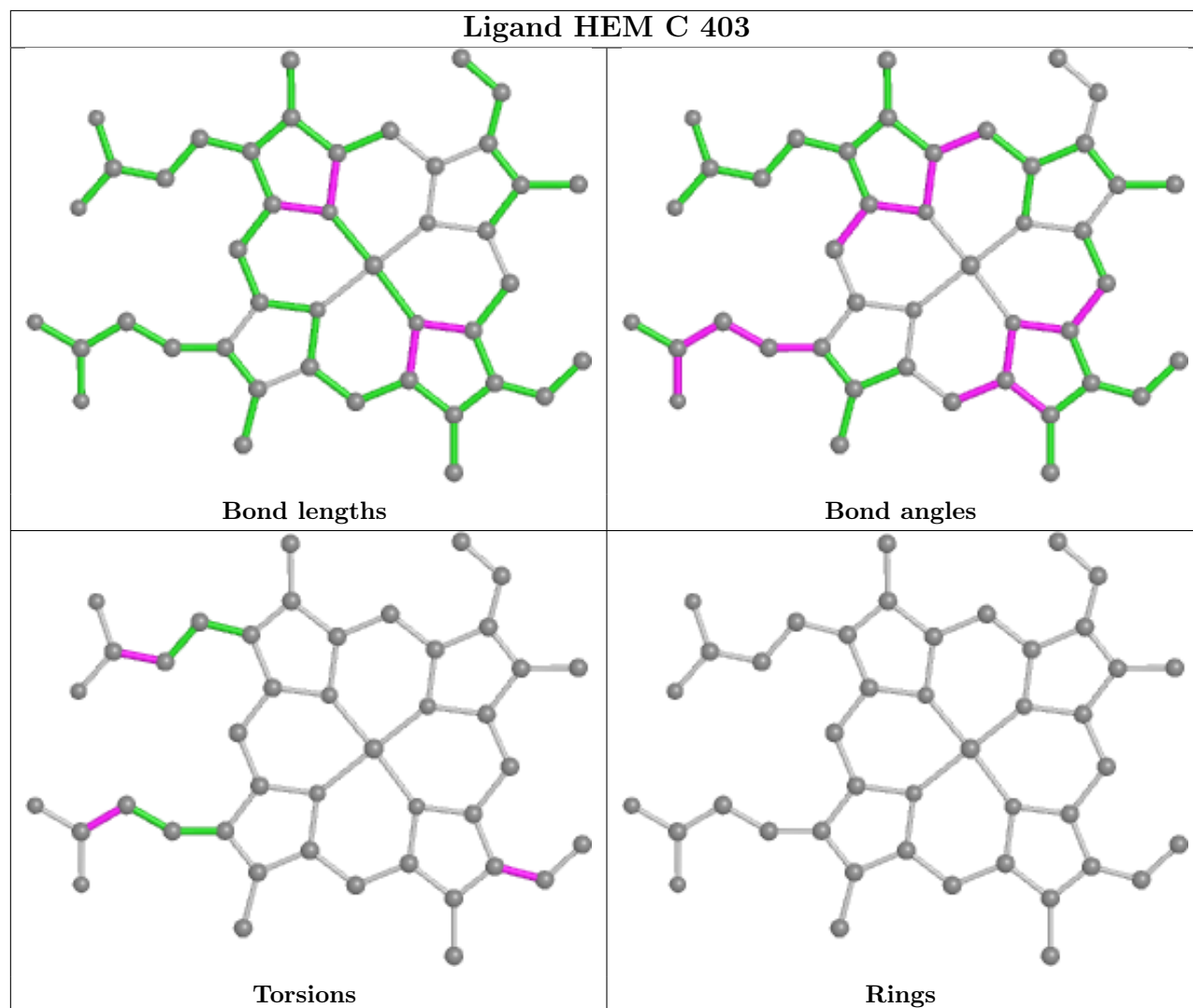
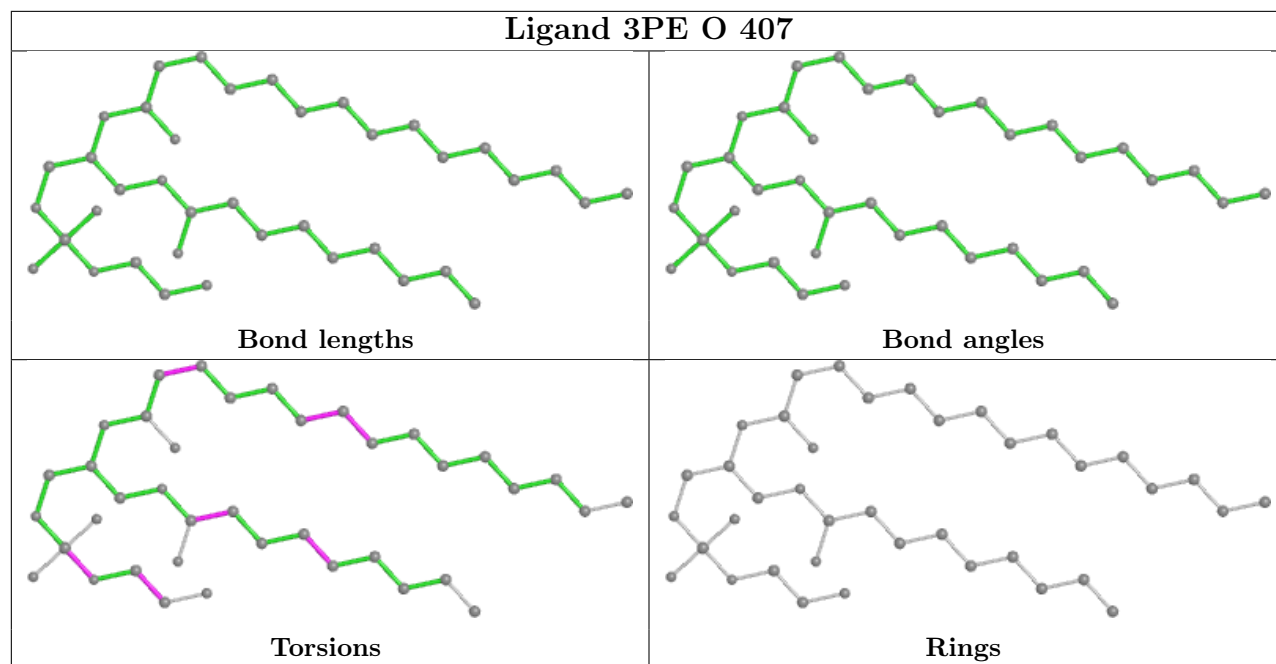
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

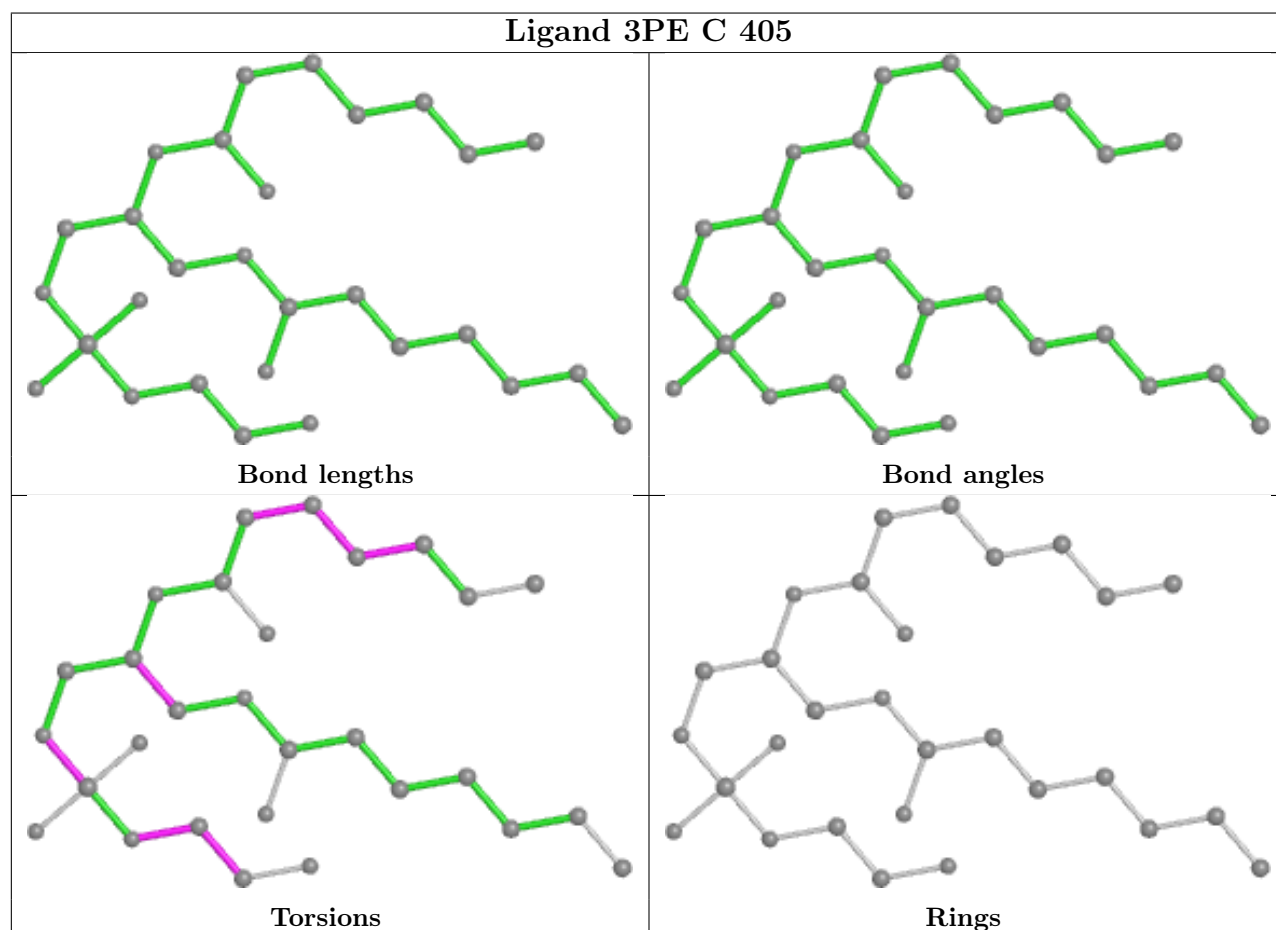
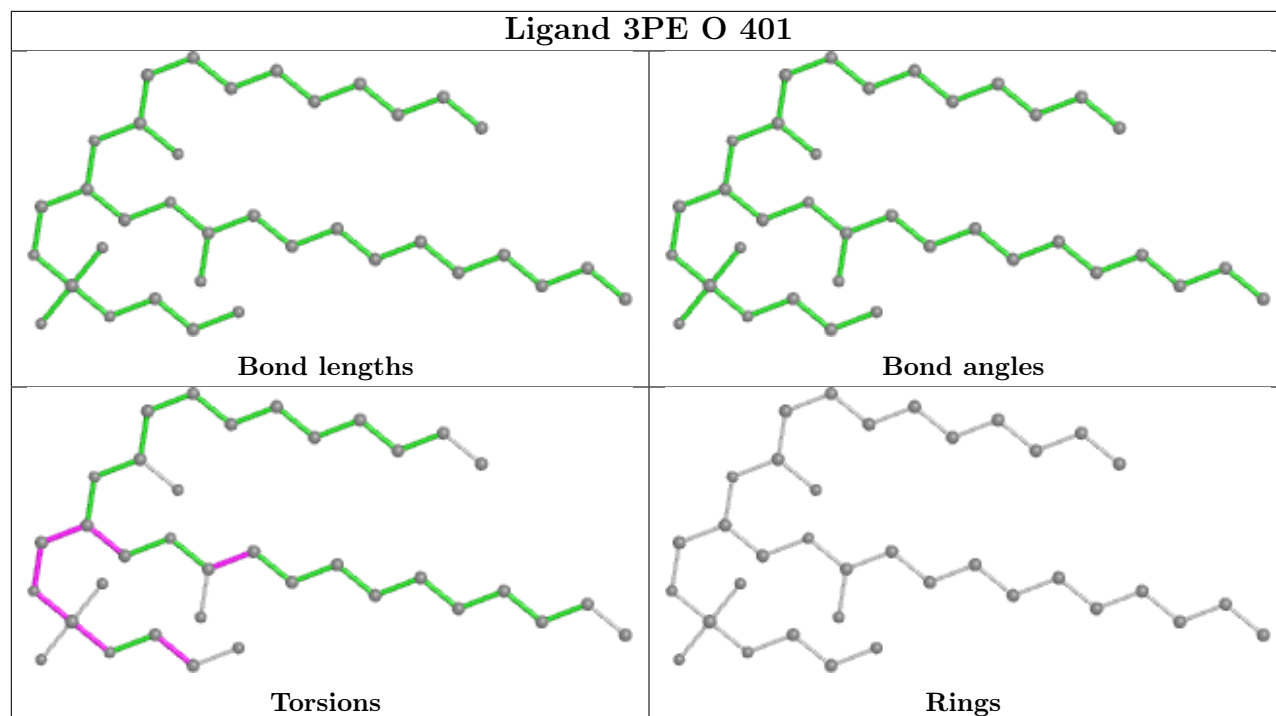


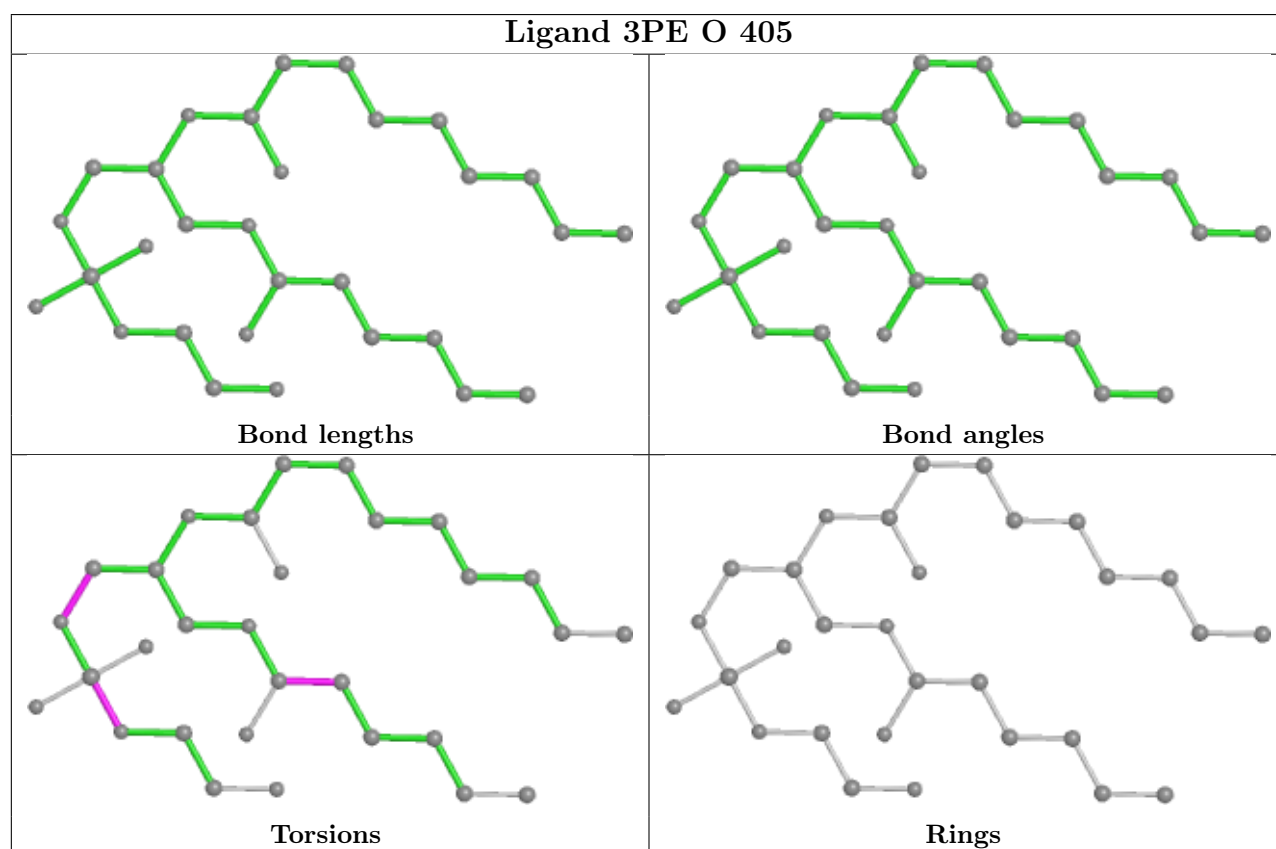
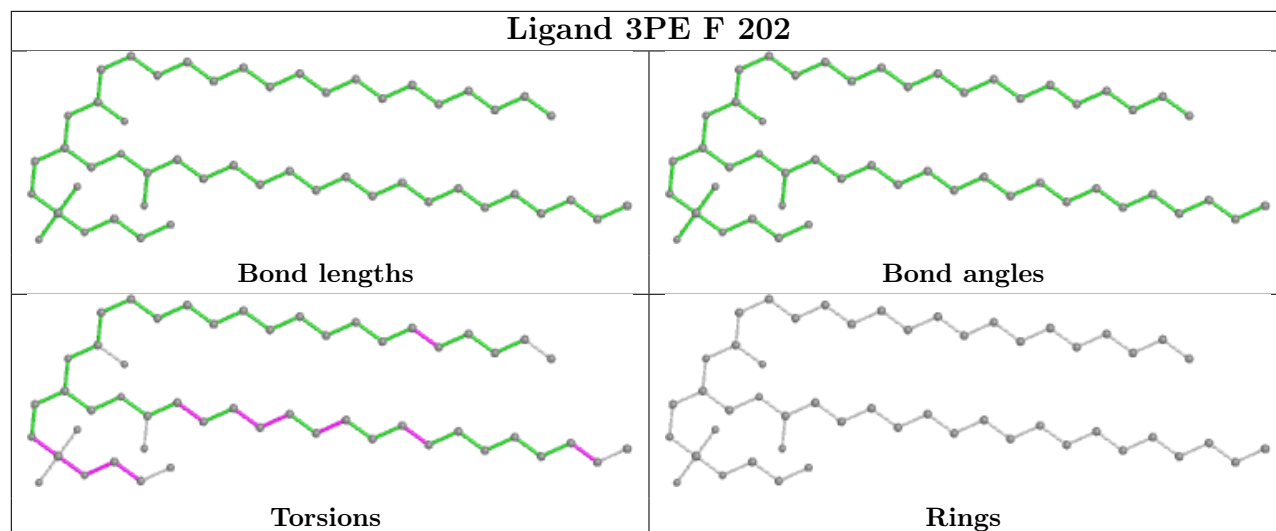


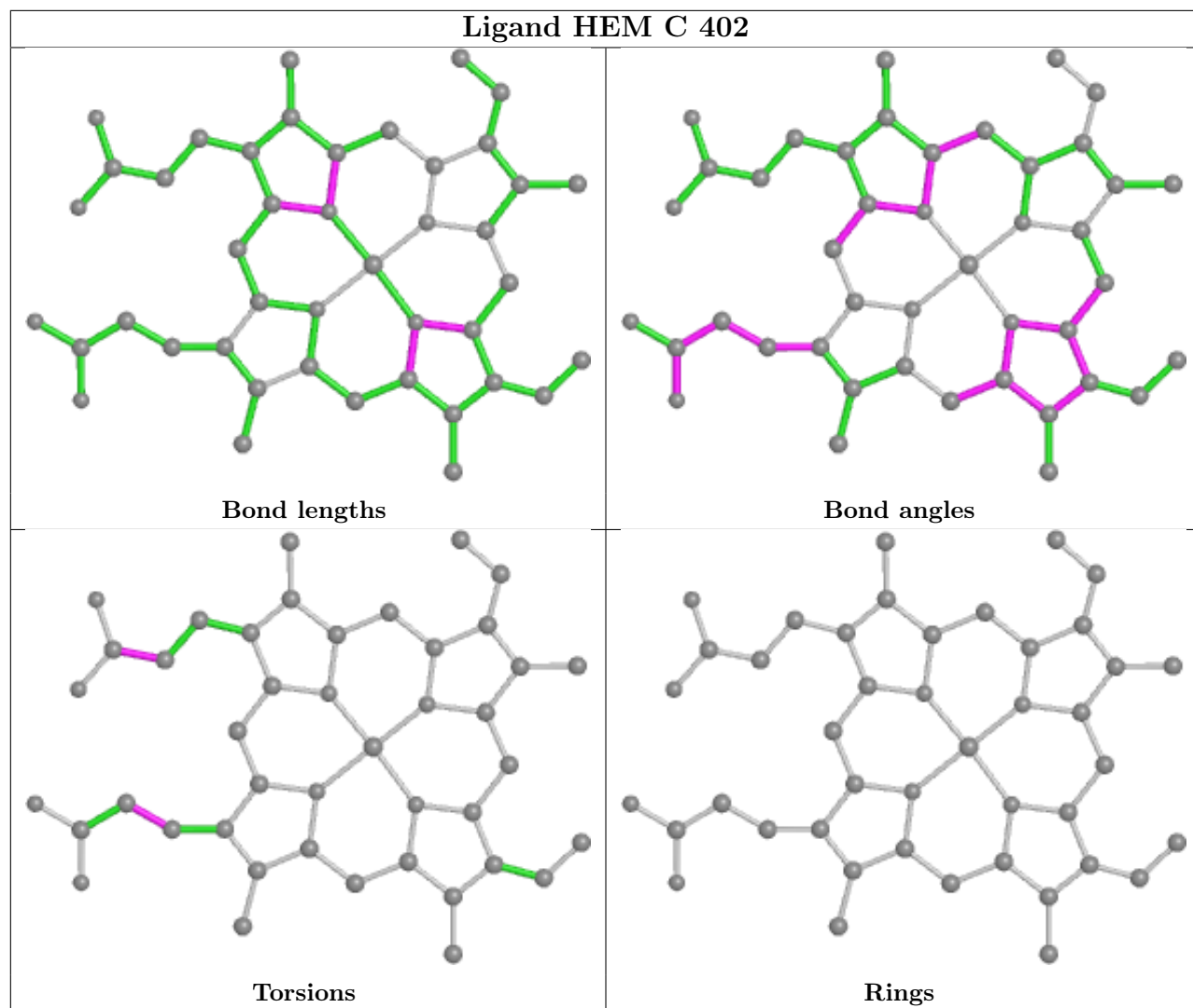


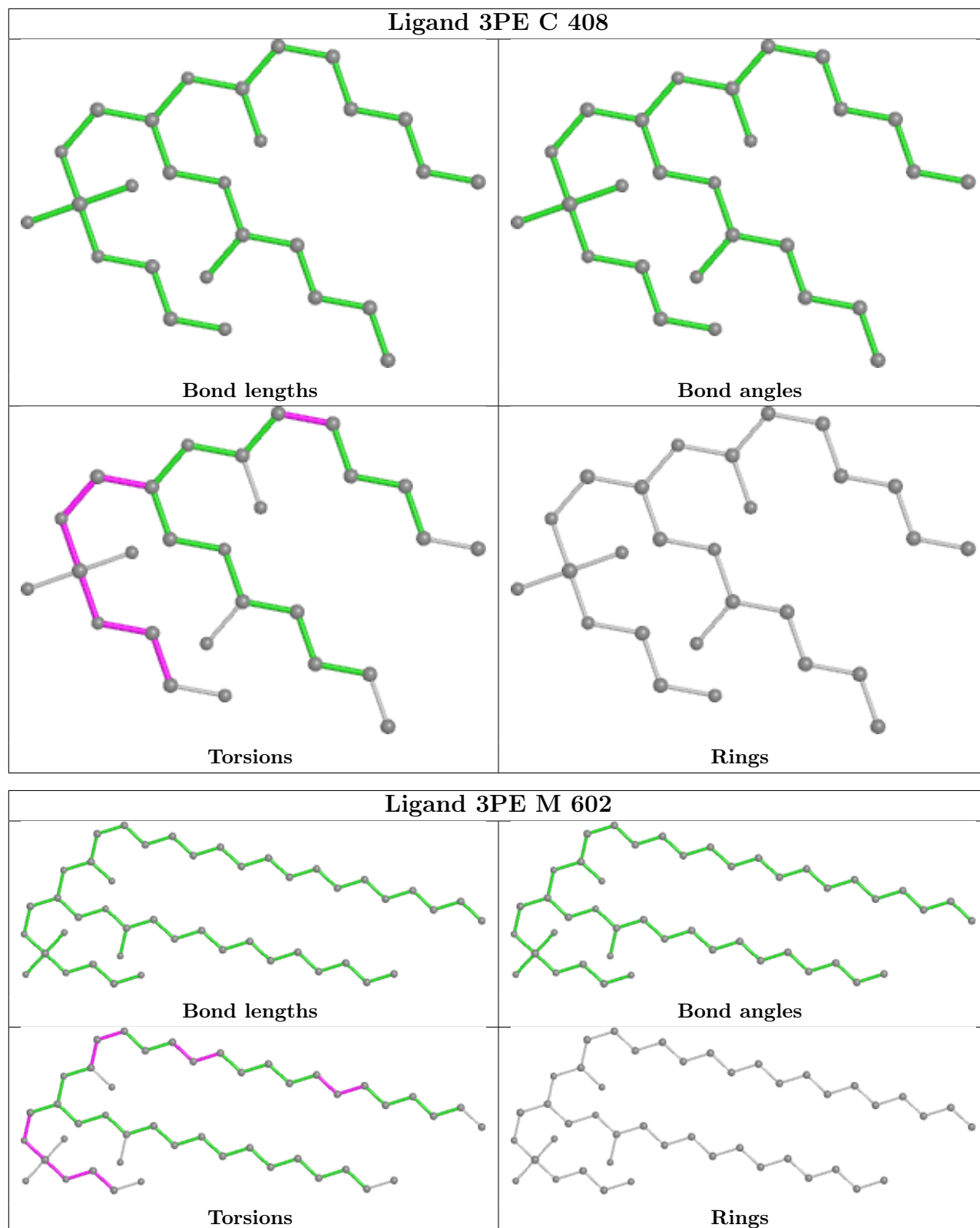


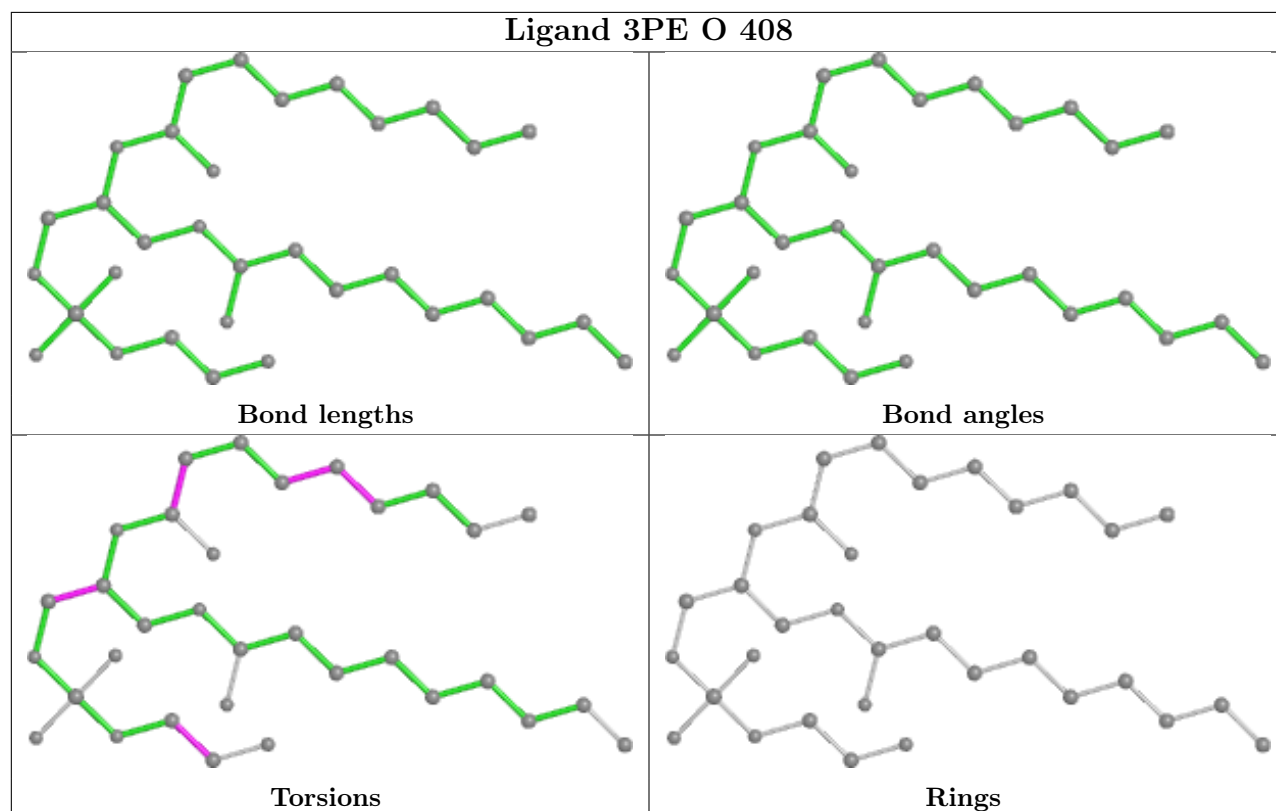
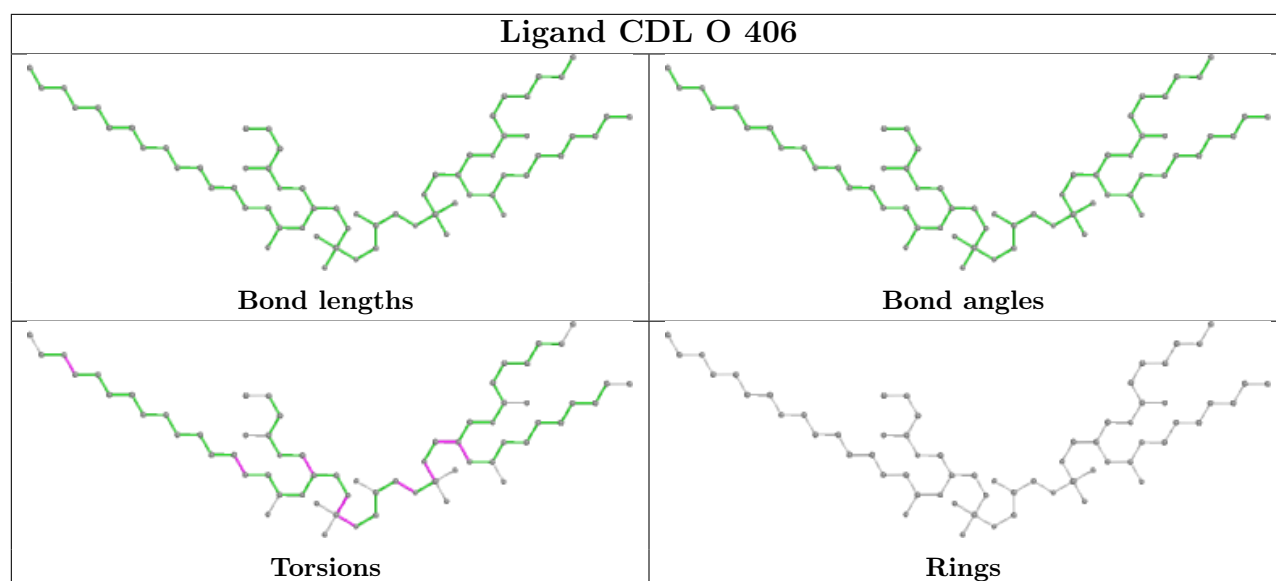


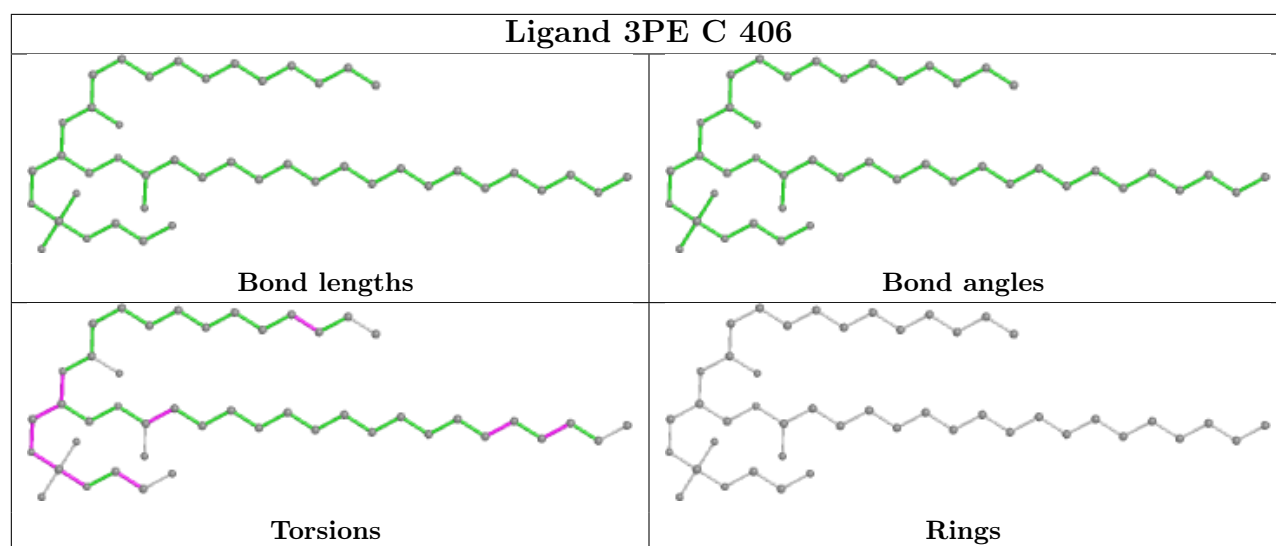
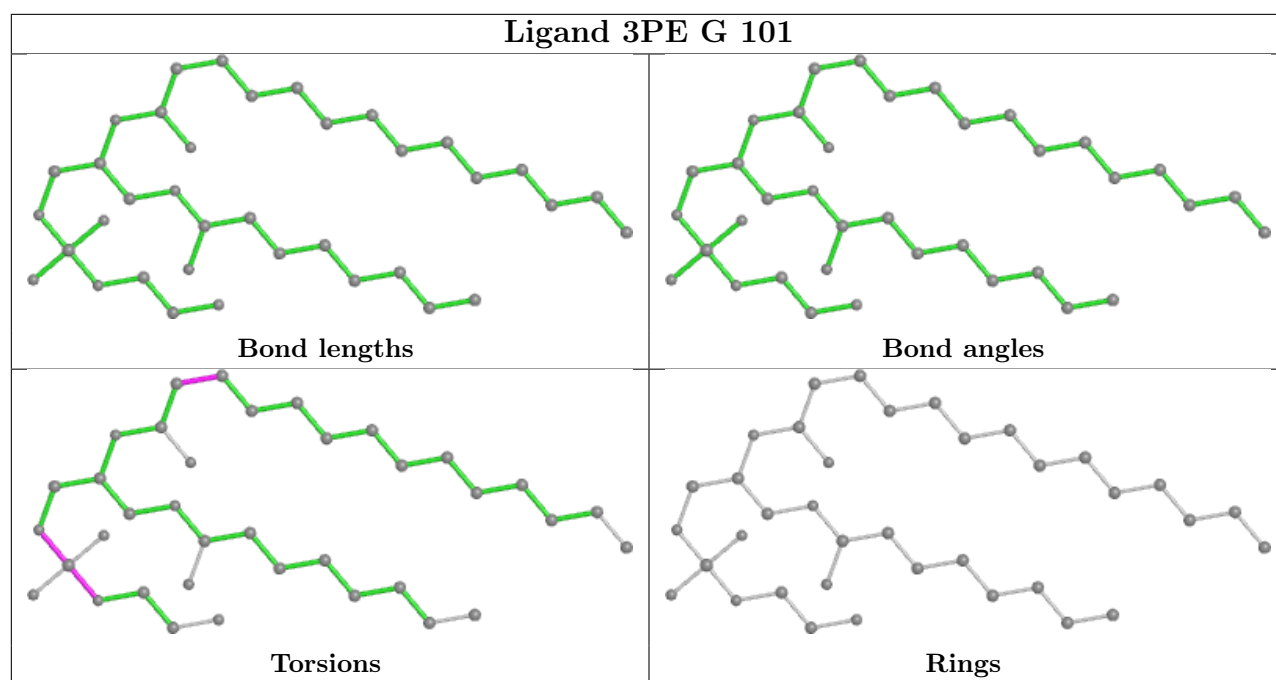


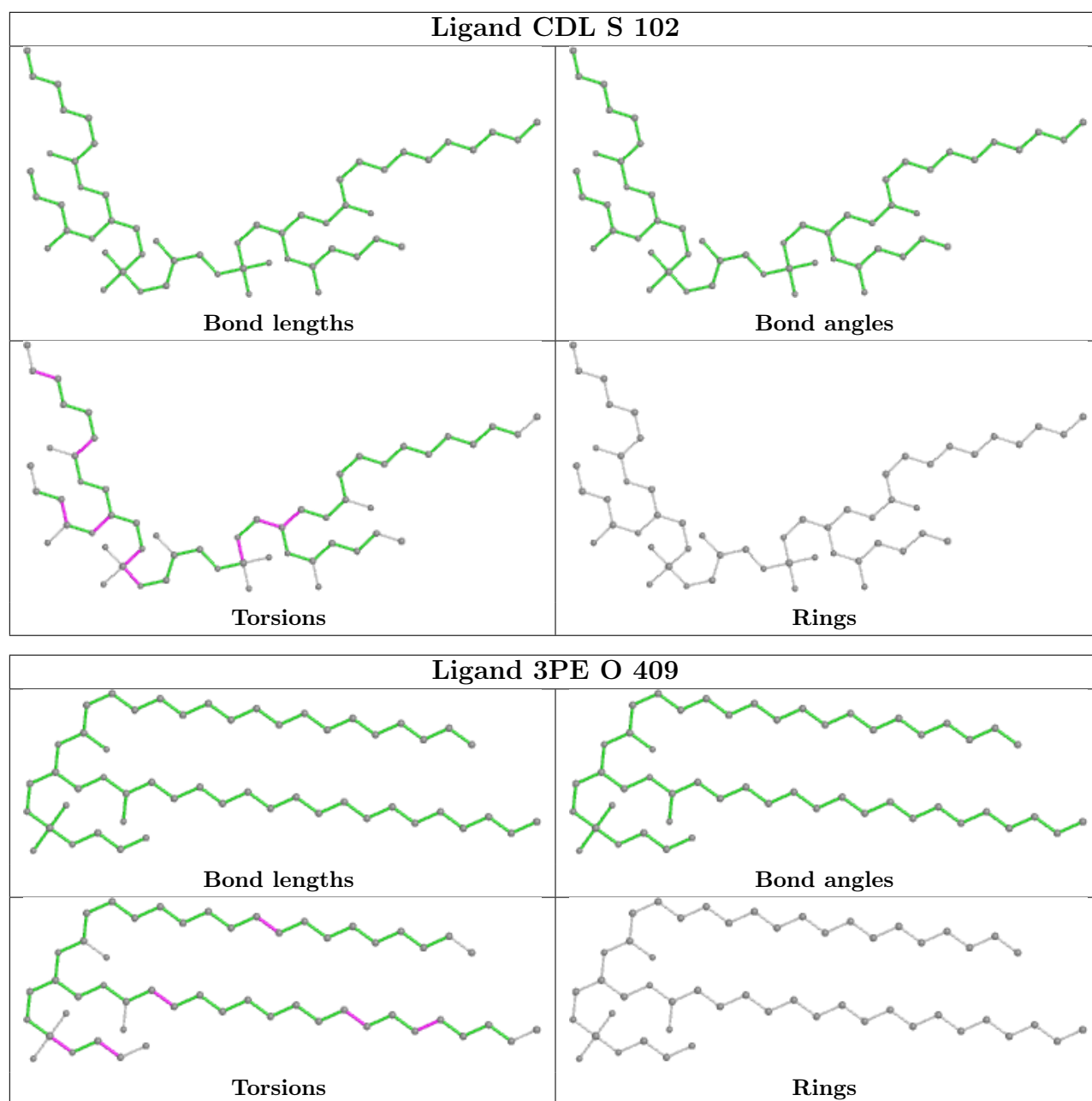


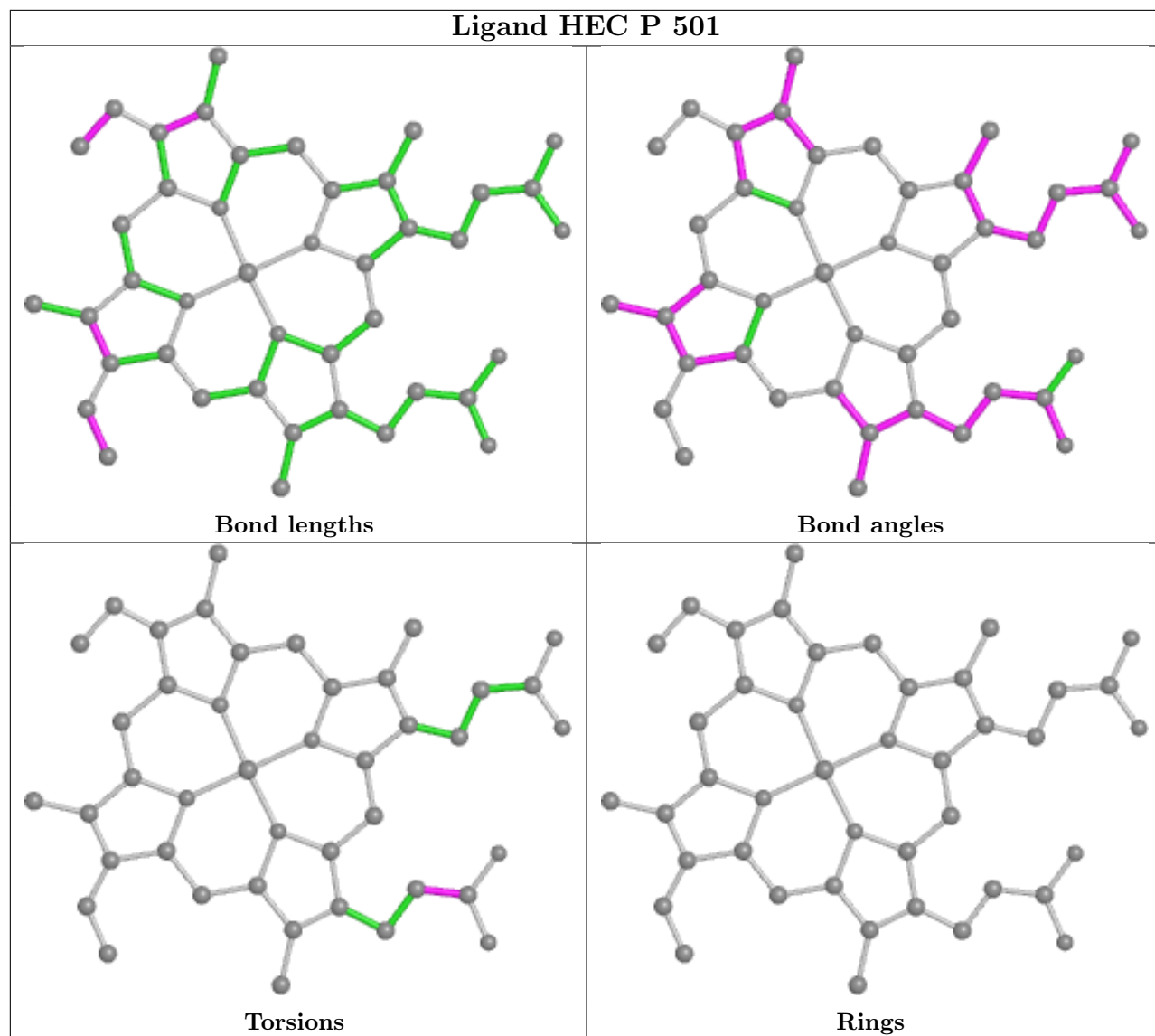


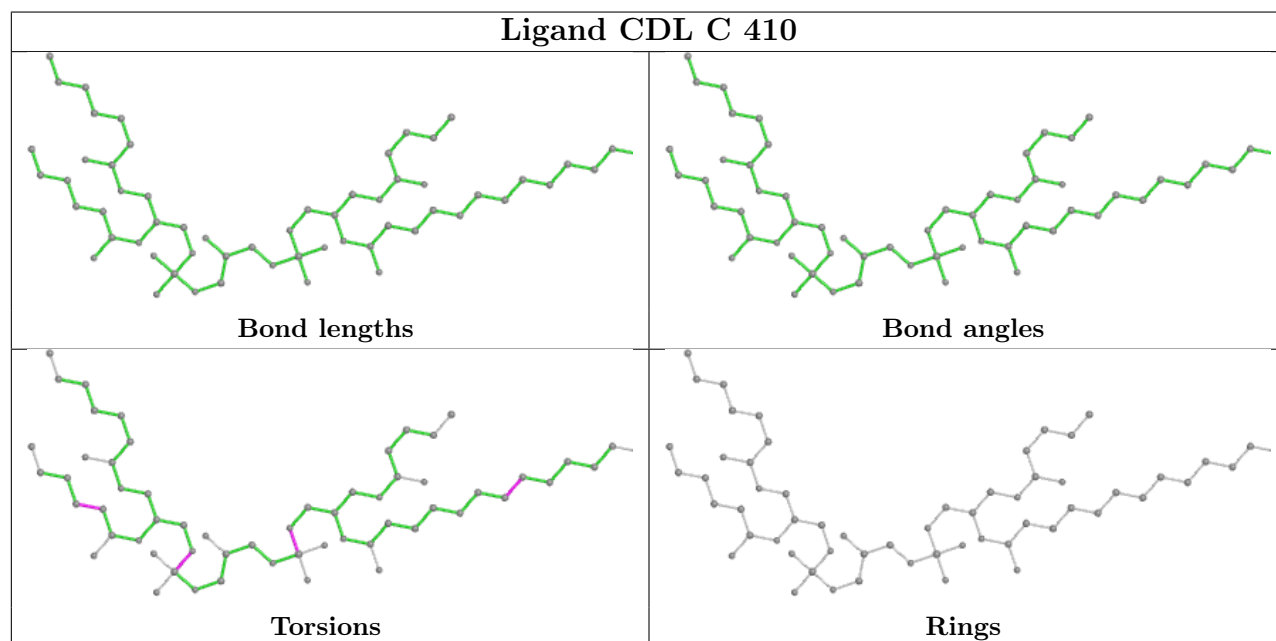
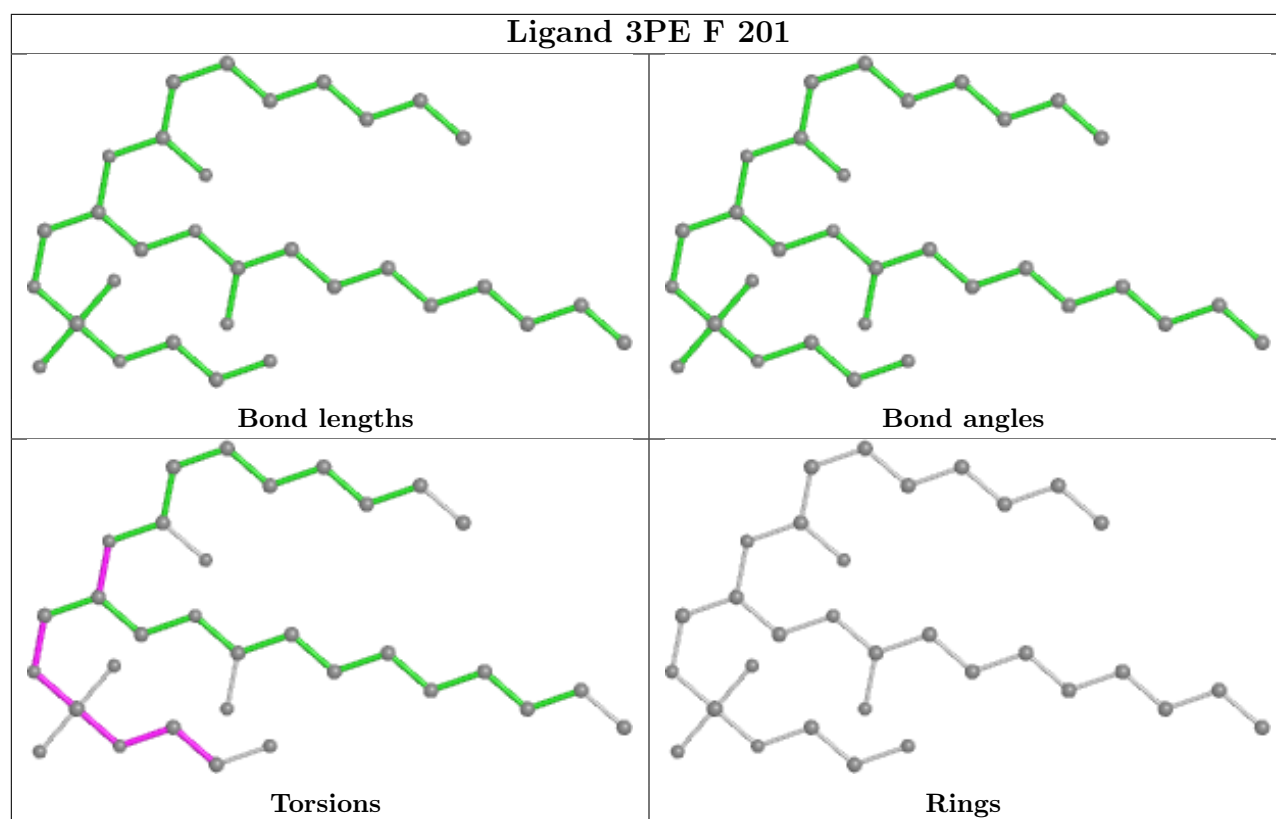


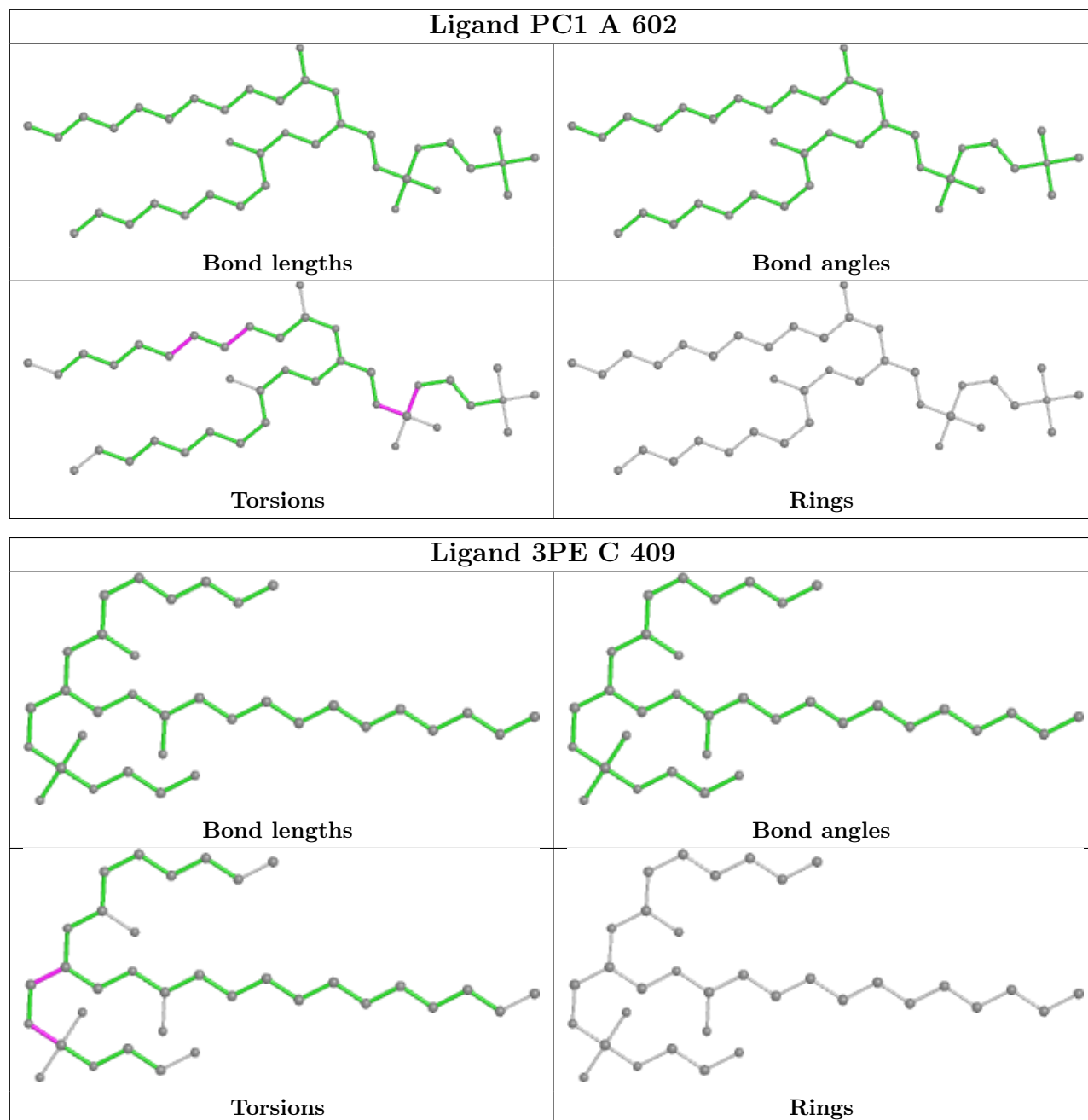


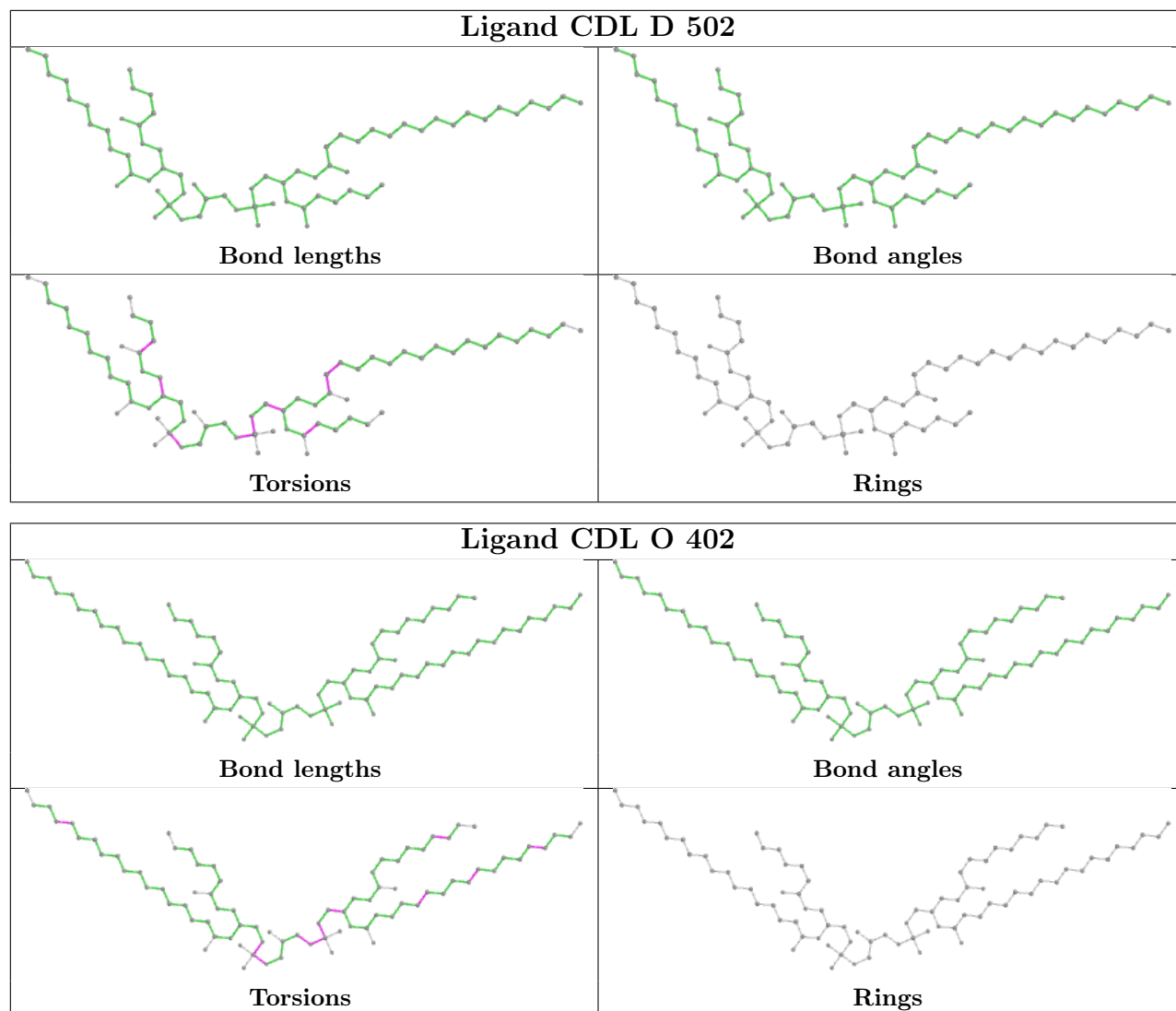


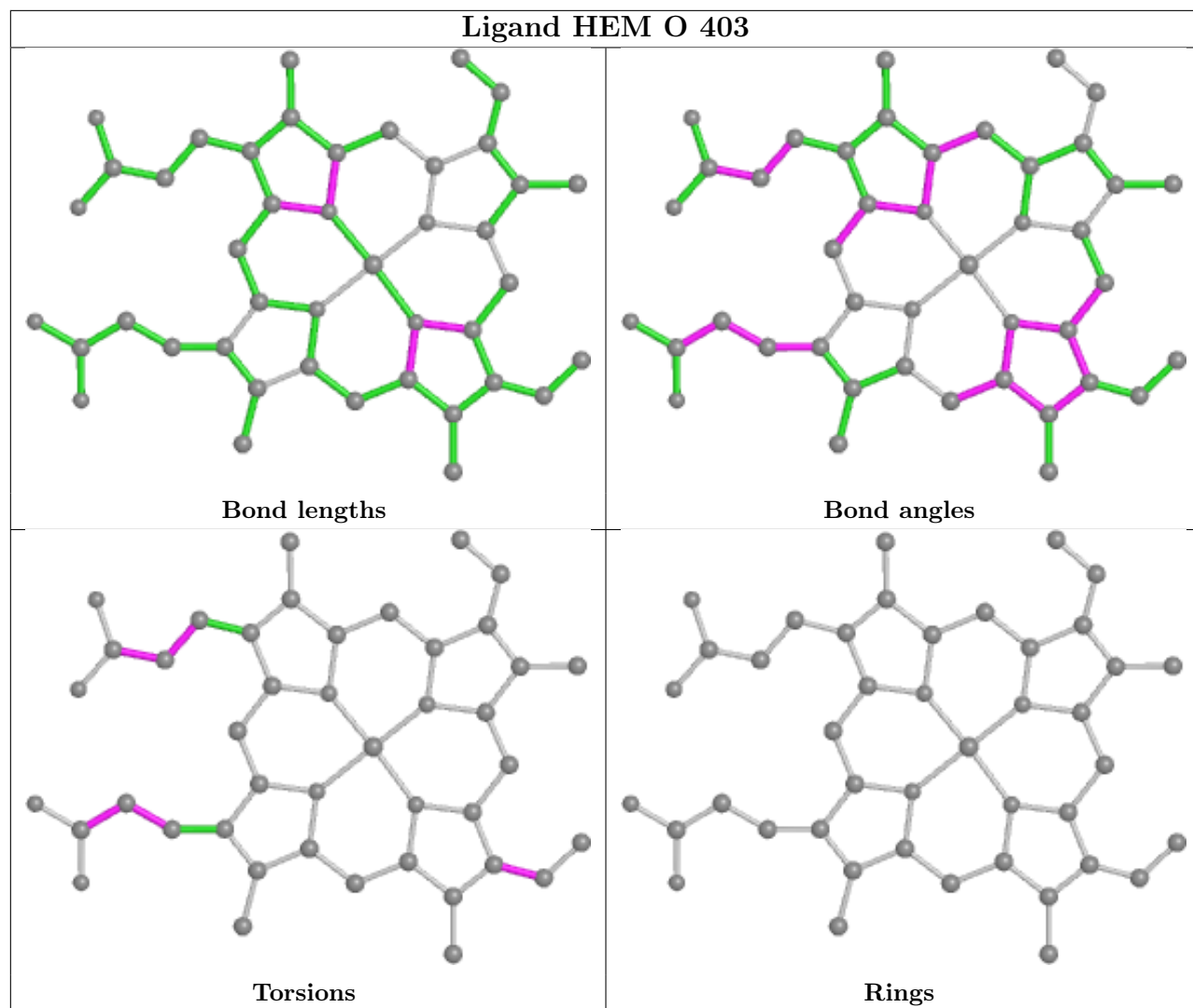


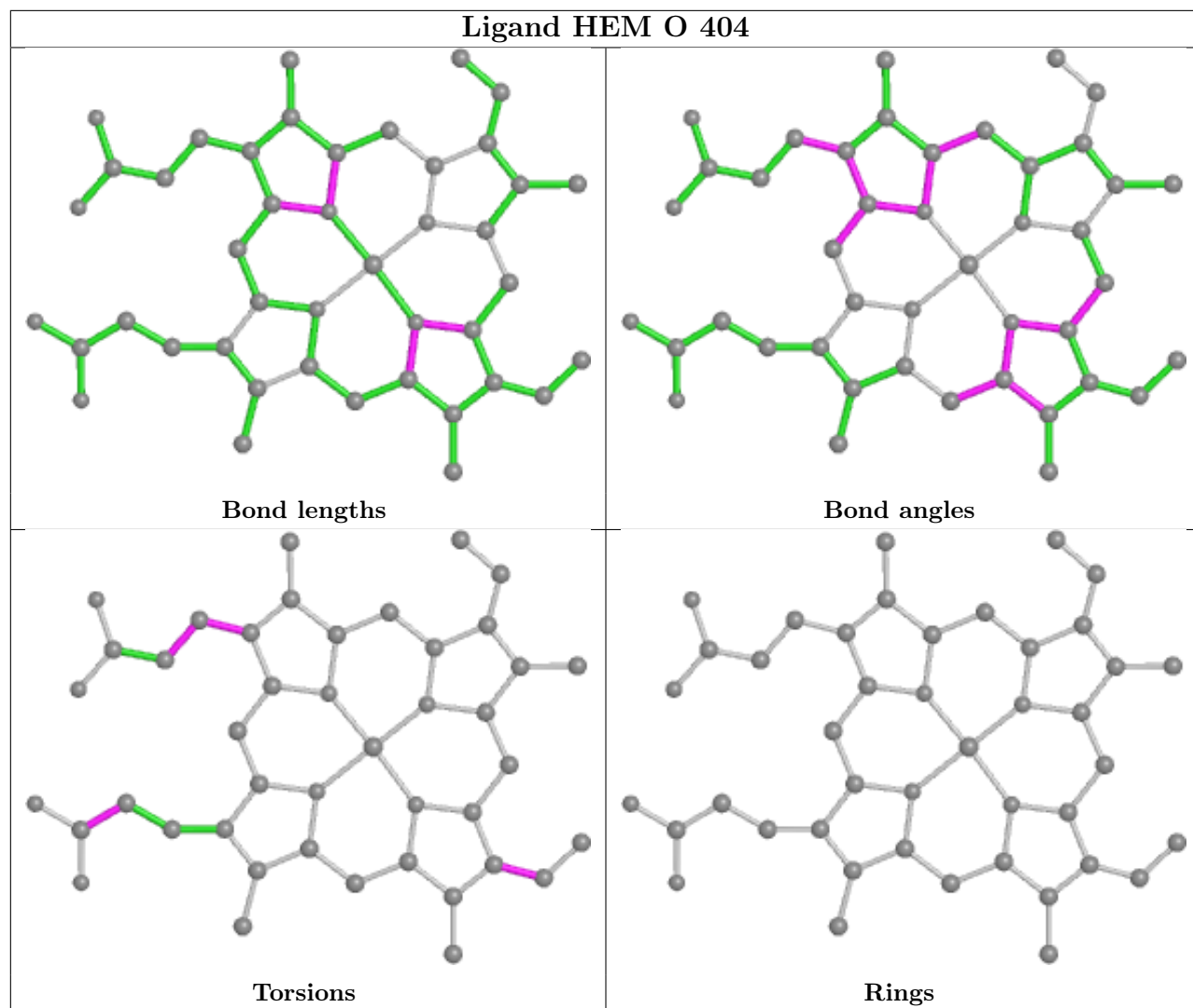


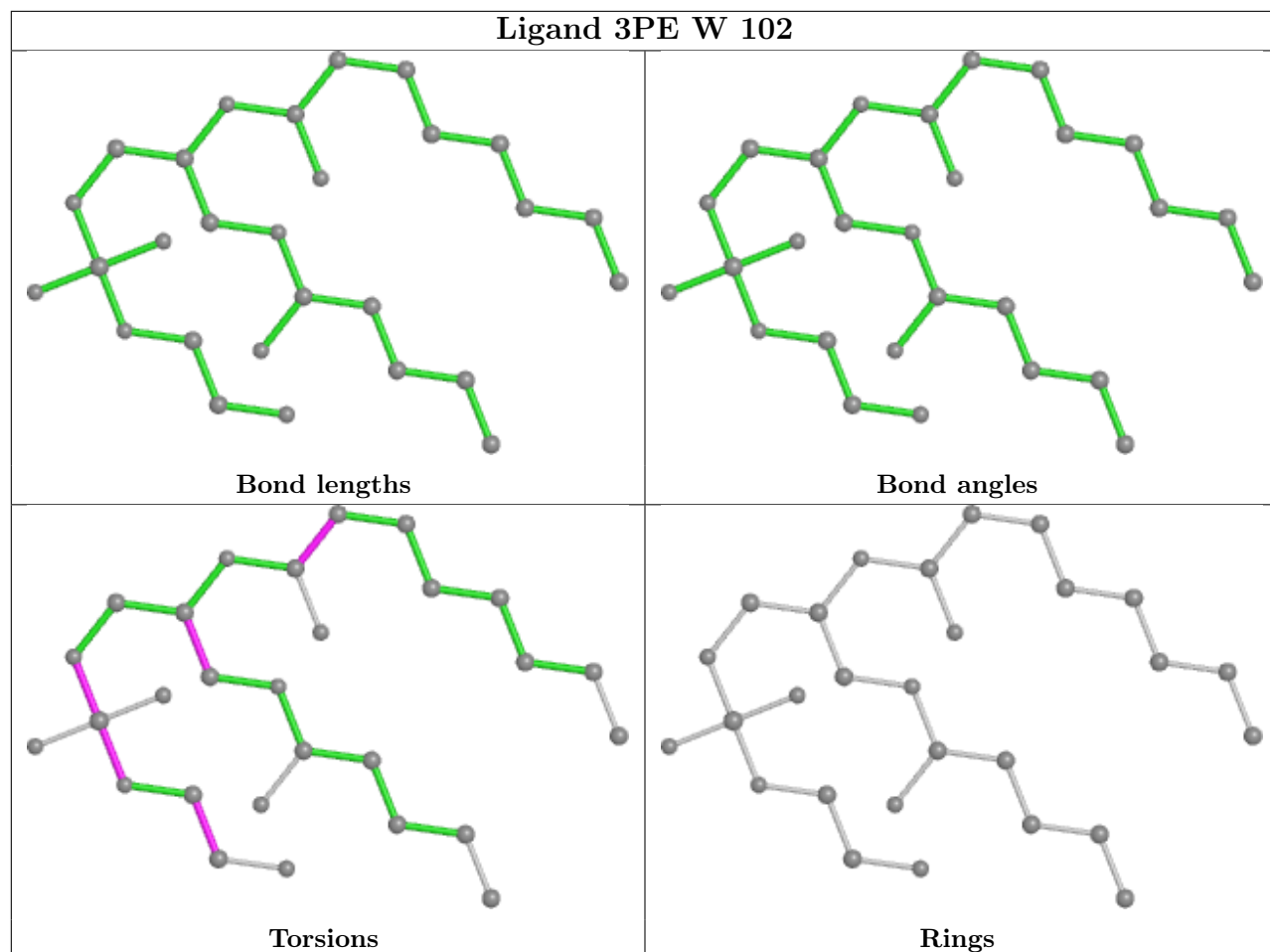


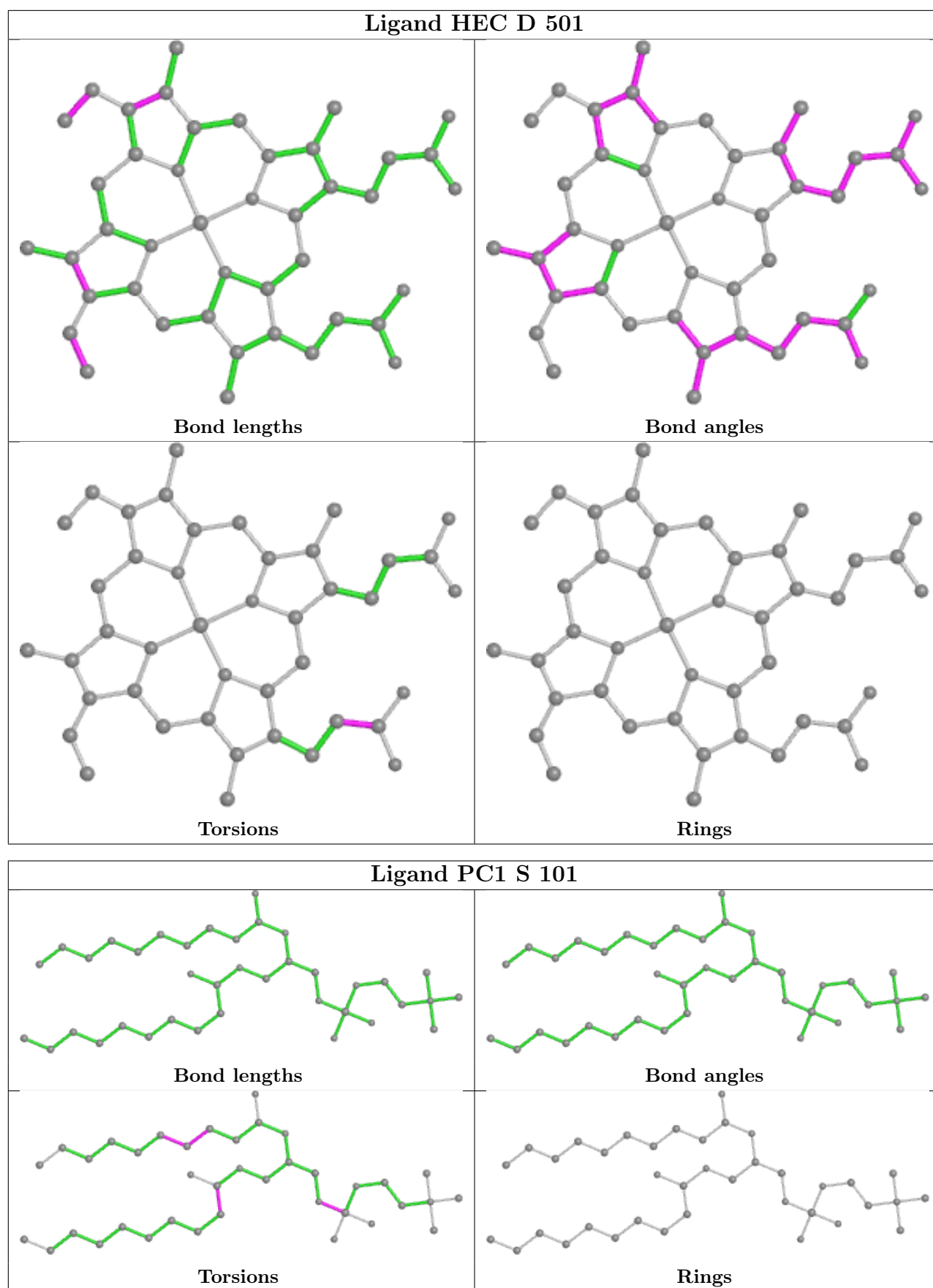


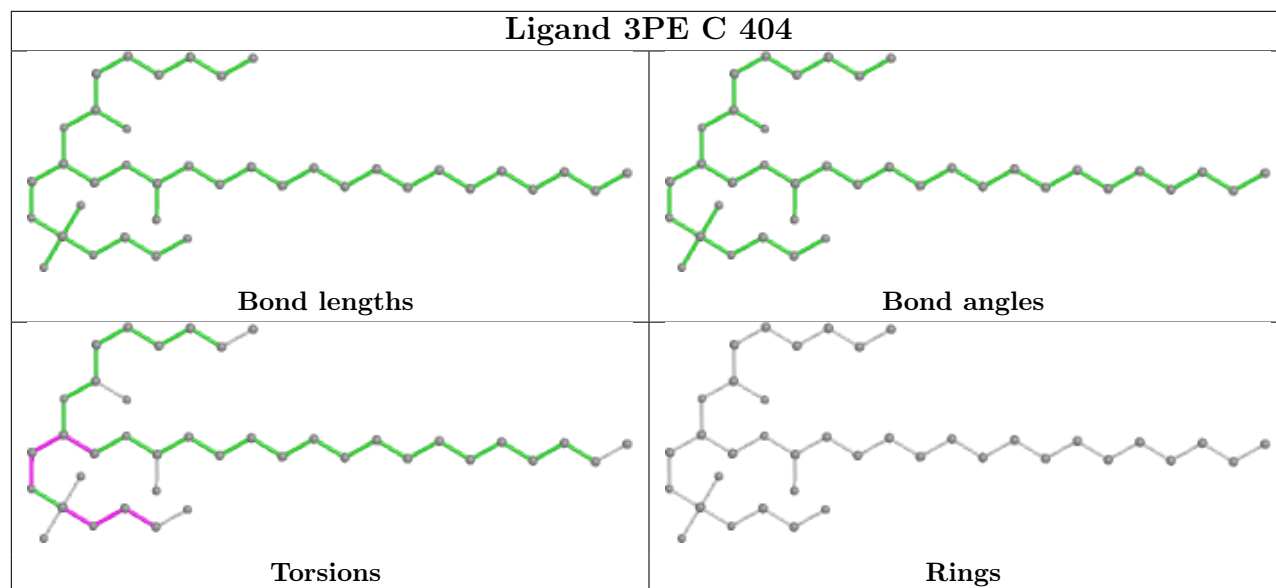












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

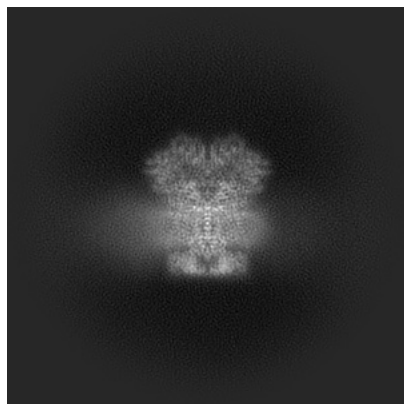
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22445. These allow visual inspection of the internal detail of the map and identification of artifacts.

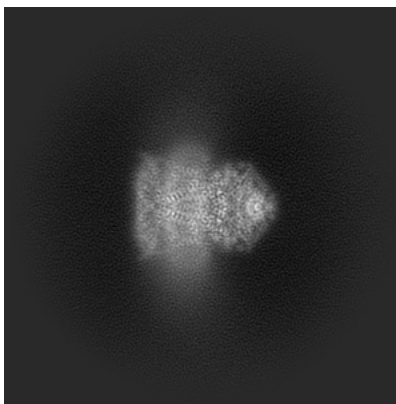
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

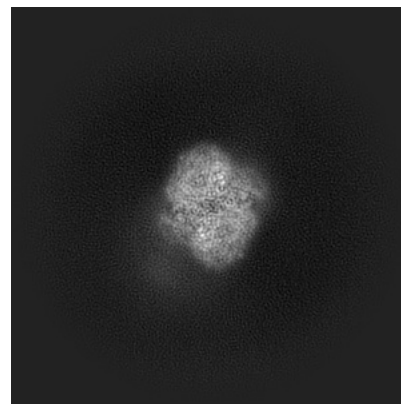
6.1.1 Primary map



X

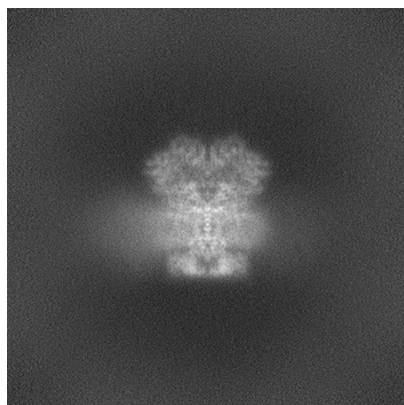


Y

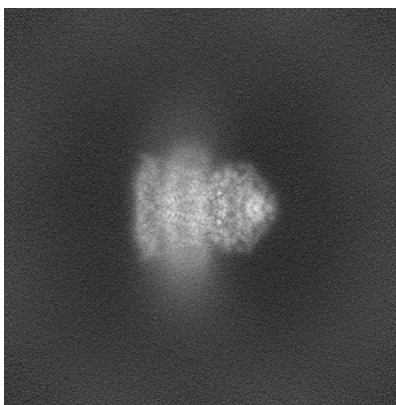


Z

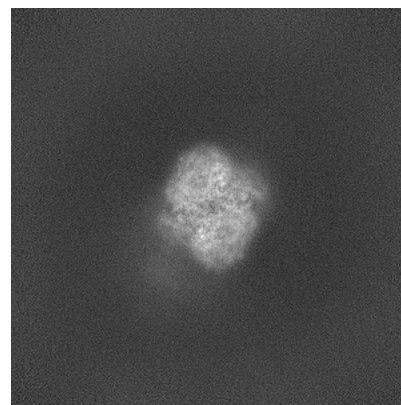
6.1.2 Raw map



X



Y

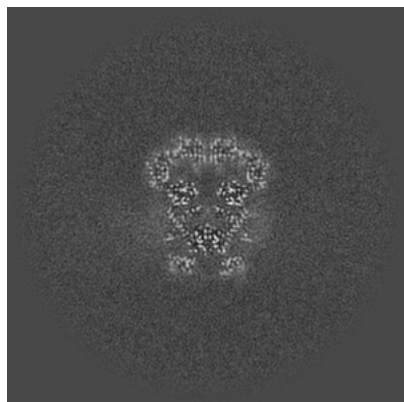


Z

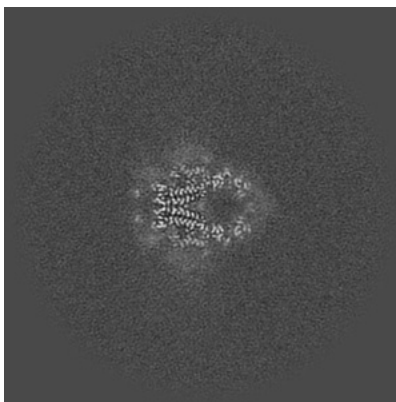
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

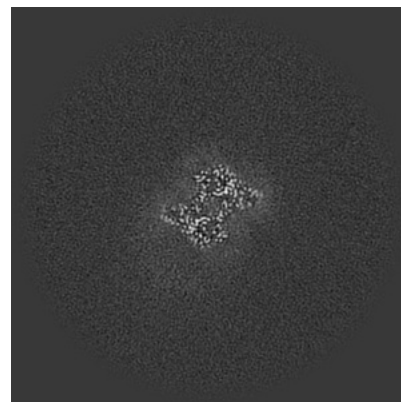
6.2.1 Primary map



X Index: 256

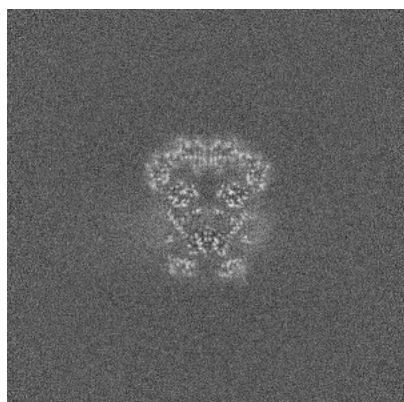


Y Index: 256

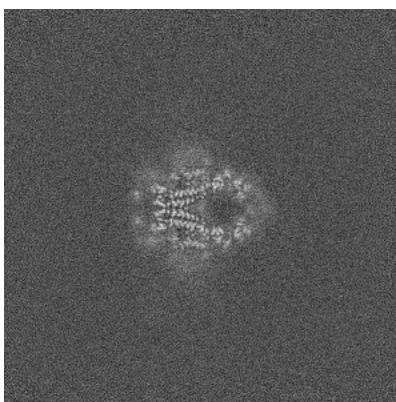


Z Index: 256

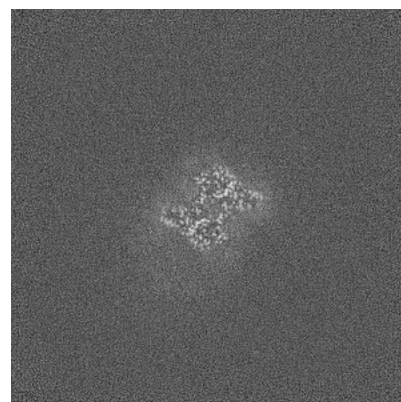
6.2.2 Raw map



X Index: 256



Y Index: 256

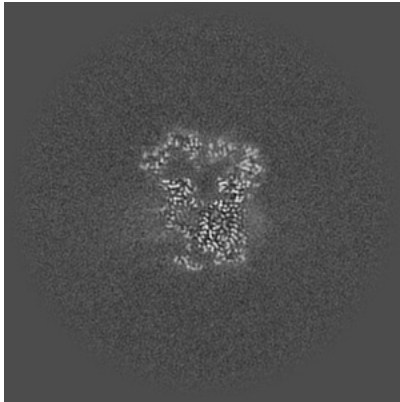


Z Index: 256

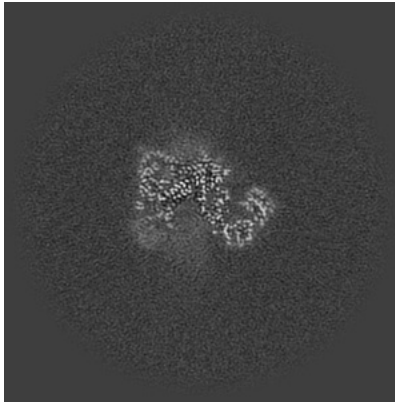
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

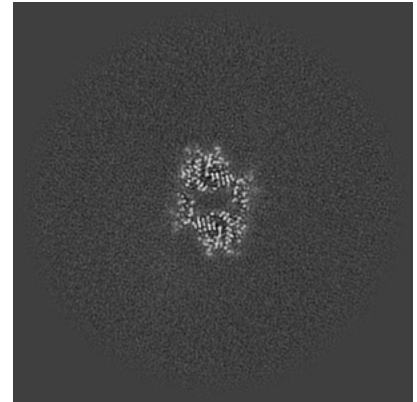
6.3.1 Primary map



X Index: 264

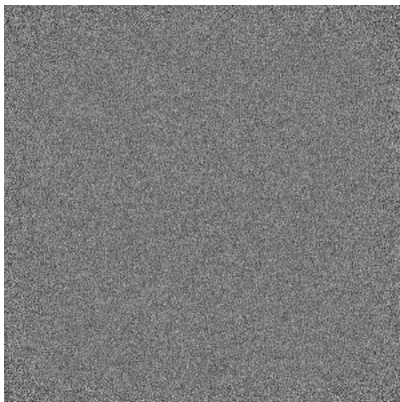


Y Index: 273

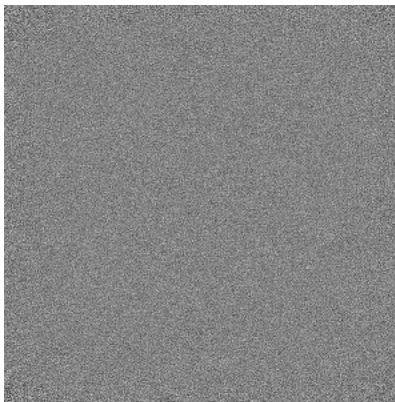


Z Index: 276

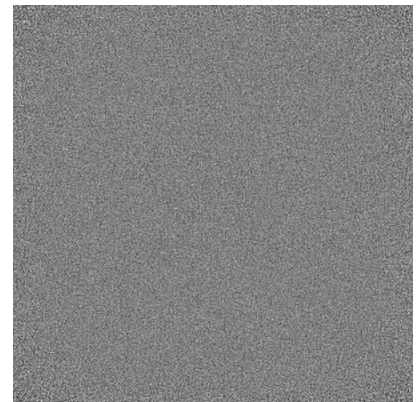
6.3.2 Raw map



X Index: 0



Y Index: 0

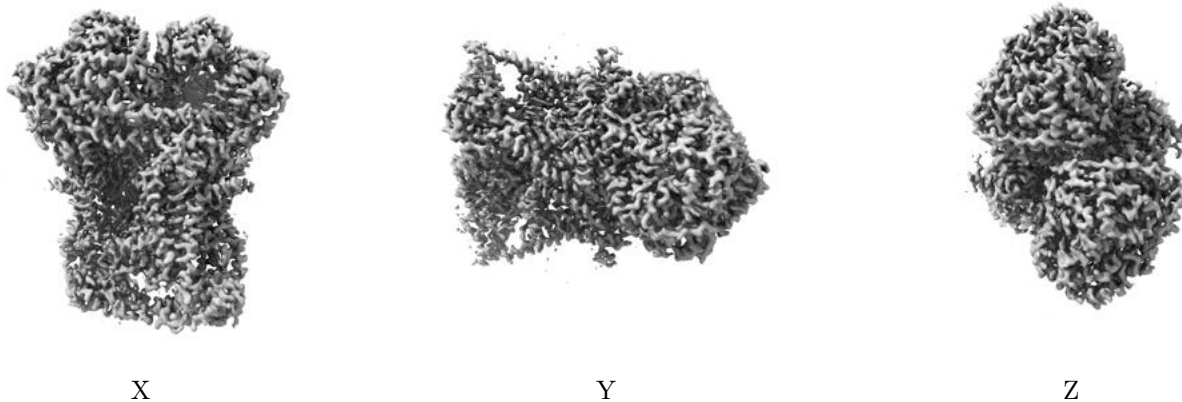


Z Index: 0

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

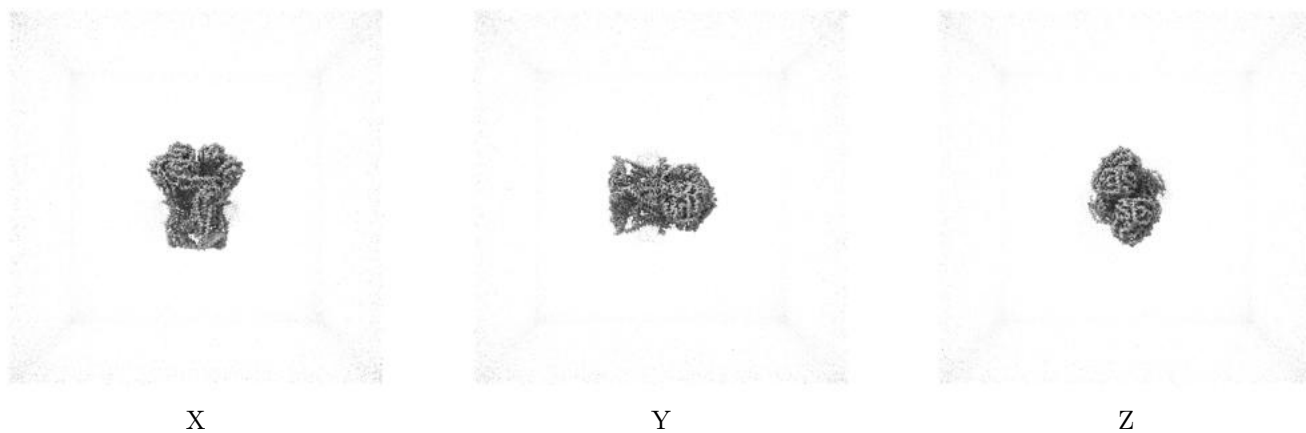
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

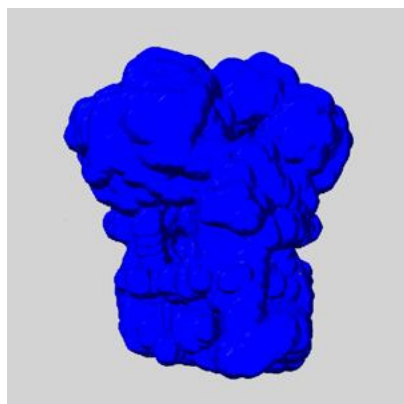
6.5 Mask visualisation [i](#)

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

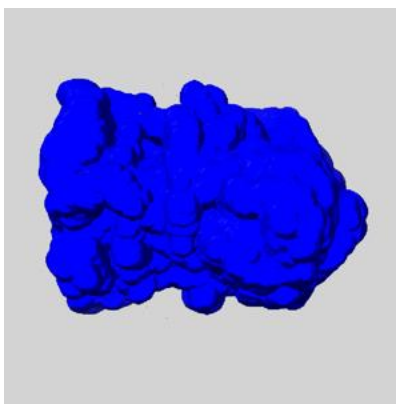
A mask typically either:

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

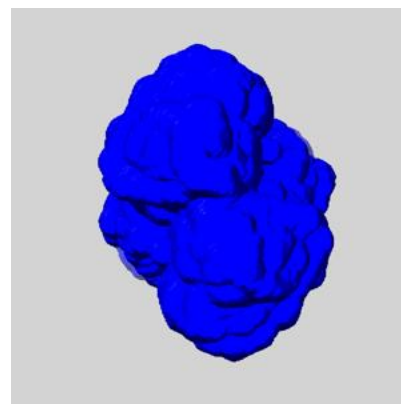
6.5.1 emd_22445_msk_1.map [i](#)



X



Y

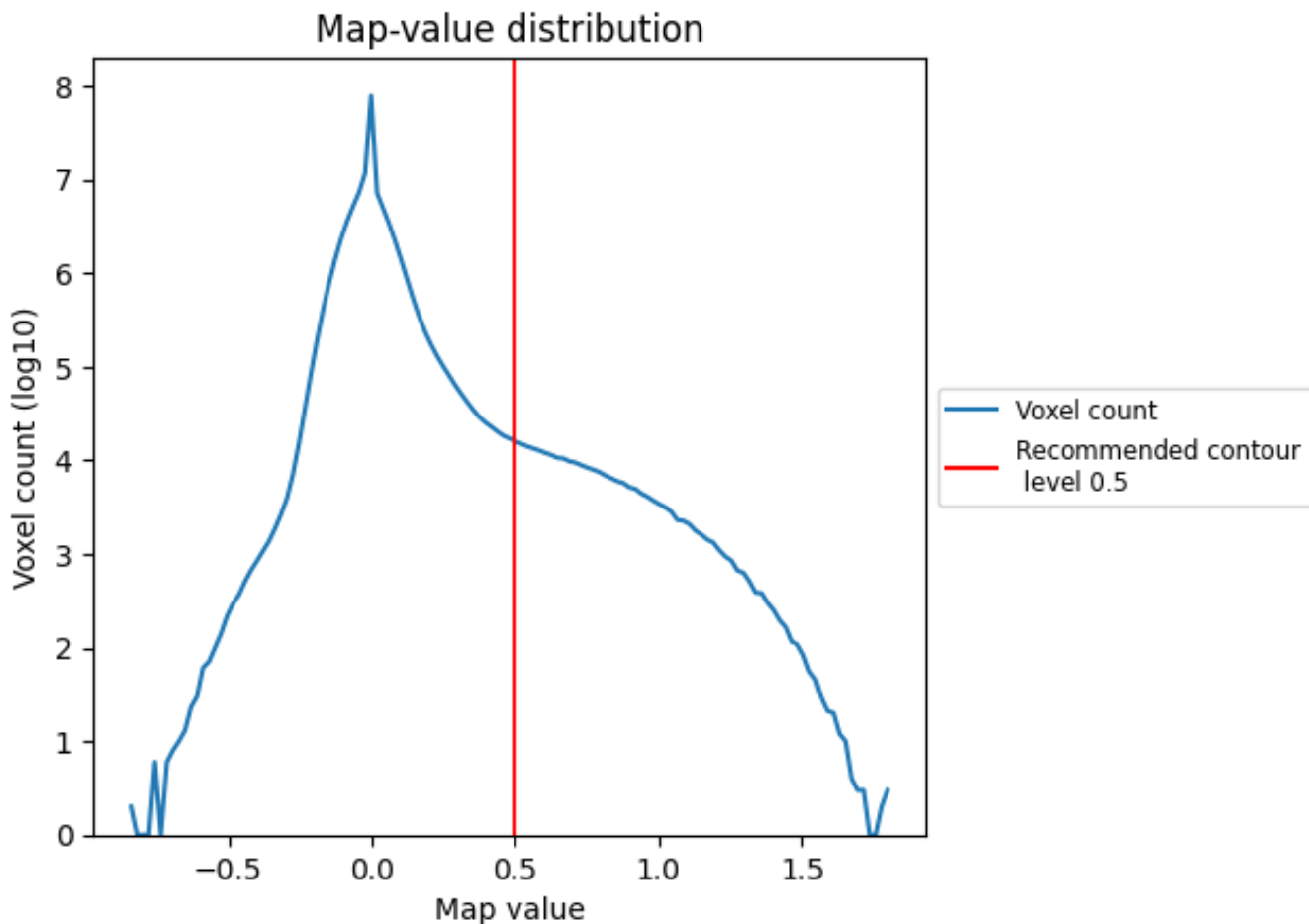


Z

7 Map analysis [i](#)

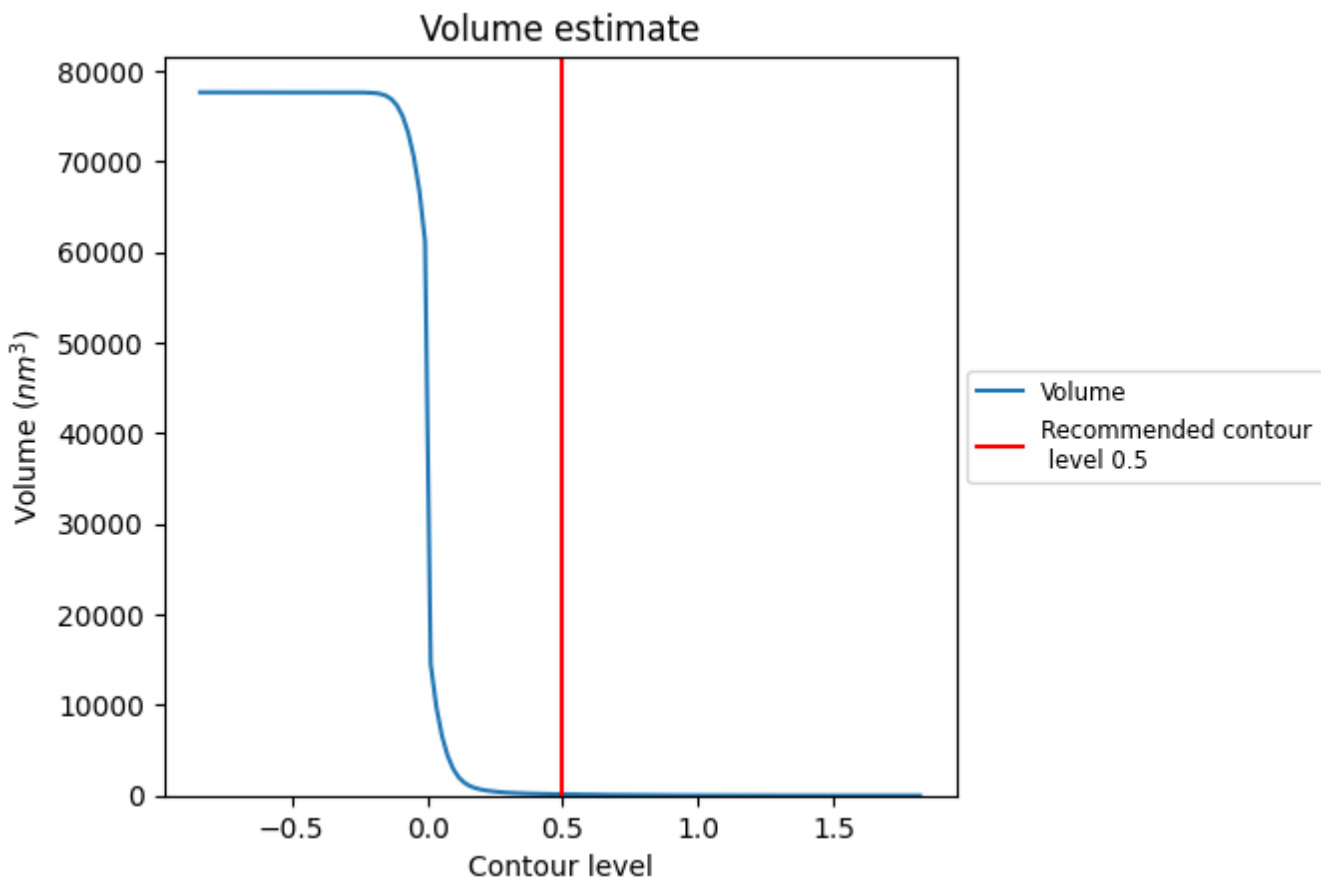
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

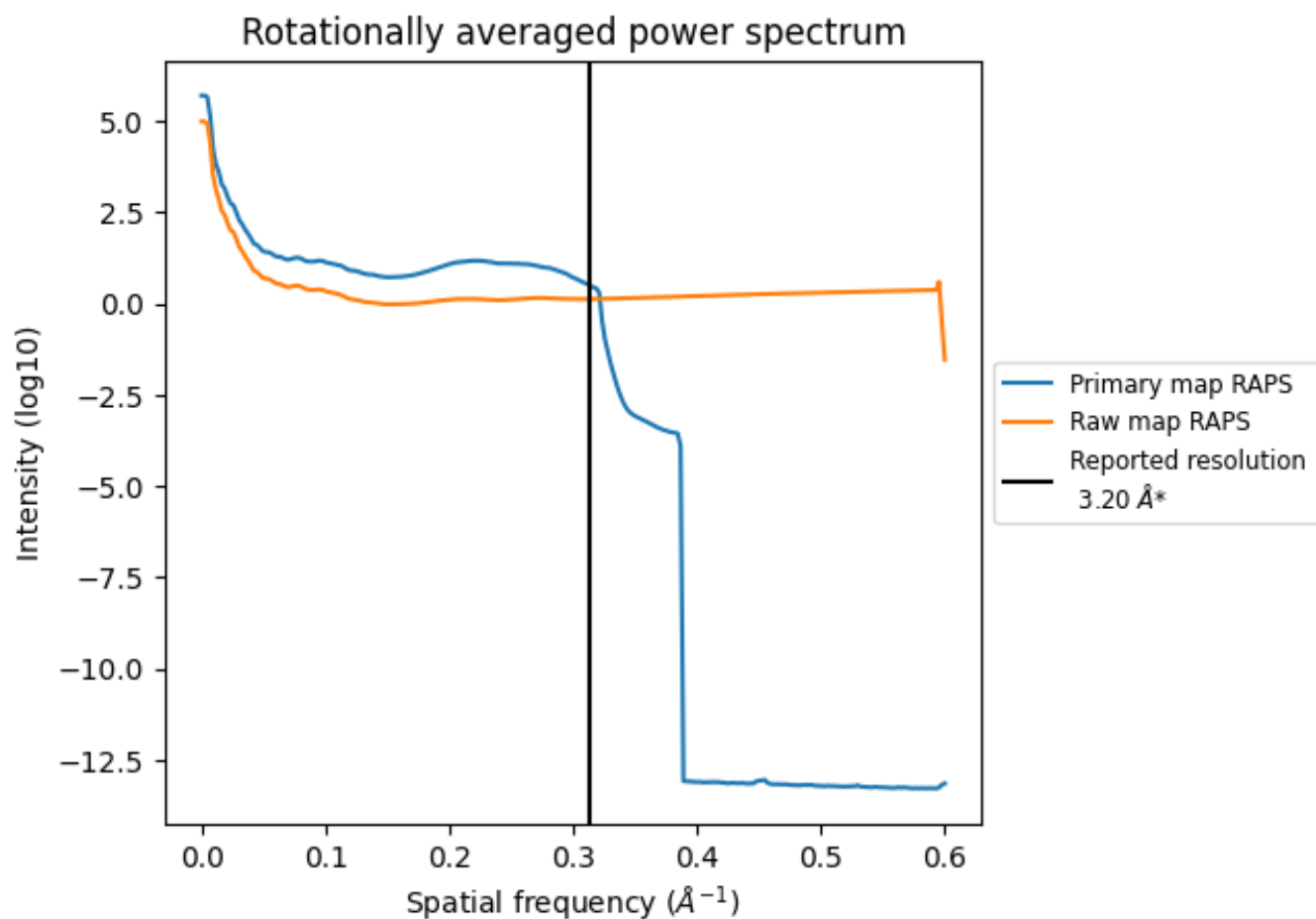
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 128 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](#)

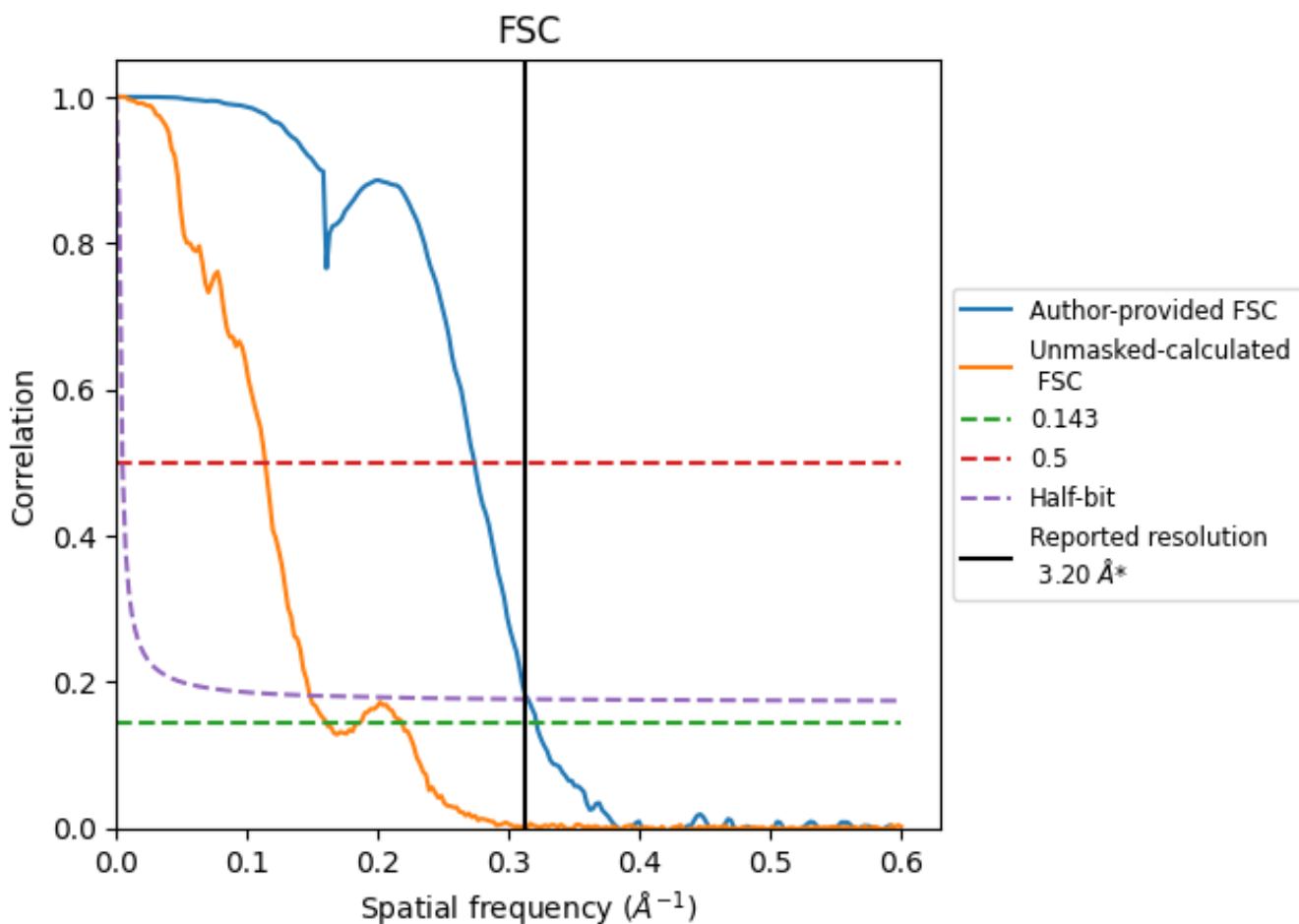


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

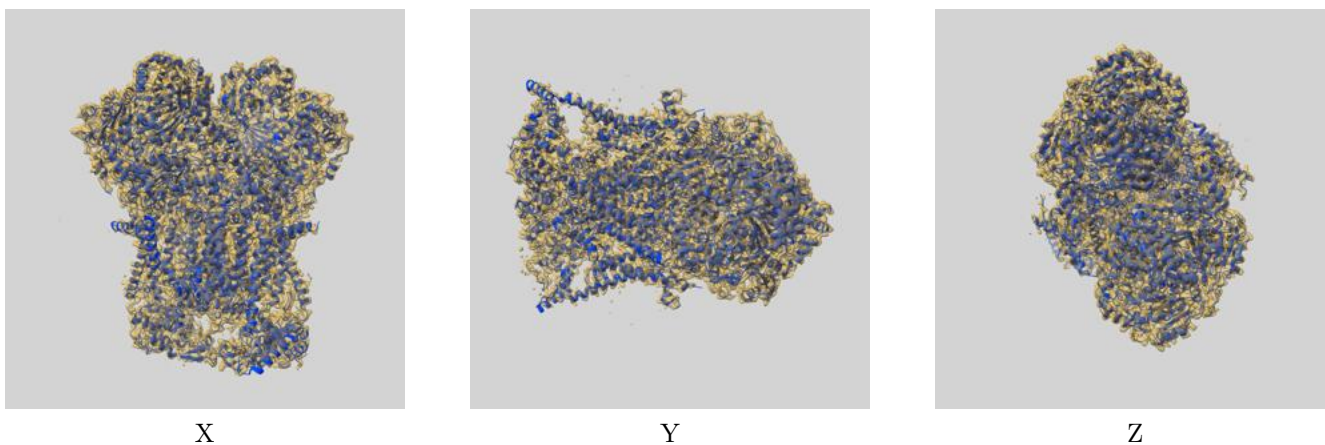
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.11	3.65	3.18
Unmasked-calculated*	6.23	8.79	6.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.23 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

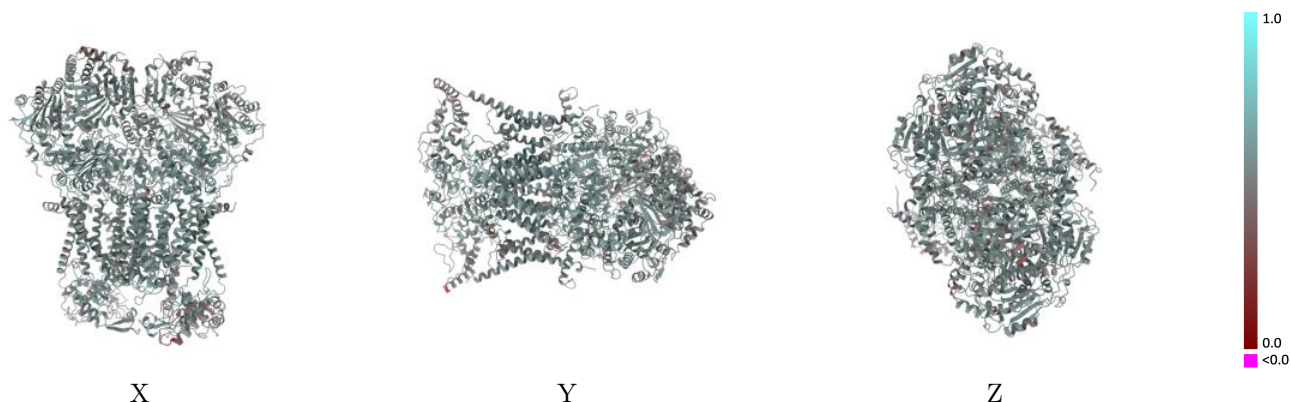
This section contains information regarding the fit between EMDB map EMD-22445 and PDB model 7JRG. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



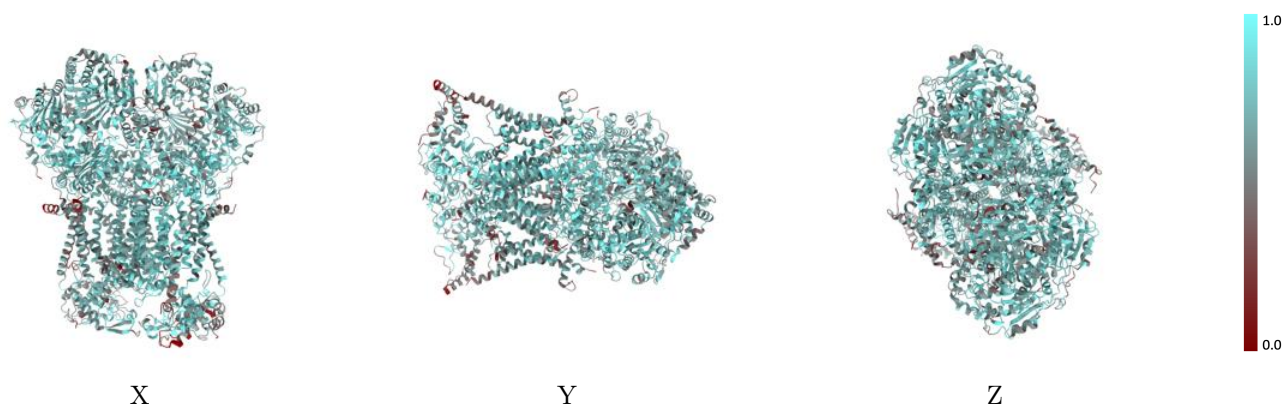
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



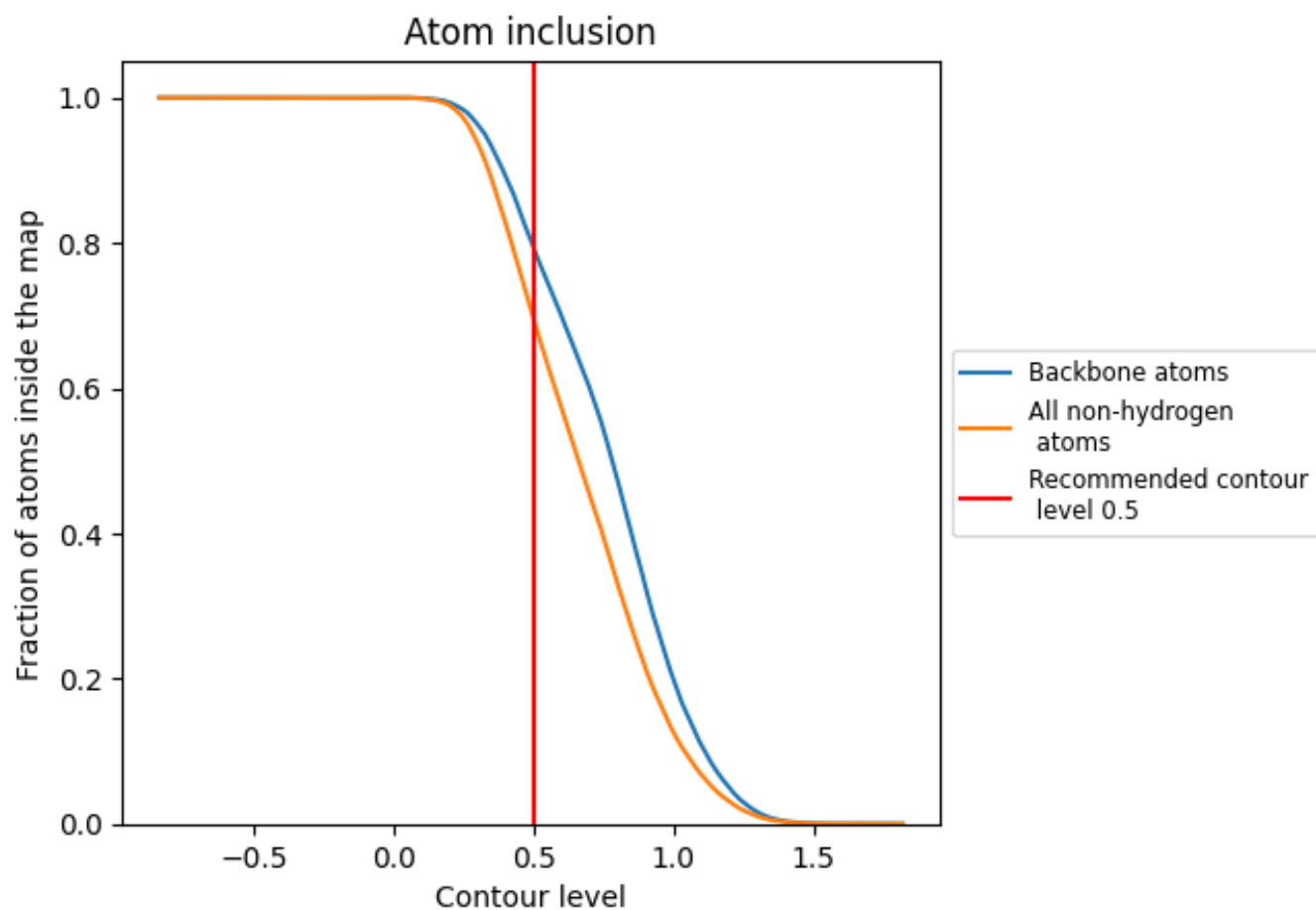
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 70% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6953	 0.5430
A	 0.7396	 0.5500
B	 0.6734	 0.5180
C	 0.7381	 0.5670
D	 0.7235	 0.5520
E	 0.5819	 0.5370
F	 0.6995	 0.5660
G	 0.5429	 0.5240
H	 0.4288	 0.4610
J	 0.5139	 0.5210
K	 0.3843	 0.4960
M	 0.7330	 0.5490
N	 0.6914	 0.5220
O	 0.7459	 0.5690
P	 0.7558	 0.5530
Q	 0.6661	 0.5420
R	 0.7608	 0.5620
S	 0.5393	 0.5330
T	 0.4556	 0.4520
V	 0.6199	 0.5390
W	 0.4714	 0.5040

