



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 01:14 PM UTC

PDB ID : 8BEL / pdb_00008bel
EMDB ID : EMD-16007
Title : Cryo-EM structure of the Arabidopsis thaliana I+III2 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

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:

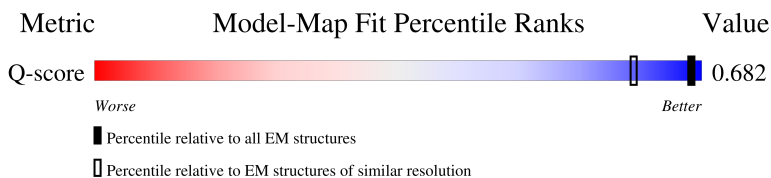
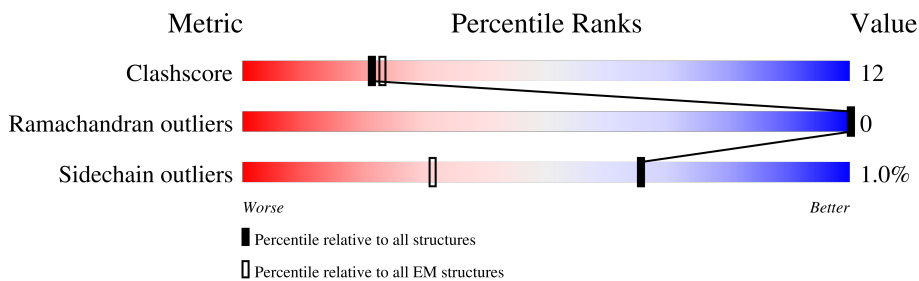
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.






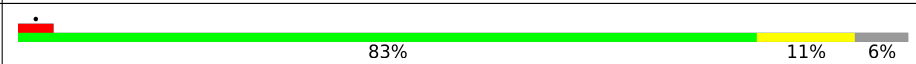
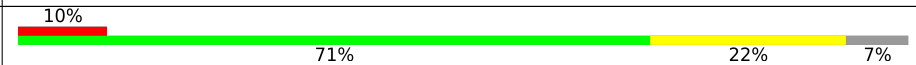

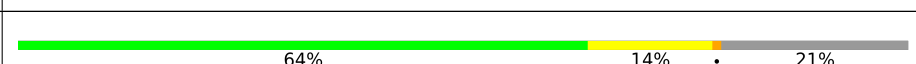
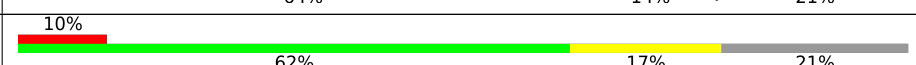
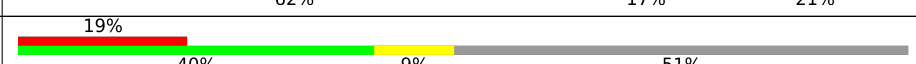
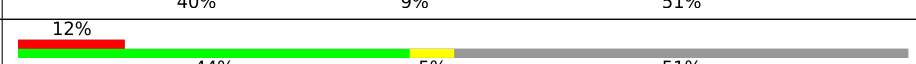
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3458 (1.75 - 2.75)

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	C	393	
1	M	393	
2	D	272	
2	N	272	

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Mol	Chain	Length	Quality of chain
3	E	307	
3	O	307	
4	G	72	
4	Q	72	
5	H	69	
5	R	69	
6	I	72	
6	S	72	
7	J	57	
7	T	57	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	FES	N	301	-	-	X	-

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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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		

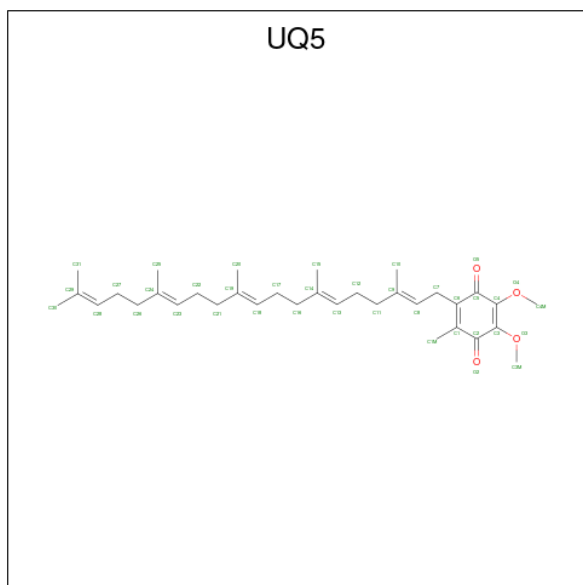
- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

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.

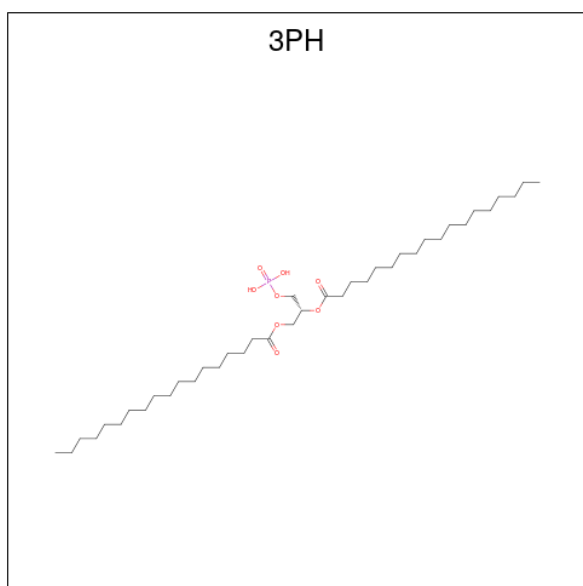
Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	28	Total	C	N	O	0	0
			203	137	33	33		
7	T	28	Total	C	N	O	0	0
			205	139	34	32		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



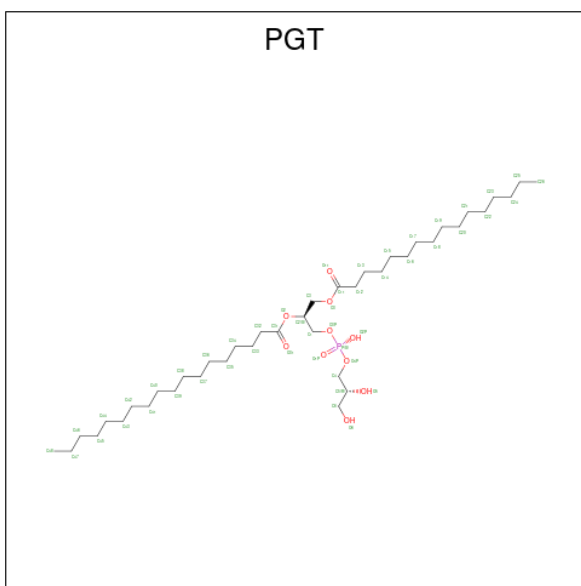
Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			38	34	4	
9	C	1	Total	C	O	0
			38	34	4	
9	M	1	Total	C	O	0
			38	34	4	

- Molecule 10 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 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	

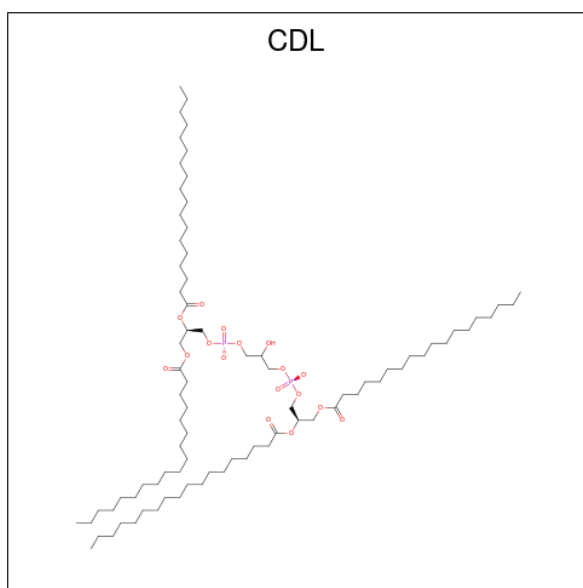
- Molecule 11 is (1S)-2-{{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



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	

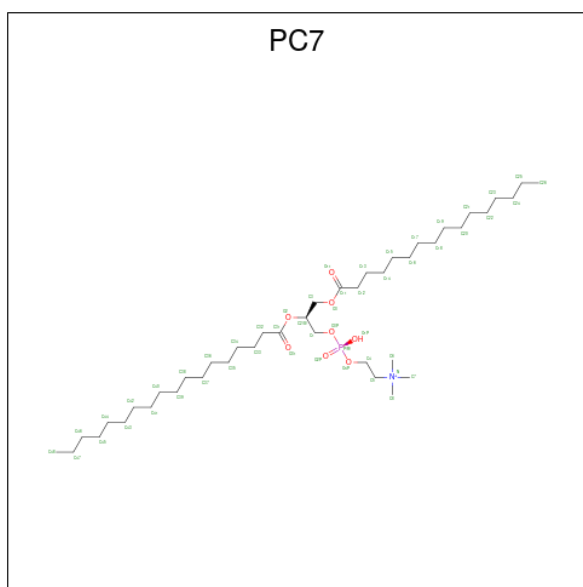
- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand

of Interest" by depositor).



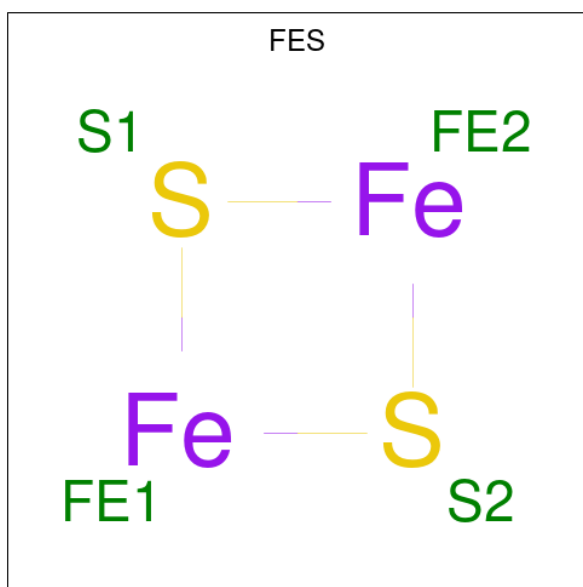
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	C	1	81	62	17	2	0
12	C	1	85	66	17	2	0
12	G	1	85	66	17	2	0
12	M	1	77	58	17	2	0
12	N	1	81	62	17	2	0
12	O	1	88	69	17	2	0
12	Q	1	70	51	17	2	0

- 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 (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P) (labeled as "Ligand of Interest" by depositor).



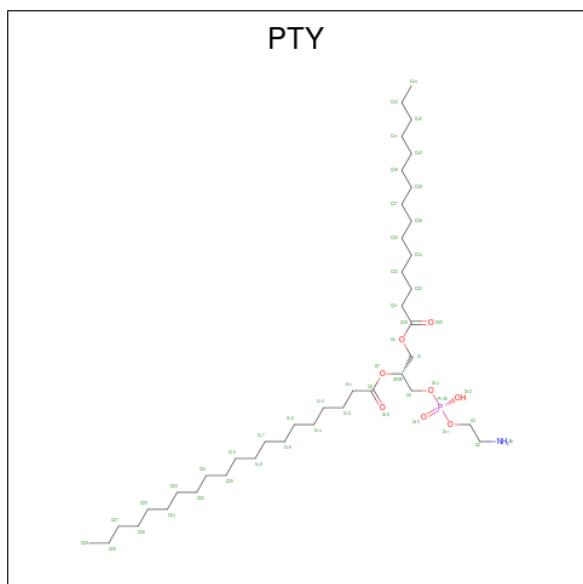
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	C	1	51	41	1	8	1	0
13	D	1	34	24	1	8	1	0
13	G	1	52	42	1	8	1	0
13	M	1	45	35	1	8	1	0
13	N	1	39	29	1	8	1	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (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 (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



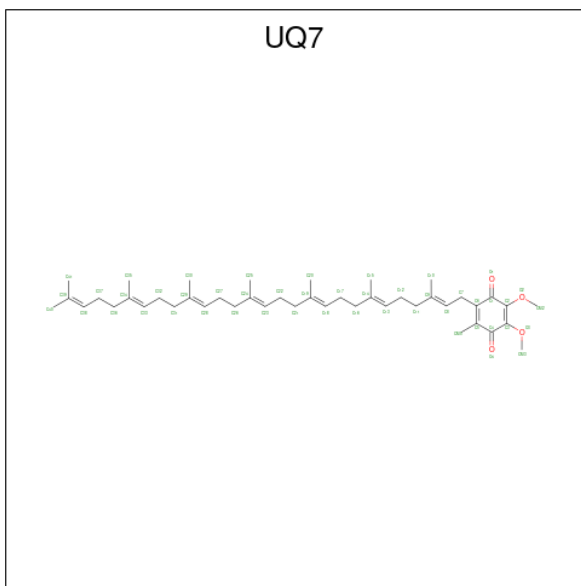
Mol	Chain	Residues	Atoms				AltConf	
15	J	1	Total	C	N	O	P	0
			41	31	1	8	1	

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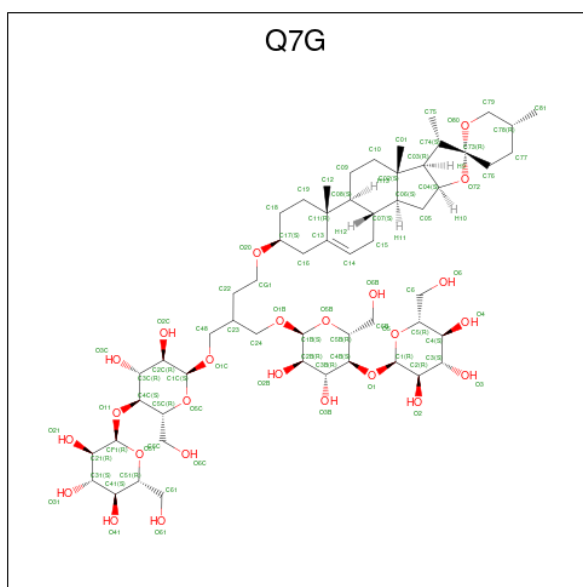
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	M	1	40	30	1	8	1	0
15	T	1	29	19	1	8	1	0

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



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

- 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 (CCD ID: 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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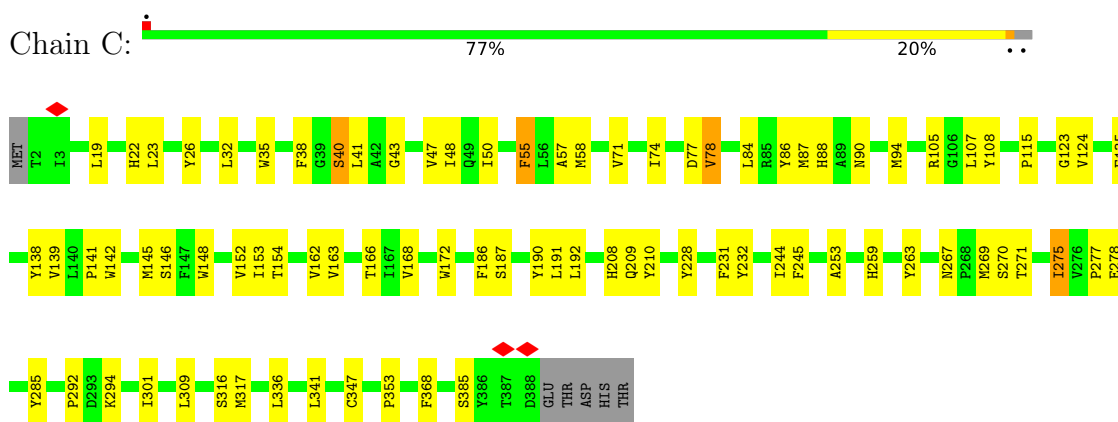
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Mol	Chain	Residues	Atoms		AltConf
18	R	2	Total 2	O 2	0
18	S	13	Total 13	O 13	0
18	T	1	Total 1	O 1	0

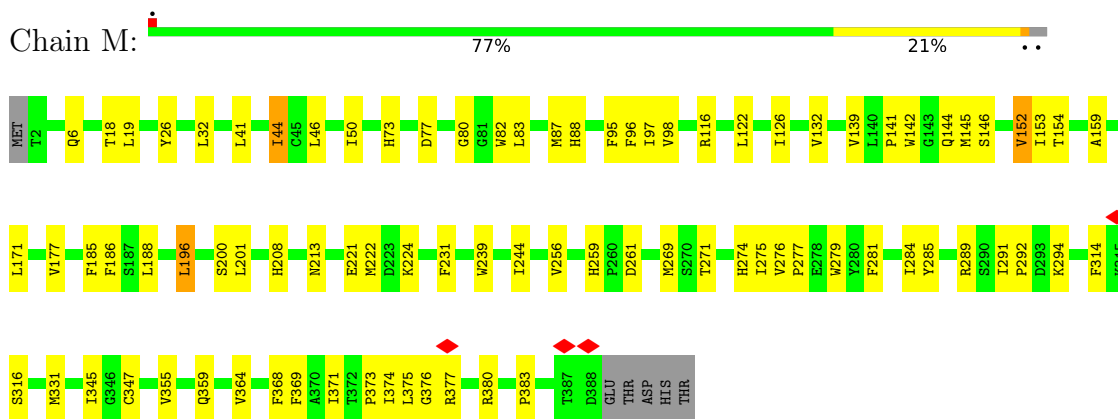
3 Residue-property plots [i](#)

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

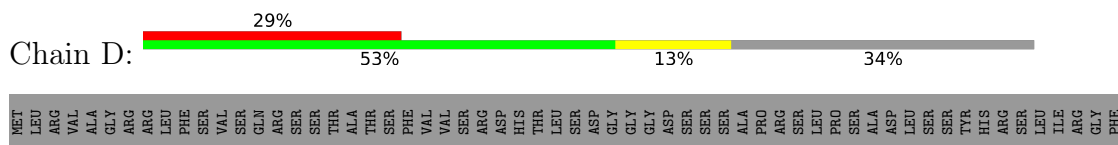
- Molecule 1: Cytochrome b

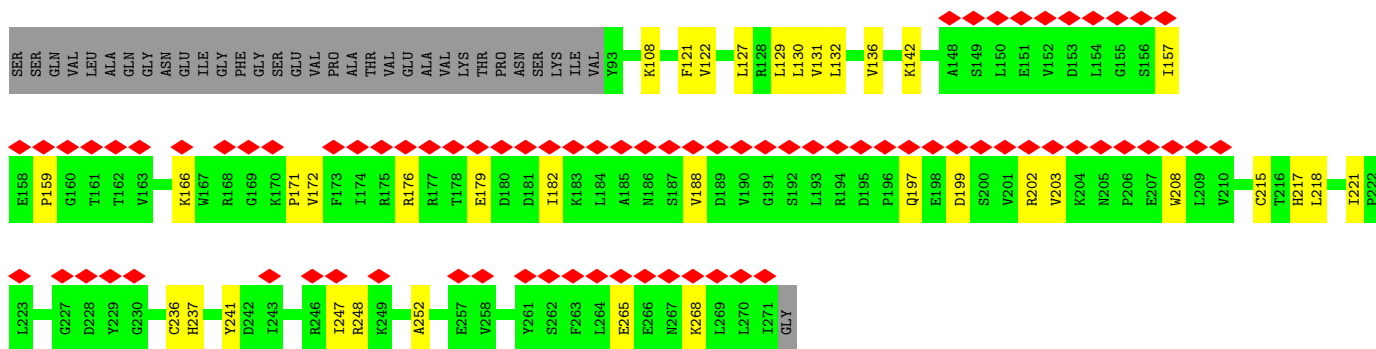


- Molecule 1: Cytochrome b

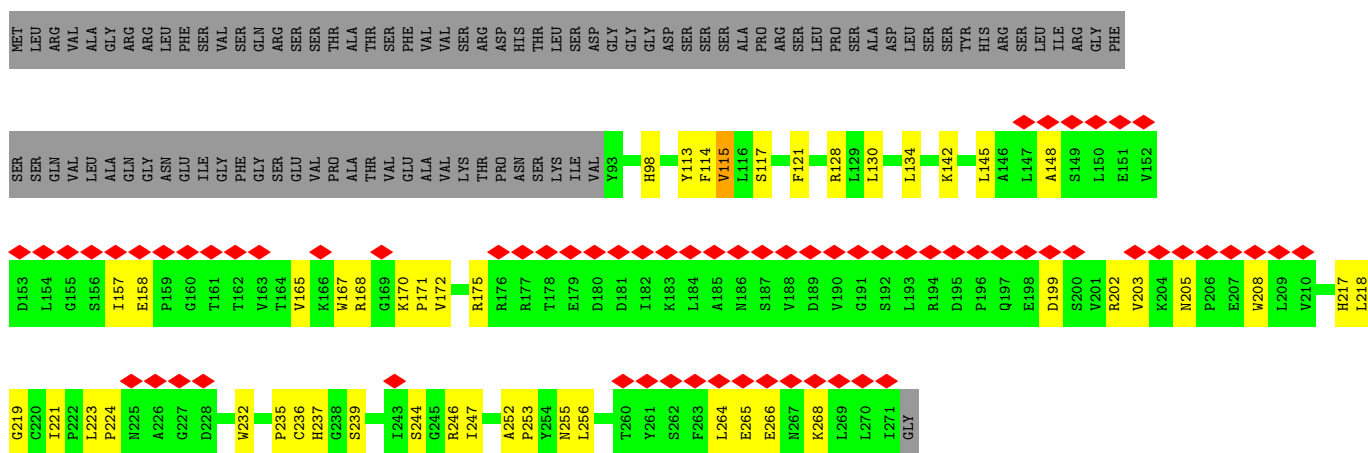


- Molecule 2: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

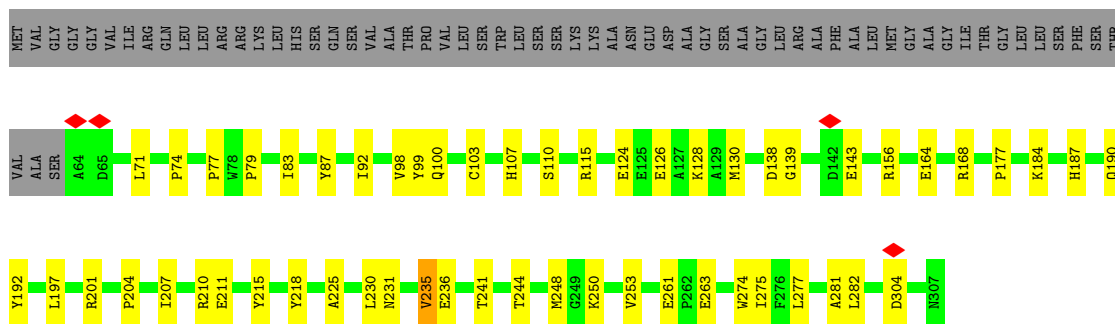




• Molecule 2: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

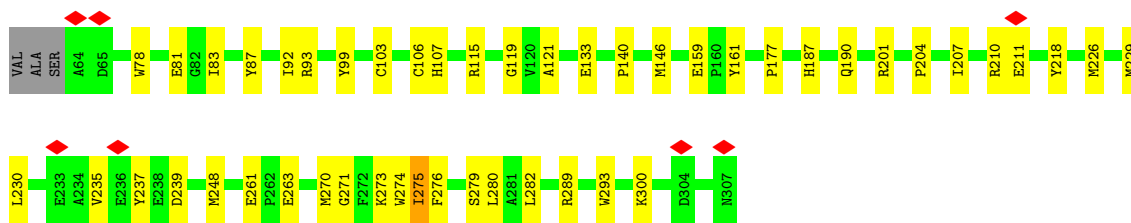


• Molecule 3: Cytochrome c1 2, heme protein, mitochondrial



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

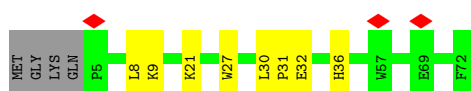
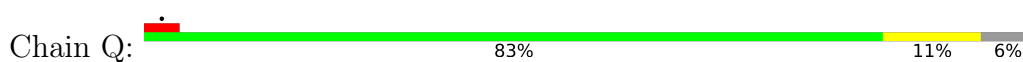




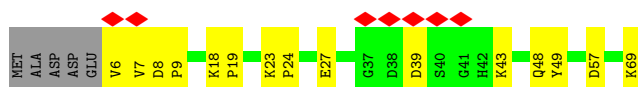
- Molecule 4: Cytochrome b-c1 complex subunit 8-1, mitochondrial



- 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

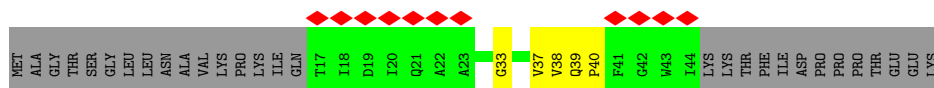
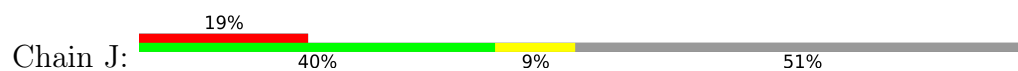


- Molecule 6: Cytochrome b-c1 complex subunit 9, mitochondrial

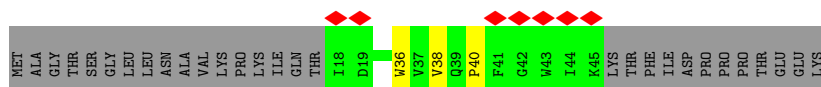




- Molecule 7: Cytochrome b-c1 complex subunit 10, mitochondrial



- 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: FES, PTY, HEM, 3PH, PC7, Q7G, UQ5, UQ7, CDL, PGT

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	0.68	13/3208 (0.4%)	0.75	8/4395 (0.2%)
1	M	0.63	7/3208 (0.2%)	0.77	5/4395 (0.1%)
2	D	0.34	0/1441	0.47	0/1961
2	N	0.48	0/1441	0.67	4/1961 (0.2%)
3	E	0.40	0/1968	0.57	2/2672 (0.1%)
3	O	0.44	0/1968	0.55	2/2672 (0.1%)
4	G	0.50	1/600 (0.2%)	0.47	1/815 (0.1%)
4	Q	0.37	0/591	0.69	0/802
5	H	0.26	0/531	0.43	0/713
5	R	0.64	2/524 (0.4%)	0.80	2/703 (0.3%)
6	I	0.96	4/488 (0.8%)	0.90	0/655
6	S	0.48	0/488	0.77	2/655 (0.3%)
7	J	0.66	0/210	1.14	4/290 (1.4%)
7	T	0.15	0/212	0.34	0/291
All	All	0.55	27/16878 (0.2%)	0.68	30/22980 (0.1%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	88	HIS	C-O	-9.52	1.13	1.24
1	C	192	LEU	C-O	-9.17	1.15	1.24
1	M	87	MET	C-O	-8.34	1.14	1.24
4	G	7	LYS	C-O	-7.99	1.14	1.24
1	C	190	TYR	C-O	-7.29	1.15	1.24

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	175	ARG	CB-CA-C	-9.53	98.94	111.42
1	M	96	PHE	CA-C-O	-7.37	112.74	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	96	PHE	CB-CA-C	7.37	123.02	110.79
7	J	38	VAL	N-CA-C	-7.27	99.32	109.21
3	E	304	ASP	CA-CB-CG	6.38	118.98	112.60

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	C	3093	0	3074	77	0
1	M	3093	0	3074	95	0
2	D	1404	0	1395	32	0
2	N	1404	0	1395	41	0
3	E	1917	0	1844	48	0
3	O	1917	0	1844	39	0
4	G	581	0	589	17	0
4	Q	572	0	582	9	0
5	H	518	0	518	14	0
5	R	511	0	511	13	0
6	I	476	0	469	11	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	6	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	2	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	11	0
17	M	78	0	0	0	0
18	C	179	0	0	17	0
18	D	32	0	0	0	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	2	0
18	S	13	0	0	5	0
18	T	1	0	0	0	0
All	All	18929	0	18363	430	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 430 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 [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	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 [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	C	330/336 (98%)	327 (99%)	3 (1%)	70	79
1	M	330/336 (98%)	323 (98%)	7 (2%)	47	58
2	D	155/232 (67%)	153 (99%)	2 (1%)	61	72
2	N	155/232 (67%)	154 (99%)	1 (1%)	78	84
3	E	200/247 (81%)	199 (100%)	1 (0%)	81	87
3	O	200/247 (81%)	198 (99%)	2 (1%)	68	77
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%)	56 (98%)	1 (2%)	51	63
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%)	1721 (99%)	17 (1%)	65	77

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	235	VAL
5	R	27	GLU
1	M	98	VAL
1	M	122	LEU
1	M	256	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
1	M	274	HIS

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Mol	Chain	Res	Type
2	N	96	HIS
5	R	54	GLN
3	O	163	ASN
1	M	144	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
13	PC7	C	410	-	50,50,51	0.99	4 (8%)	56,58,59	1.08	3 (5%)
11	PGT	M	406	-	36,36,50	1.22	4 (11%)	39,42,56	1.13	2 (5%)
8	HEM	C	401	1	50,50,50	1.48	8 (16%)	67,82,82	1.16	5 (7%)
9	UQ5	C	404	-	38,38,38	0.46	0	48,49,49	0.84	2 (4%)
10	3PH	M	405	-	43,43,47	0.66	1 (2%)	46,48,52	0.63	1 (2%)
11	PGT	G	102	-	50,50,50	1.09	4 (8%)	53,56,56	1.07	2 (3%)
15	PTY	M	407	-	39,39,49	0.99	4 (10%)	42,44,54	1.07	2 (4%)
12	CDL	N	302	-	80,80,99	0.97	8 (10%)	86,92,111	1.17	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	UQ5	C	403	-	38,38,38	0.96	2 (5%)	48,49,49	0.91	1 (2%)
10	3PH	C	405	12	32,32,47	0.74	1 (3%)	35,37,52	0.78	1 (2%)
12	CDL	C	408	-	80,80,99	0.38	0	86,92,111	0.57	2 (2%)
14	FES	N	301	2	0,4,4	-	-	-	-	-
12	CDL	O	402	-	87,87,99	0.94	8 (9%)	93,99,111	1.12	4 (4%)
14	FES	D	301	2	0,4,4	-	-	-	-	-
12	CDL	M	408	-	76,76,99	1.01	8 (10%)	82,88,111	1.12	4 (4%)
15	PTY	T	103	-	28,28,49	1.14	4 (14%)	31,33,54	1.19	2 (6%)
11	PGT	C	406	-	40,40,50	0.39	0	43,46,56	0.44	0
13	PC7	M	409	-	43,43,51	1.05	4 (9%)	48,50,59	1.14	3 (6%)
10	3PH	T	102	-	47,47,47	0.64	1 (2%)	50,52,52	0.59	1 (2%)
13	PC7	D	302	-	33,33,51	1.20	4 (12%)	39,41,59	1.09	2 (5%)
10	3PH	I	101	-	31,31,47	0.77	1 (3%)	34,36,52	0.77	2 (5%)
8	HEM	C	402	1	50,50,50	2.01	13 (26%)	67,82,82	1.62	11 (16%)
13	PC7	N	303	-	38,38,51	0.40	0	44,46,59	0.65	1 (2%)
10	3PH	T	101	-	40,40,47	0.68	1 (2%)	43,45,52	0.65	1 (2%)
12	CDL	C	409	10	84,84,99	0.96	8 (9%)	90,96,111	1.11	4 (4%)
17	Q7G	M	410	-	44,44,90	0.75	1 (2%)	64,68,138	1.40	12 (18%)
16	UQ7	M	404	-	48,48,48	0.67	2 (4%)	60,61,61	0.76	2 (3%)
12	CDL	Q	101	-	69,69,99	1.05	8 (11%)	75,81,111	1.18	5 (6%)
10	3PH	G	101	-	32,32,47	0.76	1 (3%)	35,37,52	0.68	1 (2%)
11	PGT	C	407	-	50,50,50	1.11	4 (8%)	53,56,56	1.05	2 (3%)
8	HEM	E	400	3	50,50,50	1.45	7 (14%)	67,82,82	1.17	8 (11%)
8	HEM	M	402	1	50,50,50	2.10	13 (26%)	67,82,82	1.68	16 (23%)
8	HEM	O	401	3	50,50,50	2.04	16 (32%)	67,82,82	2.04	20 (29%)
12	CDL	G	103	-	84,84,99	0.97	8 (9%)	90,96,111	1.12	4 (4%)
9	UQ5	M	403	-	38,38,38	0.49	0	48,49,49	0.62	1 (2%)
17	Q7G	M	411	-	44,44,90	0.79	1 (2%)	64,68,138	1.40	11 (17%)
8	HEM	M	401	1	50,50,50	2.02	18 (36%)	67,82,82	1.70	20 (29%)
13	PC7	G	104	-	51,51,51	0.99	4 (7%)	57,59,59	1.02	2 (3%)
15	PTY	J	101	-	40,40,49	0.34	0	43,45,54	0.38	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	PC7	C	410	-	-	19/54/54/55	-
11	PGT	M	406	-	-	20/41/41/55	-
8	HEM	C	401	1	-	2/14/54/54	-
9	UQ5	C	404	-	-	13/33/57/57	0/1/1/1
10	3PH	M	405	-	-	20/45/45/49	-
11	PGT	G	102	-	-	37/55/55/55	-
15	PTY	M	407	-	-	18/43/43/53	-
12	CDL	N	302	-	-	34/91/91/110	-
9	UQ5	C	403	-	-	11/33/57/57	0/1/1/1
10	3PH	C	405	12	-	17/34/34/49	-
12	CDL	C	408	-	-	47/91/91/110	-
14	FES	N	301	2	-	-	0/1/1/1
12	CDL	O	402	-	-	33/98/98/110	-
14	FES	D	301	2	-	-	0/1/1/1
12	CDL	M	408	-	-	42/87/87/110	-
15	PTY	T	103	-	-	17/32/32/53	-
11	PGT	C	406	-	-	12/45/45/55	-
13	PC7	M	409	-	-	19/45/45/55	-
10	3PH	T	102	-	-	13/49/49/49	-
13	PC7	D	302	-	-	15/37/37/55	-
10	3PH	I	101	-	-	15/33/33/49	-
8	HEM	C	402	1	-	6/14/54/54	-
13	PC7	N	303	-	-	10/42/42/55	-
10	3PH	T	101	-	-	14/42/42/49	-
12	CDL	C	409	10	-	40/95/95/110	-
17	Q7G	M	410	-	-	3/12/100/200	0/6/6/10
16	UQ7	M	404	-	-	19/45/69/69	0/1/1/1
12	CDL	Q	101	-	-	37/80/80/110	-
10	3PH	G	101	-	-	16/34/34/49	-
11	PGT	C	407	-	-	22/55/55/55	-
8	HEM	E	400	3	-	2/14/54/54	-
8	HEM	M	402	1	-	4/14/54/54	-
8	HEM	O	401	3	-	4/14/54/54	-
12	CDL	G	103	-	-	30/95/95/110	-
9	UQ5	M	403	-	-	9/33/57/57	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Q7G	M	411	-	-	0/12/100/200	0/6/6/10
8	HEM	M	401	1	-	2/14/54/54	-
13	PC7	G	104	-	-	21/55/55/55	-
15	PTY	J	101	-	-	5/44/44/53	-

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	402	HEM	FE-NB	7.17	2.17	1.94
8	M	402	HEM	C1B-NB	-6.33	1.29	1.40
8	C	402	HEM	FE-NB	6.13	2.13	1.94
8	C	402	HEM	FE-NC	5.81	2.14	1.95
8	O	401	HEM	C1B-NB	-5.52	1.30	1.40

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	401	HEM	CHC-C4B-NB	8.02	133.06	124.42
8	M	402	HEM	C1B-NB-C4B	5.26	111.44	105.21
8	O	401	HEM	CHD-C1D-ND	5.22	130.04	124.42
8	C	402	HEM	C1B-NB-C4B	5.21	111.38	105.21
8	O	401	HEM	C1B-NB-C4B	4.81	110.91	105.21

There are no chirality outliers.

5 of 648 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	402	HEM	C2C-C3C-CAC-CBC
9	C	403	UQ5	C17-C18-C19-C20
9	C	403	UQ5	C17-C18-C19-C21
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 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	410	PC7	9	0
11	M	406	PGT	4	0
8	C	401	HEM	1	0

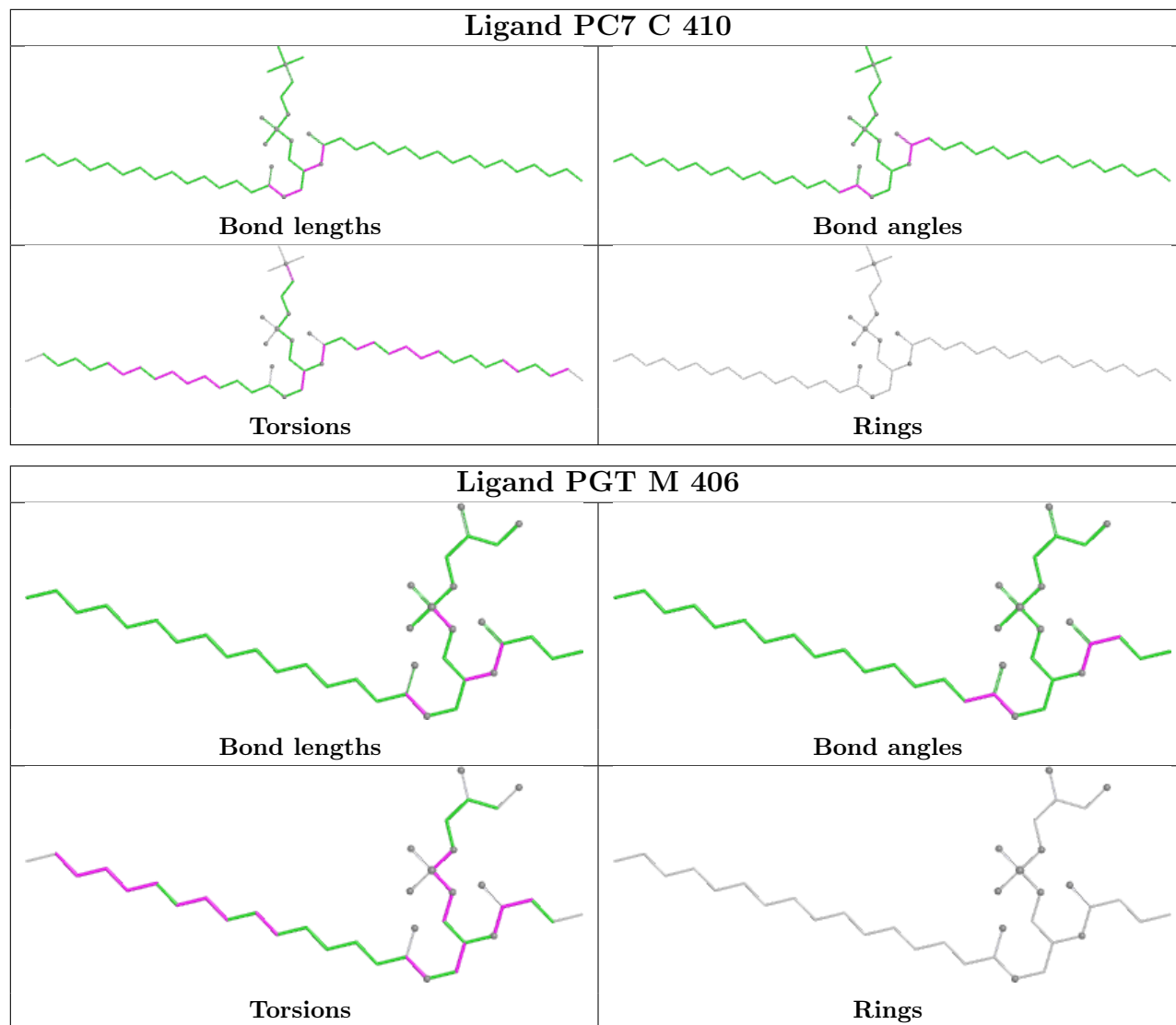
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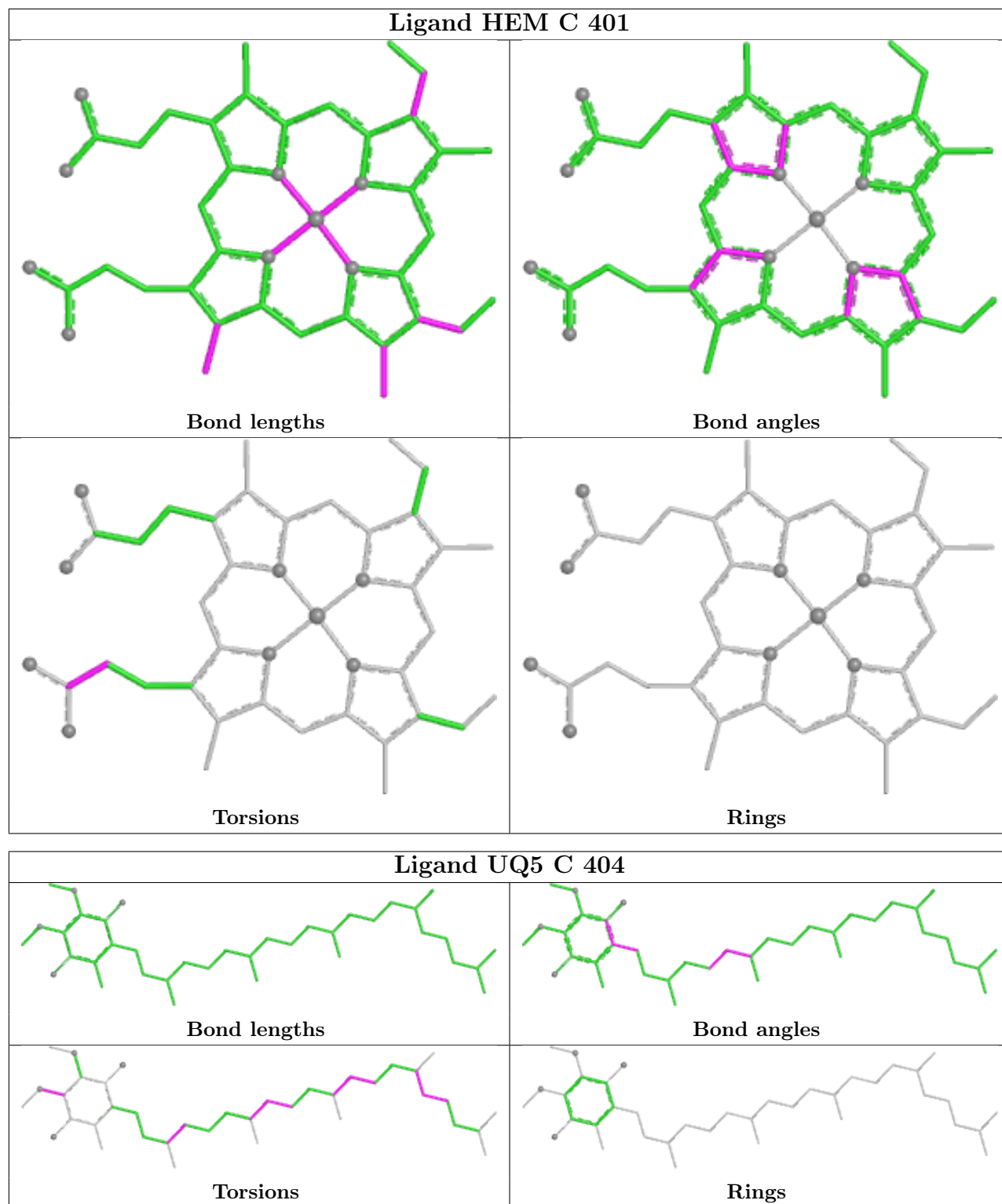
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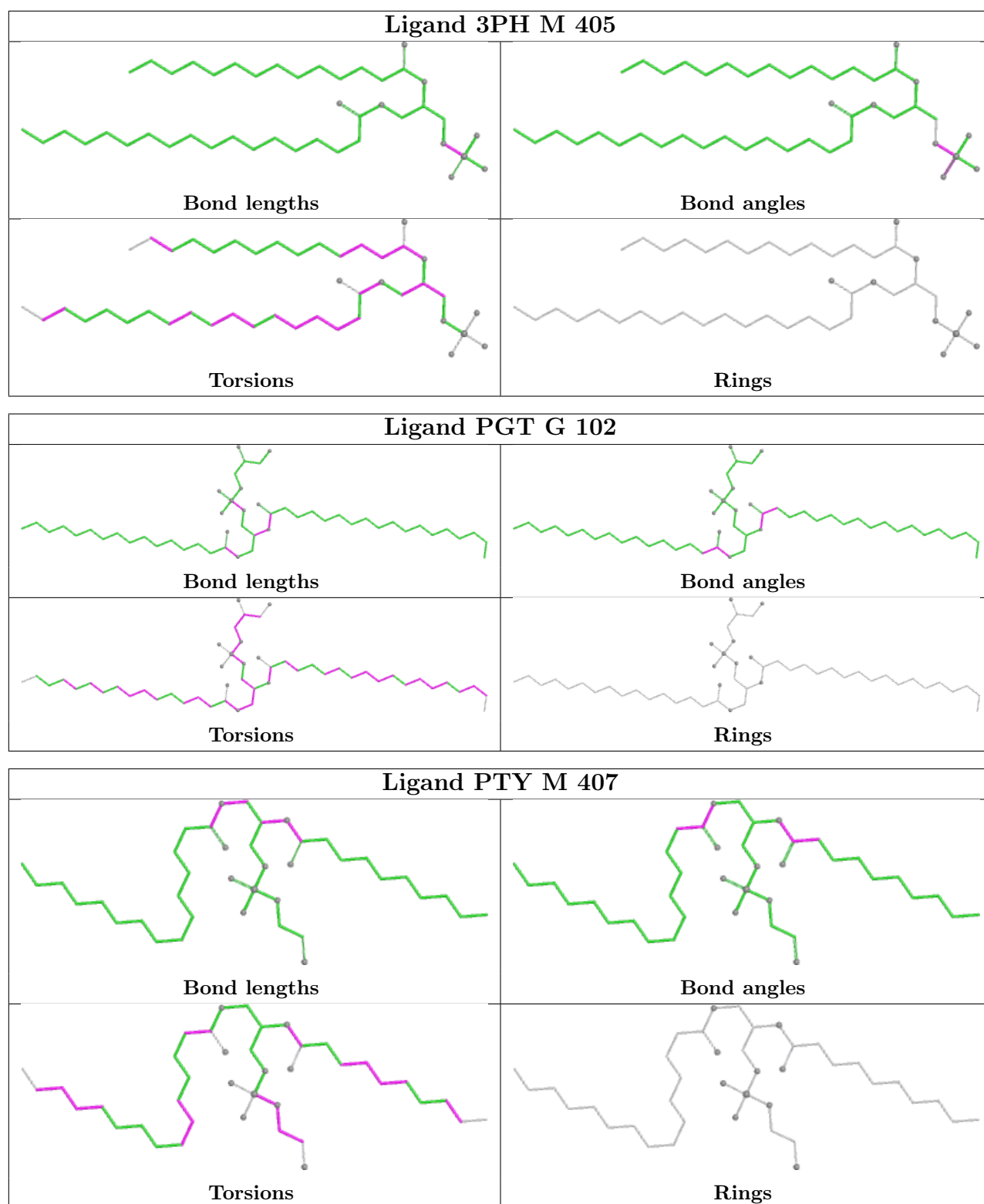
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	404	UQ5	6	0
10	M	405	3PH	6	0
11	G	102	PGT	2	0
15	M	407	PTY	2	0
12	N	302	CDL	3	0
9	C	403	UQ5	11	0
10	C	405	3PH	1	0
12	C	408	CDL	9	0
14	N	301	FES	2	0
12	O	402	CDL	7	0
12	M	408	CDL	8	0
15	T	103	PTY	1	0
11	C	406	PGT	6	0
13	M	409	PC7	2	0
10	T	102	3PH	1	0
13	D	302	PC7	1	0
10	I	101	3PH	3	0
8	C	402	HEM	1	0
13	N	303	PC7	6	0
10	T	101	3PH	2	0
12	C	409	CDL	10	0
16	M	404	UQ7	11	0
12	Q	101	CDL	6	0
10	G	101	3PH	1	0
11	C	407	PGT	4	0
8	E	400	HEM	5	0
8	M	402	HEM	1	0
8	O	401	HEM	6	0
12	G	103	CDL	6	0
9	M	403	UQ5	8	0
13	G	104	PC7	5	0

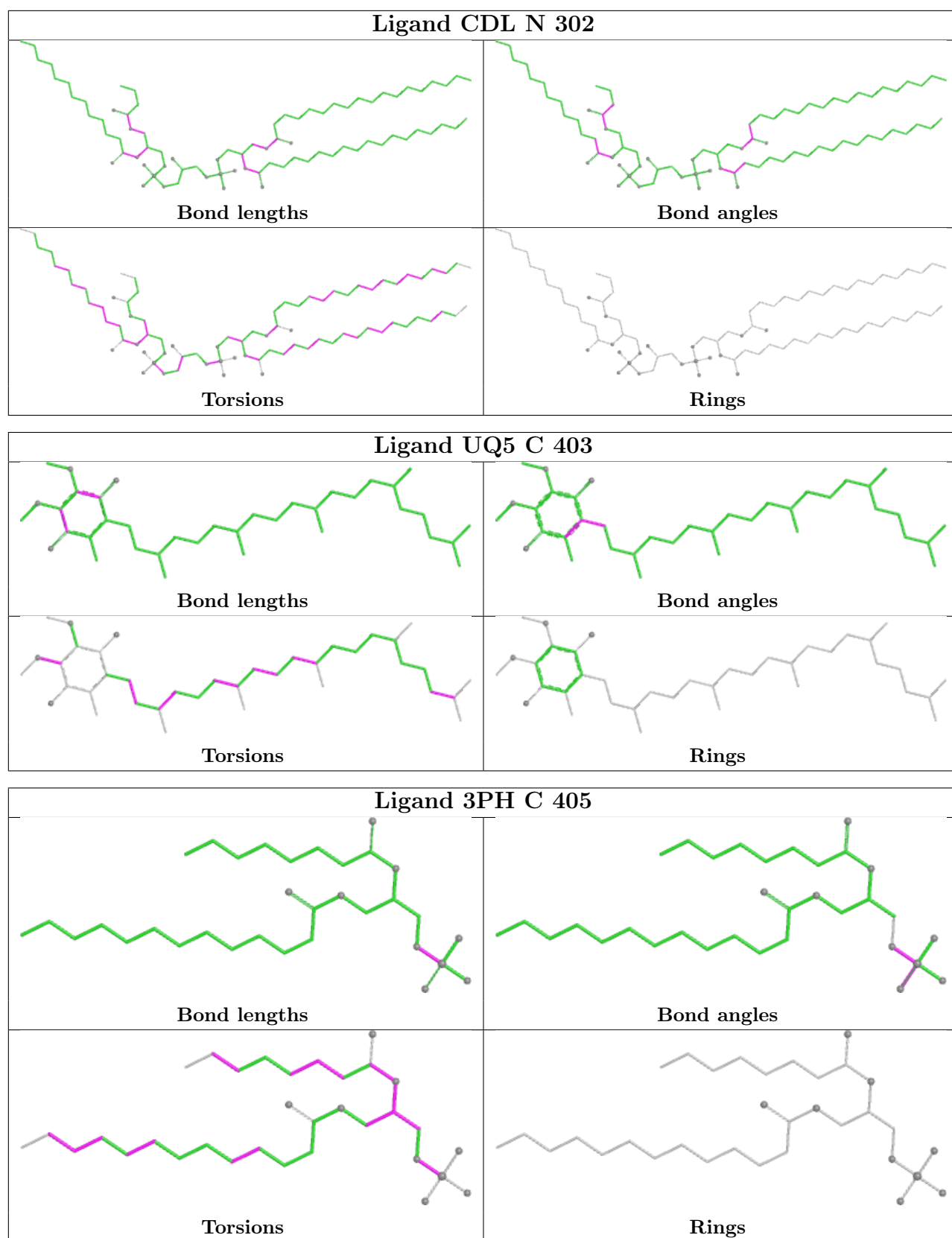
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

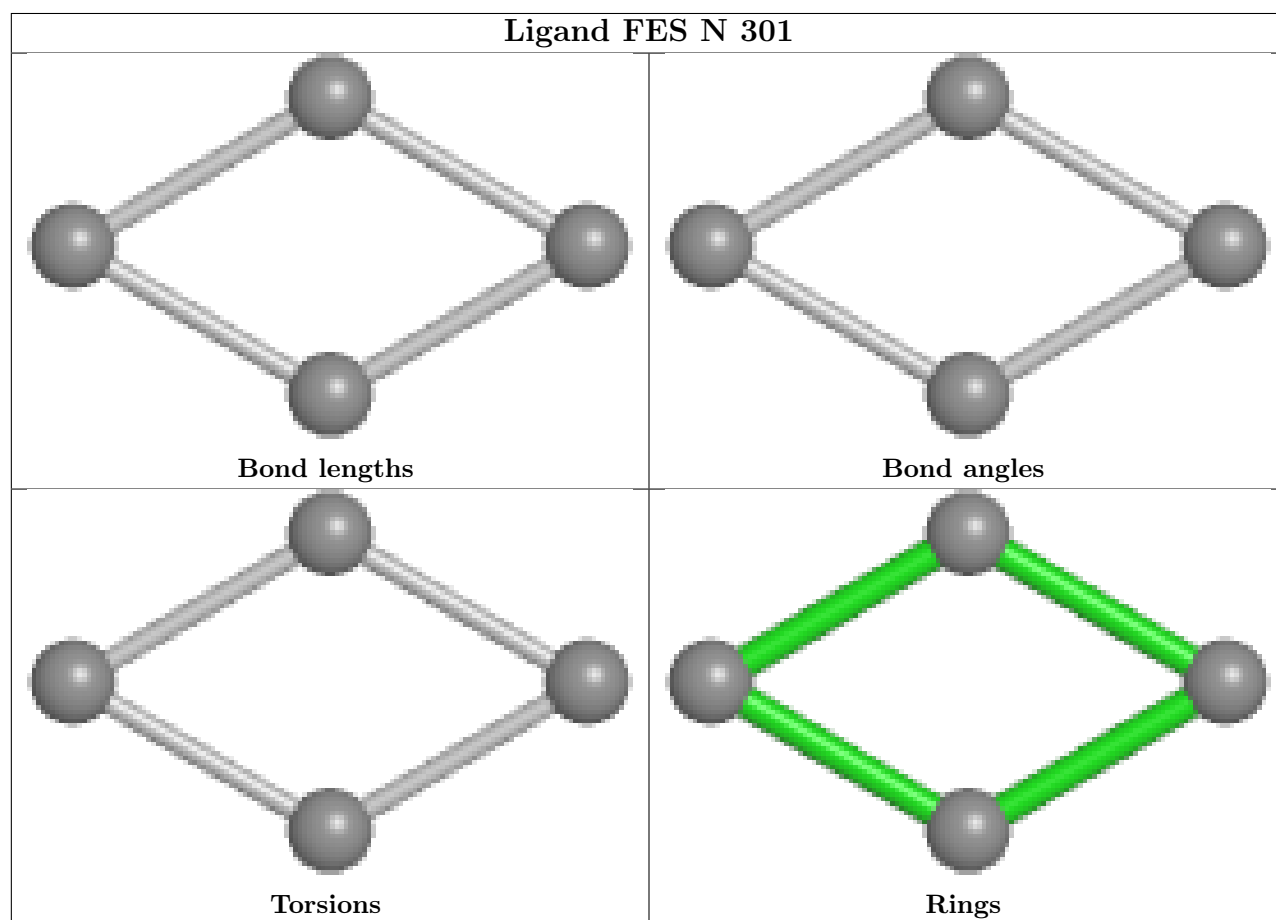
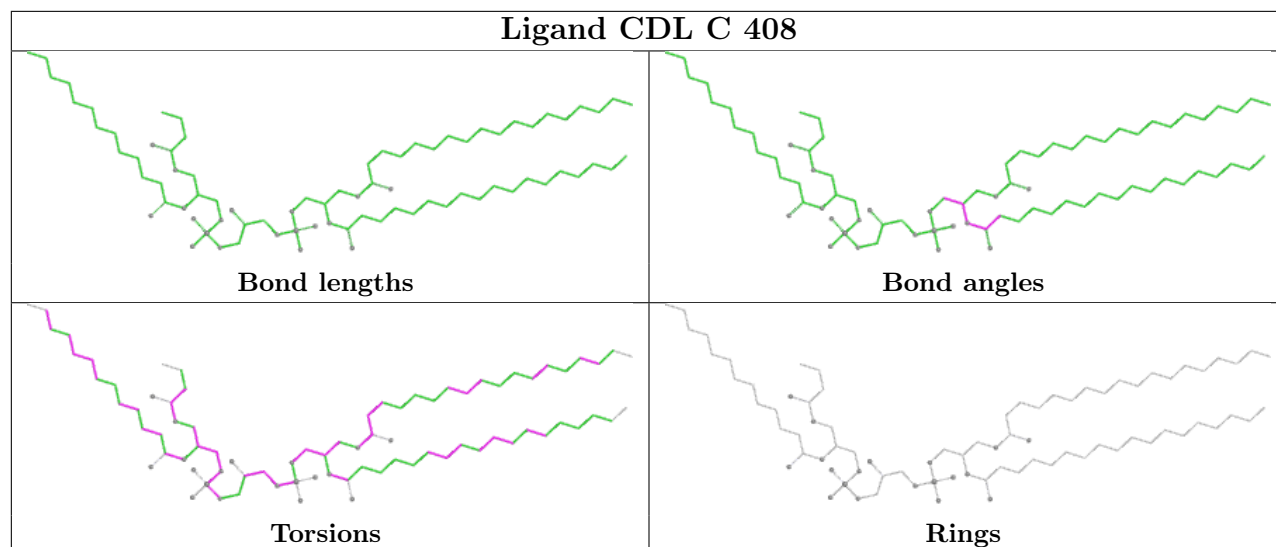
equivalents in the CSD to analyse the geometry.

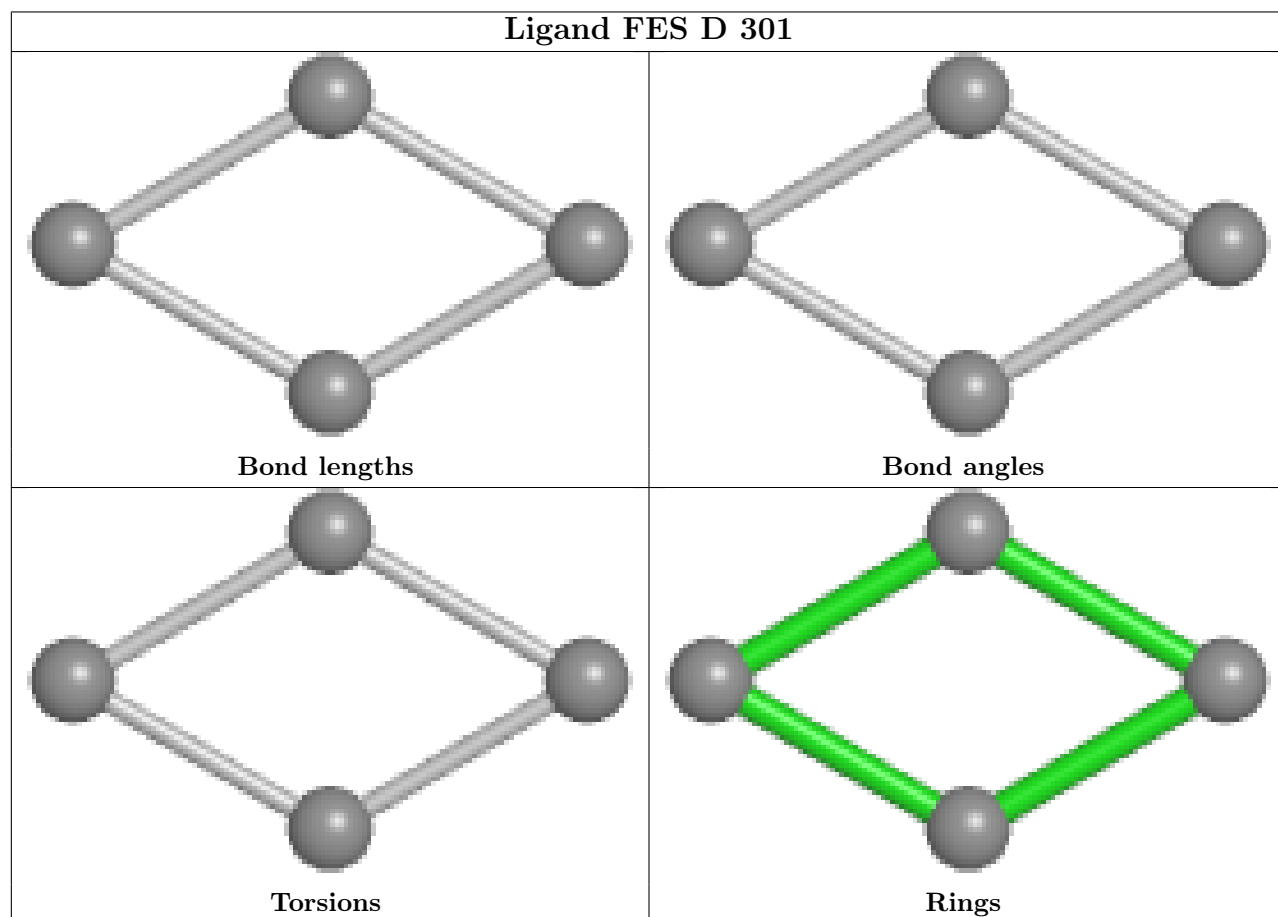
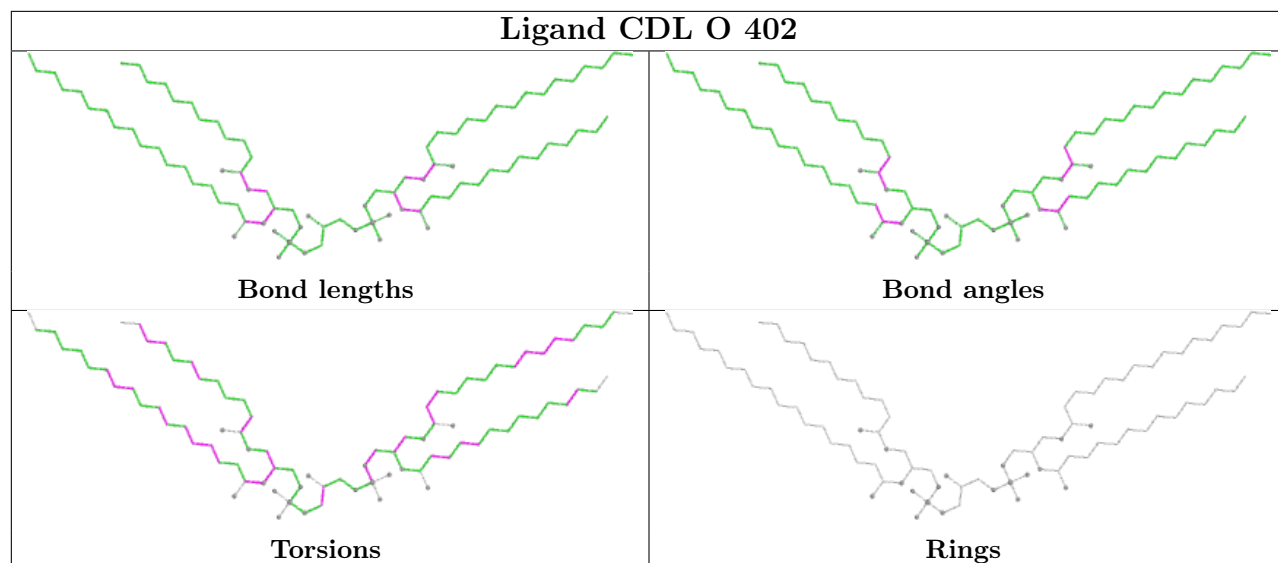


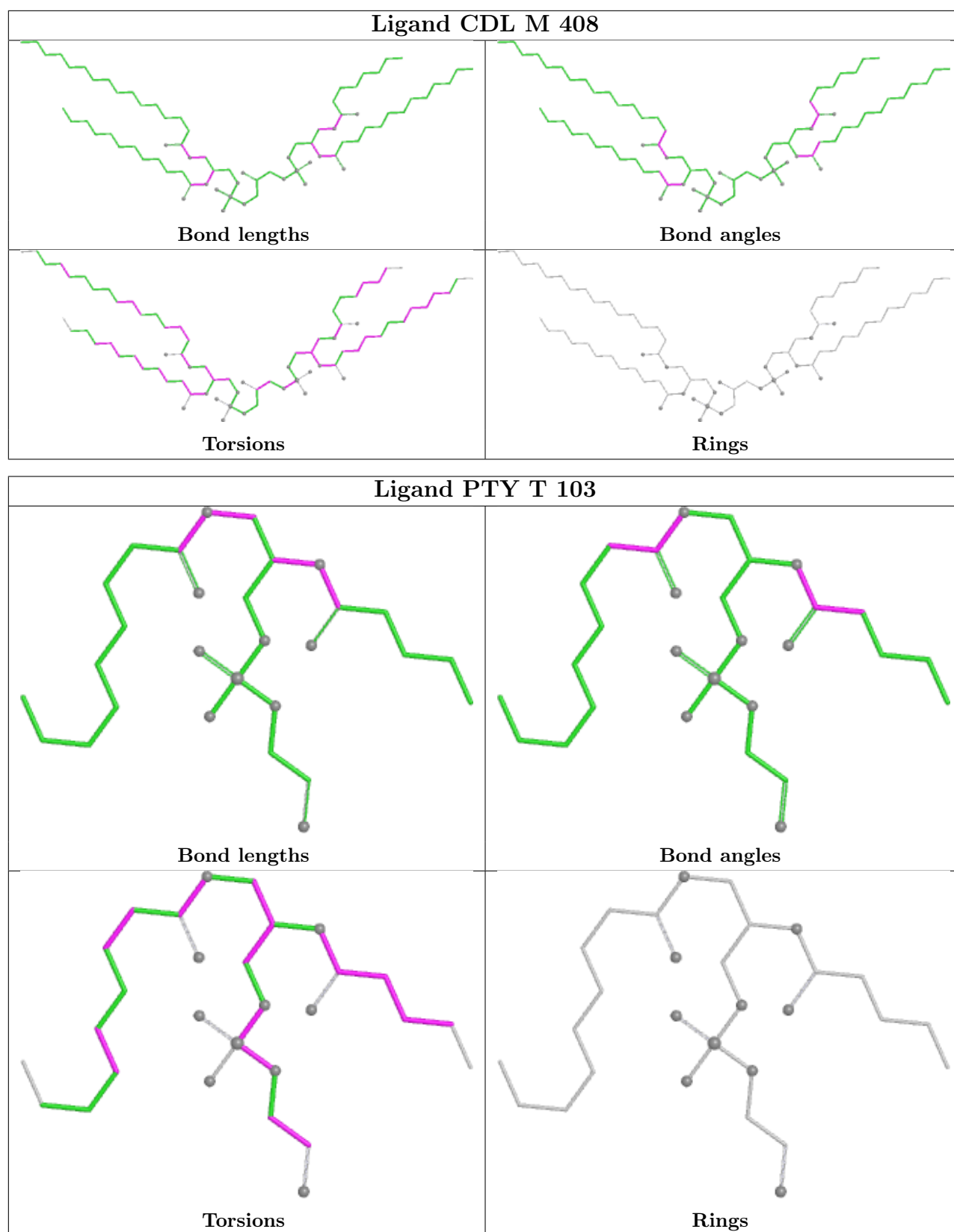


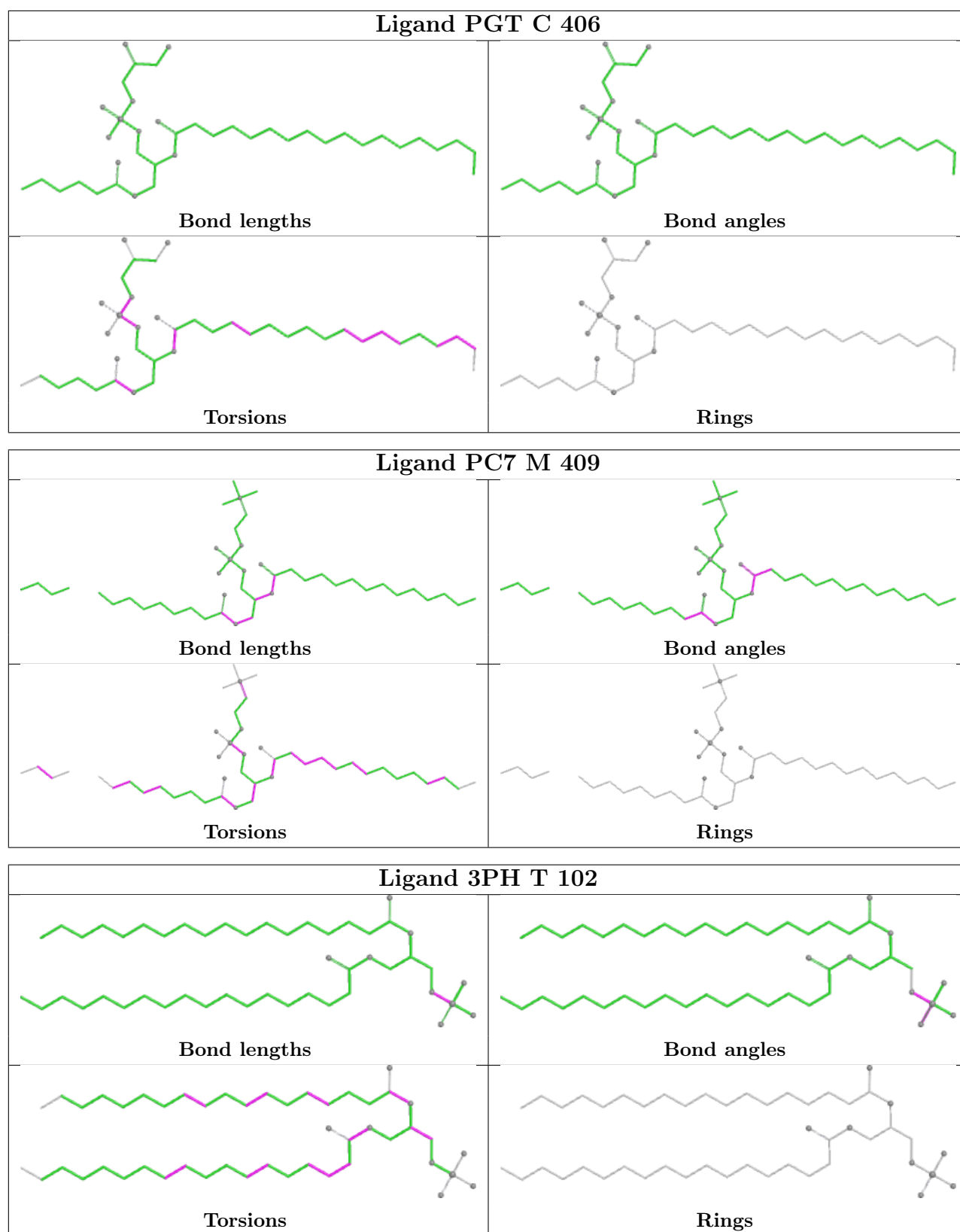


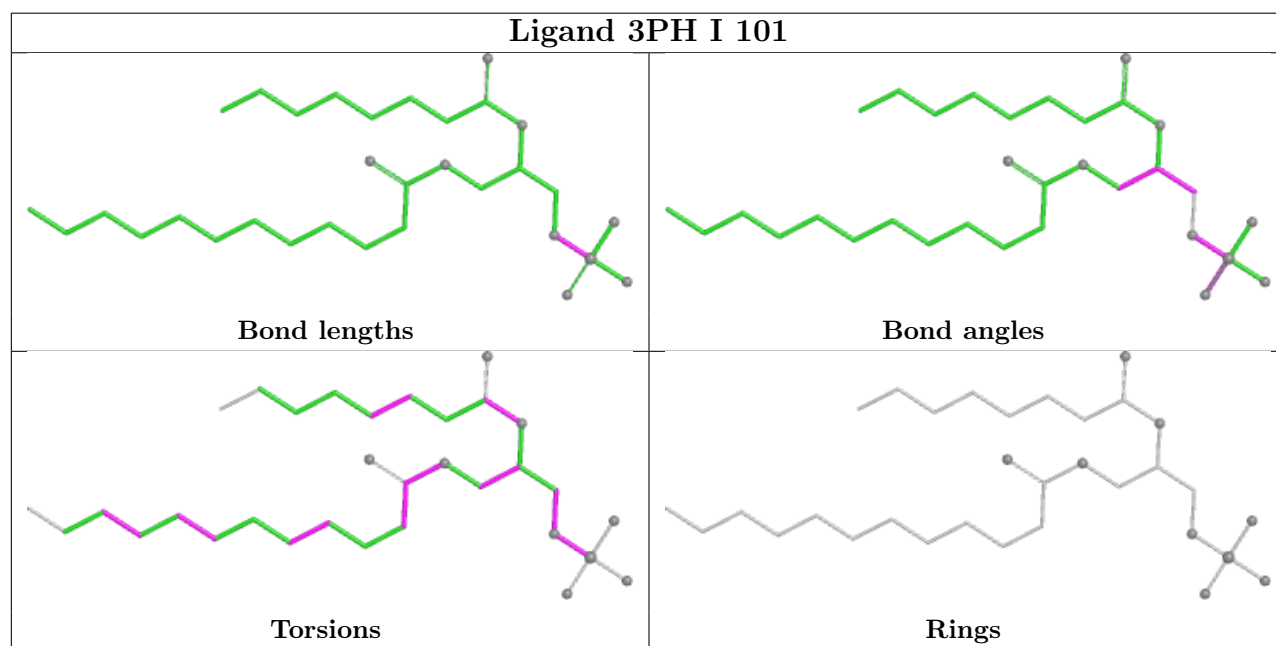
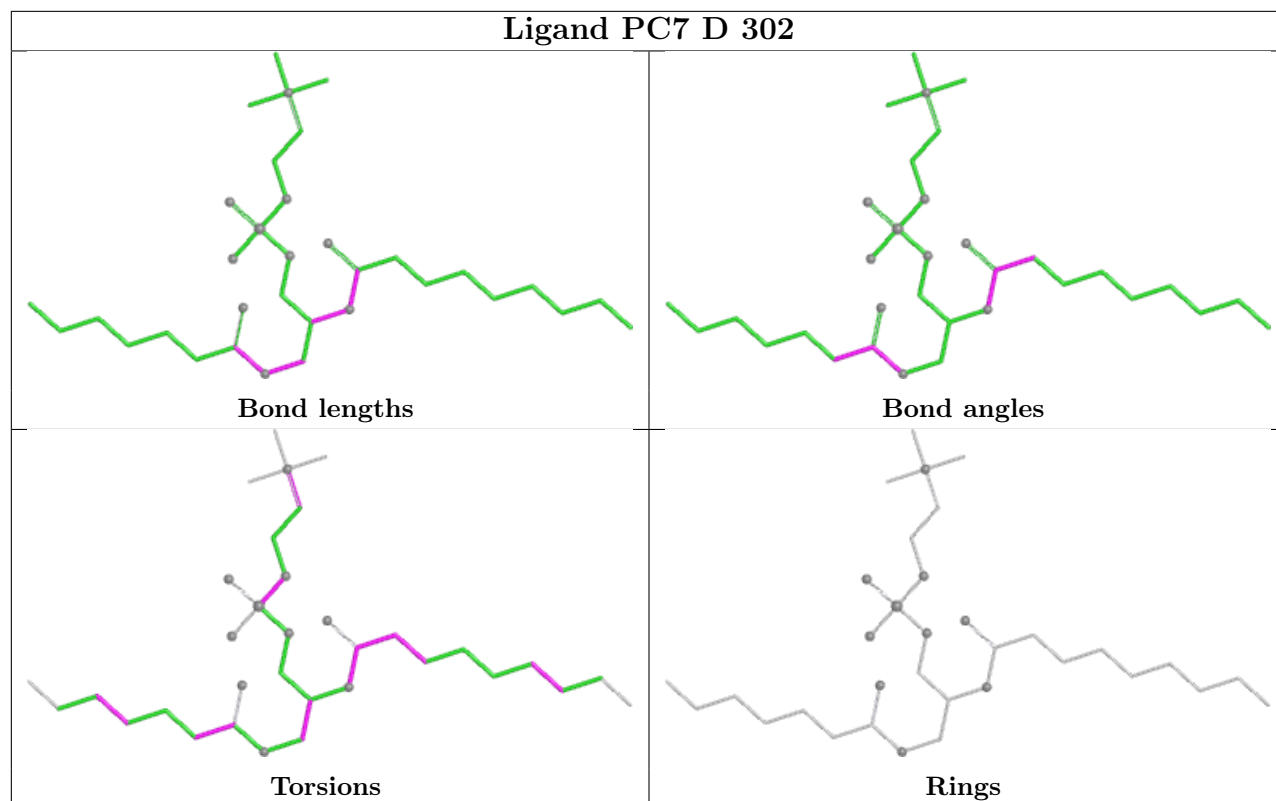


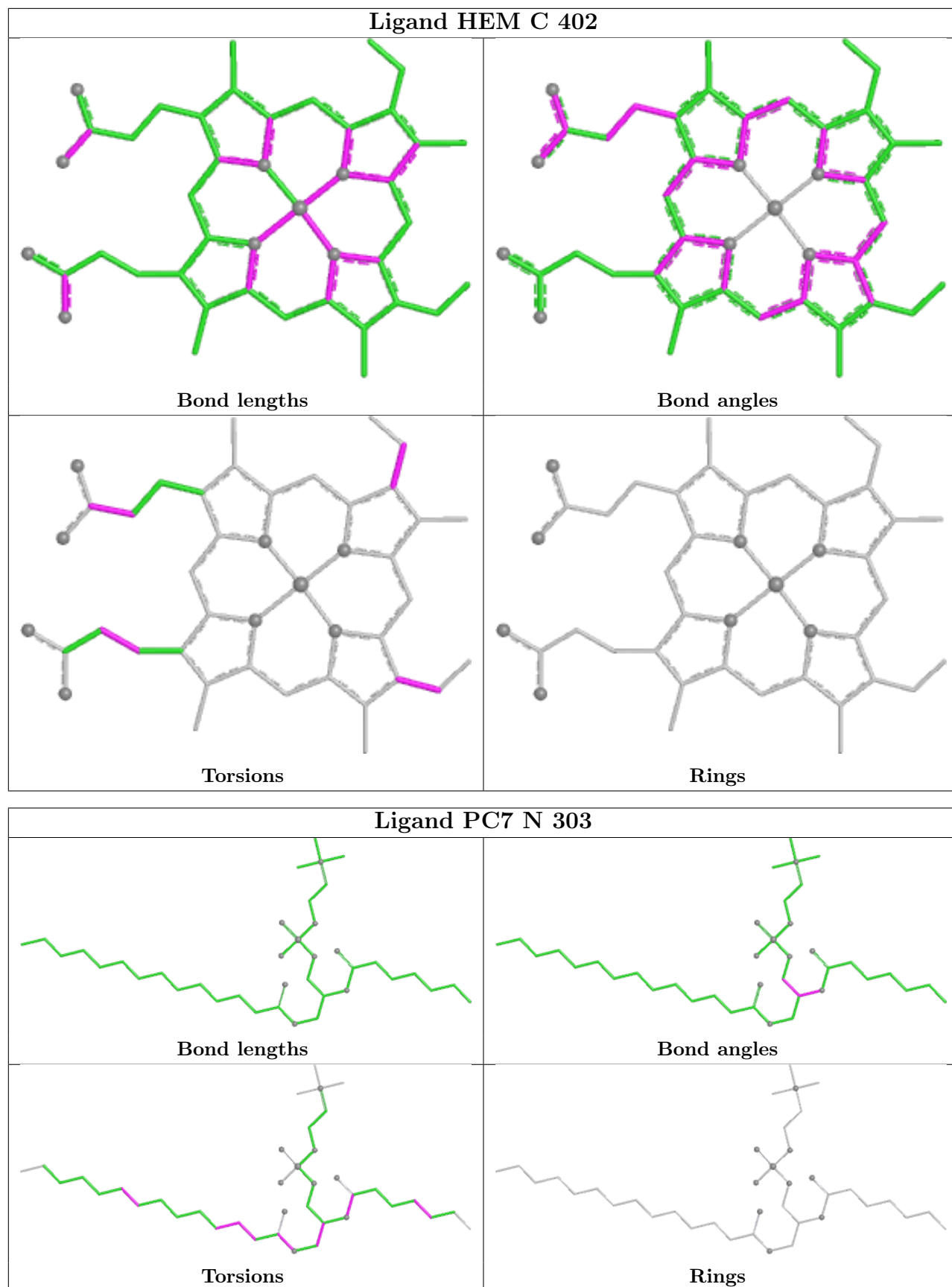


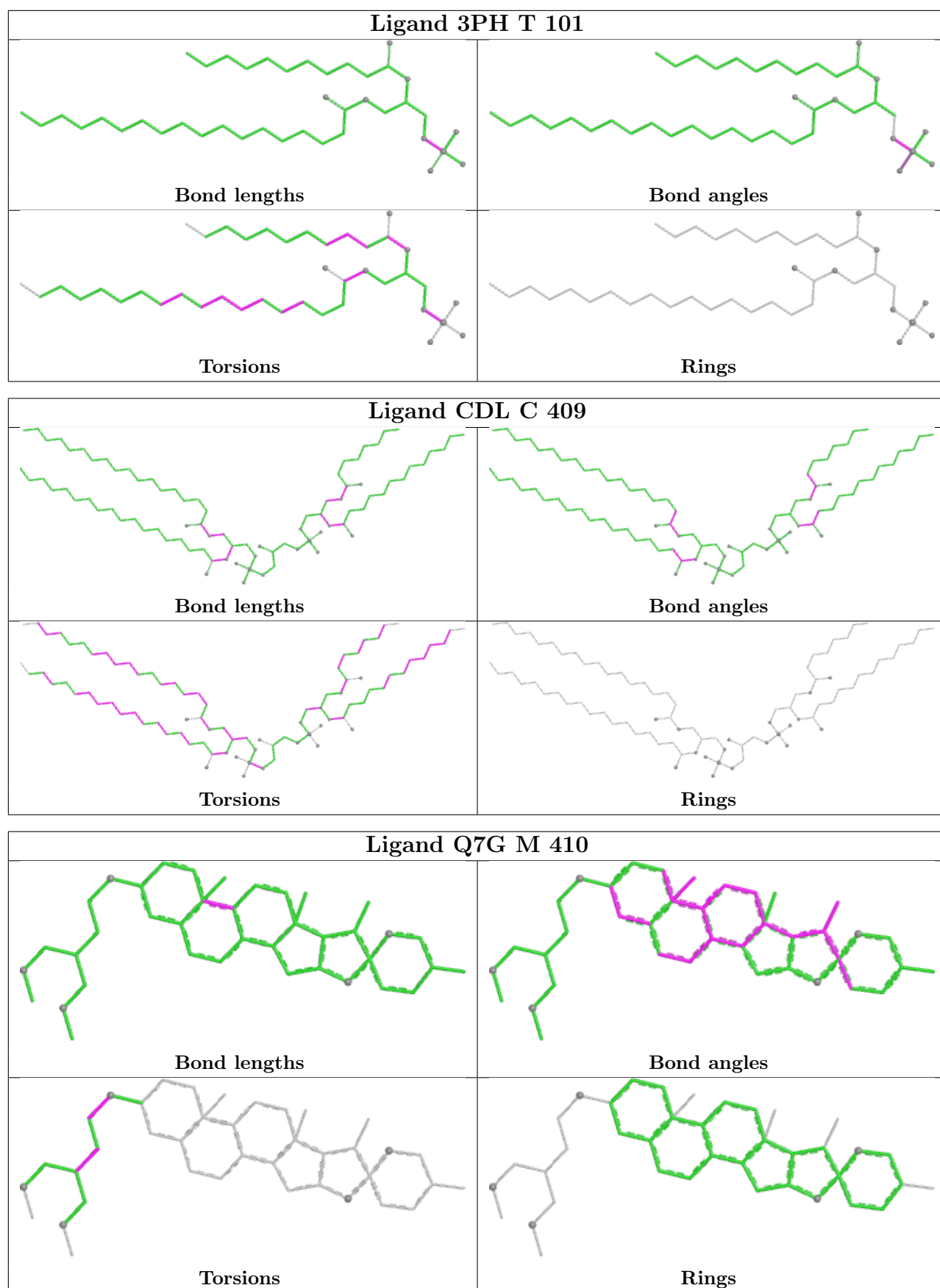


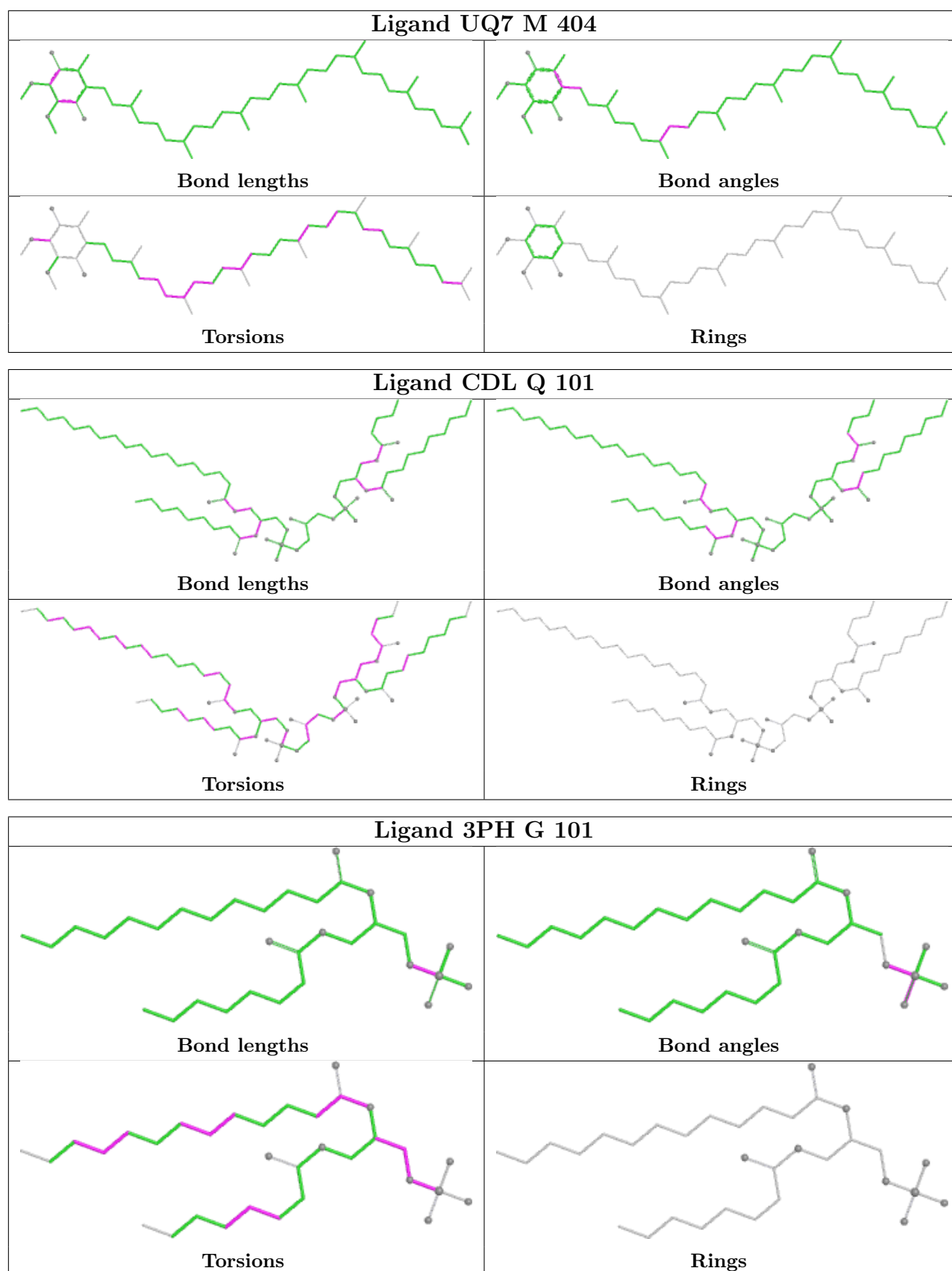


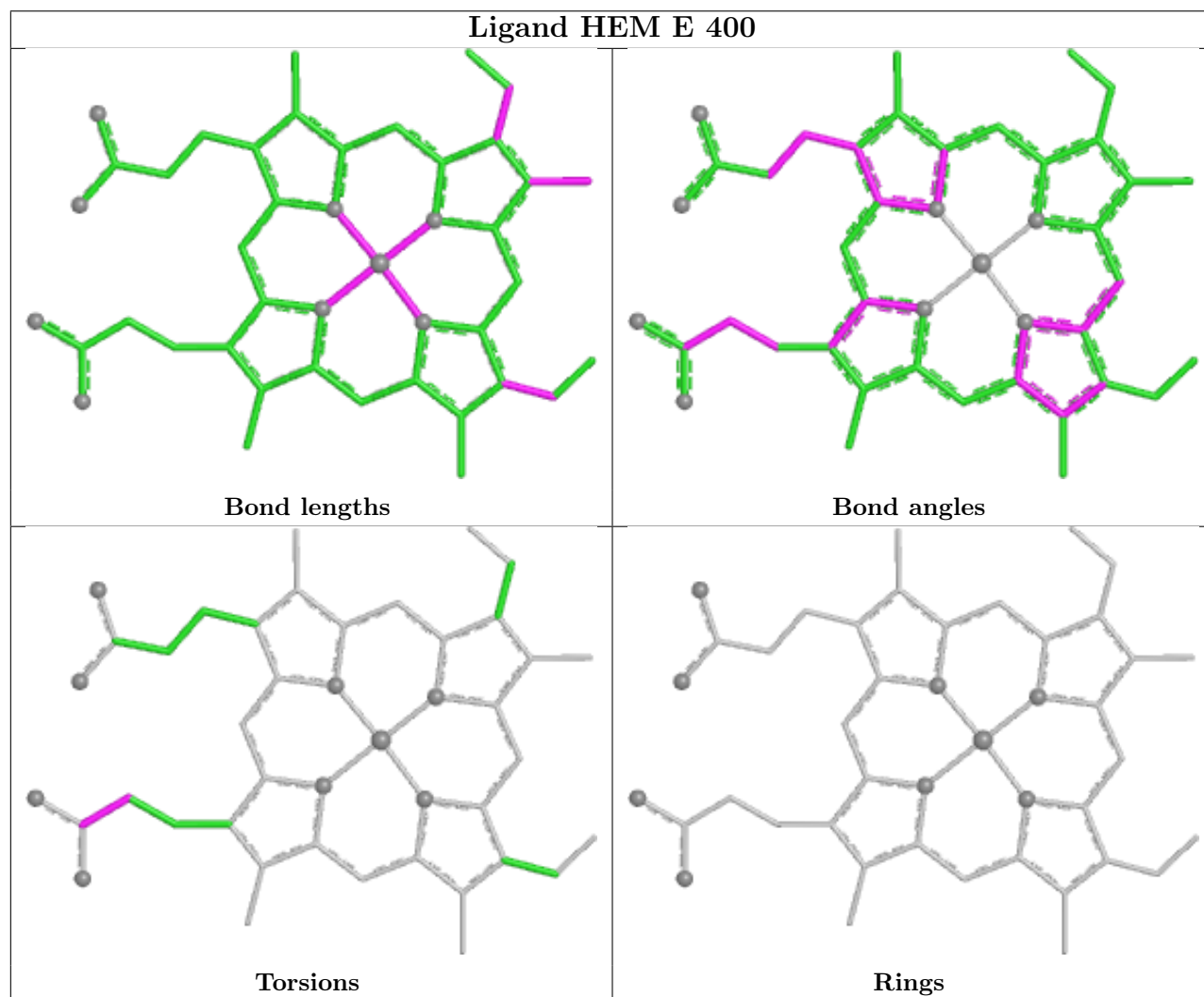
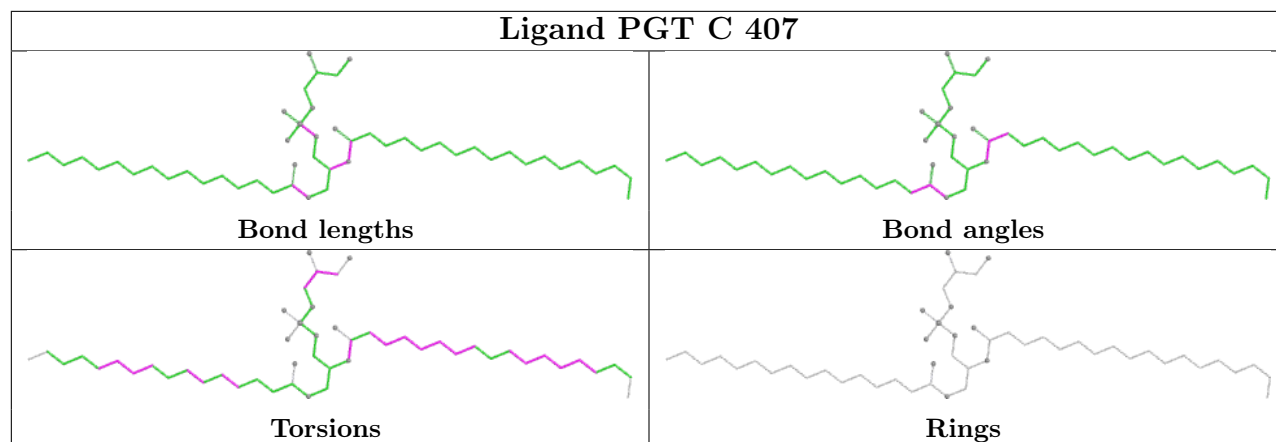


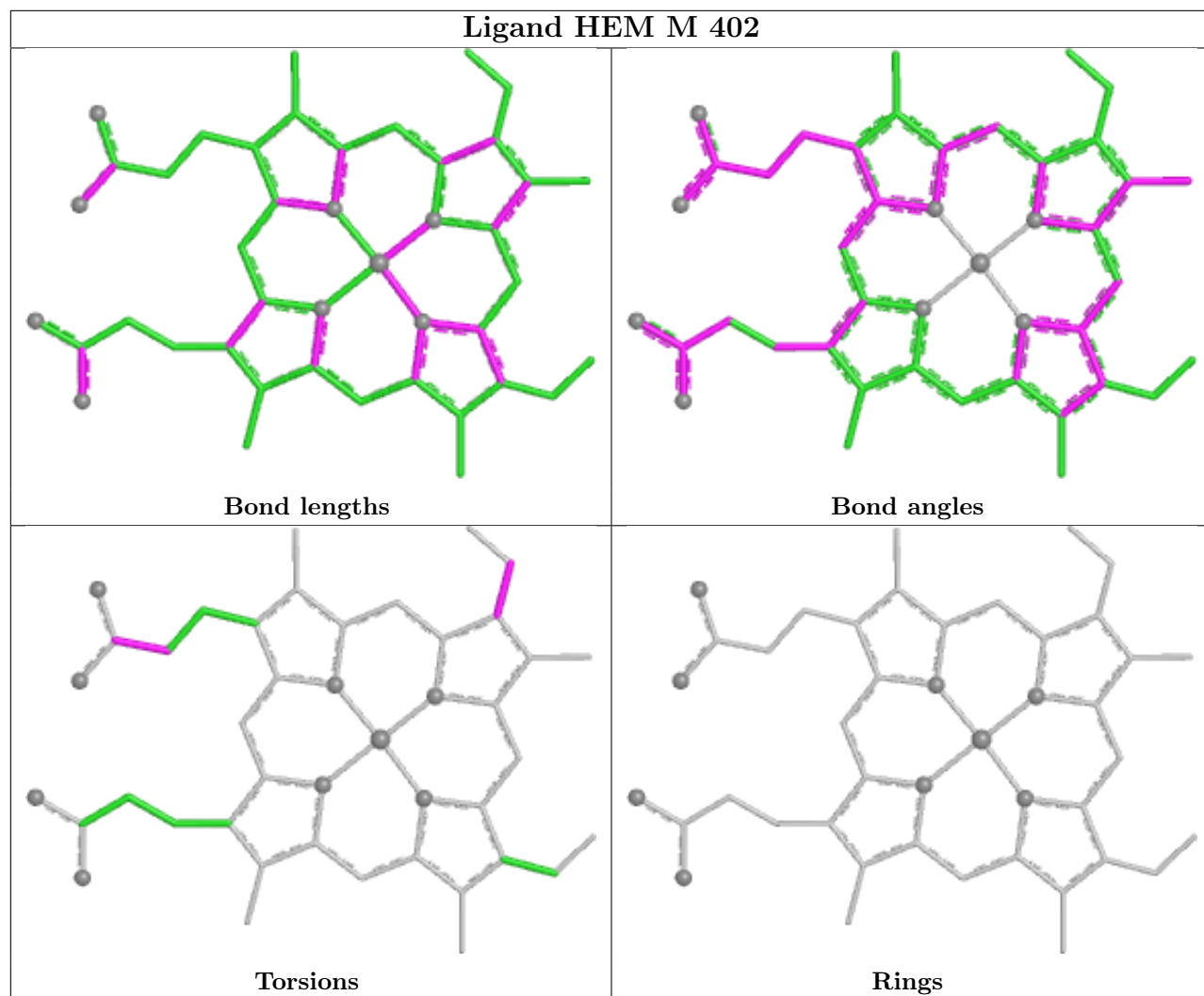


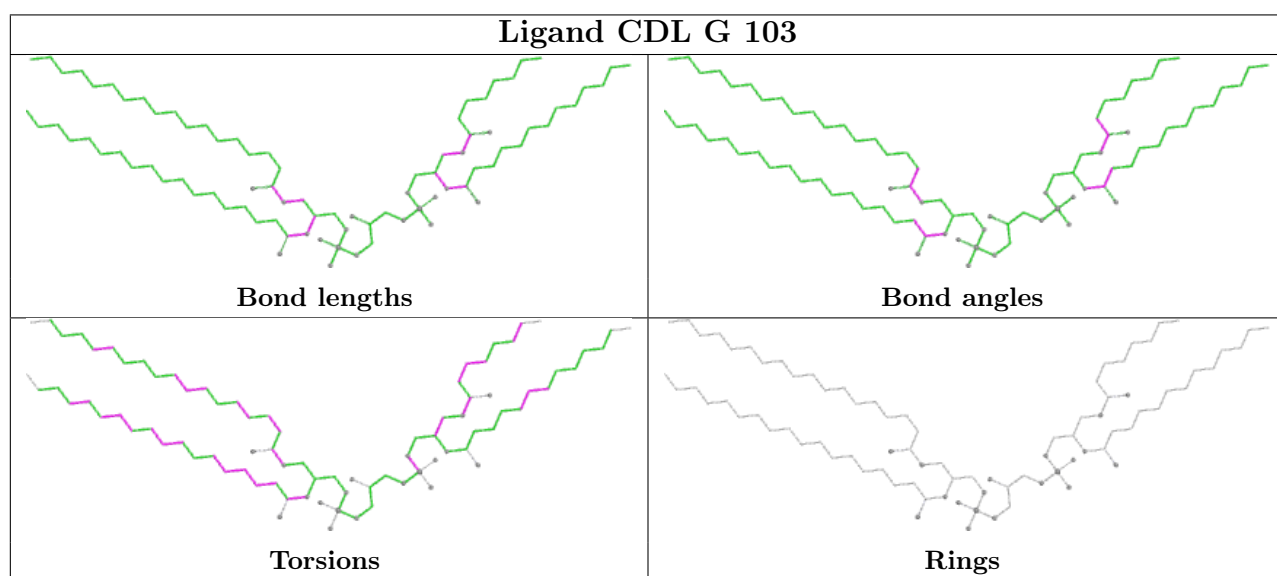
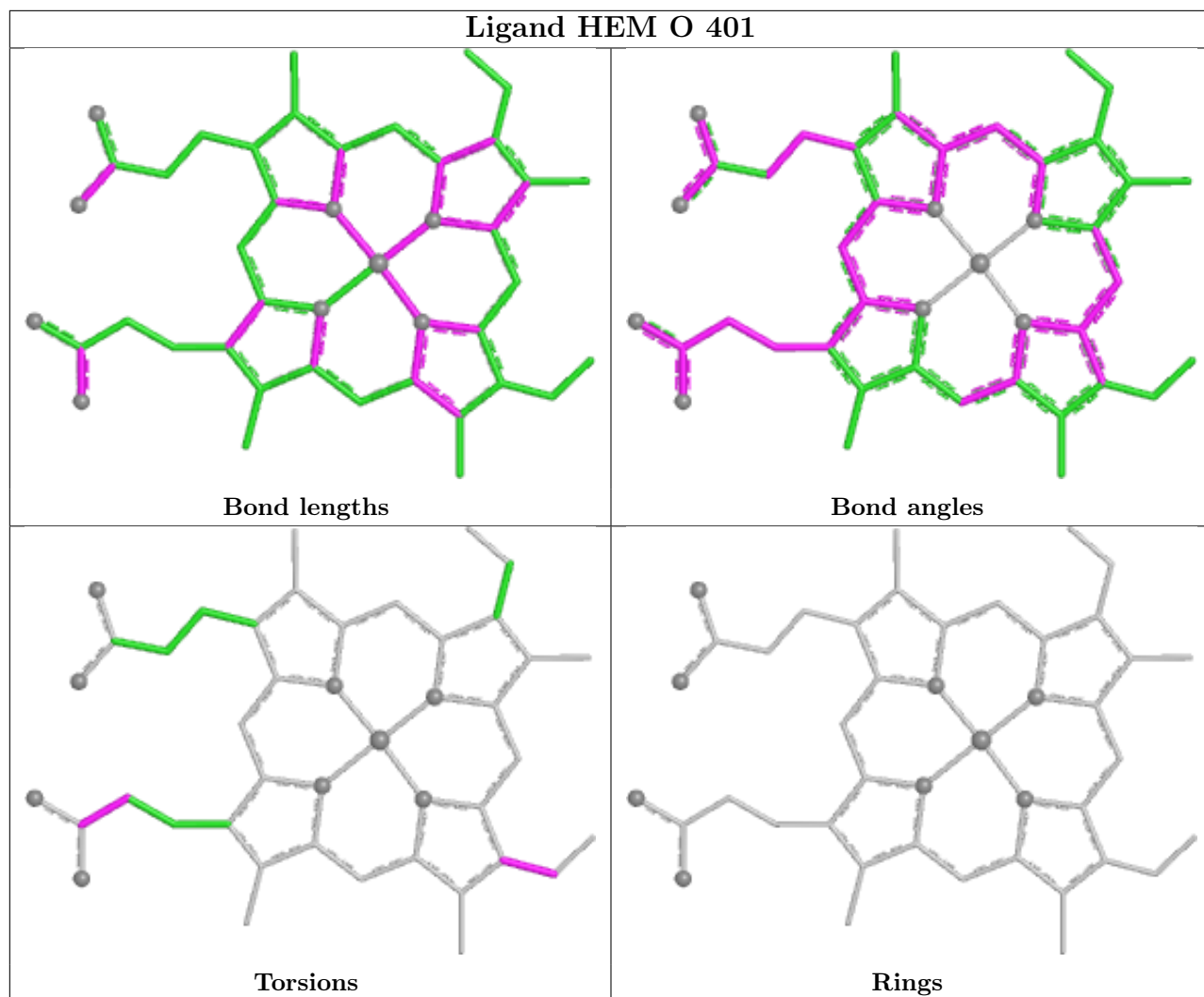


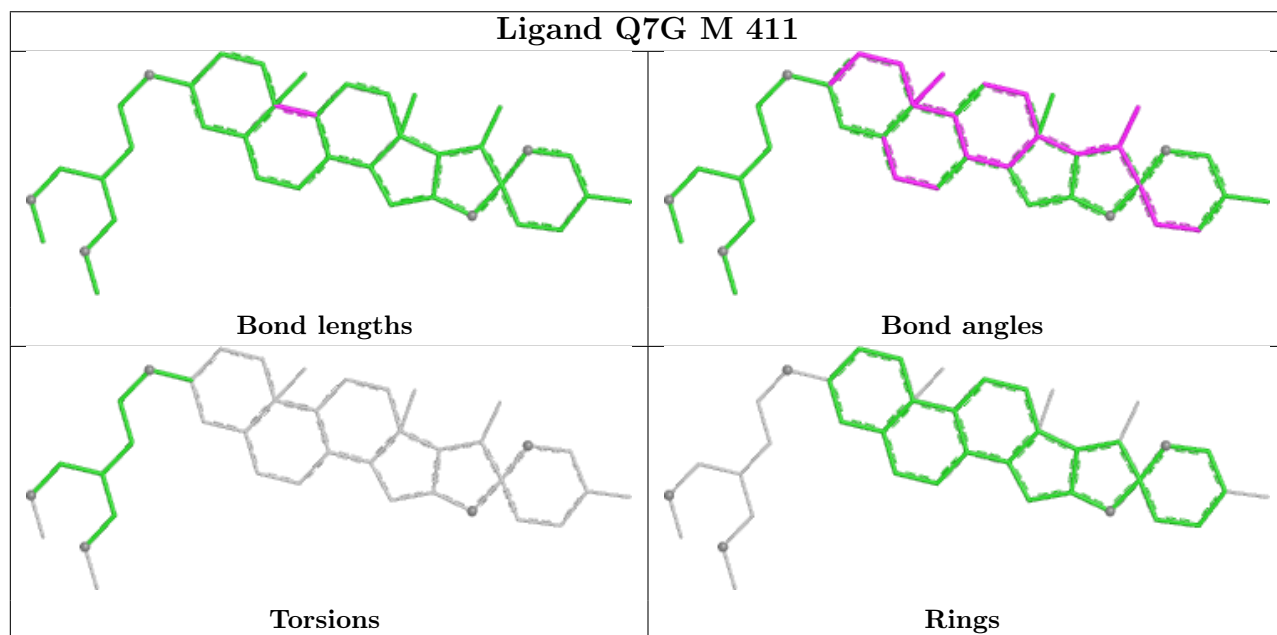
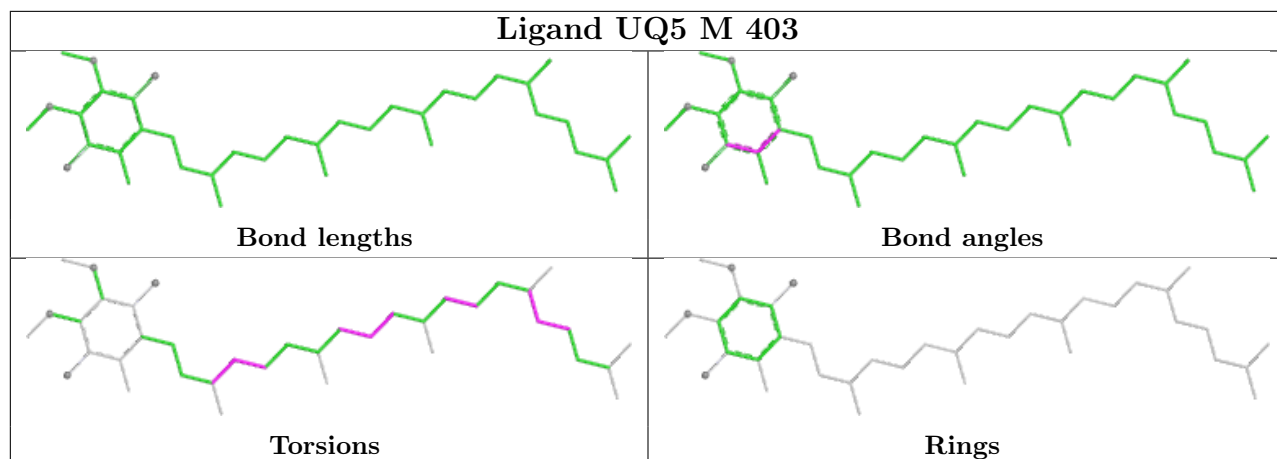


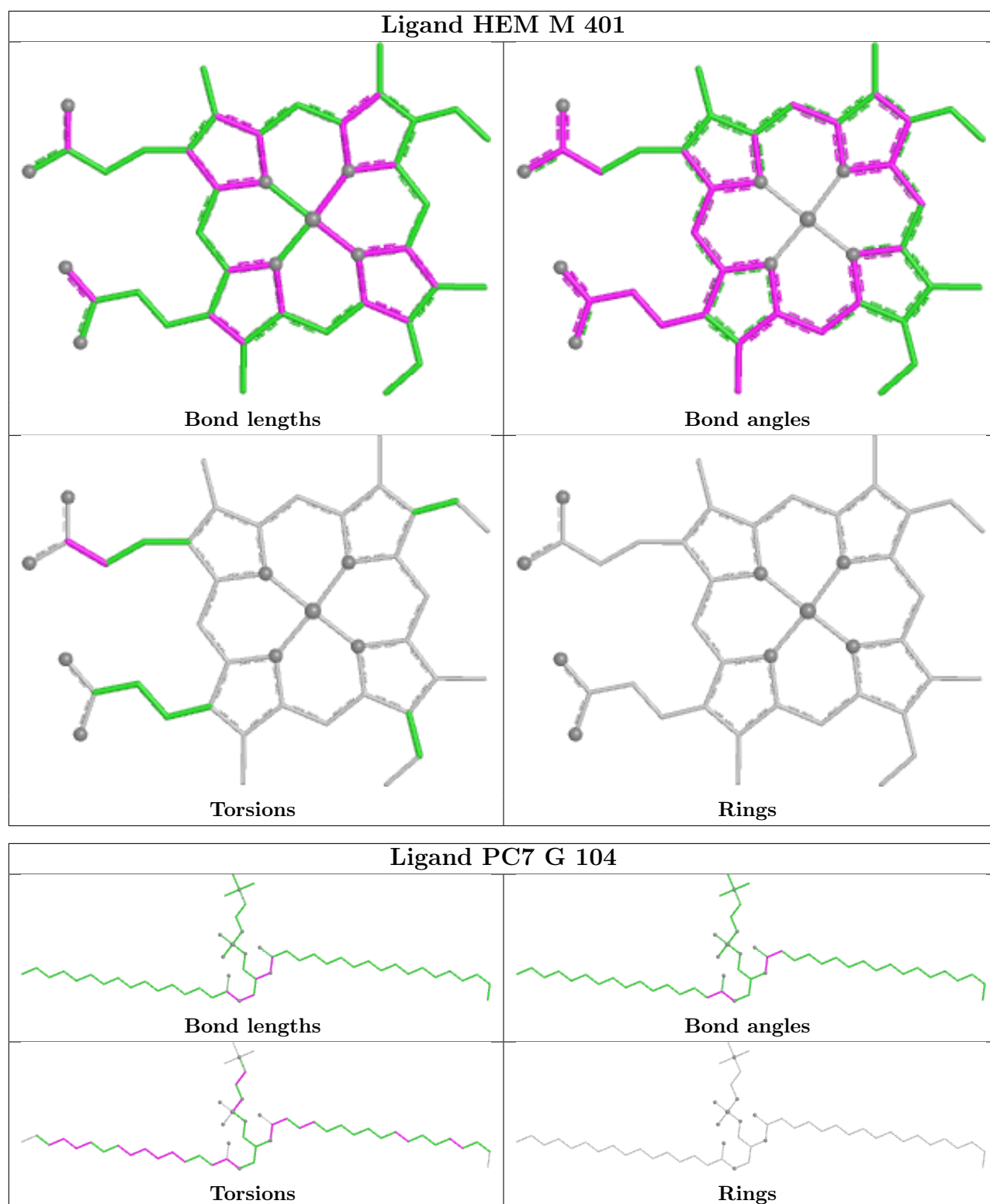


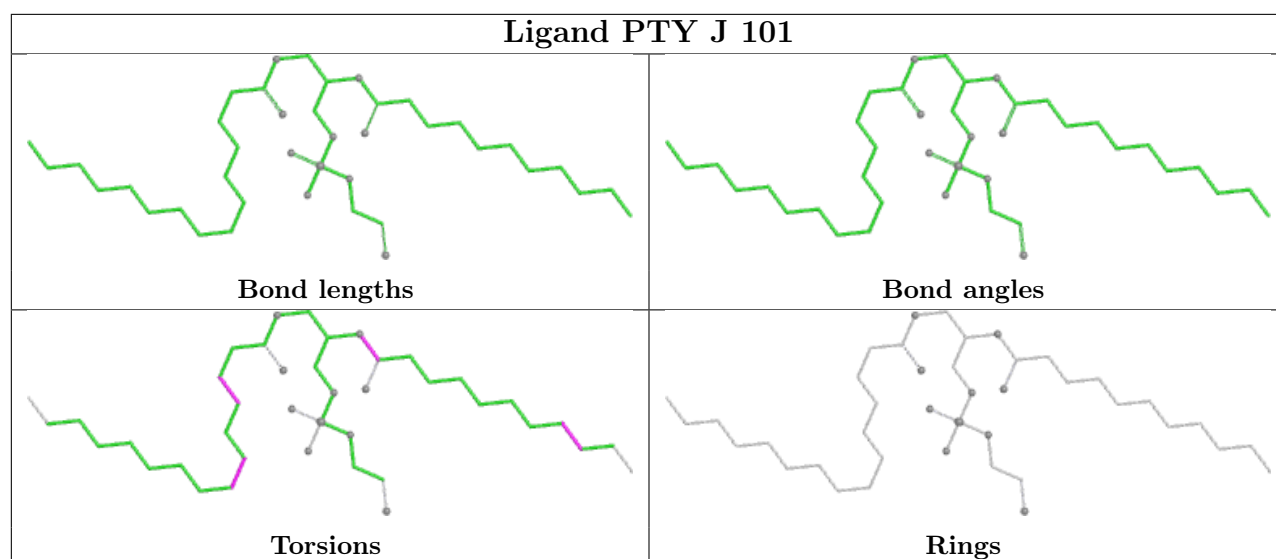












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

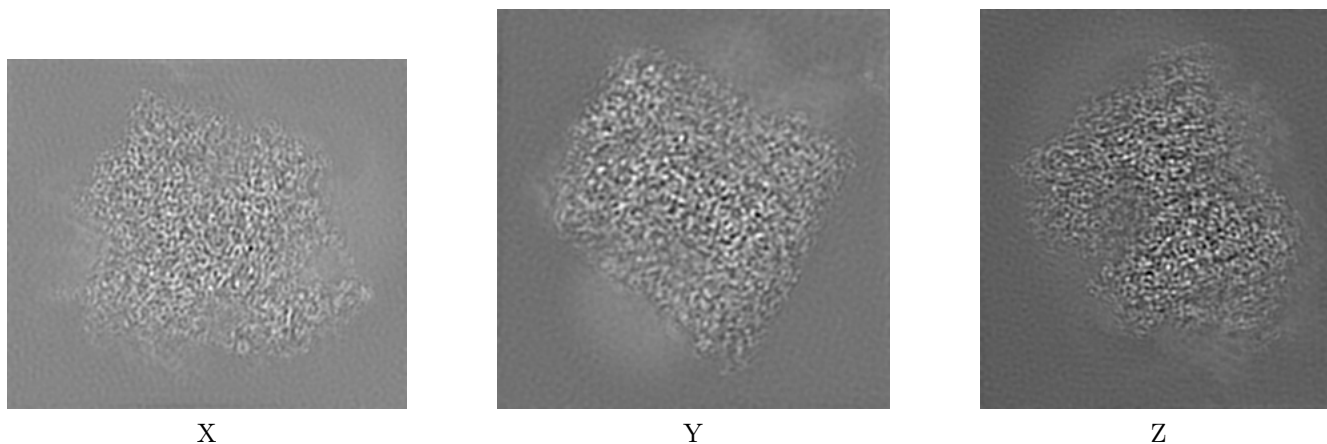
6 Map visualisation [i](#)

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

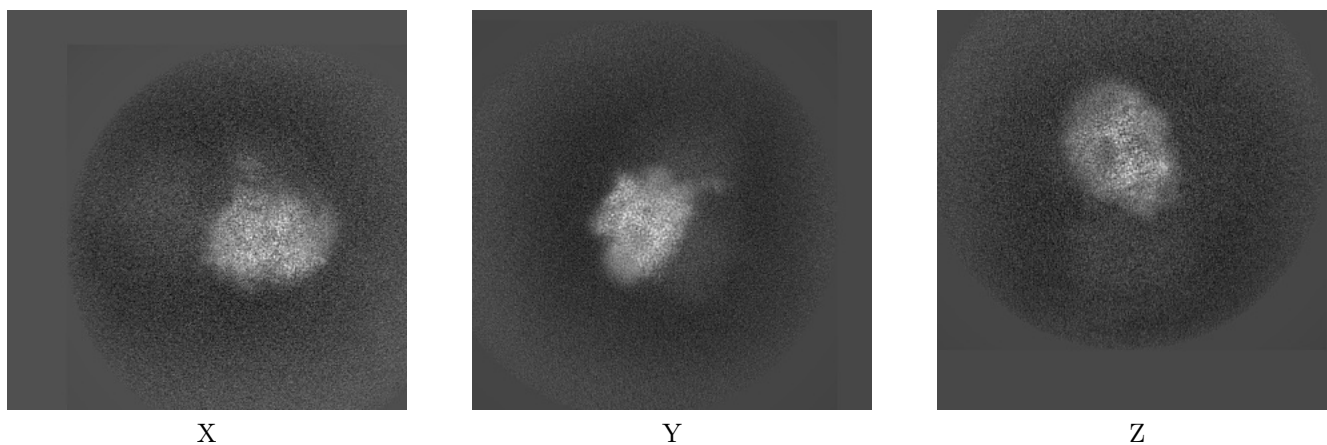
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



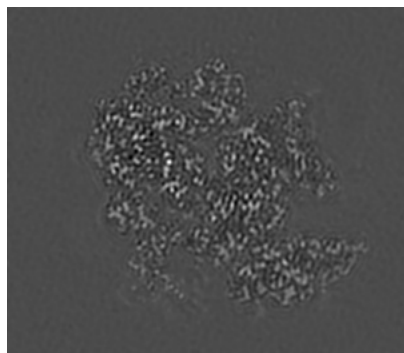
6.1.2 Raw map



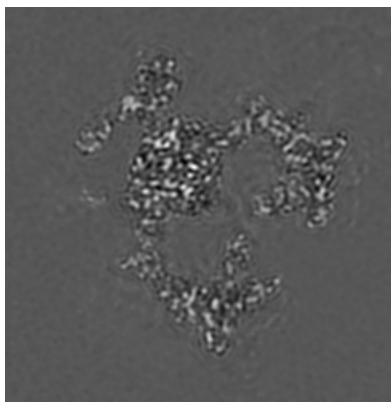
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

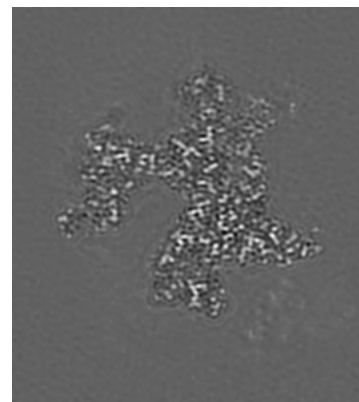
6.2.1 Primary map



X Index: 127

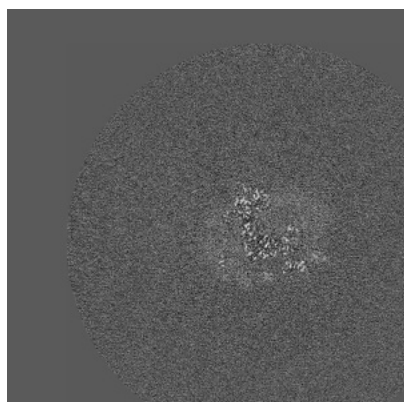


Y Index: 142

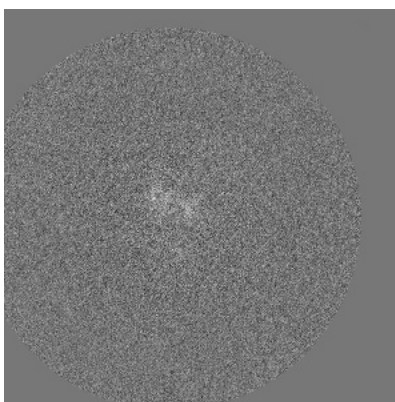


Z Index: 124

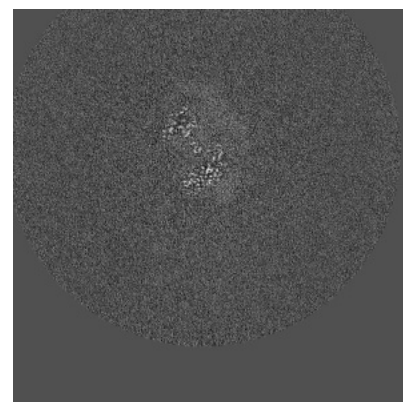
6.2.2 Raw map



X Index: 375



Y Index: 375

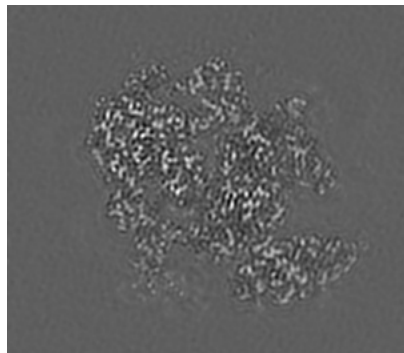


Z Index: 375

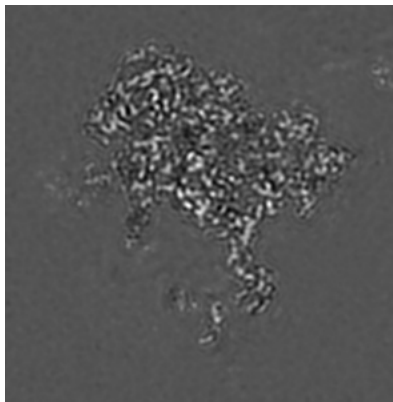
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

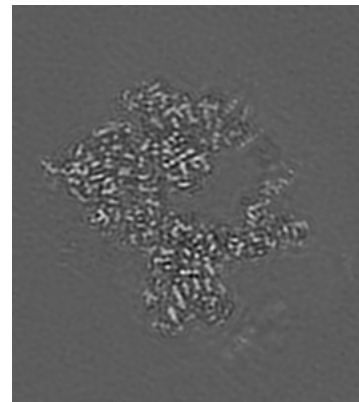
6.3.1 Primary map



X Index: 126

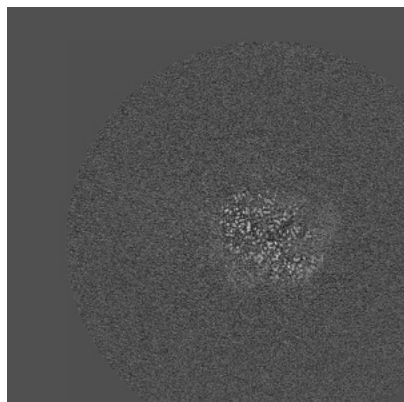


Y Index: 121

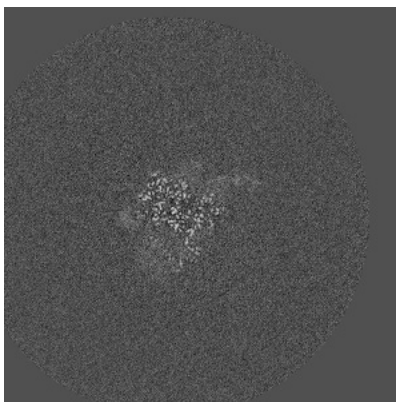


Z Index: 146

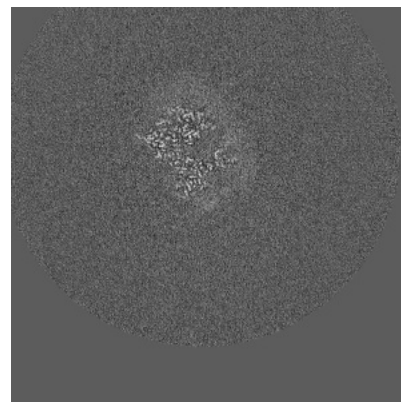
6.3.2 Raw map



X Index: 343



Y Index: 458

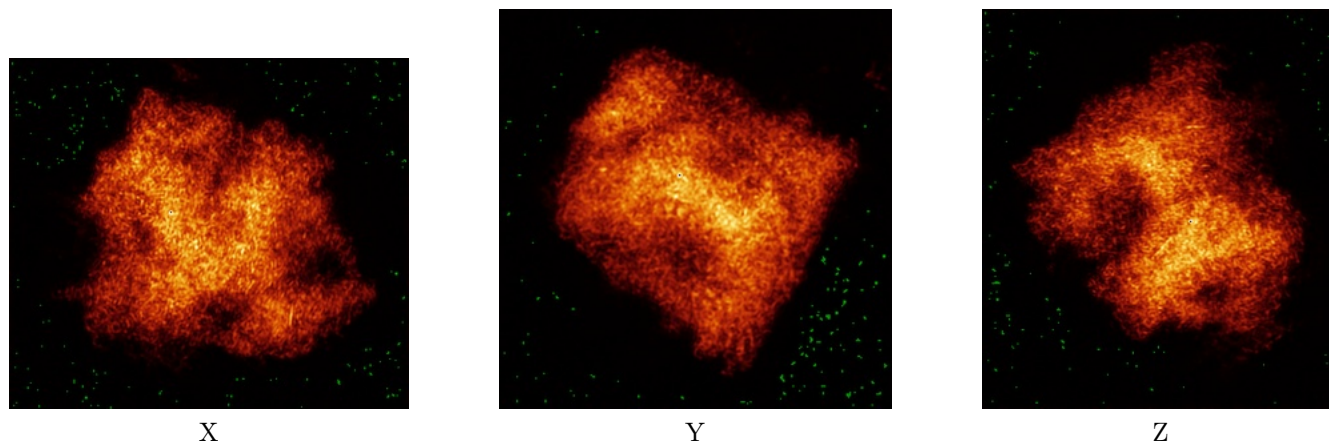


Z Index: 344

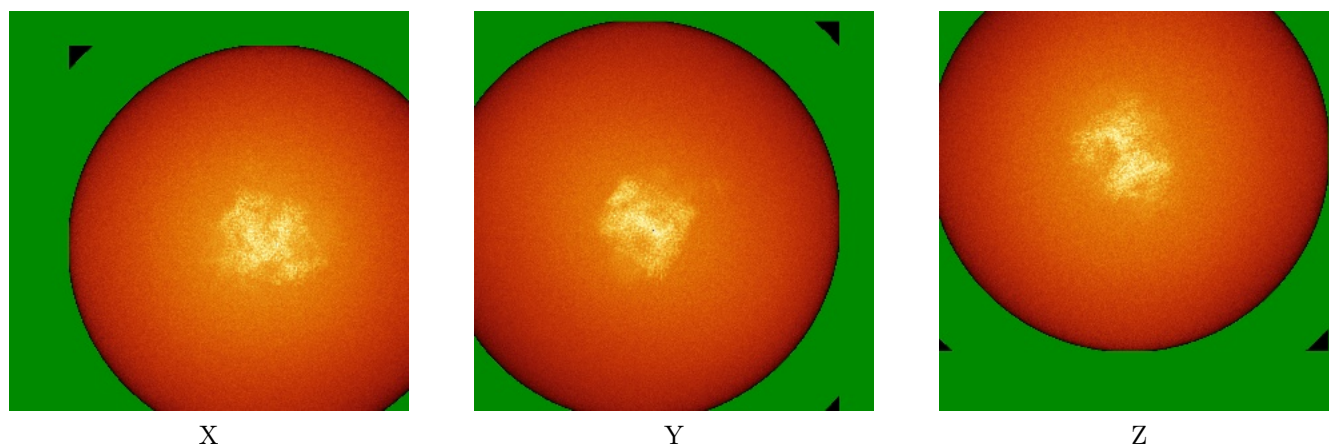
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



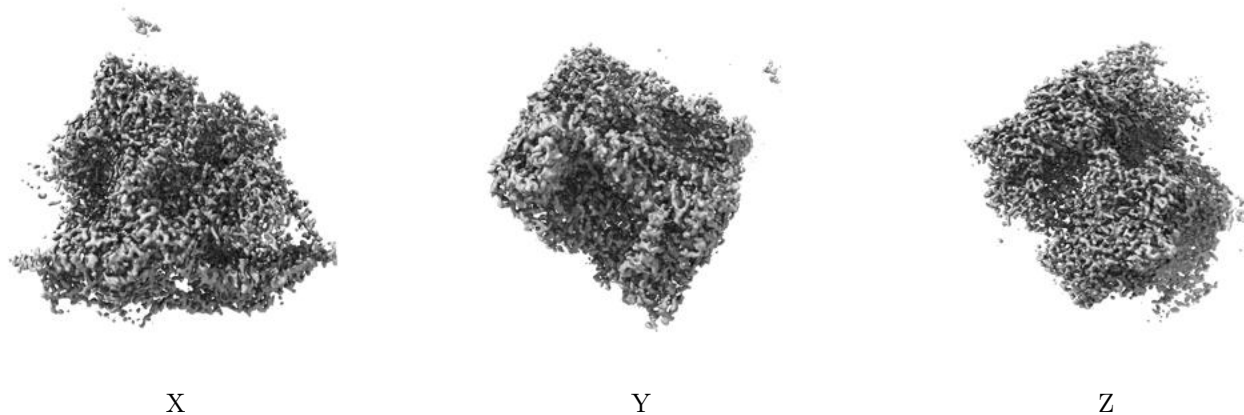
6.4.2 Raw map



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.

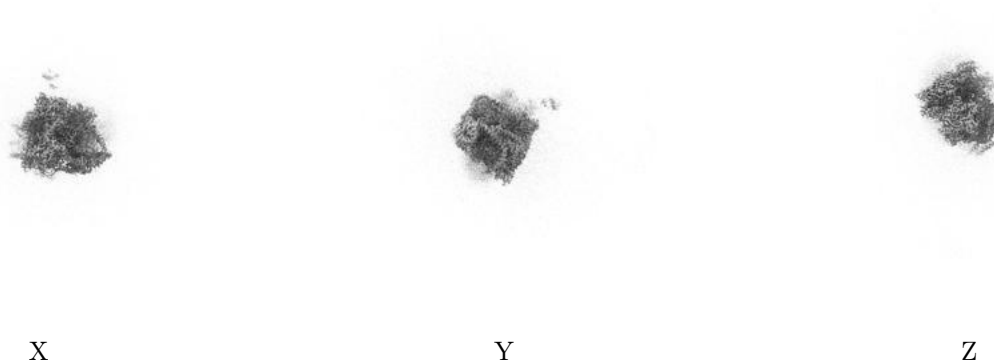
6.5 Orthogonal surface views [i](#)

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.

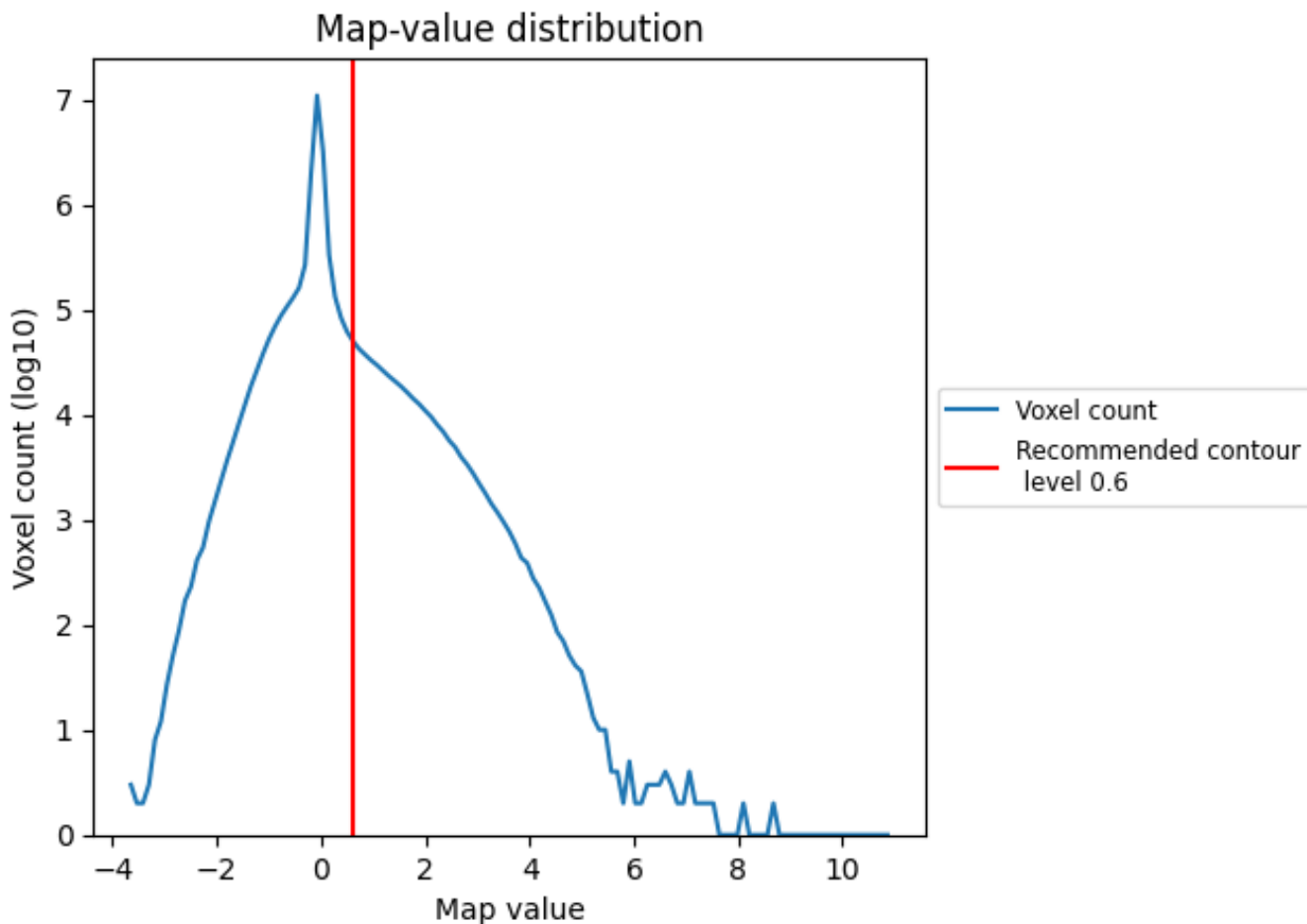
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

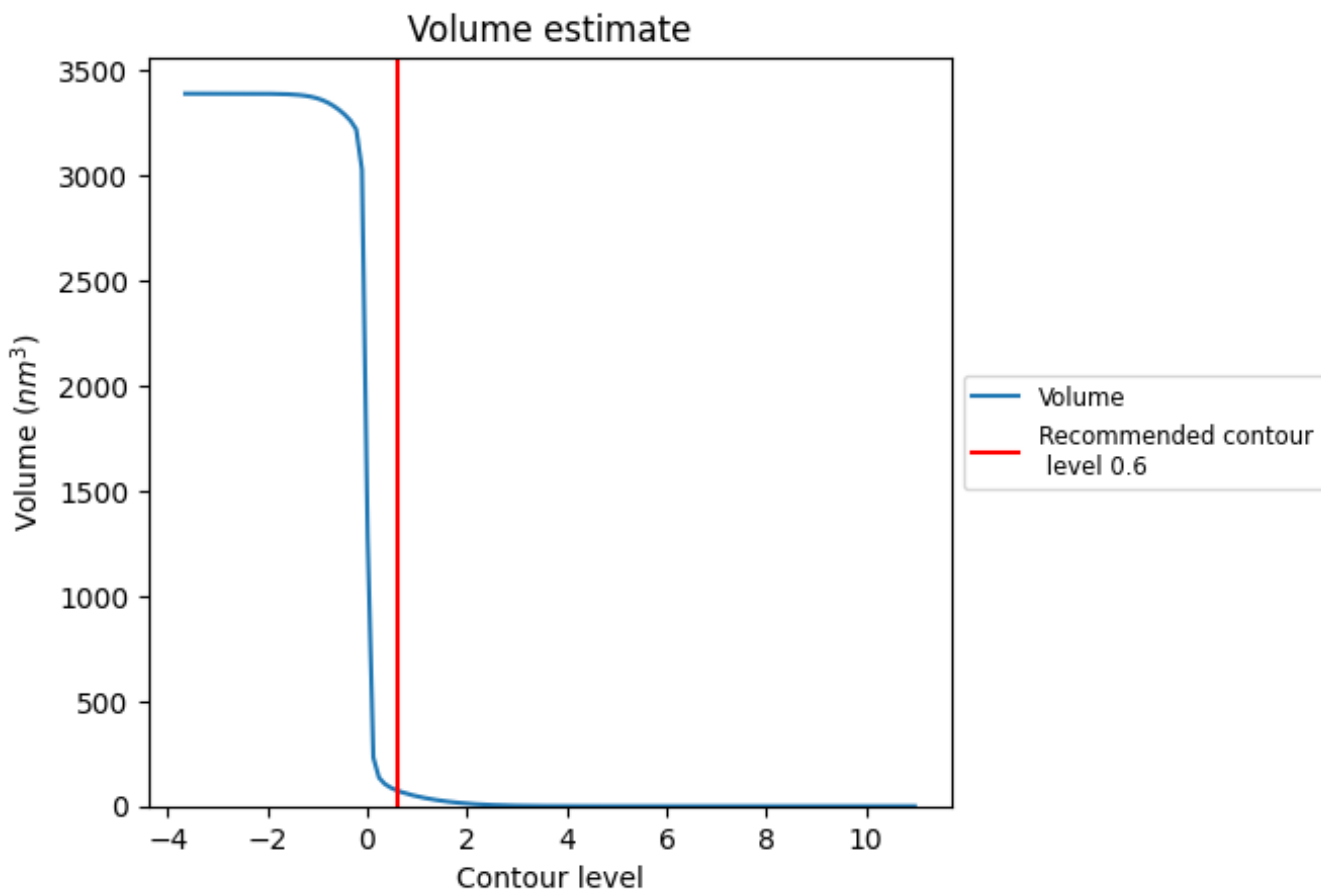
This section contains the results of statistical analysis of the map.

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 nm³; 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.

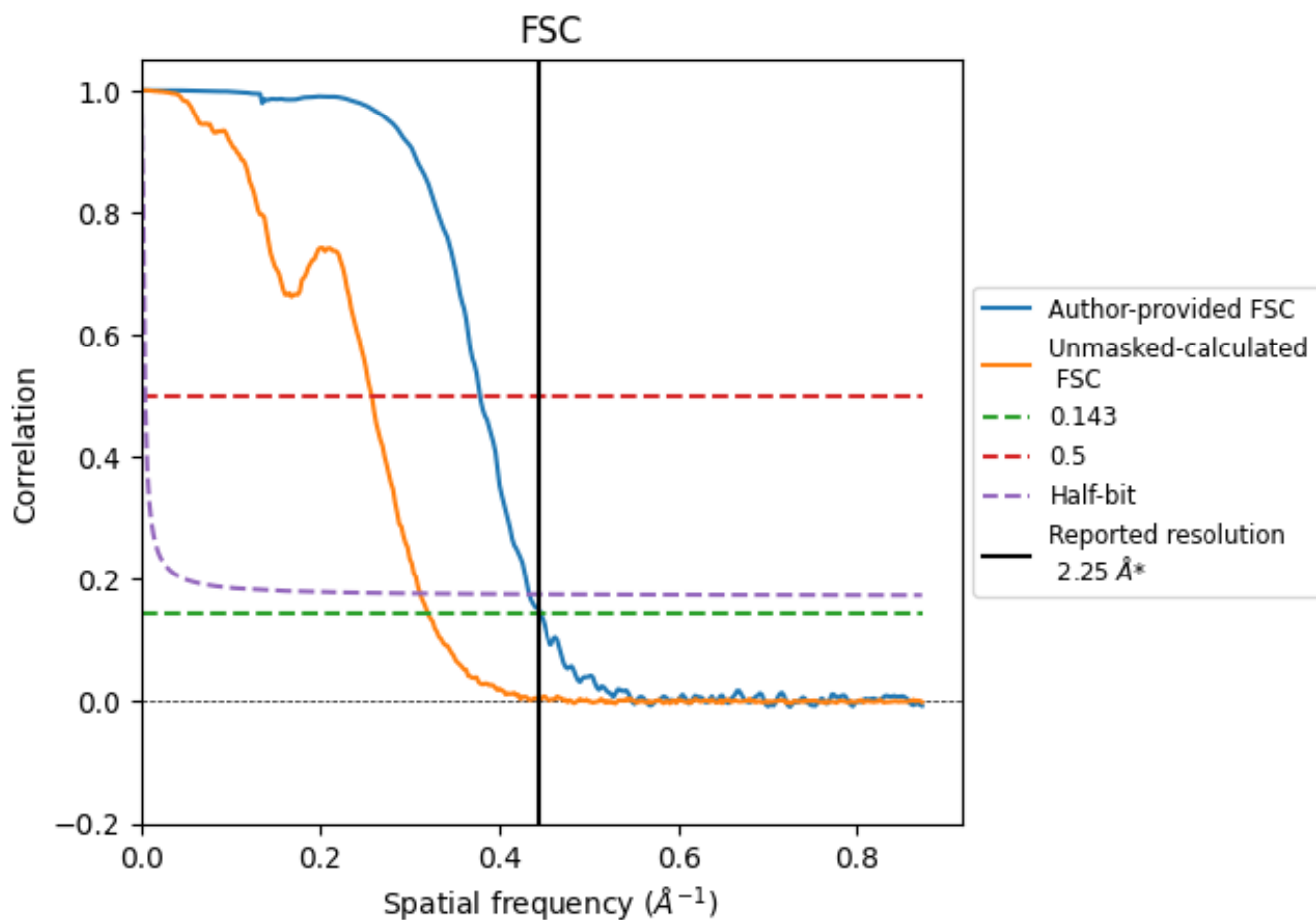
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [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 0.444 Å⁻¹

8.2 Resolution estimates [i](#)

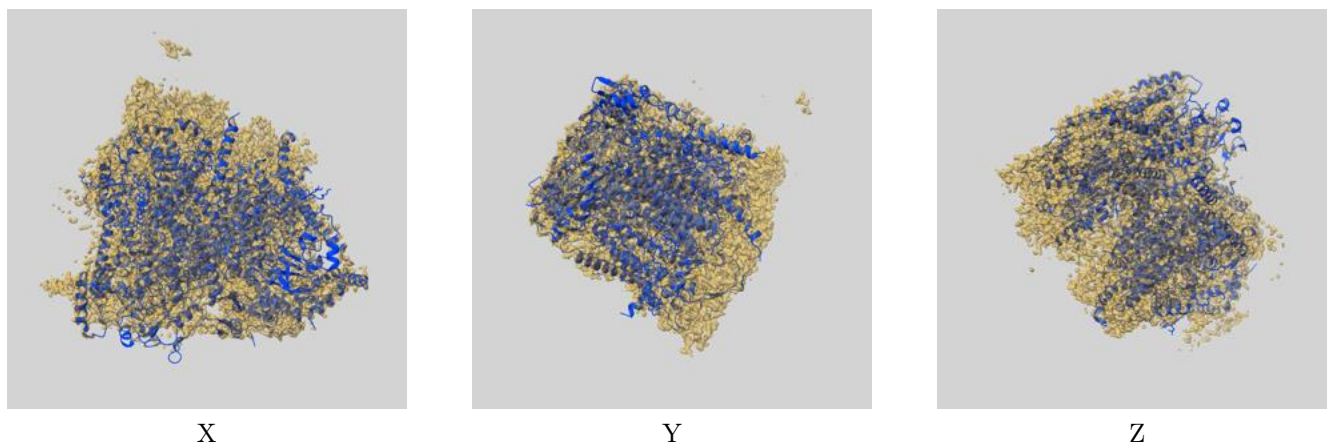
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.24	2.64	2.31
Unmasked-calculated*	3.12	3.88	3.21

*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 3.12 differs from the reported value 2.25 by more than 10 %

9 Map-model fit [i](#)

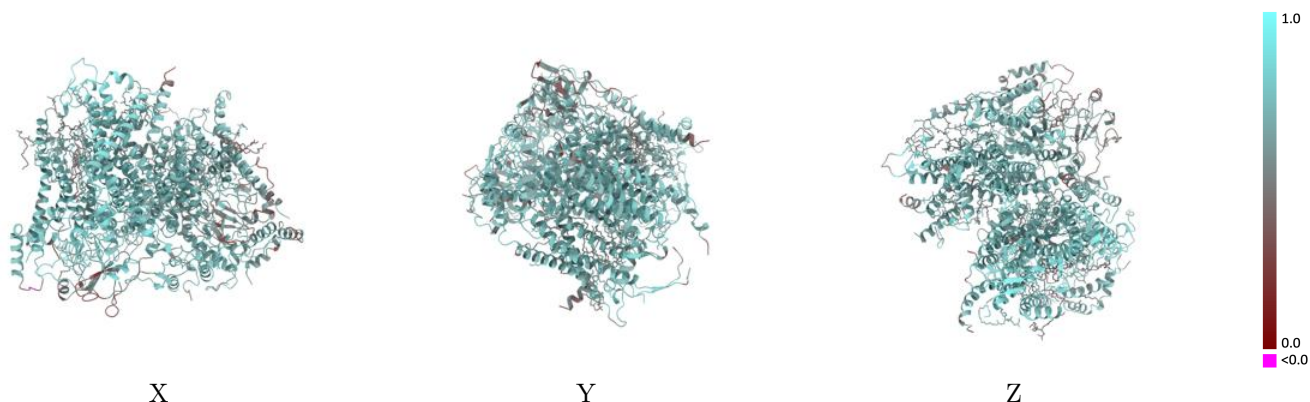
This section contains information regarding the fit between EMDB map EMD-16007 and PDB model 8BEL. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



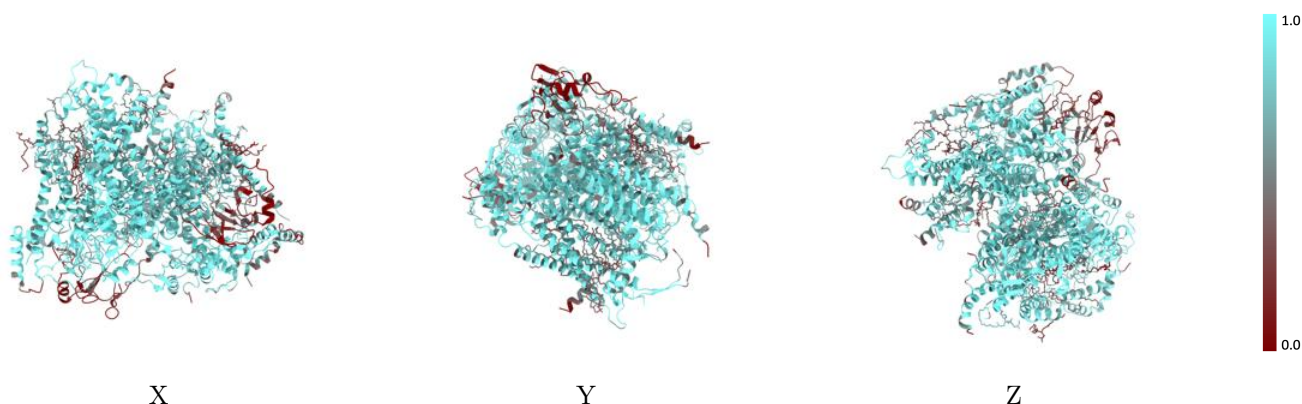
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



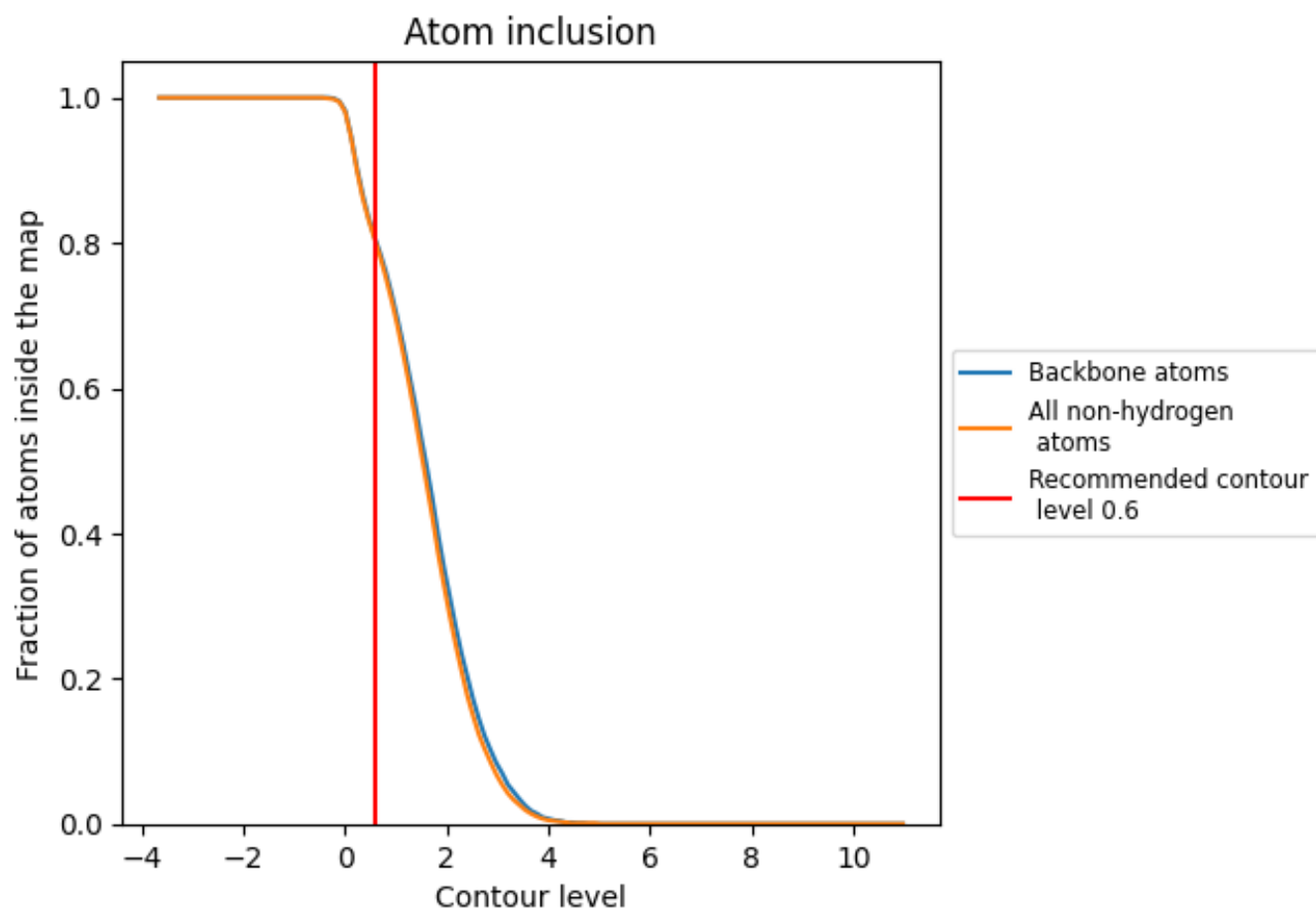
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8020	 0.6820
C	 0.9050	 0.7310
D	 0.5210	 0.5940
E	 0.9330	 0.7410
G	 0.7630	 0.6610
H	 0.7980	 0.6640
I	 0.8270	 0.7040
J	 0.4560	 0.5700
M	 0.8830	 0.7050
N	 0.5570	 0.5950
O	 0.8840	 0.7010
Q	 0.7650	 0.6440
R	 0.6490	 0.5850
S	 0.7690	 0.6440
T	 0.5490	 0.6090

