



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 06:39 PM UTC

PDB ID : 9HZL / pdb\_00009hzl  
EMDB ID : EMD-52525  
Title : High resolution cryo-EM structure of human complex III in mitochondria  
Authors : Nguyen, M.D.; Khawaja, A.; Rorbach, J.  
Deposited on : 2025-01-14  
Resolution : 2.52 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : **FAILED**  
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

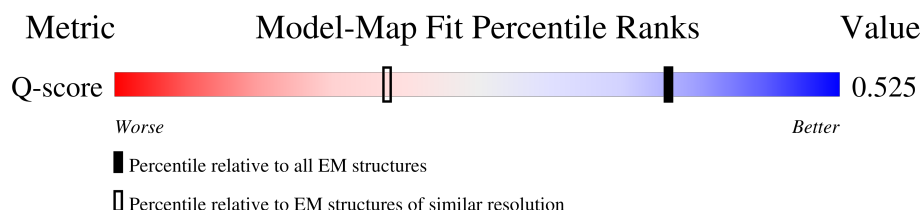
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.52 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	7226 ( 2.02 - 3.02 )

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
18	U10	J	406	-	X	-	-
18	U10	V	403	-	X	-	-
18	U10	V	404	-	X	-	-

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 68729 atoms, of which 34115 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-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	81	Total	C	H	N	O	S	0	0
			1377	450	683	126	117	1		
1	N	81	Total	C	H	N	O	S	0	0
			1377	450	683	126	117	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	48	Total	C	H	N	O	S	0	0
			714	218	370	63	62	1		
2	C	187	Total	C	H	N	O	S	0	0
			2898	922	1441	255	274	6		
2	O	57	Total	C	H	N	O	S	0	0
			841	259	432	74	75	1		
2	P	196	Total	C	H	N	O	S	0	0
			3026	960	1505	264	290	7		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	62	Total	C	H	N	O	S	0	0
			1020	332	511	87	89	1		
3	Q	62	Total	C	H	N	O	S	0	0
			1020	332	511	87	89	1		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	73	Total	C	H	N	O	S	0	0
			1132	357	544	107	119	5		
4	R	74	Total	C	H	N	O	S	0	0
			1106	351	526	108	116	5		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	106	Total	C	H	N	O	S	0	0
			1831	589	910	162	168	2		
5	S	106	Total	C	H	N	O	S	0	0
			1831	589	910	162	168	2		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	52	Total	C	H	N	O		0	0
			869	293	435	74	67			
6	T	51	Total	C	H	N	O		0	0
			847	287	422	72	66			

- Molecule 7 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	241	Total	C	H	N	O	S	0	0
			3798	1231	1874	329	349	15		
7	U	241	Total	C	H	N	O	S	0	0
			3798	1231	1874	329	349	15		

- Molecule 8 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	379	Total	C	H	N	O	S	0	0
			6093	2022	3077	468	509	17		
8	V	379	Total	C	H	N	O	S	0	0
			6093	2022	3077	468	509	17		

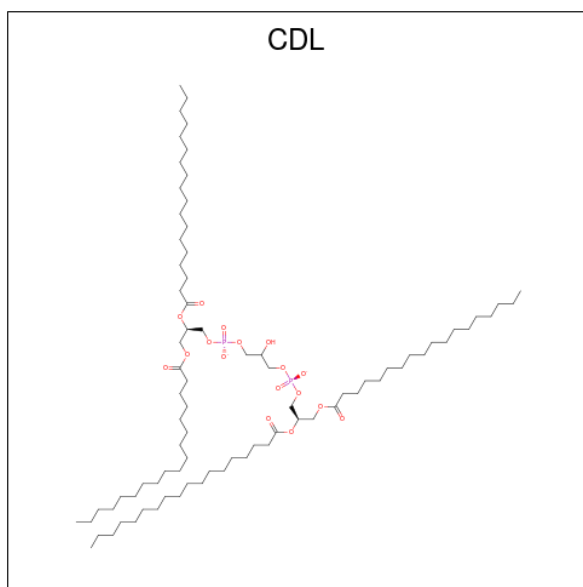
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	422	Total	C	H	N	O	S	0	0
			6315	1995	3141	556	613	10		
9	W	419	Total	C	H	N	O	S	0	0
			6301	1989	3139	553	610	10		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

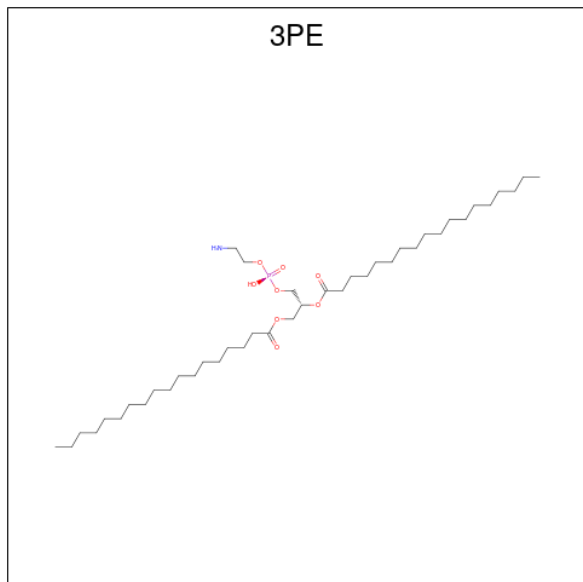
Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	446	Total	C	H	N	O	S	0	0
			6823	2169	3370	603	661	20		
10	Y	446	Total	C	H	N	O	S	0	0
			6823	2169	3370	603	661	20		

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



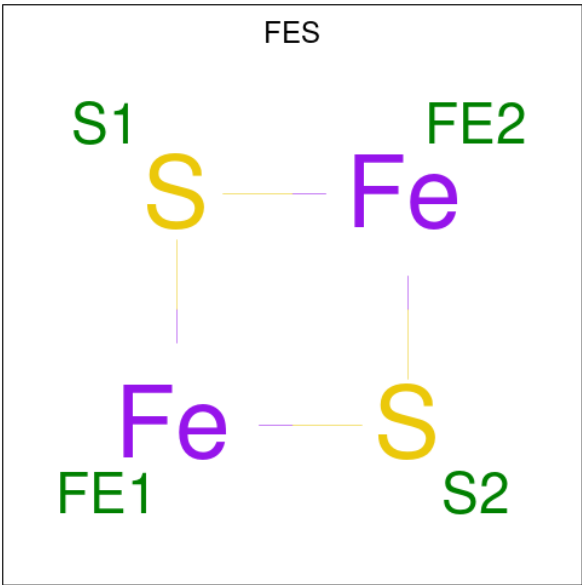
Mol	Chain	Residues	Atoms						AltConf
11	A	1	Total	C	H	O	P		0
			112	45	48	17	2		
11	G	1	Total	C	H	O	P		0
			112	45	48	17	2		
11	H	1	Total	C	H	O	P		0
			112	45	48	17	2		
11	J	1	Total	C	H	O	P		0
			112	45	48	17	2		
11	J	1	Total	C	H	O	P		0
			112	45	48	17	2		
11	T	1	Total	C	H	O	P		0
			112	45	48	17	2		
11	U	1	Total	C	H	O	P		0
			112	45	48	17	2		
11	V	1	Total	C	H	O	P		0
			112	45	48	17	2		
11	Y	1	Total	C	H	O	P		0
			112	45	48	17	2		

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



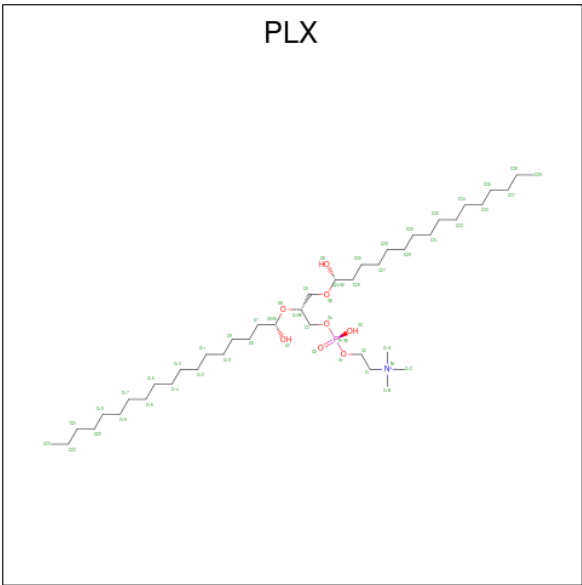
Mol	Chain	Residues	Atoms						AltConf
12	C	1	Total	C	H	N	O	P	0
			51	19	22	1	8	1	
12	C	1	Total	C	H	N	O	P	0
			53	23	20	1	8	1	
12	L	1	Total	C	H	N	O	P	0
			43	17	16	1	8	1	
12	U	1	Total	C	H	N	O	P	0
			103	37	56	1	8	1	
12	V	1	Total	C	H	N	O	P	0
			49	23	16	1	8	1	
12	Y	1	Total	C	H	N	O	P	0
			37	15	12	1	8	1	

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $Fe_2S_2$ ).



Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	Fe	S	0
			4	2	2	
13	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 14 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms						AltConf
14	D	1	Total	C	H	N	O	P	0
			122	42	70	1	8	1	

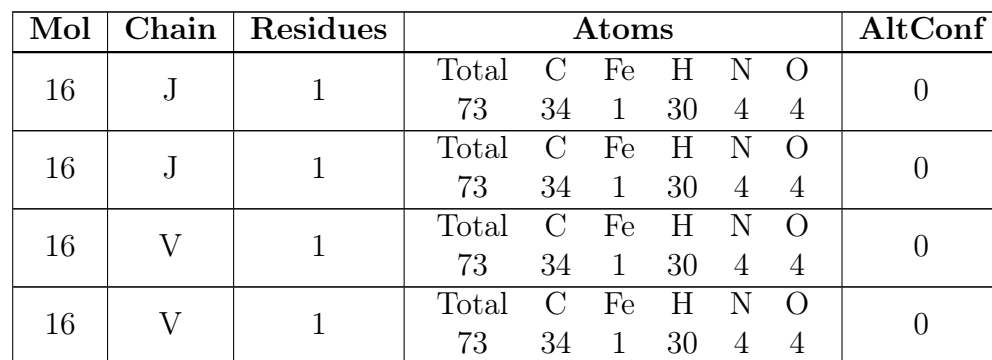
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Mol	Chain	Residues	Atoms					AltConf	
14	T	1	Total	C	H	N	O	P	0
			122	42	70	1	8	1	

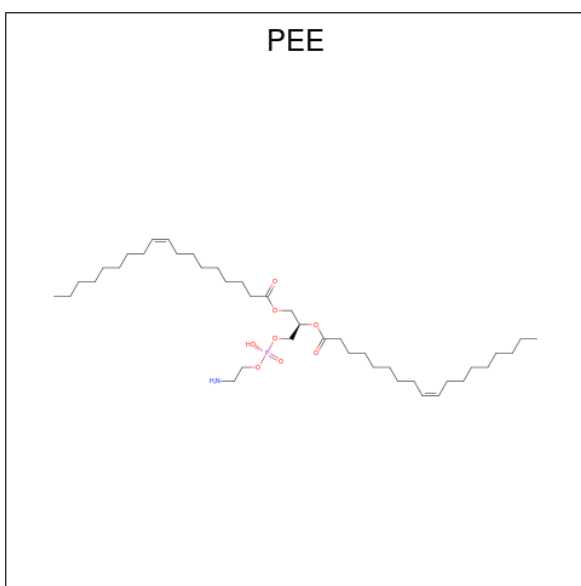
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- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



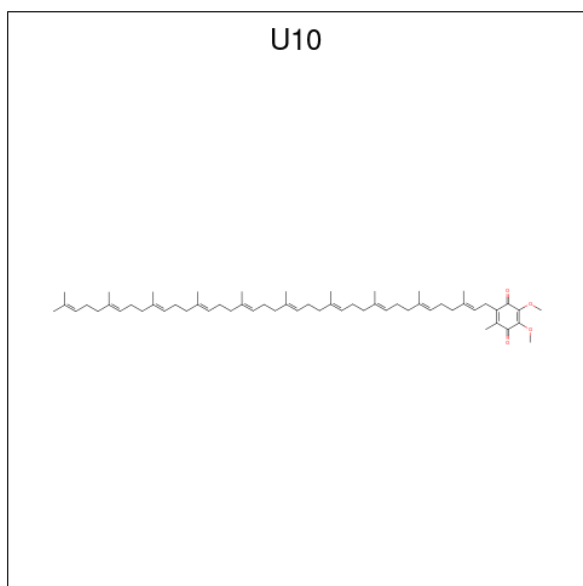


- Molecule 17 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



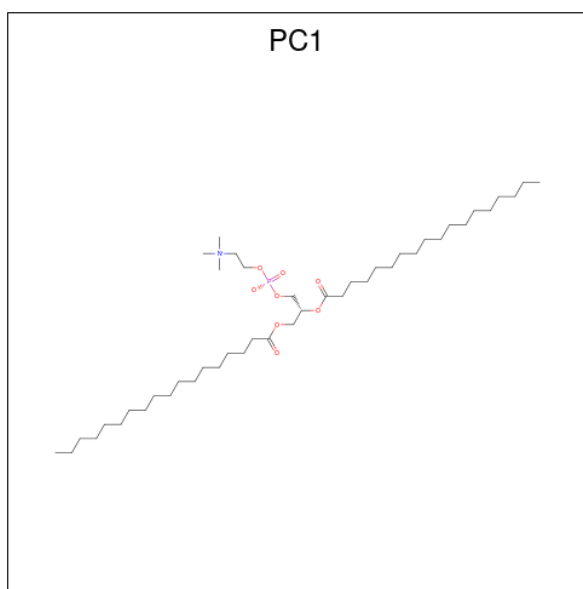
Mol	Chain	Residues	Atoms					AltConf
17	J	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 18 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	J	1	Total	C	H	O	0
			150	59	87	4	
18	J	1	Total	C	H	O	0
			150	59	87	4	
18	V	1	Total	C	H	O	0
			150	59	87	4	
18	V	1	Total	C	H	O	0
			150	59	87	4	

- Molecule 19 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
19	P	1	109	35	64	1	8	1	0

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### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	37.643	Depositor
Minimum map value	-14.750	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.54	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.875, 0.875, 0.875	Depositor

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

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### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

31 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
11	CDL	G	101	-	63,63,99	1.43	7 (11%)	69,75,111	1.05	4 (5%)
18	U10	J	406	-	63,63,63	2.90	35 (55%)	78,79,79	7.92	43 (55%)
14	PLX	D	101	-	51,51,51	1.03	4 (7%)	53,59,59	0.75	0
13	FES	C	302	2	0,4,4	-	-	-	-	-
18	U10	V	403	-	63,63,63	2.83	30 (47%)	78,79,79	7.50	44 (56%)
16	HEM	V	401	8	50,50,50	1.45	8 (16%)	67,82,82	1.09	2 (2%)
16	HEM	V	402	8	50,50,50	1.42	7 (14%)	67,82,82	1.23	6 (8%)
11	CDL	U	403	-	63,63,99	1.43	8 (12%)	69,75,111	1.17	4 (5%)
11	CDL	Y	501	-	63,63,99	1.43	7 (11%)	69,75,111	1.17	4 (5%)
18	U10	J	405	-	63,63,63	2.97	30 (47%)	78,79,79	8.16	38 (48%)
12	3PE	C	303	-	32,32,50	1.21	4 (12%)	35,37,55	1.10	2 (5%)
12	3PE	C	301	-	28,28,50	1.28	4 (14%)	31,33,55	1.13	2 (6%)
12	3PE	L	501	-	26,26,50	1.32	3 (11%)	29,31,55	1.14	2 (6%)
12	3PE	U	401	-	46,46,50	1.07	4 (8%)	49,51,55	0.99	2 (4%)
11	CDL	A	101	-	63,63,99	1.42	7 (11%)	69,75,111	1.09	4 (5%)
16	HEM	J	401	8	50,50,50	1.47	7 (14%)	67,82,82	1.04	2 (2%)
18	U10	V	404	-	63,63,63	2.92	35 (55%)	78,79,79	7.49	37 (47%)
11	CDL	J	404	-	63,63,99	1.42	8 (12%)	69,75,111	1.14	4 (5%)
15	HEC	H	401	-	46,50,50	1.83	6 (13%)	58,82,82	1.91	5 (8%)
13	FES	P	301	2	0,4,4	-	-	-	-	-
12	3PE	Y	502	-	24,24,50	1.34	3 (12%)	27,29,55	1.22	2 (7%)
11	CDL	V	406	-	63,63,99	1.44	8 (12%)	69,75,111	1.03	3 (4%)
12	3PE	V	405	-	32,32,50	1.21	3 (9%)	35,37,55	1.10	2 (5%)
19	PC1	P	302	-	44,44,53	1.41	7 (15%)	50,52,61	0.70	1 (2%)
11	CDL	H	402	-	63,63,99	1.42	8 (12%)	69,75,111	1.12	4 (5%)
17	PEE	J	403	-	48,48,50	1.19	3 (6%)	51,53,55	1.01	2 (3%)
14	PLX	T	102	-	51,51,51	1.05	5 (9%)	53,59,59	0.73	0
15	HEC	U	402	7	46,50,50	1.84	5 (10%)	58,82,82	1.96	6 (10%)
16	HEM	J	402	8	50,50,50	1.40	6 (12%)	67,82,82	1.18	5 (7%)
11	CDL	J	407	-	63,63,99	1.43	8 (12%)	69,75,111	1.05	4 (5%)
11	CDL	T	101	-	63,63,99	1.42	8 (12%)	69,75,111	1.13	5 (7%)

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
11	CDL	G	101	-	-	31/74/74/110	-
18	U10	J	406	-	-	18/63/87/87	0/1/1/1
14	PLX	D	101	-	-	8/55/55/55	-
13	FES	C	302	2	-	-	0/1/1/1
18	U10	V	403	-	-	25/63/87/87	0/1/1/1
16	HEM	V	401	8	-	5/14/54/54	-
16	HEM	V	402	8	-	5/14/54/54	-
11	CDL	U	403	-	-	12/74/74/110	-
11	CDL	Y	501	-	-	19/74/74/110	-
18	U10	J	405	-	-	19/63/87/87	0/1/1/1
12	3PE	C	303	-	-	6/36/36/54	-
12	3PE	C	301	-	-	11/32/32/54	-
12	3PE	L	501	-	-	9/30/30/54	-
12	3PE	U	401	-	-	12/50/50/54	-
11	CDL	A	101	-	-	21/74/74/110	-
16	HEM	J	401	8	-	2/14/54/54	-
18	U10	V	404	-	-	20/63/87/87	0/1/1/1
11	CDL	J	404	-	-	28/74/74/110	-
15	HEC	H	401	-	-	6/14/54/54	-
13	FES	P	301	2	-	-	0/1/1/1
12	3PE	Y	502	-	-	6/28/28/54	-
11	CDL	V	406	-	-	27/74/74/110	-
12	3PE	V	405	-	-	14/36/36/54	-
19	PC1	P	302	-	-	10/48/48/57	-
11	CDL	H	402	-	-	21/74/74/110	-
17	PEE	J	403	-	-	11/52/52/54	-
14	PLX	T	102	-	-	8/55/55/55	-
15	HEC	U	402	7	-	9/14/54/54	-
16	HEM	J	402	8	-	4/14/54/54	-
11	CDL	J	407	-	-	18/74/74/110	-
11	CDL	T	101	-	-	20/74/74/110	-

The worst 5 of 278 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	404	U10	C6-C1	11.16	1.55	1.35
18	J	405	U10	C6-C1	10.44	1.53	1.35
18	J	406	U10	C6-C1	10.42	1.53	1.35
18	V	403	U10	C6-C1	9.69	1.52	1.35
15	H	401	HEC	CAB-C3B	6.19	1.55	1.35

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	J	405	U10	C10-C9-C11	-20.60	79.48	115.23
18	J	406	U10	C40-C39-C41	-19.02	82.21	115.23
18	V	403	U10	C10-C9-C8	18.63	171.47	123.63
18	J	406	U10	C40-C39-C38	18.62	171.44	123.63
18	J	405	U10	C20-C19-C18	18.43	170.95	123.63

There are no chirality outliers.

5 of 405 torsion outliers are listed below:

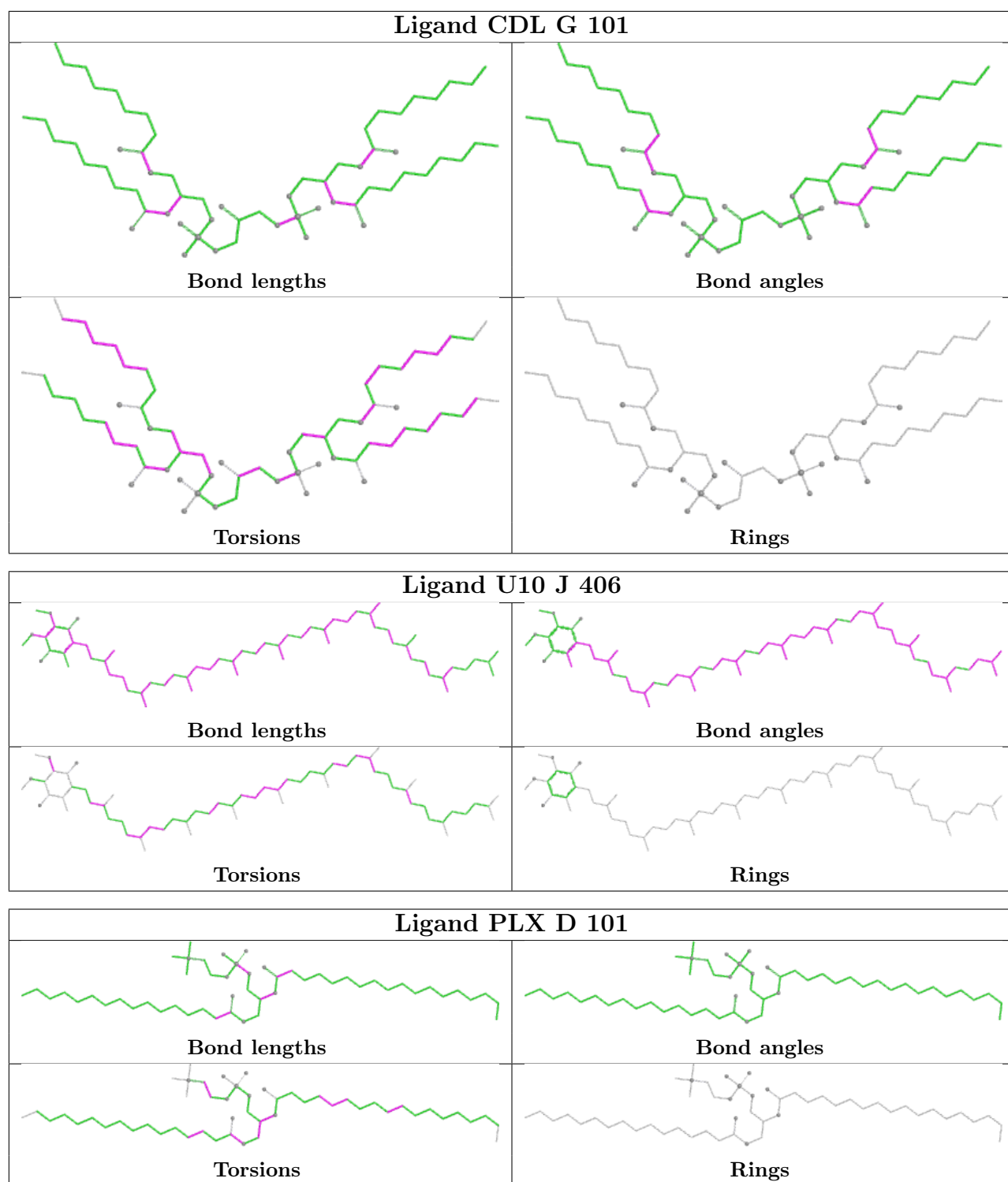
Mol	Chain	Res	Type	Atoms
11	A	101	CDL	CA2-OA2-PA1-OA4
11	A	101	CDL	CA2-OA2-PA1-OA5
11	A	101	CDL	CA3-OA5-PA1-OA2
11	A	101	CDL	C1-CB2-OB2-PB2
11	A	101	CDL	CB2-OB2-PB2-OB4

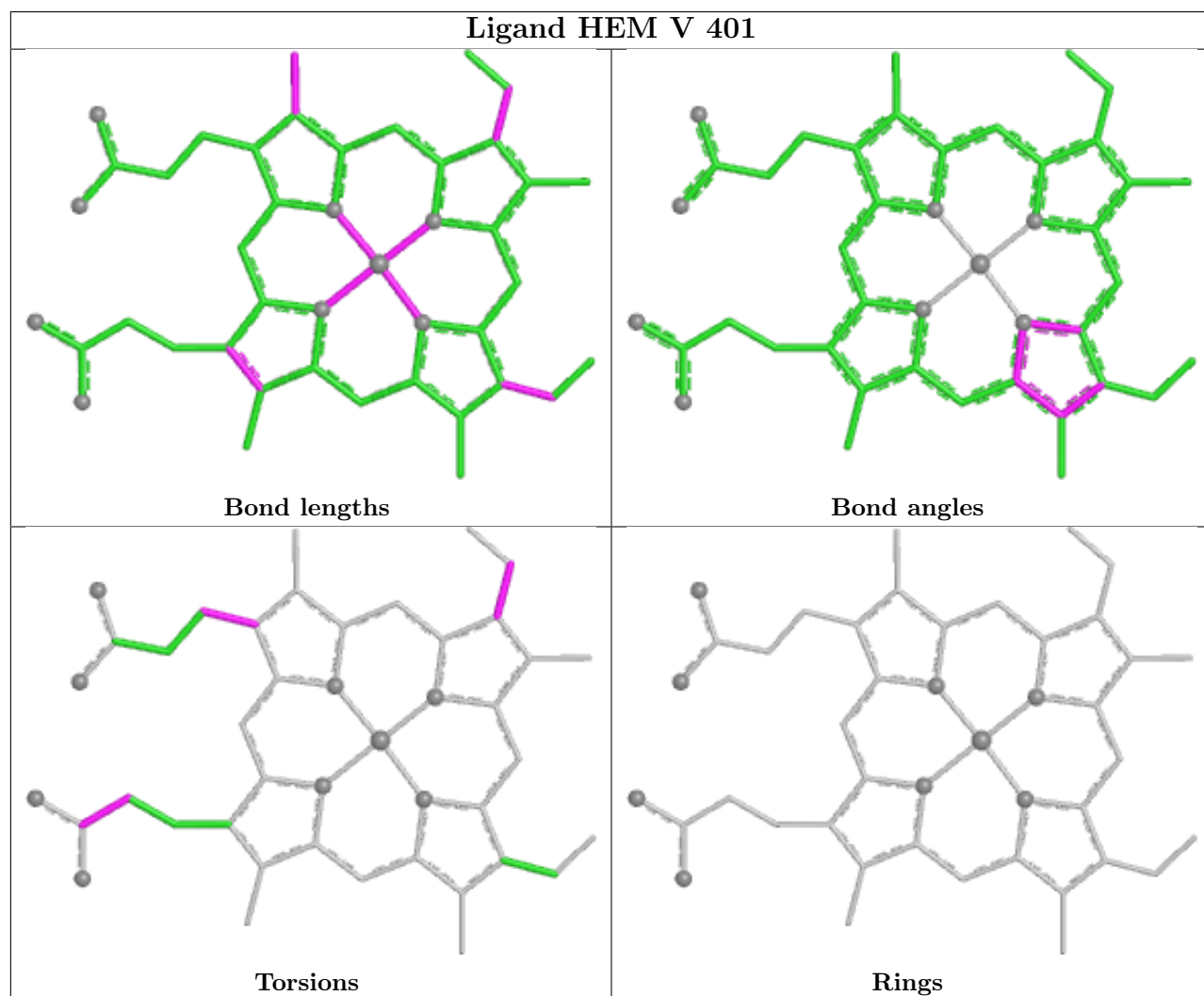
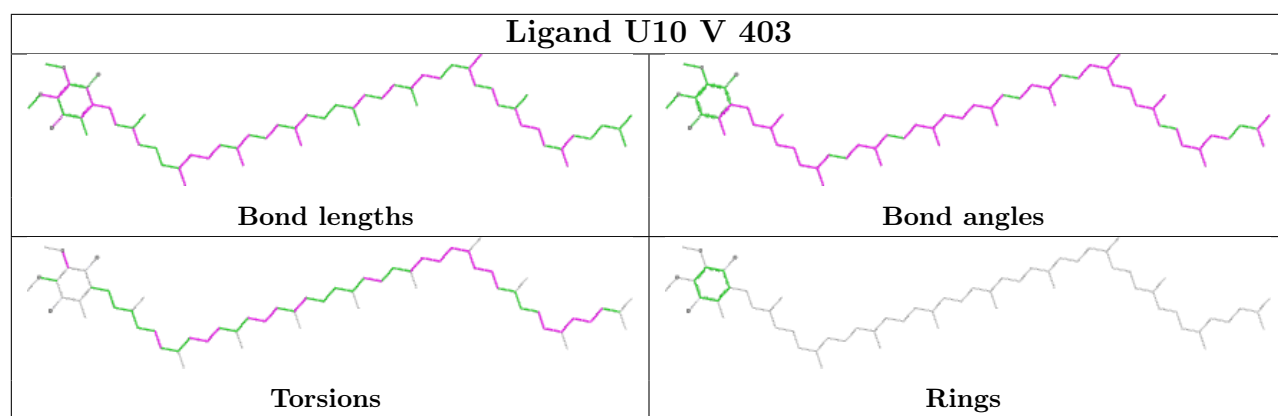
There are no ring outliers.

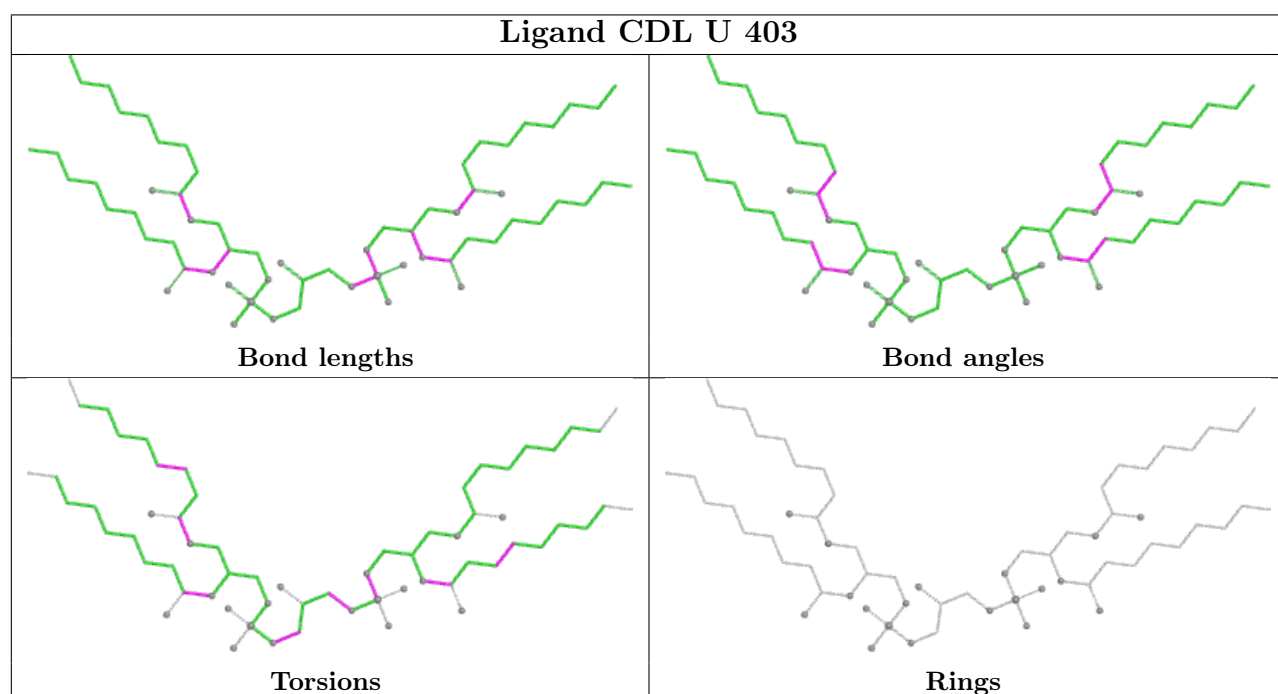
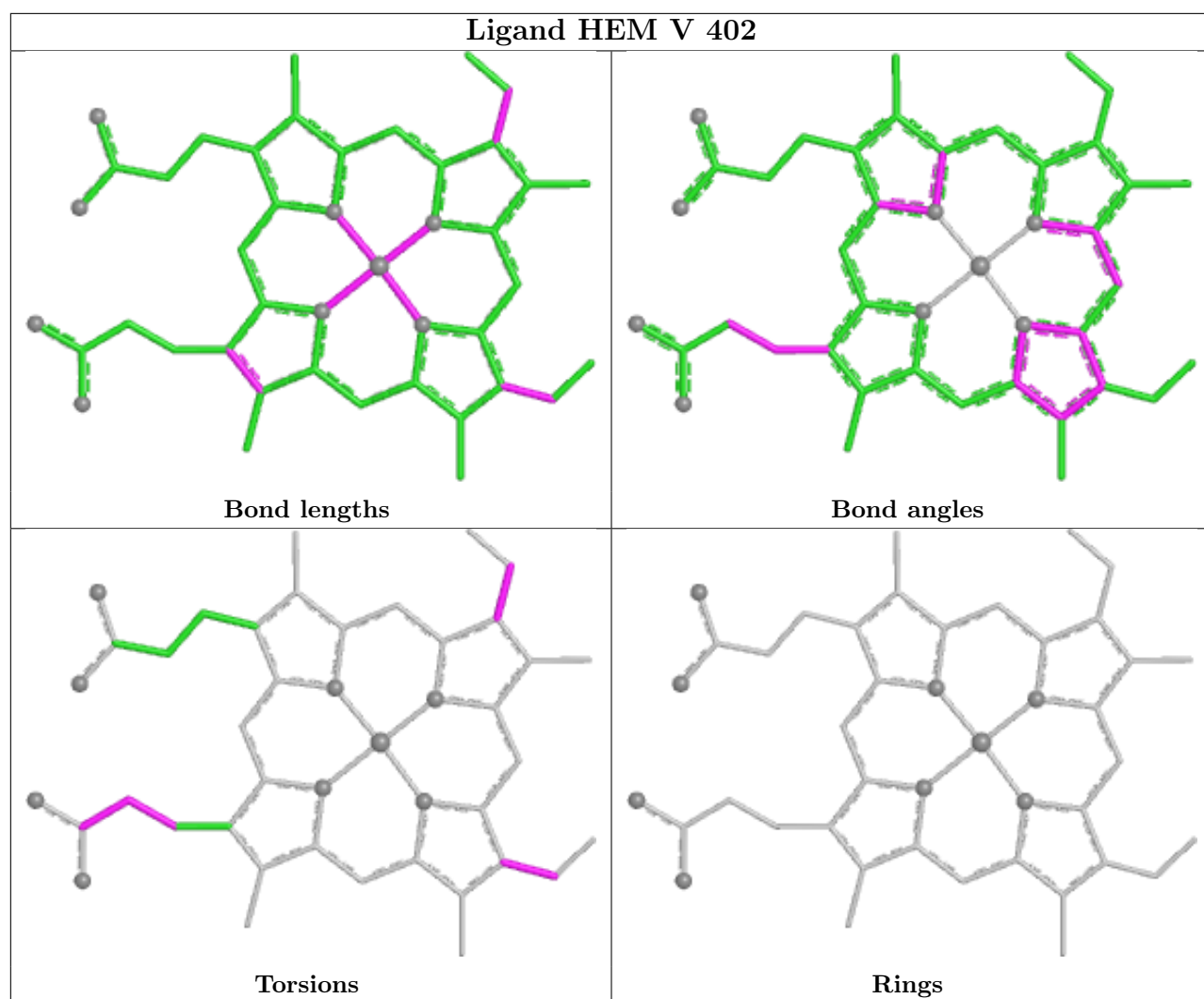
No monomer is involved in short contacts.

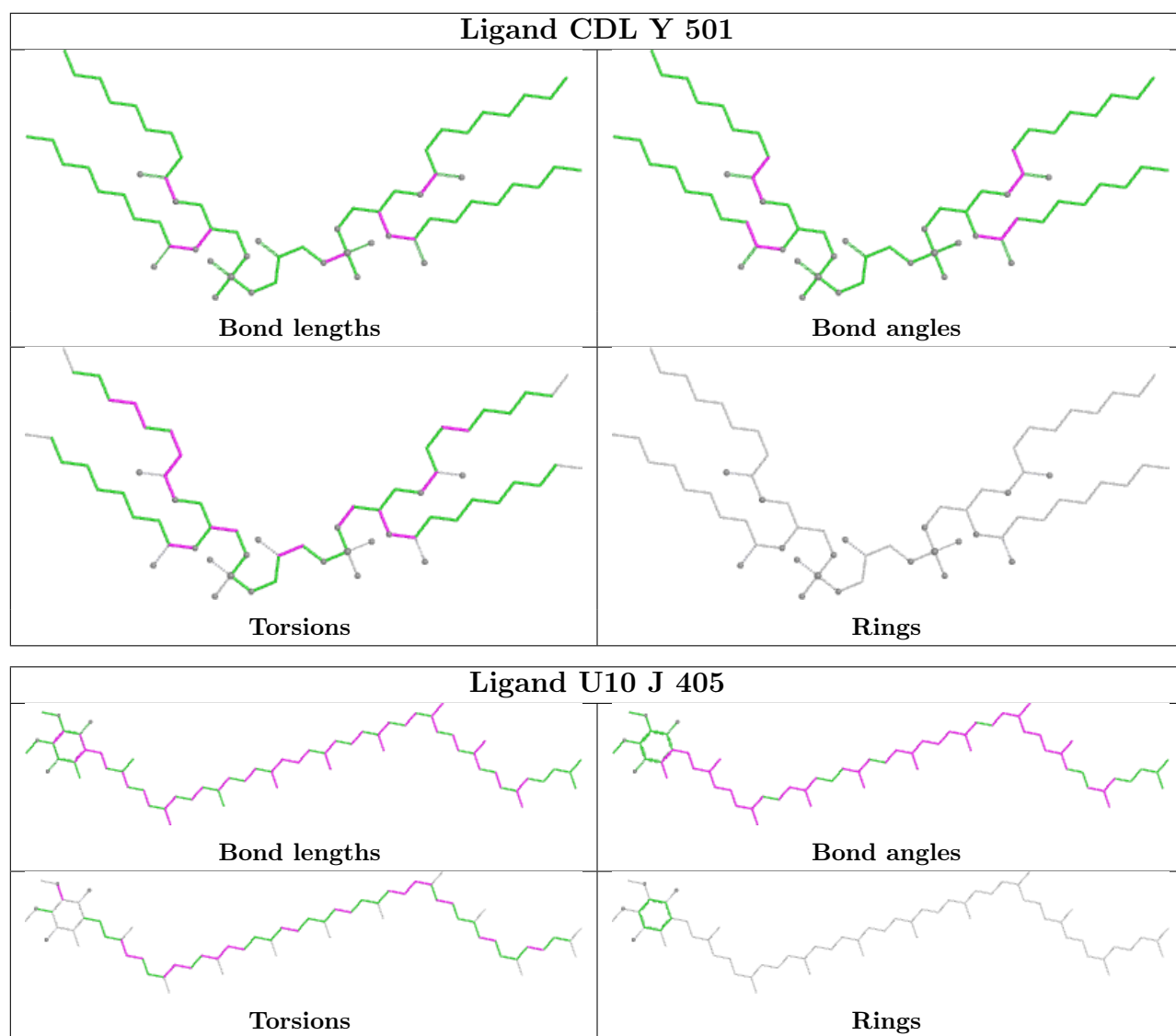
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

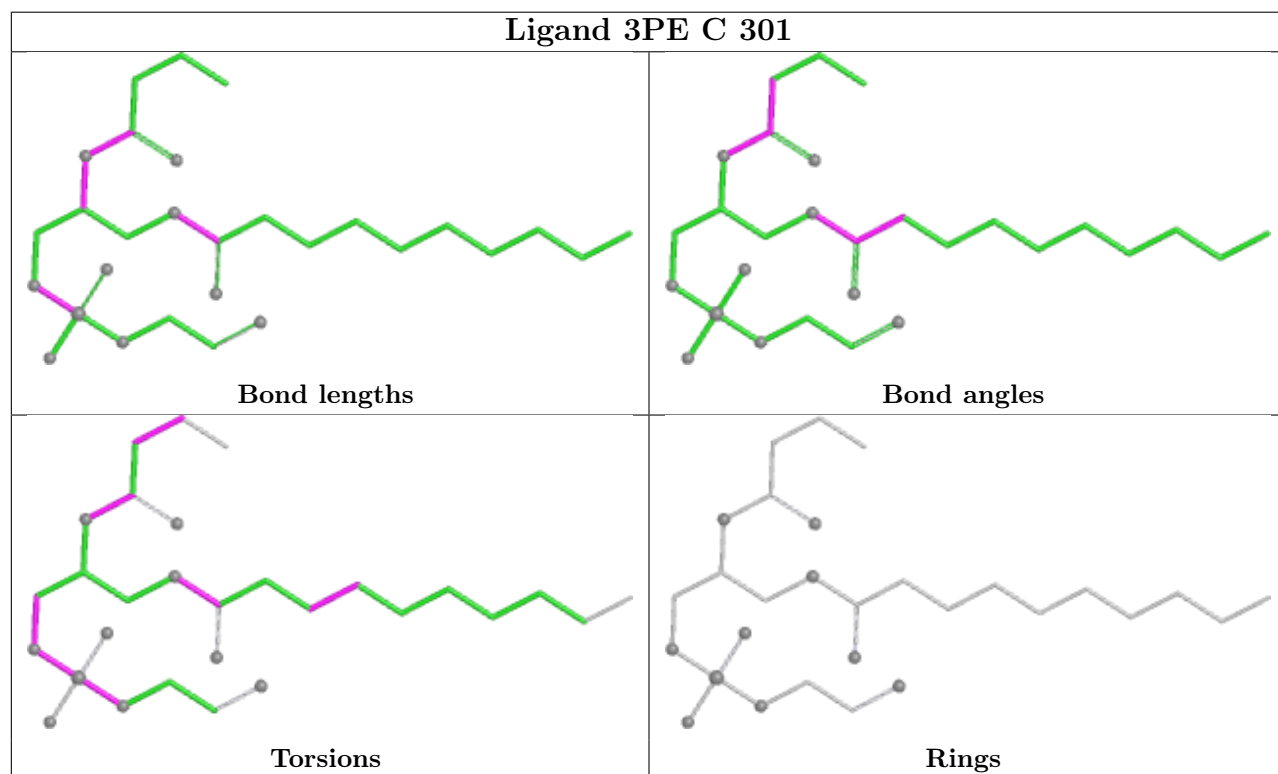
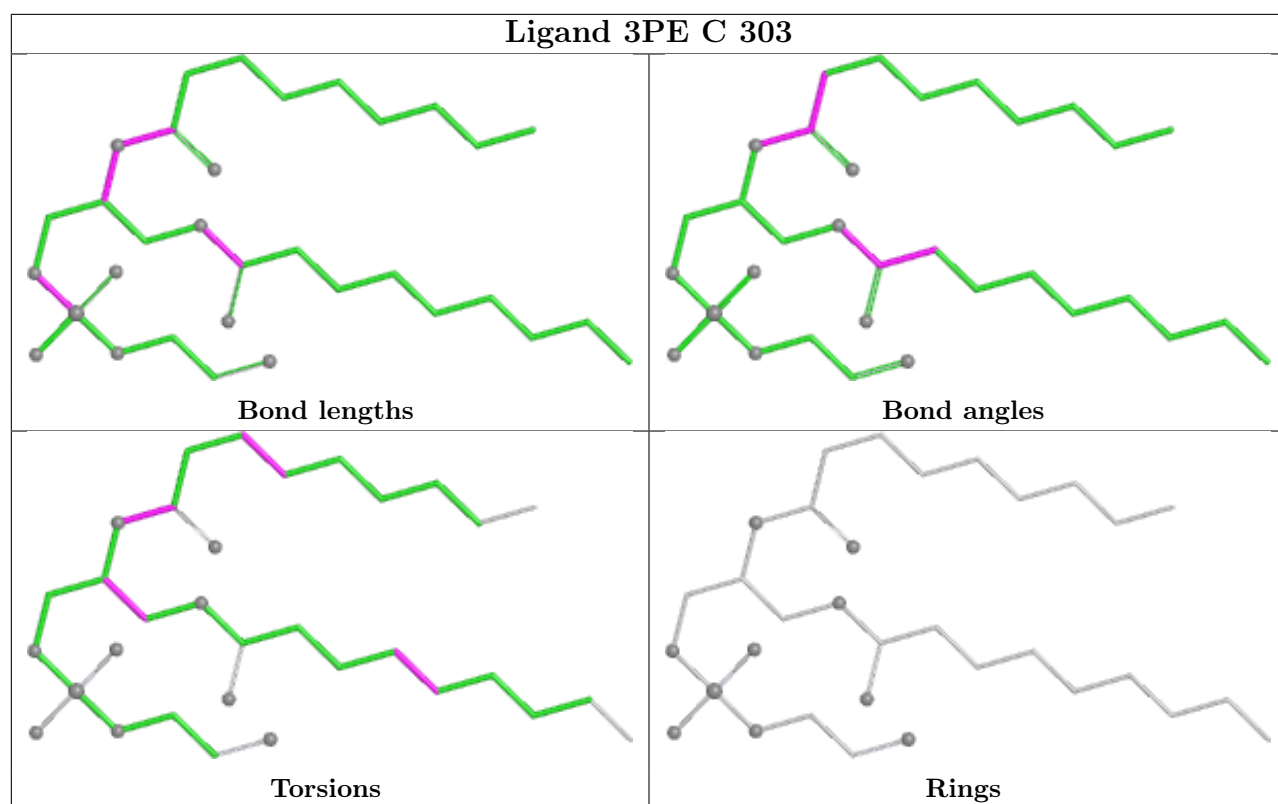




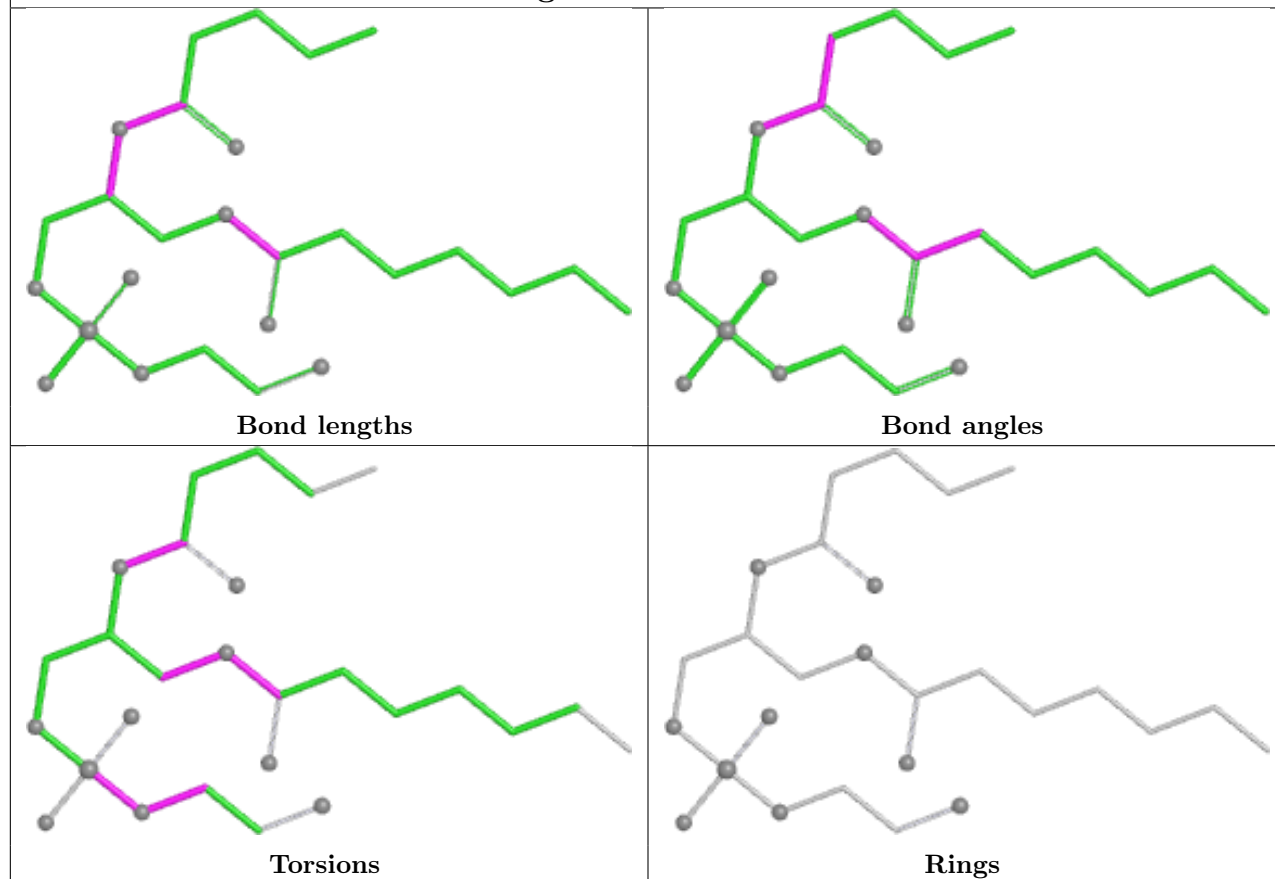




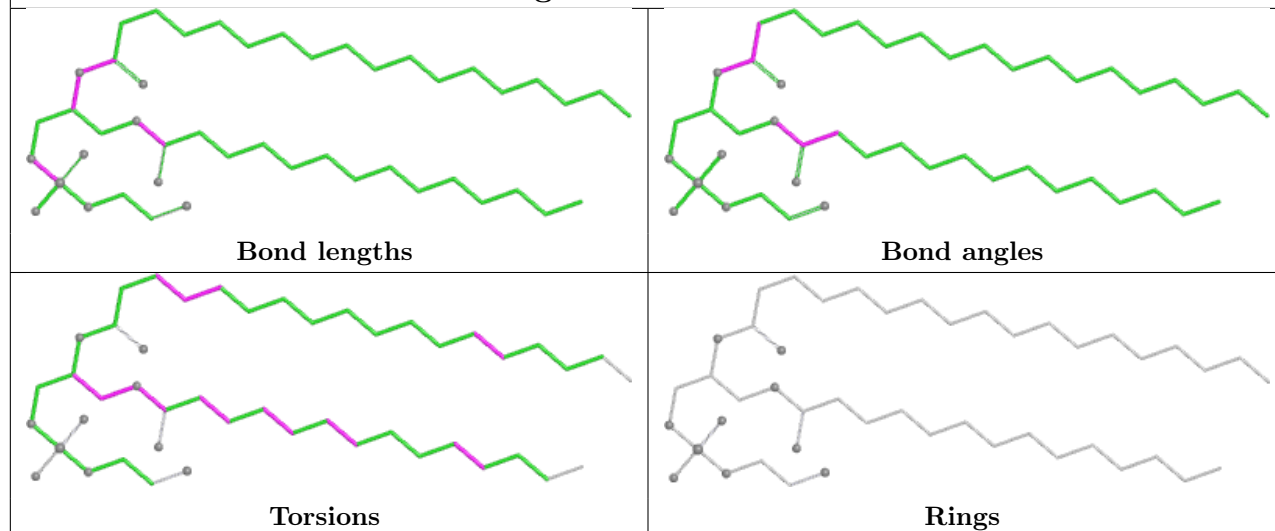


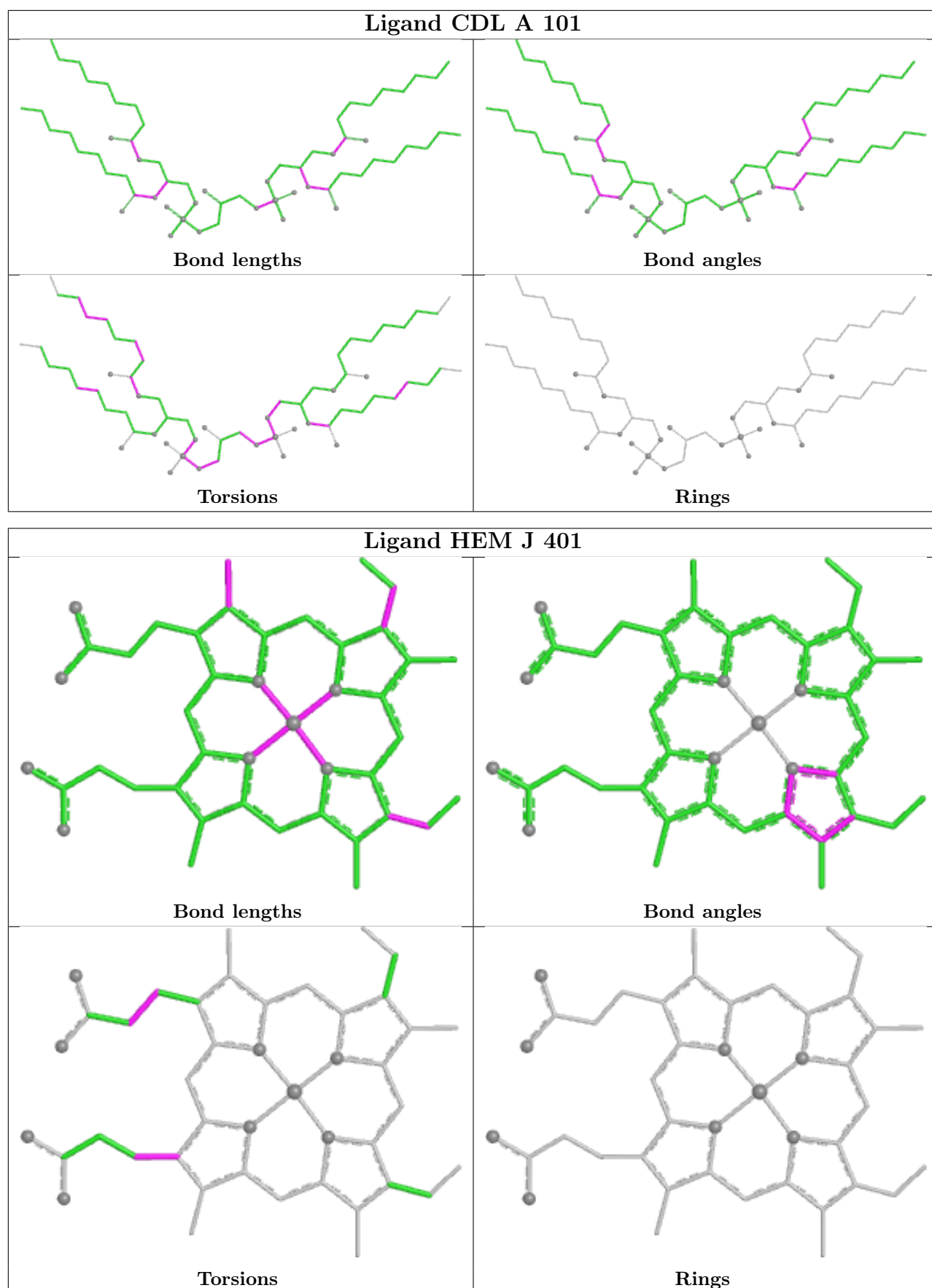


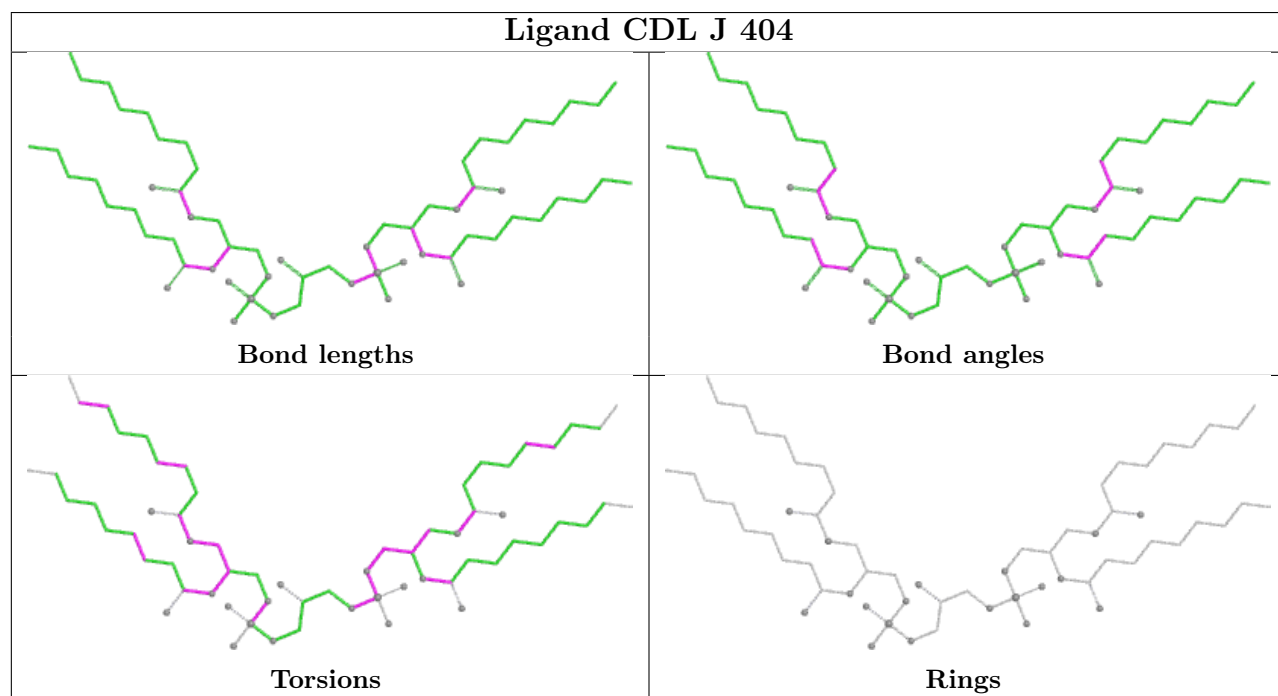
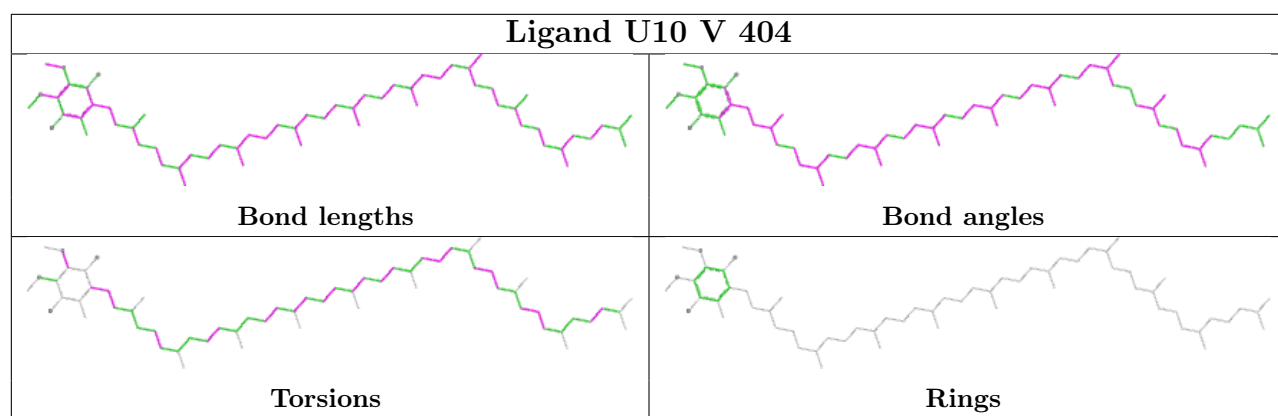
## Ligand 3PE L 501



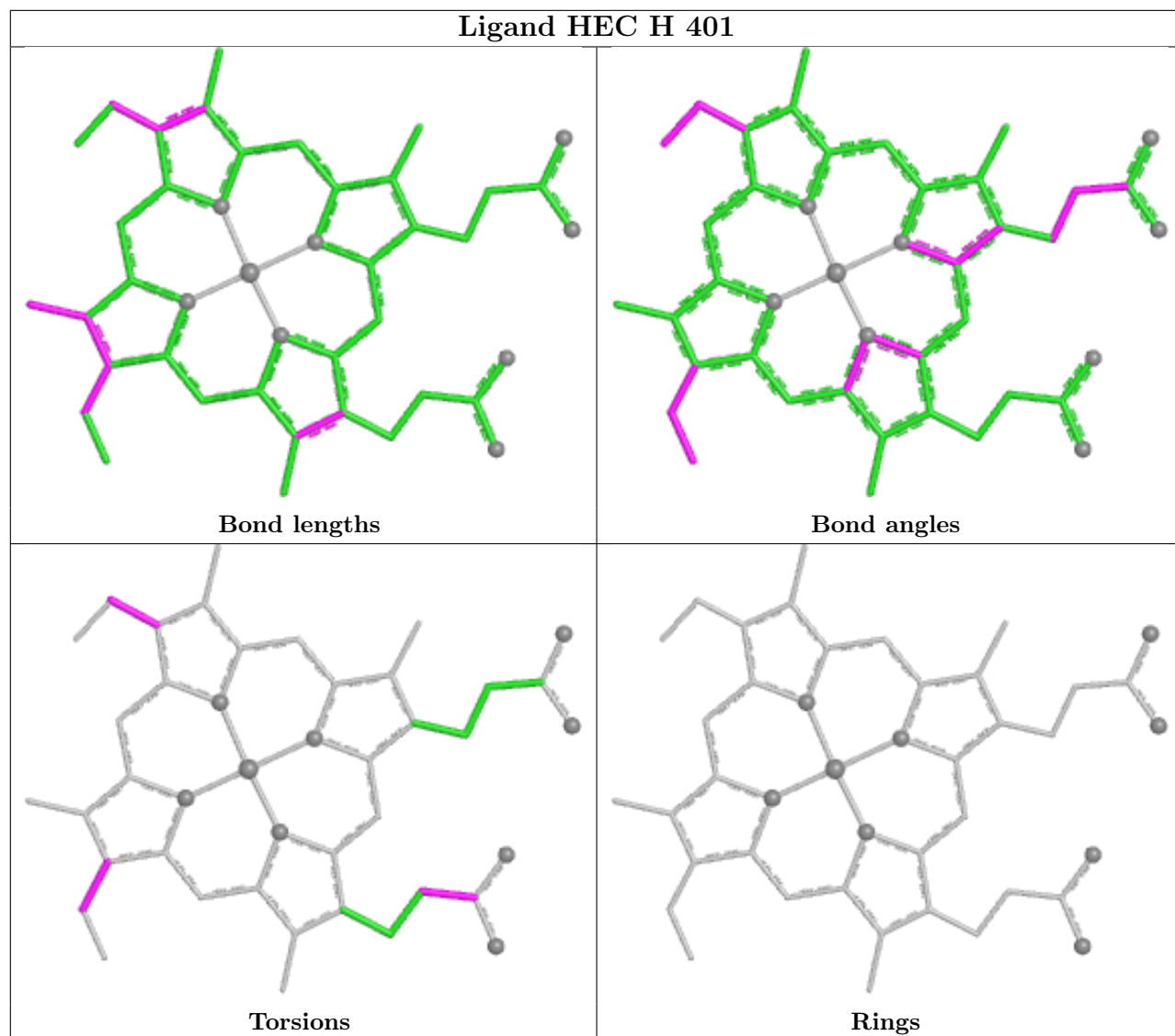
## Ligand 3PE U 401

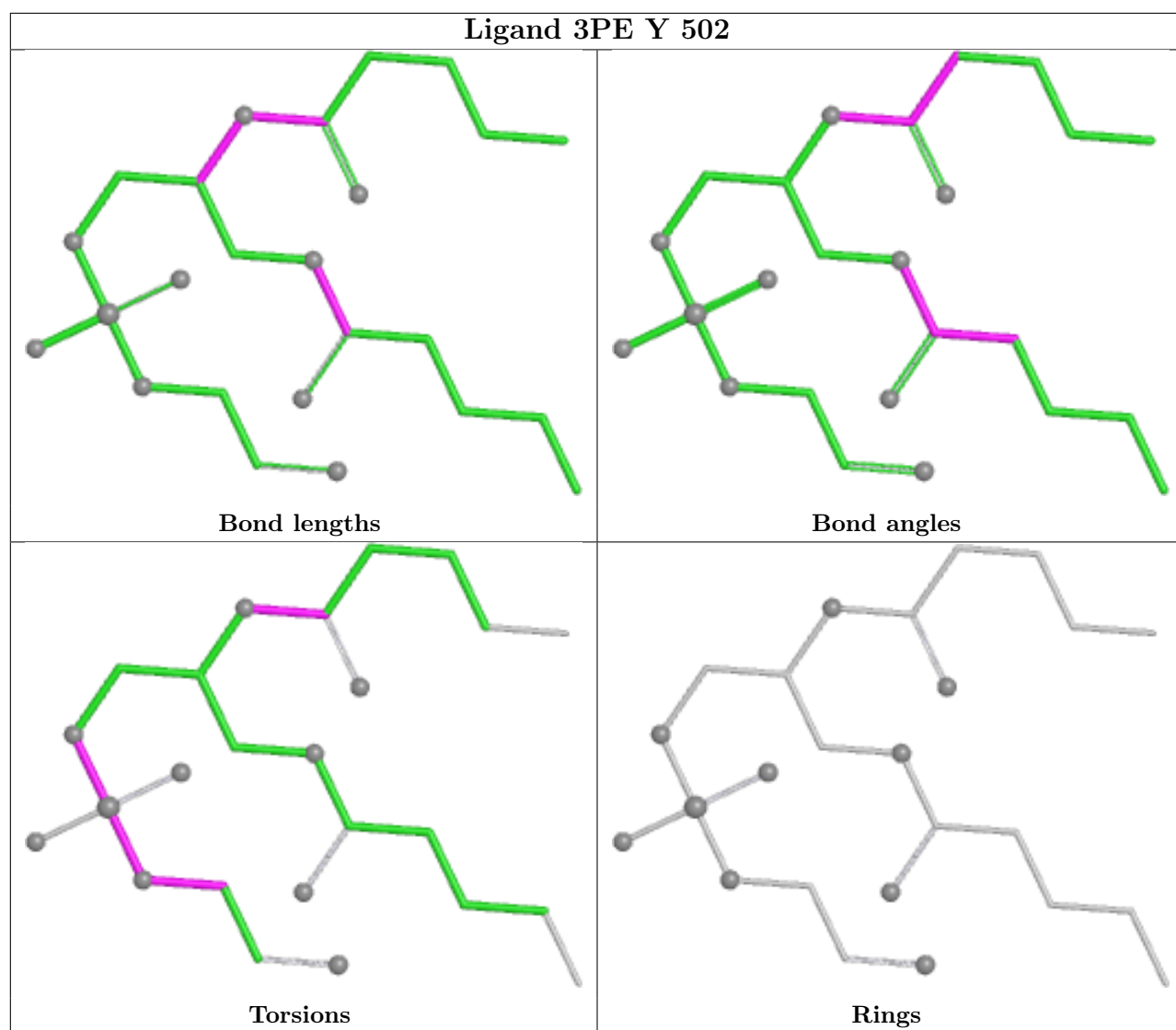


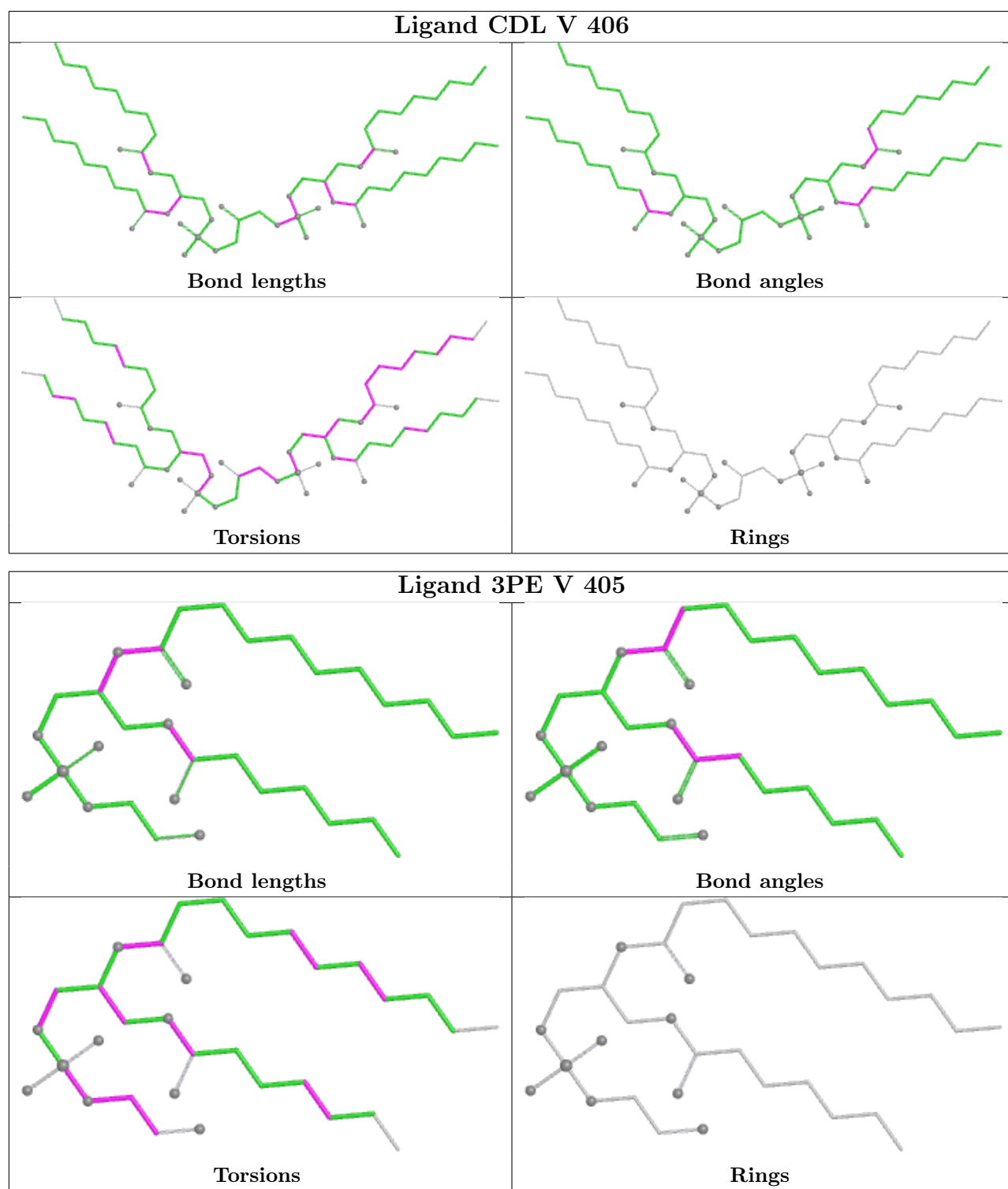


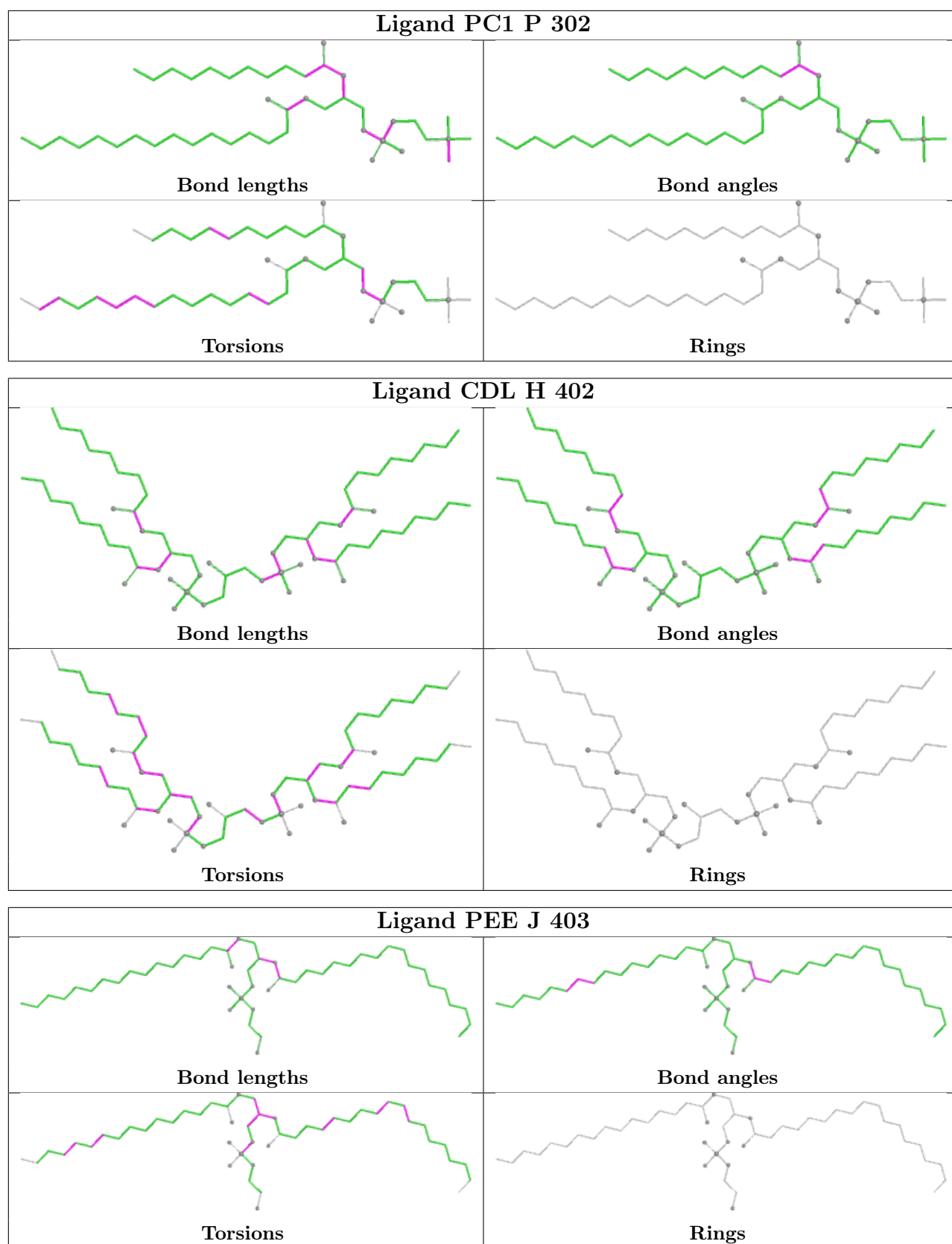




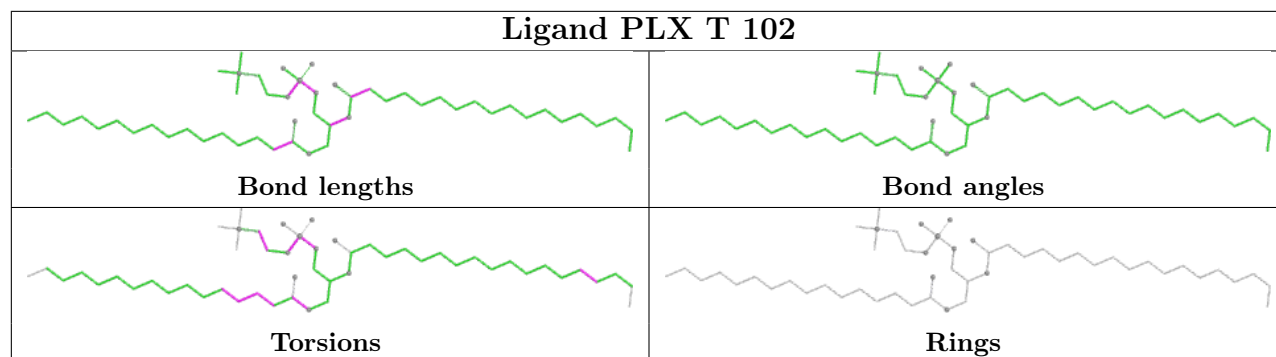




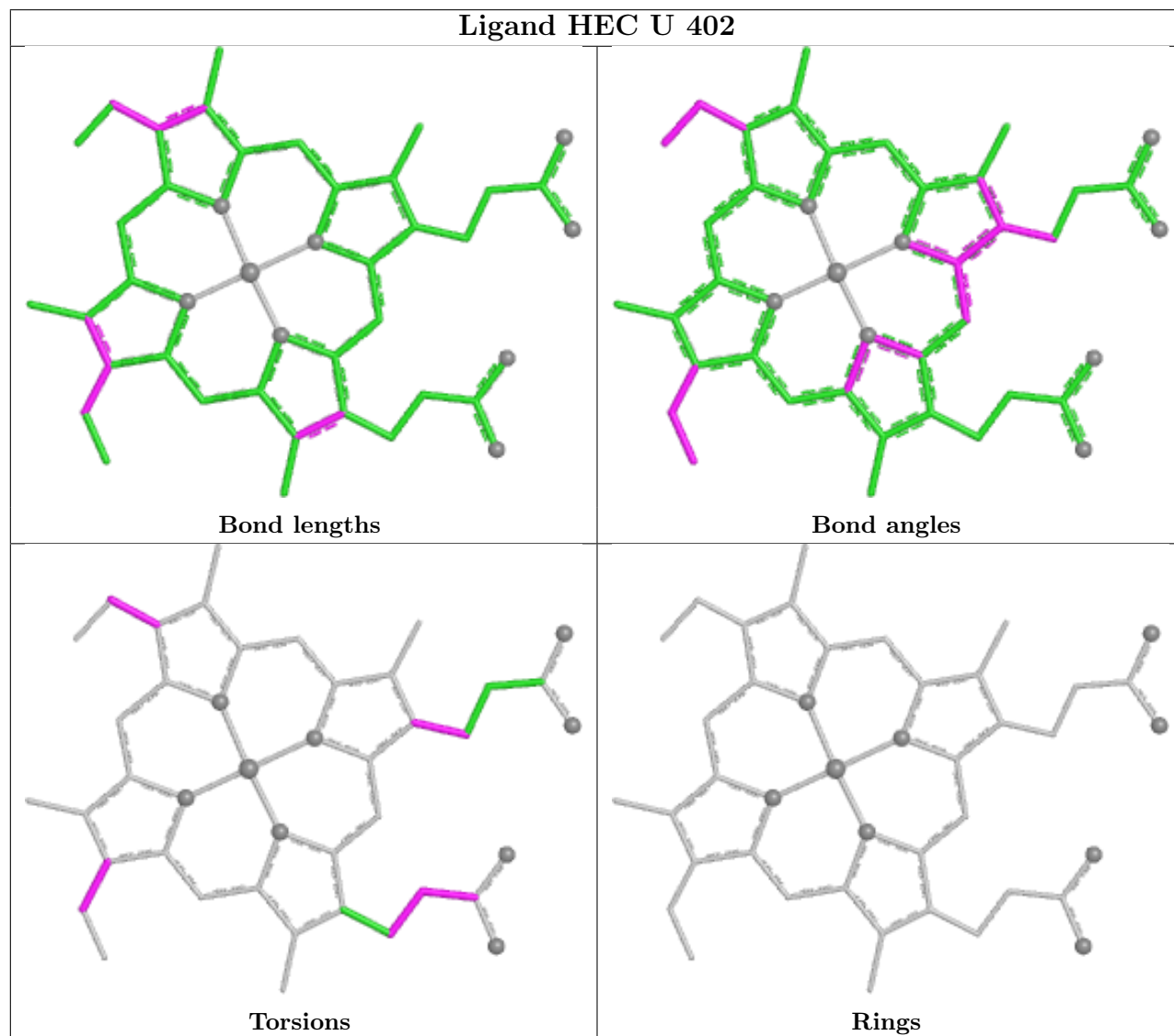


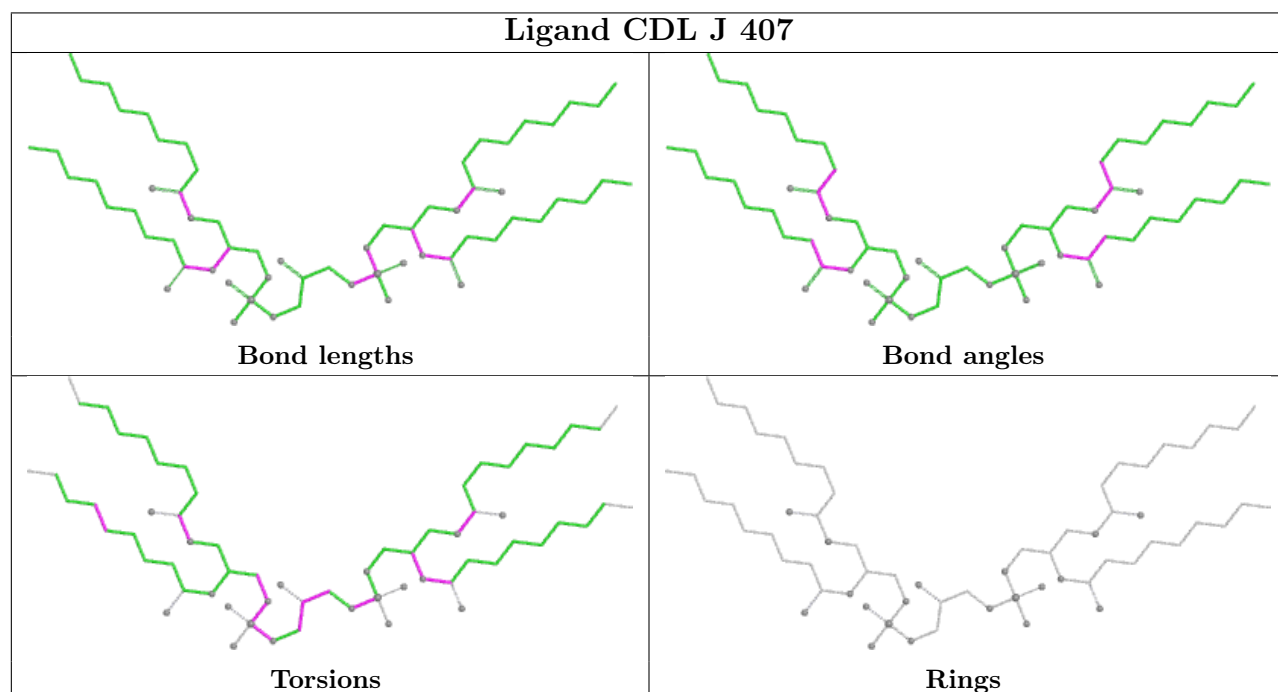
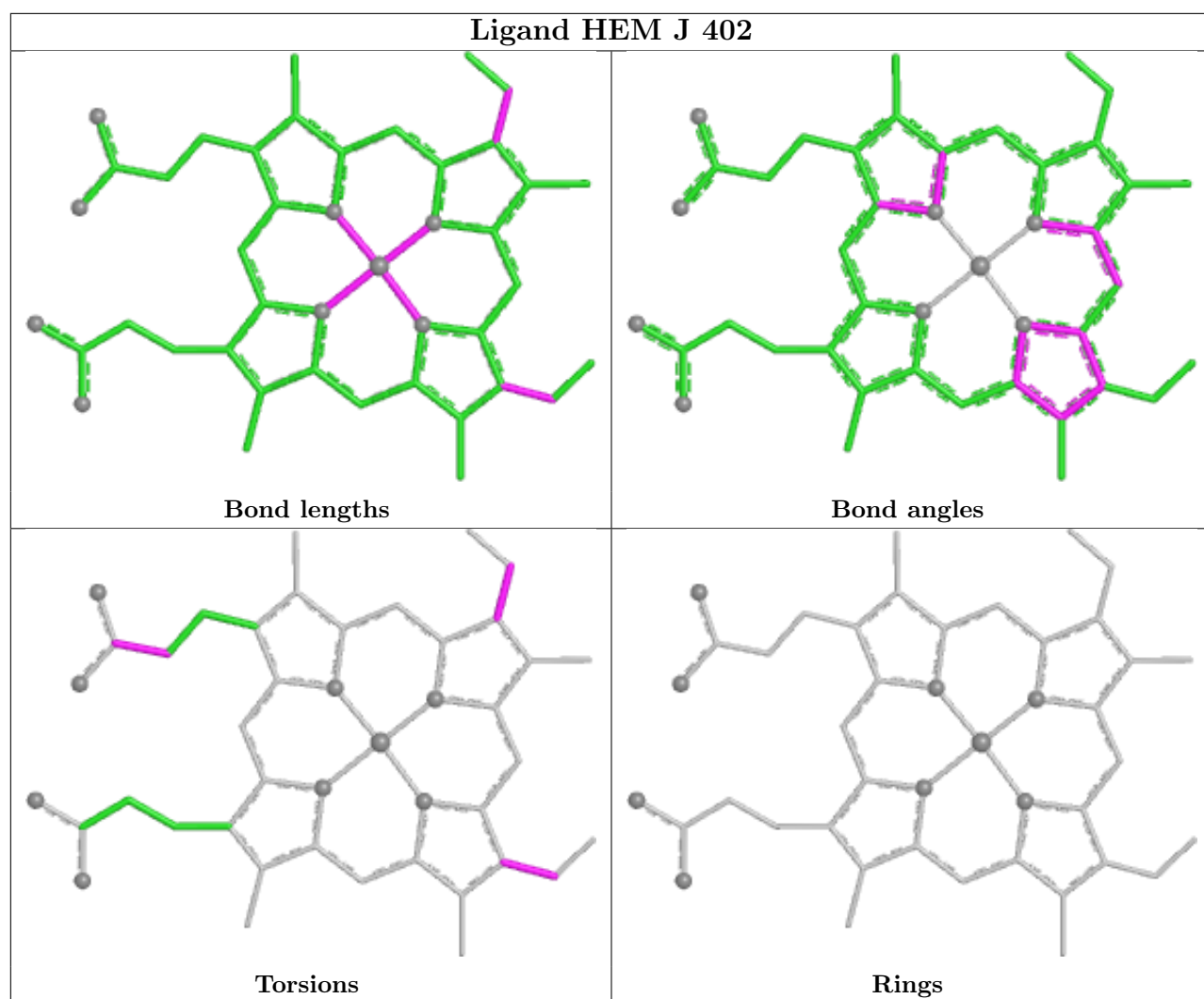


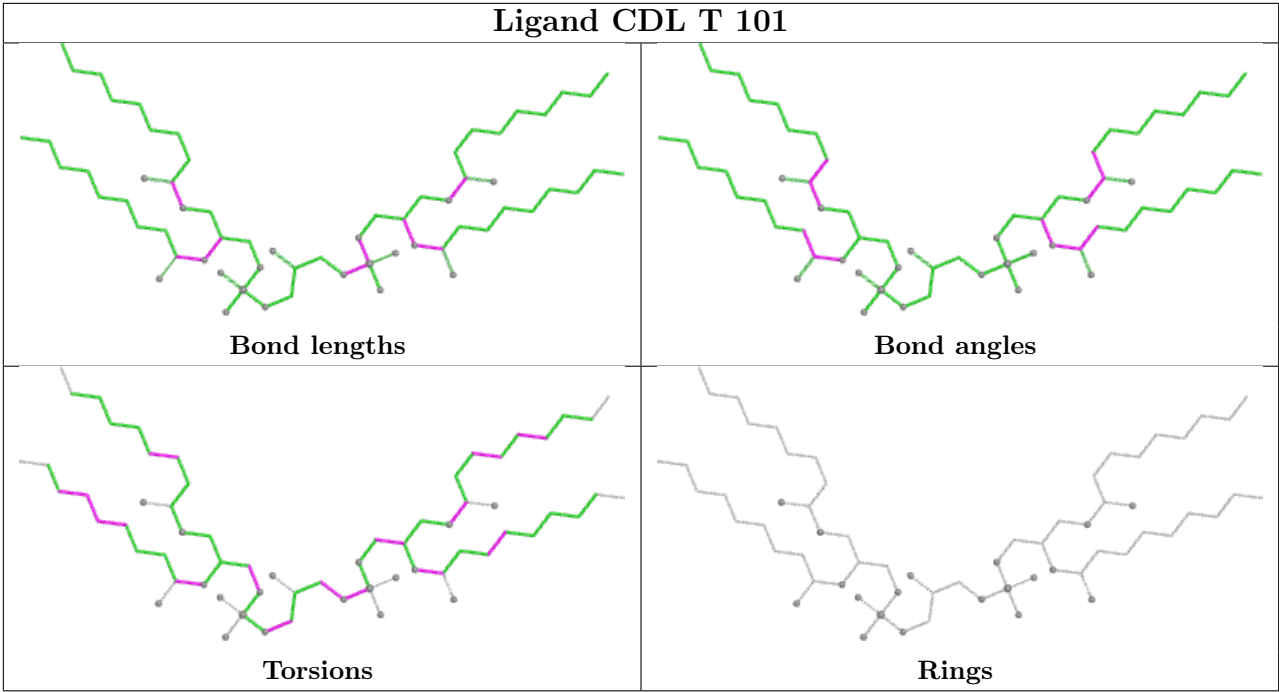
## Ligand PLX T 102



## Ligand HEC U 402







4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	52:PHE	C	57:LYS	N	3.00

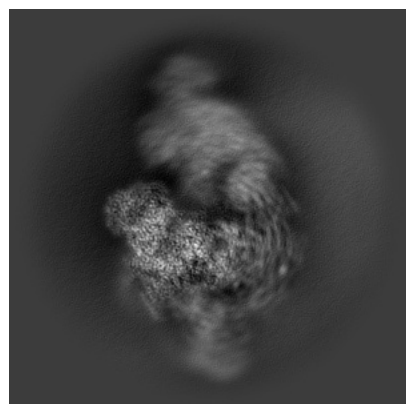
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52525. These allow visual inspection of the internal detail of the map and identification of artifacts.

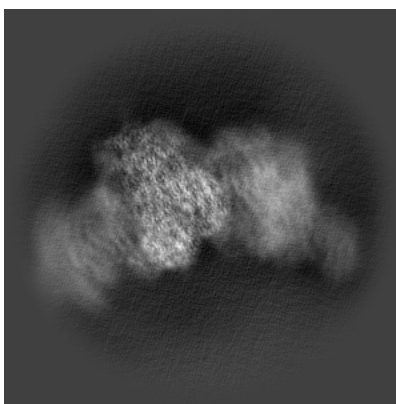
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

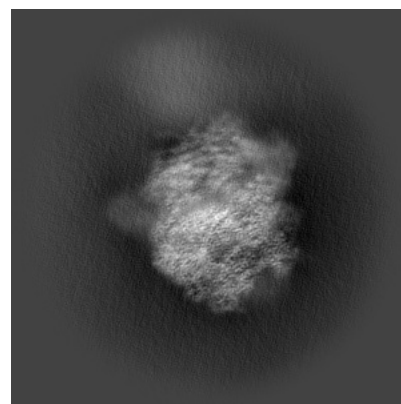
#### 5.1.1 Primary map



X

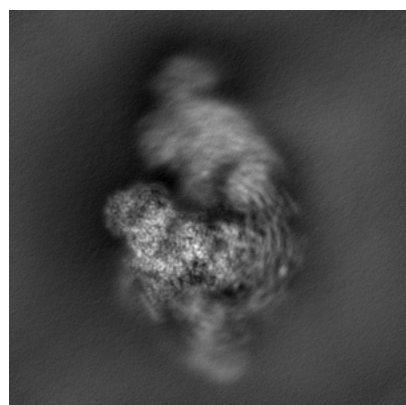


Y

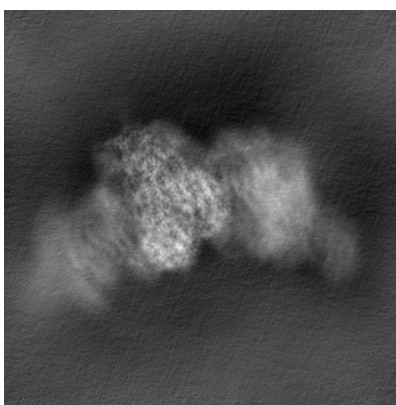


Z

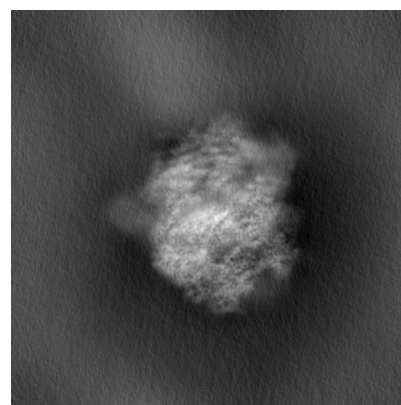
#### 5.1.2 Raw map



X



Y



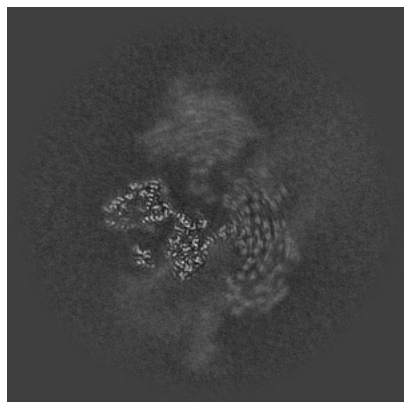
Z

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

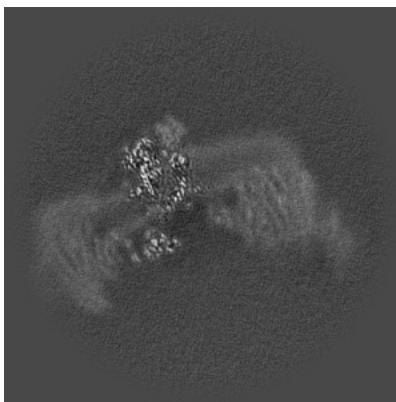


## 5.2 Central slices [i](#)

### 5.2.1 Primary map



X Index: 240

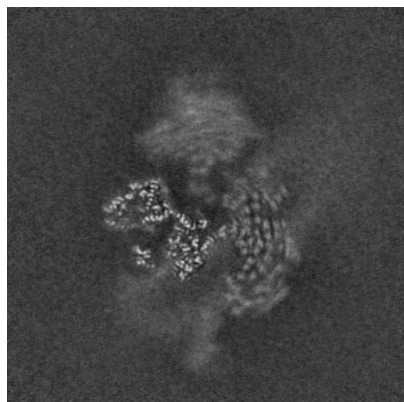


Y Index: 240

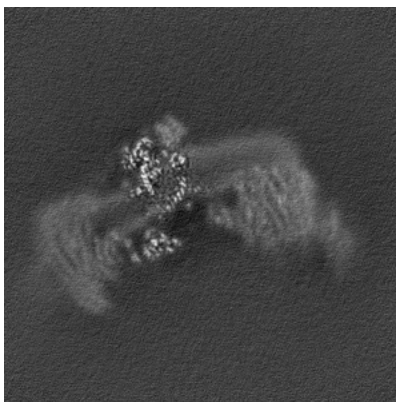


Z Index: 240

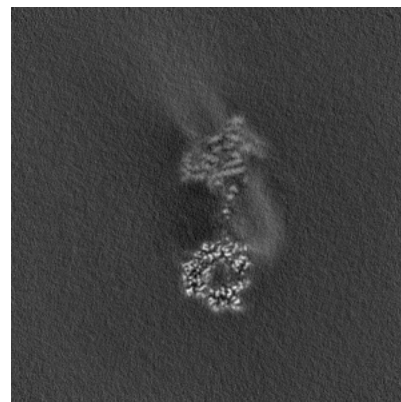
### 5.2.2 Raw map



X Index: 240



Y Index: 240

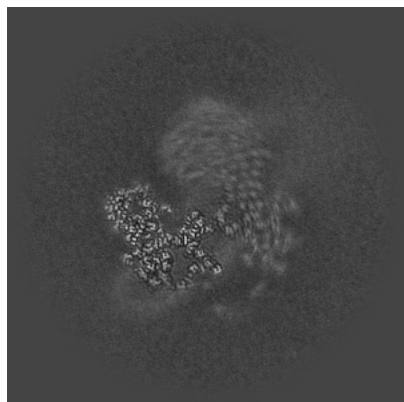


Z Index: 240

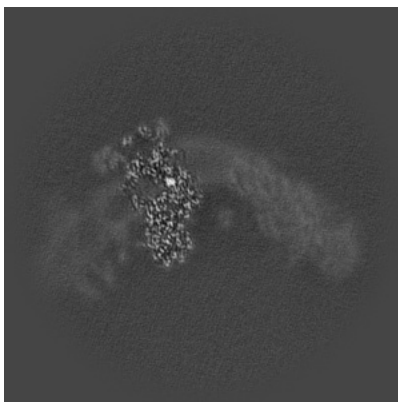
The images above show central slices of the map in three orthogonal directions.

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

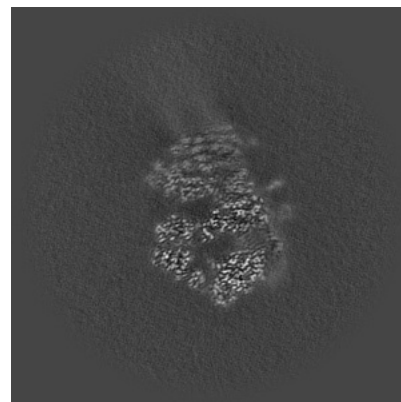
### 5.3.1 Primary map



X Index: 268

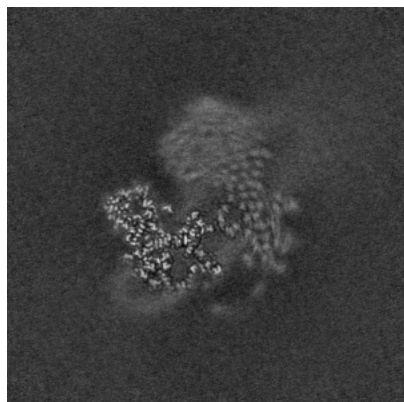


Y Index: 214

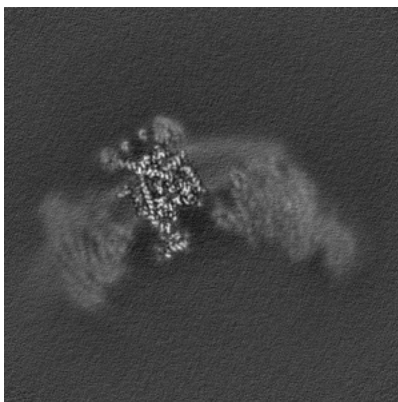


Z Index: 214

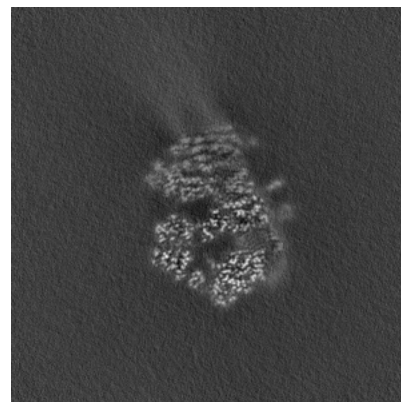
### 5.3.2 Raw map



X Index: 269



Y Index: 227

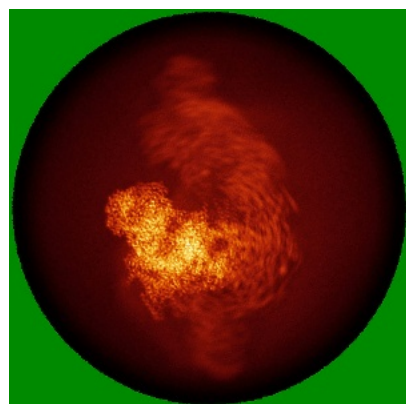


Z Index: 214

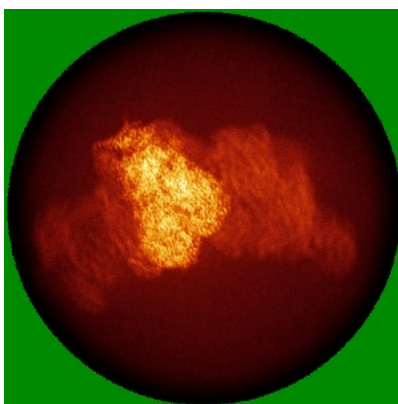
The images above show the largest variance slices of the map in three orthogonal directions.

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

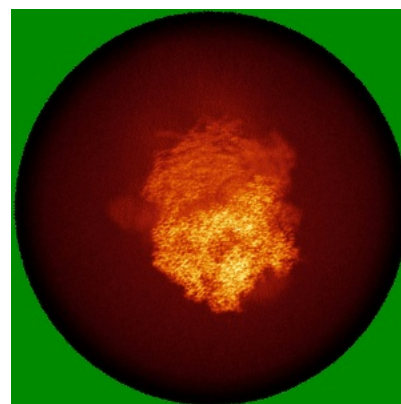
### 5.4.1 Primary map



X

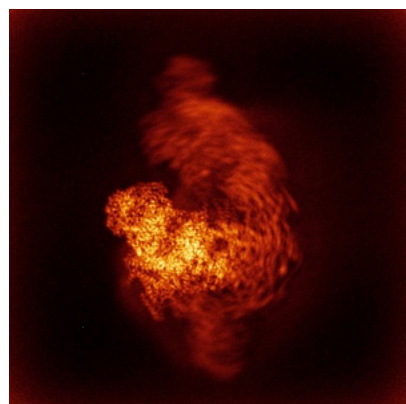


Y

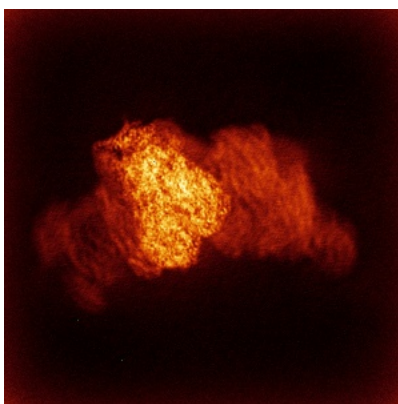


Z

### 5.4.2 Raw map



X



Y



Z

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

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

### 5.5.1 Primary map



X



Y



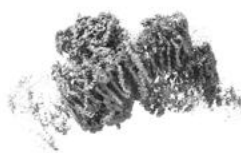
Z

The images above show the 3D surface view of the map at the recommended contour level 4.54. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 5.5.2 Raw map



X



Y



Z

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.

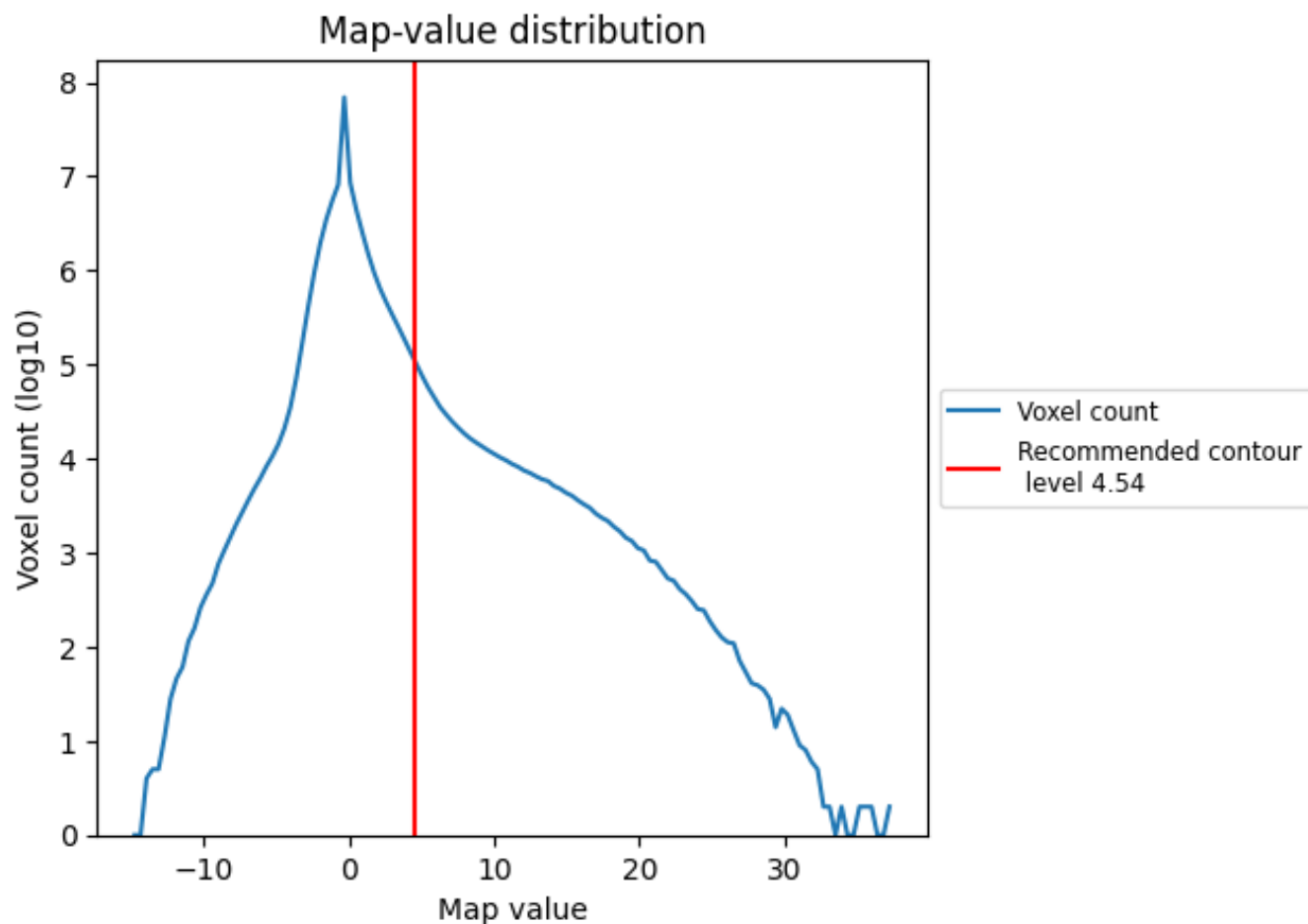
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

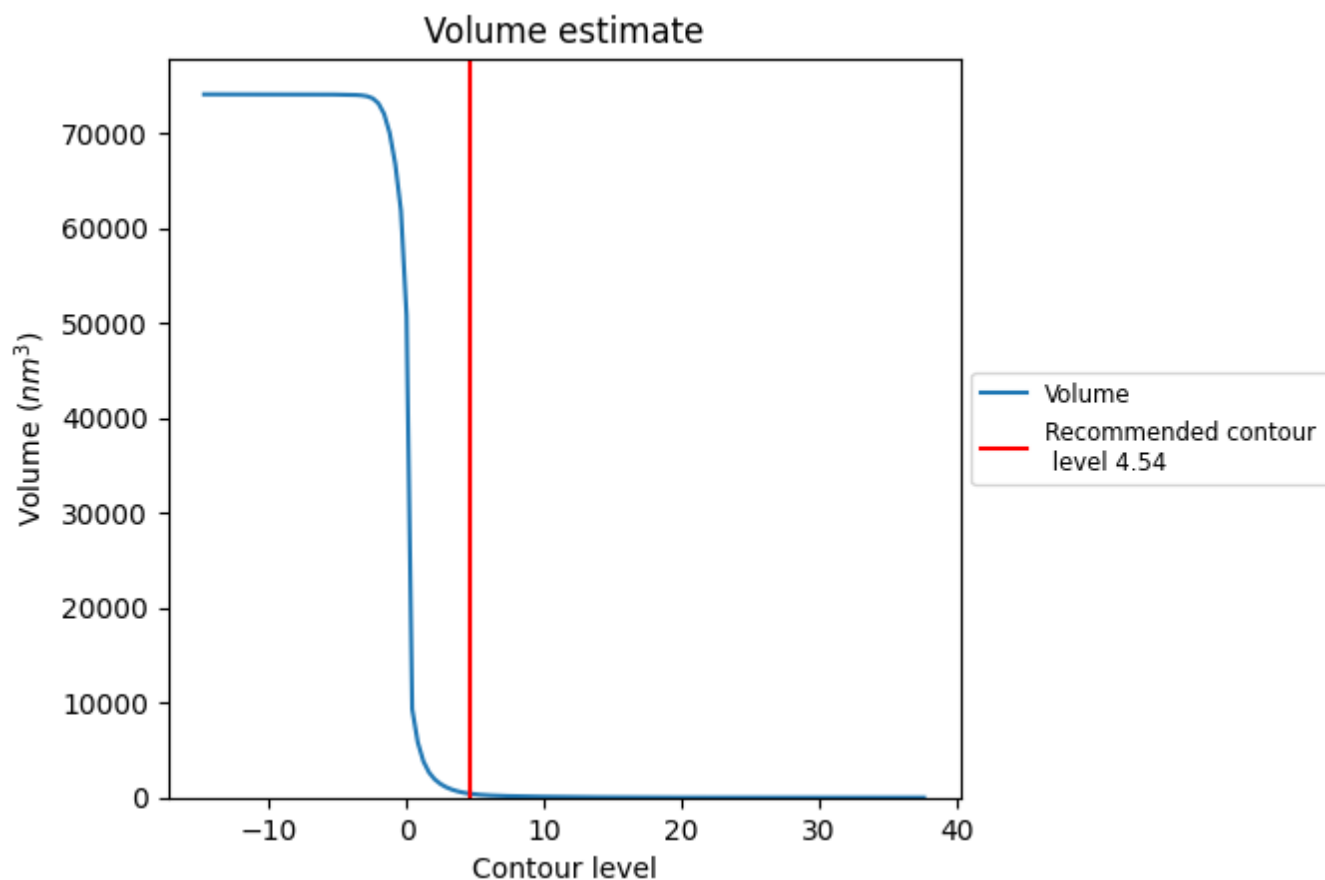
This section contains the results of statistical analysis of the map.

### 6.1 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.

## 6.2 Volume estimate [i](#)

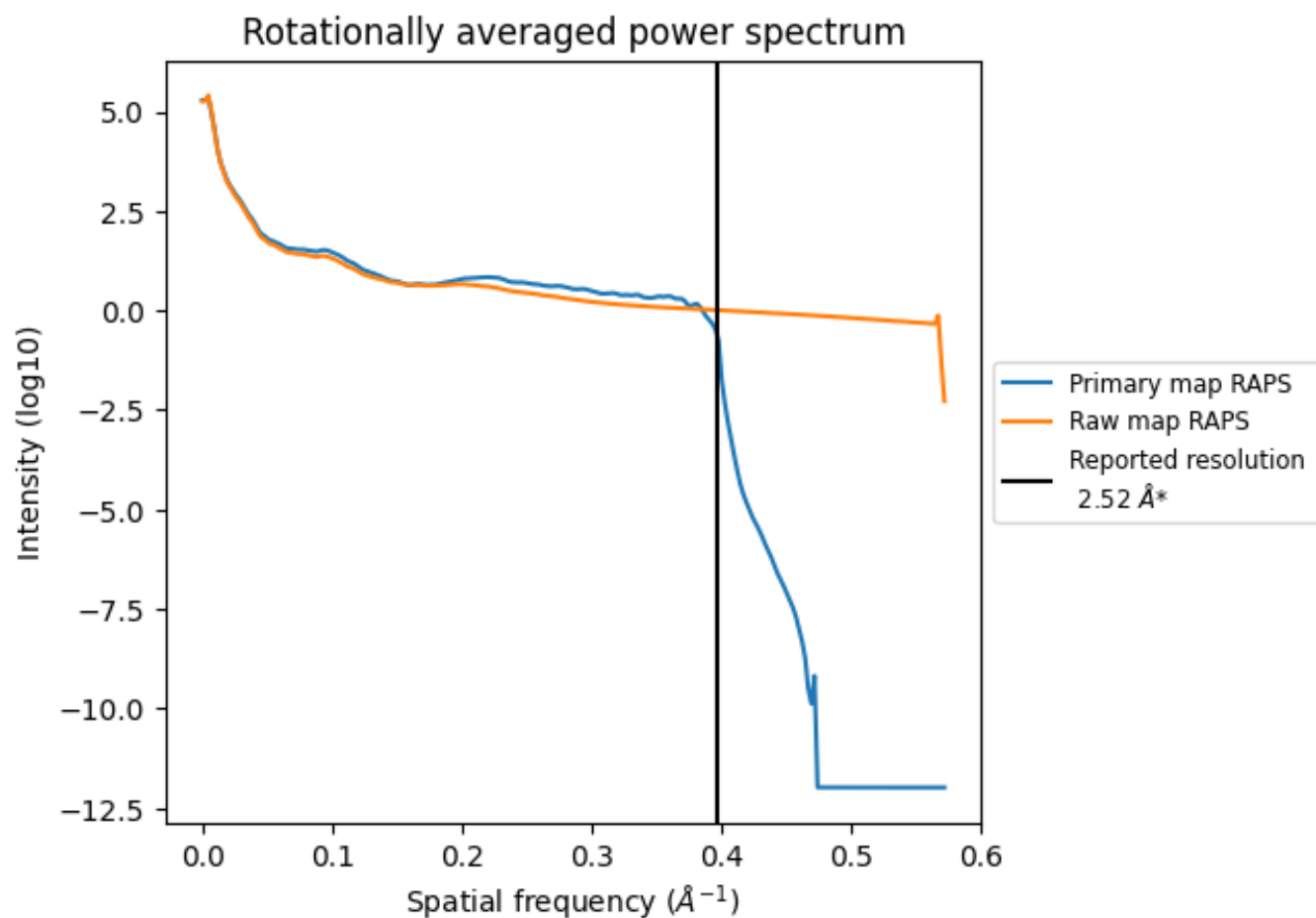


The volume at the recommended contour level is 421  $\text{nm}^3$ ; this corresponds to an approximate mass of 380 kDa.

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.



### 6.3 Rotationally averaged power spectrum ⓘ

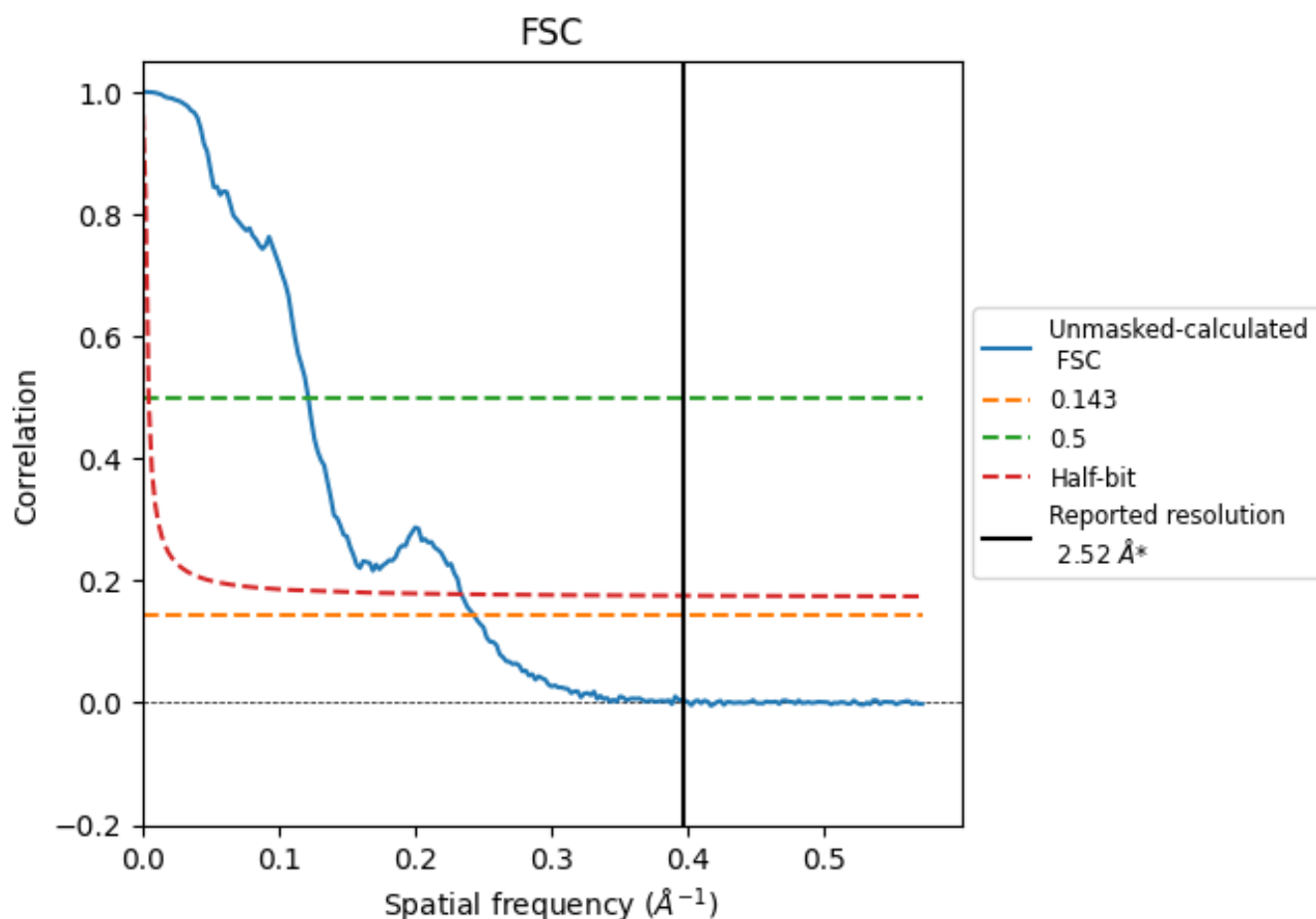


\*Reported resolution corresponds to spatial frequency of 0.397 Å<sup>-1</sup>

## 7 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.

### 7.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.397 Å<sup>-1</sup>



## 7.2 Resolution estimates [i](#)

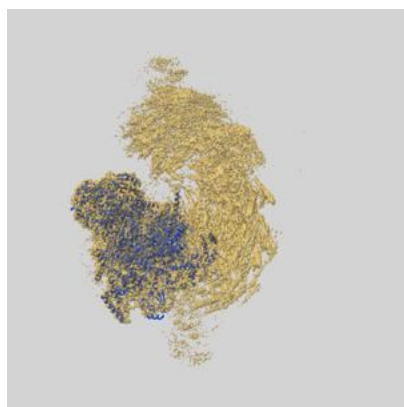
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.11	8.22	4.28

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 2.52 by more than 10 %

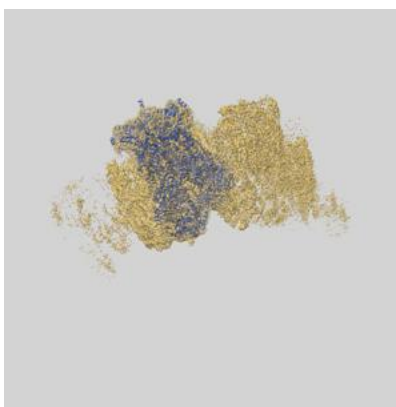
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52525 and PDB model 9HZL. Per-residue inclusion information can be found in section ?? on page ??.

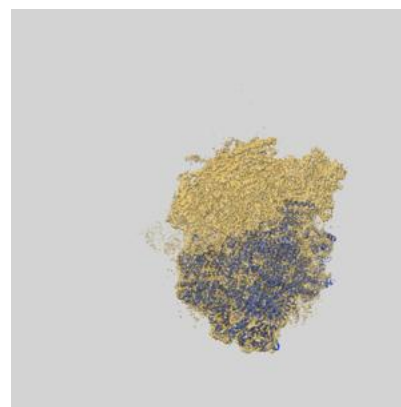
### 8.1 Map-model overlay [i](#)



X



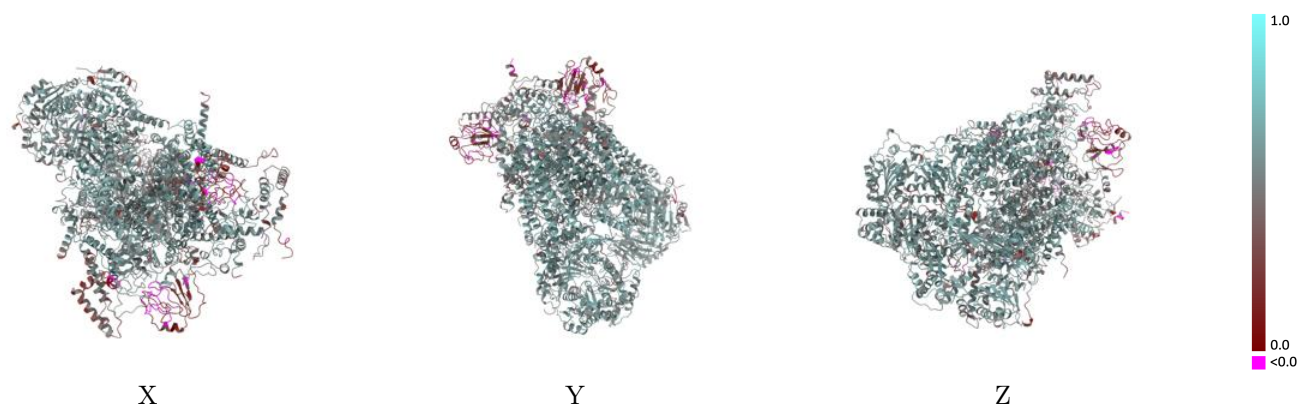
Y



Z

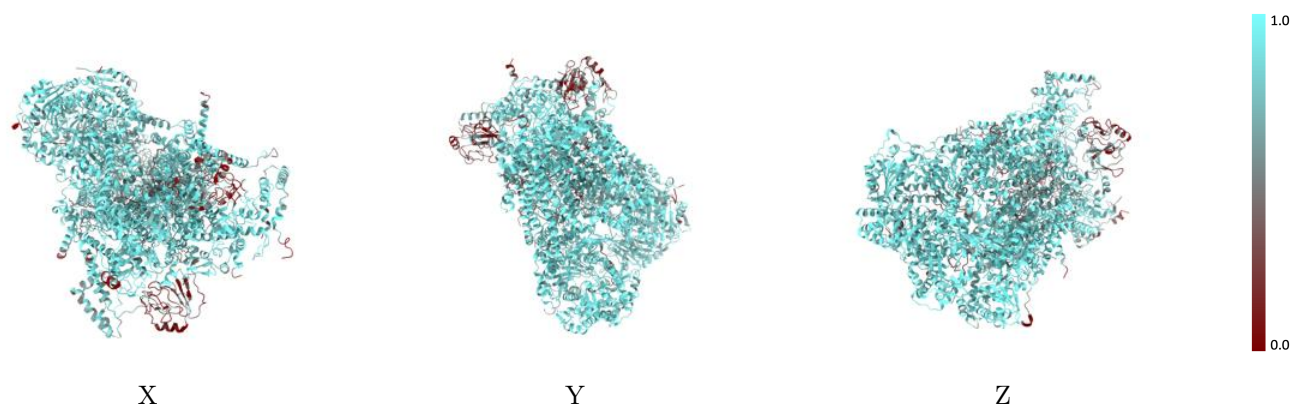
The images above show the 3D surface view of the map at the recommended contour level 4.54 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



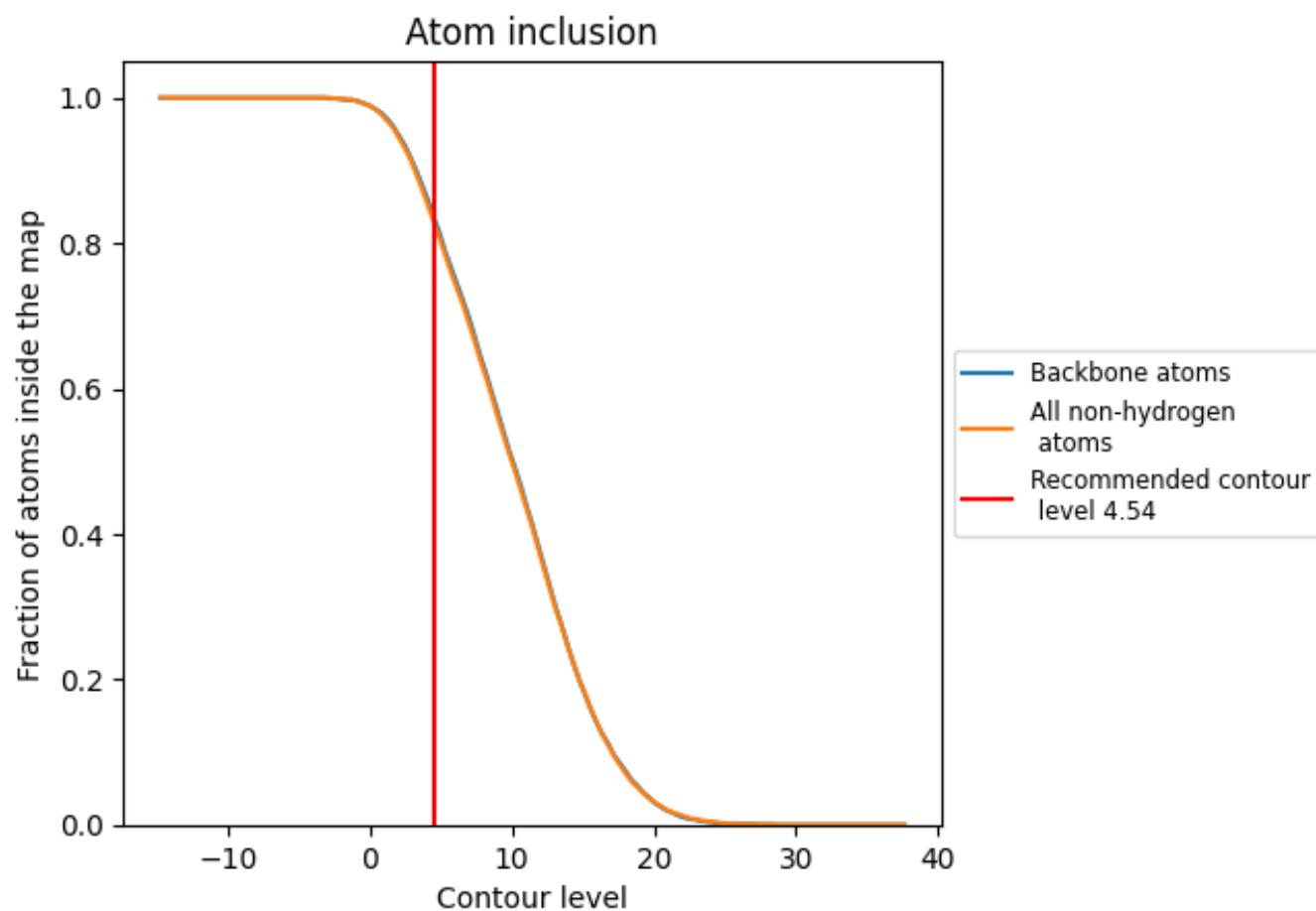
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.54).















































## 8.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

## 8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8260	 0.5250
A	 0.8270	 0.5300
B	 0.4970	 0.3540
C	 0.5170	 0.3110
D	 0.8350	 0.5630
E	 0.7100	 0.4080
F	 0.8640	 0.5740
G	 0.7760	 0.5220
H	 0.8880	 0.5500
J	 0.8770	 0.5760
K	 0.8910	 0.5420
L	 0.9110	 0.5860
N	 0.8550	 0.5210
O	 0.4010	 0.2760
P	 0.5510	 0.3220
Q	 0.8140	 0.5010
R	 0.6720	 0.3410
S	 0.8700	 0.5620
T	 0.7520	 0.4890
U	 0.8610	 0.5420
V	 0.8710	 0.5780
W	 0.8930	 0.5620
Y	 0.8800	 0.5500

