



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 06:03 pm BST

PDB ID : 6YMX / pdb_00006ymx
EMDB ID : EMD-10847
Title : CIII2/CIV respiratory supercomplex from *Saccharomyces cerevisiae*
Authors : Berndtsson, J.; Rathore, S.; Ott, M.
Deposited on : 2020-04-10
Resolution : 3.17 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

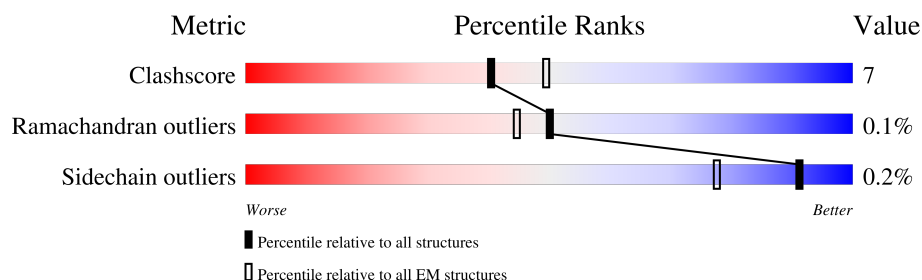
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





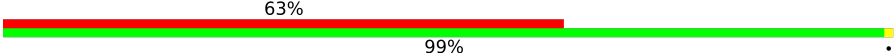
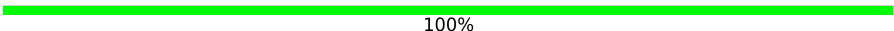




















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	530	100%
2	b	236	100%
3	c	268	6% 100%
4	d	117	10% 99% .
5	e	128	100%
6	f	99	100%
7	g	55	9% 100%
8	h	51	98% .

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Mol	Chain	Length	Quality of chain
9	i	53	 100%
10	j	78	 21% 99%
11	k	114	 63% 99%
12	m	38	 100%
13	A	431	 84% 16%
13	L	431	 89% 11%
14	B	352	 90% 10%
14	M	352	 91% 9%
15	C	385	 87% 13%
15	N	385	 89% 10%
16	D	248	 89% 11%
16	O	248	 88% 12%
17	E	185	 84% 16%
17	P	185	 8% 78% 22%
18	F	74	 85% 15%
19	G	126	 92% 8%
19	R	126	 92% 6%
20	H	93	 92% 8%
20	S	93	 87% 11%
21	I	54	 93% 7%
22	Q	75	 91% 9%
23	T	54	 87% 13%
24	U	44	 91% 9%
25	V	51	 84% 16%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	PTY	D	402	-	-	X	-
40	FES	P	301	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 47034 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	530	Total	C	N	O	S	0	0
			4126	2757	641	707	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	236	Total	C	N	O	S	0	0
			1888	1242	286	350	10		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	268	Total	C	N	O	S	0	0
			2138	1425	343	356	14		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	117	Total	C	N	O	S	0	0
			888	559	147	177	5		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	128	Total	C	N	O	S	0	0
			1008	639	175	190	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	99	Total	C	N	O	S	0	0
			828	533	134	160	1		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	g	55	Total	C	N	O	0	0
			456	310	77	69		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	51	Total	C	N	O	S	0	0
			408	278	66	63	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	53	Total	C	N	O	S	0	0
			439	290	76	70	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	78	Total	C	N	O	S	0	0
			649	414	111	119	5		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	114	Total	C	N	O	S	0	0
			941	608	163	167	3		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	38	Total	C	N	O	S	0	0
			308	207	49	51	1		

- Molecule 13 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		
13	L	431	Total	C	N	O	S	0	0
			3344	2110	576	652	6		

- Molecule 14 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
14	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 15 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
15	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 16 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		
16	O	248	Total	C	N	O	S	0	0
			1961	1249	340	363	9		

- Molecule 17 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
17	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 18 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	74	Total	C	N	O	S	0	0
			624	391	108	123	2		

- Molecule 19 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 20 is a protein called Cytochrome b-c1 complex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
20	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 21 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	I	54	Total	C	N	O	0	0
			442	295	74	73		

- Molecule 22 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 23 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	54	Total	C	N	O	0	0
			443	295	74	74		

- Molecule 24 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	44	Total	C	N	O	S	0	0
			347	230	58	57	2		

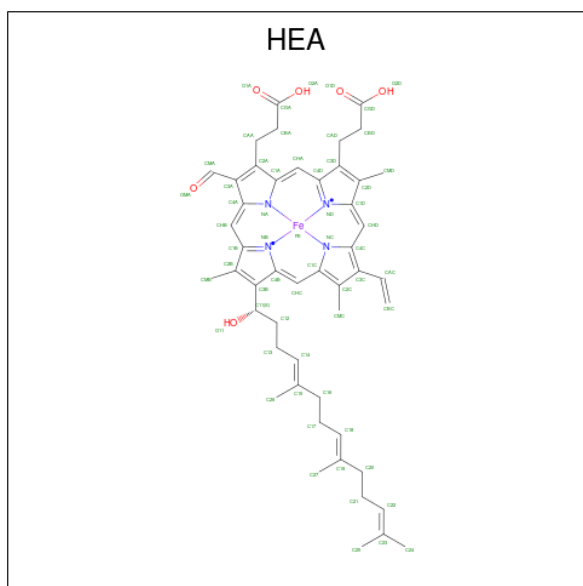
- Molecule 25 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	51	Total	C	N	O	S	0	0
			406	272	66	66	2		

- Molecule 26 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

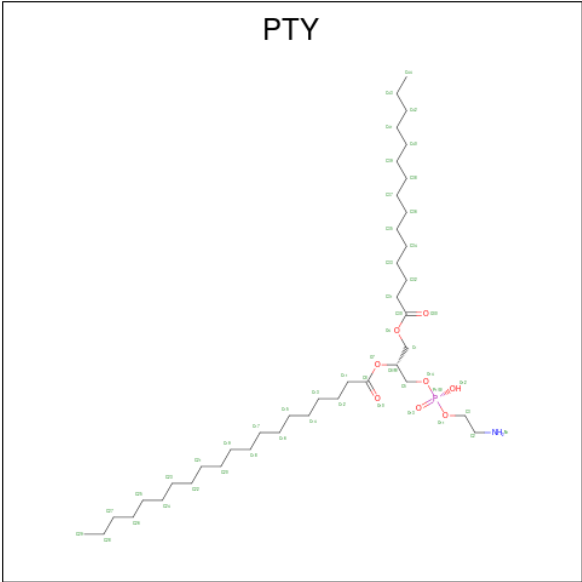
Mol	Chain	Residues	Atoms		AltConf
26	a	1	Total	Cu	0
			1	1	

- Molecule 27 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



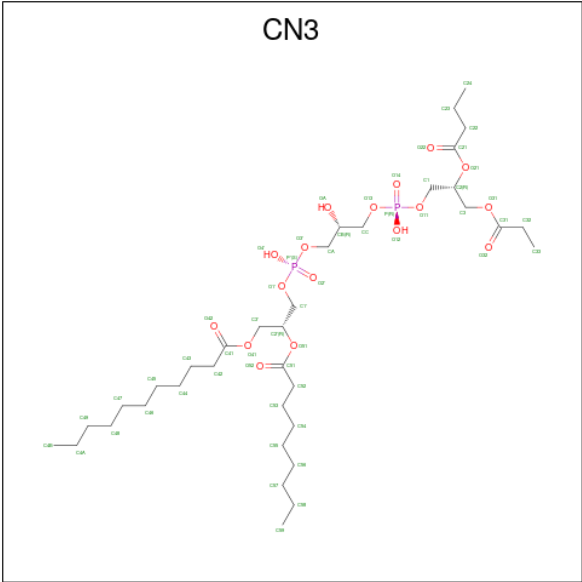
Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
27	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 28 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).



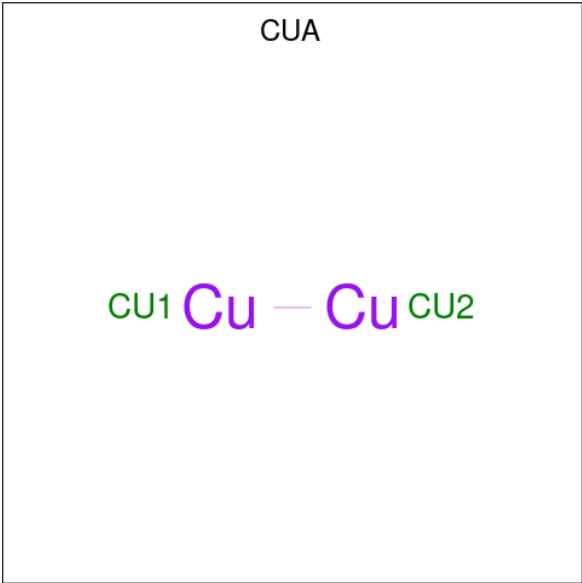
Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total	C	N	O	P	0
			34	24	1	8	1	
28	b	1	Total	C	N	O	P	0
			35	25	1	8	1	
28	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
28	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
28	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
28	m	1	Total	C	N	O	P	0
			30	20	1	8	1	
28	D	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 29 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanonadec-1-yl undecanoate (CCD ID: CN3) (formula: C₃₆H₆₈O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	C	O	P	0
			55	36	17	2	
29	N	1	Total	C	O	P	0
			55	36	17	2	

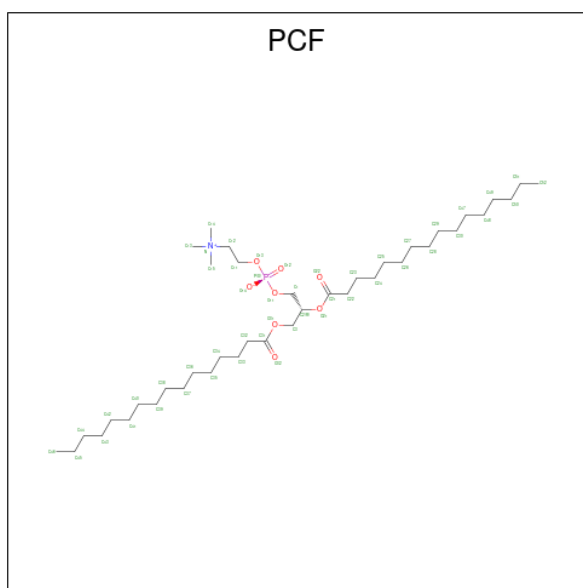
- Molecule 30 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 31 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF)

(formula: C₄₀H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).

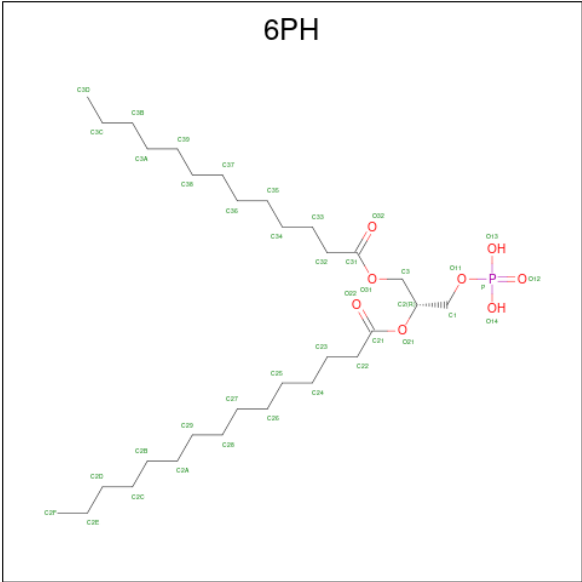


Mol	Chain	Residues	Atoms					AltConf
31	c	1	Total	C	N	O	P	0
			43	33	1	8	1	
31	e	1	Total	C	N	O	P	0
			36	26	1	8	1	
31	m	1	Total	C	N	O	P	0
			38	28	1	8	1	
31	I	1	Total	C	N	O	P	0
			35	25	1	8	1	
31	T	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

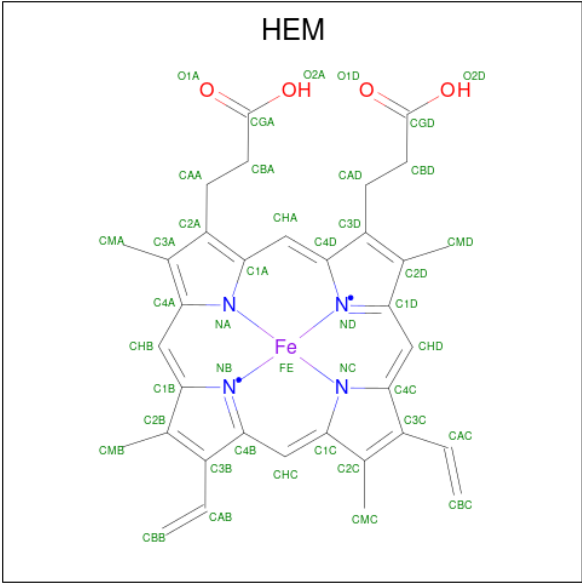
Mol	Chain	Residues	Atoms		AltConf
32	d	1	Total	Zn	0
			1	1	

- Molecule 33 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: C₃₁H₆₁O₈P).



Mol	Chain	Residues	Atoms				AltConf
33	C	1	Total	C	O	P	0
			40	31	8	1	
33	O	1	Total	C	O	P	0
			40	31	8	1	

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



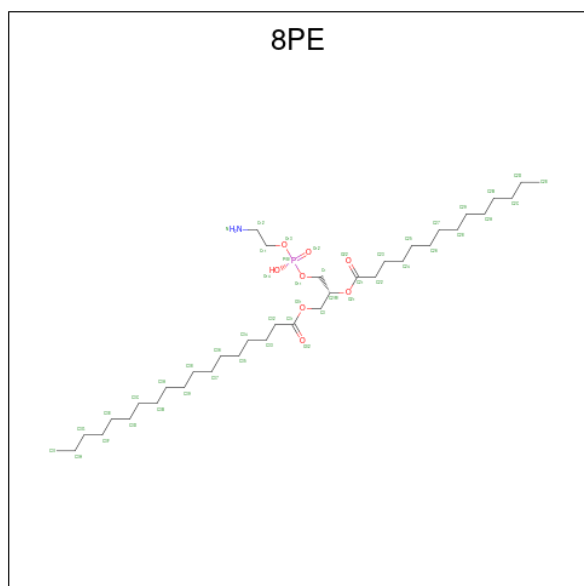
Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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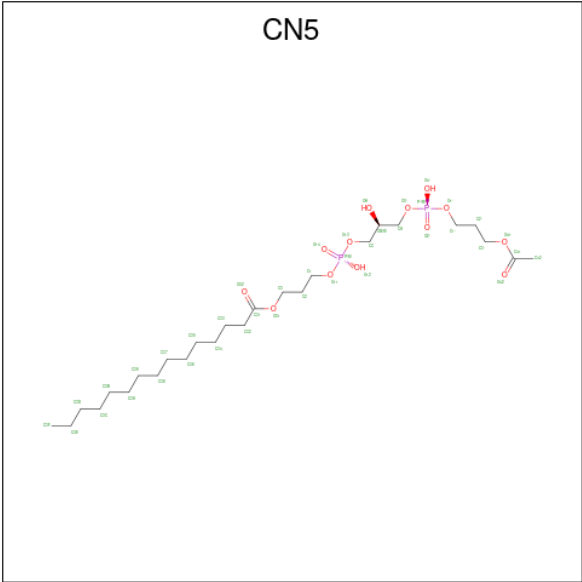
Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
34	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 35 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: $C_{37}H_{74}NO_8P$).



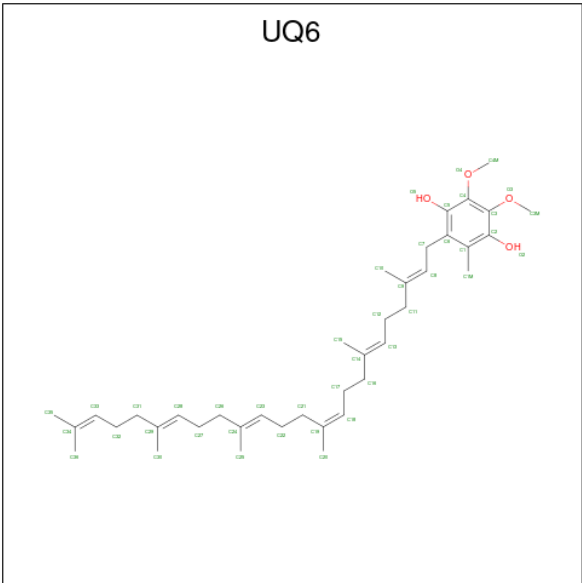
Mol	Chain	Residues	Atoms					AltConf
35	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
35	N	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 36 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-di phosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



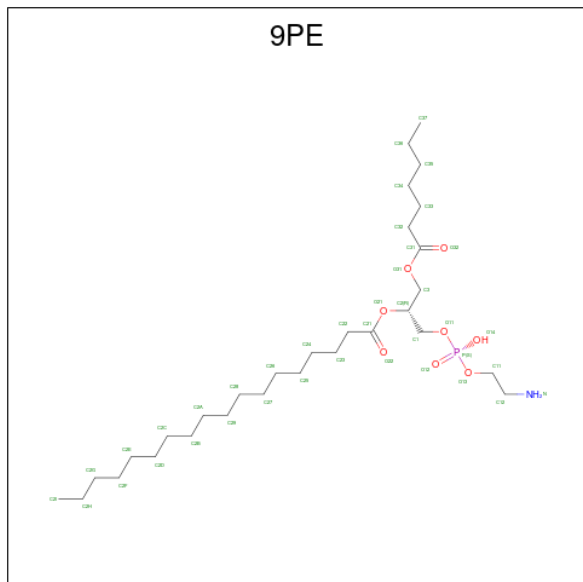
Mol	Chain	Residues	Atoms				AltConf
36	C	1	Total	C	O	P	0
			41	26	13	2	

- Molecule 37 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXA ENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: C₃₉H₆₀O₄).



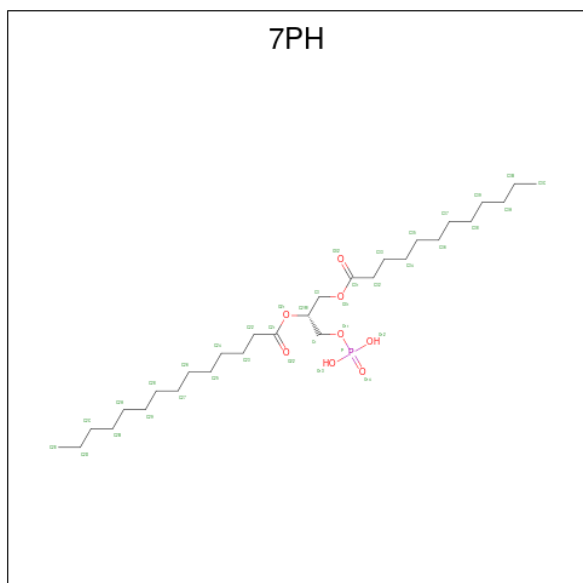
Mol	Chain	Residues	Atoms				AltConf
37	C	1	Total	C	O		0
			43	39	4		
37	N	1	Total	C	O		0
			43	39	4		

- Molecule 38 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: $C_{30}H_{60}NO_8P$).



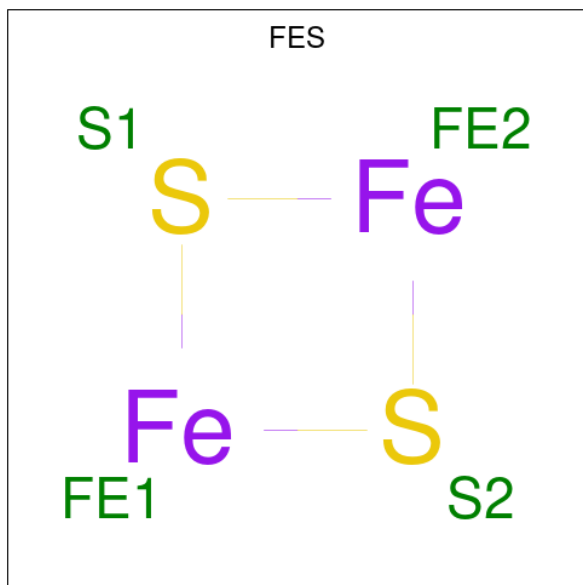
Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			40	30	1	8	1	
38	N	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 39 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: $C_{29}H_{57}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
39	E	1	Total	C	O	P	0
			38	29	8	1	
39	O	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

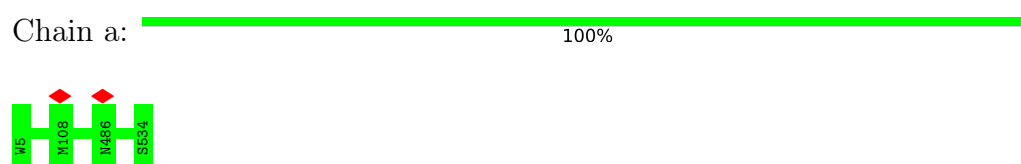


Mol	Chain	Residues	Atoms			AltConf
40	E	1	Total	Fe	S	0
			4	2	2	
40	P	1	Total	Fe	S	0
			4	2	2	

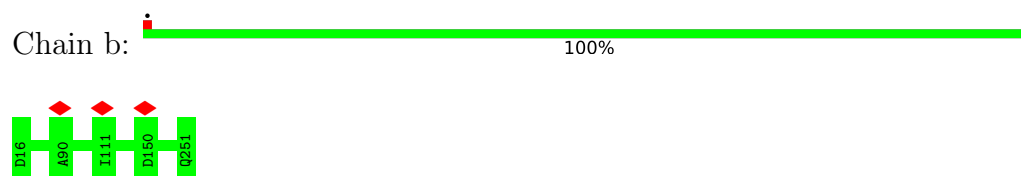
3 Residue-property plots

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

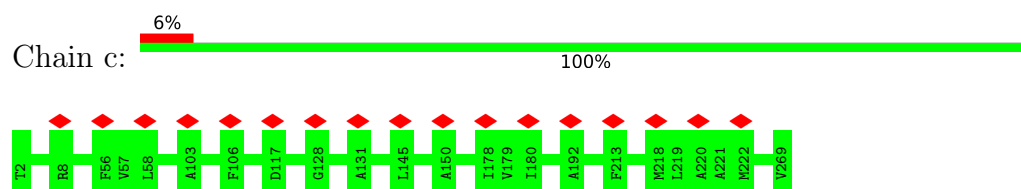
- Molecule 1: Cytochrome c oxidase subunit 1



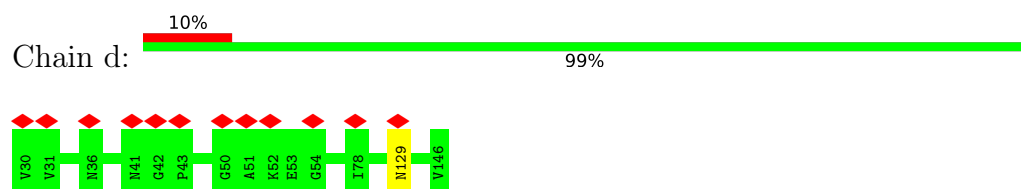
- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3



- Molecule 4: Cytochrome c oxidase subunit 4, mitochondrial



- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



There are no outlier residues recorded for this chain.

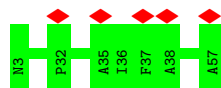
- Molecule 6: Cytochrome c oxidase subunit 6, mitochondrial

Chain f:  100%

There are no outlier residues recorded for this chain.

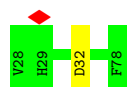
- Molecule 7: Cytochrome c oxidase subunit 7, mitochondrial

Chain g:  9% 100%



- Molecule 8: Cytochrome c oxidase subunit 8, mitochondrial

Chain h:  98%



- Molecule 9: Cytochrome c oxidase subunit 9, mitochondrial

Chain i:  100%

There are no outlier residues recorded for this chain.

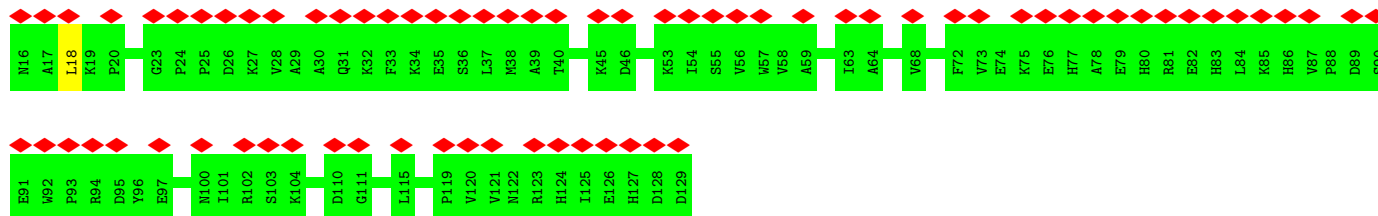
- Molecule 10: Cytochrome c oxidase subunit 12, mitochondrial

Chain j:  21% 99%



- Molecule 11: Cytochrome c oxidase subunit 13, mitochondrial

Chain k:  63% 99%




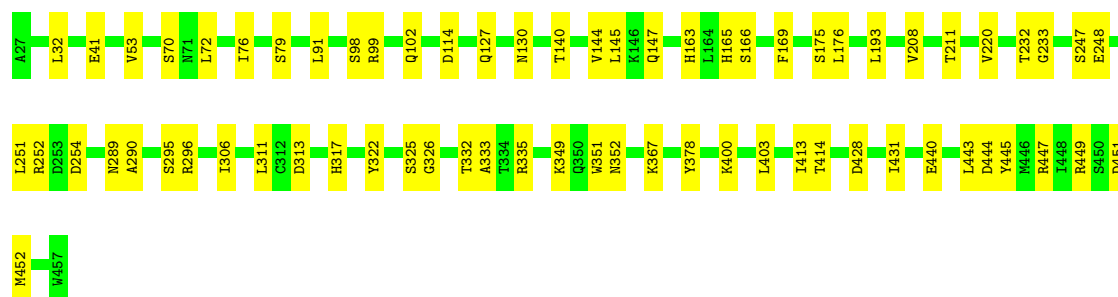
- Molecule 12: Cytochrome c oxidase subunit 26, mitochondrial

Chain m:  100%


There are no outlier residues recorded for this chain.

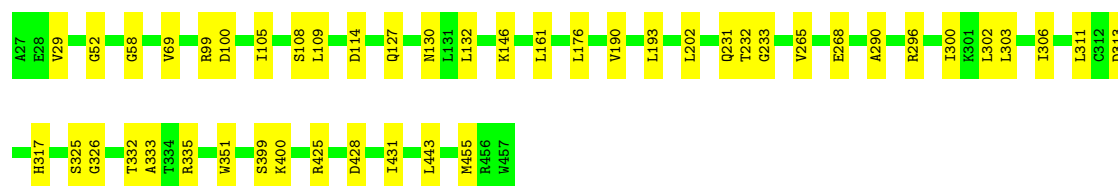
- Molecule 13: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:  84% 16%




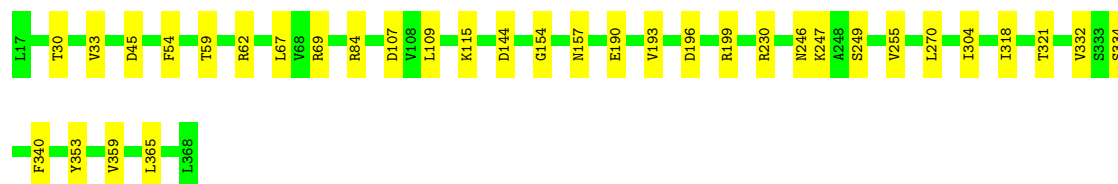
- Molecule 13: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:  89% 11%



- Molecule 14: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  90% 10%




- Molecule 14: Cytochrome b-c1 complex subunit 2, mitochondrial

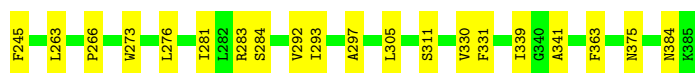
Chain M:  91% 9%



- Molecule 15: Cytochrome b

Chain C:  87% 13%





- Molecule 15: Cytochrome b

Chain N: 89% 10%



- Molecule 16: Cytochrome c1, heme protein, mitochondrial

Chain D: 89% 11%



- Molecule 16: Cytochrome c1, heme protein, mitochondrial

Chain O: 88% 12%



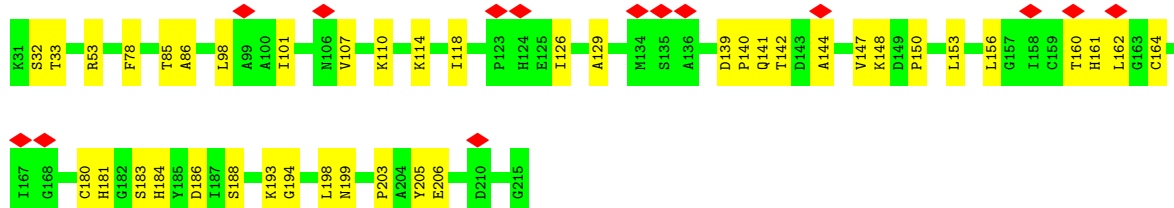
- Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 84% 16%




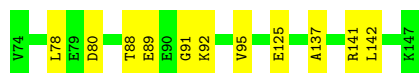
- Molecule 17: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P: 8% 78% 22%



- Molecule 18: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain F:  85% 15%



- Molecule 19: Cytochrome b-c1 complex subunit 7, mitochondrial

Chain G:  92% 8%



- Molecule 19: Cytochrome b-c1 complex subunit 7, mitochondrial

Chain R:  92% 6% .



- Molecule 20: Cytochrome b-c1 complex subunit 8, mitochondrial

Chain H:  92% 8%



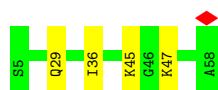
- Molecule 20: Cytochrome b-c1 complex subunit 8, mitochondrial

Chain S:  87% 11% .



- Molecule 21: Cytochrome b-c1 complex subunit 9, mitochondrial

Chain I:  93% 7%

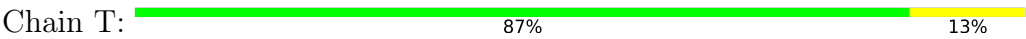


- Molecule 22: Cytochrome b-c1 complex subunit 6, mitochondrial

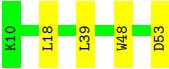
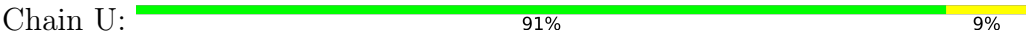
Chain Q:  91% 9%



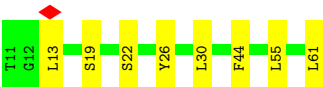
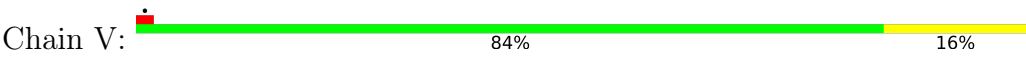
- Molecule 23: Cytochrome b-c1 complex subunit 9, mitochondrial



● Molecule 24: Cytochrome b-c1 complex subunit 10, mitochondrial



● Molecule 25: 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	201223	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-1.4	Depositor
Maximum defocus (nm)	-3.0	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.373	Depositor
Minimum map value	-1.240	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	392.2, 392.2, 392.2	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0600001, 1.0600001, 1.0600001	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, 9PE, 8PE, FES, CU, HEM, ZN, PCF, 7PH, HEA, UQ6, CN5, CN3, 6PH, CUA

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	0.36	0/4254	0.57	0/5811
2	b	0.32	0/1940	0.56	0/2653
3	c	0.28	0/2210	0.52	0/3026
4	d	0.32	0/905	0.61	0/1231
5	e	0.39	0/1032	0.56	0/1396
6	f	0.32	0/845	0.55	0/1143
7	g	0.28	0/472	0.53	0/645
8	h	0.33	0/423	0.58	0/569
9	i	0.30	0/451	0.42	0/605
10	j	0.28	0/671	0.56	1/910 (0.1%)
11	k	0.30	0/974	0.55	1/1324 (0.1%)
12	m	0.31	0/319	0.56	0/435
13	A	0.47	0/3405	0.57	1/4615 (0.0%)
13	L	0.46	0/3405	0.55	0/4615
14	B	0.49	0/2781	0.55	0/3764
14	M	0.47	0/2781	0.55	0/3764
15	C	0.55	0/3192	0.55	0/4354
15	N	0.59	0/3192	0.57	0/4354
16	D	0.50	0/2022	0.51	0/2751
16	O	0.51	0/2022	0.50	0/2751
17	E	0.34	0/1444	0.54	1/1957 (0.1%)
17	P	0.33	0/1444	0.55	0/1957
18	F	0.39	0/638	0.50	0/858
19	G	0.47	0/1040	0.56	0/1408
19	R	0.46	0/1040	0.56	0/1408
20	H	0.50	0/804	0.47	0/1088
20	S	0.50	0/804	0.52	0/1088
21	I	0.49	0/455	0.49	0/614
22	Q	0.38	0/647	0.46	0/870
23	T	0.46	0/456	0.48	0/615
24	U	0.37	0/358	0.57	1/483 (0.2%)
25	V	0.40	0/419	0.70	1/567 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.44	0/46845	0.55	6/63629 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	18	LEU	CA-CB-CG	6.35	129.91	115.30
17	E	121	ARG	C-N-CA	6.31	137.47	121.70
10	j	58	LEU	CA-CB-CG	5.78	128.60	115.30
13	A	91	LEU	CA-CB-CG	5.45	127.84	115.30
24	U	18	LEU	CA-CB-CG	5.25	127.38	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	4126	0	4149	0	0
2	b	1888	0	1867	0	0
3	c	2138	0	2125	0	0
4	d	888	0	883	0	0
5	e	1008	0	990	0	0
6	f	828	0	807	0	0
7	g	456	0	481	0	0
8	h	408	0	408	0	0
9	i	439	0	449	0	0
10	j	649	0	592	0	0
11	k	941	0	902	0	0
12	m	308	0	302	0	0
13	A	3344	0	3323	39	0
13	L	3344	0	3323	29	0
14	B	2735	0	2774	20	0
14	M	2735	0	2774	18	0
15	C	3090	0	3129	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	N	3090	0	3129	31	0
16	D	1961	0	1890	27	0
16	O	1961	0	1890	23	0
17	E	1411	0	1388	23	0
17	P	1411	0	1388	26	0
18	F	624	0	581	7	0
19	G	1019	0	1034	8	0
19	R	1019	0	1034	9	0
20	H	773	0	736	5	0
20	S	773	0	736	11	0
21	I	442	0	440	4	0
22	Q	633	0	587	5	0
23	T	443	0	440	7	0
24	U	347	0	345	3	0
25	V	406	0	414	5	0
26	a	1	0	0	0	0
27	a	120	0	108	0	0
28	D	32	0	37	33	0
28	a	34	0	41	0	0
28	b	35	0	39	0	0
28	c	40	0	51	0	0
28	i	40	0	53	0	0
28	m	71	0	88	0	0
29	N	55	0	66	2	0
29	a	55	0	66	0	0
30	b	2	0	0	0	0
31	I	35	0	44	1	0
31	T	35	0	44	2	0
31	c	43	0	60	0	0
31	e	36	0	46	0	0
31	m	38	0	50	0	0
32	d	1	0	0	0	0
33	C	40	0	59	0	0
33	O	40	0	59	3	0
34	C	86	0	60	1	0
34	D	43	0	30	3	0
34	N	86	0	60	1	0
34	O	43	0	30	3	0
35	C	47	0	73	2	0
35	N	47	0	73	2	0
36	C	41	0	50	2	0
37	C	43	0	58	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	N	43	0	58	0	0
38	C	40	0	59	0	0
38	N	40	0	59	0	0
39	E	38	0	55	2	0
39	O	38	0	55	4	0
40	E	4	0	0	1	0
40	P	4	0	0	2	0
All	All	47034	0	46941	338	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 7.

The worst 5 of 338 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)
20:S:36:PRO:O	20:S:37:LEU:HD12	1.36	1.23
16:D:82:PHE:CZ	28:D:402:PTY:H201	1.92	1.04
20:S:36:PRO:O	20:S:37:LEU:CD1	2.12	0.97
16:D:82:PHE:CE1	28:D:402:PTY:H202	2.01	0.94
15:N:272:GLU:N	15:N:272:GLU:OE1	2.06	0.89

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	528/530 (100%)	485 (92%)	43 (8%)	0	100	100
2	b	234/236 (99%)	213 (91%)	21 (9%)	0	100	100
3	c	266/268 (99%)	252 (95%)	14 (5%)	0	100	100
4	d	115/117 (98%)	94 (82%)	20 (17%)	1 (1%)	14	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	126/128 (98%)	113 (90%)	13 (10%)	0	100	100
6	f	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
7	g	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
8	h	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
9	i	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
10	j	76/78 (97%)	71 (93%)	5 (7%)	0	100	100
11	k	112/114 (98%)	93 (83%)	19 (17%)	0	100	100
12	m	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
13	A	429/431 (100%)	403 (94%)	26 (6%)	0	100	100
13	L	429/431 (100%)	400 (93%)	29 (7%)	0	100	100
14	B	350/352 (99%)	333 (95%)	17 (5%)	0	100	100
14	M	350/352 (99%)	330 (94%)	20 (6%)	0	100	100
15	C	383/385 (100%)	371 (97%)	12 (3%)	0	100	100
15	N	383/385 (100%)	370 (97%)	13 (3%)	0	100	100
16	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
16	O	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
17	E	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
17	P	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
18	F	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
19	G	124/126 (98%)	119 (96%)	4 (3%)	1 (1%)	16	49
19	R	124/126 (98%)	120 (97%)	3 (2%)	1 (1%)	16	49
20	H	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
20	S	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
21	I	52/54 (96%)	49 (94%)	3 (6%)	0	100	100
22	Q	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
23	T	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
24	U	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
25	V	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
All	All	5695/5759 (99%)	5347 (94%)	345 (6%)	3 (0%)	50	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	R	5	PHE
19	G	5	PHE
4	d	129	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	443/443 (100%)	443 (100%)	0	100	100
2	b	209/209 (100%)	209 (100%)	0	100	100
3	c	227/227 (100%)	227 (100%)	0	100	100
4	d	99/99 (100%)	99 (100%)	0	100	100
5	e	106/106 (100%)	106 (100%)	0	100	100
6	f	88/88 (100%)	88 (100%)	0	100	100
7	g	48/48 (100%)	48 (100%)	0	100	100
8	h	41/41 (100%)	40 (98%)	1 (2%)	44	69
9	i	44/44 (100%)	44 (100%)	0	100	100
10	j	70/70 (100%)	70 (100%)	0	100	100
11	k	100/100 (100%)	100 (100%)	0	100	100
12	m	32/32 (100%)	32 (100%)	0	100	100
13	A	370/370 (100%)	369 (100%)	1 (0%)	91	95
13	L	370/370 (100%)	370 (100%)	0	100	100
14	B	301/301 (100%)	300 (100%)	1 (0%)	91	95
14	M	301/301 (100%)	300 (100%)	1 (0%)	91	95
15	C	338/338 (100%)	337 (100%)	1 (0%)	91	95
15	N	338/338 (100%)	337 (100%)	1 (0%)	91	95
16	D	206/206 (100%)	206 (100%)	0	100	100
16	O	206/206 (100%)	206 (100%)	0	100	100
17	E	151/151 (100%)	151 (100%)	0	100	100
17	P	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	F	67/67 (100%)	67 (100%)	0	100	100
19	G	110/110 (100%)	110 (100%)	0	100	100
19	R	110/110 (100%)	108 (98%)	2 (2%)	54	75
20	H	77/77 (100%)	77 (100%)	0	100	100
20	S	77/77 (100%)	74 (96%)	3 (4%)	27	57
21	I	44/44 (100%)	44 (100%)	0	100	100
22	Q	68/68 (100%)	68 (100%)	0	100	100
23	T	45/45 (100%)	45 (100%)	0	100	100
24	U	35/35 (100%)	35 (100%)	0	100	100
25	V	42/42 (100%)	41 (98%)	1 (2%)	44	69
All	All	4914/4914 (100%)	4902 (100%)	12 (0%)	91	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	R	83	LEU
20	S	25	THR
25	V	55	LEU
20	S	37	LEU
15	C	384	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	177	GLN
16	O	127	ASN
19	R	79	HIS
13	A	102	GLN
11	k	122	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 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	$\# Z > 2$
31	PCF	m	103	-	37,37,49	0.66	0	43,45,57	0.60	0
34	HEM	C	403	15	41,50,50	1.47	3 (7%)	45,82,82	1.34	4 (8%)
38	9PE	C	407	-	39,39,39	0.43	0	42,44,44	1.14	2 (4%)
28	PTY	c	301	3	39,39,49	1.02	3 (7%)	42,44,54	1.25	4 (9%)
27	HEA	a	603	-	57,67,67	1.38	8 (14%)	61,103,103	1.66	18 (29%)
30	CUA	b	301	2	0,1,1	-	-	-	-	-
39	7PH	E	301	-	37,37,37	0.52	0	41,42,42	1.15	2 (4%)
31	PCF	T	101	-	34,34,49	0.62	0	40,42,57	0.67	0
39	7PH	O	403	-	37,37,37	0.52	0	41,42,42	1.14	2 (4%)
28	PTY	m	102	-	29,29,49	1.16	2 (6%)	32,34,54	1.24	4 (12%)
28	PTY	i	101	-	39,39,49	0.99	2 (5%)	42,44,54	1.08	3 (7%)
34	HEM	N	401	15	41,50,50	1.65	3 (7%)	45,82,82	1.15	5 (11%)
35	8PE	C	404	-	46,46,46	0.44	0	49,51,51	1.15	2 (4%)
28	PTY	a	604	-	33,33,49	1.06	4 (12%)	36,38,54	1.10	2 (5%)
28	PTY	b	302	2	32,32,49	1.08	2 (6%)	35,37,54	1.07	2 (5%)
33	6PH	O	401	-	39,39,39	0.49	0	43,44,44	1.16	2 (4%)
40	FES	E	302	-	0,4,4	-	-	-	-	-
33	6PH	C	401	-	39,39,39	0.49	0	43,44,44	1.19	2 (4%)
34	HEM	C	402	15	41,50,50	1.57	6 (14%)	45,82,82	1.97	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	D	401	16	41,50,50	1.57	3 (7%)	45,82,82	1.32	5 (11%)
34	HEM	O	402	16	41,50,50	1.58	3 (7%)	45,82,82	1.42	6 (13%)
40	FES	P	301	-	0,4,4	-	-	-	-	-
38	9PE	N	405	-	39,39,39	0.44	0	42,44,44	1.13	2 (4%)
29	CN3	a	605	-	54,54,54	0.51	0	60,66,66	1.14	4 (6%)
28	PTY	D	402	-	31,31,49	1.08	2 (6%)	34,36,54	1.21	3 (8%)
35	8PE	N	404	-	46,46,46	0.42	0	49,51,51	1.15	2 (4%)
31	PCF	I	101	-	34,34,49	0.63	0	40,42,57	0.61	0
37	UQ6	N	403	-	43,43,43	0.51	0	51,55,55	1.59	12 (23%)
27	HEA	a	602	1	57,67,67	1.34	7 (12%)	61,103,103	1.71	16 (26%)
34	HEM	N	402	15	41,50,50	1.48	4 (9%)	45,82,82	1.37	6 (13%)
31	PCF	e	201	-	35,35,49	0.69	0	41,43,57	0.56	0
29	CN3	N	406	-	54,54,54	0.51	0	60,66,66	1.30	4 (6%)
28	PTY	m	101	-	40,40,49	1.04	2 (5%)	43,45,54	1.20	4 (9%)
31	PCF	c	302	-	42,42,49	0.64	0	48,50,57	0.61	0
37	UQ6	C	406	-	43,43,43	0.46	0	51,55,55	1.59	13 (25%)
36	CN5	C	405	-	40,40,40	1.04	2 (5%)	44,48,48	0.96	2 (4%)

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
31	PCF	m	103	-	-	17/41/41/53	-
34	HEM	C	403	15	-	4/12/54/54	-
38	9PE	C	407	-	-	14/43/43/43	-
28	PTY	c	301	3	-	18/43/43/53	-
27	HEA	a	603	-	-	10/32/76/76	-
39	7PH	E	301	-	-	12/39/39/39	-
31	PCF	T	101	-	-	14/38/38/53	-
39	7PH	O	403	-	-	14/39/39/39	-
28	PTY	m	102	-	-	16/33/33/53	-
28	PTY	i	101	-	-	14/43/43/53	-
34	HEM	N	401	15	-	2/12/54/54	-
35	8PE	C	404	-	-	22/50/50/50	-
28	PTY	a	604	-	-	15/37/37/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PTY	b	302	2	-	9/36/36/53	-
33	6PH	O	401	-	-	9/41/41/41	-
40	FES	E	302	-	-	-	0/1/1/1
33	6PH	C	401	-	-	13/41/41/41	-
34	HEM	C	402	15	-	6/12/54/54	-
34	HEM	D	401	16	-	0/12/54/54	-
34	HEM	O	402	16	-	0/12/54/54	-
40	FES	P	301	-	-	-	0/1/1/1
38	9PE	N	405	-	-	19/43/43/43	-
29	CN3	a	605	-	-	25/65/65/65	-
28	PTY	D	402	-	-	11/35/35/53	-
35	8PE	N	404	-	-	23/50/50/50	-
31	PCF	I	101	-	-	12/38/38/53	-
37	UQ6	N	403	-	-	7/39/39/39	0/1/1/1
27	HEA	a	602	1	-	13/32/76/76	-
34	HEM	N	402	15	-	2/12/54/54	-
31	PCF	e	201	-	-	11/39/39/53	-
29	CN3	N	406	-	-	34/65/65/65	-
28	PTY	m	101	-	-	18/44/44/53	-
31	PCF	c	302	-	-	15/46/46/53	-
37	UQ6	C	406	-	-	13/39/39/39	0/1/1/1
36	CN5	C	405	-	-	18/44/44/44	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	N	401	HEM	C3C-C2C	-6.94	1.30	1.40
34	O	402	HEM	C3C-C2C	-6.32	1.31	1.40
34	D	401	HEM	C3C-C2C	-6.20	1.31	1.40
34	C	403	HEM	C3C-C2C	-4.68	1.33	1.40
34	C	402	HEM	C3C-C2C	-4.62	1.34	1.40

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	402	HEM	CAD-C3D-C4D	6.18	135.46	124.66
34	C	402	HEM	CAD-C3D-C2D	-5.41	117.80	127.88
37	N	403	UQ6	C7-C8-C9	-5.19	119.18	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	406	UQ6	C7-C8-C9	-4.93	119.59	127.24
29	N	406	CN3	O51-C51-C52	4.57	121.36	111.50

There are no chirality outliers.

5 of 430 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	a	602	HEA	C13-C14-C15-C26
27	a	602	HEA	C21-C22-C23-C25
28	a	604	PTY	C11-C8-O7-C6
28	c	301	PTY	O4-C1-C6-O7
28	c	301	PTY	C3-O11-P1-O13

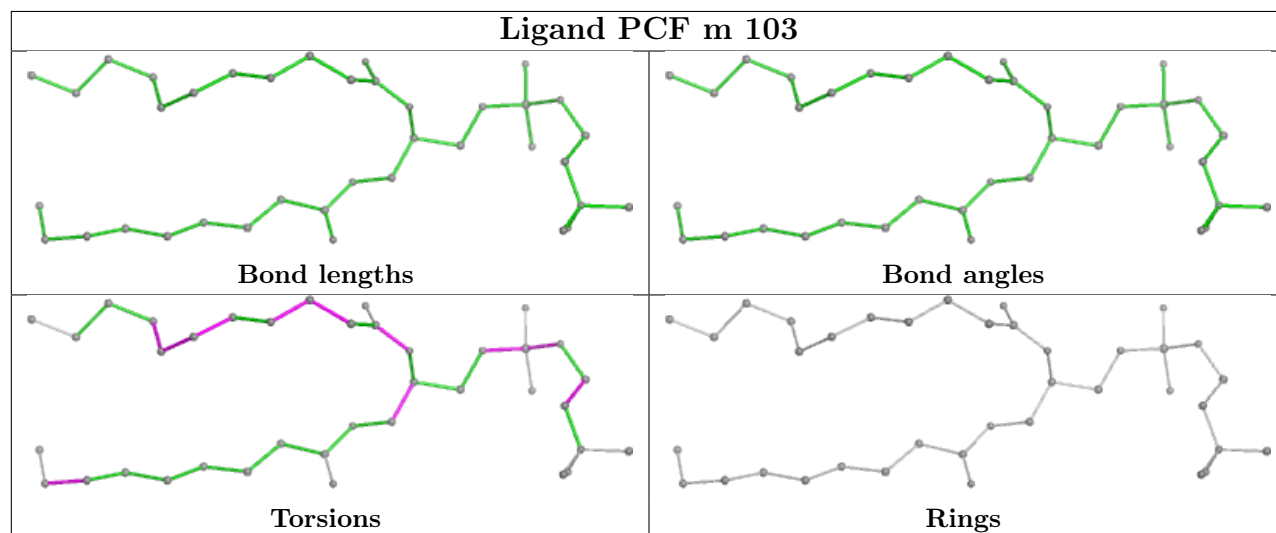
There are no ring outliers.

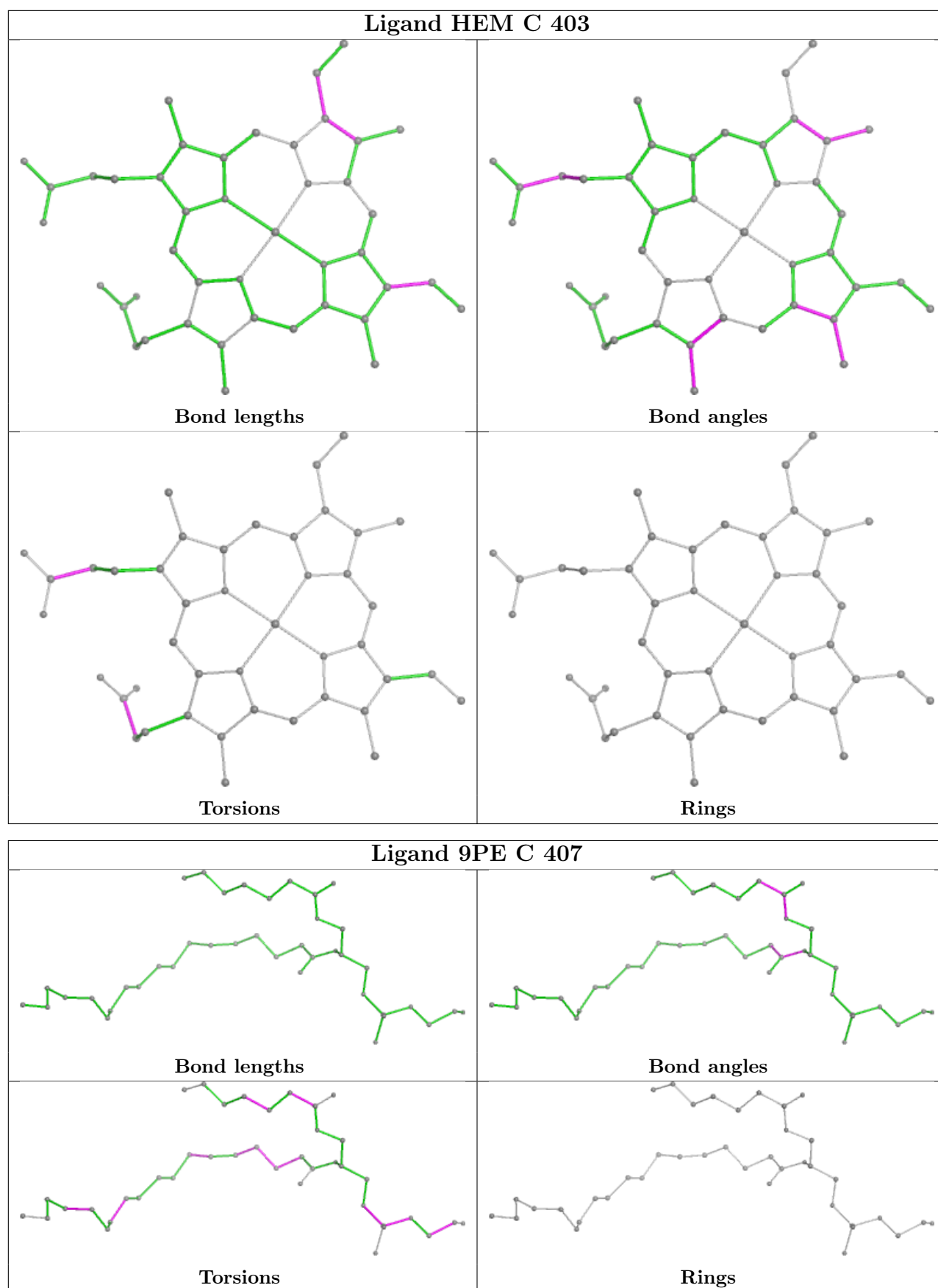
17 monomers are involved in 66 short contacts:

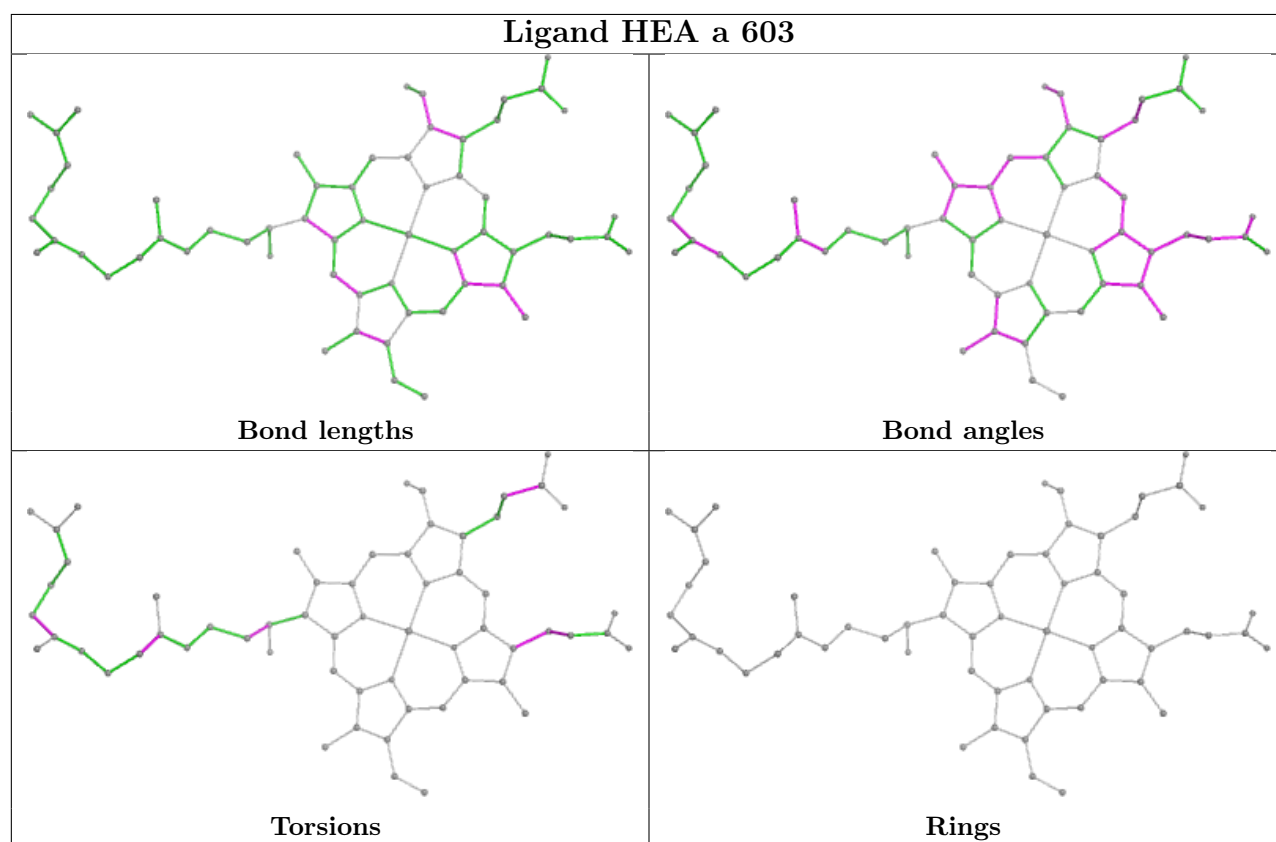
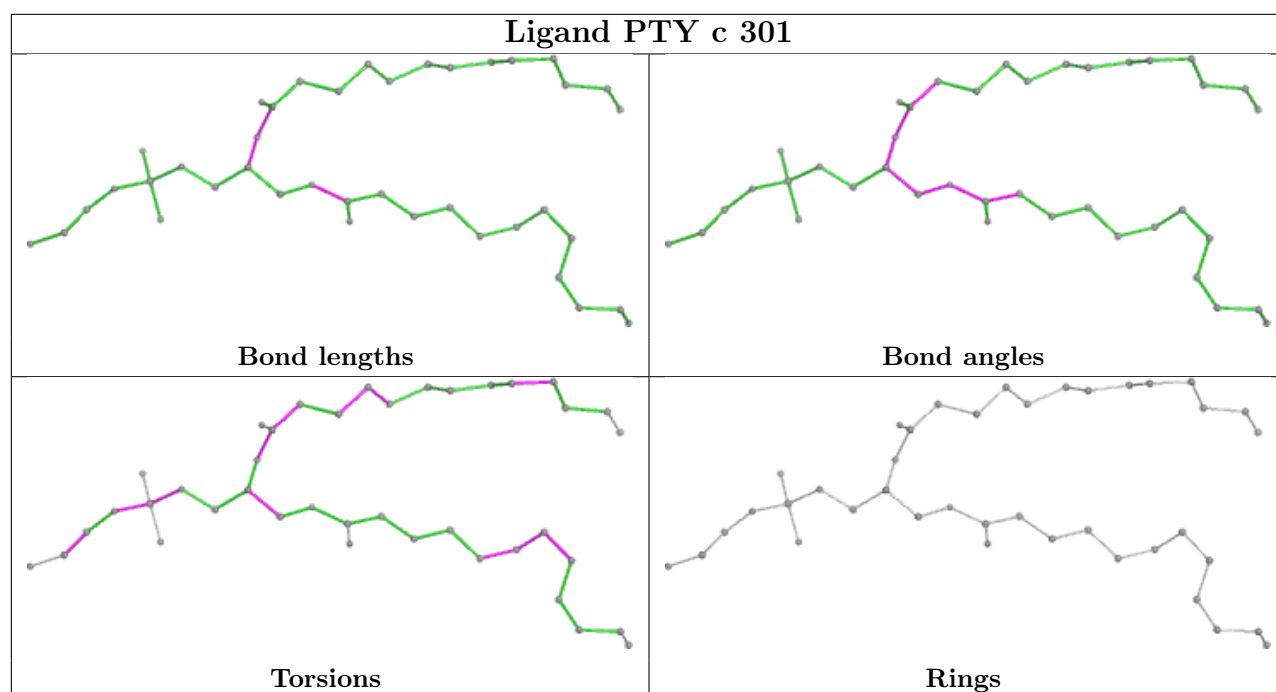
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	403	HEM	1	0
39	E	301	7PH	2	0
31	T	101	PCF	2	0
39	O	403	7PH	4	0
34	N	401	HEM	1	0
35	C	404	8PE	2	0
33	O	401	6PH	3	0
40	E	302	FES	1	0
34	D	401	HEM	3	0
34	O	402	HEM	3	0
40	P	301	FES	2	0
28	D	402	PTY	33	0
35	N	404	8PE	2	0
31	I	101	PCF	1	0
29	N	406	CN3	2	0
37	C	406	UQ6	3	0
36	C	405	CN5	2	0

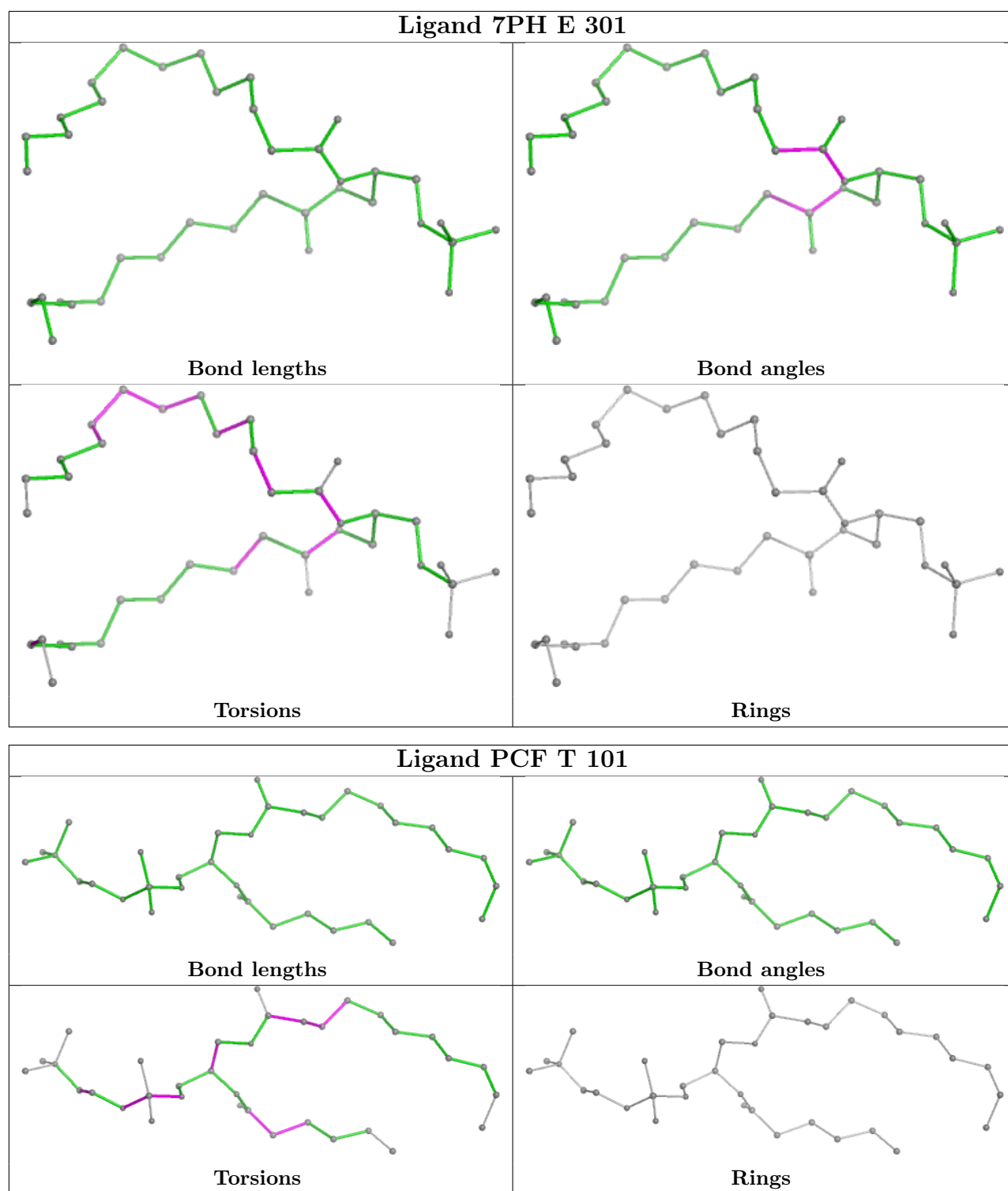
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

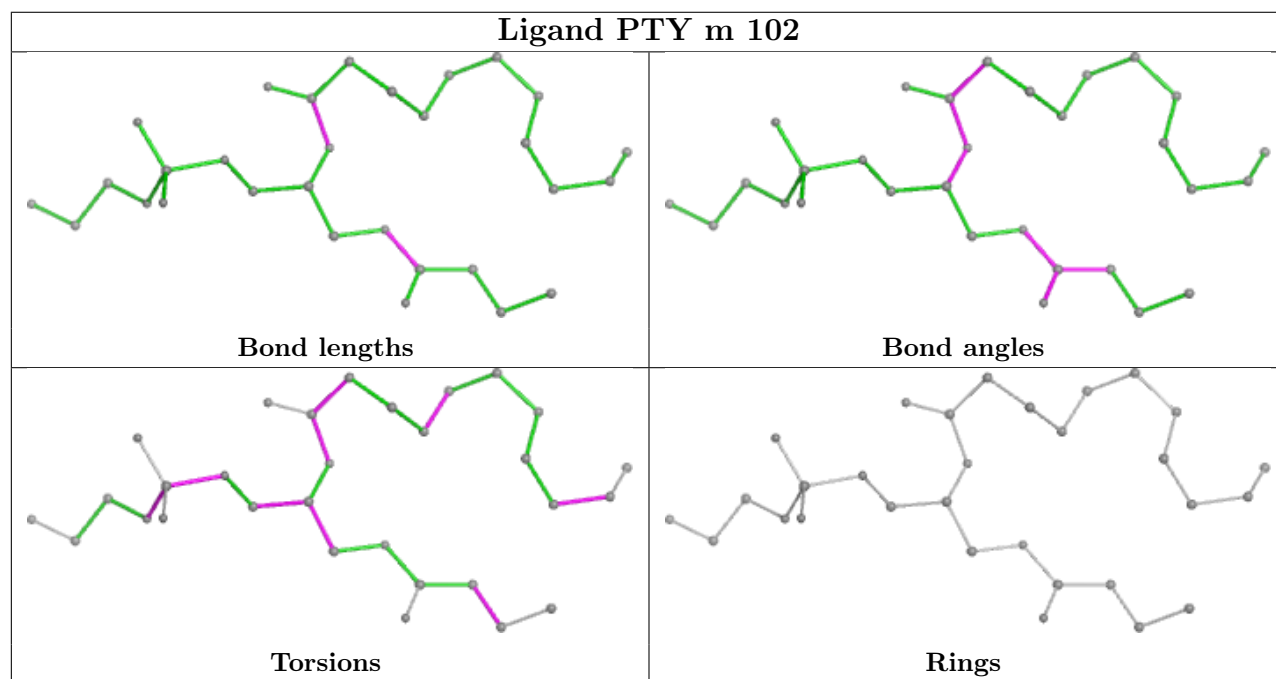
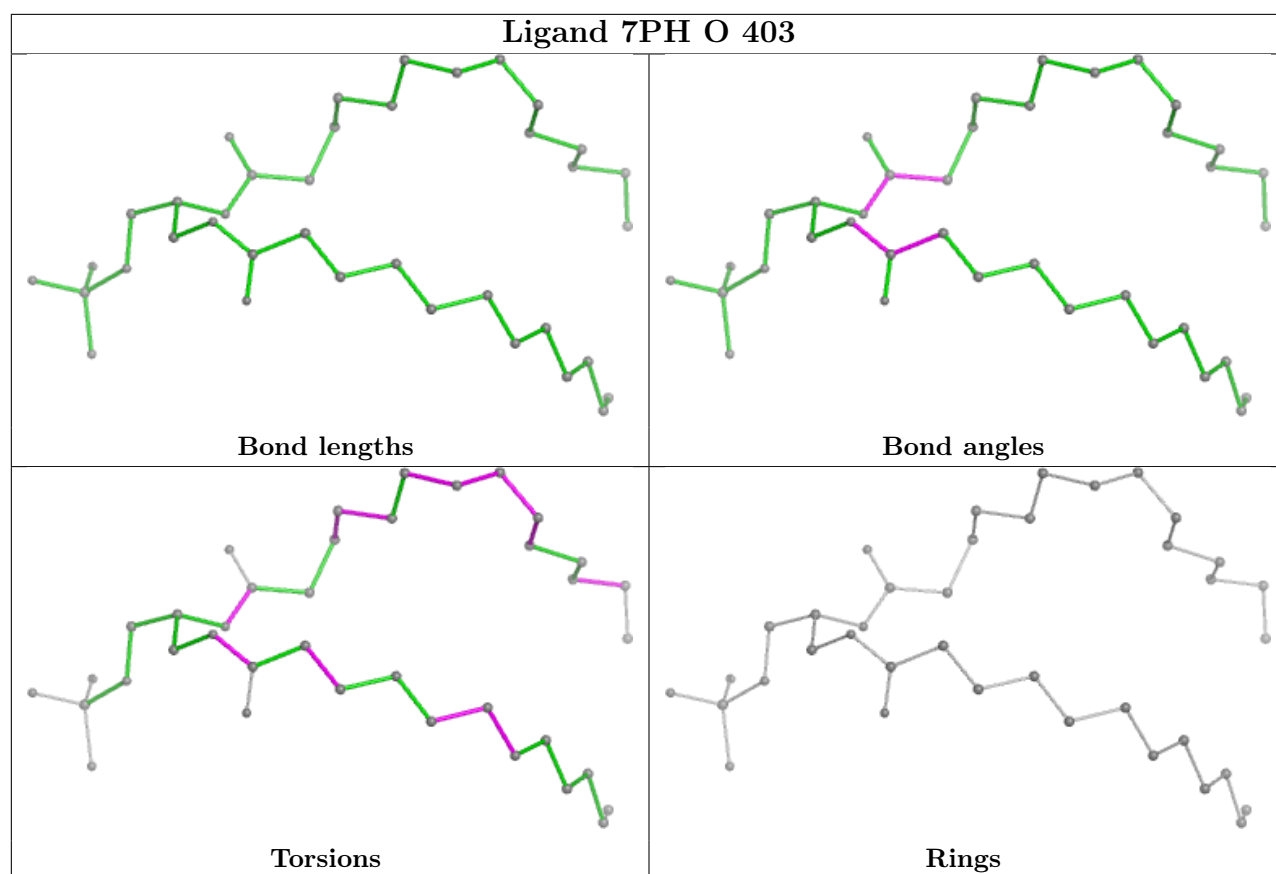
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

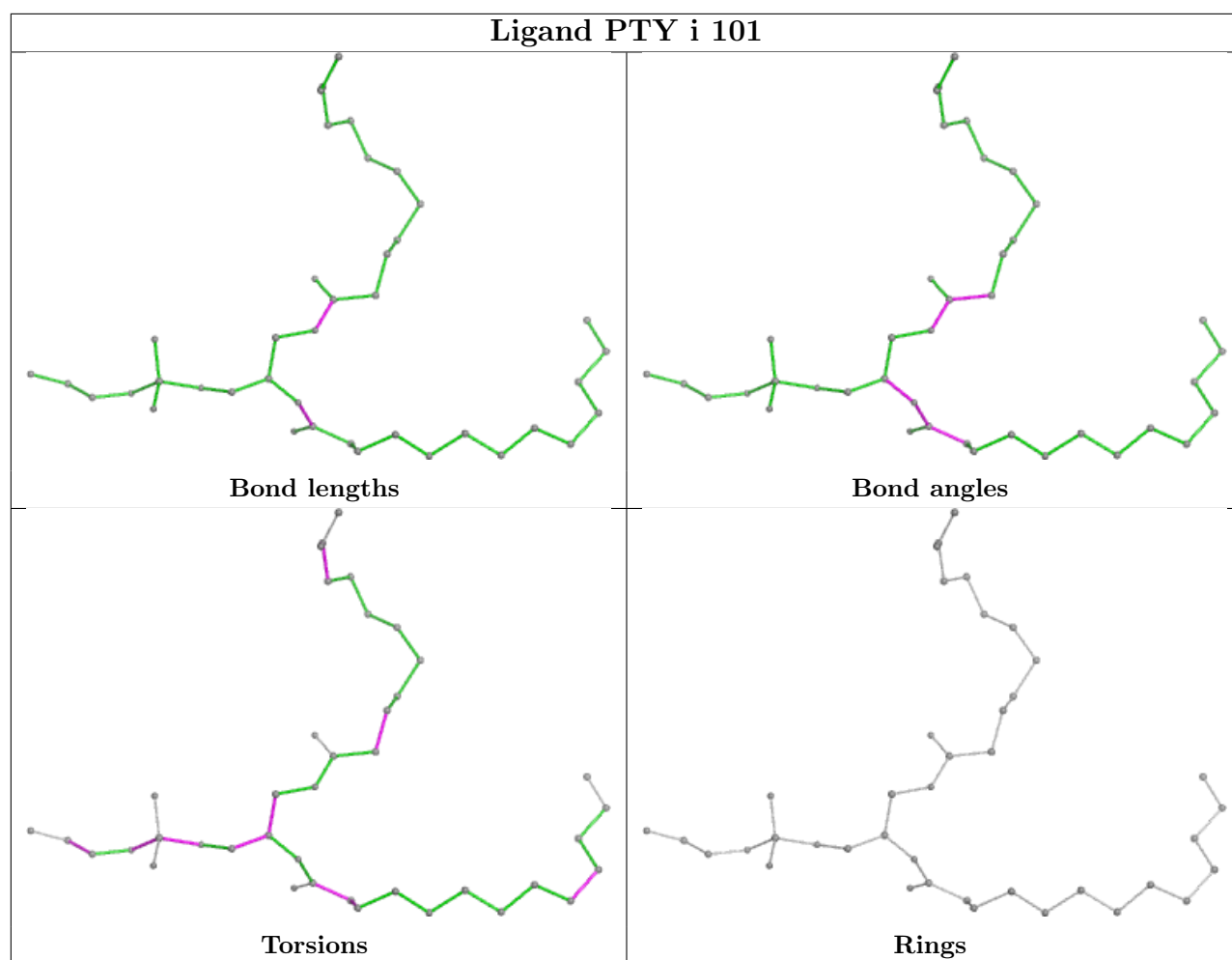


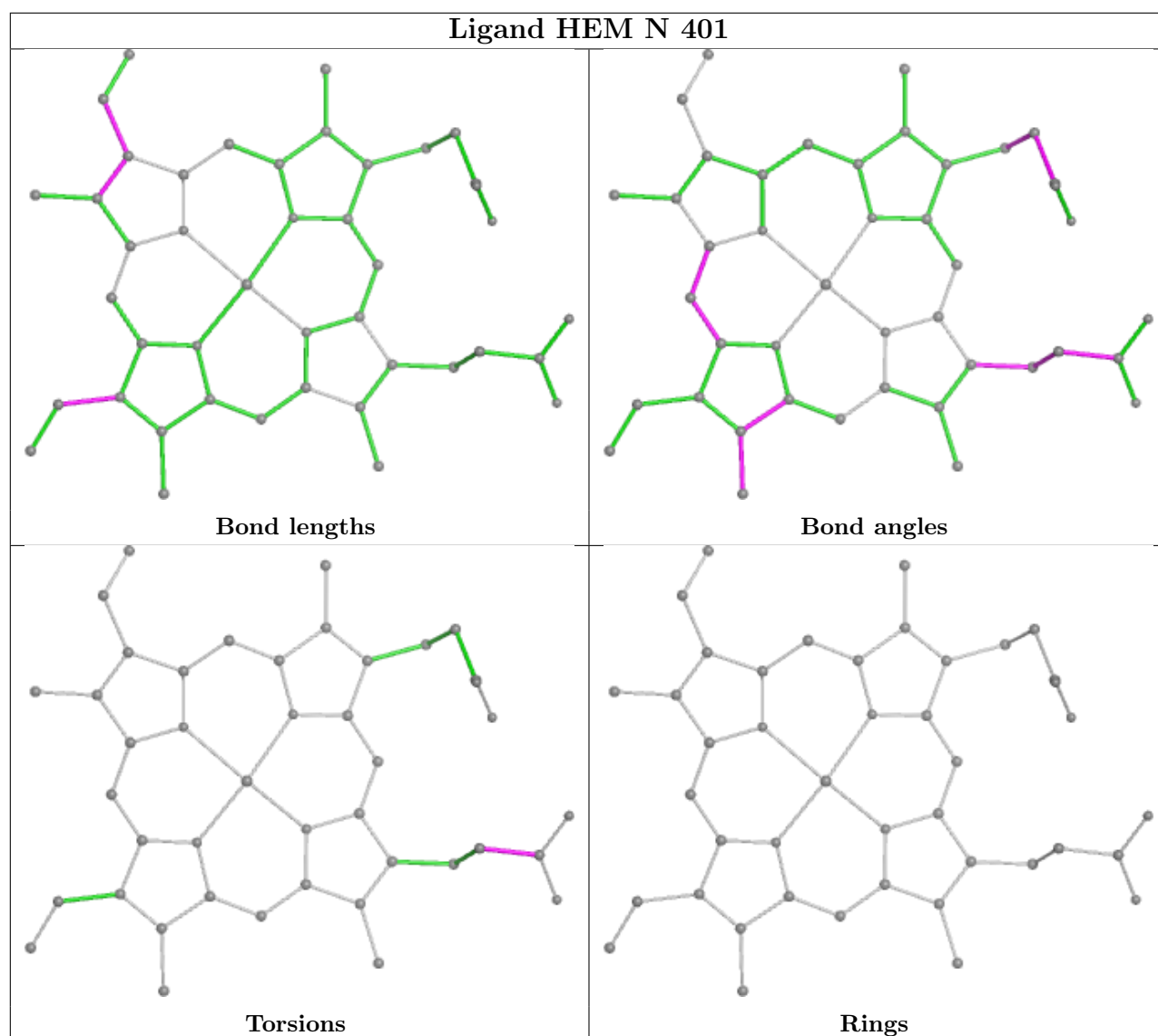


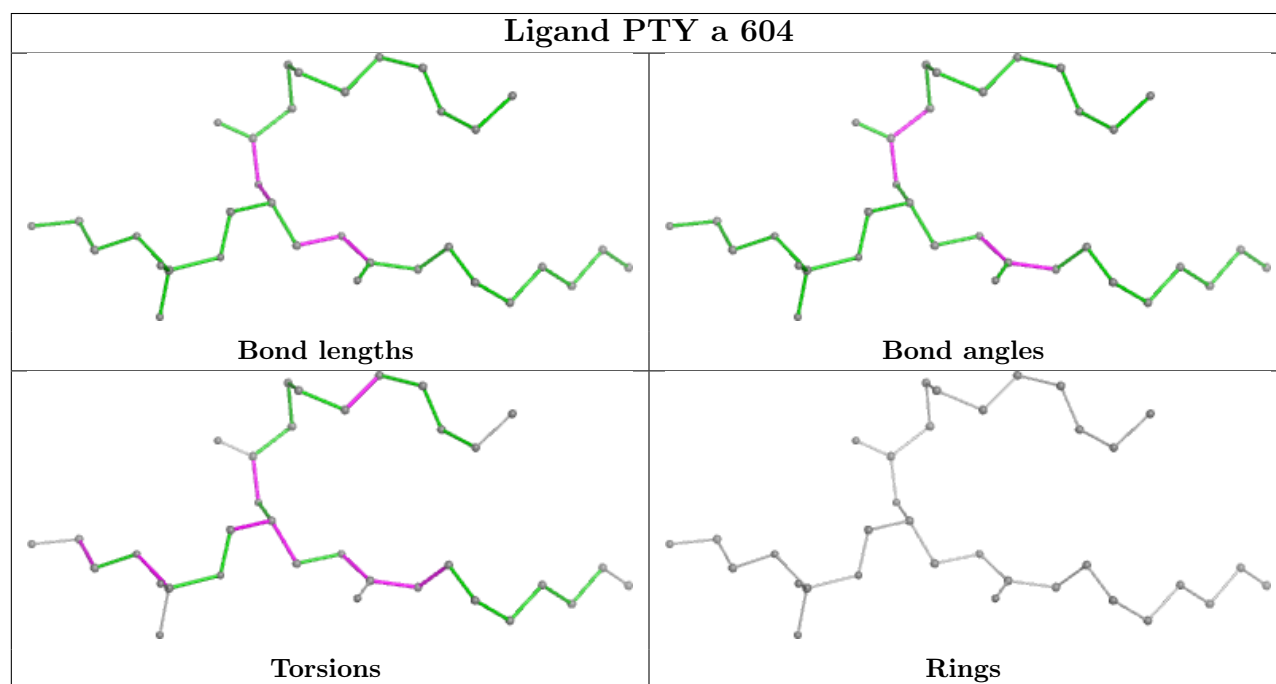
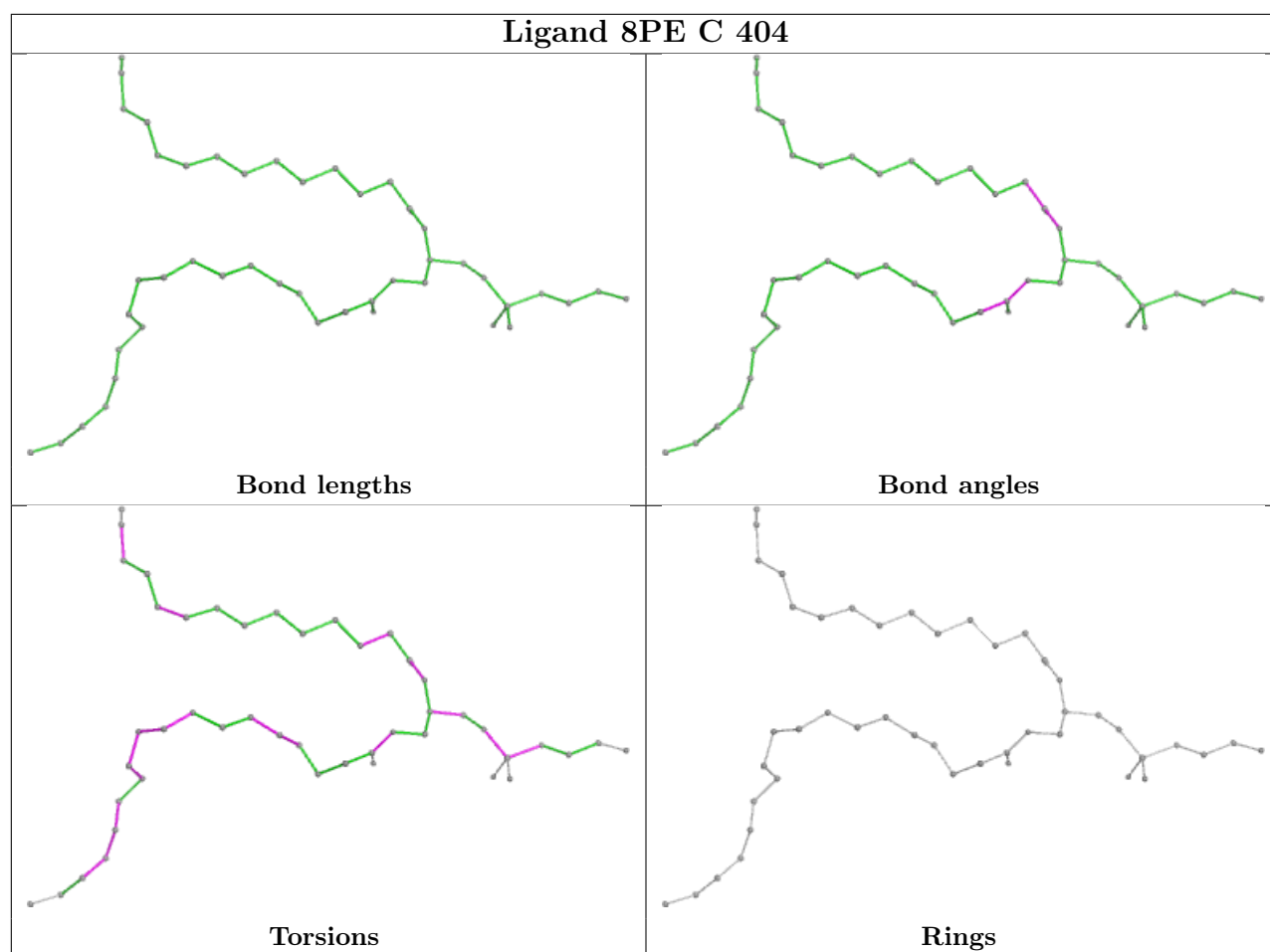


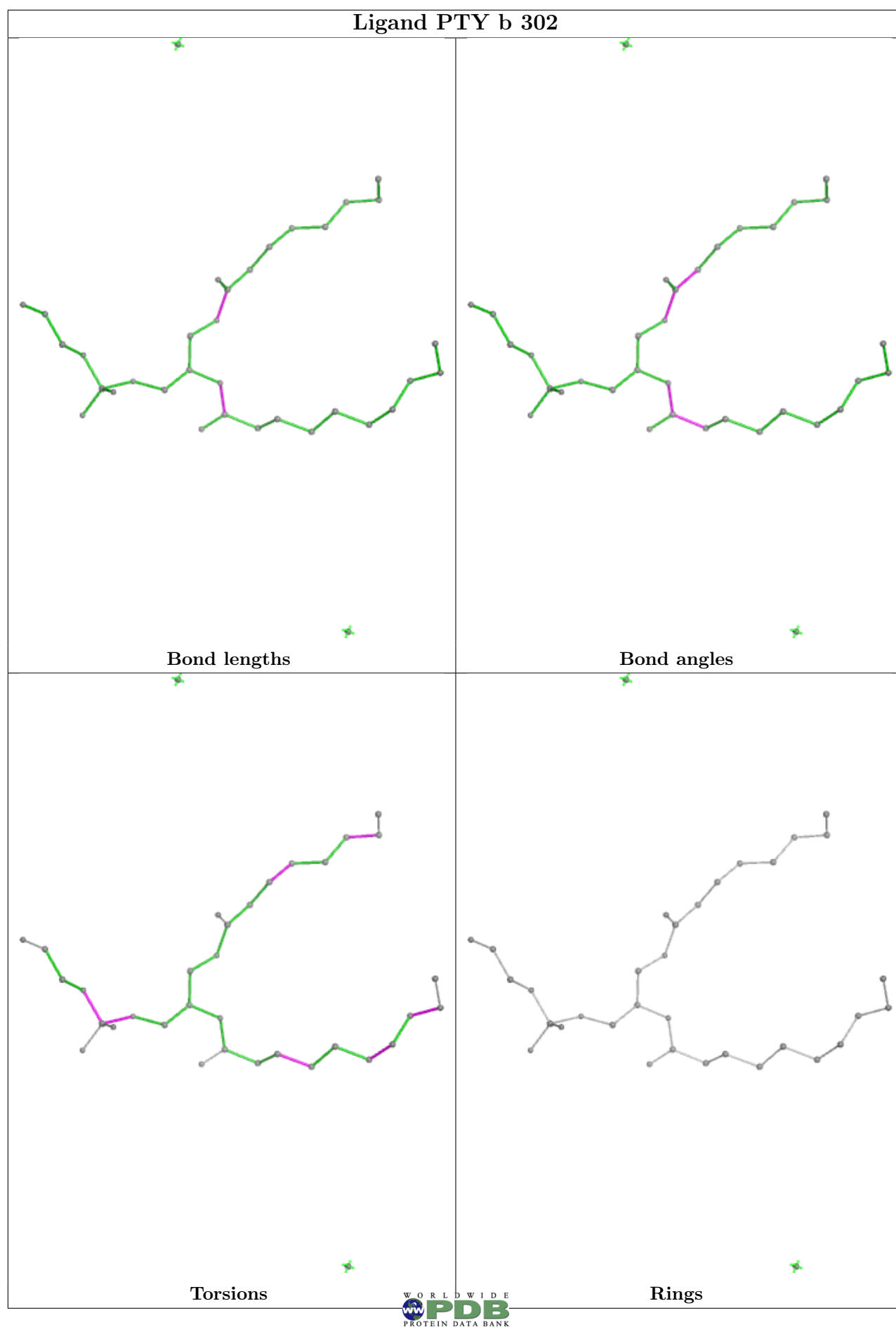


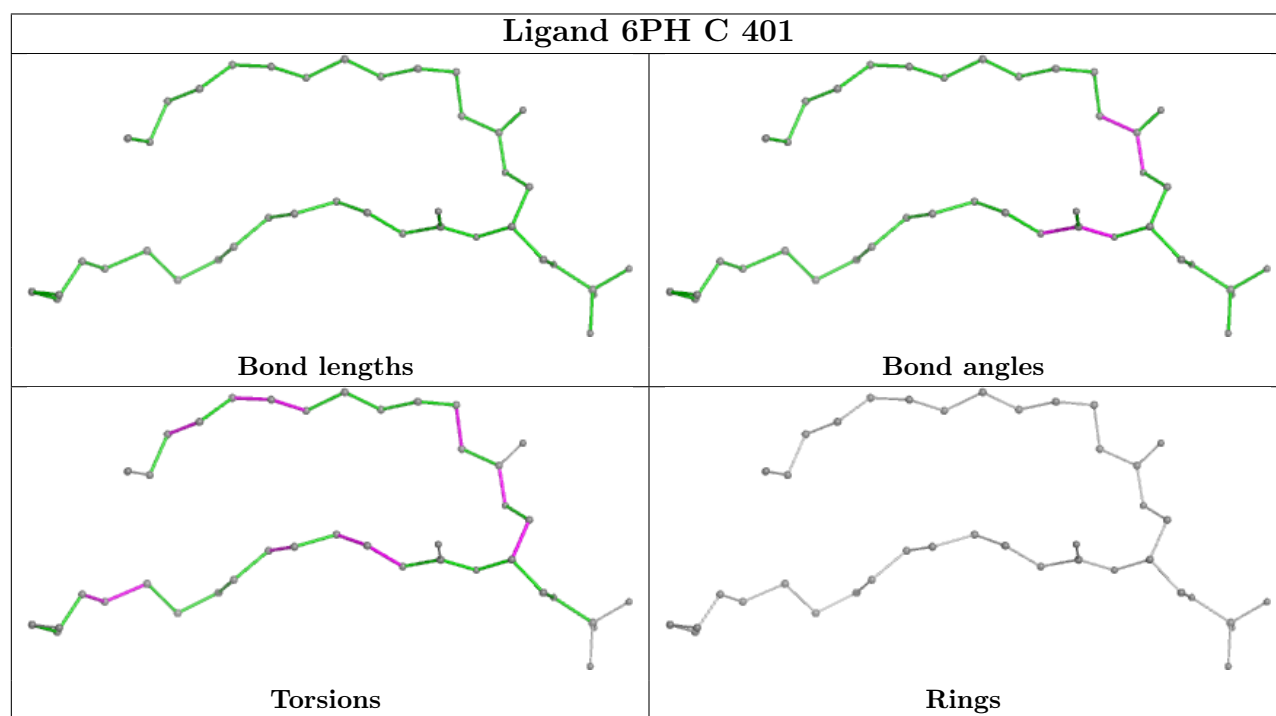
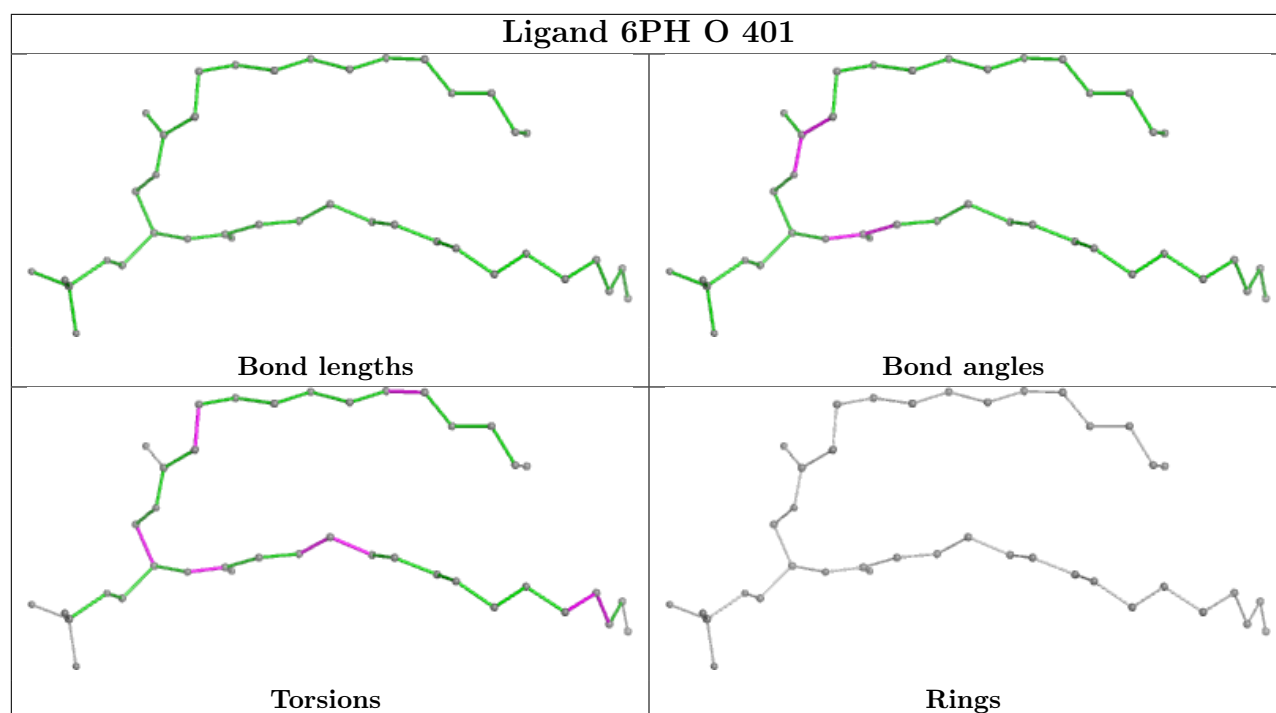


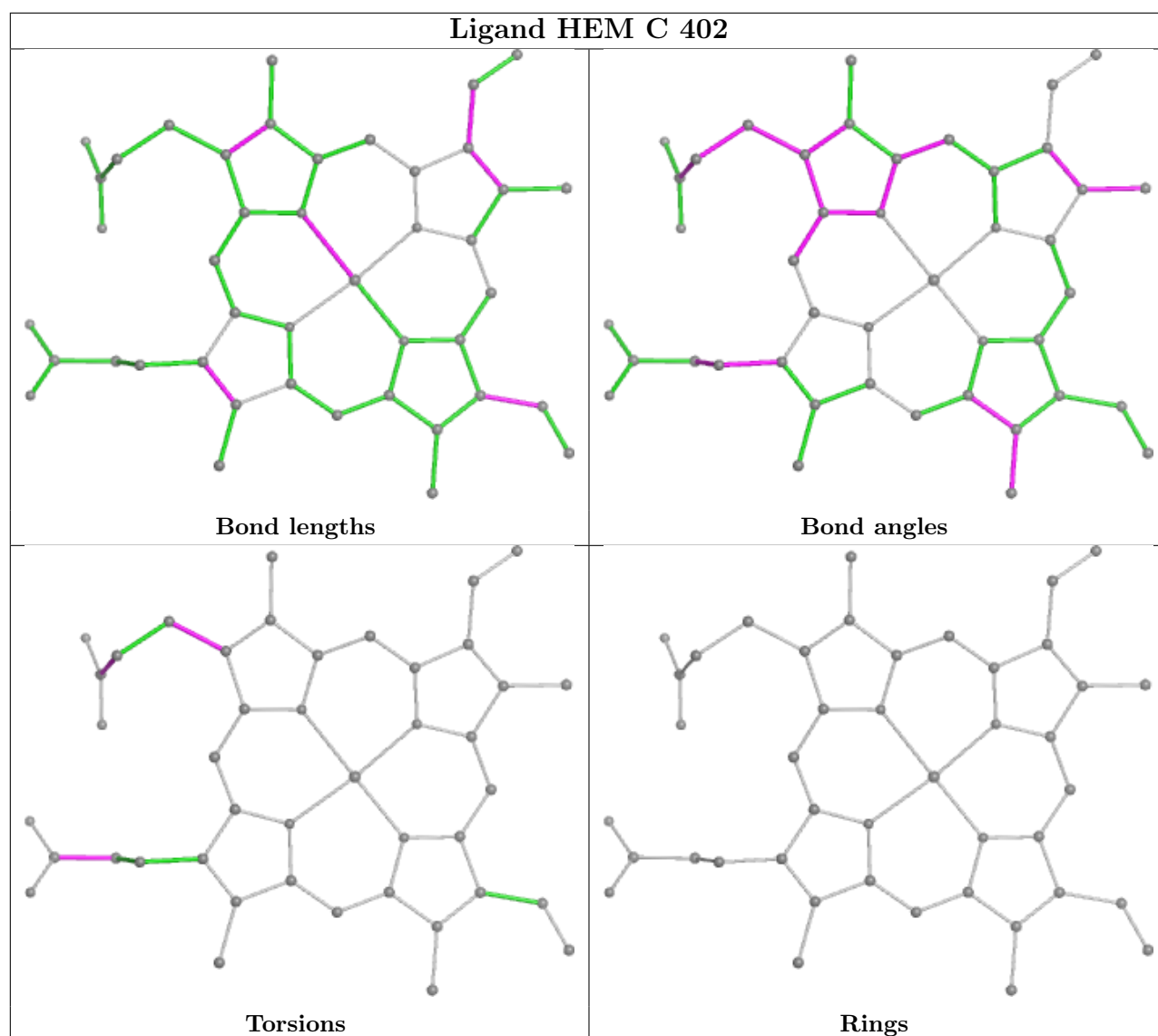


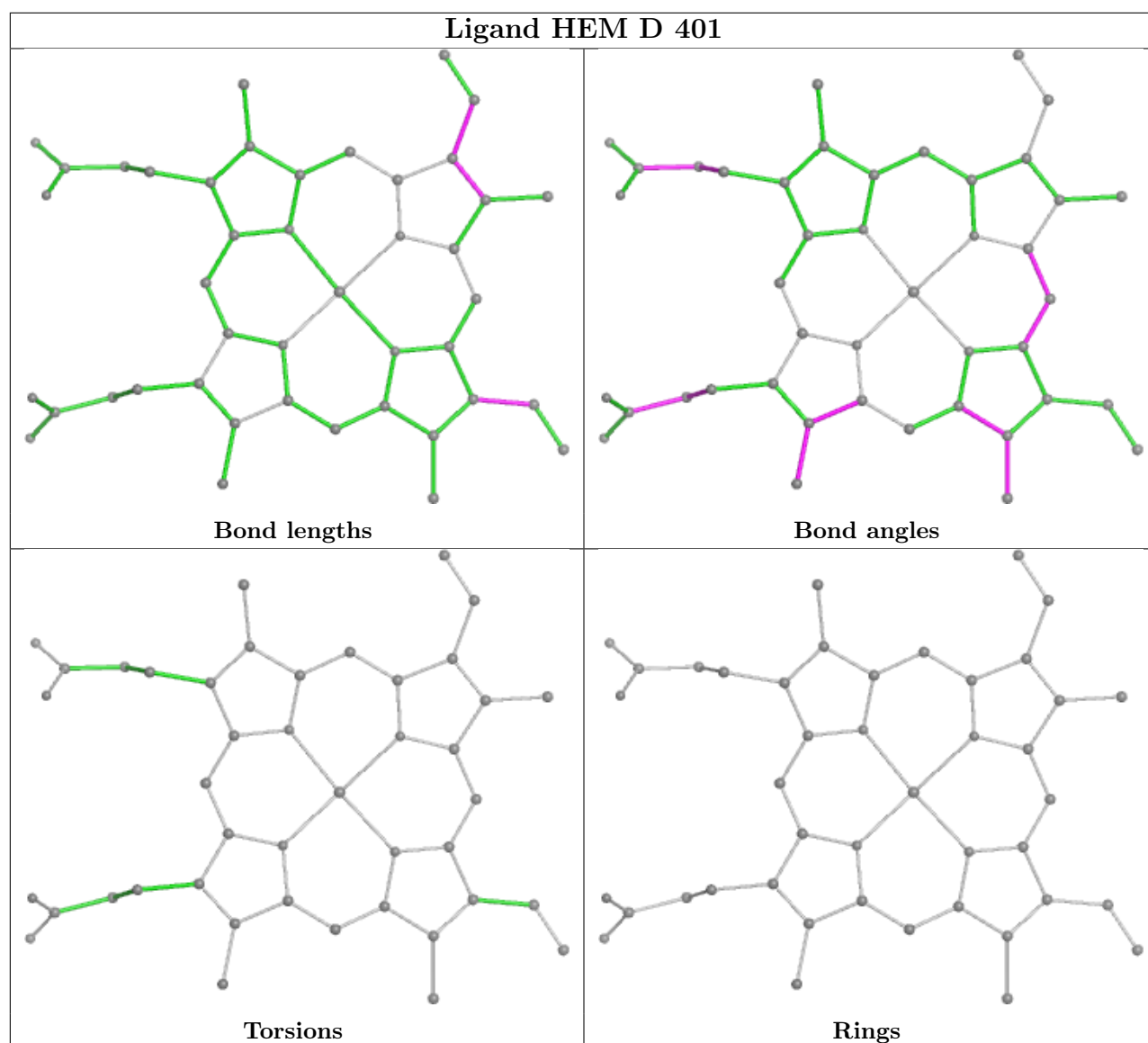


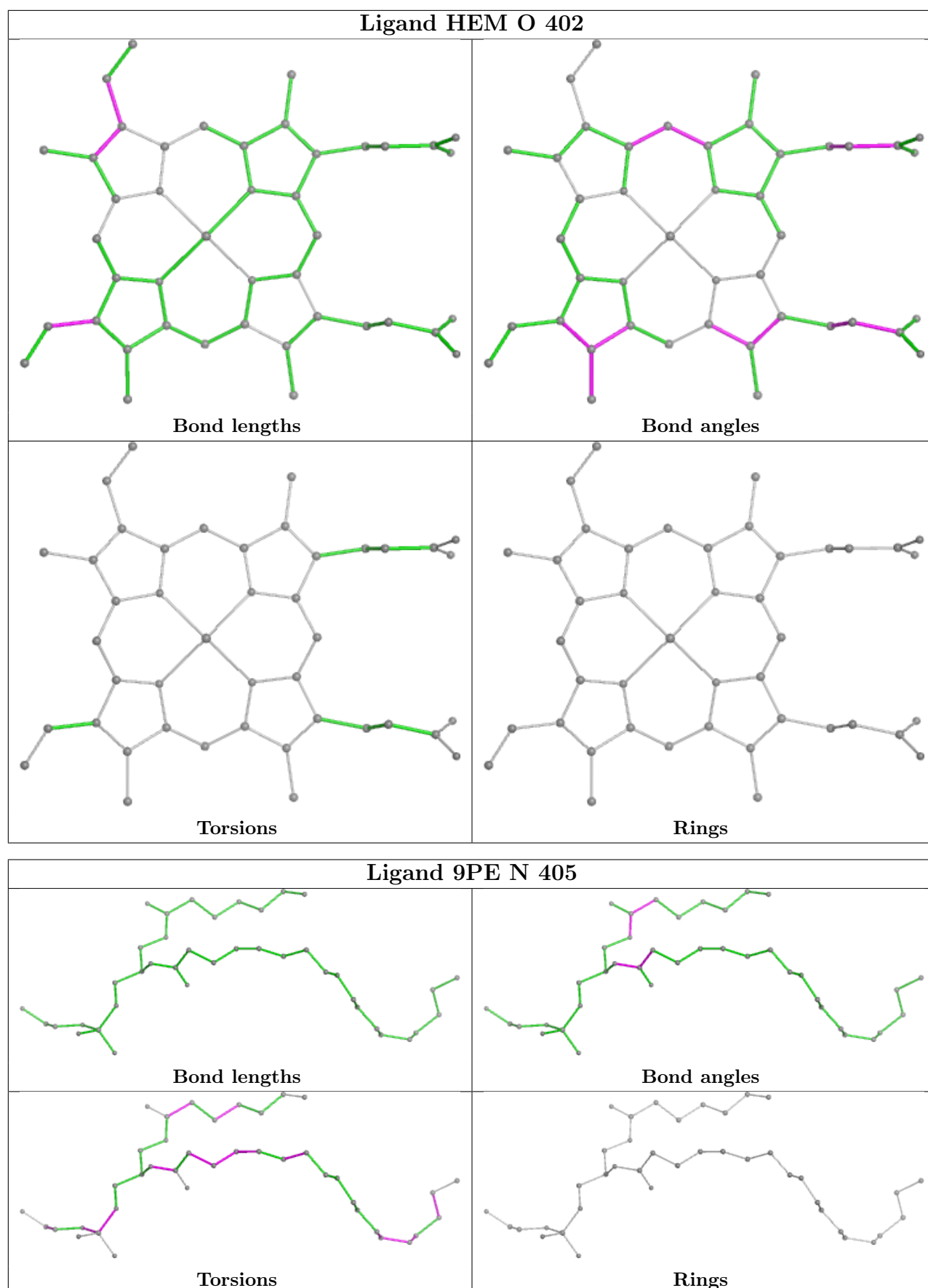


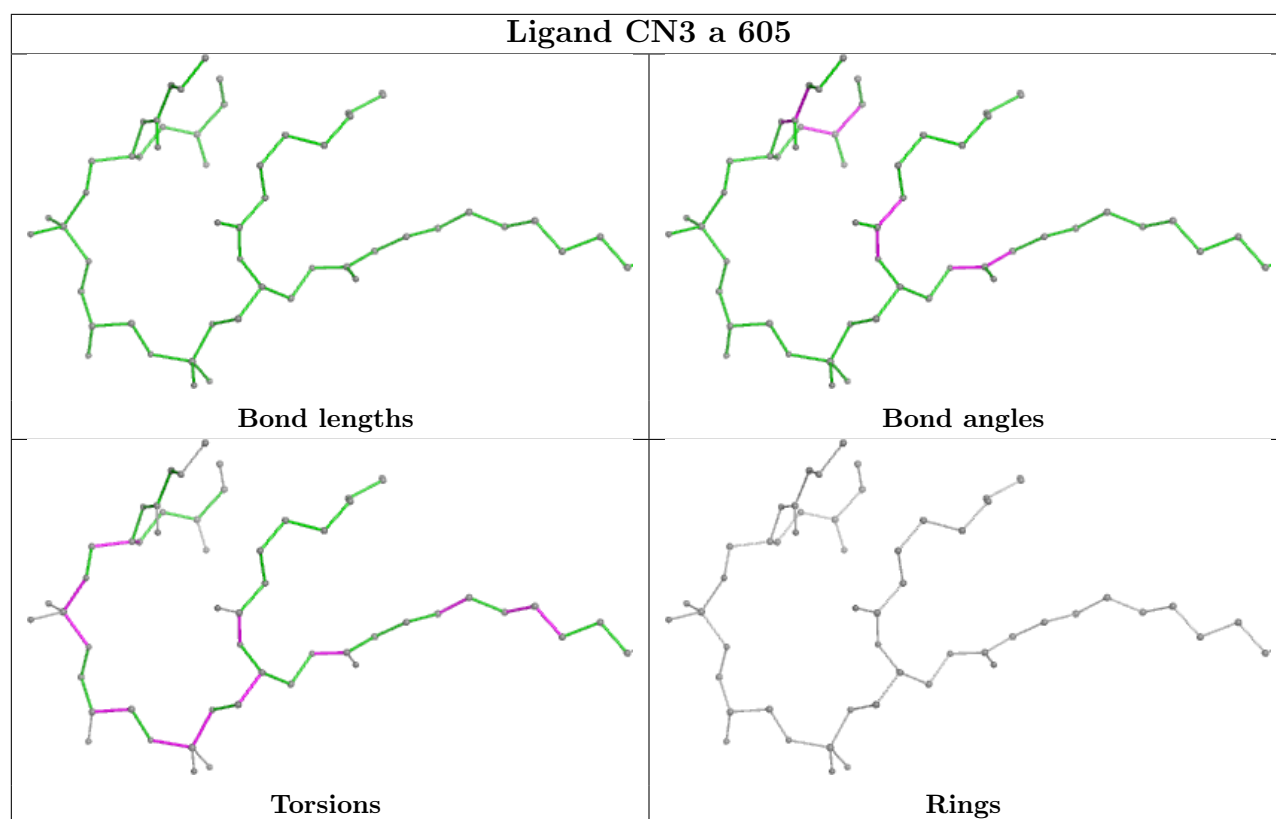


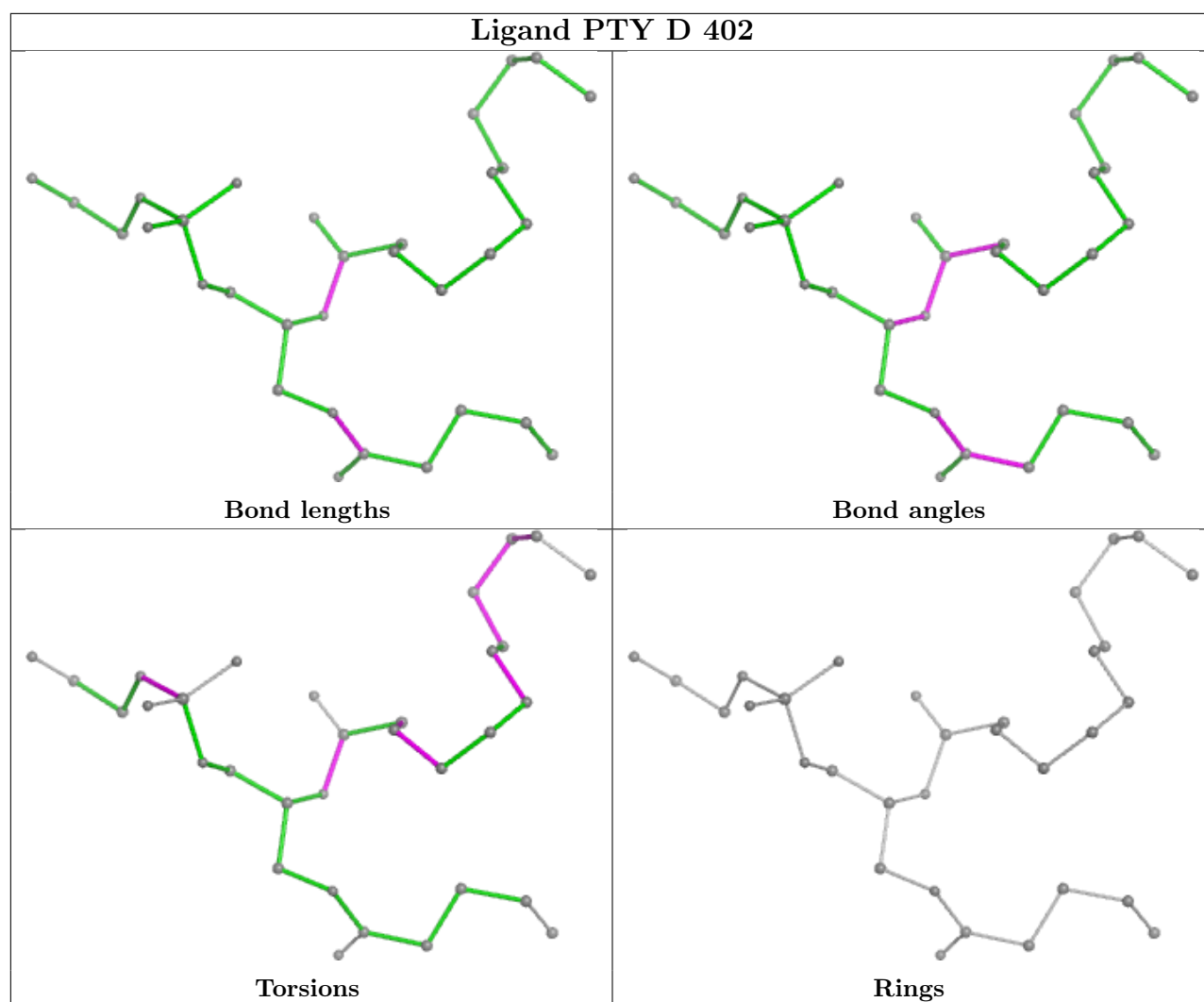


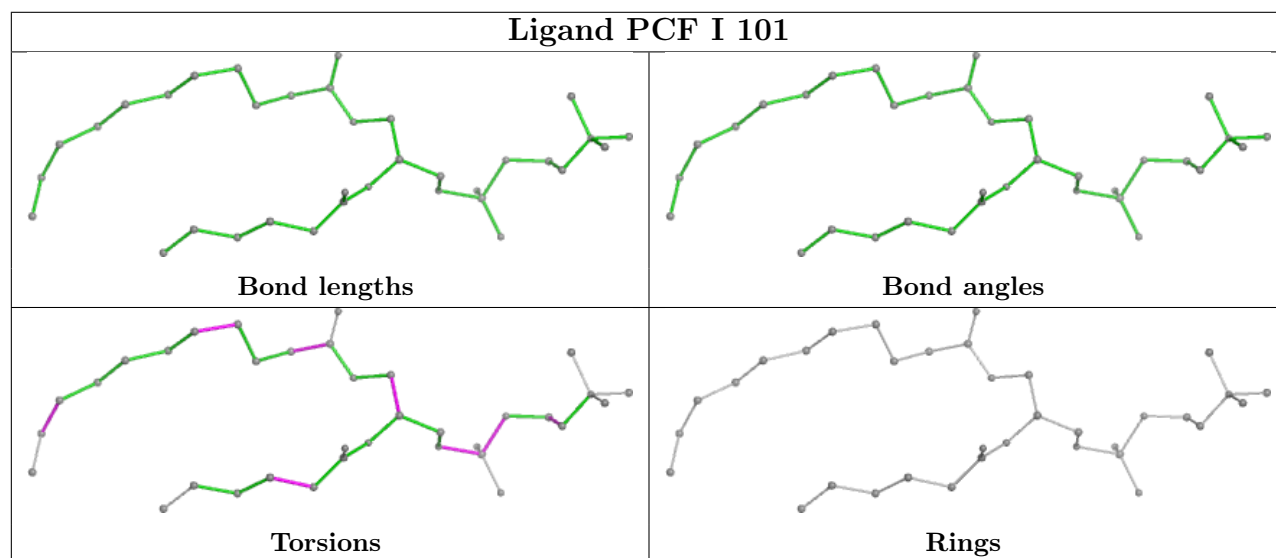
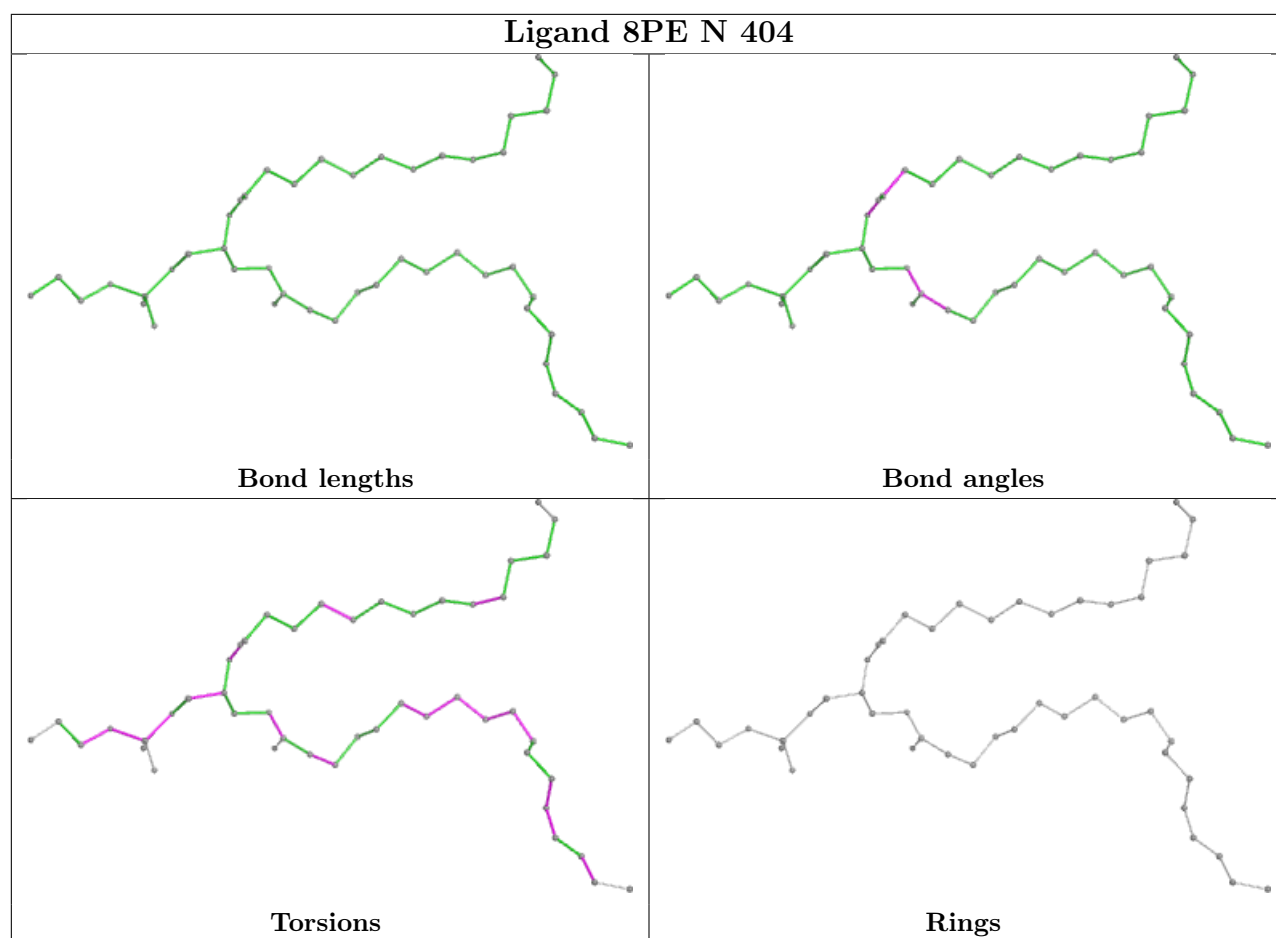


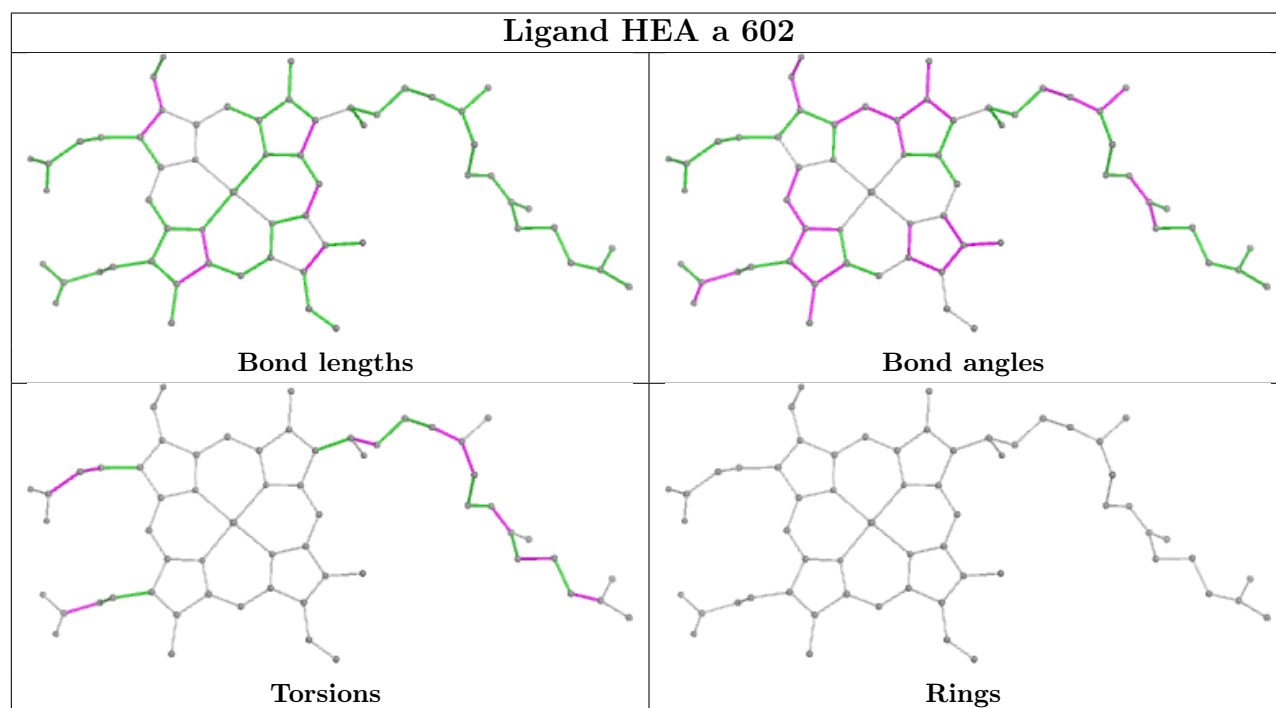
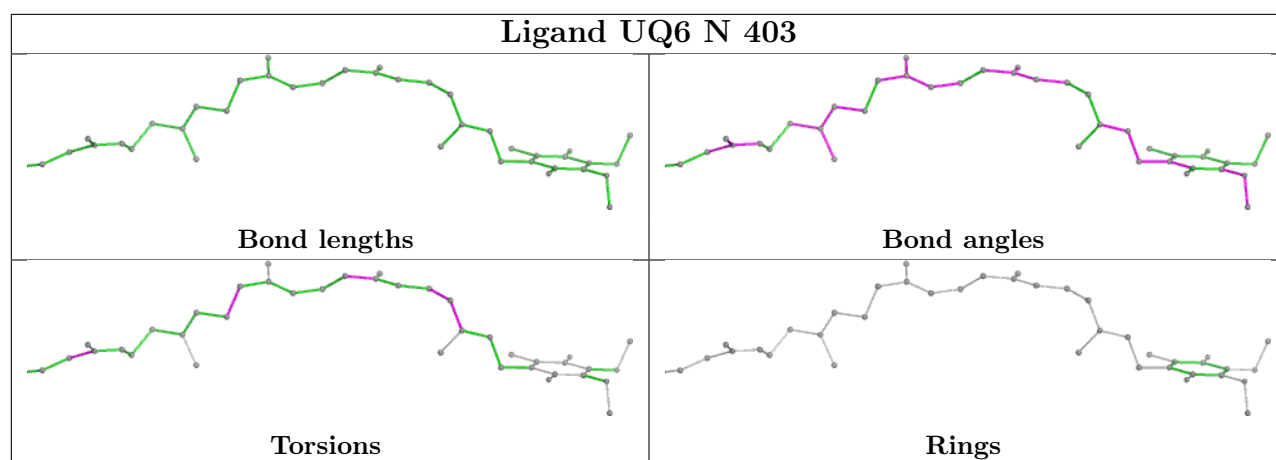


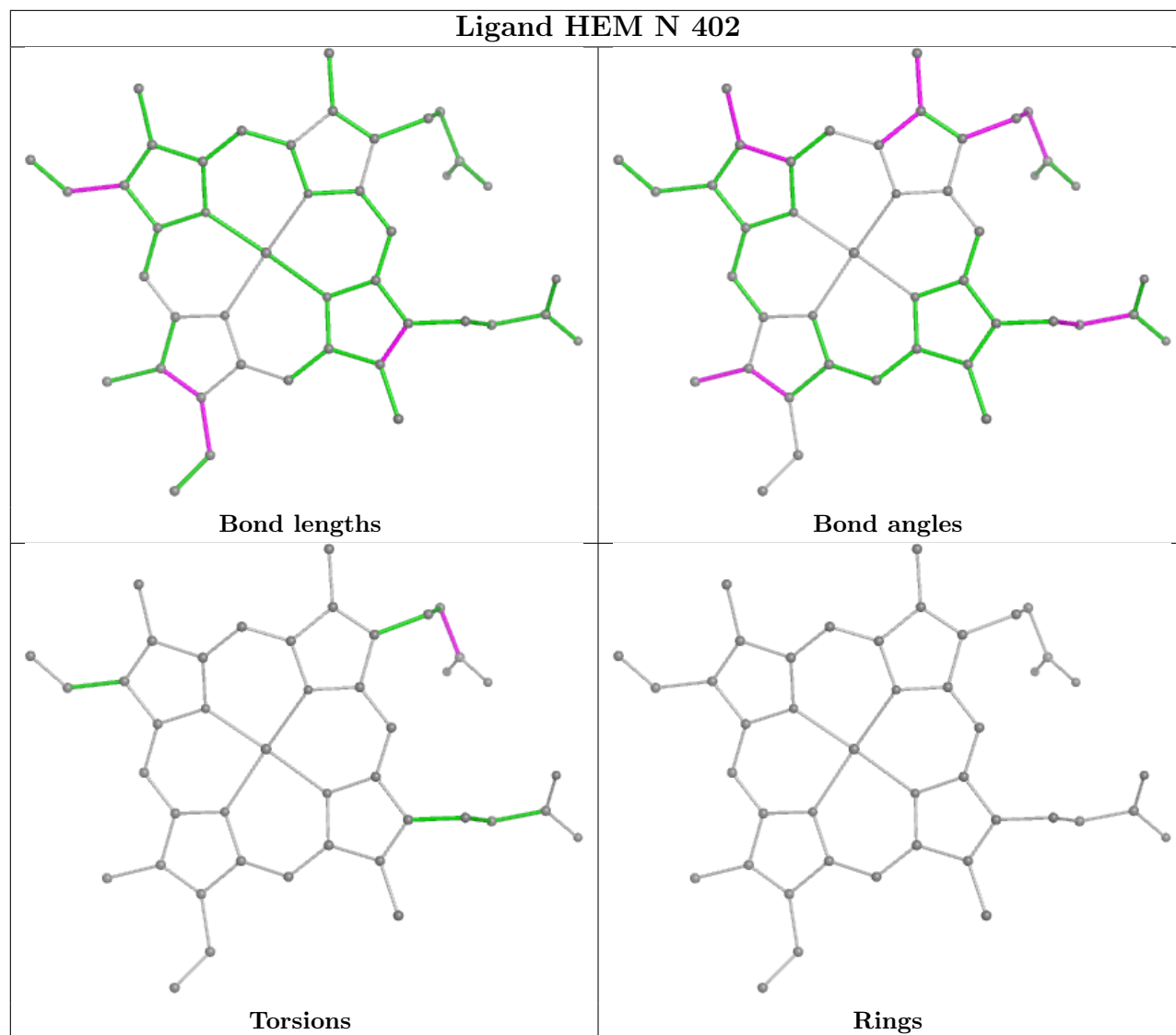


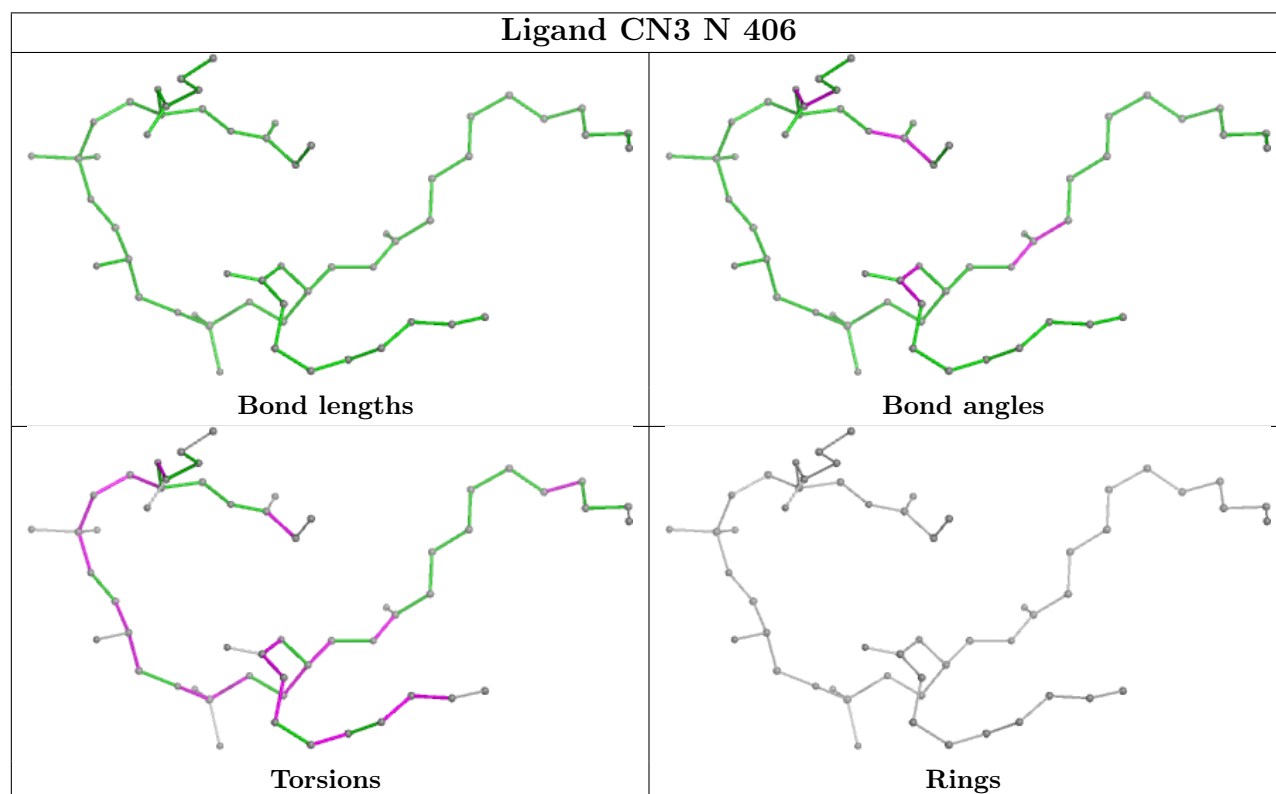
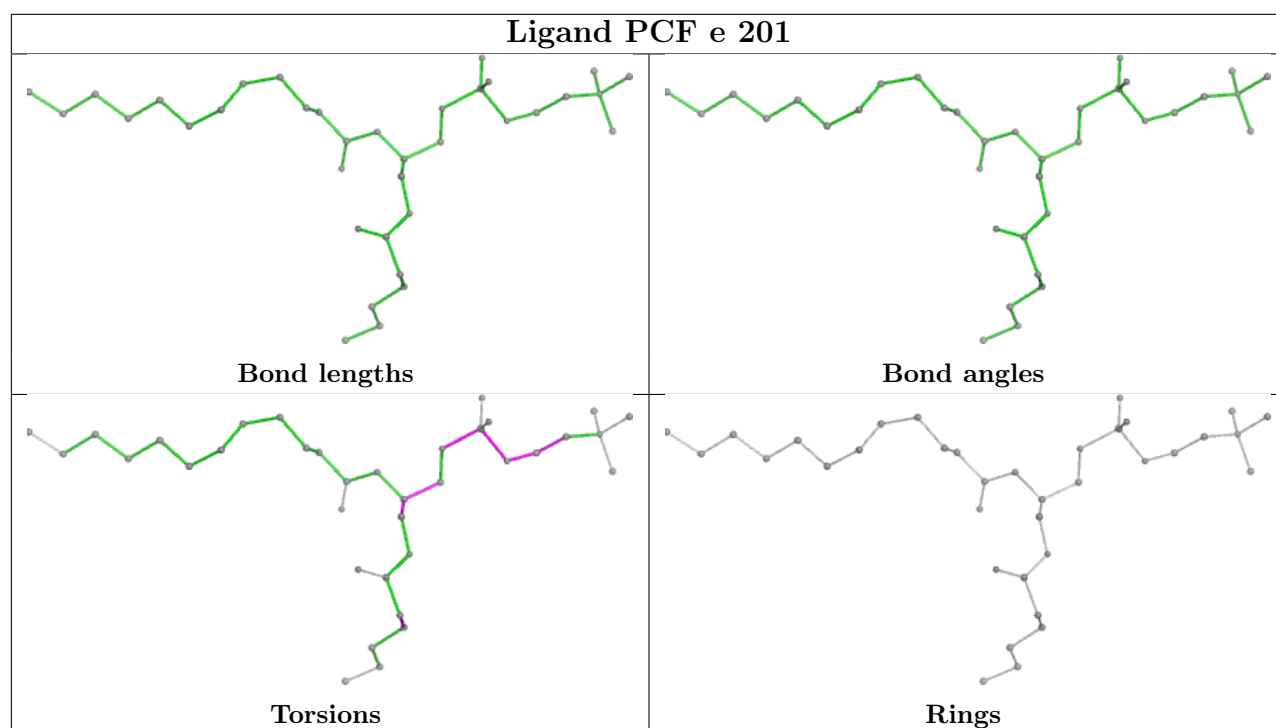


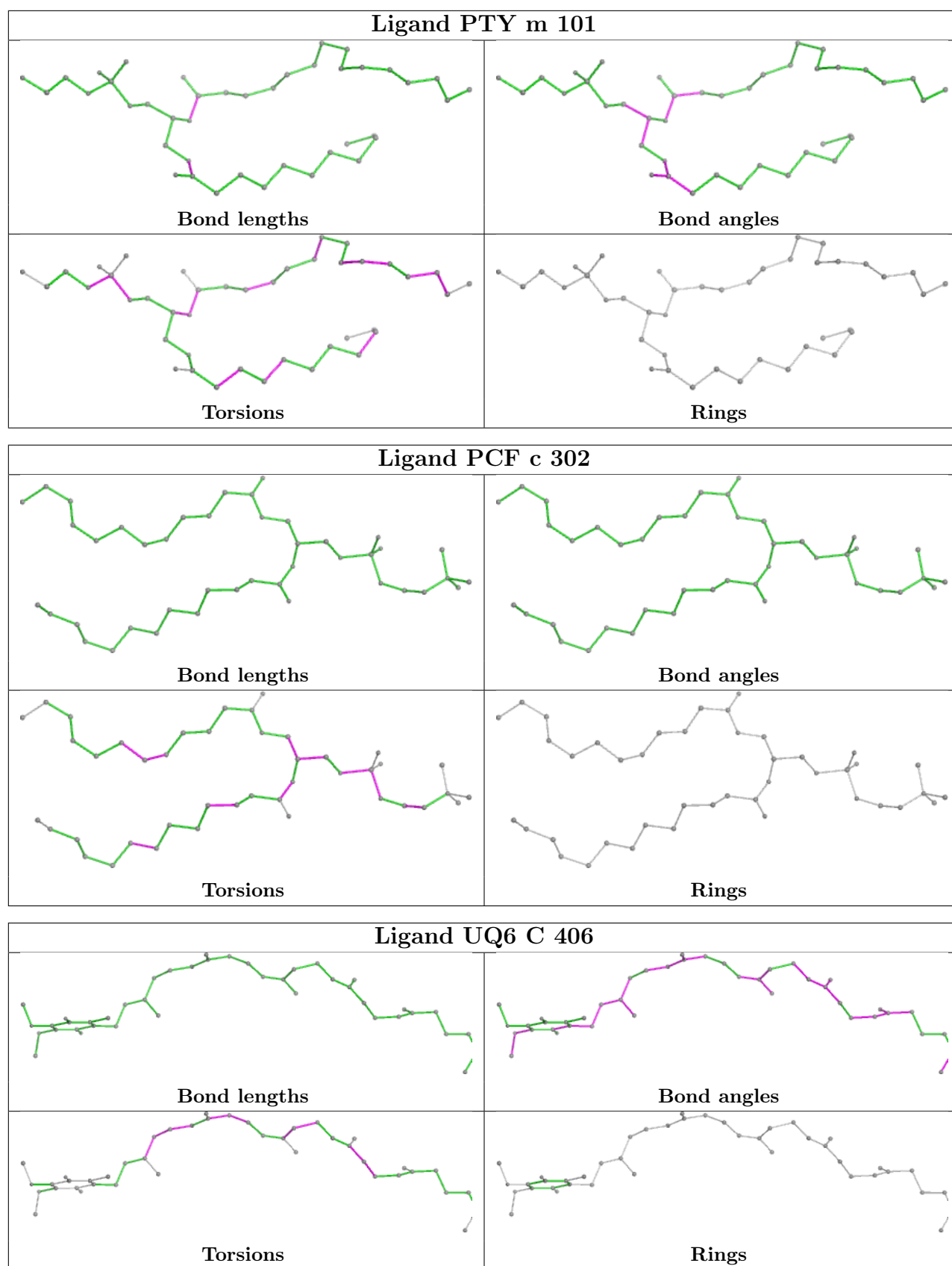


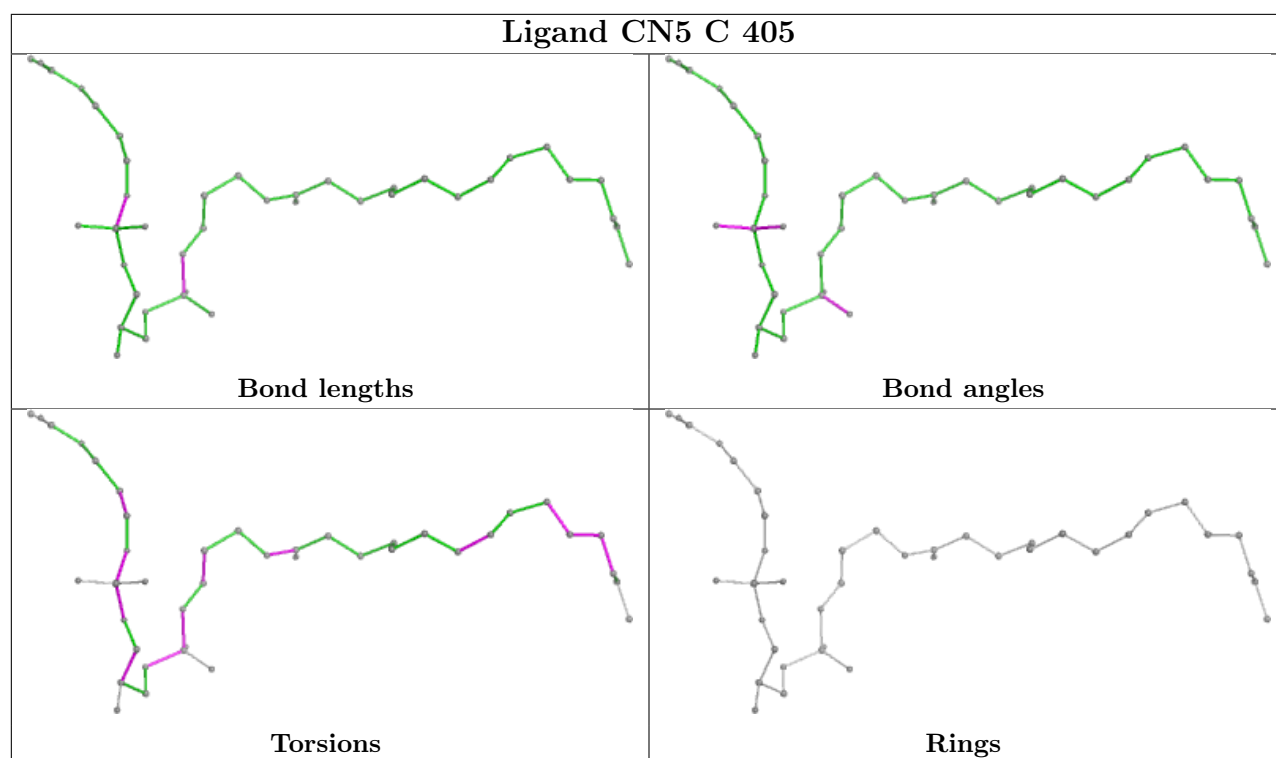












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

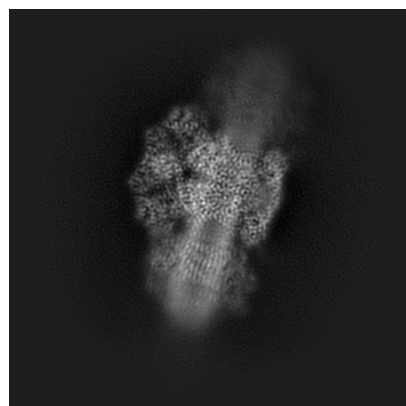
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10847. These allow visual inspection of the internal detail of the map and identification of artifacts.

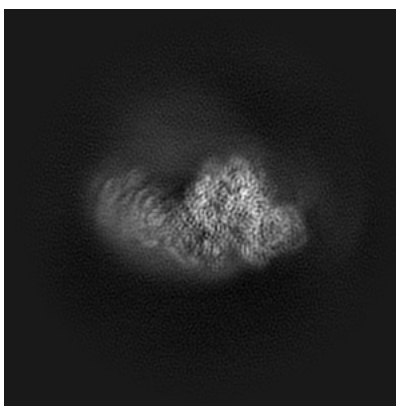
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

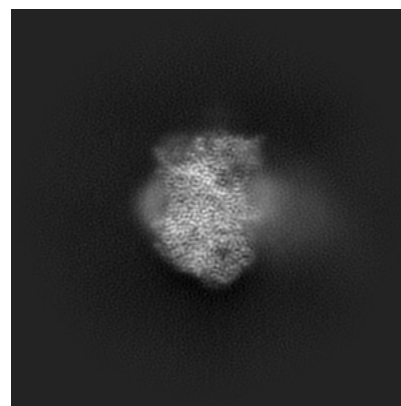
6.1.1 Primary map



X

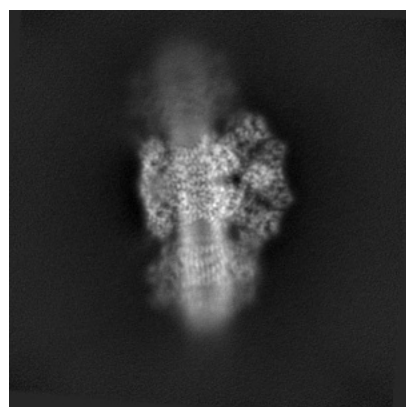


Y

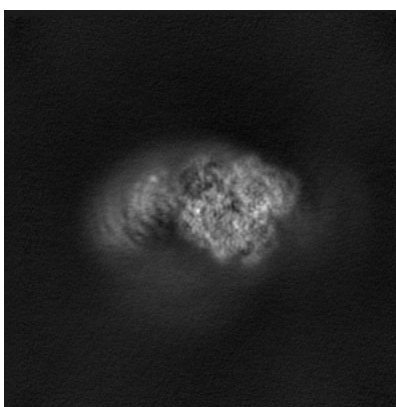


Z

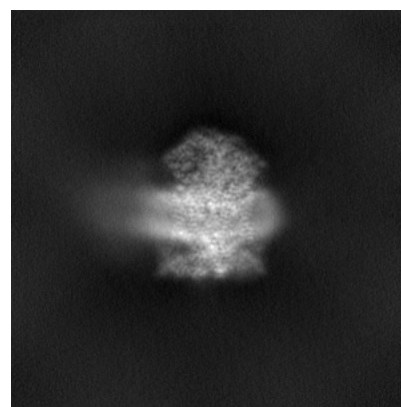
6.1.2 Raw map



X



Y

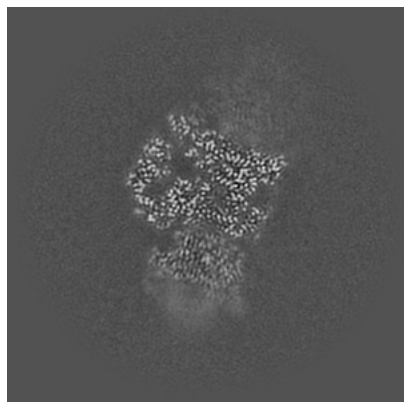


Z

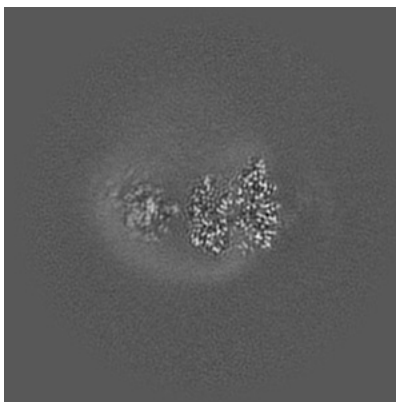
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

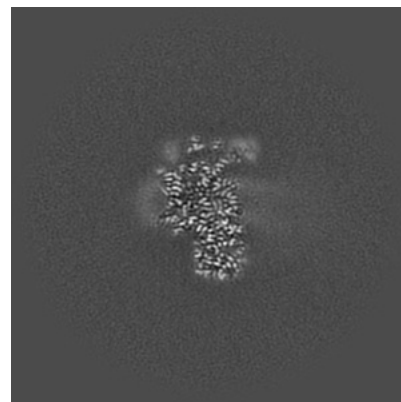
6.2.1 Primary map



X Index: 185

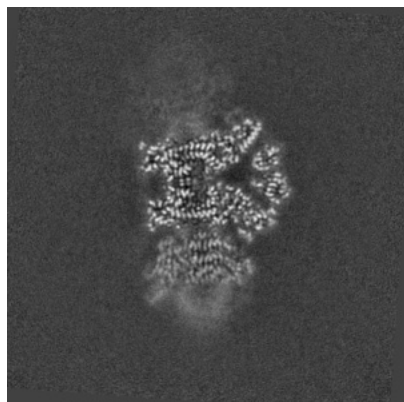


Y Index: 185

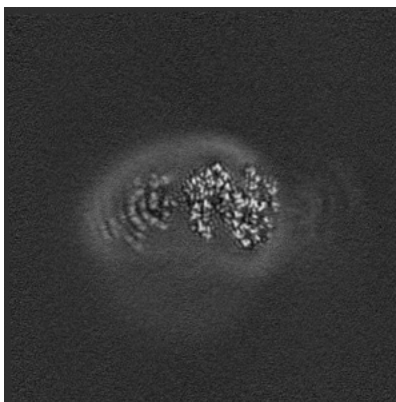


Z Index: 185

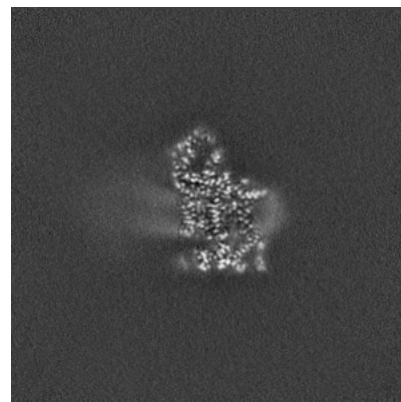
6.2.2 Raw map



X Index: 185



Y Index: 185

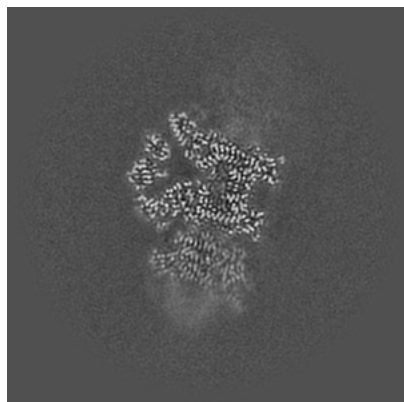


Z Index: 185

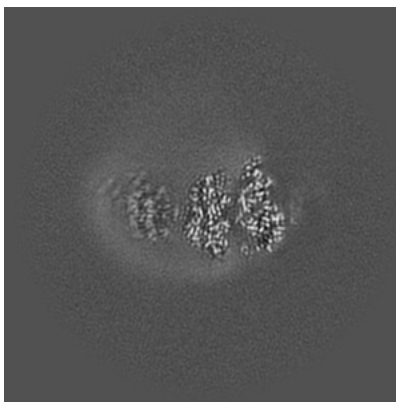
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

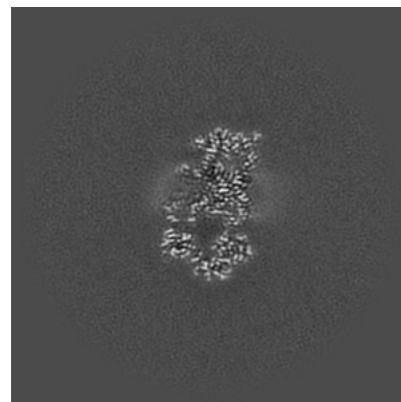
6.3.1 Primary map



X Index: 182

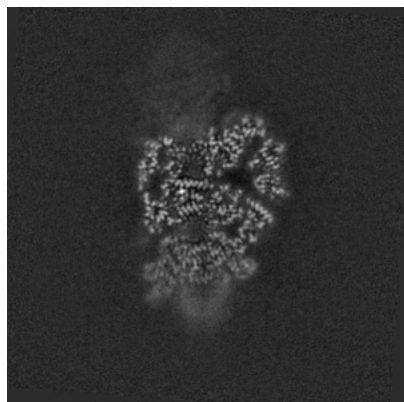


Y Index: 180

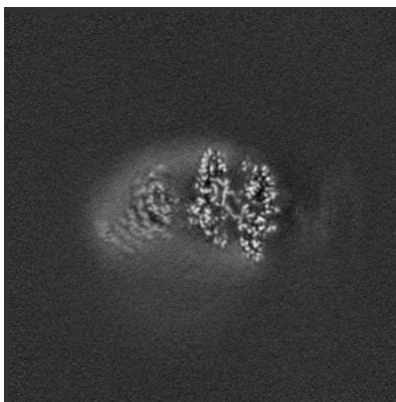


Z Index: 221

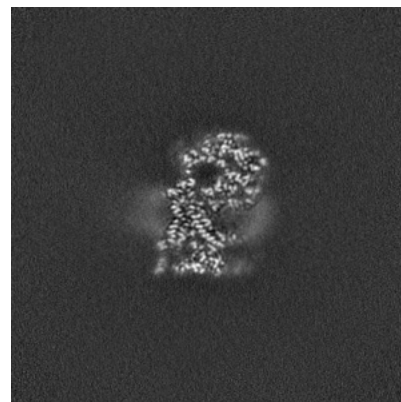
6.3.2 Raw map



X Index: 191



Y Index: 197

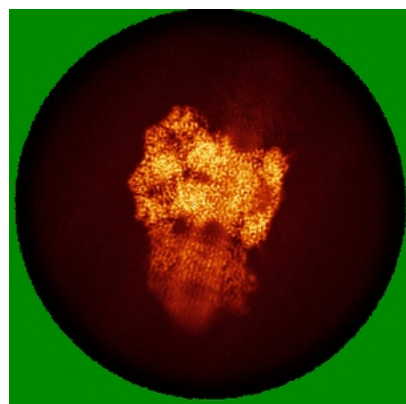


Z Index: 223

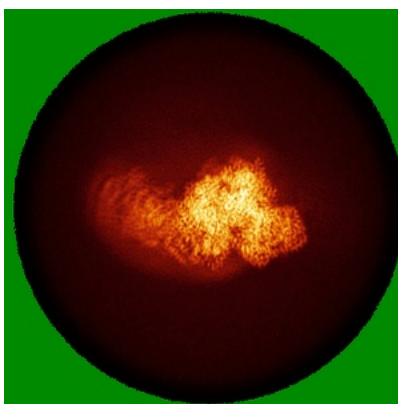
The images above show the largest variance slices of the map in three orthogonal directions.

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

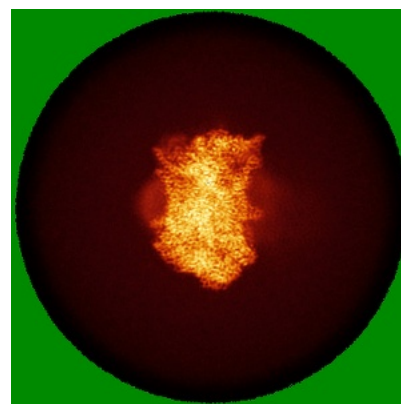
6.4.1 Primary map



X

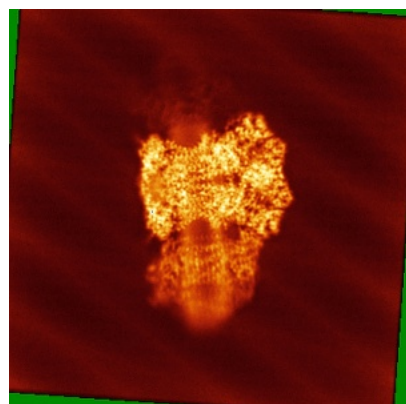


Y

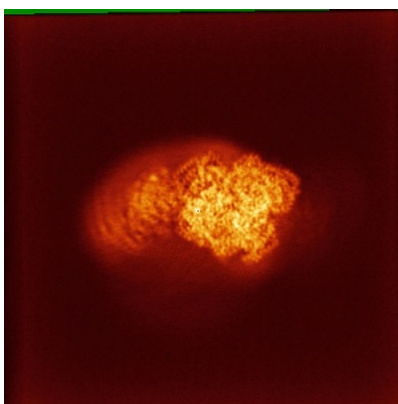


Z

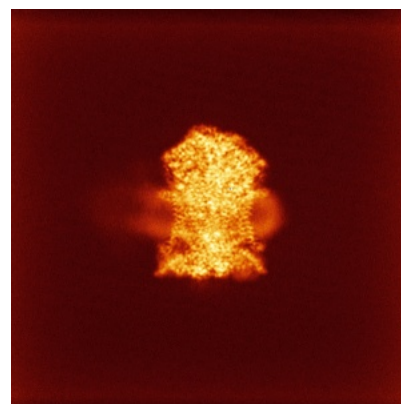
6.4.2 Raw map



X



Y

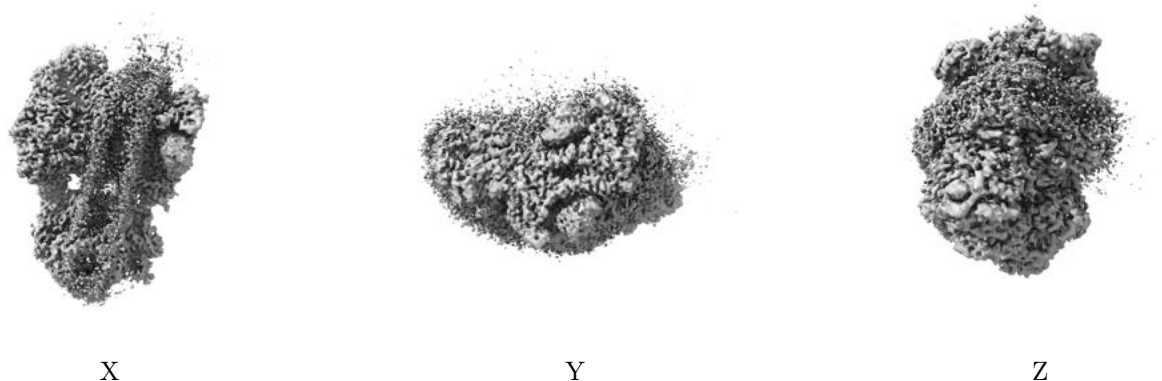


Z

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.

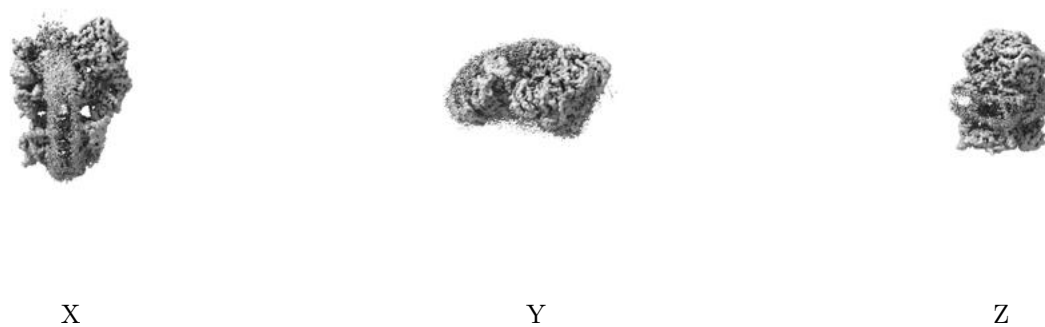
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

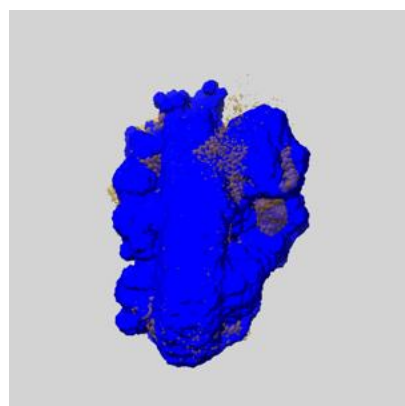
6.6 Mask visualisation [i](#)

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

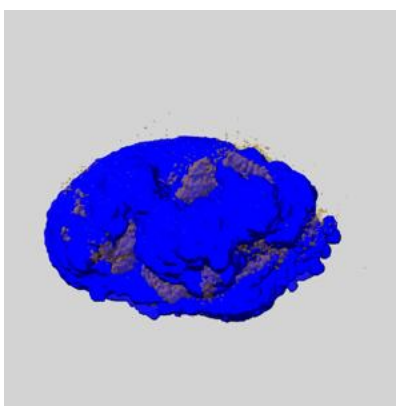
A mask typically either:

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

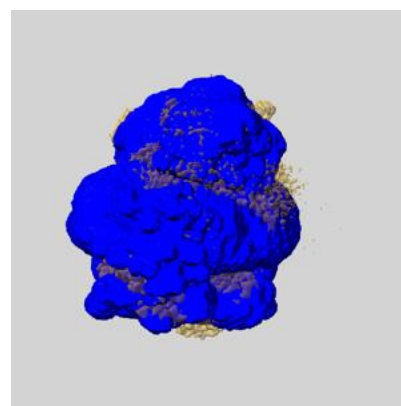
6.6.1 emd_10847_msk_1.map [i](#)



X



Y

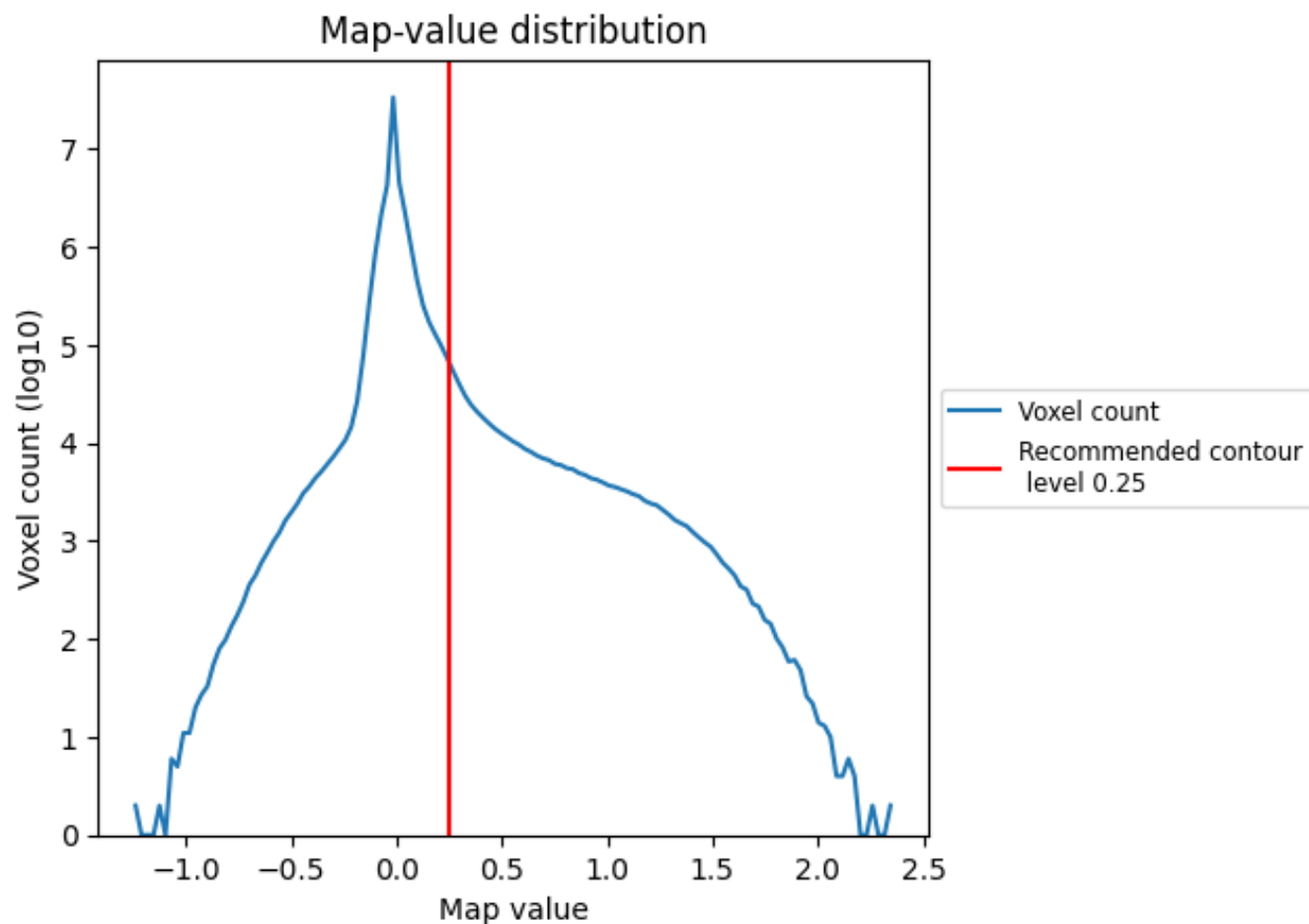


Z

7 Map analysis [i](#)

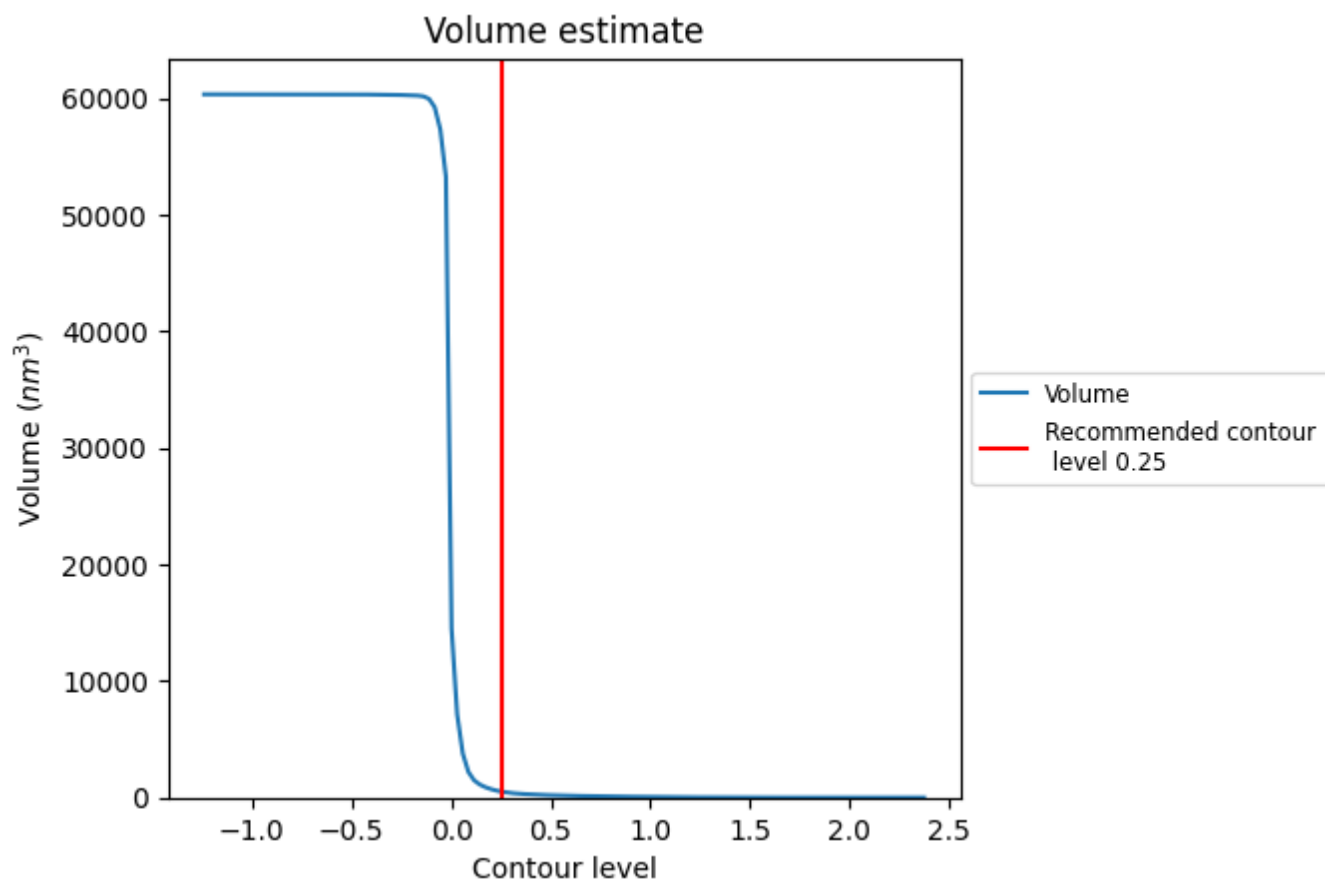
This section contains the results of statistical analysis of the map.

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.

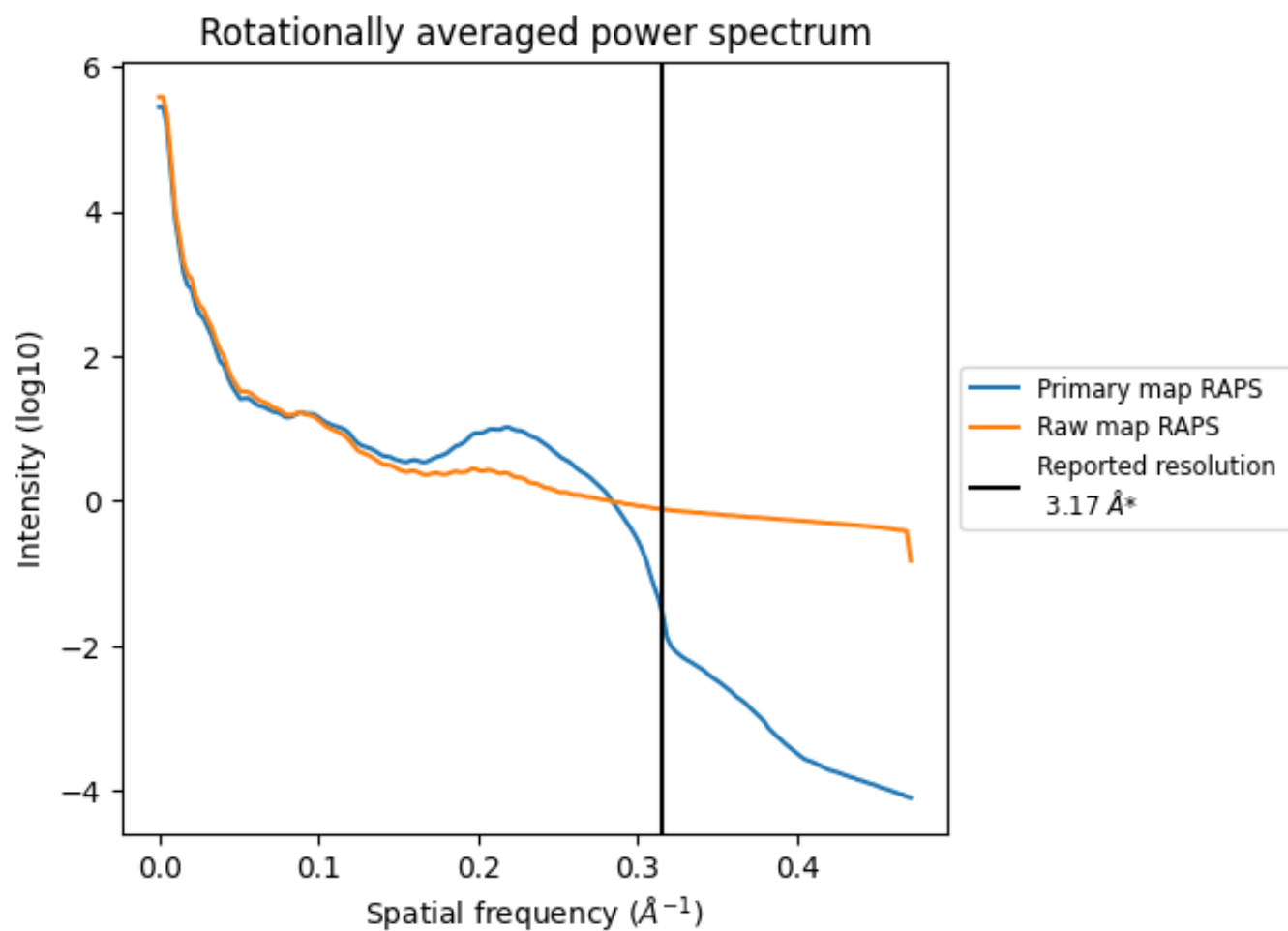
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm³; this corresponds to an approximate mass of 467 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

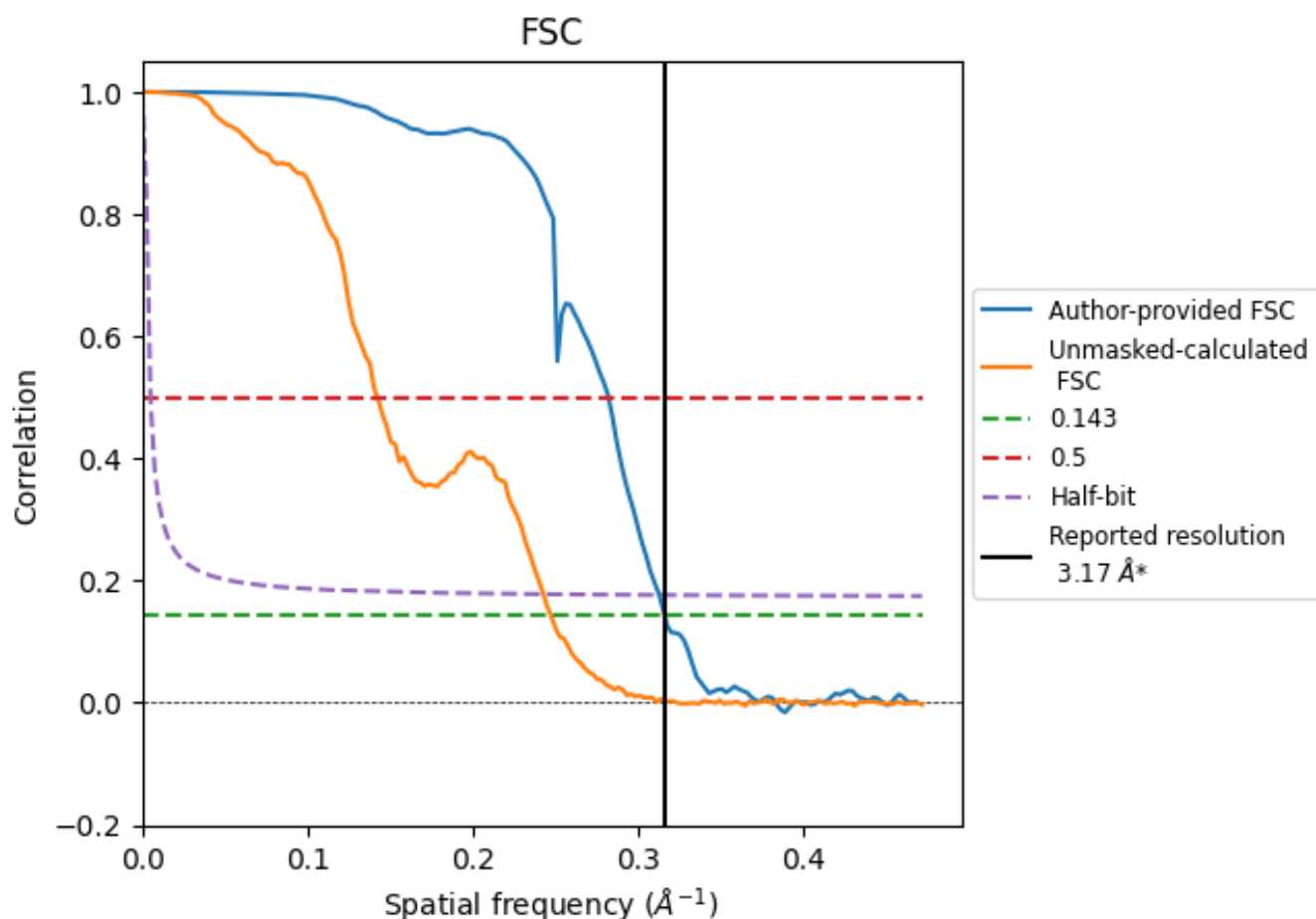


*Reported resolution corresponds to spatial frequency of 0.315 \AA^{-1}

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 0.315 \AA^{-1}

8.2 Resolution estimates [i](#)

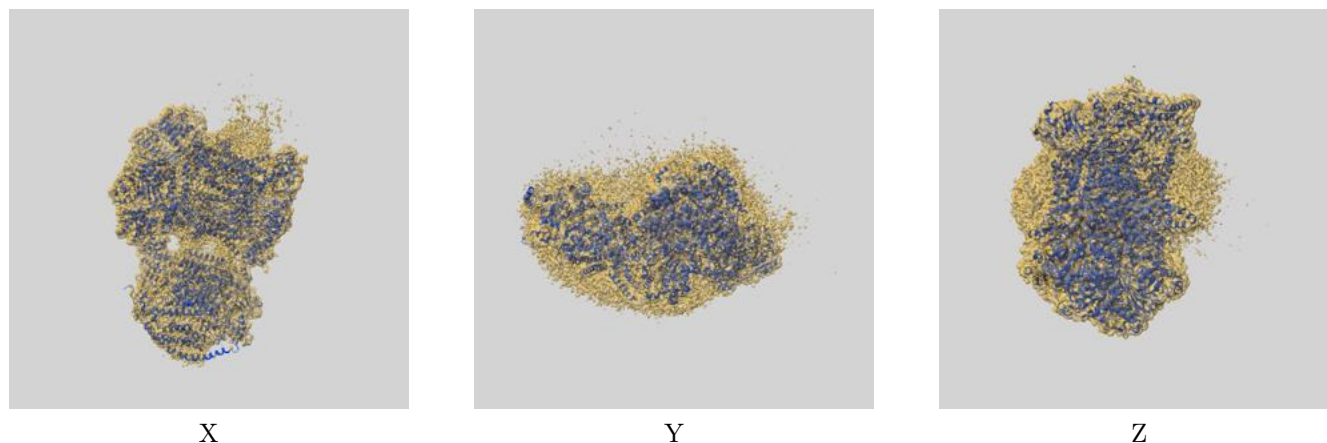
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.16	3.55	3.20
Unmasked-calculated*	4.05	7.03	4.12

*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 4.05 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

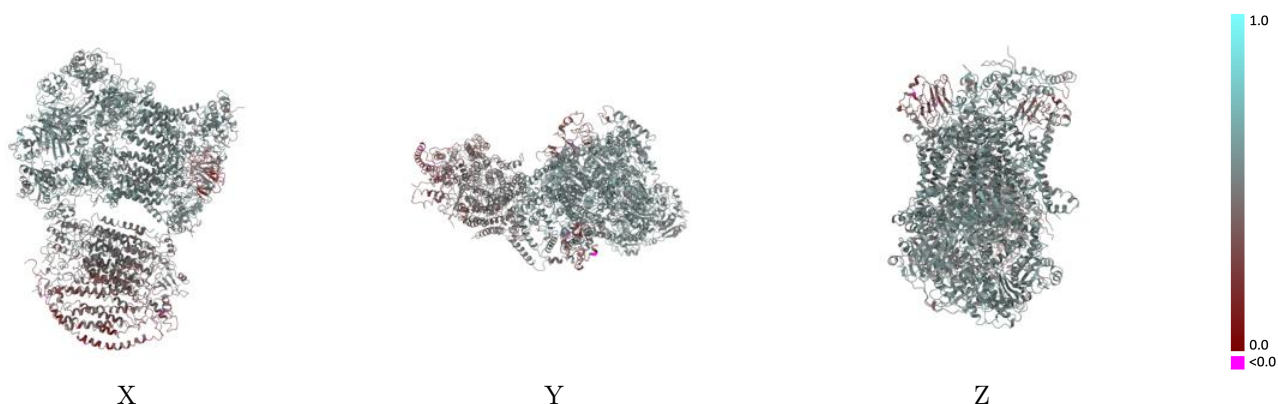
This section contains information regarding the fit between EMDB map EMD-10847 and PDB model 6YMX. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



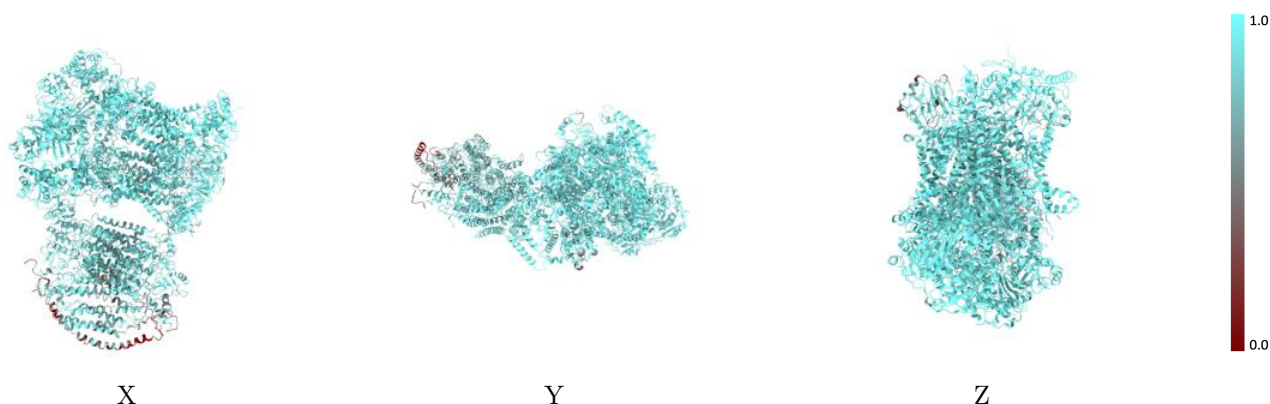
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



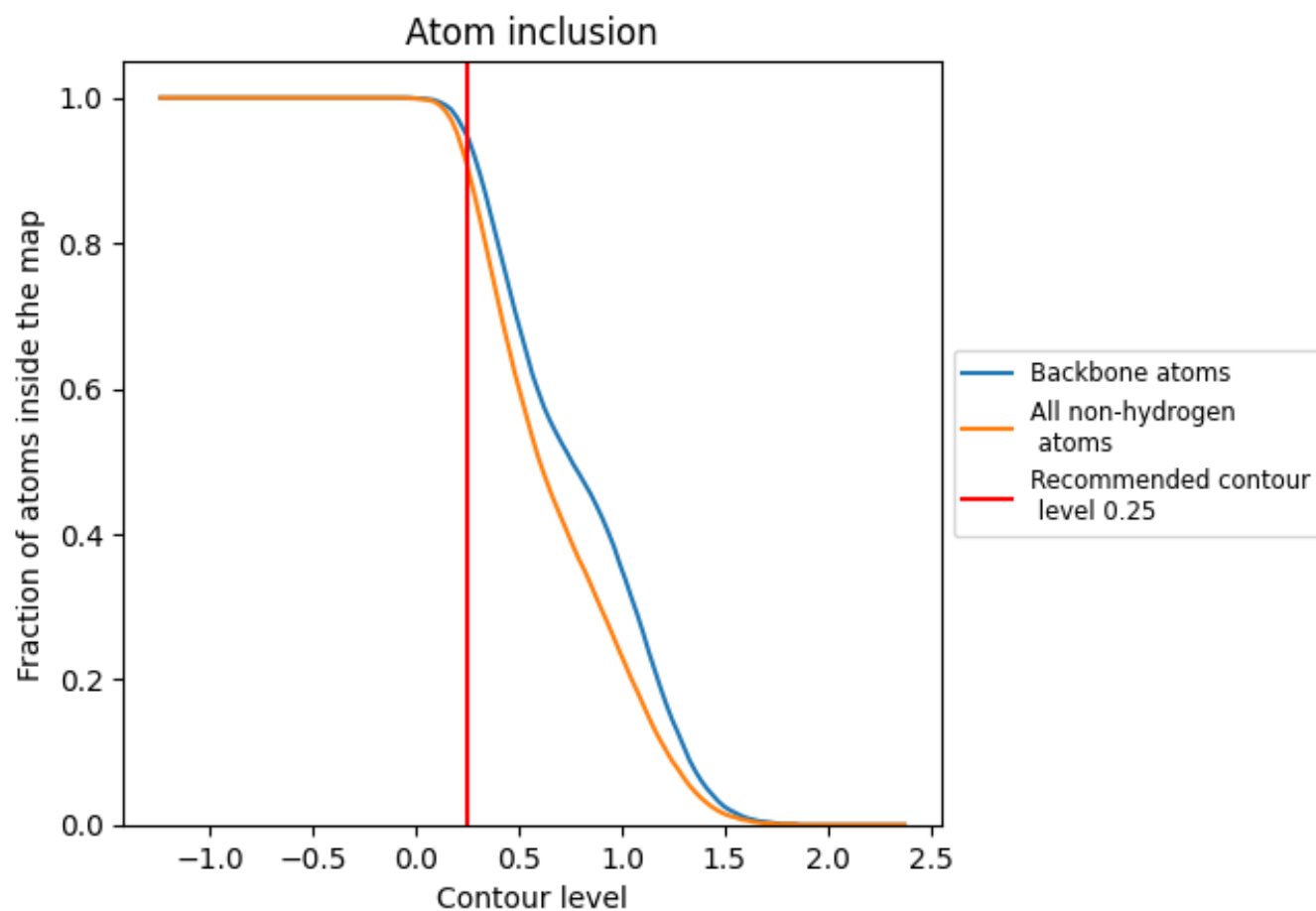
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.4950
A	 0.9640	 0.5440
B	 0.9640	 0.5480
C	 0.9550	 0.5530
D	 0.9490	 0.5420
E	 0.9030	 0.4140
F	 0.9400	 0.5010
G	 0.9540	 0.5420
H	 0.9590	 0.5410
I	 0.9490	 0.5450
L	 0.9640	 0.5370
M	 0.9670	 0.5430
N	 0.9600	 0.5550
O	 0.9660	 0.5490
P	 0.8230	 0.3840
Q	 0.9500	 0.4930
R	 0.9610	 0.5480
S	 0.9570	 0.5330
T	 0.9680	 0.5420
U	 0.9740	 0.5350
V	 0.9170	 0.5200
a	 0.8710	 0.4650
b	 0.8660	 0.4320
c	 0.7780	 0.3600
d	 0.7970	 0.4140
e	 0.8960	 0.4860
f	 0.9280	 0.4360
g	 0.7460	 0.3590
h	 0.8060	 0.4330
i	 0.8800	 0.4280
j	 0.6680	 0.3610
k	 0.3500	 0.2600
m	 0.8170	 0.4300

