



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 08:47 pm GMT

PDB ID : 6ET5
EMDB ID : EMD-3951
Title : Reaction centre light harvesting complex 1 from Blc. viridis
Authors : Qian, P.; Siebert, C.A.; Canniffe, D.P.; Wang, P.; Hunter, C.N.
Deposited on : 2017-10-25
Resolution : 3.00 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:

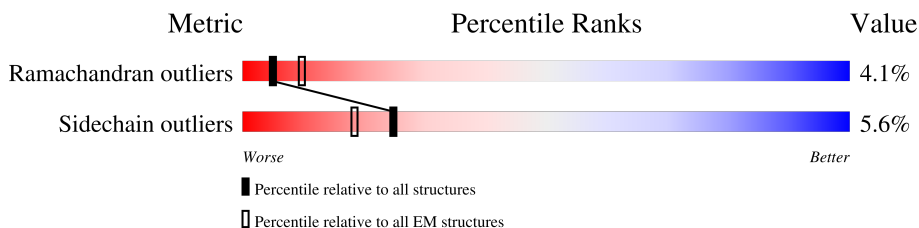
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



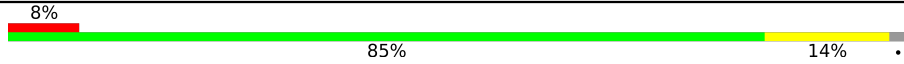

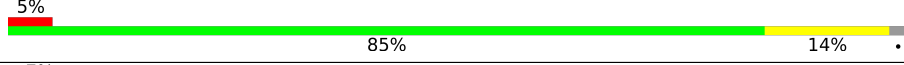

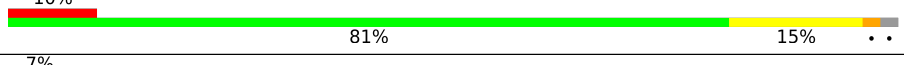
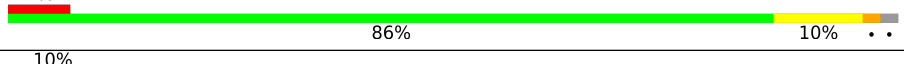
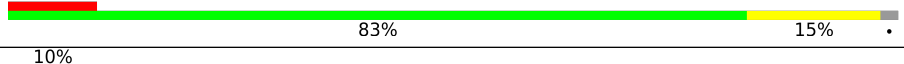

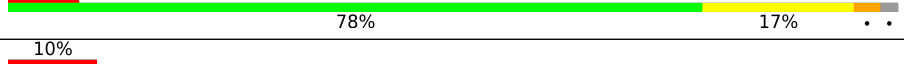


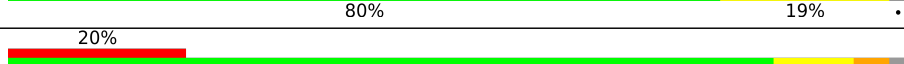
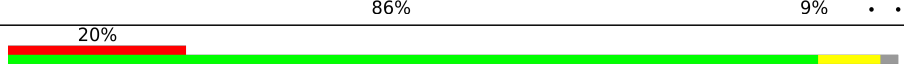
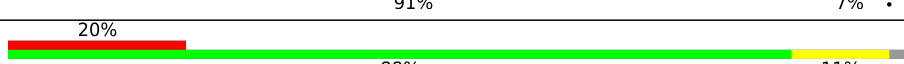

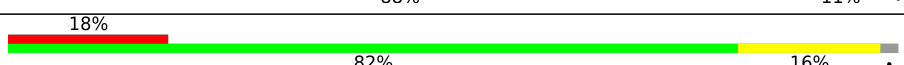
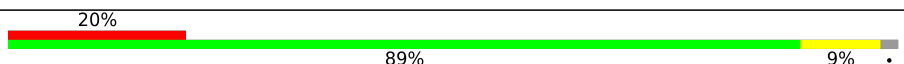
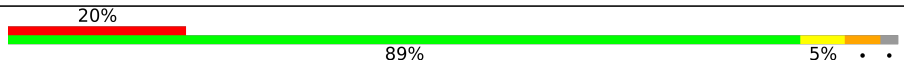
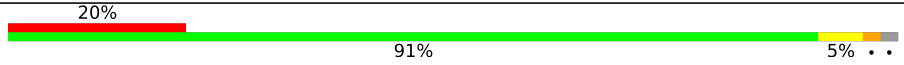
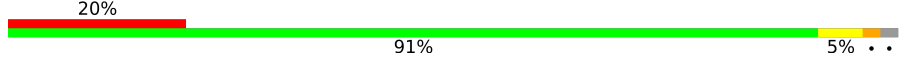
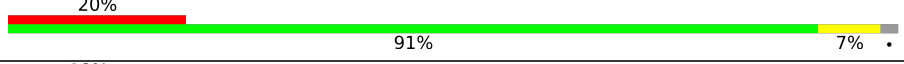
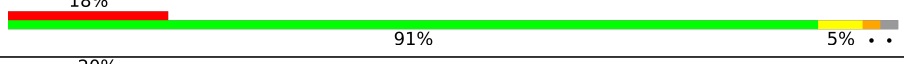
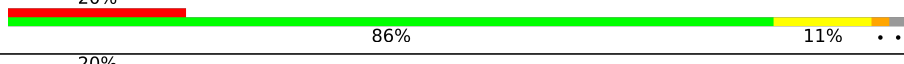


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	C	333	96% .
2	L	274	93% 6% .
3	M	323	96% .
4	H	258	9% 91% 8% .
5	3	59	7% 83% 14% . .
5	6	59	10% 80% 19% .
5	F	59	12% 81% 17% .
5	K	59	10% 85% 14% .
5	P	59	8% 83% 15% .

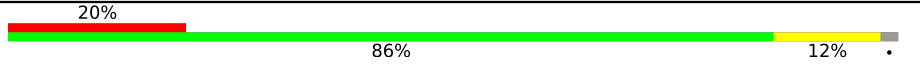

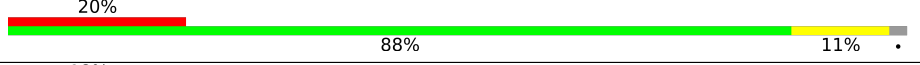



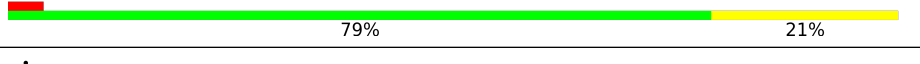

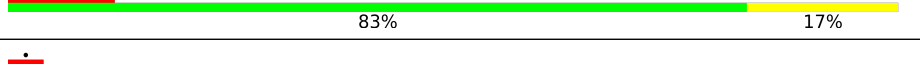


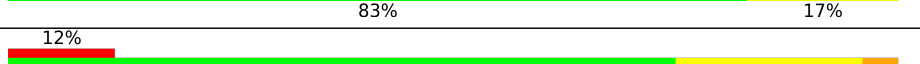

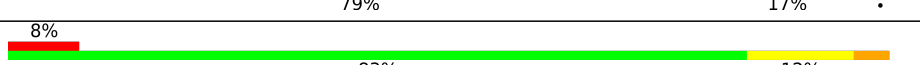

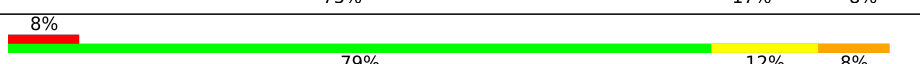
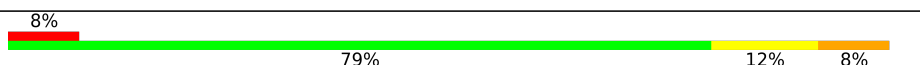
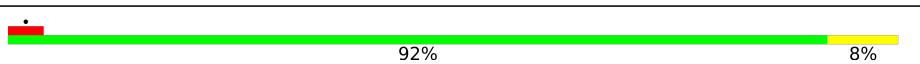
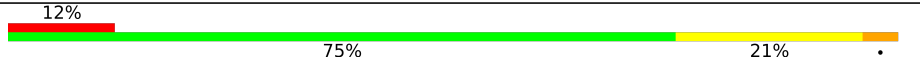

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Mol	Chain	Length	Quality of chain
5	S	59	 8% 85% 14%
5	V	59	 8% 86% 12%
5	Y	59	 5% 85% 14%
5	b	59	 7% 83% 14%
5	e	59	 10% 81% 15%
5	h	59	 7% 86% 10%
5	k	59	 10% 83% 15%
5	n	59	 10% 85% 14%
5	q	59	 8% 78% 17%
5	t	59	 10% 85% 14%
5	w	59	 7% 80% 19%
5	z	59	 7% 80% 19%
6	1	56	 20% 86% 9%
6	4	56	 20% 91% 7%
6	7	56	 20% 88% 11%
6	G	56	 20% 88% 11%
6	N	56	 18% 82% 16%
6	Q	56	 20% 89% 9%
6	T	56	 20% 89% 5%
6	W	56	 20% 91% 5%
6	Z	56	 20% 91% 5%
6	c	56	 20% 91% 7%
6	f	56	 18% 91% 5%
6	i	56	 20% 86% 11%
6	l	56	 20% 86% 12%

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Mol	Chain	Length	Quality of chain
6	o	56	
6	r	56	
6	u	56	
6	x	56	
7	2	24	
7	5	24	
7	I	24	
7	O	24	
7	R	24	
7	U	24	
7	X	24	
7	a	24	
7	d	24	
7	g	24	
7	j	24	
7	m	24	
7	p	24	
7	s	24	
7	v	24	
7	y	24	

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
10	BPB	L	303	X	-	-	-
10	BPB	M	407	X	-	-	-
17	NS0	1	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	NS0	4	102	-	X	-	-
17	NS0	7	102	-	X	-	-
17	NS0	G	102	-	X	-	-
17	NS0	N	102	-	X	-	-
17	NS0	Q	102	-	X	-	-
17	NS0	T	102	-	X	-	-
17	NS0	W	102	-	X	-	-
17	NS0	Z	102	-	X	-	-
17	NS0	c	102	-	X	-	-
17	NS0	f	102	-	X	-	-
17	NS0	i	102	-	X	-	-
17	NS0	l	102	-	X	-	-
17	NS0	o	102	-	X	-	-
17	NS0	r	102	-	X	-	-
17	NS0	u	102	-	X	-	-
17	NS0	x	102	-	X	-	-

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31994 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	333	2603	1640	467	478	18	0	1

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	273	2171	1459	350	355	7	0	0

- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	323	2555	1702	419	423	11	0	0

- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	258	2018	1292	344	380	2	0	0

- Molecule 5 is a protein called Light-harvesting protein B-1015 alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	z	58	487	327	83	77	0	0
5	F	58	487	327	83	77	0	0
5	K	58	487	327	83	77	0	0
5	P	58	487	327	83	77	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	58	Total 487	C 327	N 83	O 77	0	0
5	V	58	Total 487	C 327	N 83	O 77	0	0
5	Y	58	Total 487	C 327	N 83	O 77	0	0
5	b	58	Total 487	C 327	N 83	O 77	0	0
5	e	58	Total 487	C 327	N 83	O 77	0	0
5	h	58	Total 487	C 327	N 83	O 77	0	0
5	k	58	Total 487	C 327	N 83	O 77	0	0
5	n	58	Total 487	C 327	N 83	O 77	0	0
5	q	58	Total 487	C 327	N 83	O 77	0	0
5	t	58	Total 487	C 327	N 83	O 77	0	0
5	w	58	Total 487	C 327	N 83	O 77	0	0
5	3	58	Total 487	C 327	N 83	O 77	0	0
5	6	58	Total 487	C 327	N 83	O 77	0	0

- Molecule 6 is a protein called Light-harvesting protein B-1015 beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	1	55	Total 436	C 293	N 68	O 75	0	0
6	G	55	Total 436	C 293	N 68	O 75	0	0
6	N	55	Total 436	C 293	N 68	O 75	0	0
6	Q	55	Total 436	C 293	N 68	O 75	0	0
6	T	55	Total 436	C 293	N 68	O 75	0	0
6	W	55	Total 436	C 293	N 68	O 75	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	Z	55	Total	C	N	O	0	0
			436	293	68	75		
6	c	55	Total	C	N	O	0	0
			436	293	68	75		
6	f	55	Total	C	N	O	0	0
			436	293	68	75		
6	i	55	Total	C	N	O	0	0
			436	293	68	75		
6	l	55	Total	C	N	O	0	0
			436	293	68	75		
6	o	55	Total	C	N	O	0	0
			436	293	68	75		
6	r	55	Total	C	N	O	0	0
			436	293	68	75		
6	u	55	Total	C	N	O	0	0
			436	293	68	75		
6	x	55	Total	C	N	O	0	0
			436	293	68	75		
6	4	55	Total	C	N	O	0	0
			436	293	68	75		
6	7	55	Total	C	N	O	0	0
			436	293	68	75		

- Molecule 7 is a protein called Light-harvesting protein B-1015 gamma chain.

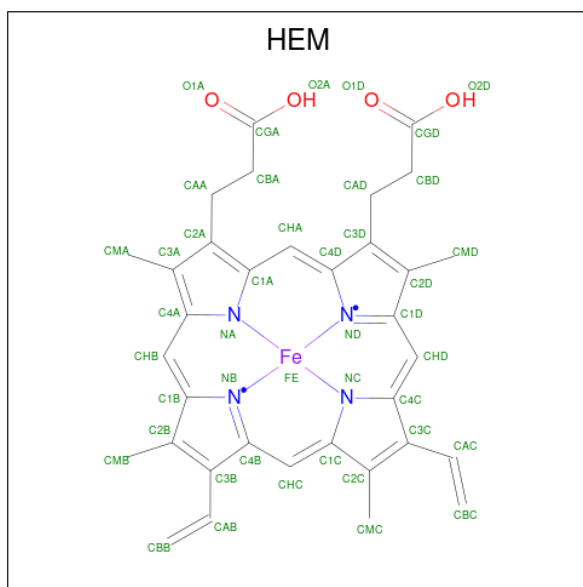
Mol	Chain	Residues	Atoms				AltConf	Trace
7	2	24	Total	C	N	O	0	0
			199	137	31	31		
7	I	24	Total	C	N	O	0	0
			199	137	31	31		
7	O	24	Total	C	N	O	0	0
			199	137	31	31		
7	R	24	Total	C	N	O	0	0
			199	137	31	31		
7	U	24	Total	C	N	O	0	0
			199	137	31	31		
7	X	24	Total	C	N	O	0	0
			199	137	31	31		
7	a	24	Total	C	N	O	0	0
			199	137	31	31		
7	d	24	Total	C	N	O	0	0
			199	137	31	31		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	g	24	Total 199	C 137	N 31	O 31	0	0
7	j	24	Total 199	C 137	N 31	O 31	0	0
7	m	24	Total 199	C 137	N 31	O 31	0	0
7	p	24	Total 199	C 137	N 31	O 31	0	0
7	s	24	Total 199	C 137	N 31	O 31	0	0
7	v	24	Total 199	C 137	N 31	O 31	0	0
7	y	24	Total 199	C 137	N 31	O 31	0	0
7	5	24	Total 199	C 137	N 31	O 31	0	0

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



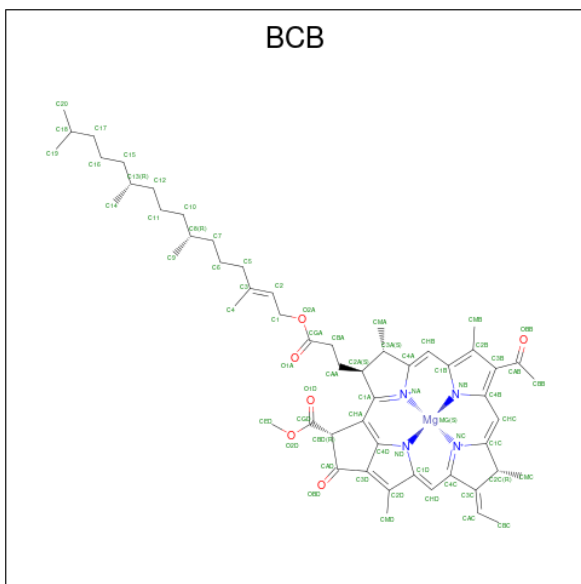
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
8	C	1	Total 172	C 136	Fe 4	N 16	O 16	0
8	C	1	Total 172	C 136	Fe 4	N 16	O 16	0
8	C	1	Total 172	C 136	Fe 4	N 16	O 16	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
8	C	1	172	136	4	16	16	0

- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	L	1	132	110	2	8	12	0
9	L	1	132	110	2	8	12	0
9	M	1	132	110	2	8	12	0
9	M	1	132	110	2	8	12	0
9	z	1	66	55	1	4	6	0
9	1	1	66	55	1	4	6	0
9	F	1	66	55	1	4	6	0
9	K	1	66	55	1	4	6	0
9	P	1	66	55	1	4	6	0
9	S	1	66	55	1	4	6	0

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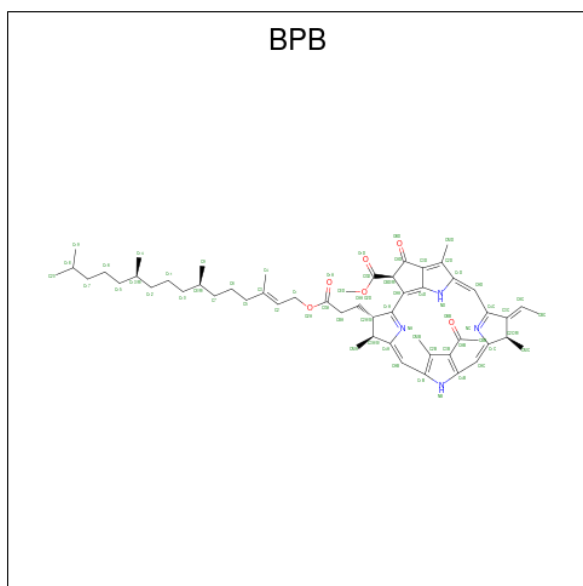
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	V	1	66	55	1	4	6	0
9	Y	1	66	55	1	4	6	0
9	b	1	66	55	1	4	6	0
9	e	1	66	55	1	4	6	0
9	h	1	66	55	1	4	6	0
9	k	1	66	55	1	4	6	0
9	n	1	66	55	1	4	6	0
9	q	1	66	55	1	4	6	0
9	t	1	66	55	1	4	6	0
9	w	1	66	55	1	4	6	0
9	3	1	66	55	1	4	6	0
9	6	1	66	55	1	4	6	0
9	G	1	66	55	1	4	6	0
9	N	1	66	55	1	4	6	0
9	Q	1	66	55	1	4	6	0
9	T	1	66	55	1	4	6	0
9	W	1	66	55	1	4	6	0
9	Z	1	66	55	1	4	6	0
9	c	1	66	55	1	4	6	0
9	f	1	66	55	1	4	6	0
9	i	1	66	55	1	4	6	0

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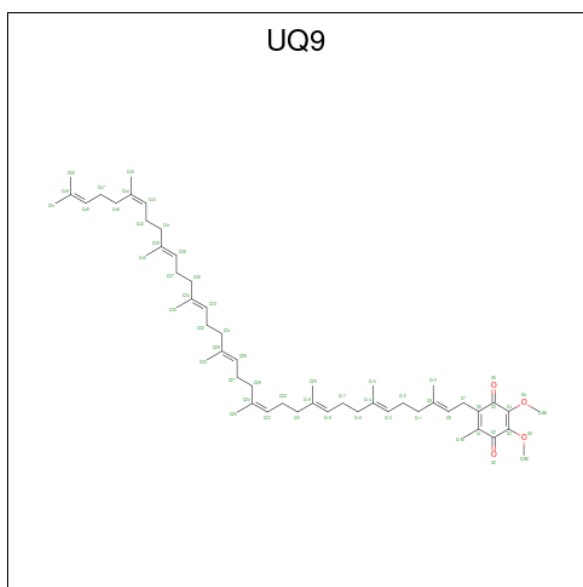
Mol	Chain	Residues	Atoms				AltConf	
9	l	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	x	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



Mol	Chain	Residues	Atoms			AltConf	
10	L	1	Total	C	N	O	0
			65	55	4	6	
10	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 11 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$).

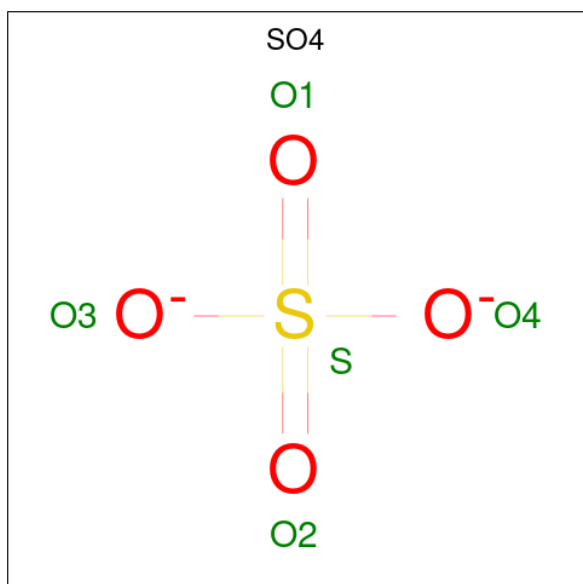


Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			58	54	4	
11	6	1	Total	C	O	0
			58	54	4	

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

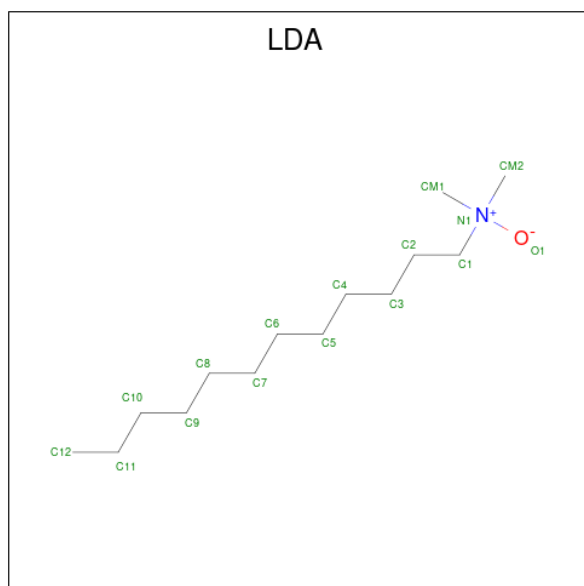
Mol	Chain	Residues	Atoms		AltConf
12	L	1	Total	Fe	0
			1	1	

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



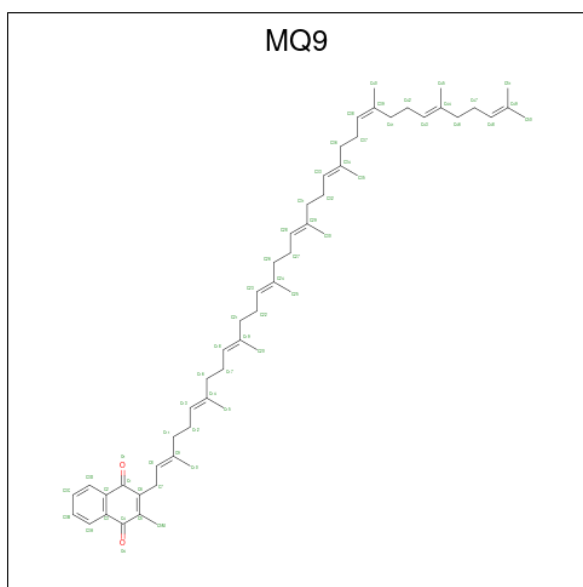
Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	O	S	0
			20	16	4	
13	M	1	Total	O	S	0
			20	16	4	
13	M	1	Total	O	S	0
			20	16	4	
13	M	1	Total	O	S	0
			20	16	4	
13	H	1	Total	O	S	0
			15	12	3	
13	H	1	Total	O	S	0
			15	12	3	
13	H	1	Total	O	S	0
			15	12	3	

- Molecule 14 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



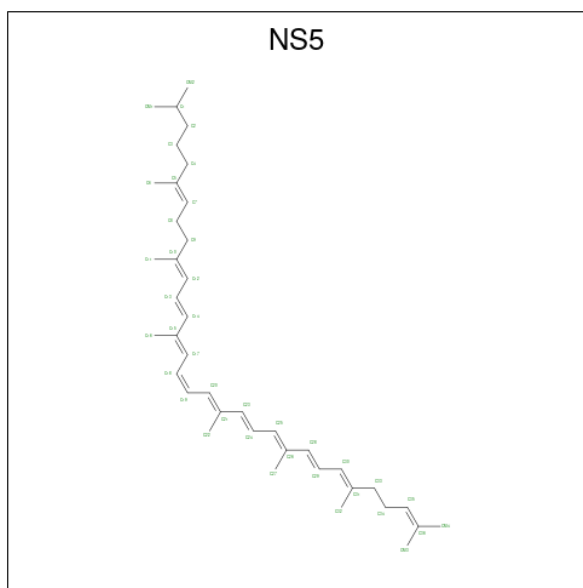
Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	N	O	0
			16	14	1	1	
14	H	1	Total	C	N	O	0
			16	14	1	1	

- Molecule 15 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



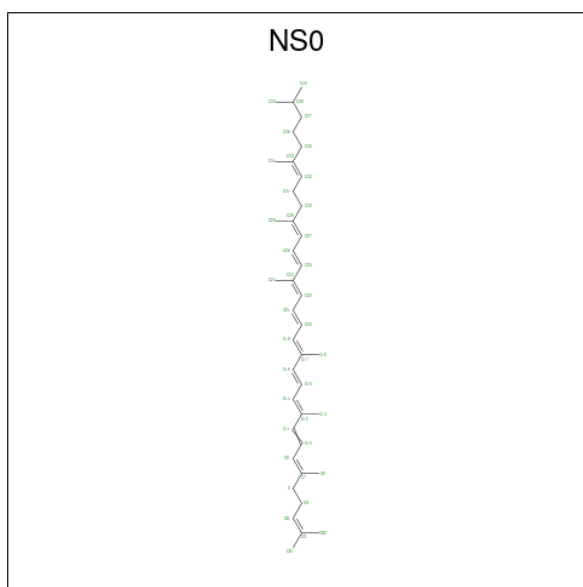
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	M	1	58	56	2	0

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
16	M	1	40	40	0

- Molecule 17 is all-trans-1,2-dihydroneurosporene (three-letter code: NS0) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms	AltConf
17	1	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	N	1	Total C 40 40	0
17	Q	1	Total C 40 40	0
17	T	1	Total C 40 40	0
17	W	1	Total C 40 40	0
17	Z	1	Total C 40 40	0
17	c	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	o	1	Total C 40 40	0
17	r	1	Total C 40 40	0
17	u	1	Total C 40 40	0

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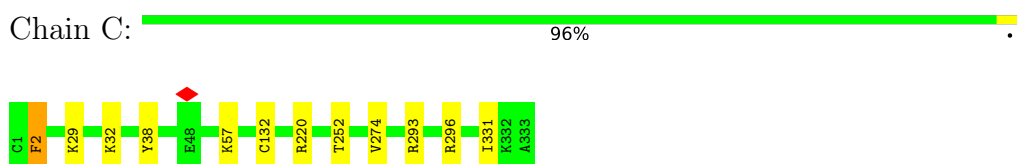
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Mol	Chain	Residues	Atoms	AltConf
17	x	1	Total C 40 40	0
17	4	1	Total C 40 40	0
17	7	1	Total C 40 40	0

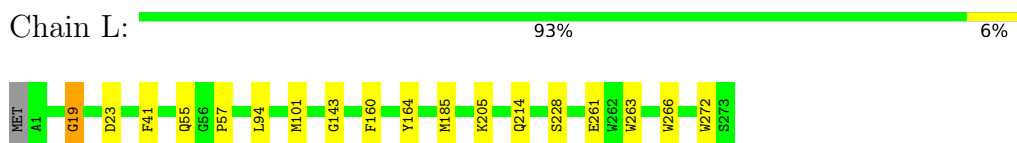
3 Residue-property plots [i](#)

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

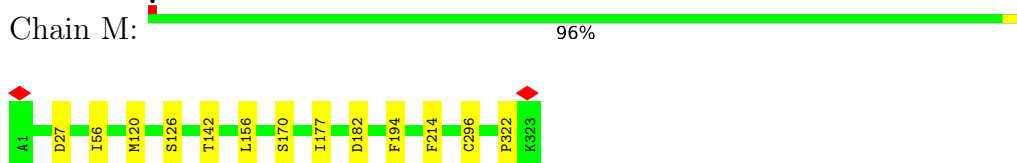
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



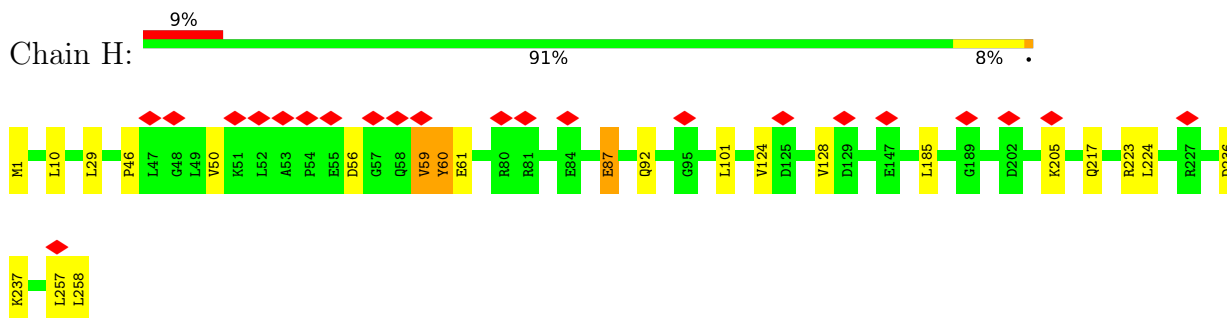
- Molecule 2: Reaction center protein L chain



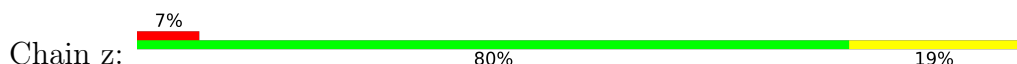
- Molecule 3: Reaction center protein M chain



- Molecule 4: Reaction center protein H chain

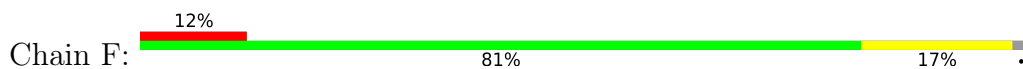


- Molecule 5: Light-harvesting protein B-1015 alpha chain

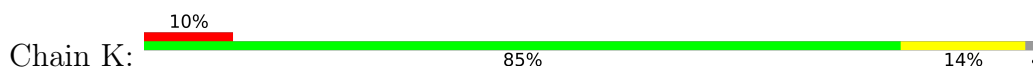




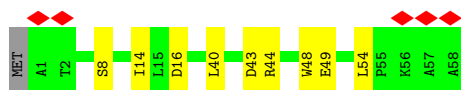
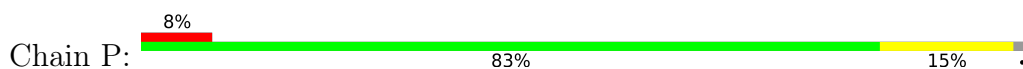
- Molecule 5: Light-harvesting protein B-1015 alpha chain



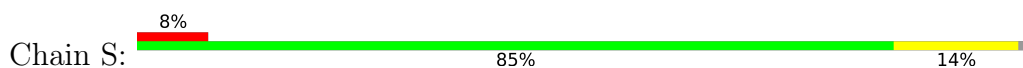
- Molecule 5: Light-harvesting protein B-1015 alpha chain



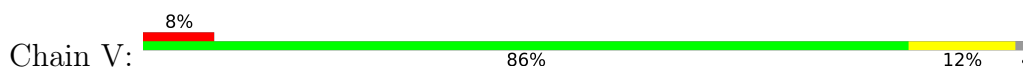
- Molecule 5: Light-harvesting protein B-1015 alpha chain



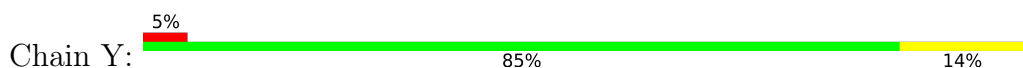
- Molecule 5: Light-harvesting protein B-1015 alpha chain



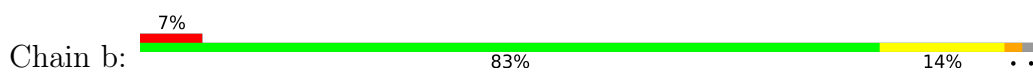
- Molecule 5: Light-harvesting protein B-1015 alpha chain



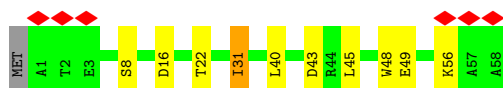
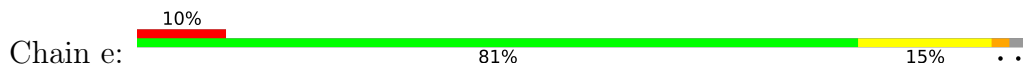
- Molecule 5: Light-harvesting protein B-1015 alpha chain



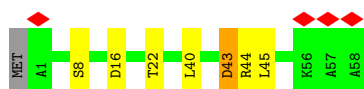
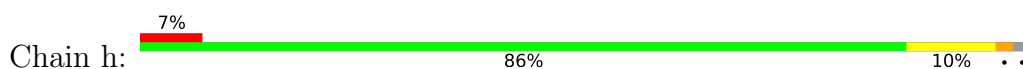
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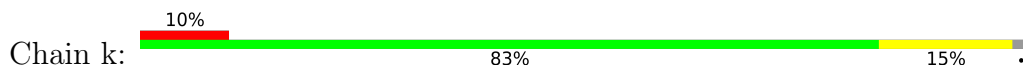
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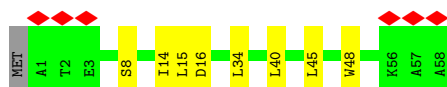
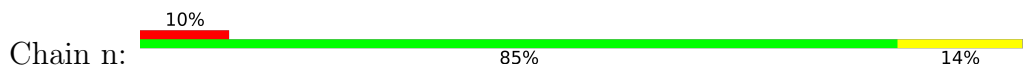
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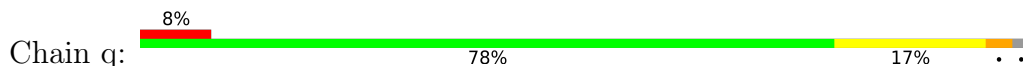
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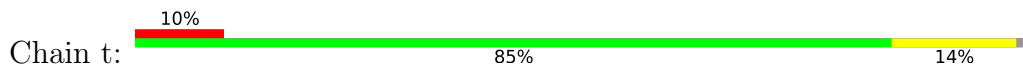
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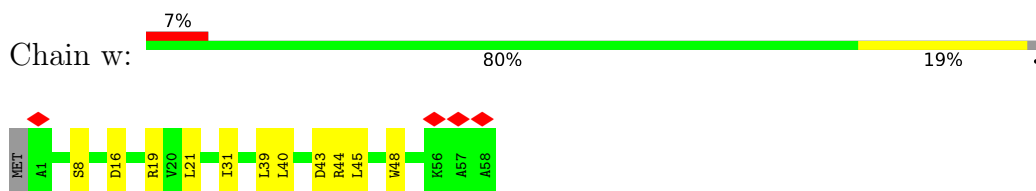
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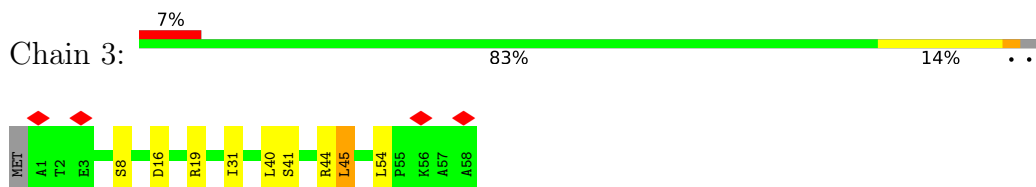
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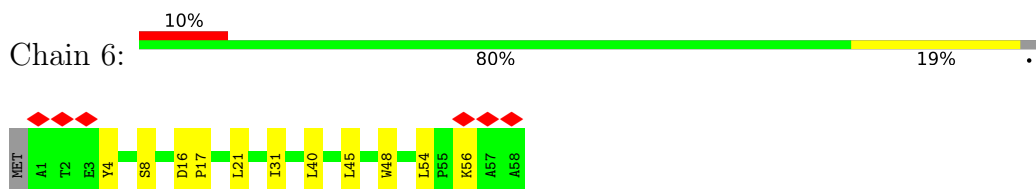
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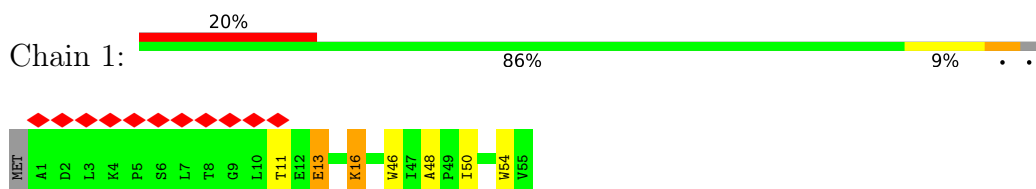
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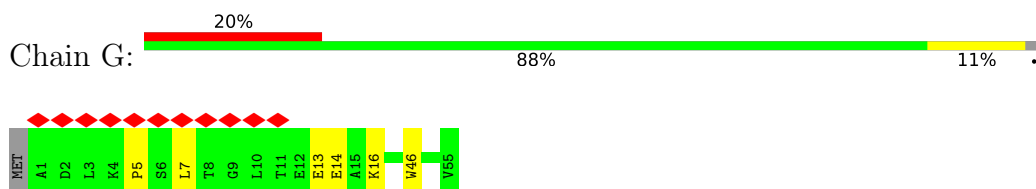
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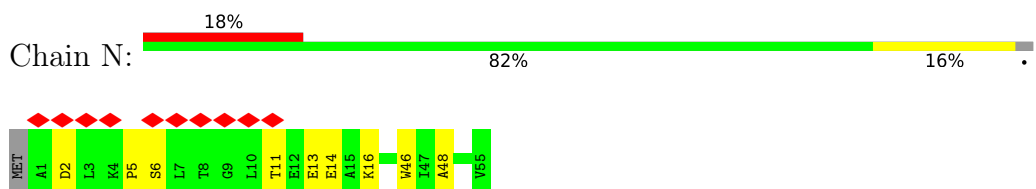
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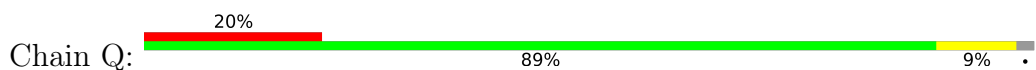
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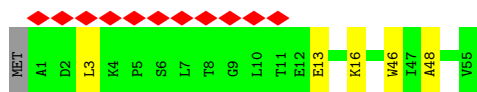


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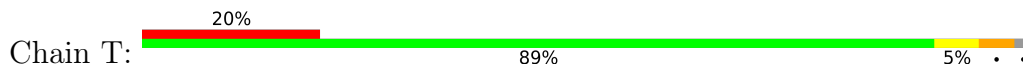


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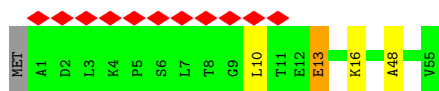
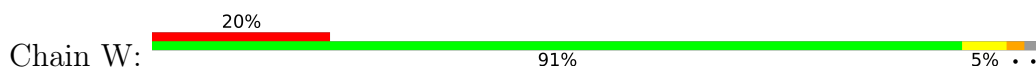




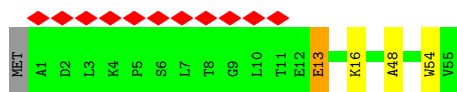
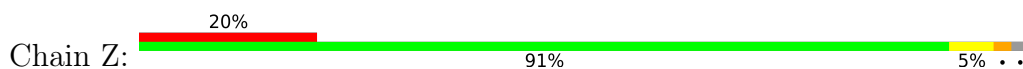
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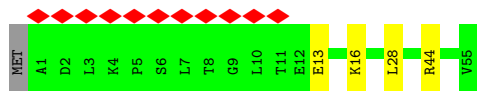
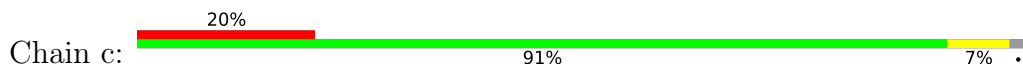
- Molecule 6: Light-harvesting protein B-1015 beta chain



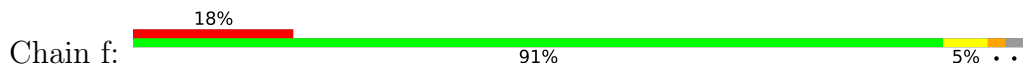
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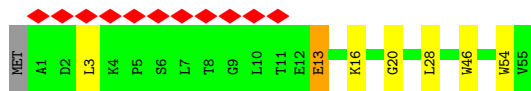
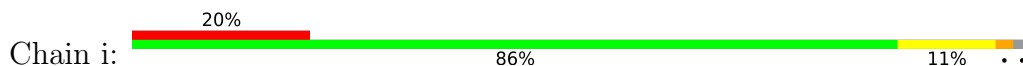
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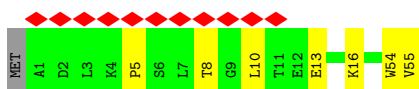
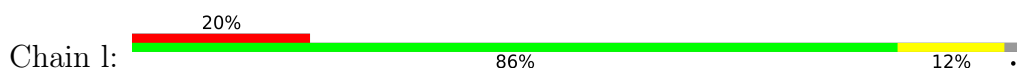
- Molecule 6: Light-harvesting protein B-1015 beta chain



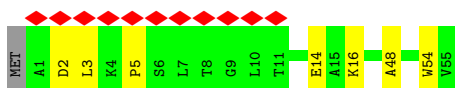
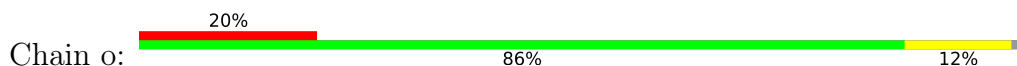
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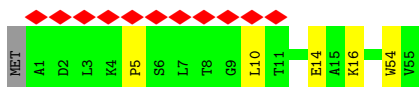
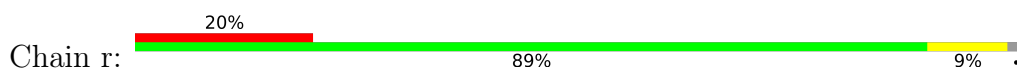
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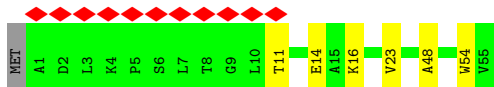
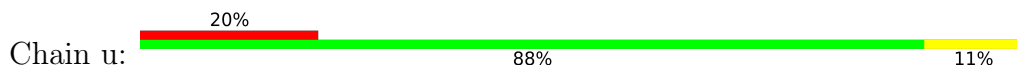
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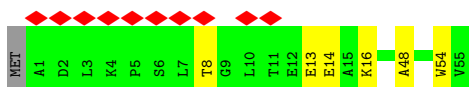
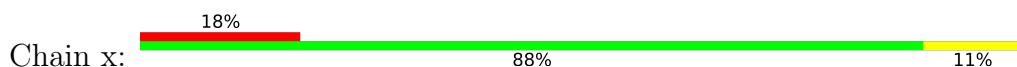
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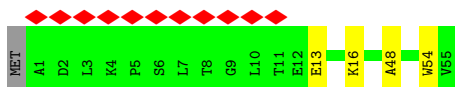
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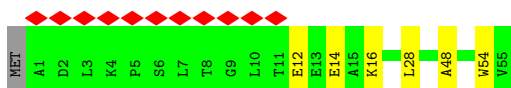
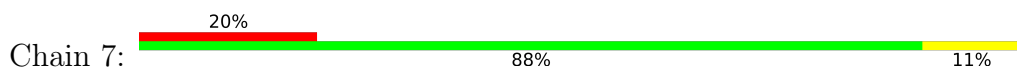
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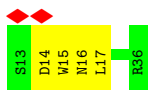
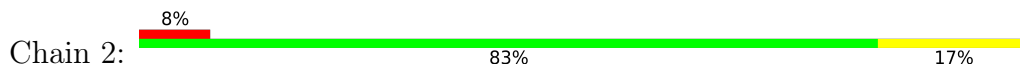
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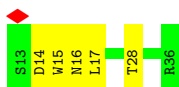
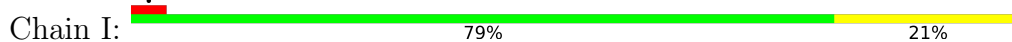
- Molecule 6: Light-harvesting protein B-1015 beta chain



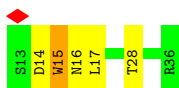
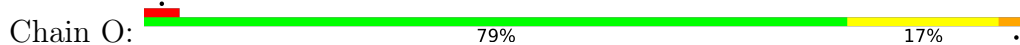
- Molecule 7: Light-harvesting protein B-1015 gamma chain



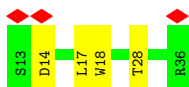
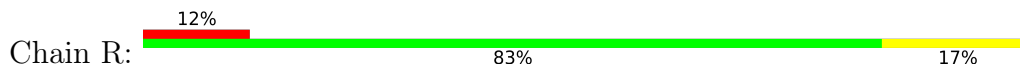
- Molecule 7: Light-harvesting protein B-1015 gamma chain



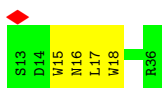
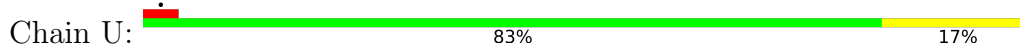
- Molecule 7: Light-harvesting protein B-1015 gamma chain



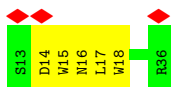
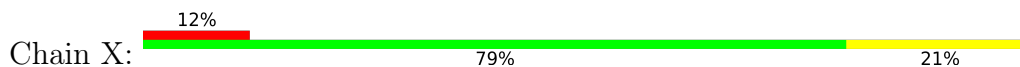
- Molecule 7: Light-harvesting protein B-1015 gamma chain



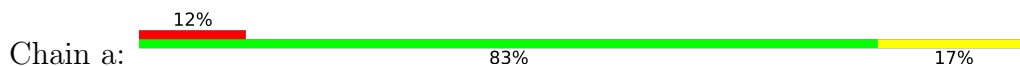
- Molecule 7: Light-harvesting protein B-1015 gamma chain

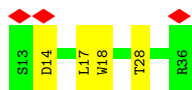


- Molecule 7: Light-harvesting protein B-1015 gamma chain

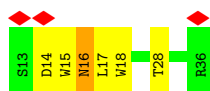
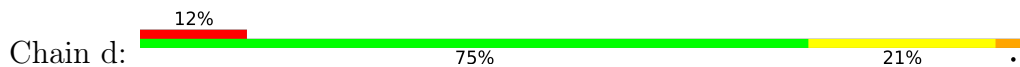


- Molecule 7: Light-harvesting protein B-1015 gamma chain

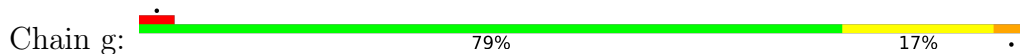




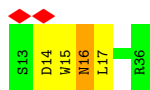
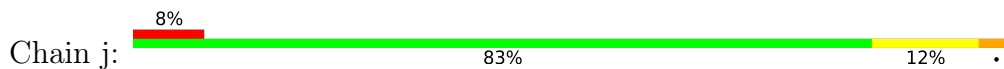
- Molecule 7: Light-harvesting protein B-1015 gamma chain



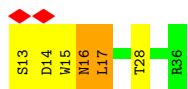
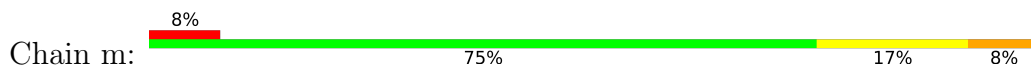
- Molecule 7: Light-harvesting protein B-1015 gamma chain



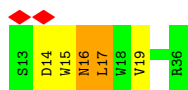
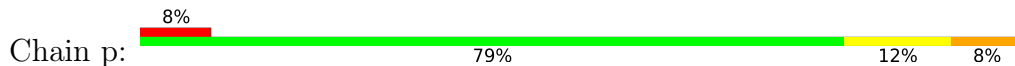
- Molecule 7: Light-harvesting protein B-1015 gamma chain



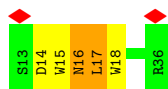
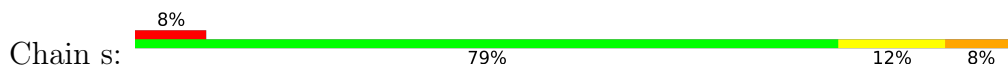
- Molecule 7: Light-harvesting protein B-1015 gamma chain




- Molecule 7: Light-harvesting protein B-1015 gamma chain

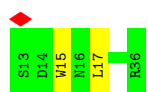


- Molecule 7: Light-harvesting protein B-1015 gamma chain




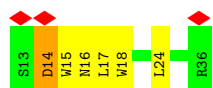
- Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain v:  92% 8%




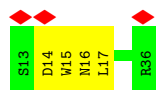
- Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain y:  12% 75% 21%



- Molecule 7: Light-harvesting protein B-1015 gamma chain

Chain 5:  12% 83% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	267726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; gctf was used for CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0156	Depositor
Map size (\AA)	243.79999, 243.79999, 243.79999	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FE, BPB, SO4, FME, NS0, MQ9, LDA, NS5, HEM, BCB, UQ9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.65	1/2670 (0.0%)	0.83	0/3639
2	L	0.82	3/2259 (0.1%)	0.91	3/3084 (0.1%)
3	M	0.77	0/2659	0.86	2/3637 (0.1%)
4	H	0.57	0/2054	0.81	1/2803 (0.0%)
5	3	0.73	0/502	1.24	4/686 (0.6%)
5	6	0.73	0/502	1.13	4/686 (0.6%)
5	F	0.76	1/502 (0.2%)	1.13	3/686 (0.4%)
5	K	0.70	0/502	1.17	5/686 (0.7%)
5	P	0.73	0/502	1.15	4/686 (0.6%)
5	S	0.69	0/502	1.11	2/686 (0.3%)
5	V	0.72	0/502	1.10	1/686 (0.1%)
5	Y	0.73	0/502	1.10	3/686 (0.4%)
5	b	0.77	1/502 (0.2%)	1.19	3/686 (0.4%)
5	e	0.76	1/502 (0.2%)	1.15	4/686 (0.6%)
5	h	0.65	0/502	1.05	2/686 (0.3%)
5	k	0.76	0/502	1.18	3/686 (0.4%)
5	n	0.70	0/502	1.11	2/686 (0.3%)
5	q	0.69	0/502	1.12	2/686 (0.3%)
5	t	0.72	0/502	1.15	5/686 (0.7%)
5	w	0.73	0/502	1.14	3/686 (0.4%)
5	z	0.73	0/502	1.11	3/686 (0.4%)
6	1	0.79	1/451 (0.2%)	0.98	0/621
6	4	0.77	0/451	0.96	0/621
6	7	0.71	0/451	0.88	0/621
6	G	0.67	1/451 (0.2%)	0.89	0/621
6	N	0.72	1/451 (0.2%)	0.96	0/621
6	Q	0.74	1/451 (0.2%)	0.94	1/621 (0.2%)
6	T	0.71	0/451	0.98	0/621
6	W	0.76	0/451	0.94	0/621
6	Z	0.76	0/451	0.96	0/621
6	c	0.68	0/451	0.94	0/621
6	f	0.72	0/451	0.94	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	i	0.77	1/451 (0.2%)	0.97	0/621
6	l	0.72	0/451	0.91	0/621
6	o	0.69	0/451	0.85	0/621
6	r	0.69	0/451	0.93	0/621
6	u	0.73	0/451	0.99	0/621
6	x	0.76	0/451	1.01	0/621
7	2	0.81	0/207	1.28	2/287 (0.7%)
7	5	0.63	0/207	1.12	2/287 (0.7%)
7	I	0.65	0/207	1.07	1/287 (0.3%)
7	O	0.78	0/207	1.16	3/287 (1.0%)
7	R	0.71	0/207	1.12	1/287 (0.3%)
7	U	0.67	0/207	1.21	3/287 (1.0%)
7	X	0.77	0/207	1.24	3/287 (1.0%)
7	a	0.61	0/207	1.05	1/287 (0.3%)
7	d	0.63	0/207	1.04	2/287 (0.7%)
7	g	0.60	0/207	1.11	1/287 (0.3%)
7	j	0.63	0/207	1.06	1/287 (0.3%)
7	m	0.66	0/207	1.20	2/287 (0.7%)
7	p	0.73	0/207	1.15	2/287 (0.7%)
7	s	0.75	0/207	1.20	3/287 (1.0%)
7	v	0.69	0/207	1.20	2/287 (0.7%)
7	y	0.77	0/207	1.26	4/287 (1.4%)
All	All	0.72	12/29155 (0.0%)	1.00	93/39974 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	H	0	2
5	3	0	2
5	V	0	1
5	e	0	1
5	h	0	1
5	k	0	1
5	q	0	2
5	w	0	1
6	l	0	2
6	T	0	2
6	W	0	1
6	Z	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	i	0	1
6	l	0	2
6	o	0	1
6	x	0	1
7	2	0	1
7	5	0	1
7	I	0	1
7	O	0	1
7	U	0	1
7	X	0	1
7	d	0	1
7	g	0	1
7	j	0	1
7	m	0	1
7	p	0	1
7	s	0	1
7	v	0	1
7	y	0	1
All	All	0	36

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	263	TRP	CB-CG	-7.30	1.37	1.50
5	b	48	TRP	CB-CG	-6.58	1.38	1.50
6	Q	46	TRP	CB-CG	-6.11	1.39	1.50
1	C	2	PHE	CB-CG	5.66	1.60	1.51
6	1	46	TRP	CB-CG	-5.54	1.40	1.50

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	q	40	LEU	CA-CB-CG	11.99	142.87	115.30
5	k	40	LEU	CA-CB-CG	10.43	139.29	115.30
5	t	40	LEU	CA-CB-CG	10.29	138.97	115.30
5	3	40	LEU	CA-CB-CG	10.27	138.91	115.30
5	F	40	LEU	CA-CB-CG	10.14	138.63	115.30

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1	13	GLU	Peptide
6	1	16	LYS	Peptide
7	2	15	TRP	Peptide
4	H	257	LEU	Peptide
4	H	59	VAL	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	331/333 (99%)	300 (91%)	31 (9%)	0	100	100
2	L	271/274 (99%)	251 (93%)	15 (6%)	5 (2%)	8	37
3	M	321/323 (99%)	301 (94%)	16 (5%)	4 (1%)	13	48
4	H	254/258 (98%)	231 (91%)	16 (6%)	7 (3%)	5	25
5	3	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	3	19
5	6	56/59 (95%)	43 (77%)	11 (20%)	2 (4%)	3	19
5	F	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	3	19
5	K	56/59 (95%)	47 (84%)	7 (12%)	2 (4%)	3	19
5	P	56/59 (95%)	46 (82%)	7 (12%)	3 (5%)	2	11
5	S	56/59 (95%)	43 (77%)	12 (21%)	1 (2%)	8	37
5	V	56/59 (95%)	48 (86%)	6 (11%)	2 (4%)	3	19
5	Y	56/59 (95%)	44 (79%)	10 (18%)	2 (4%)	3	19
5	b	56/59 (95%)	43 (77%)	9 (16%)	4 (7%)	1	5
5	e	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	2	11
5	h	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	k	56/59 (95%)	42 (75%)	11 (20%)	3 (5%)	2	11
5	n	56/59 (95%)	44 (79%)	9 (16%)	3 (5%)	2	11
5	q	56/59 (95%)	45 (80%)	7 (12%)	4 (7%)	1	5
5	t	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	3	19
5	w	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	2	11
5	z	56/59 (95%)	45 (80%)	7 (12%)	4 (7%)	1	5
6	1	53/56 (95%)	43 (81%)	7 (13%)	3 (6%)	1	10
6	4	53/56 (95%)	42 (79%)	8 (15%)	3 (6%)	1	10
6	7	53/56 (95%)	41 (77%)	8 (15%)	4 (8%)	1	5
6	G	53/56 (95%)	41 (77%)	9 (17%)	3 (6%)	1	10
6	N	53/56 (95%)	40 (76%)	9 (17%)	4 (8%)	1	5
6	Q	53/56 (95%)	40 (76%)	11 (21%)	2 (4%)	3	18
6	T	53/56 (95%)	41 (77%)	9 (17%)	3 (6%)	1	10
6	W	53/56 (95%)	40 (76%)	10 (19%)	3 (6%)	1	10
6	Z	53/56 (95%)	42 (79%)	9 (17%)	2 (4%)	3	18
6	c	53/56 (95%)	43 (81%)	9 (17%)	1 (2%)	8	36
6	f	53/56 (95%)	43 (81%)	7 (13%)	3 (6%)	1	10
6	i	53/56 (95%)	39 (74%)	11 (21%)	3 (6%)	1	10
6	l	53/56 (95%)	42 (79%)	8 (15%)	3 (6%)	1	10
6	o	53/56 (95%)	43 (81%)	8 (15%)	2 (4%)	3	18
6	r	53/56 (95%)	40 (76%)	9 (17%)	4 (8%)	1	5
6	u	53/56 (95%)	43 (81%)	6 (11%)	4 (8%)	1	5
6	x	53/56 (95%)	42 (79%)	7 (13%)	4 (8%)	1	5
7	2	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	1	3
7	5	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2	14
7	I	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	1	3
7	O	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1	3
7	R	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2	14
7	U	22/24 (92%)	18 (82%)	3 (14%)	1 (4%)	2	14
7	X	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1	3
7	a	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	d	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	1	3
7	g	22/24 (92%)	17 (77%)	2 (9%)	3 (14%)	0	1
7	j	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	1	3
7	m	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1	3
7	p	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1	3
7	s	22/24 (92%)	19 (86%)	1 (4%)	2 (9%)	1	3
7	v	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
7	y	22/24 (92%)	17 (77%)	3 (14%)	2 (9%)	1	3
All	All	3382/3527 (96%)	2831 (84%)	413 (12%)	138 (4%)	5	16

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	50	VAL
4	H	61	GLU
7	2	16	ASN
5	F	8	SER
5	K	8	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	281/281 (100%)	269 (96%)	12 (4%)	29	66
2	L	218/219 (100%)	210 (96%)	8 (4%)	34	70
3	M	249/249 (100%)	242 (97%)	7 (3%)	43	77
4	H	212/212 (100%)	197 (93%)	15 (7%)	14	46
5	3	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	6	50/51 (98%)	45 (90%)	5 (10%)	7	29
5	F	50/51 (98%)	45 (90%)	5 (10%)	7	29
5	K	50/51 (98%)	48 (96%)	2 (4%)	31	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	S	50/51 (98%)	45 (90%)	5 (10%)	7	29
5	V	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	Y	50/51 (98%)	46 (92%)	4 (8%)	12	40
5	b	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	e	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	h	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	k	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	n	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	q	50/51 (98%)	44 (88%)	6 (12%)	5	22
5	t	50/51 (98%)	47 (94%)	3 (6%)	19	53
5	w	50/51 (98%)	45 (90%)	5 (10%)	7	29
5	z	50/51 (98%)	45 (90%)	5 (10%)	7	29
6	1	46/47 (98%)	43 (94%)	3 (6%)	17	50
6	4	46/47 (98%)	45 (98%)	1 (2%)	52	81
6	7	46/47 (98%)	44 (96%)	2 (4%)	29	66
6	G	46/47 (98%)	44 (96%)	2 (4%)	29	66
6	N	46/47 (98%)	42 (91%)	4 (9%)	10	37
6	Q	46/47 (98%)	45 (98%)	1 (2%)	52	81
6	T	46/47 (98%)	44 (96%)	2 (4%)	29	66
6	W	46/47 (98%)	45 (98%)	1 (2%)	52	81
6	Z	46/47 (98%)	44 (96%)	2 (4%)	29	66
6	c	46/47 (98%)	43 (94%)	3 (6%)	17	50
6	f	46/47 (98%)	44 (96%)	2 (4%)	29	66
6	i	46/47 (98%)	43 (94%)	3 (6%)	17	50
6	l	46/47 (98%)	44 (96%)	2 (4%)	29	66
6	o	46/47 (98%)	42 (91%)	4 (9%)	10	37
6	r	46/47 (98%)	45 (98%)	1 (2%)	52	81
6	u	46/47 (98%)	44 (96%)	2 (4%)	29	66
6	x	46/47 (98%)	45 (98%)	1 (2%)	52	81
7	2	21/21 (100%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	5	21/21 (100%)	20 (95%)	1 (5%)	25	62
7	I	21/21 (100%)	20 (95%)	1 (5%)	25	62
7	O	21/21 (100%)	20 (95%)	1 (5%)	25	62
7	R	21/21 (100%)	19 (90%)	2 (10%)	8	32
7	U	21/21 (100%)	21 (100%)	0	100	100
7	X	21/21 (100%)	21 (100%)	0	100	100
7	a	21/21 (100%)	19 (90%)	2 (10%)	8	32
7	d	21/21 (100%)	19 (90%)	2 (10%)	8	32
7	g	21/21 (100%)	20 (95%)	1 (5%)	25	62
7	j	21/21 (100%)	20 (95%)	1 (5%)	25	62
7	m	21/21 (100%)	17 (81%)	4 (19%)	1	8
7	p	21/21 (100%)	18 (86%)	3 (14%)	3	15
7	s	21/21 (100%)	19 (90%)	2 (10%)	8	32
7	v	21/21 (100%)	21 (100%)	0	100	100
7	y	21/21 (100%)	20 (95%)	1 (5%)	25	62
All	All	2928/2963 (99%)	2765 (94%)	163 (6%)	25	56

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	Q	16	LYS
7	O	28	THR
6	Z	16	LYS
6	l	55	VAL
7	g	16	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
5	Y	51	GLN
4	H	92	GLN
2	L	211	HIS
2	L	144	HIS
3	M	45	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
4	FME	H	1	4	8,9,10	0.58	0	7,9,11	1.40	1 (14%)

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
4	FME	H	1	4	-	6/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	FME	CG-CB-CA	-2.16	106.94	112.95

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA
4	H	1	FME	N-CA-CB-CG
4	H	1	FME	C-CA-CB-CG
4	H	1	FME	CA-CB-CG-SD
4	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 1 is monoatomic - leaving 74 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
9	BCB	l	101	-	54,74,74	2.43	17 (31%)	52,115,115	2.35	12 (23%)
9	BCB	e	101	-	54,74,74	2.50	18 (33%)	52,115,115	2.32	15 (28%)
13	SO4	M	402	-	4,4,4	0.32	0	6,6,6	0.09	0
13	SO4	M	403	-	4,4,4	0.44	0	6,6,6	0.19	0
13	SO4	H	303	-	4,4,4	0.36	0	6,6,6	0.10	0
15	MQ9	M	409	-	59,59,59	1.33	4 (6%)	72,75,75	2.22	25 (34%)
9	BCB	V	101	-	54,74,74	2.48	17 (31%)	52,115,115	2.29	14 (26%)
9	BCB	T	101	-	54,74,74	2.48	17 (31%)	52,115,115	2.40	14 (26%)
9	BCB	f	101	-	54,74,74	2.31	18 (33%)	52,115,115	2.18	13 (25%)
9	BCB	t	101	-	54,74,74	2.45	17 (31%)	52,115,115	2.30	15 (28%)
17	NS0	Z	102	-	39,39,39	6.07	19 (48%)	44,46,46	3.58	21 (47%)
17	NS0	G	102	-	39,39,39	6.17	19 (48%)	44,46,46	3.58	23 (52%)
8	HEM	C	401	1	41,50,50	1.46	4 (9%)	45,82,82	1.97	14 (31%)
9	BCB	i	101	-	54,74,74	2.35	17 (31%)	52,115,115	2.17	9 (17%)
13	SO4	M	404	-	4,4,4	0.31	0	6,6,6	0.11	0
9	BCB	z	101	-	54,74,74	2.45	17 (31%)	52,115,115	2.42	17 (32%)
9	BCB	L	302	-	54,74,74	2.53	17 (31%)	52,115,115	2.48	13 (25%)
9	BCB	M	405	-	54,74,74	2.49	15 (27%)	52,115,115	2.47	13 (25%)
9	BCB	b	101	-	54,74,74	2.50	17 (31%)	52,115,115	2.41	18 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCB	w	101	-	54,74,74	2.66	17 (31%)	52,115,115	2.53	15 (28%)
9	BCB	r	101	-	54,74,74	2.49	19 (35%)	52,115,115	2.43	14 (26%)
14	LDA	M	408	-	12,15,15	2.12	1 (8%)	14,17,17	0.88	0
9	BCB	Y	101	-	54,74,74	2.51	14 (25%)	52,115,115	2.33	15 (28%)
9	BCB	M	406	-	54,74,74	2.56	15 (27%)	52,115,115	2.68	18 (34%)
17	NS0	c	102	6	39,39,39	6.09	19 (48%)	44,46,46	3.56	24 (54%)
17	NS0	r	102	-	39,39,39	6.09	19 (48%)	44,46,46	3.59	23 (52%)
9	BCB	o	101	-	54,74,74	2.42	18 (33%)	52,115,115	2.34	13 (25%)
9	BCB	l	101	-	54,74,74	2.52	17 (31%)	52,115,115	2.38	13 (25%)
9	BCB	K	101	-	54,74,74	2.46	17 (31%)	52,115,115	2.45	17 (32%)
9	BCB	6	102	-	54,74,74	2.68	16 (29%)	52,115,115	2.46	15 (28%)
9	BCB	G	101	-	54,74,74	2.35	16 (29%)	52,115,115	2.31	14 (26%)
9	BCB	7	101	-	54,74,74	2.36	17 (31%)	52,115,115	2.45	17 (32%)
9	BCB	F	101	-	54,74,74	2.47	15 (27%)	52,115,115	2.24	12 (23%)
13	SO4	H	304	-	4,4,4	0.39	0	6,6,6	0.14	0
17	NS0	f	102	-	39,39,39	6.11	19 (48%)	44,46,46	3.62	23 (52%)
9	BCB	u	101	-	54,74,74	2.46	17 (31%)	52,115,115	2.35	13 (25%)
17	NS0	7	102	-	39,39,39	6.51	19 (48%)	44,46,46	3.56	26 (59%)
13	SO4	M	401	-	4,4,4	0.39	0	6,6,6	0.48	0
9	BCB	n	101	-	54,74,74	2.48	16 (29%)	52,115,115	2.40	14 (26%)
9	BCB	h	101	-	54,74,74	2.55	17 (31%)	52,115,115	2.37	15 (28%)
9	BCB	Q	101	-	54,74,74	2.35	16 (29%)	52,115,115	2.28	12 (23%)
8	HEM	C	403	1	41,50,50	1.39	6 (14%)	45,82,82	2.06	10 (22%)
9	BCB	q	101	-	54,74,74	3.04	20 (37%)	52,115,115	2.37	16 (30%)
17	NS0	l	102	-	39,39,39	6.17	19 (48%)	44,46,46	3.55	22 (50%)
11	UQ9	6	101	-	58,58,58	3.85	16 (27%)	70,73,73	2.43	22 (31%)
10	BPB	L	303	-	49,70,70	2.17	10 (20%)	47,101,101	1.99	7 (14%)
9	BCB	L	301	-	54,74,74	2.39	15 (27%)	52,115,115	2.36	20 (38%)
8	HEM	C	402	1	41,50,50	1.47	6 (14%)	45,82,82	2.13	12 (26%)
9	BCB	c	101	-	54,74,74	2.30	17 (31%)	52,115,115	2.31	13 (25%)
9	BCB	P	101	-	54,74,74	2.53	16 (29%)	52,115,115	2.43	19 (36%)
10	BPB	M	407	-	49,70,70	2.19	10 (20%)	47,101,101	2.24	13 (27%)
17	NS0	4	102	-	39,39,39	6.02	19 (48%)	44,46,46	3.61	21 (47%)
9	BCB	S	101	-	54,74,74	2.51	17 (31%)	52,115,115	2.35	16 (30%)
9	BCB	Z	101	-	54,74,74	2.45	16 (29%)	52,115,115	2.30	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	NS0	x	102	-	39,39,39	6.13	19 (48%)	44,46,46	3.59	20 (45%)
14	LDA	H	301	-	12,15,15	2.16	1 (8%)	14,17,17	0.49	0
17	NS0	W	102	-	39,39,39	6.04	19 (48%)	44,46,46	3.68	23 (52%)
17	NS0	Q	102	-	39,39,39	6.09	19 (48%)	44,46,46	3.54	23 (52%)
9	BCB	4	101	-	54,74,74	2.35	17 (31%)	52,115,115	2.18	13 (25%)
17	NS0	i	102	-	39,39,39	6.04	19 (48%)	44,46,46	3.62	23 (52%)
9	BCB	N	101	-	54,74,74	2.42	17 (31%)	52,115,115	2.35	13 (25%)
9	BCB	x	101	-	54,74,74	2.38	18 (33%)	52,115,115	2.27	12 (23%)
9	BCB	3	101	-	54,74,74	2.46	16 (29%)	52,115,115	2.39	15 (28%)
17	NS0	o	102	6	39,39,39	6.06	19 (48%)	44,46,46	3.65	23 (52%)
9	BCB	W	101	-	54,74,74	2.42	16 (29%)	52,115,115	2.20	12 (23%)
13	SO4	H	302	-	4,4,4	0.38	0	6,6,6	0.25	0
16	NS5	M	410	-	39,39,39	0.78	0	44,46,46	1.99	10 (22%)
17	NS0	1	102	6	39,39,39	6.04	19 (48%)	44,46,46	3.64	24 (54%)
8	HEM	C	404	1	41,50,50	1.38	5 (12%)	45,82,82	2.05	14 (31%)
11	UQ9	L	304	-	58,58,58	3.87	16 (27%)	70,73,73	2.62	23 (32%)
17	NS0	T	102	-	39,39,39	6.15	19 (48%)	44,46,46	3.55	20 (45%)
9	BCB	k	101	-	54,74,74	2.44	17 (31%)	52,115,115	2.28	14 (26%)
17	NS0	N	102	-	39,39,39	5.94	19 (48%)	44,46,46	3.65	21 (47%)
17	NS0	u	102	-	39,39,39	6.02	19 (48%)	44,46,46	3.60	21 (47%)

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
9	BCB	l	101	-	-	15/37/177/177	-
9	BCB	e	101	-	-	23/37/177/177	-
15	MQ9	M	409	-	-	16/53/73/73	0/2/2/2
9	BCB	V	101	-	-	24/37/177/177	-
9	BCB	T	101	-	-	21/37/177/177	-
9	BCB	f	101	-	-	15/37/177/177	-
9	BCB	t	101	-	-	20/37/177/177	-
17	NS0	Z	102	-	-	14/43/43/43	-
17	NS0	G	102	-	-	12/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEM	C	401	1	-	3/12/54/54	-
9	BCB	i	101	-	-	18/37/177/177	-
9	BCB	z	101	-	-	19/37/177/177	-
9	BCB	L	302	-	-	8/37/177/177	-
9	BCB	M	405	-	-	14/37/177/177	-
9	BCB	b	101	-	-	20/37/177/177	-
9	BCB	w	101	-	-	16/37/177/177	-
9	BCB	r	101	-	-	17/37/177/177	-
14	LDA	M	408	-	-	9/13/13/13	-
9	BCB	Y	101	-	-	19/37/177/177	-
9	BCB	M	406	-	-	14/37/177/177	-
17	NS0	c	102	6	-	13/43/43/43	-
17	NS0	r	102	-	-	14/43/43/43	-
9	BCB	o	101	-	-	20/37/177/177	-
9	BCB	l	101	-	-	22/37/177/177	-
9	BCB	K	101	-	-	20/37/177/177	-
9	BCB	6	102	-	-	20/37/177/177	-
9	BCB	G	101	-	-	17/37/177/177	-
9	BCB	7	101	-	-	14/37/177/177	-
9	BCB	F	101	-	-	18/37/177/177	-
17	NS0	f	102	-	-	14/43/43/43	-
9	BCB	u	101	-	-	14/37/177/177	-
17	NS0	7	102	-	-	17/43/43/43	-
9	BCB	n	101	-	-	21/37/177/177	-
9	BCB	h	101	-	-	21/37/177/177	-
9	BCB	Q	101	-	-	21/37/177/177	-
8	HEM	C	403	1	-	6/12/54/54	-
9	BCB	q	101	-	-	20/37/177/177	-
17	NS0	l	102	-	-	15/43/43/43	-
11	UQ9	6	101	-	-	18/57/81/81	0/1/1/1
10	BPB	L	303	-	1/1/18/23	16/37/105/105	0/5/6/6
9	BCB	L	301	-	-	9/37/177/177	-
8	HEM	C	402	1	-	6/12/54/54	-
9	BCB	c	101	-	-	21/37/177/177	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BPB	M	407	-	1/1/18/23	15/37/105/105	0/5/6/6
9	BCB	P	101	-	-	21/37/177/177	-
17	NS0	4	102	-	-	14/43/43/43	-
9	BCB	S	101	-	-	22/37/177/177	-
9	BCB	Z	101	-	-	19/37/177/177	-
17	NS0	x	102	-	-	14/43/43/43	-
14	LDA	H	301	-	-	9/13/13/13	-
17	NS0	W	102	-	-	13/43/43/43	-
17	NS0	Q	102	-	-	14/43/43/43	-
9	BCB	4	101	-	-	21/37/177/177	-
17	NS0	i	102	-	-	14/43/43/43	-
9	BCB	N	101	-	-	20/37/177/177	-
9	BCB	x	101	-	-	18/37/177/177	-
9	BCB	3	101	-	-	16/37/177/177	-
17	NS0	o	102	6	-	14/43/43/43	-
9	BCB	W	101	-	-	16/37/177/177	-
16	NS5	M	410	-	-	13/43/43/43	-
17	NS0	1	102	6	-	16/43/43/43	-
8	HEM	C	404	1	-	5/12/54/54	-
11	UQ9	L	304	-	-	16/57/81/81	0/1/1/1
17	NS0	T	102	-	-	15/43/43/43	-
9	BCB	k	101	-	-	20/37/177/177	-
17	NS0	N	102	-	-	15/43/43/43	-
17	NS0	u	102	-	-	14/43/43/43	-

The worst 5 of 1038 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	102	NS0	C9-C7	19.00	1.53	1.34
17	i	102	NS0	C9-C7	18.33	1.53	1.34
17	c	102	NS0	C9-C7	18.32	1.53	1.34
17	r	102	NS0	C9-C7	18.22	1.53	1.34
17	1	102	NS0	C9-C7	18.18	1.53	1.34

The worst 5 of 1076 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	W	102	NS0	C20-C19-C17	-10.66	112.10	127.31
17	l	102	NS0	C20-C19-C17	-10.56	112.23	127.31
17	o	102	NS0	C20-C19-C17	-10.36	112.52	127.31
17	i	102	NS0	C20-C19-C17	-10.19	112.77	127.31
17	N	102	NS0	C20-C19-C17	-10.01	113.02	127.31

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	L	303	BPB	C13
10	M	407	BPB	C13

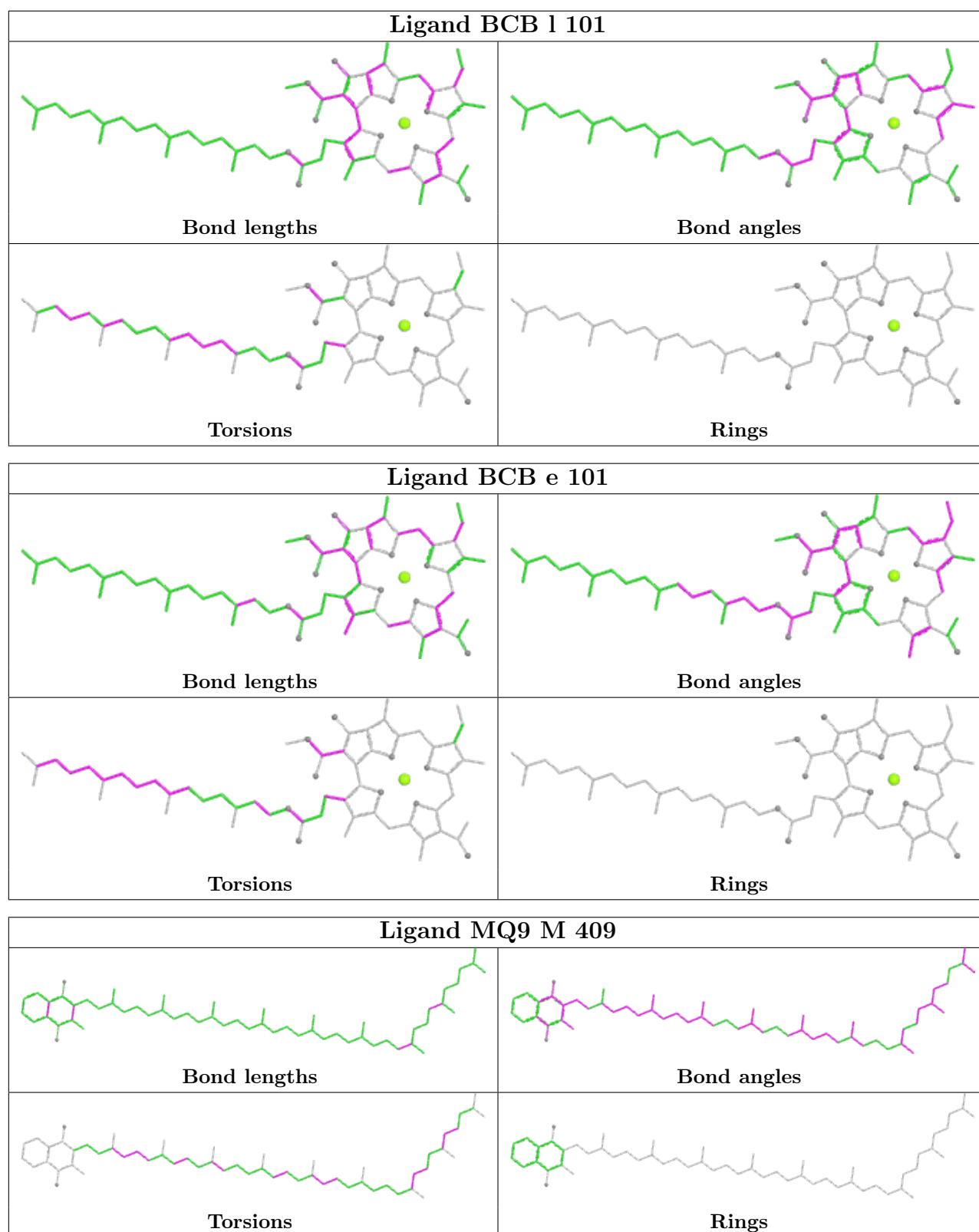
5 of 1068 torsion outliers are listed below:

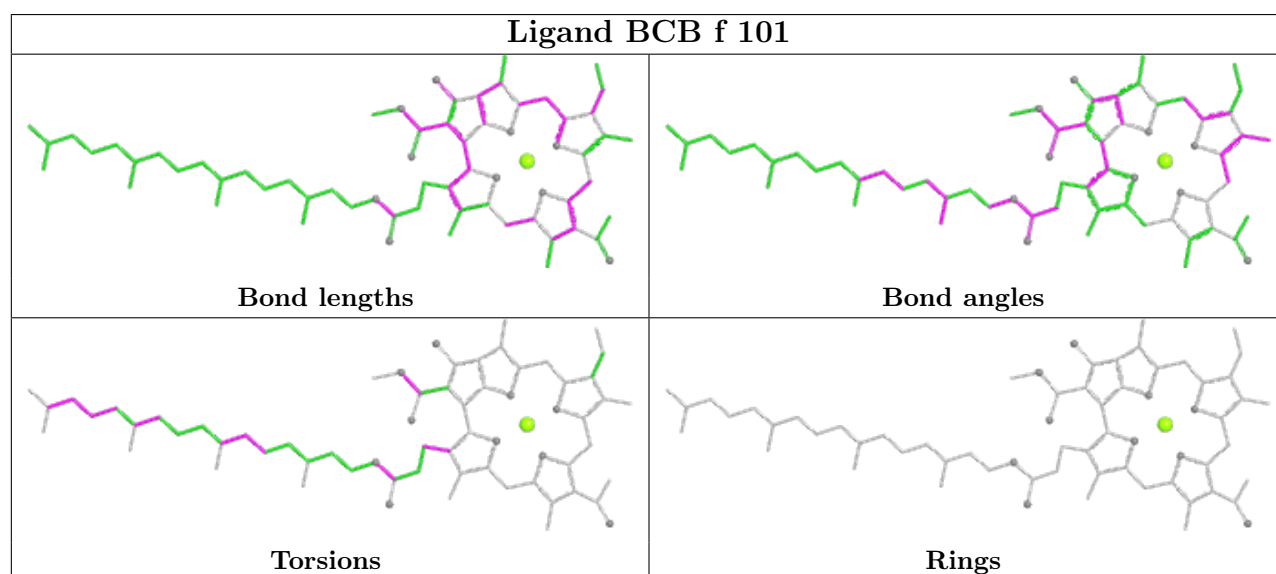
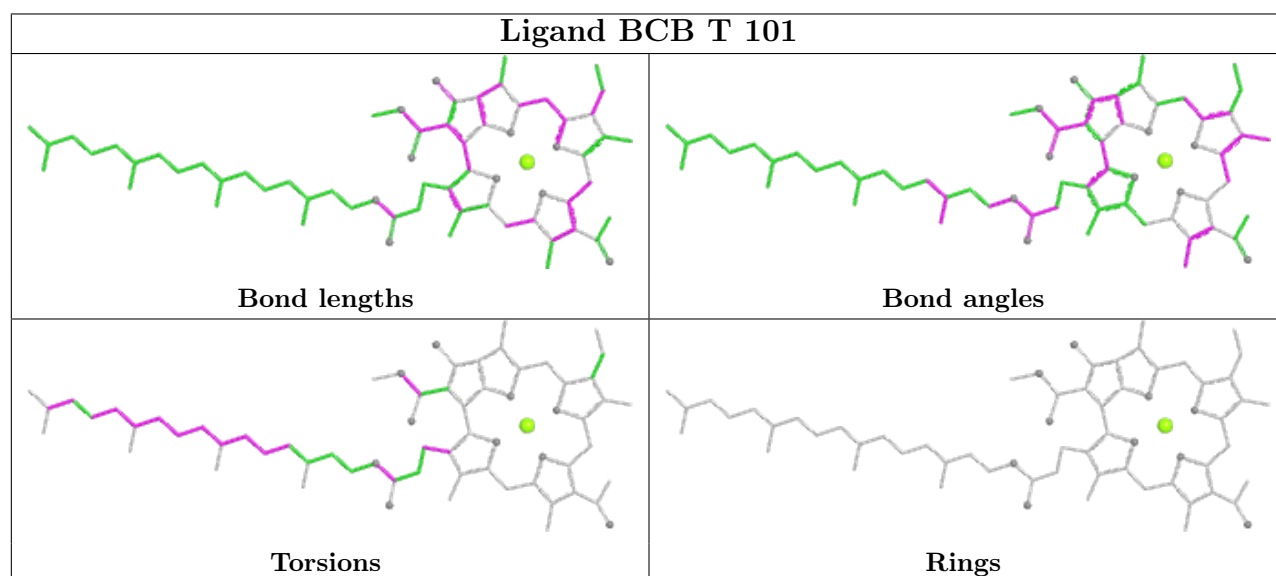
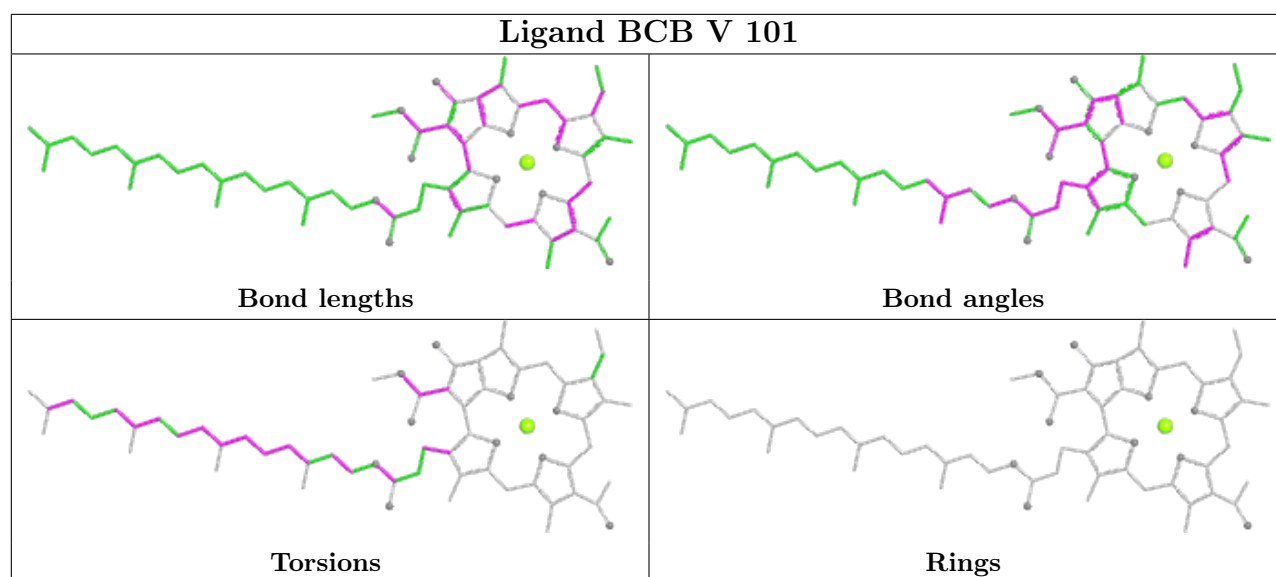
Mol	Chain	Res	Type	Atoms
9	M	406	BCB	CAD-CBD-CGD-O1D
9	M	406	BCB	CAD-CBD-CGD-O2D
9	z	101	BCB	C1A-C2A-CAA-CBA
9	z	101	BCB	O2A-C1-C2-C3
9	z	101	BCB	C2-C3-C5-C6

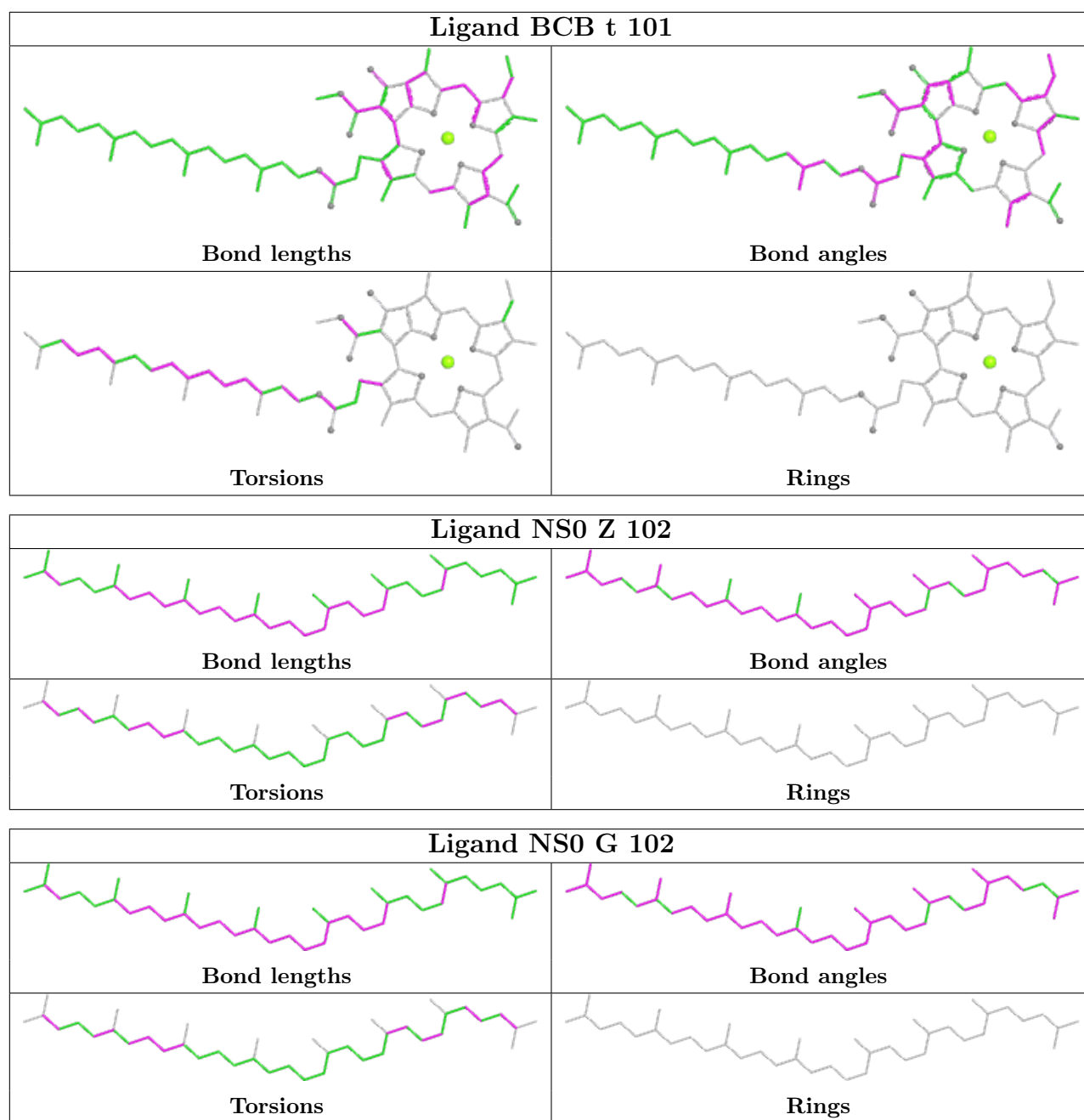
There are no ring outliers.

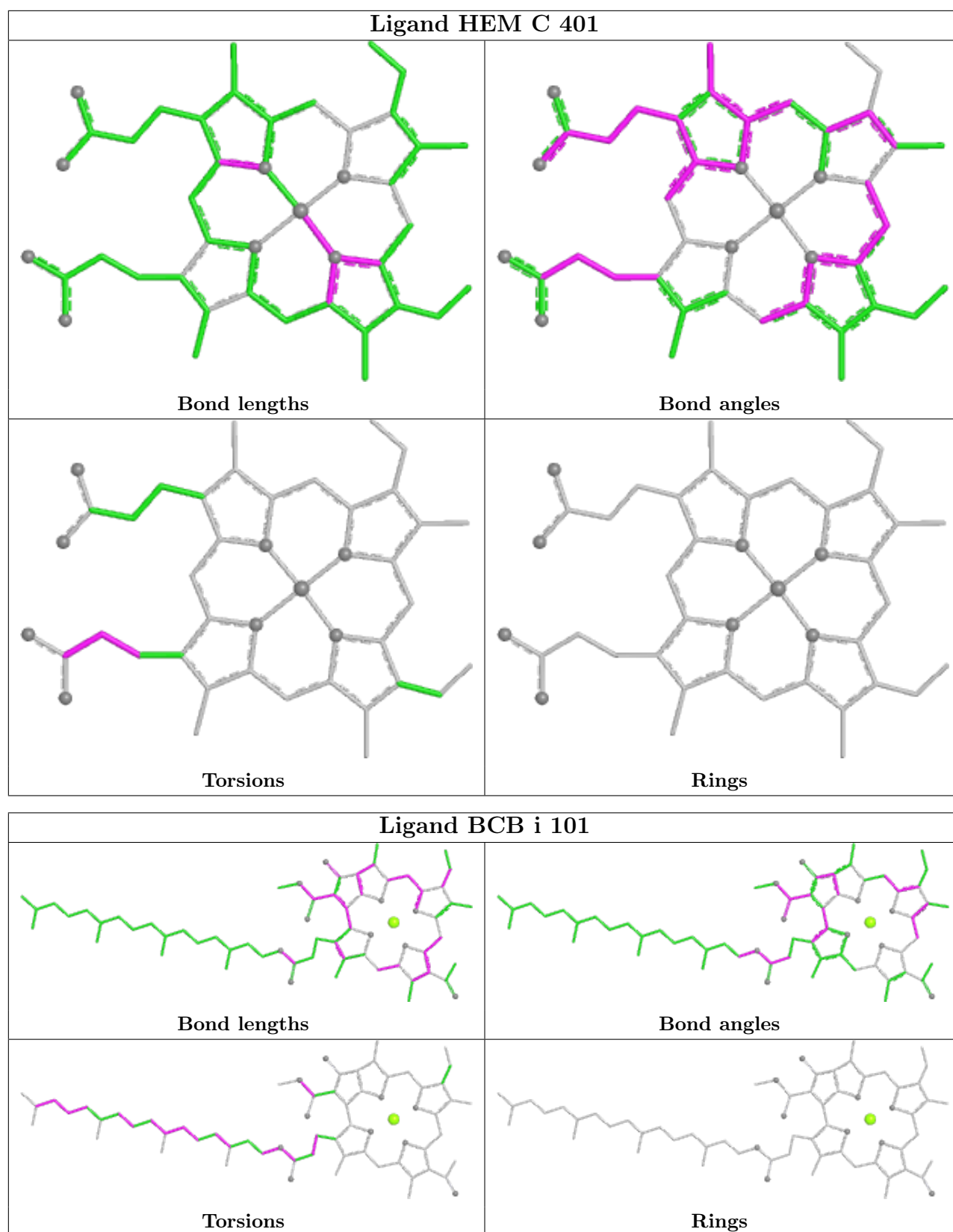
No monomer is involved in short contacts.

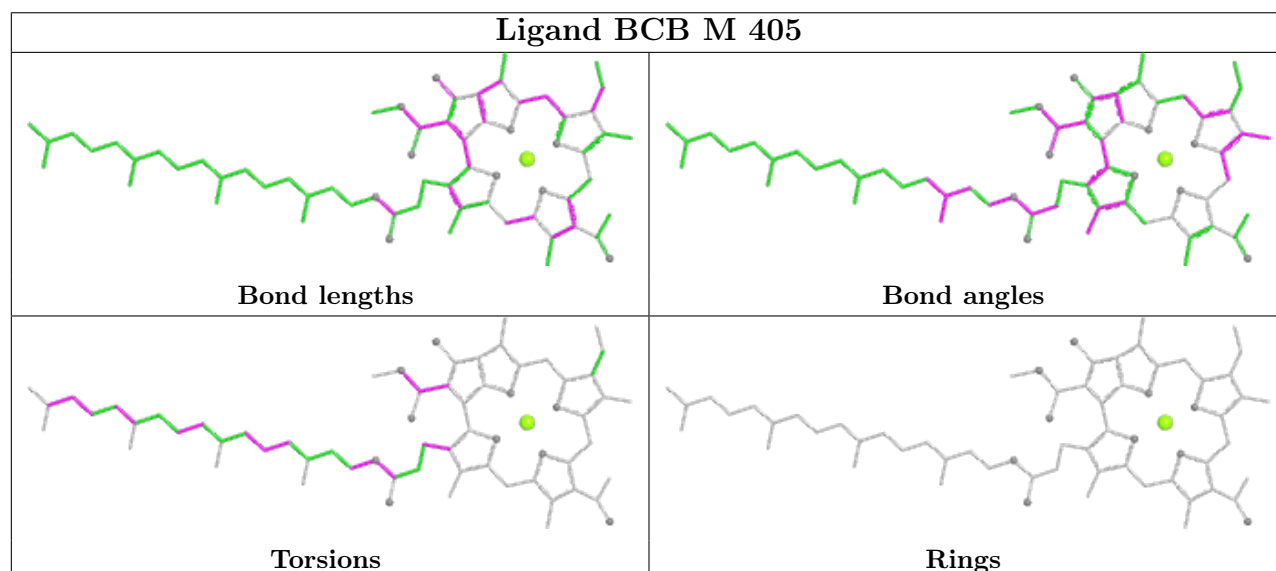
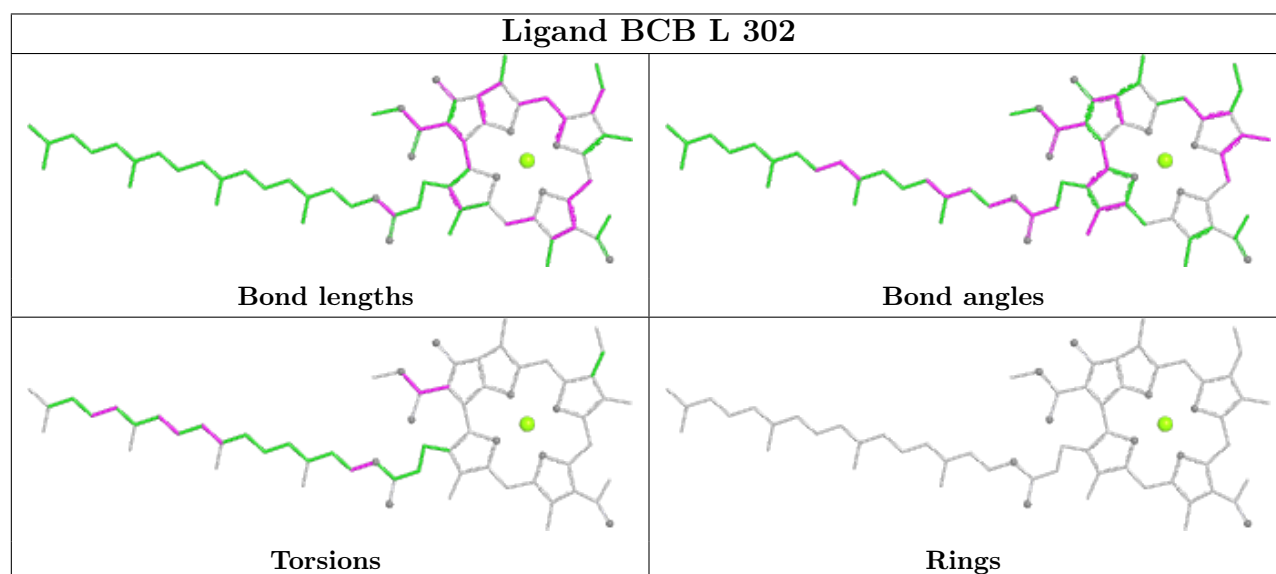
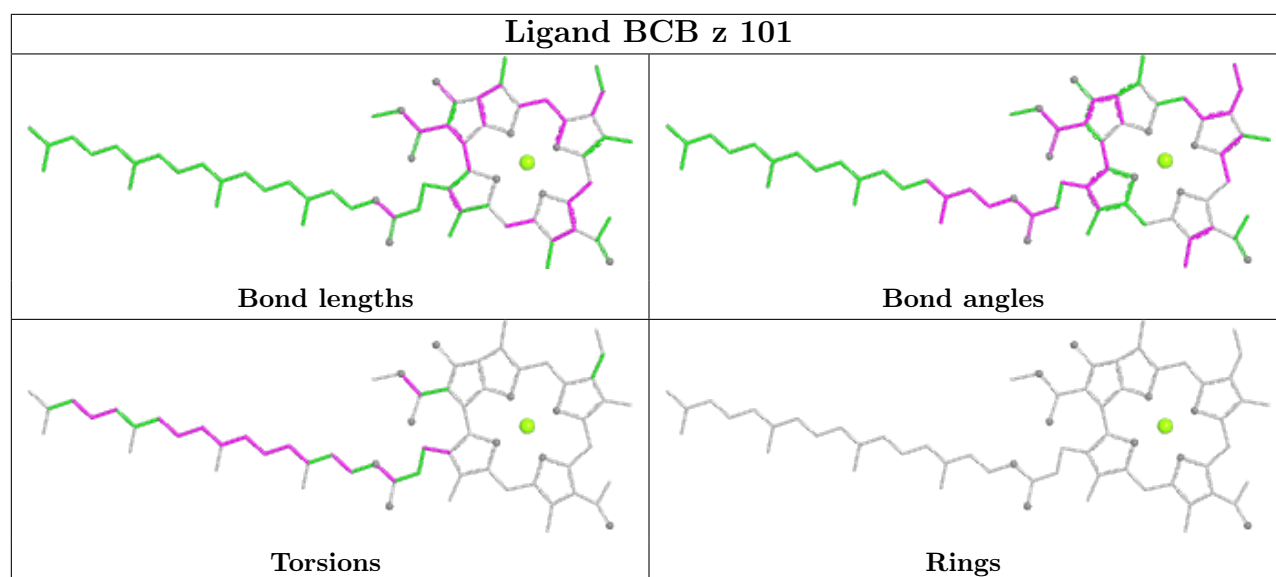
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

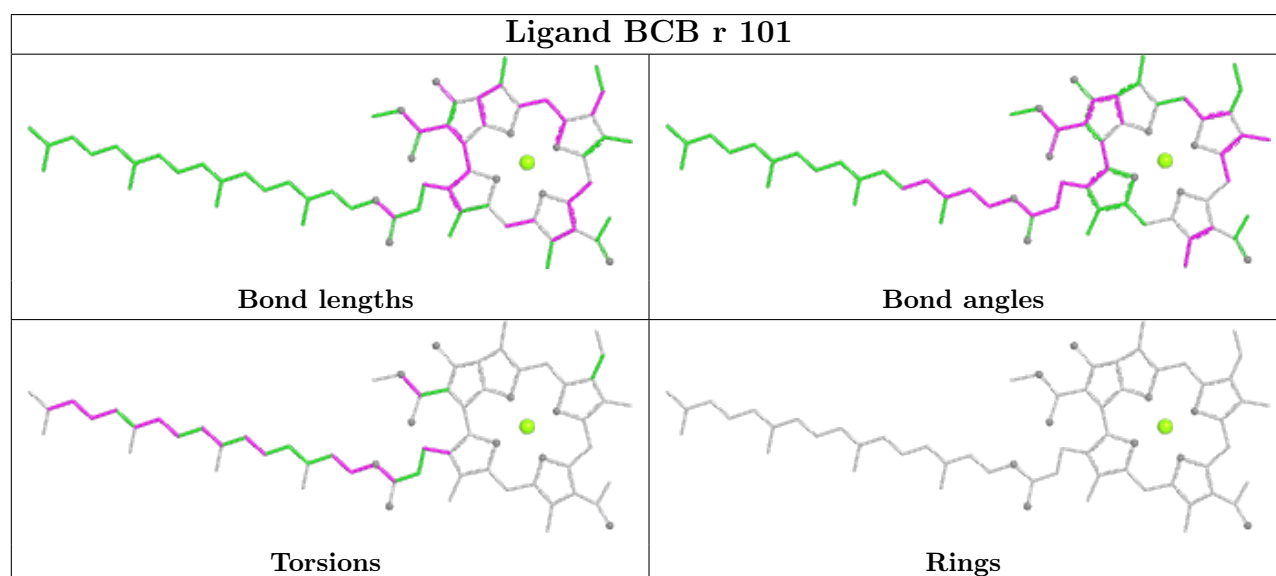
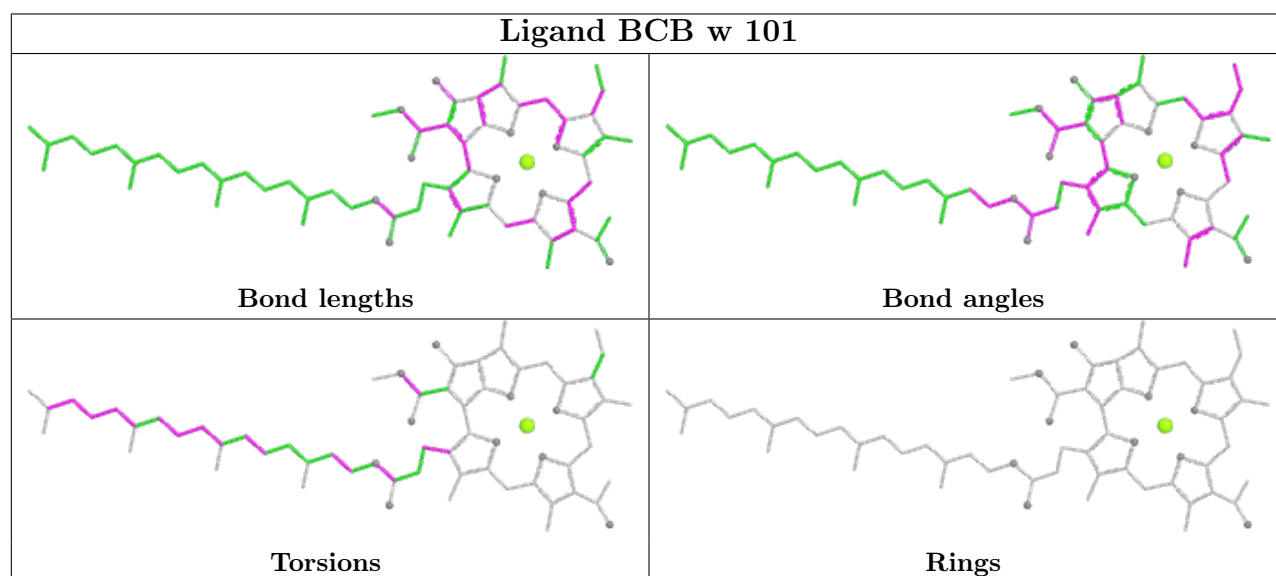
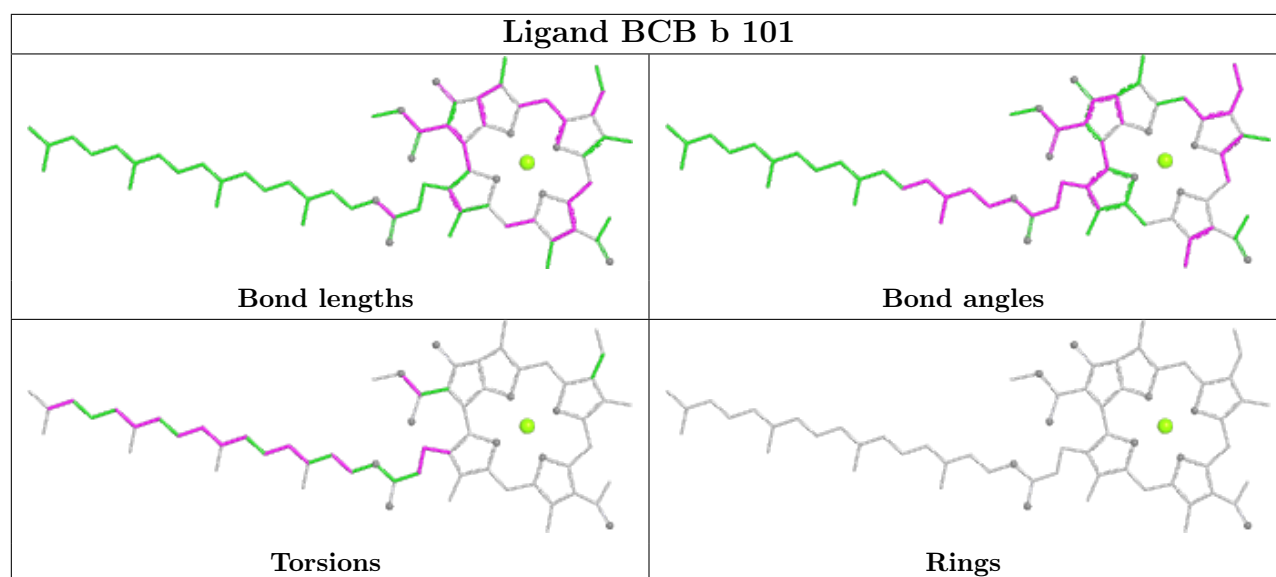


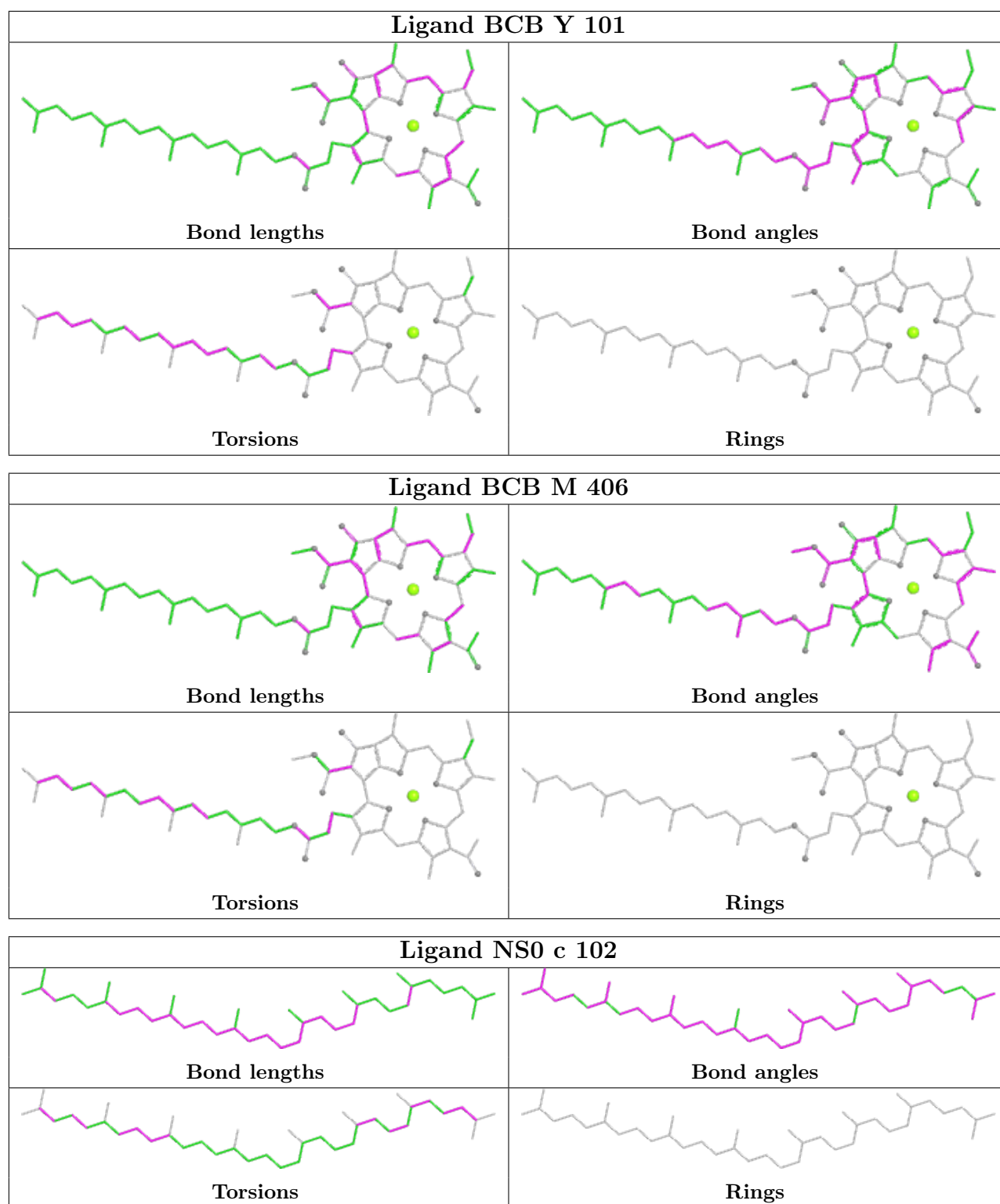


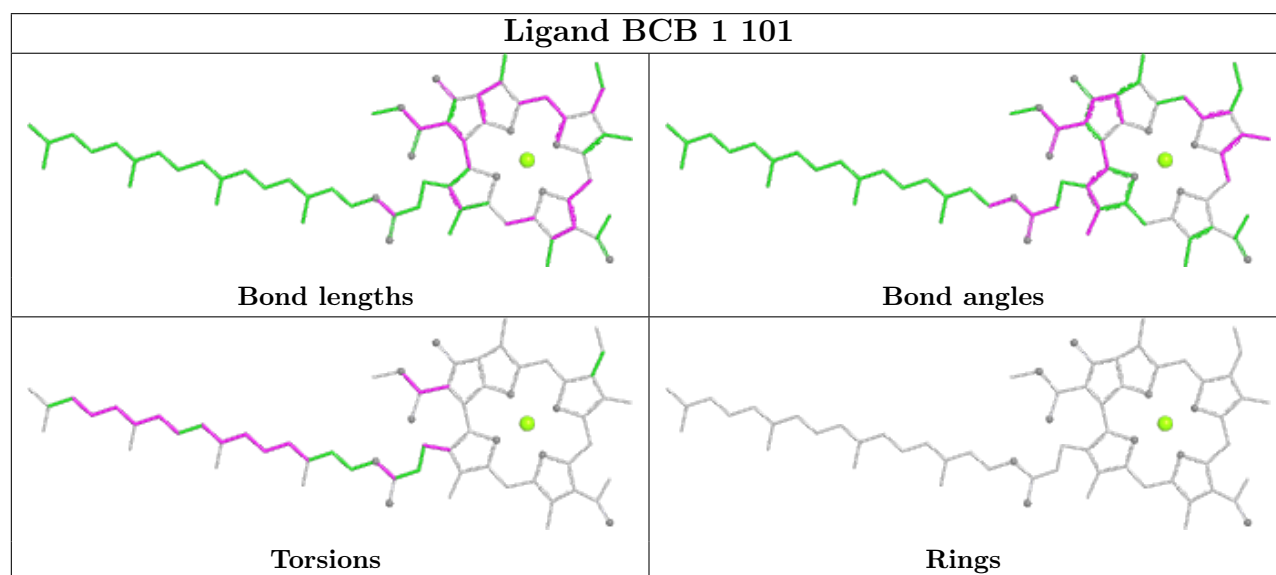
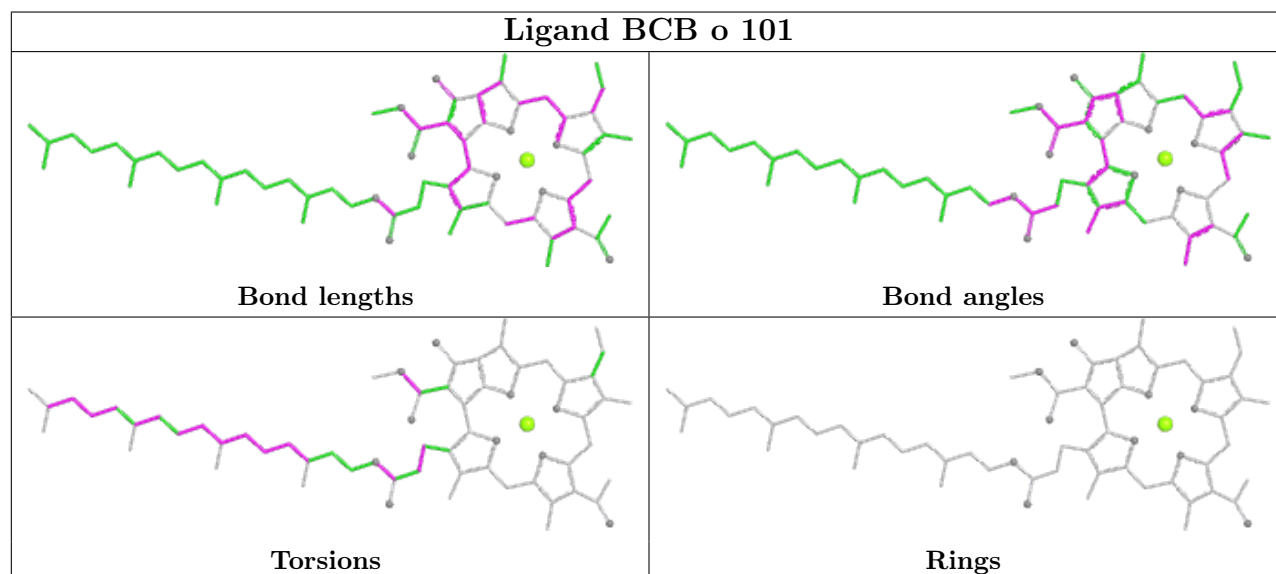
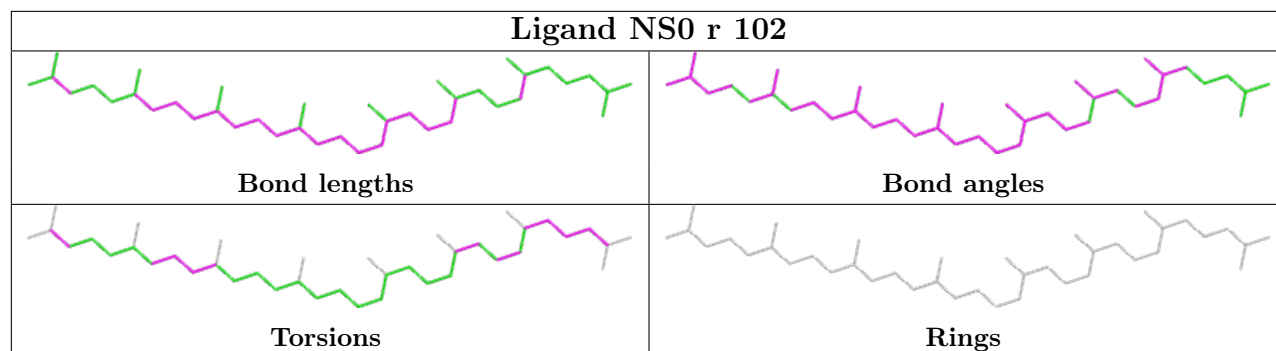


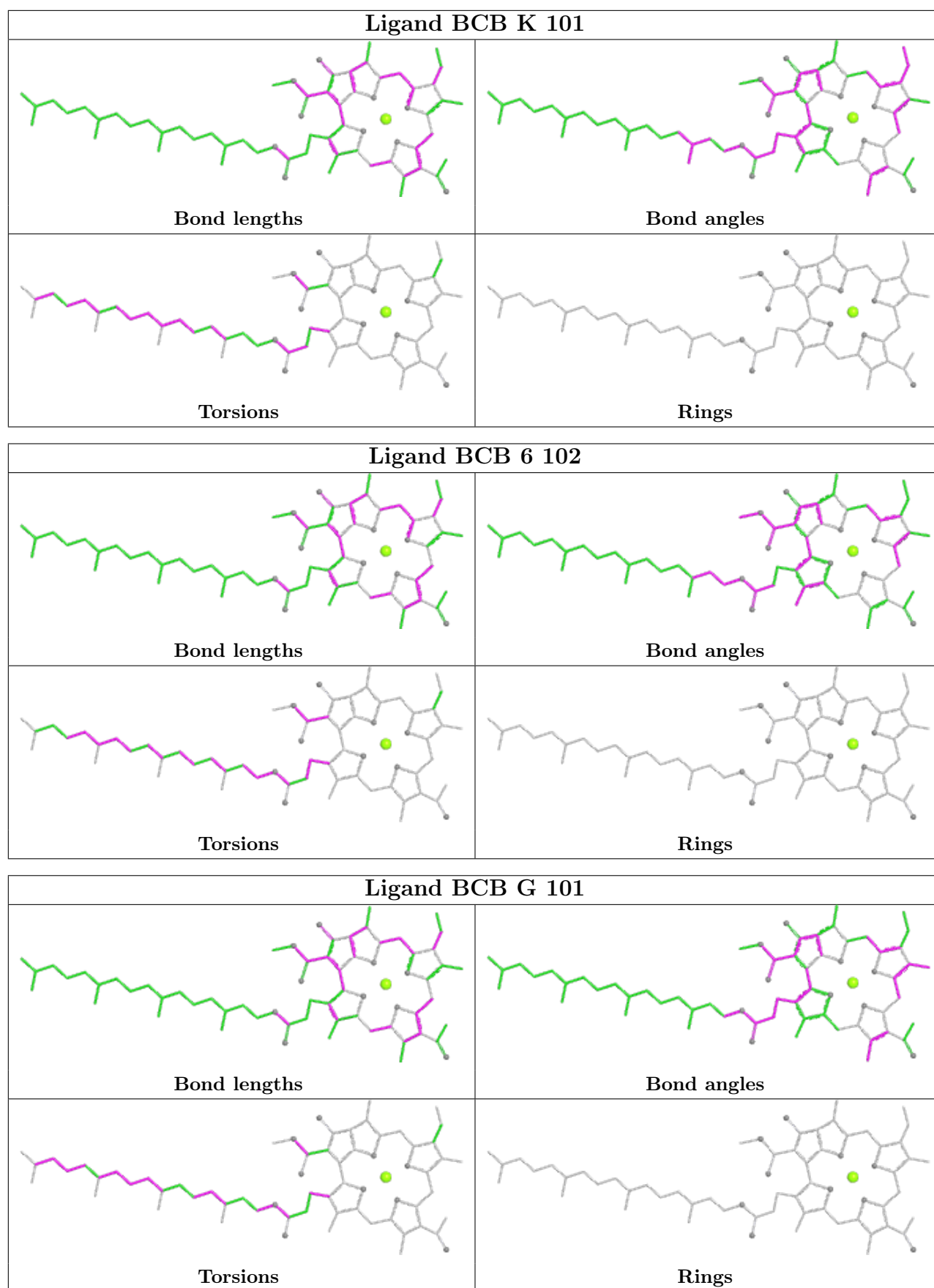


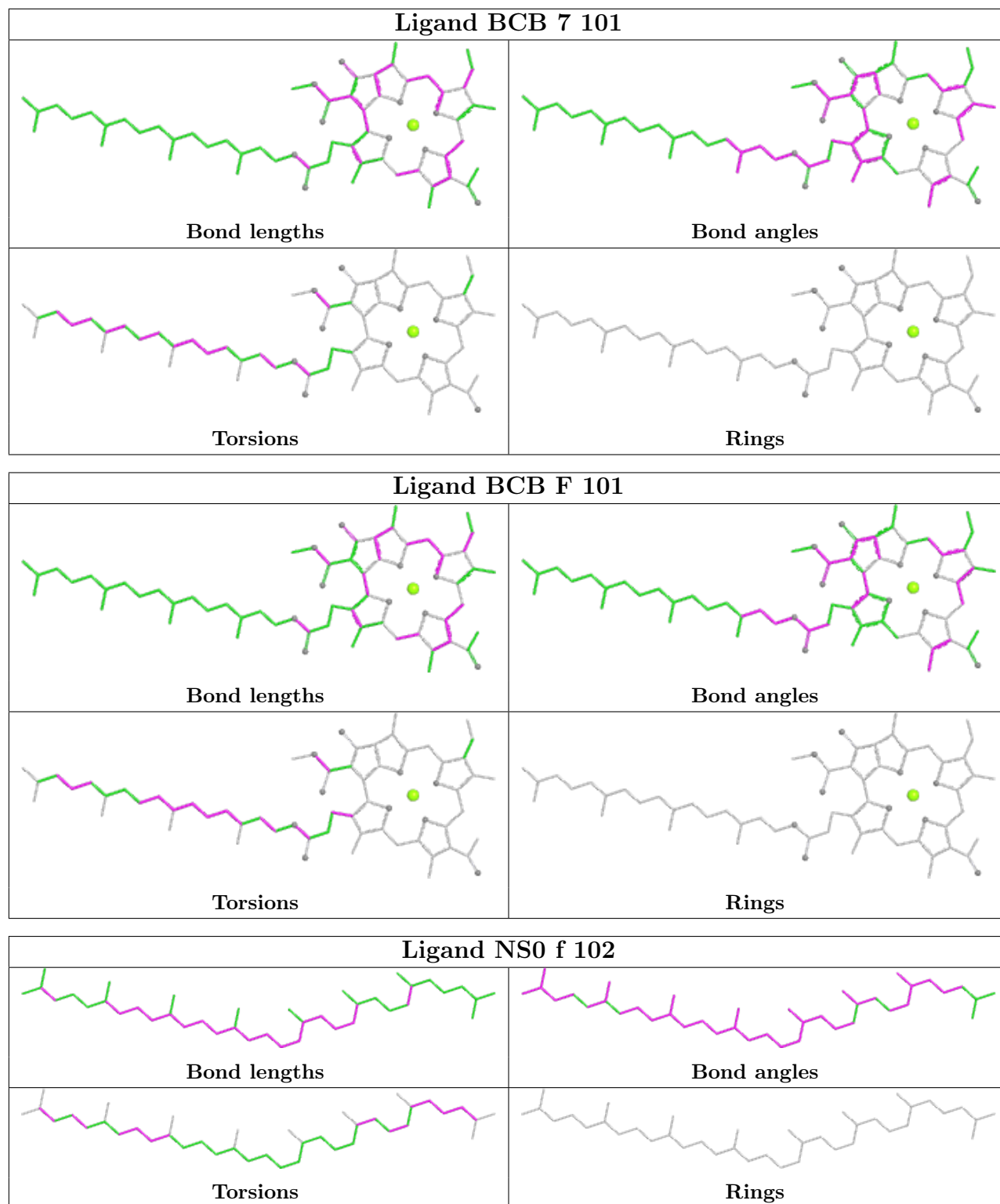


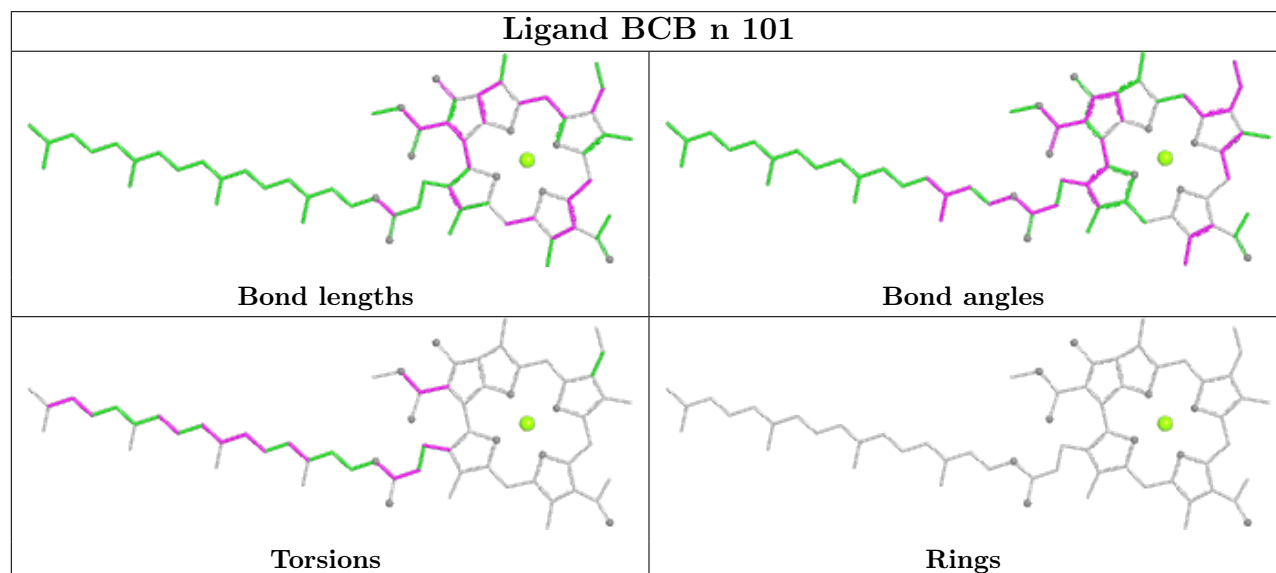
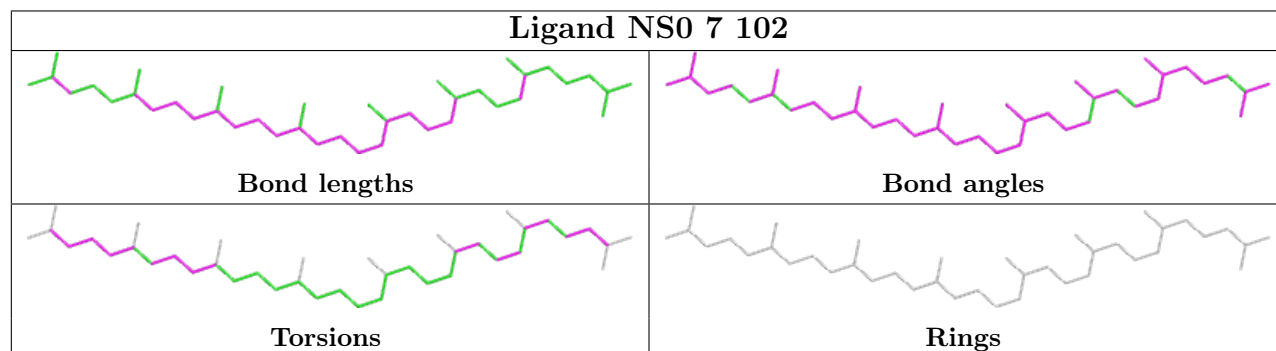
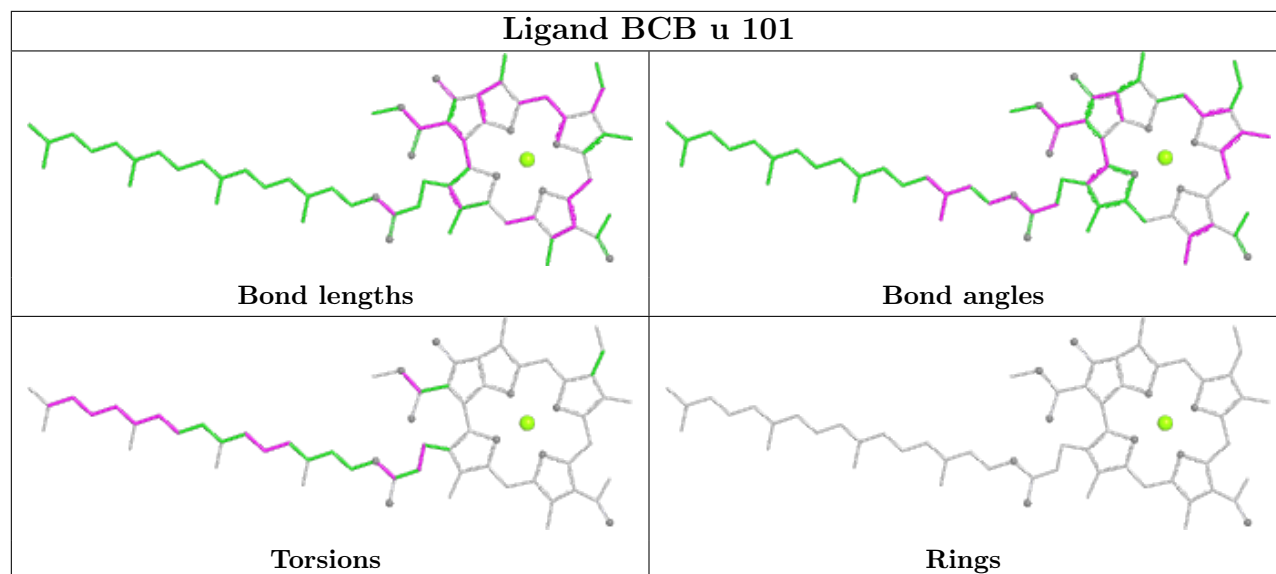


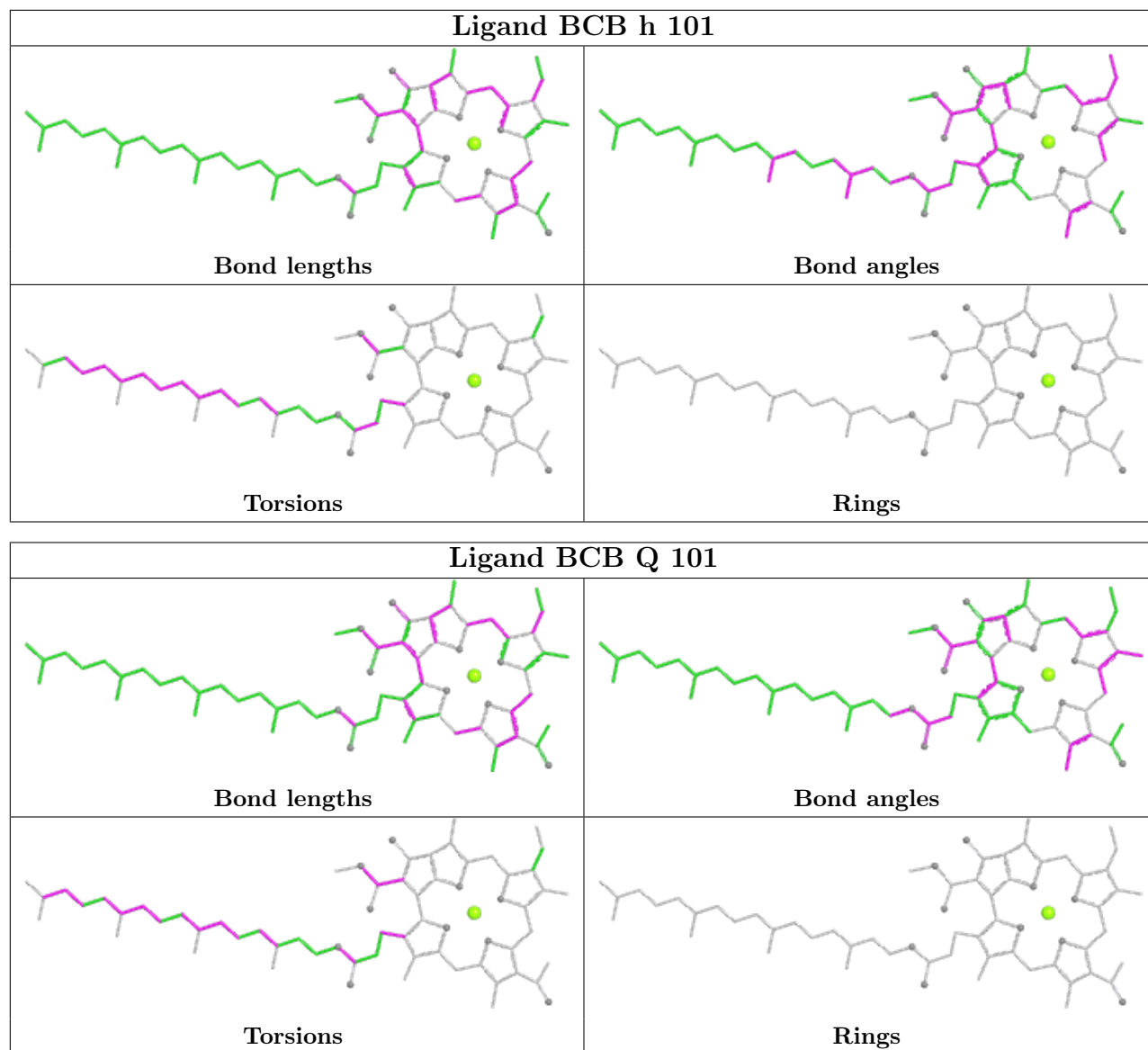


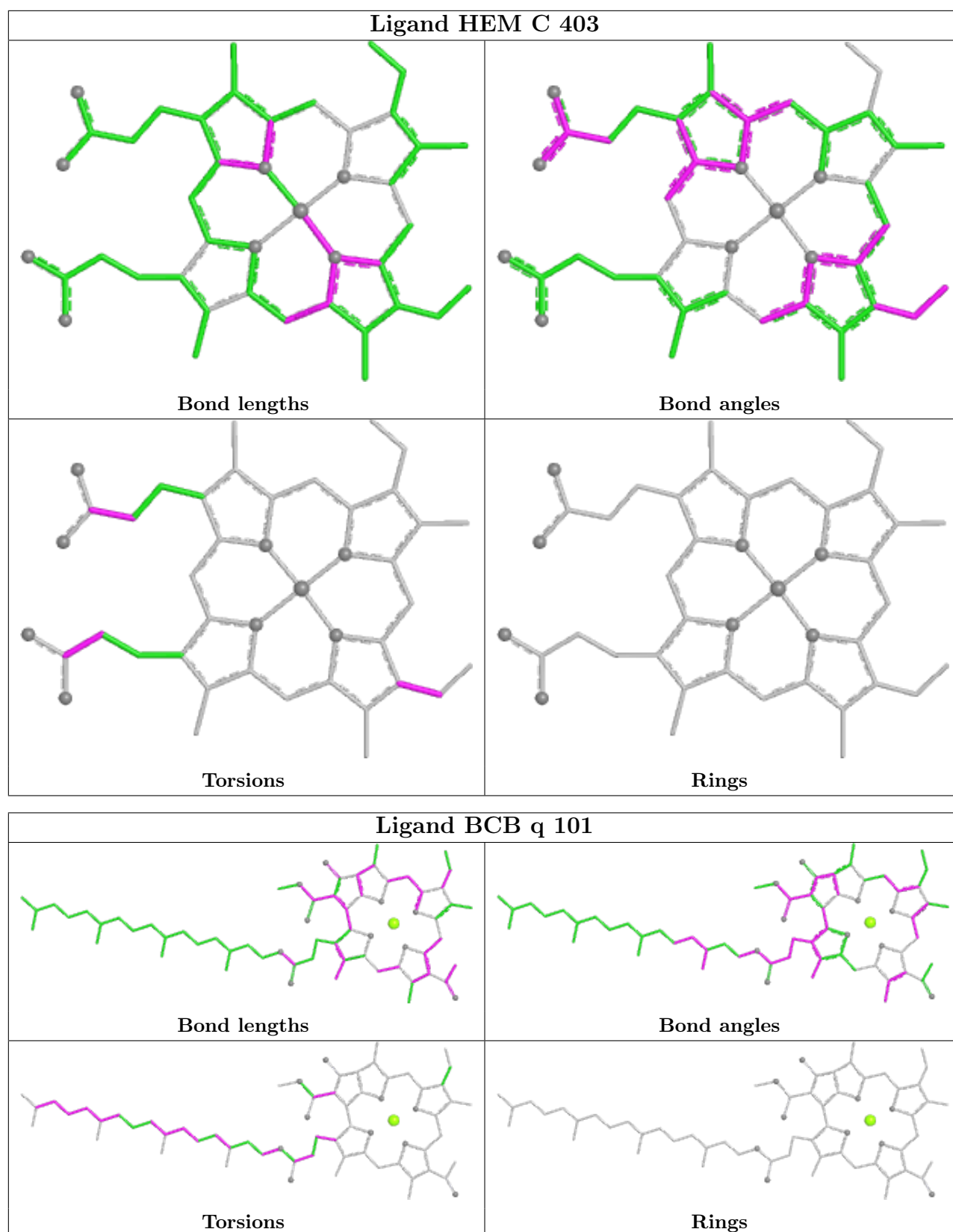


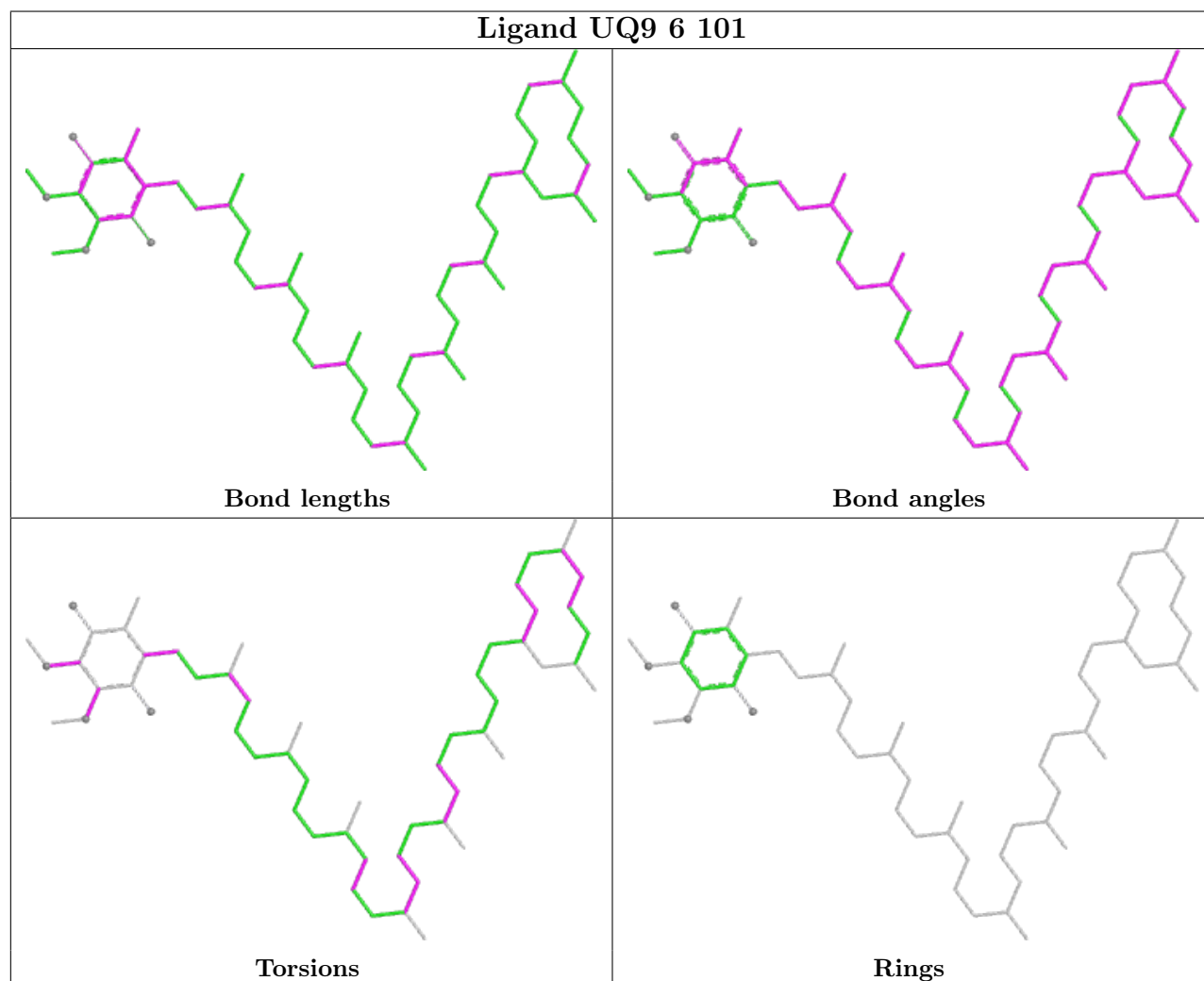
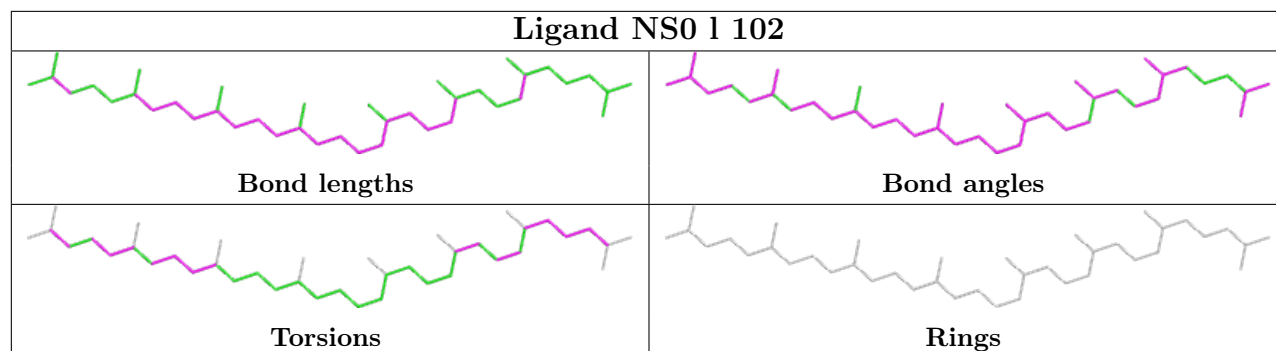


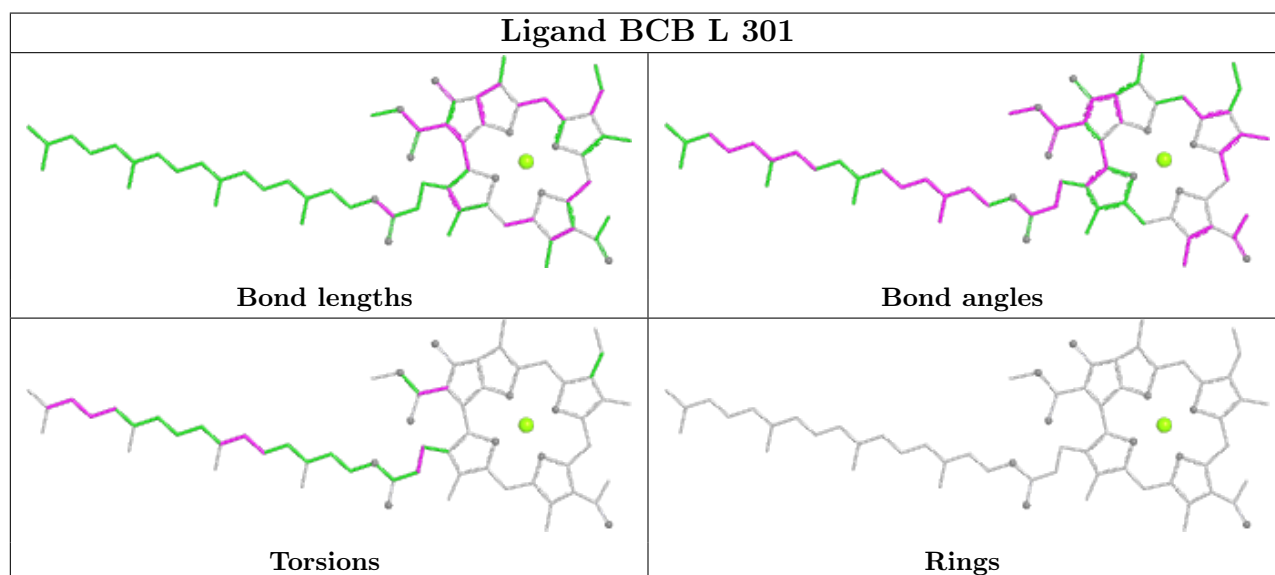
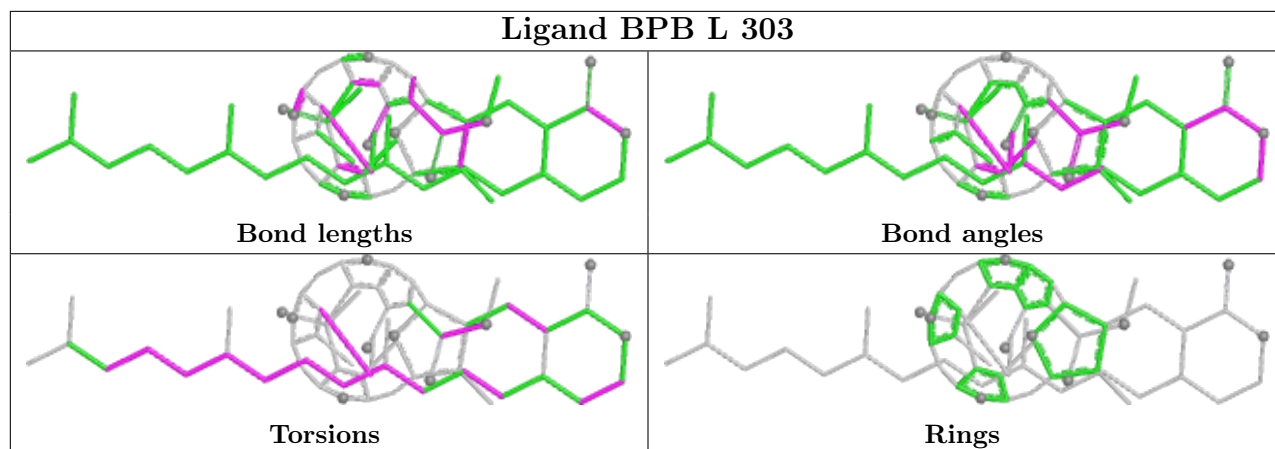


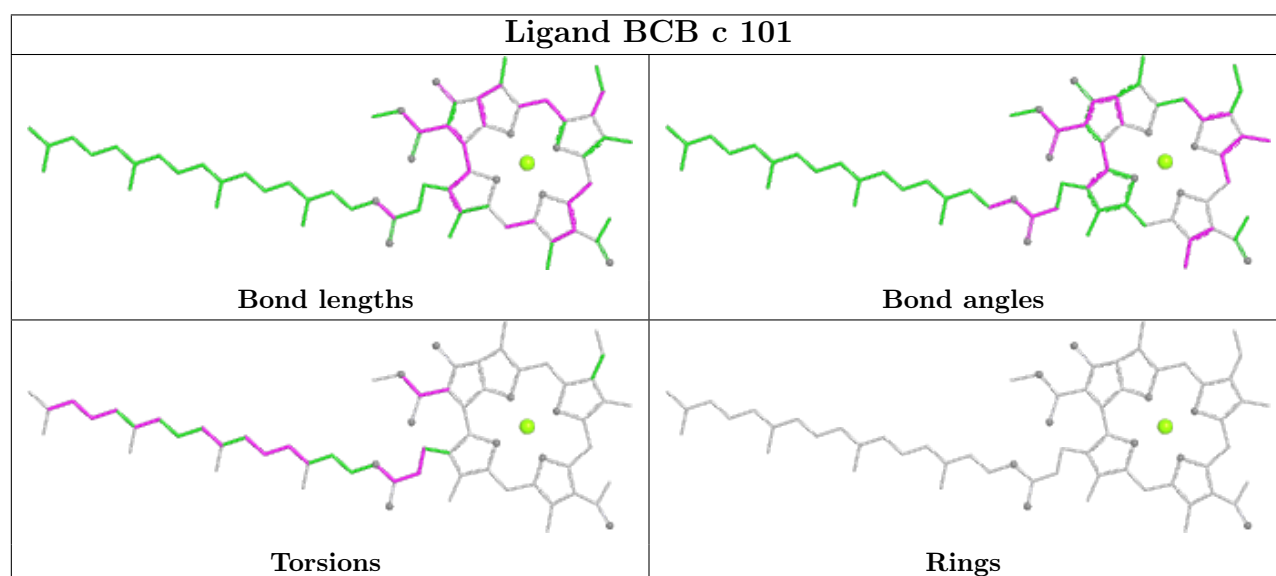
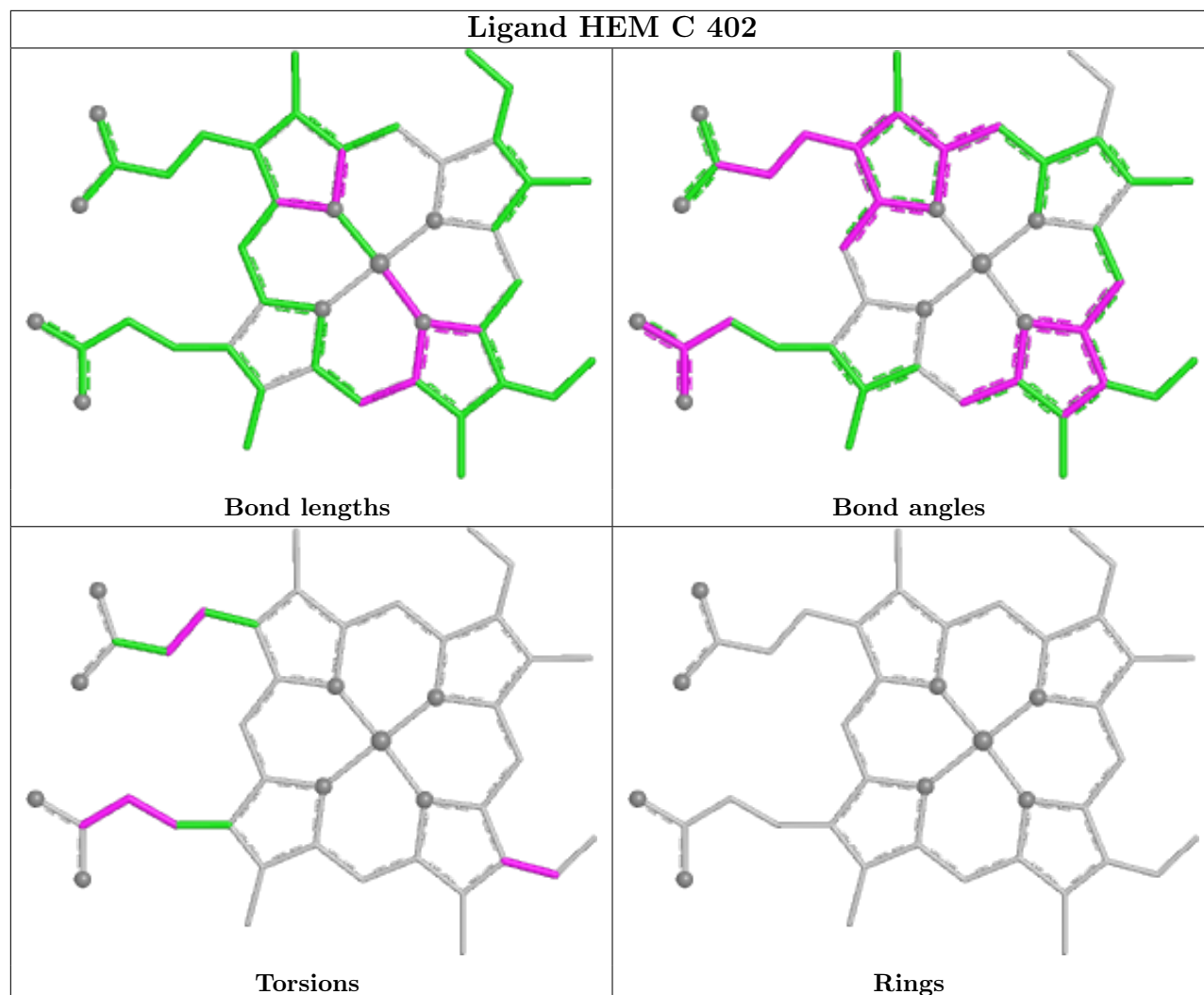


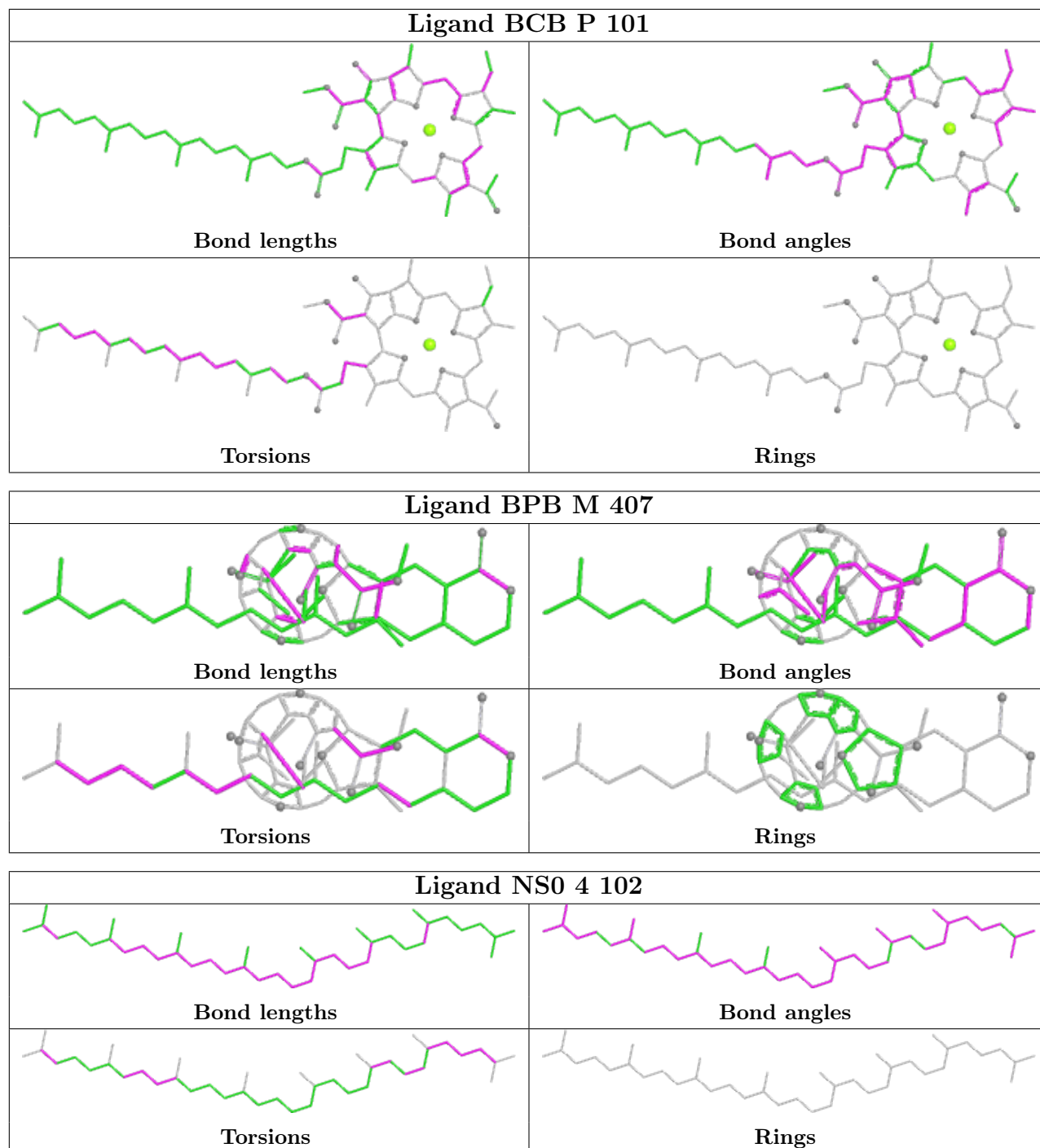


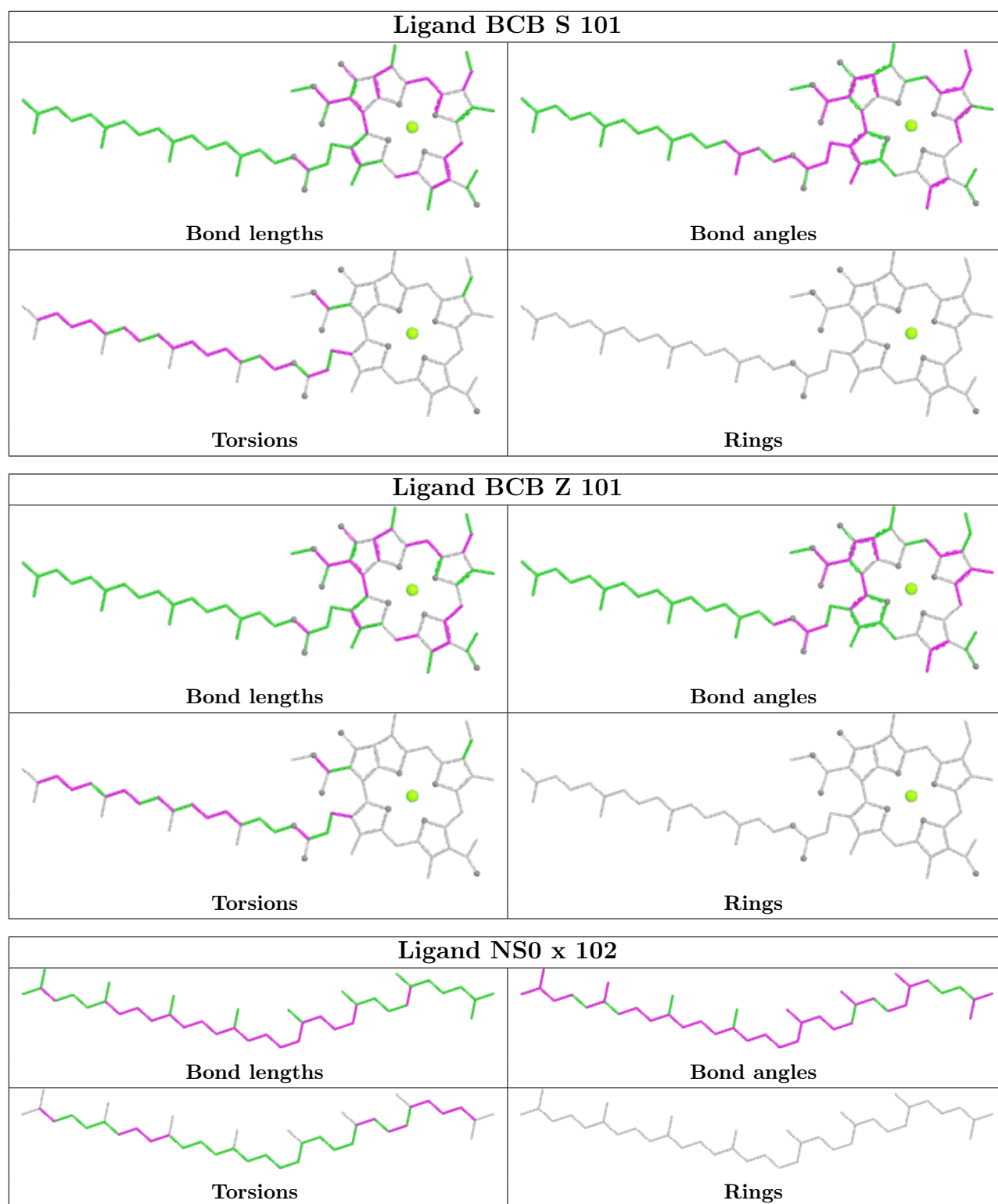


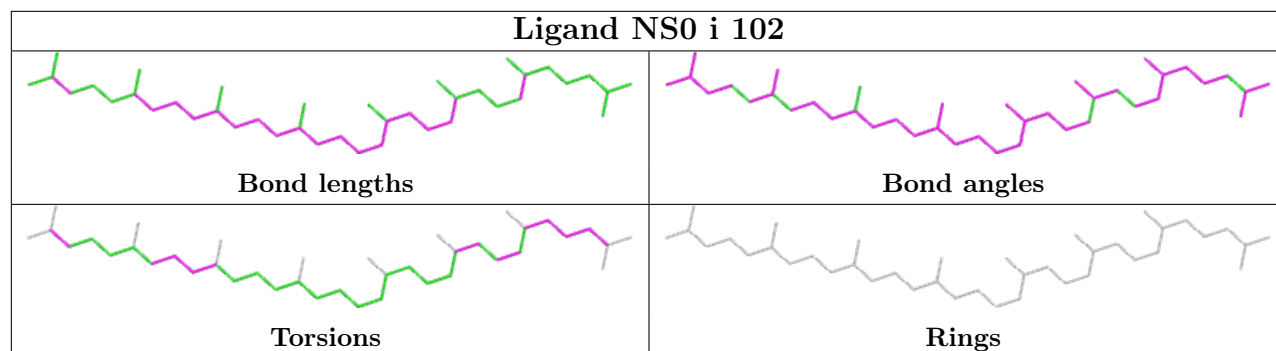
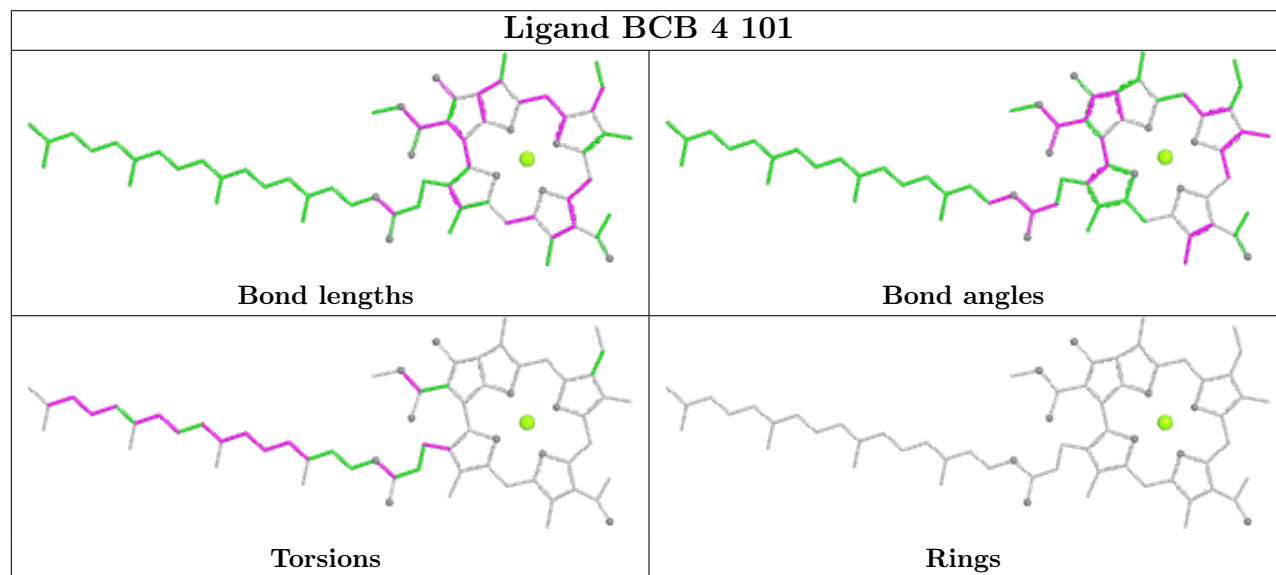
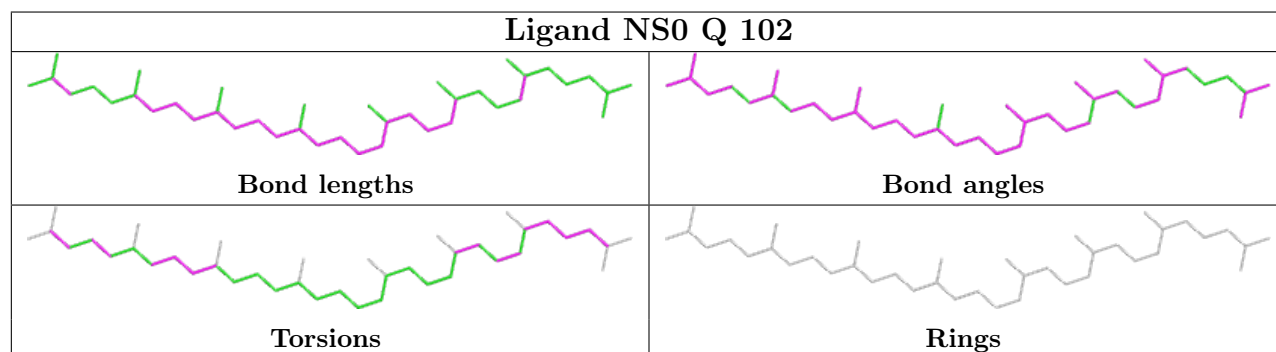
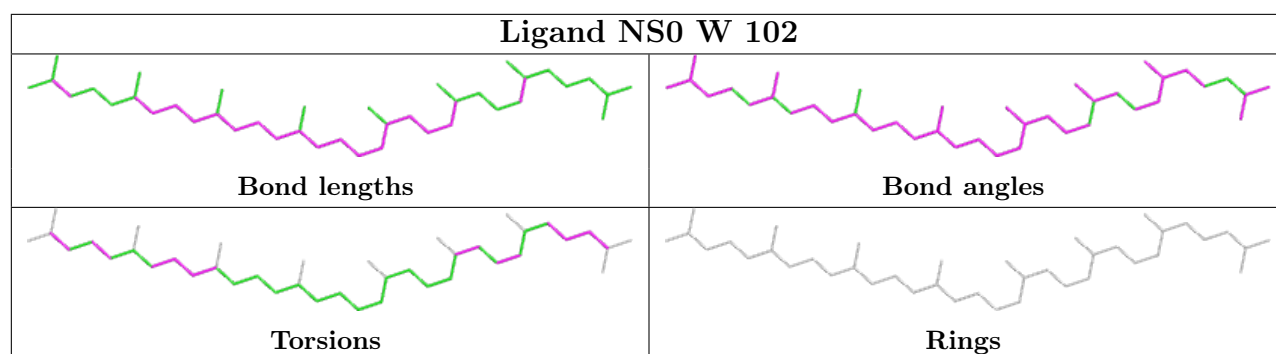


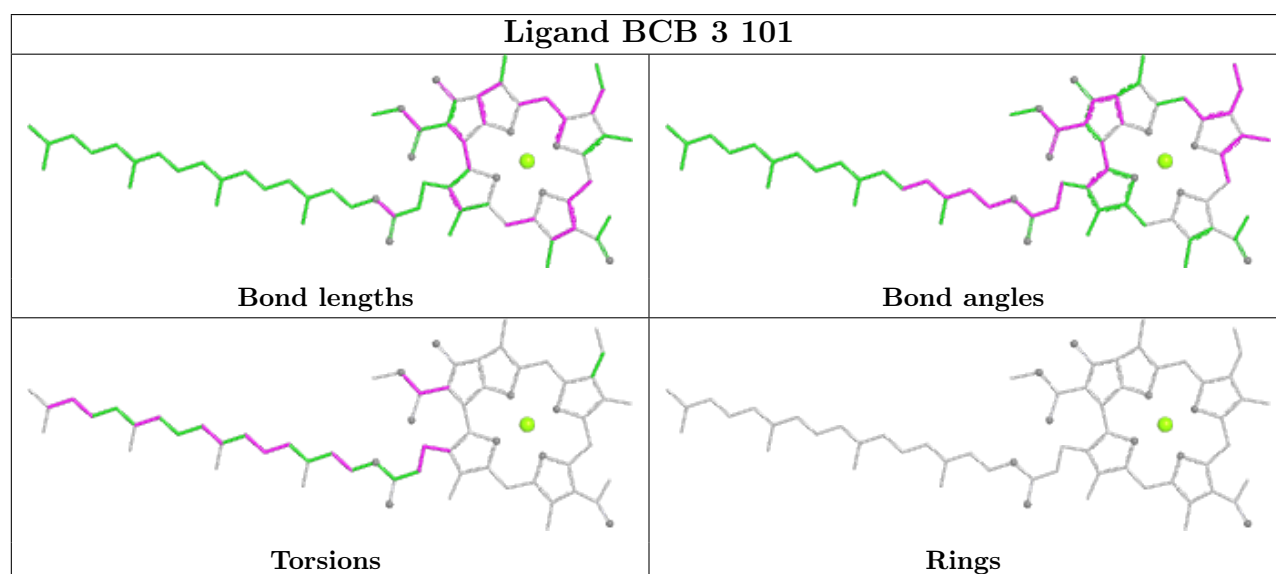
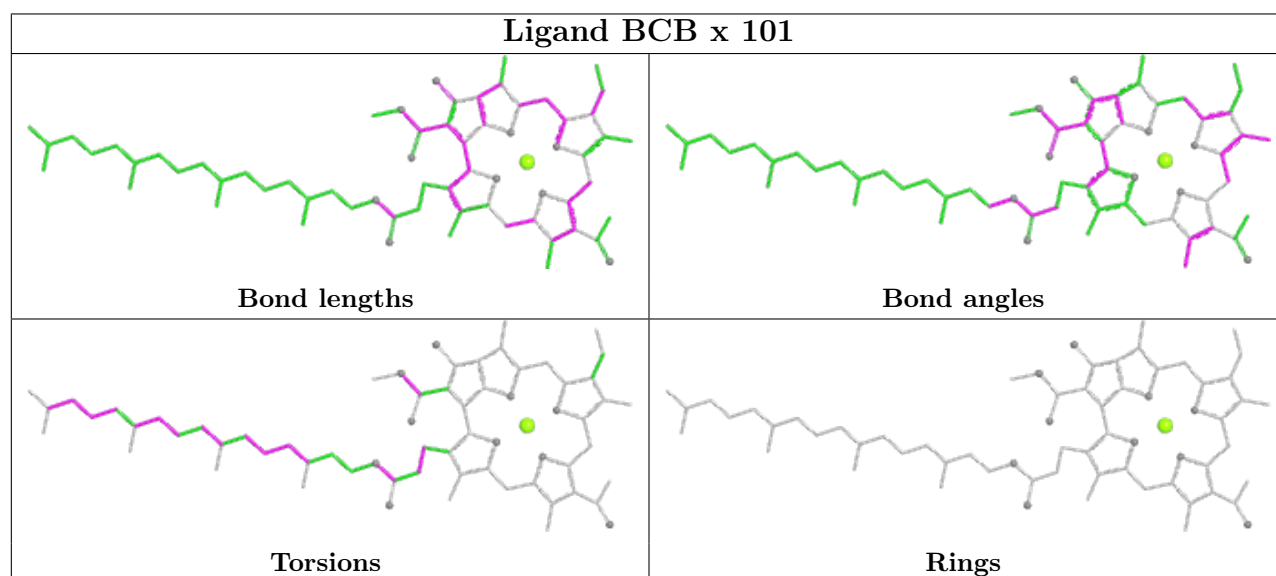
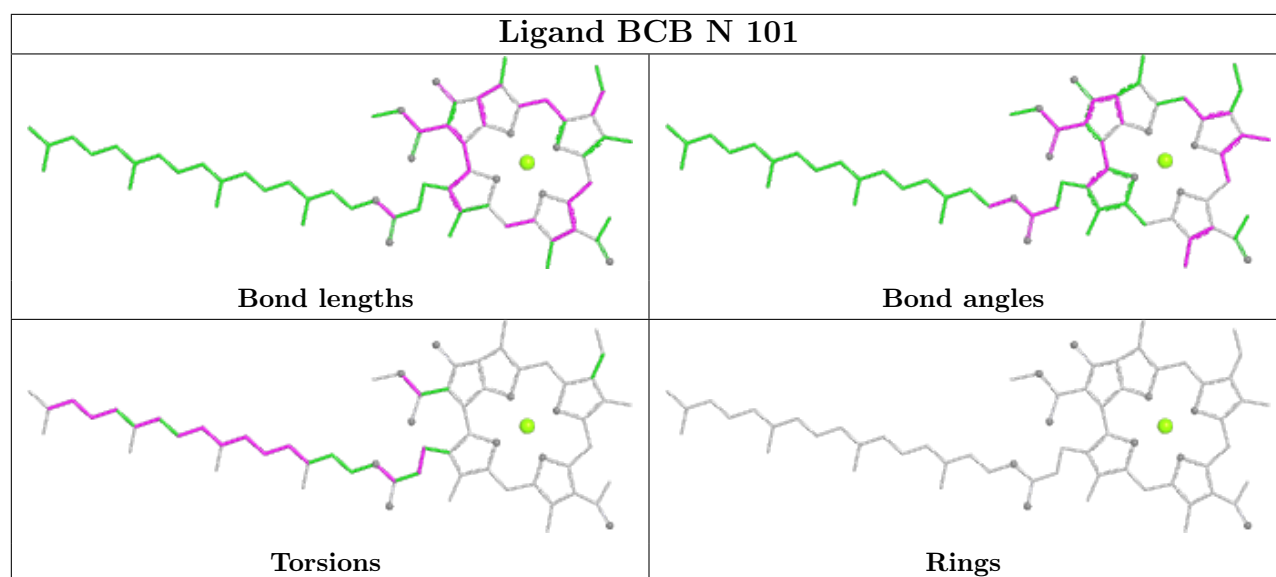


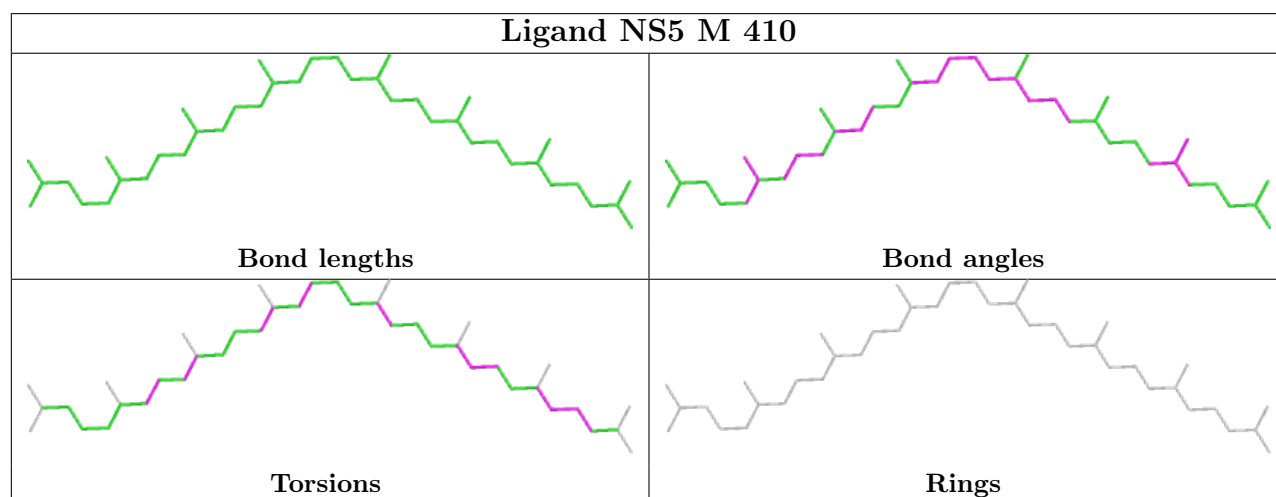
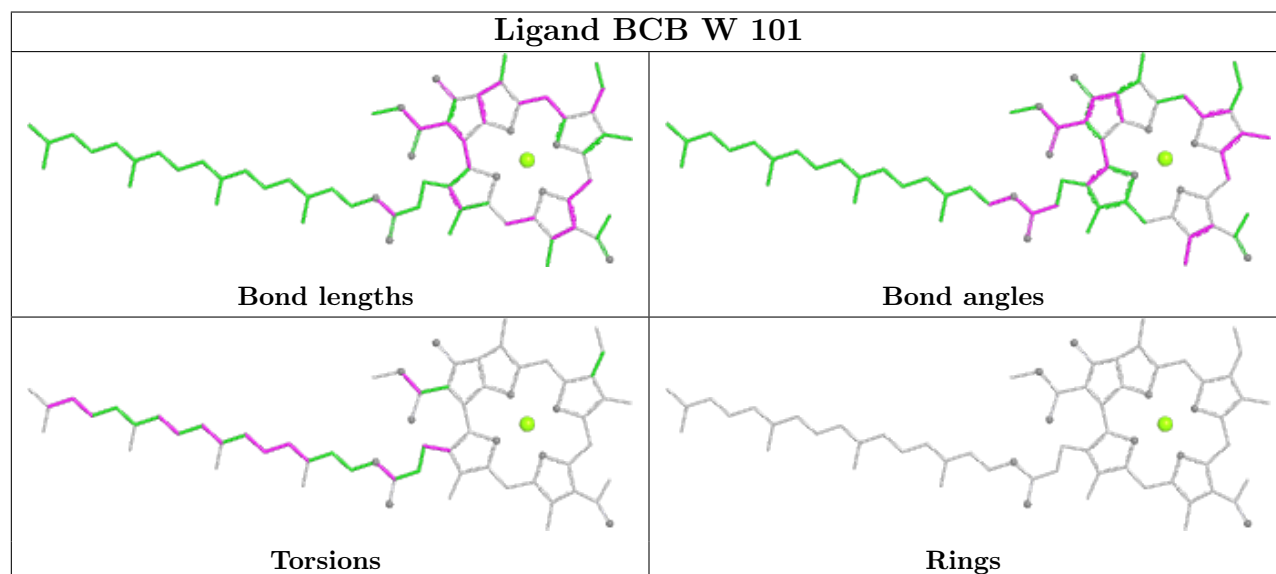
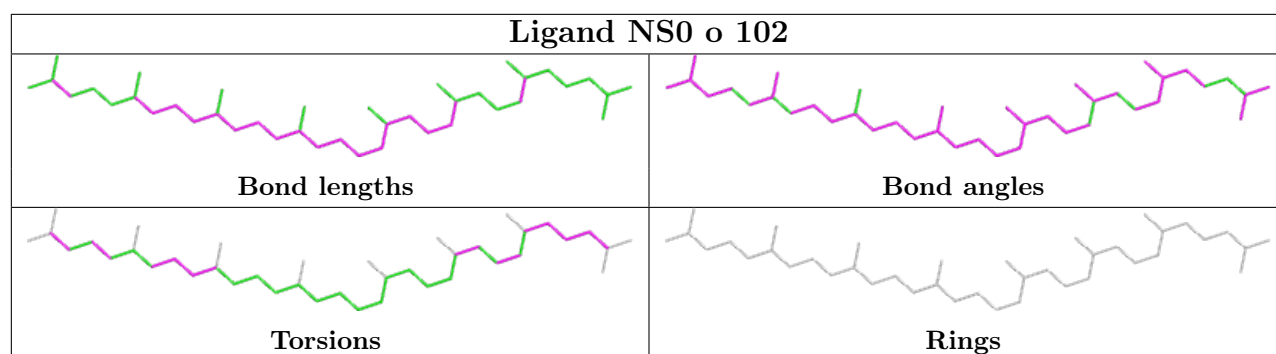


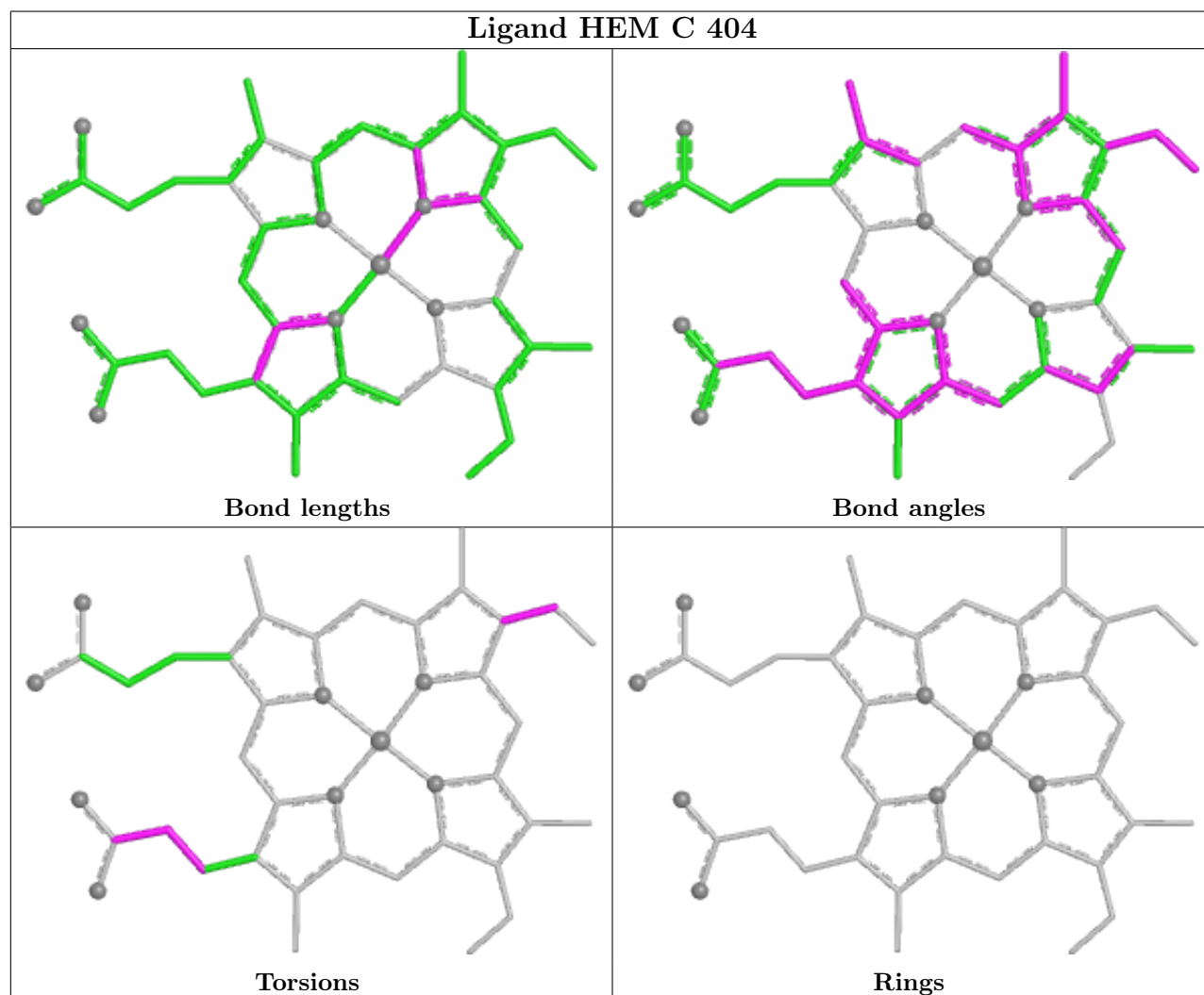
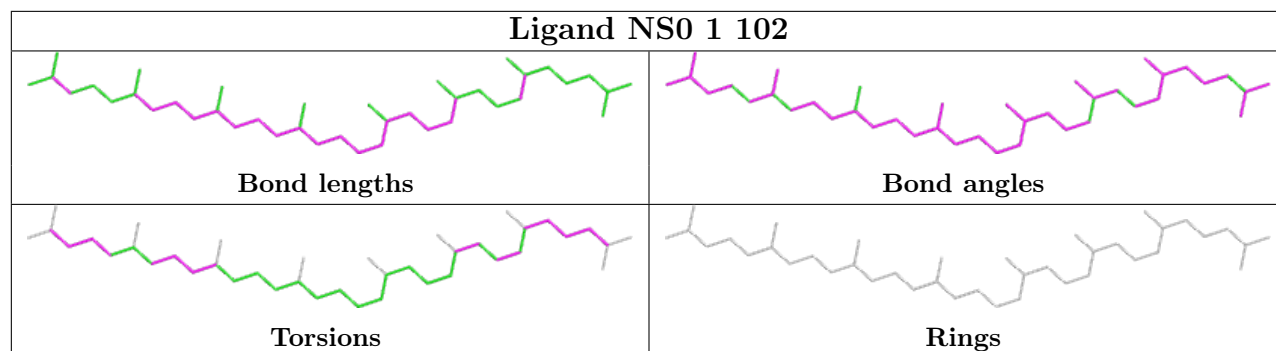


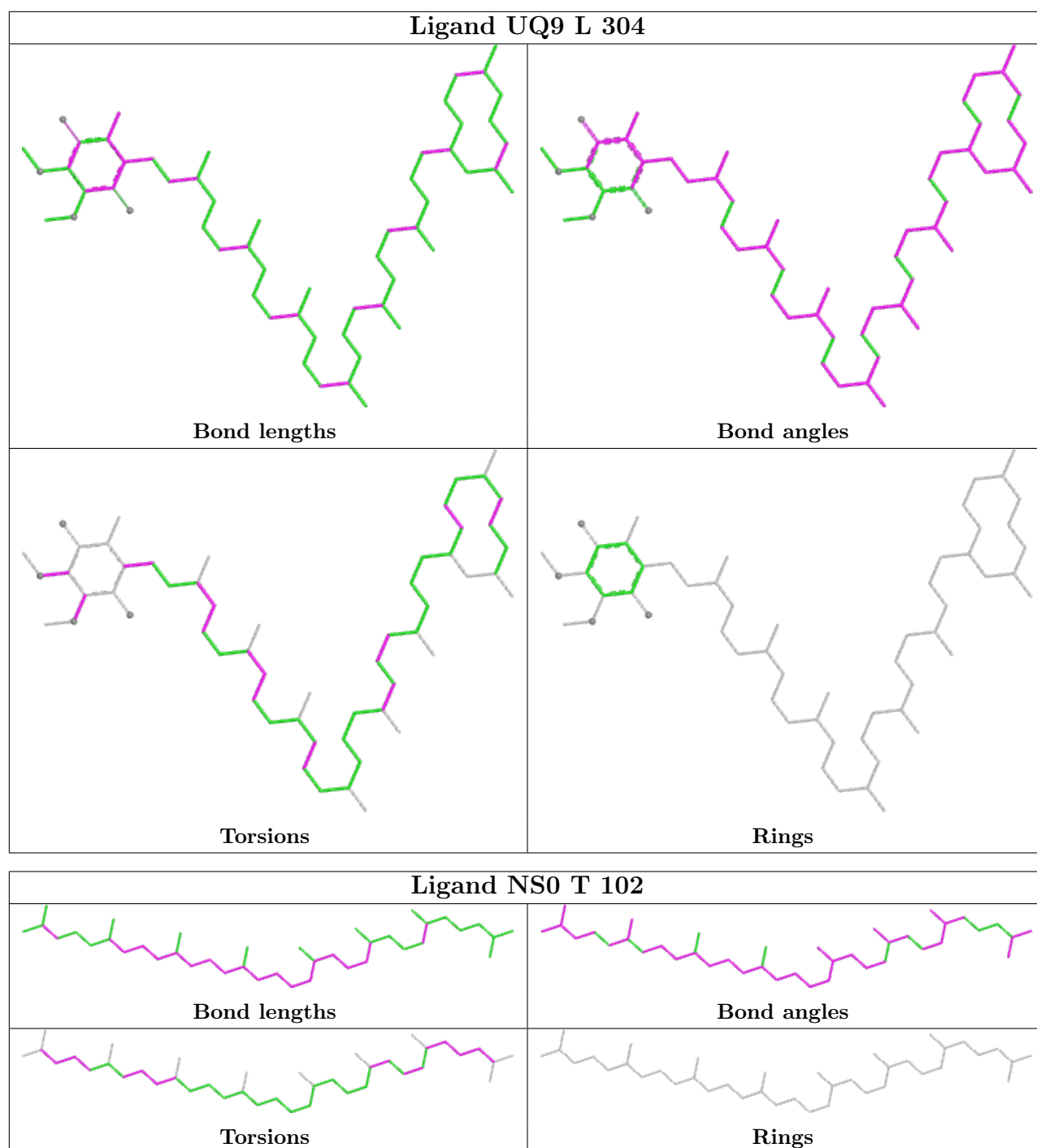


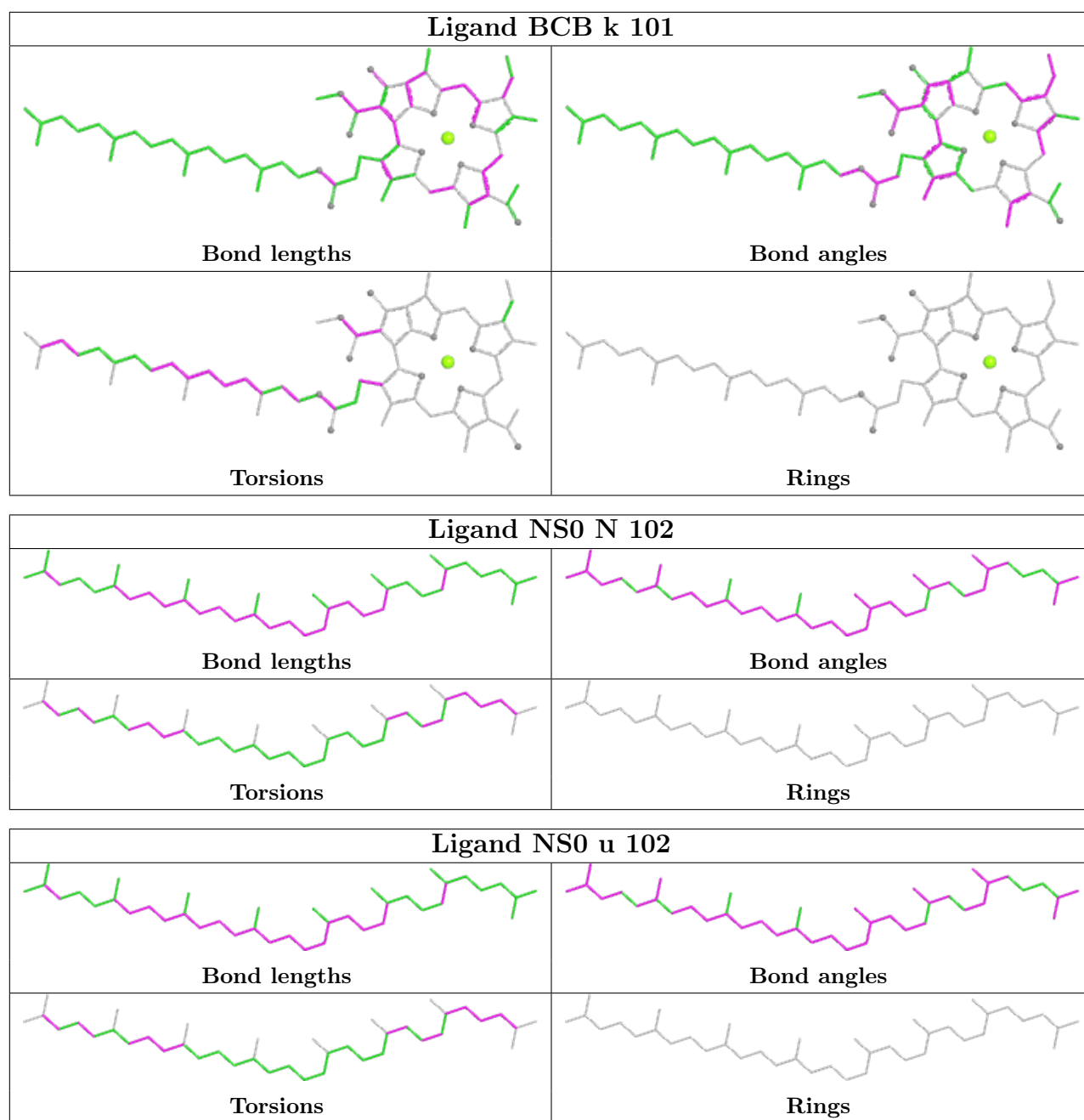












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
-----	-------	------------------

Mol	Chain	Number of breaks
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	53:ALA	C	54:PRO	N	3.10

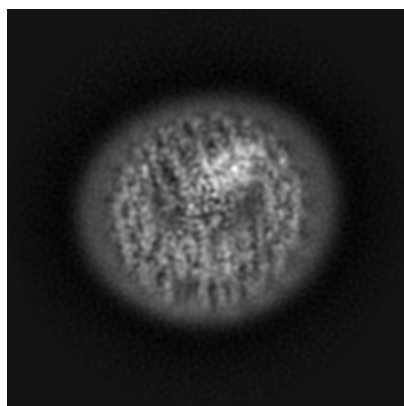
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3951. These allow visual inspection of the internal detail of the map and identification of artifacts.

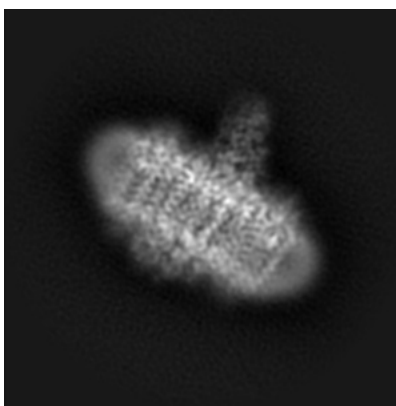
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

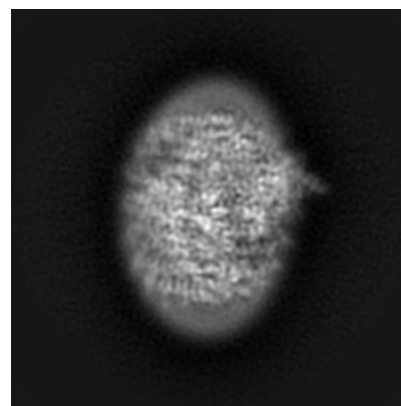
6.1.1 Primary map



X

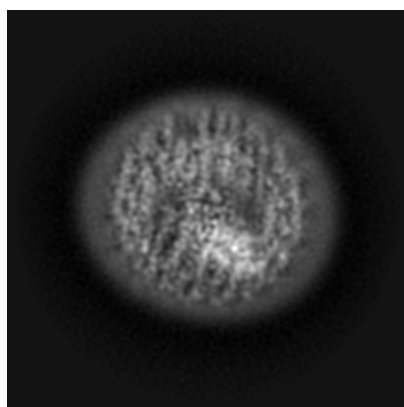


Y

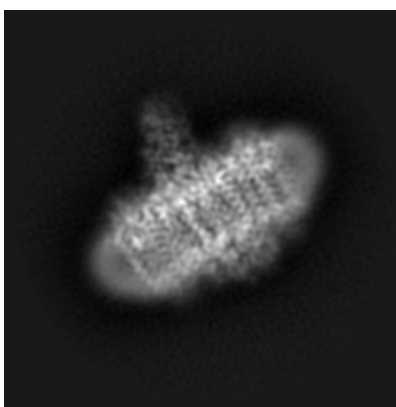


Z

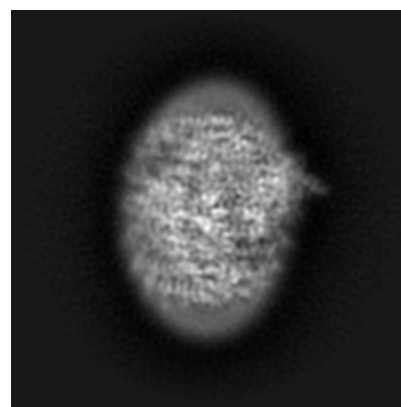
6.1.2 Raw map



X



Y

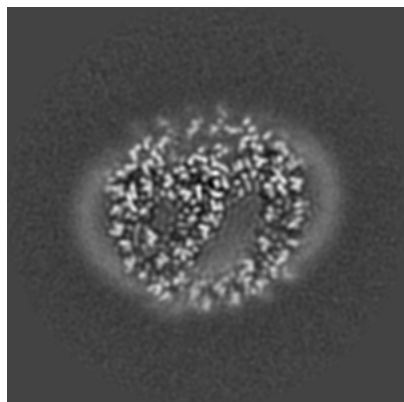


Z

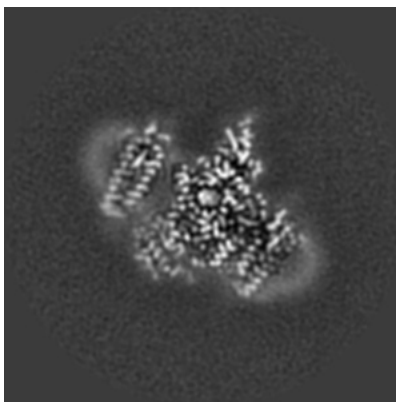
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

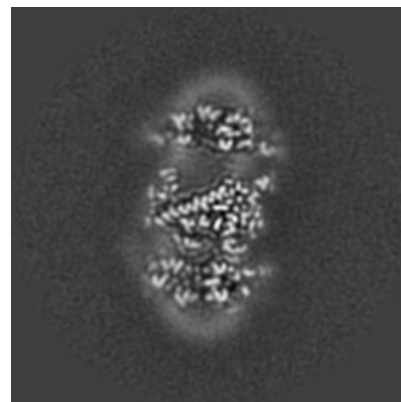
6.2.1 Primary map



X Index: 115

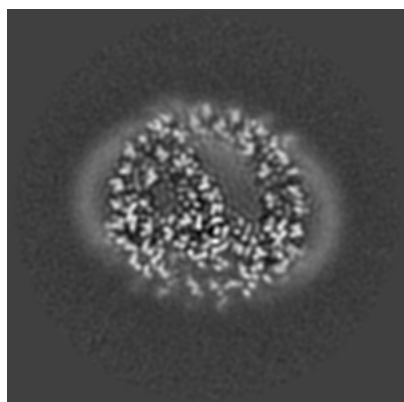


Y Index: 115

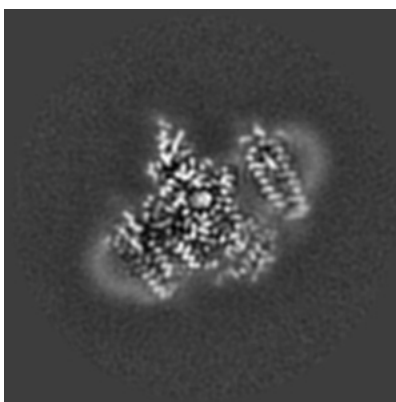


Z Index: 115

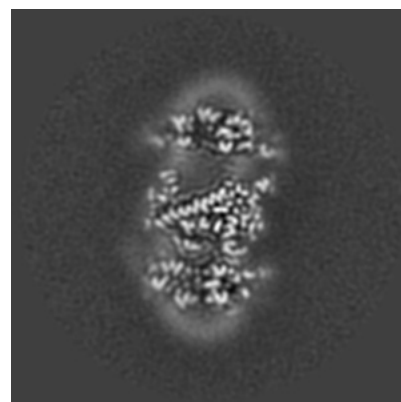
6.2.2 Raw map



X Index: 115



Y Index: 115

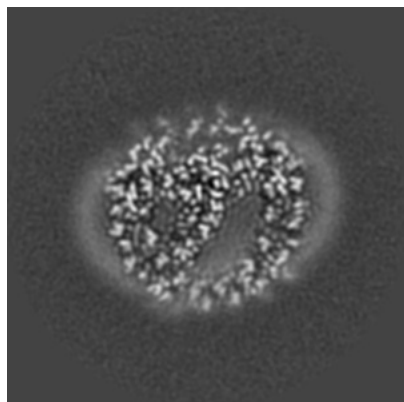


Z Index: 115

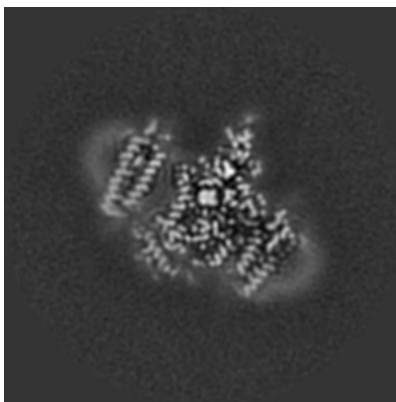
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

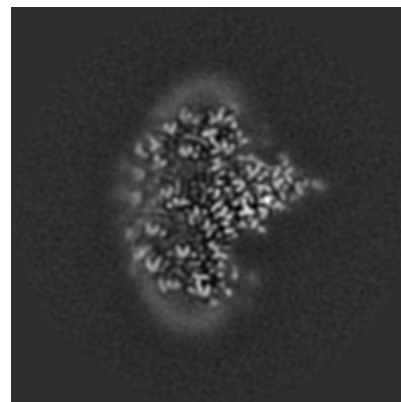
6.3.1 Primary map



X Index: 115

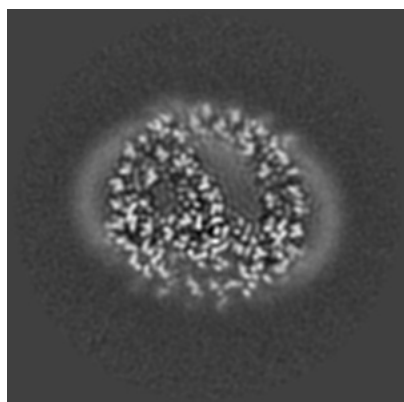


Y Index: 114

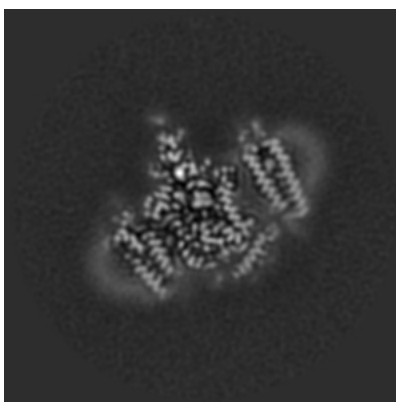


Z Index: 131

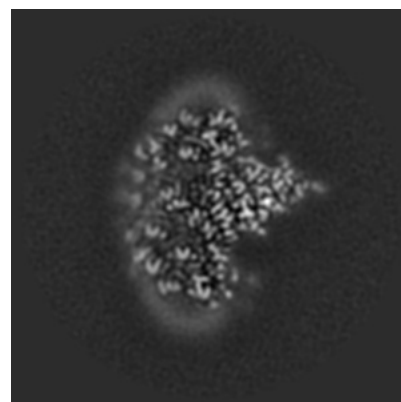
6.3.2 Raw map



X Index: 115



Y Index: 113

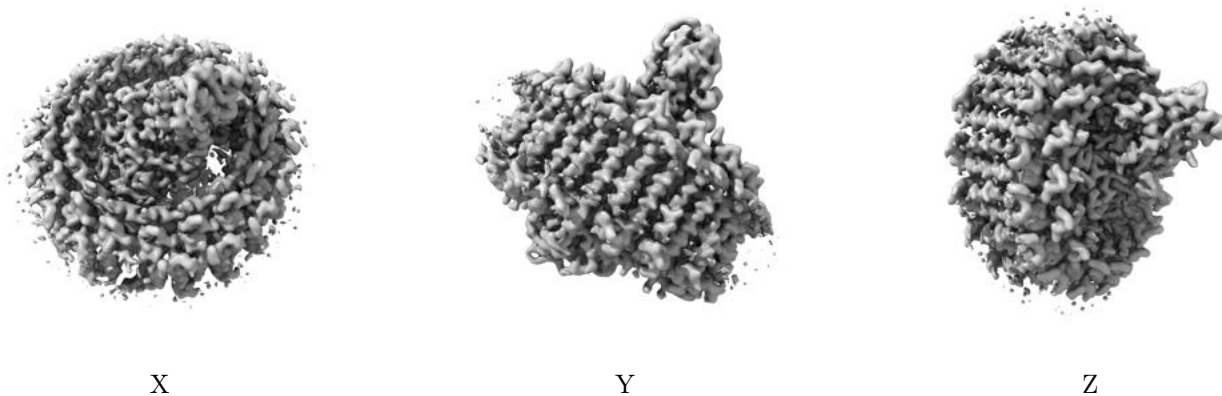


Z Index: 99

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

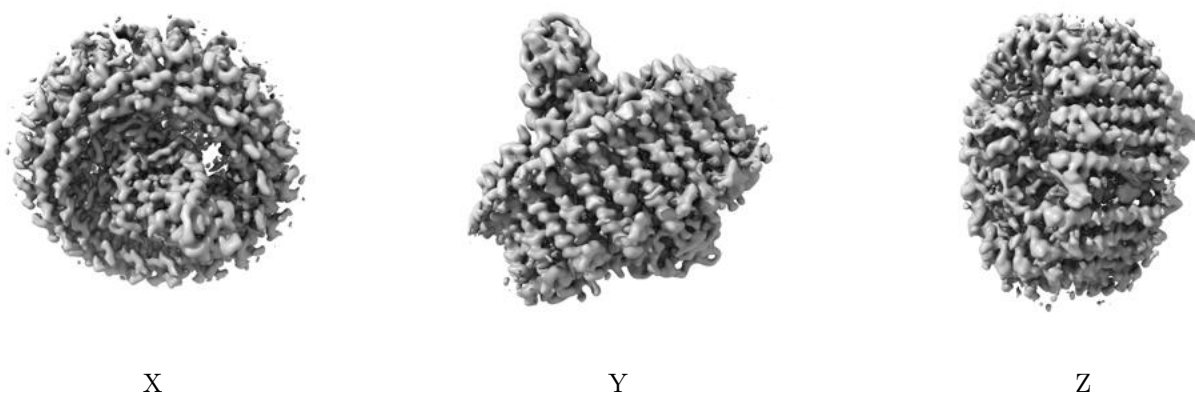
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

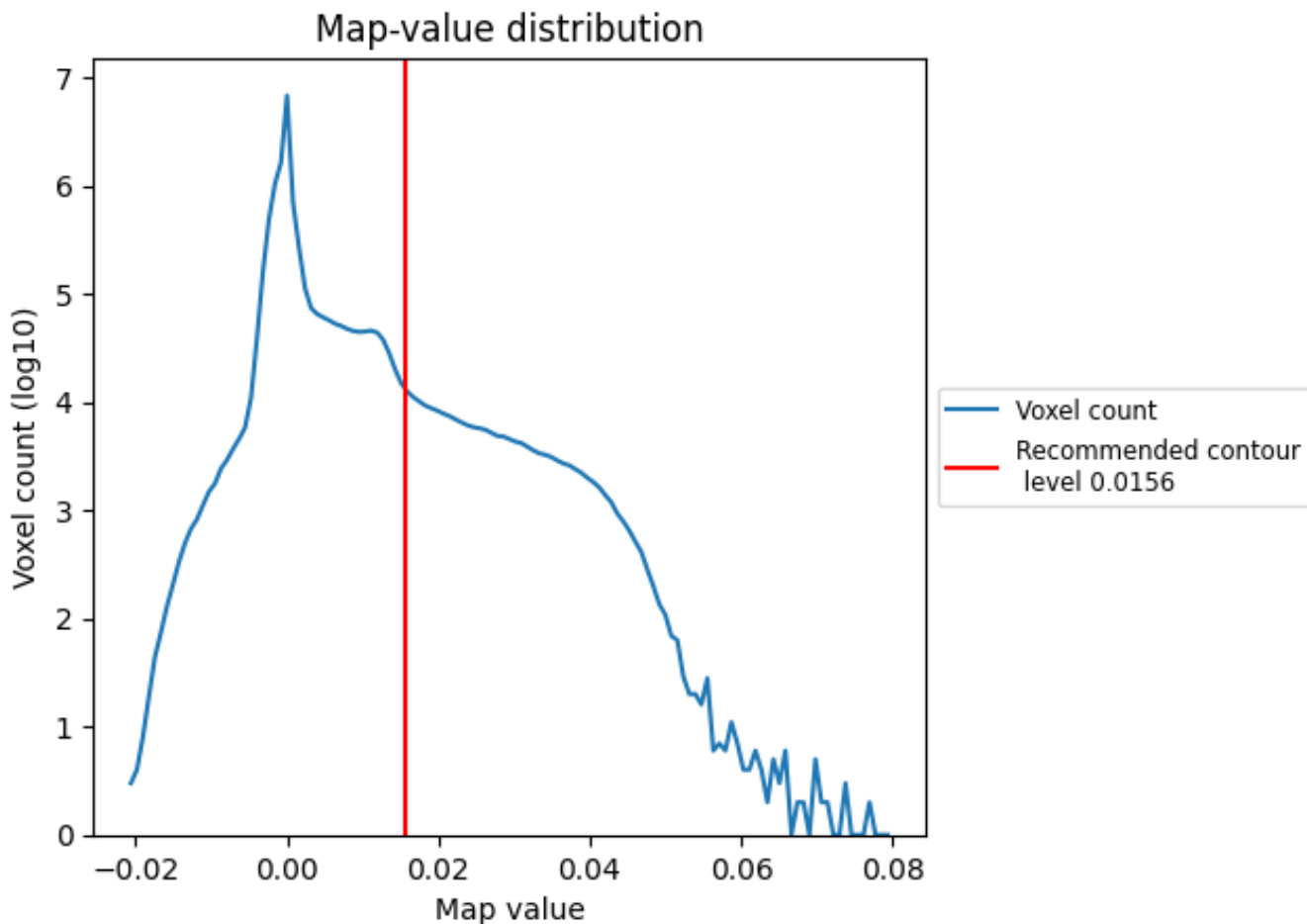
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

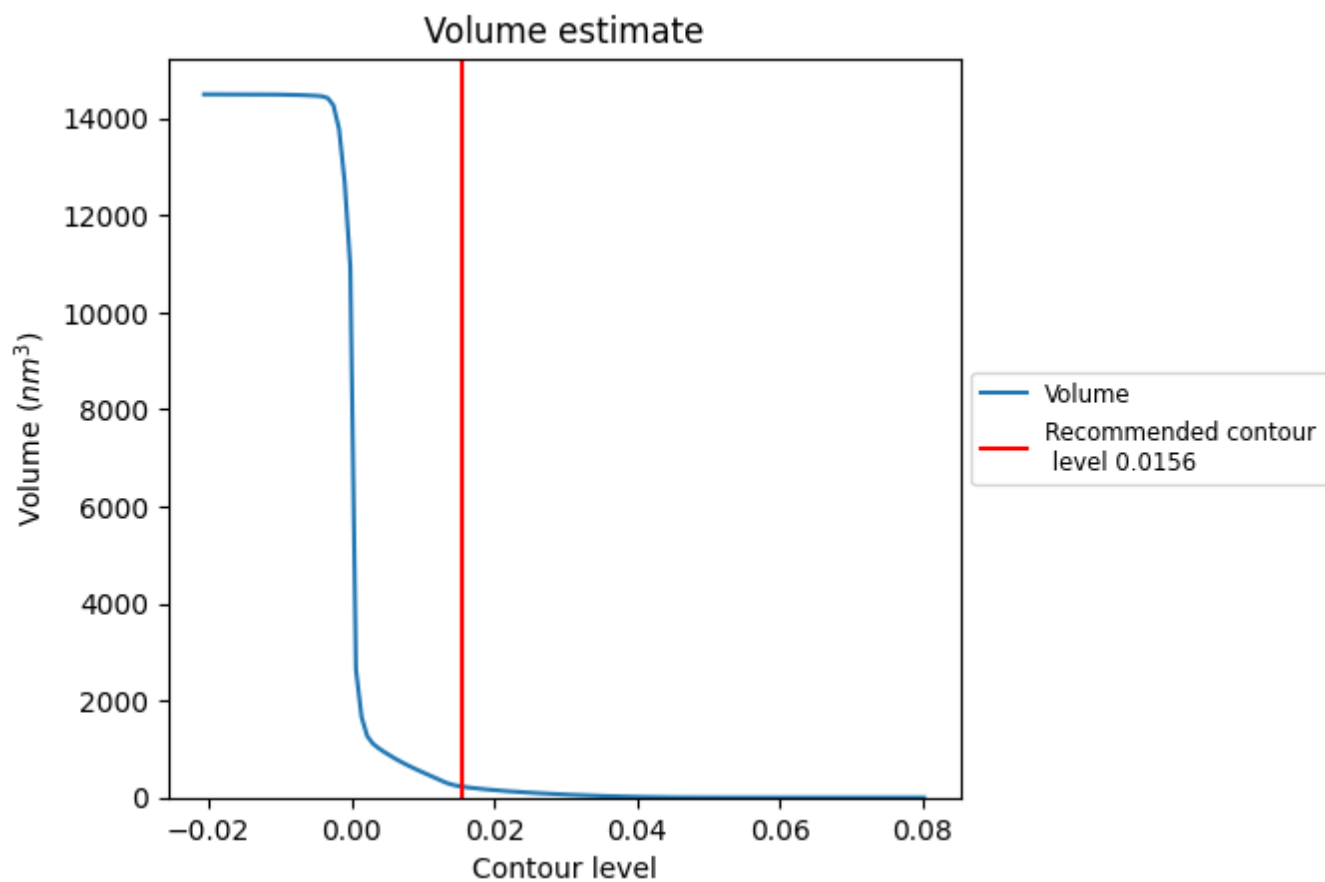
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

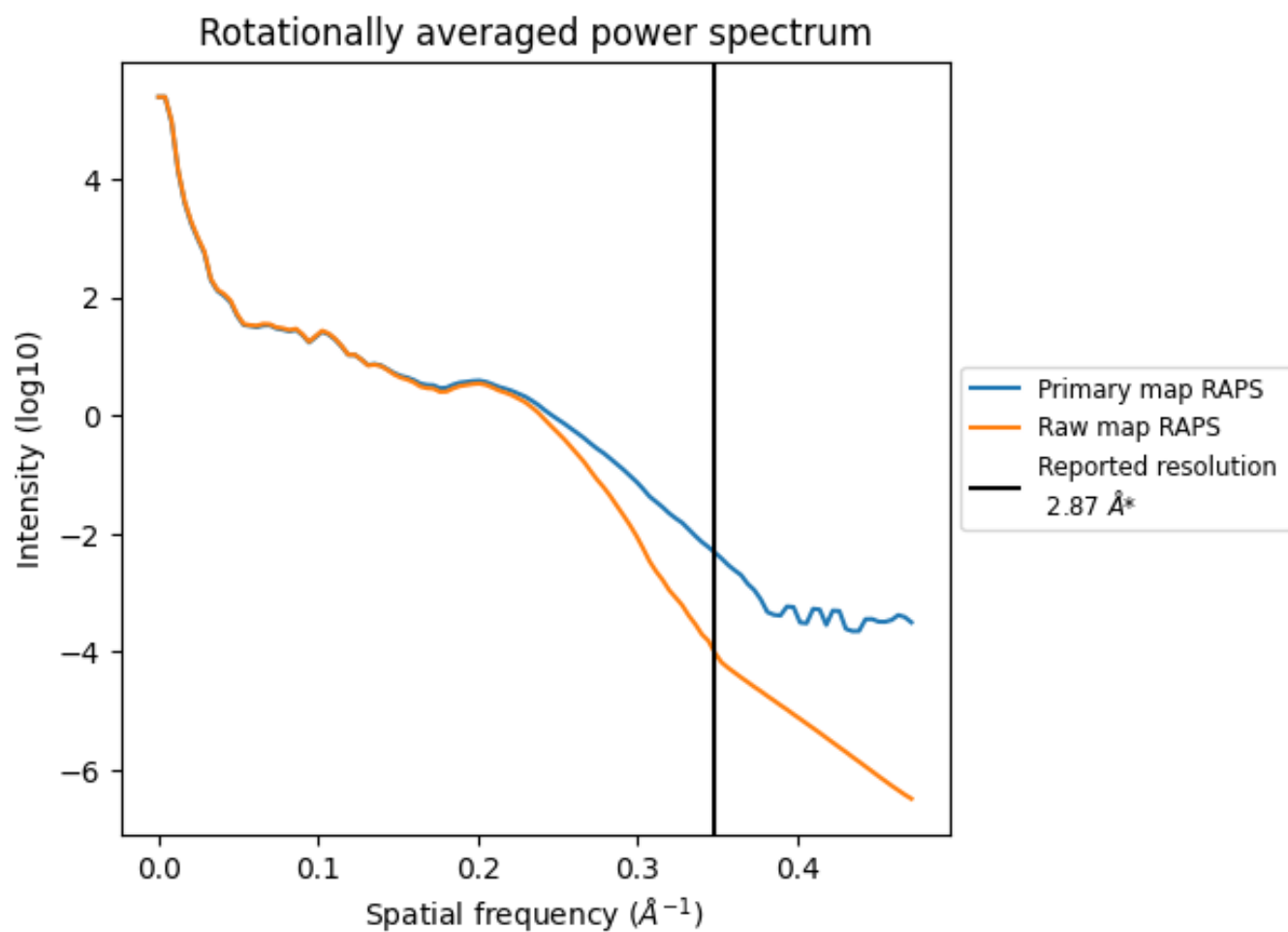
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 202 kDa.

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

7.3 Rotationally averaged power spectrum i

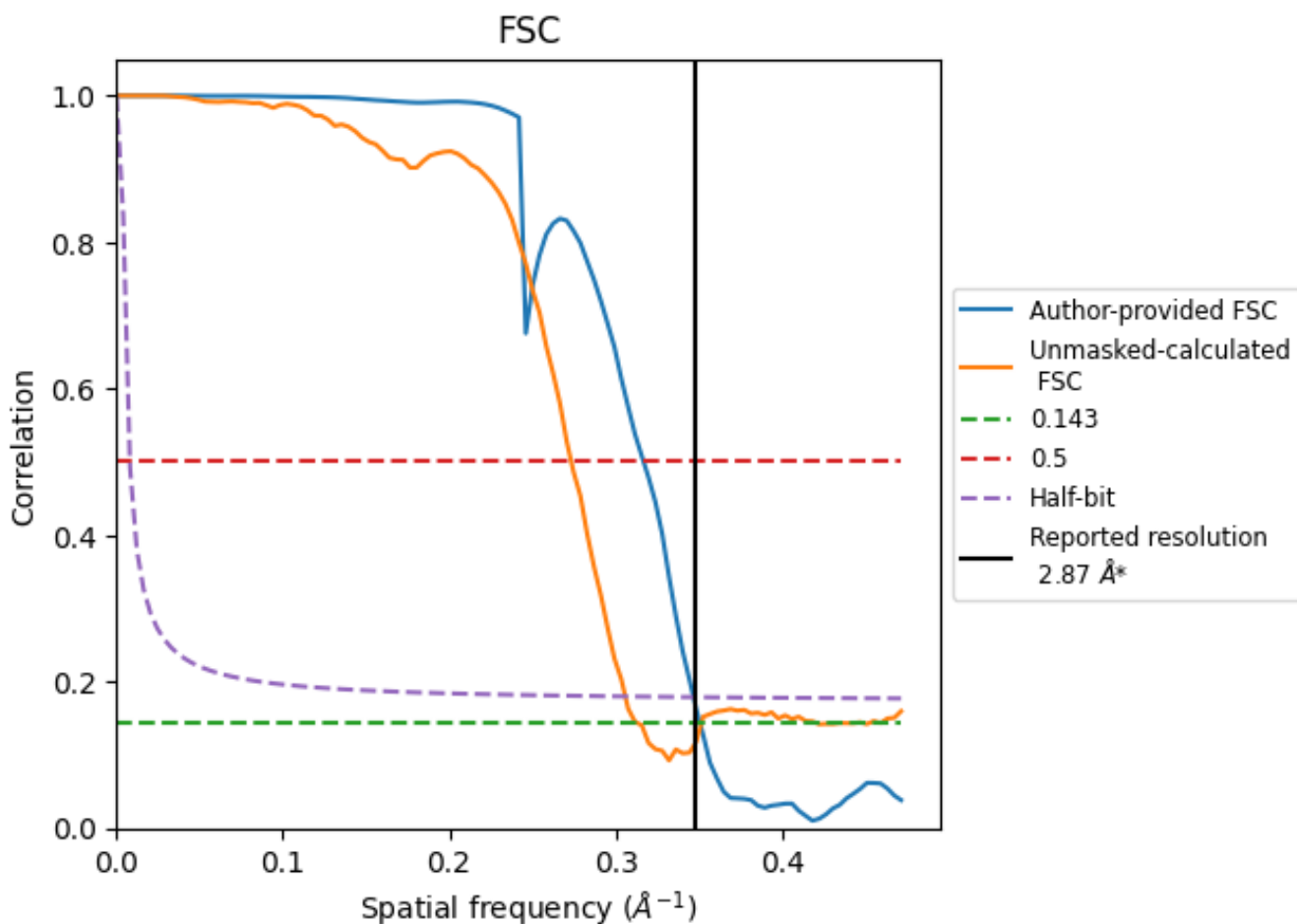


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

8.2 Resolution estimates [i](#)

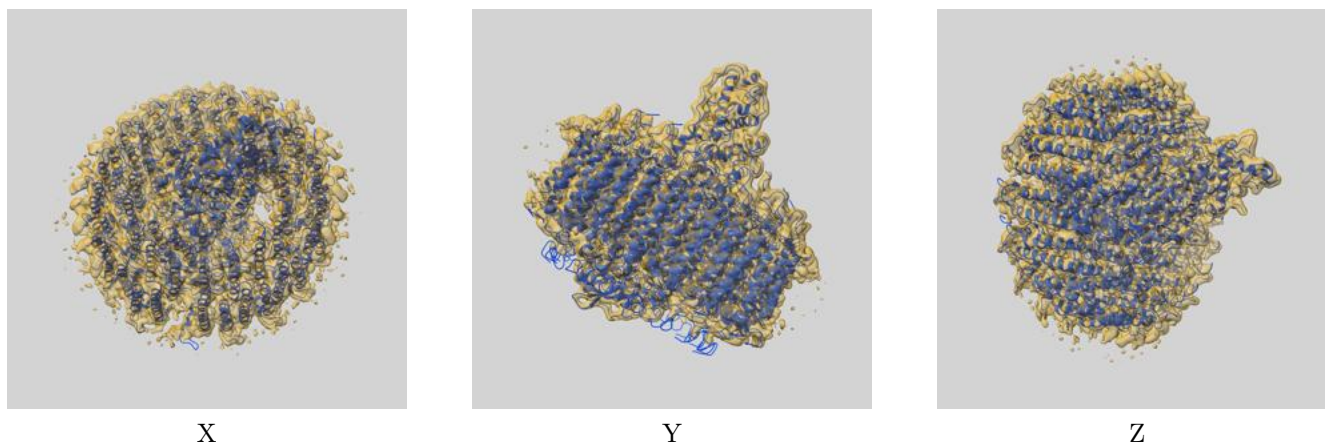
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.85	3.16	2.88
Unmasked-calculated*	3.19	3.66	3.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

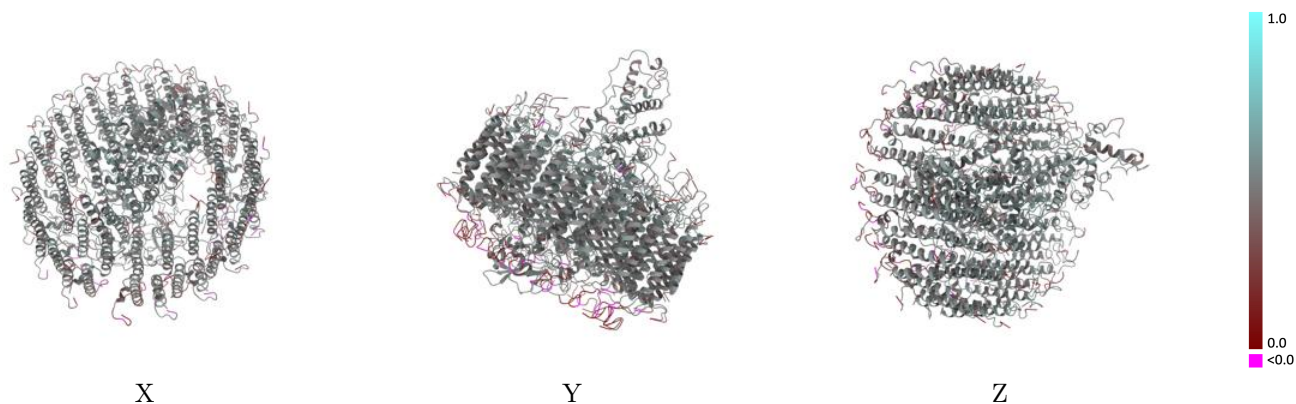
This section contains information regarding the fit between EMDB map EMD-3951 and PDB model 6ET5. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



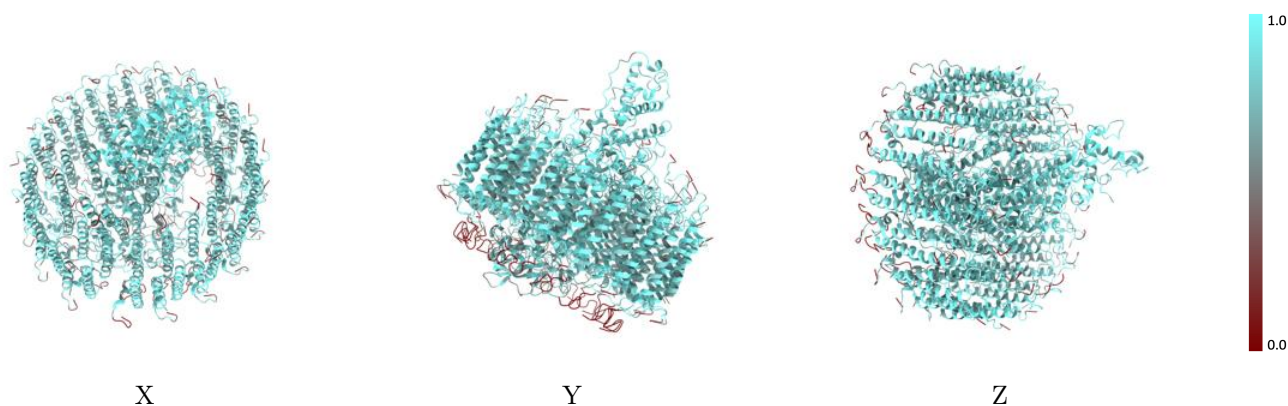
The images above show the 3D surface view of the map at the recommended contour level 0.0156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



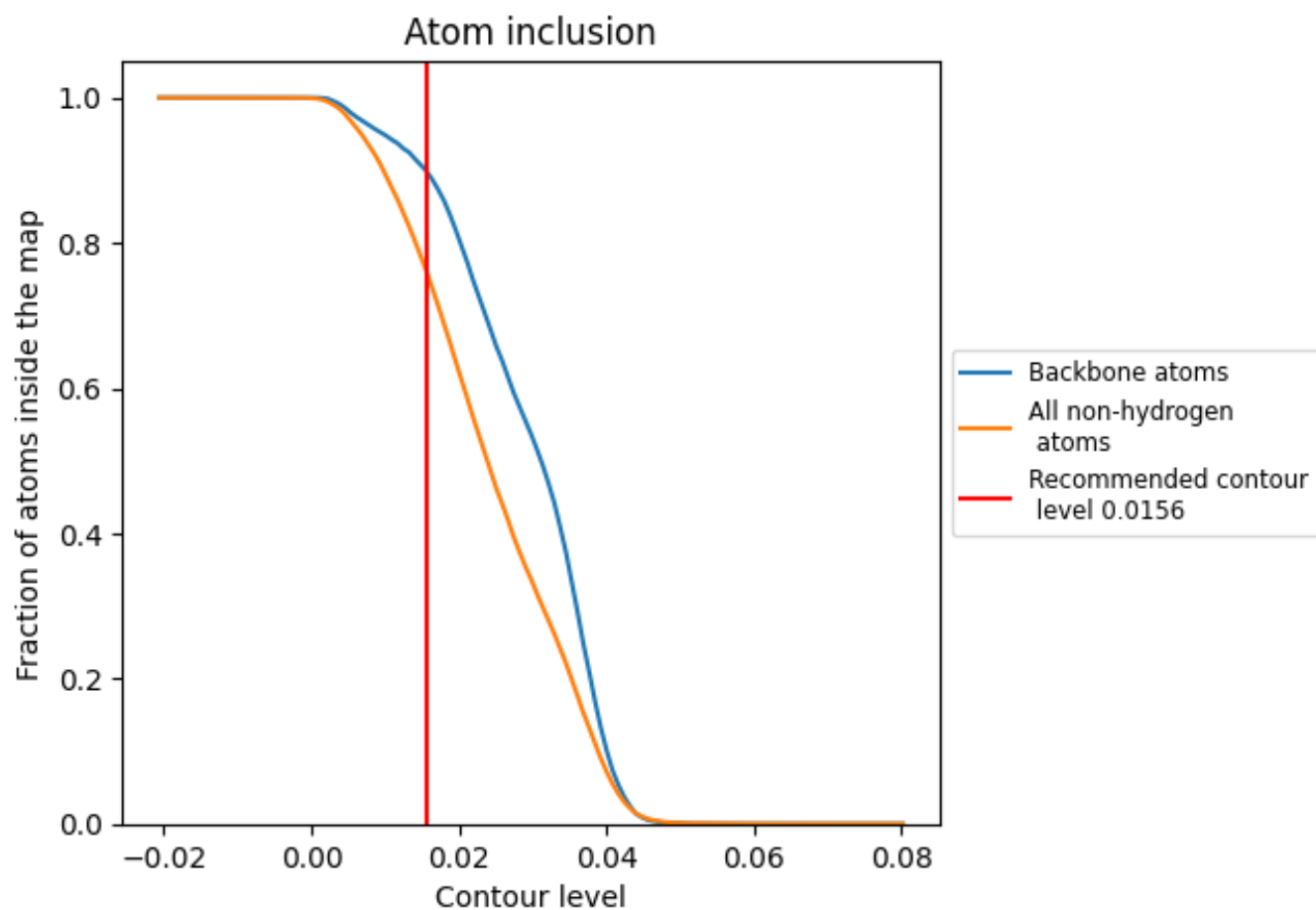
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0156).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.0156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7607	 0.4690
1	 0.6930	 0.4460
2	 0.8083	 0.4560
3	 0.7880	 0.4780
4	 0.6893	 0.4410
5	 0.7306	 0.4390
6	 0.7022	 0.4620
7	 0.6535	 0.4290
C	 0.8859	 0.5100
F	 0.7129	 0.4330
G	 0.6441	 0.4030
H	 0.7061	 0.4740
I	 0.7927	 0.4380
K	 0.7636	 0.4710
L	 0.8381	 0.5230
M	 0.8377	 0.5190
N	 0.6911	 0.4340
O	 0.8187	 0.4540
P	 0.7767	 0.4740
Q	 0.6893	 0.4420
R	 0.7824	 0.4430
S	 0.7749	 0.4760
T	 0.7043	 0.4310
U	 0.8083	 0.4460
V	 0.7767	 0.4840
W	 0.6949	 0.4290
X	 0.7979	 0.4380
Y	 0.7842	 0.4810
Z	 0.6930	 0.4240
a	 0.6891	 0.4280
b	 0.7767	 0.4800
c	 0.6817	 0.4320
d	 0.7150	 0.4370
e	 0.7598	 0.4720
f	 0.7024	 0.4280



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Chain	Atom inclusion	Q-score
g	 0.7668	 0.4430
h	 0.7655	 0.4820
i	 0.6930	 0.4330
j	 0.6891	 0.4310
k	 0.7598	 0.4730
l	 0.6798	 0.4370
m	 0.7409	 0.4320
n	 0.7430	 0.4710
o	 0.6704	 0.4190
p	 0.7720	 0.4490
q	 0.7617	 0.4670
r	 0.6817	 0.4260
s	 0.8135	 0.4490
t	 0.7617	 0.4760
u	 0.6987	 0.4280
v	 0.7772	 0.4320
w	 0.7749	 0.4780
x	 0.7081	 0.4330
y	 0.8135	 0.4540
z	 0.7842	 0.4870