



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:19 PM UTC

PDB ID : 6ET5 / pdb_00006et5
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 : 2.87 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

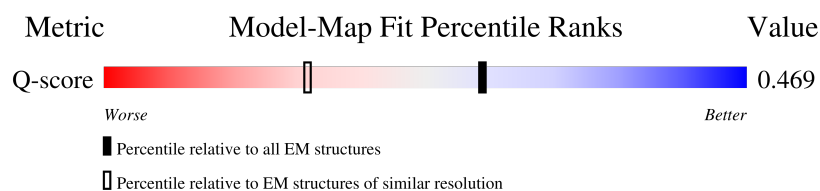
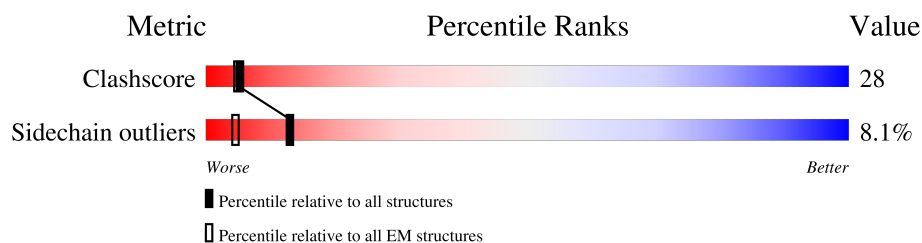
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	 77% 21% .
2	L	274	 69% 27% .
3	M	323	 81% 18% .
4	H	258	 9% 74% 22% .
5	3	59	 7% 53% 34% 12% .

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Mol	Chain	Length	Quality of chain
5	6	59	
5	F	59	
5	K	59	
5	P	59	
5	S	59	
5	V	59	
5	Y	59	
5	b	59	
5	e	59	
5	h	59	
5	k	59	
5	n	59	
5	q	59	
5	t	59	
5	w	59	
5	z	59	
6	1	56	
6	4	56	
6	7	56	
6	G	56	
6	N	56	
6	Q	56	
6	T	56	
6	W	56	
6	Z	56	

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Mol	Chain	Length	Quality of chain
6	c	56	
6	f	56	
6	i	56	
6	l	56	
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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BPB	L	303	X	-	-	-
10	BPB	M	408	X	-	-	-
11	UQ9	6	101	-	-	X	-
11	UQ9	L	304	-	-	X	-
17	NS0	1	102	-	X	-	-
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	-	-
9	BCB	1	101	X	-	-	-
9	BCB	3	101	X	-	-	-
9	BCB	4	101	X	-	-	-
9	BCB	6	102	X	-	-	-
9	BCB	7	101	X	-	-	-
9	BCB	F	101	X	-	-	-
9	BCB	G	101	X	-	-	-
9	BCB	K	101	X	-	-	-
9	BCB	L	301	X	-	-	-
9	BCB	L	302	X	-	-	-
9	BCB	M	406	X	-	-	-
9	BCB	M	407	X	-	-	-
9	BCB	N	101	X	-	-	-
9	BCB	P	101	X	-	-	-
9	BCB	Q	101	X	-	-	-
9	BCB	S	101	X	-	-	-
9	BCB	T	101	X	-	-	-
9	BCB	V	101	X	-	-	-
9	BCB	W	101	X	-	-	-
9	BCB	Y	101	X	-	-	-
9	BCB	Z	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCB	b	101	X	-	-	-
9	BCB	c	101	X	-	-	-
9	BCB	e	101	X	-	-	-
9	BCB	f	101	X	-	-	-
9	BCB	h	101	X	-	-	-
9	BCB	i	101	X	-	-	-
9	BCB	k	101	X	-	-	-
9	BCB	l	101	X	-	-	-
9	BCB	n	101	X	-	-	-
9	BCB	o	101	X	-	-	-
9	BCB	q	101	X	-	-	-
9	BCB	r	101	X	-	-	-
9	BCB	t	101	X	-	-	-
9	BCB	u	101	X	-	-	-
9	BCB	w	101	X	-	-	-
9	BCB	x	101	X	-	-	-
9	BCB	z	101	X	-	-	-

2 Entry composition

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
1	C	333	Total	C	N	O	S	0	1
			2603	1640	467	478	18		

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

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

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

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

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

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

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

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

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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 436	C 293	N 68	O 75	0	0
6	c	55	Total 436	C 293	N 68	O 75	0	0
6	f	55	Total 436	C 293	N 68	O 75	0	0
6	i	55	Total 436	C 293	N 68	O 75	0	0
6	l	55	Total 436	C 293	N 68	O 75	0	0
6	o	55	Total 436	C 293	N 68	O 75	0	0
6	r	55	Total 436	C 293	N 68	O 75	0	0
6	u	55	Total 436	C 293	N 68	O 75	0	0
6	x	55	Total 436	C 293	N 68	O 75	0	0
6	4	55	Total 436	C 293	N 68	O 75	0	0
6	7	55	Total 436	C 293	N 68	O 75	0	0

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

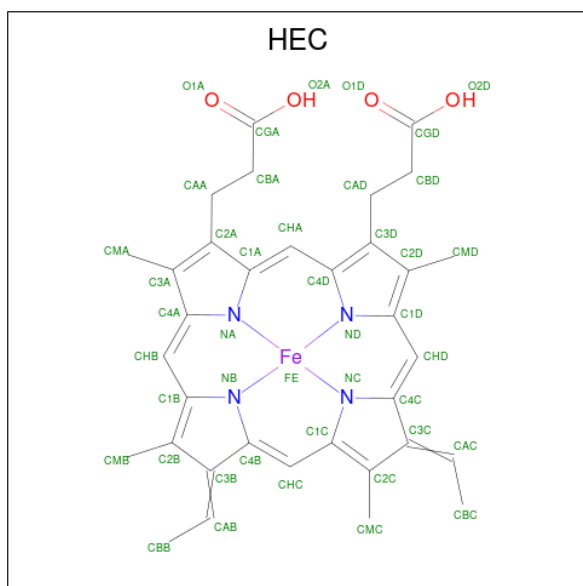
Mol	Chain	Residues	Atoms				AltConf	Trace
7	2	24	Total 199	C 137	N 31	O 31	0	0
7	I	24	Total 199	C 137	N 31	O 31	0	0
7	O	24	Total 199	C 137	N 31	O 31	0	0
7	R	24	Total 199	C 137	N 31	O 31	0	0
7	U	24	Total 199	C 137	N 31	O 31	0	0
7	X	24	Total 199	C 137	N 31	O 31	0	0
7	a	24	Total 199	C 137	N 31	O 31	0	0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

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

- Molecule 8 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



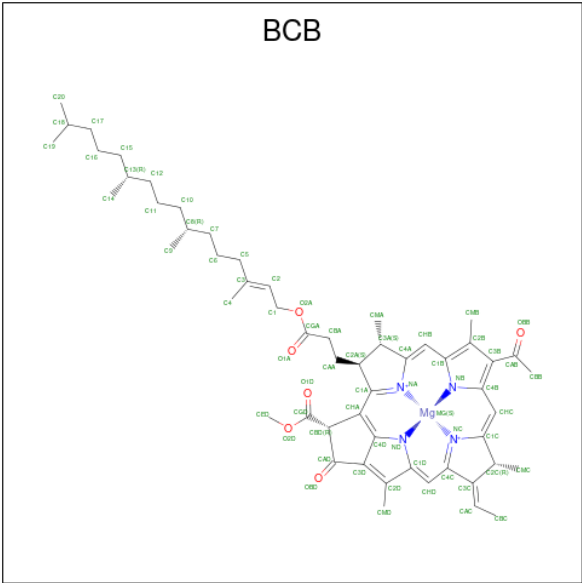
Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	Fe	N	O
			43	34	1	4	4
8	C	1	Total	C	Fe	N	O
			43	34	1	4	4
8	C	1	Total	C	Fe	N	O
			43	34	1	4	4

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

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



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

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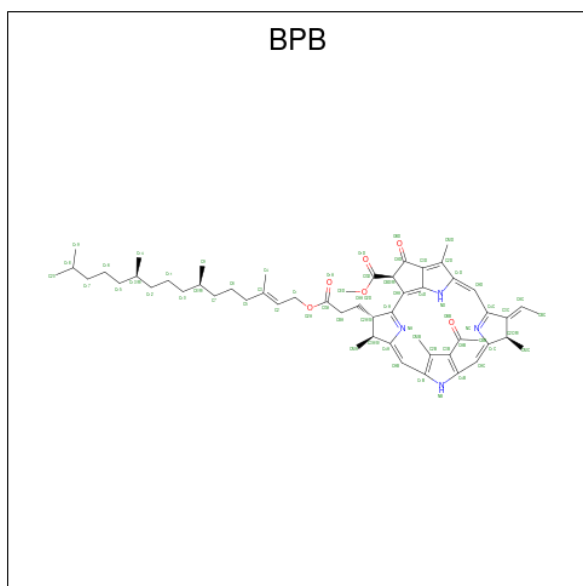
Mol	Chain	Residues	Atoms					AltConf
9	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	h	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
9	q	1	Total 66	C 55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

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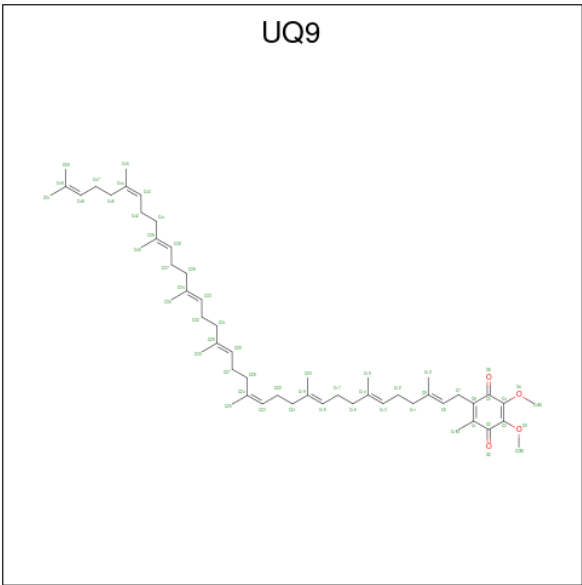
Mol	Chain	Residues	Atoms					AltConf
9	l	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	o	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	x	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55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

- Molecule 10 is BACTERIOPHEOPHYTIN B (CCD ID: 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 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).

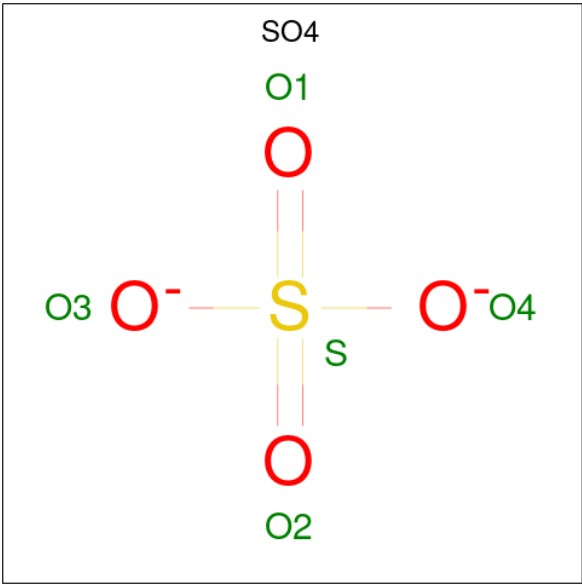


Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			58	54	4	
11	6	1	Total	C	O	0
			58	54	4	

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

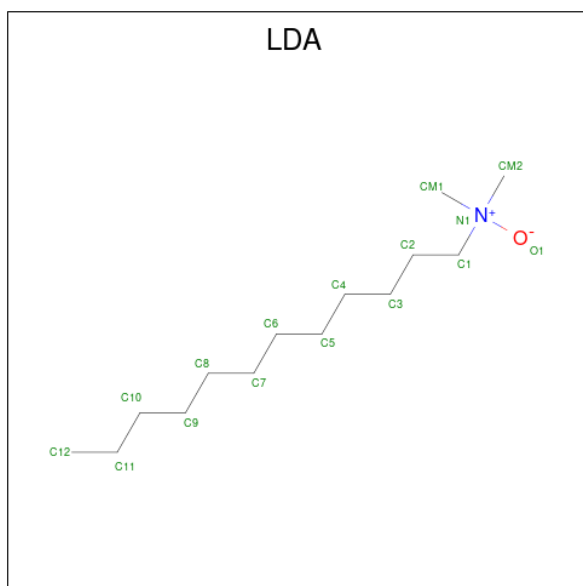
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Fe	0
			1	1	

- Molecule 13 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



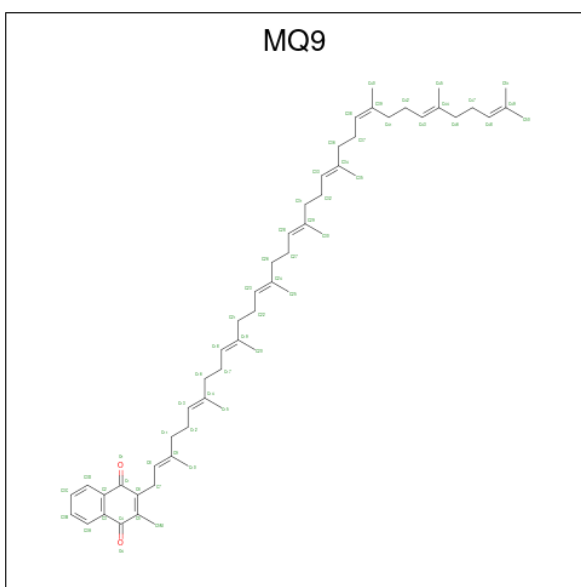
Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	O	S	0
			5	4	1	
13	M	1	Total	O	S	0
			5	4	1	
13	M	1	Total	O	S	0
			5	4	1	
13	M	1	Total	O	S	0
			5	4	1	
13	H	1	Total	O	S	0
			5	4	1	
13	H	1	Total	O	S	0
			5	4	1	
13	H	1	Total	O	S	0
			5	4	1	

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



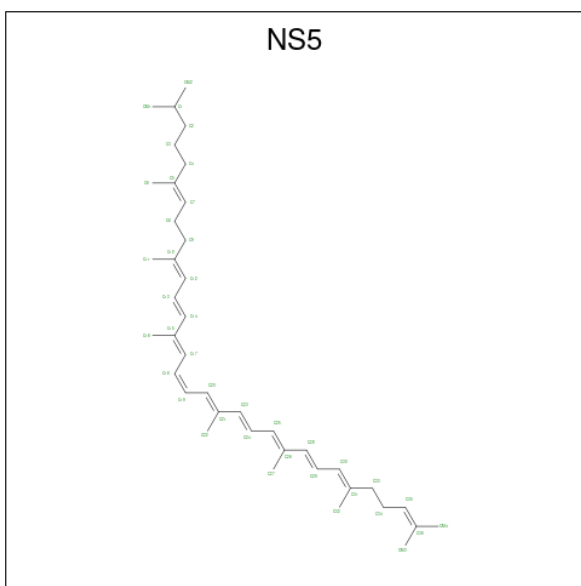
Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	N	O	0
			16	14	1	1	
14	H	1	Total	C	N	O	0
			16	14	1	1	

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



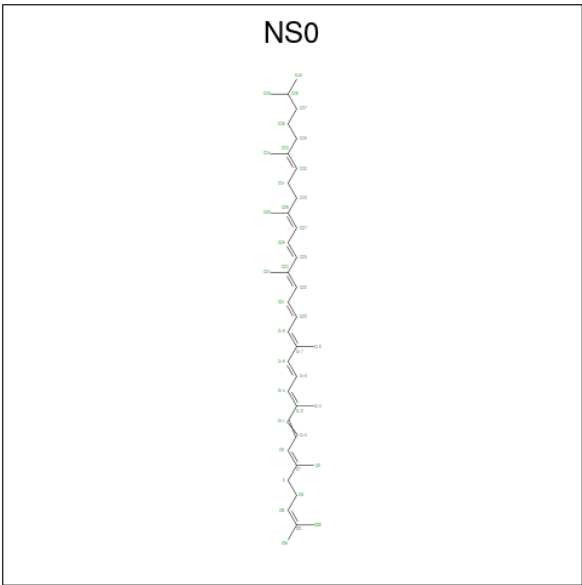
Mol	Chain	Residues	Atoms			AltConf
15	M	1	Total	C	O	0
			58	56	2	

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).



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

- Molecule 17 is all-trans-1,2-dihydroneurosporene (CCD ID: NS0) (formula: $C_{40}H_{60}$).



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

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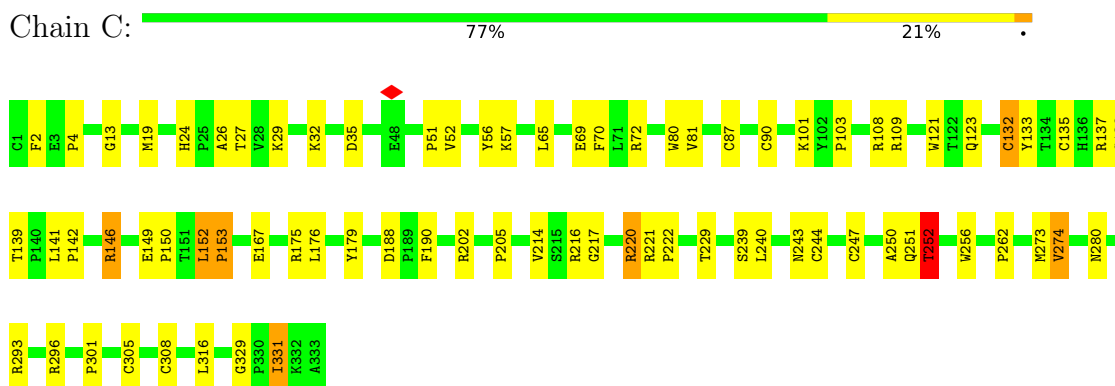
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Mol	Chain	Residues	Atoms		AltConf
17	x	1	Total 40	C 40	0
17	4	1	Total 40	C 40	0
17	7	1	Total 40	C 40	0

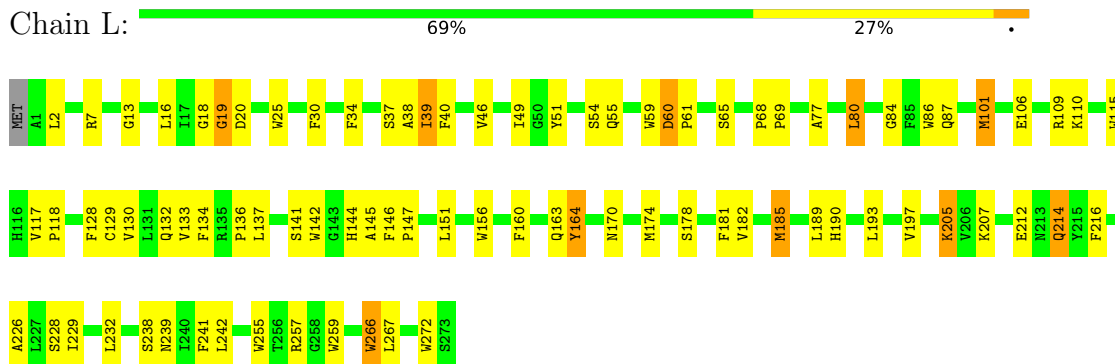
3 Residue-property plots

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

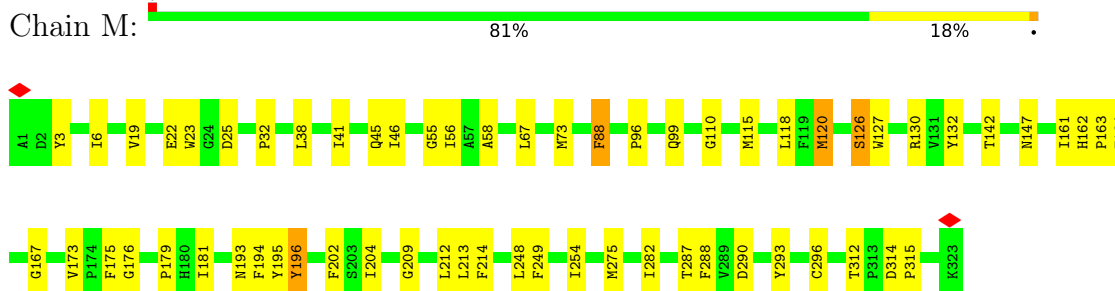
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



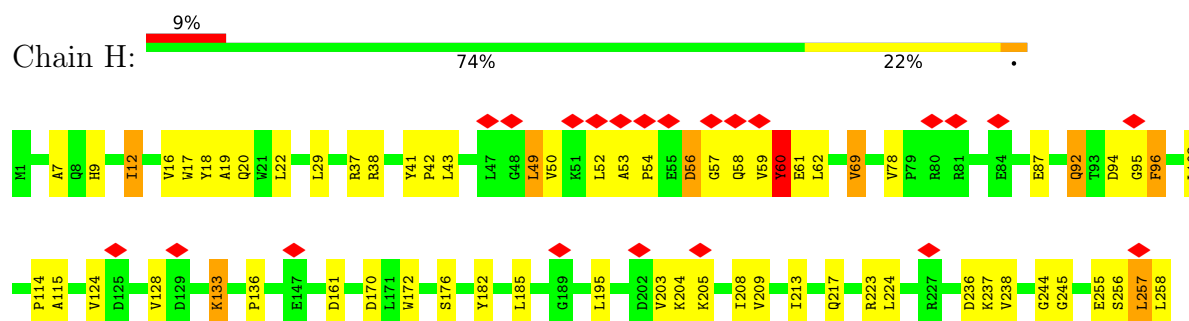
- Molecule 2: Reaction center protein L chain



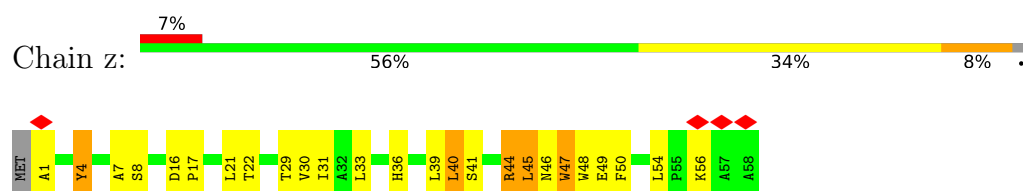
- Molecule 3: Reaction center protein M chain



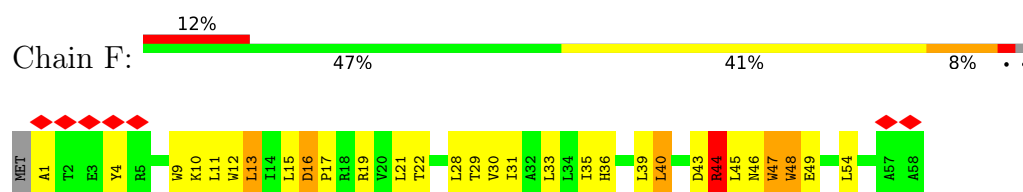
- Molecule 4: Reaction center protein H chain



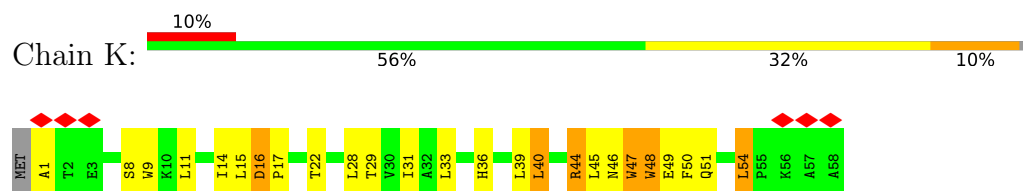
- Molecule 5: Light-harvesting protein B-1015 alpha chain



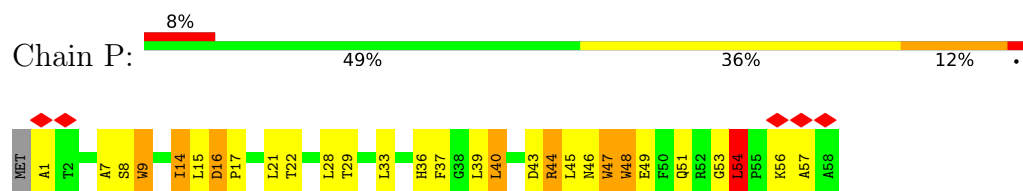
- Molecule 5: Light-harvesting protein B-1015 alpha chain



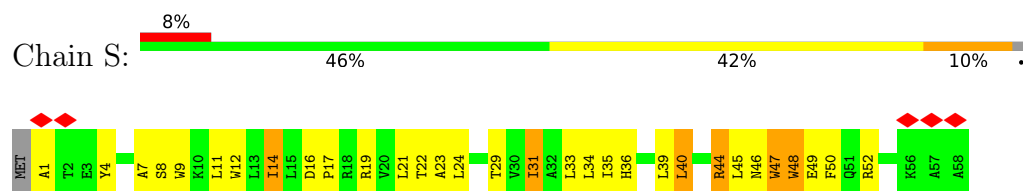
- Molecule 5: Light-harvesting protein B-1015 alpha chain



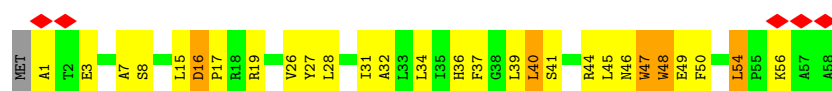
- Molecule 5: Light-harvesting protein B-1015 alpha chain



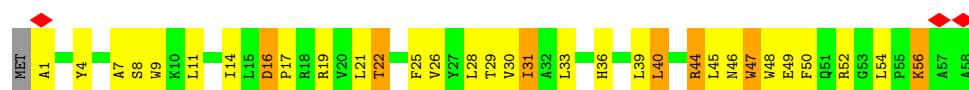
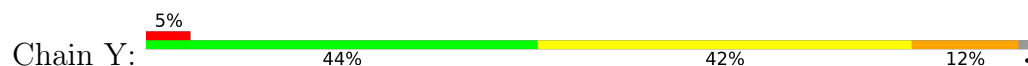
- Molecule 5: Light-harvesting protein B-1015 alpha chain



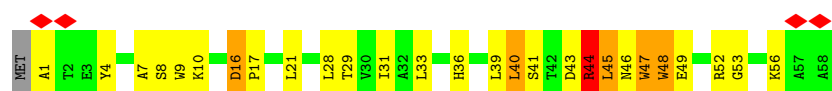
- Molecule 5: Light-harvesting protein B-1015 alpha chain



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



- 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



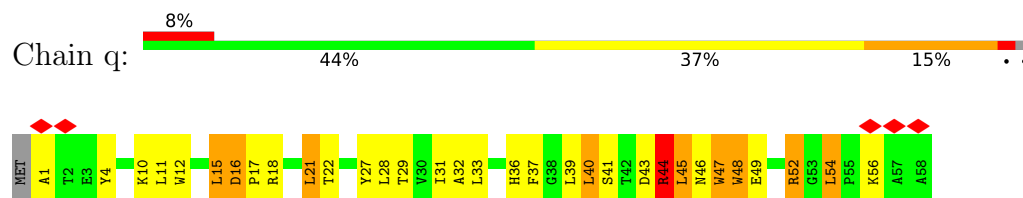
- Molecule 5: Light-harvesting protein B-1015 alpha chain



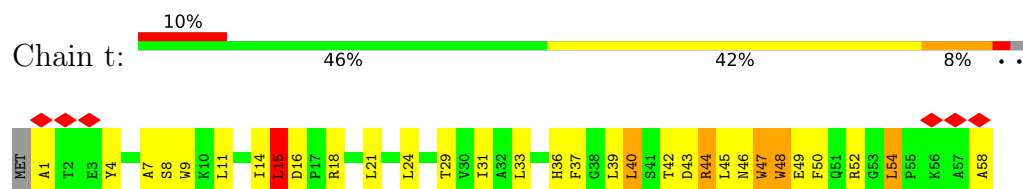
- Molecule 5: Light-harvesting protein B-1015 alpha chain



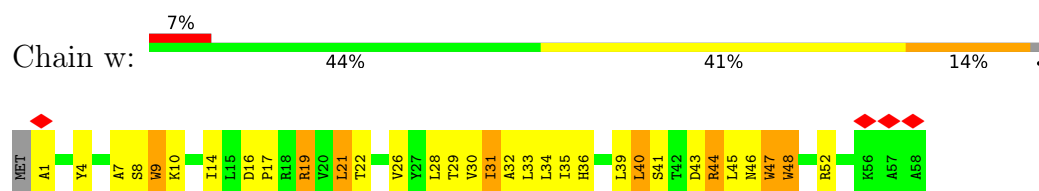
- Molecule 5: Light-harvesting protein B-1015 alpha chain



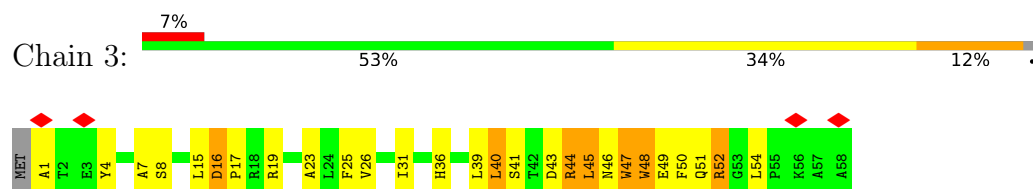
- Molecule 5: Light-harvesting protein B-1015 alpha chain



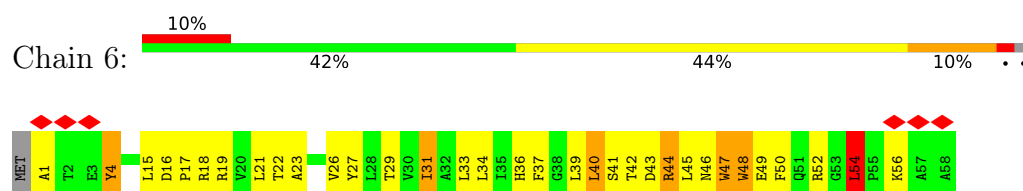
- Molecule 5: Light-harvesting protein B-1015 alpha chain



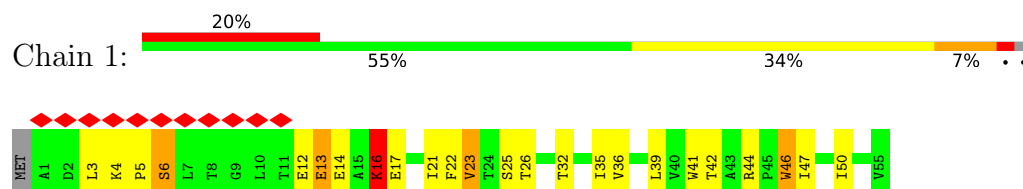
- Molecule 5: Light-harvesting protein B-1015 alpha chain



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



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

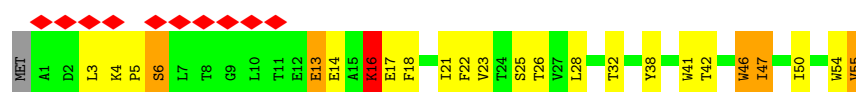


- Molecule 6: Light-harvesting protein B-1015 beta chain





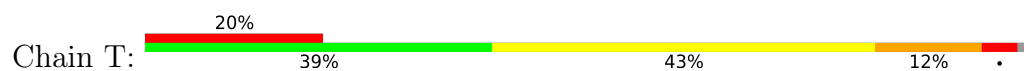
- Molecule 6: Light-harvesting protein B-1015 beta chain



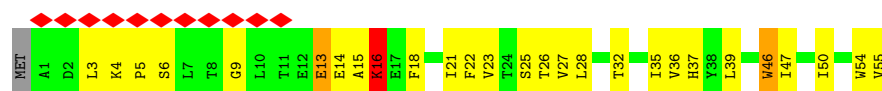
- Molecule 6: Light-harvesting protein B-1015 beta chain



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



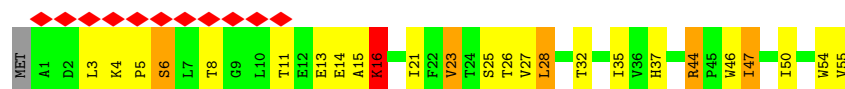
- Molecule 6: Light-harvesting protein B-1015 beta chain



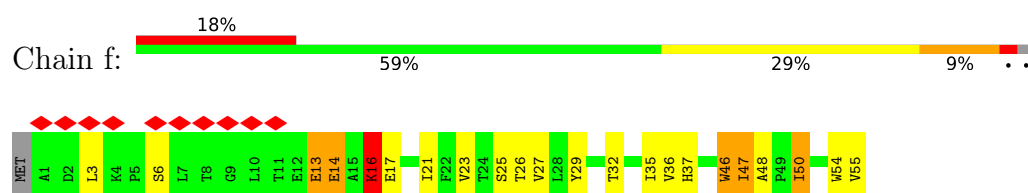
- Molecule 6: Light-harvesting protein B-1015 beta chain



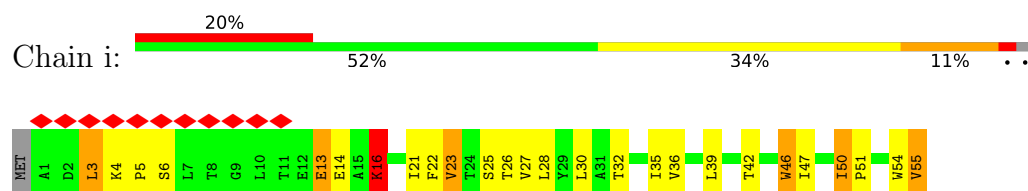
- Molecule 6: Light-harvesting protein B-1015 beta chain



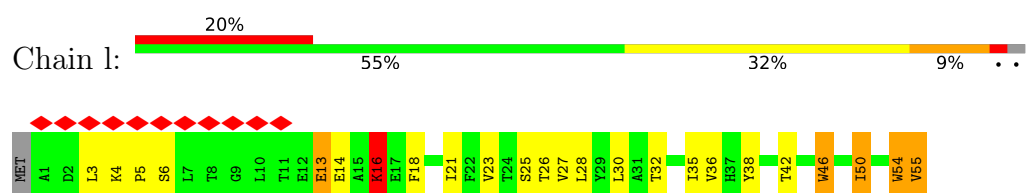
- Molecule 6: Light-harvesting protein B-1015 beta chain



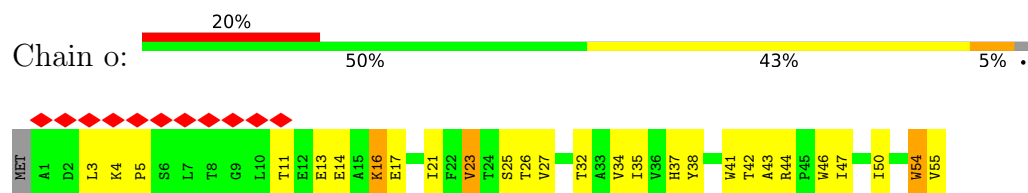
- Molecule 6: Light-harvesting protein B-1015 beta chain



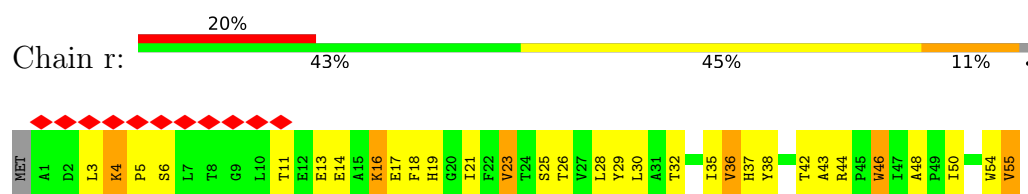
- Molecule 6: Light-harvesting protein B-1015 beta chain



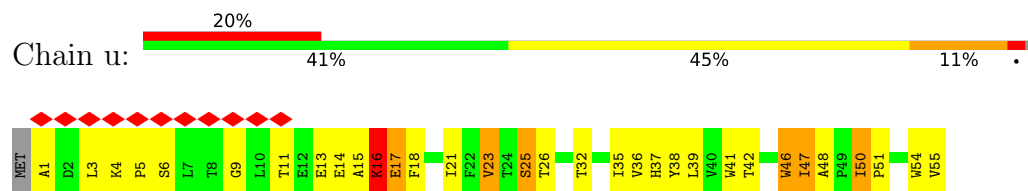
- Molecule 6: Light-harvesting protein B-1015 beta chain



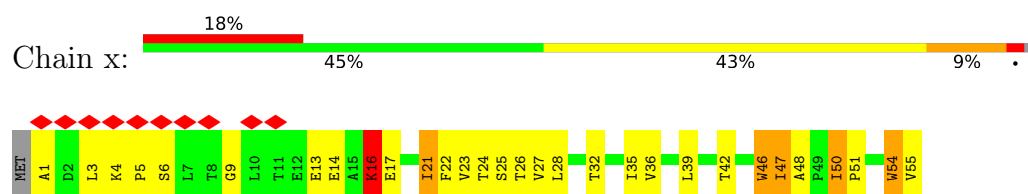
- Molecule 6: Light-harvesting protein B-1015 beta chain



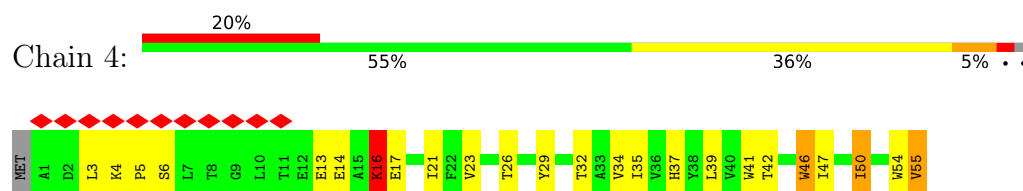
- Molecule 6: Light-harvesting protein B-1015 beta chain



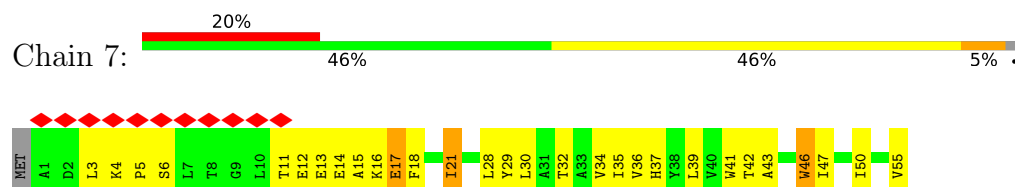
- Molecule 6: Light-harvesting protein B-1015 beta chain



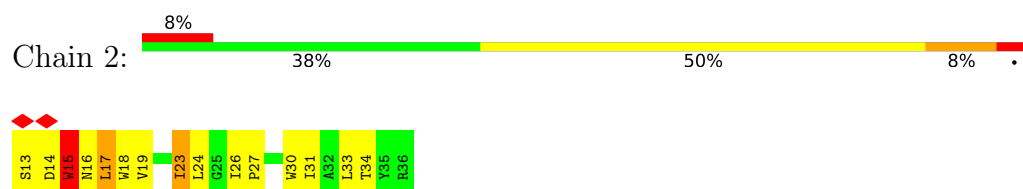
- Molecule 6: Light-harvesting protein B-1015 beta chain



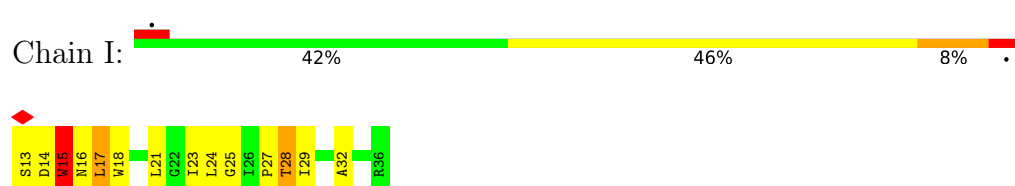
- Molecule 6: Light-harvesting protein B-1015 beta chain



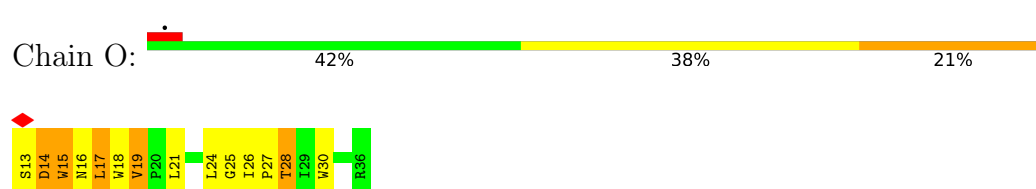
- Molecule 7: Light-harvesting protein B-1015 gamma chain



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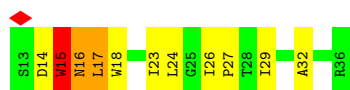


- Molecule 7: Light-harvesting protein B-1015 gamma chain



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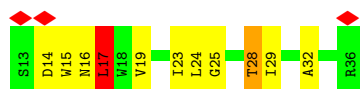




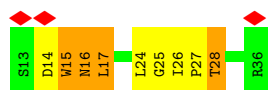
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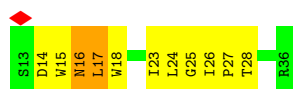
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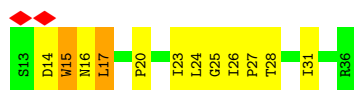
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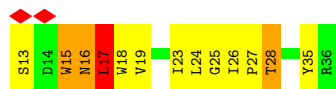
- Molecule 7: Light-harvesting protein B-1015 gamma chain



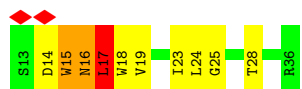
- Molecule 7: Light-harvesting protein B-1015 gamma chain



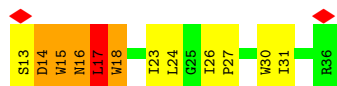
- Molecule 7: Light-harvesting protein B-1015 gamma chain



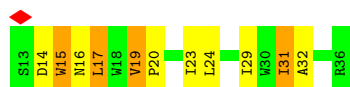
- Molecule 7: Light-harvesting protein B-1015 gamma chain



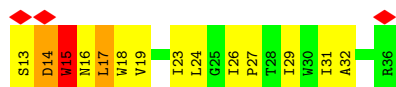
- Molecule 7: Light-harvesting protein B-1015 gamma chain



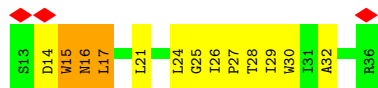
- Molecule 7: Light-harvesting protein B-1015 gamma chain



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



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



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 (Å)	243.79999, 243.79999, 243.79999	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.83	2/2670 (0.1%)	1.16	10/3639 (0.3%)
2	L	0.99	1/2259 (0.0%)	1.19	9/3084 (0.3%)
3	M	0.92	0/2659	1.14	7/3637 (0.2%)
4	H	0.72	0/2054	1.04	7/2803 (0.2%)
5	3	0.94	0/502	1.51	10/686 (1.5%)
5	6	0.92	0/502	1.39	9/686 (1.3%)
5	F	0.93	0/502	1.42	8/686 (1.2%)
5	K	0.91	0/502	1.47	9/686 (1.3%)
5	P	0.95	0/502	1.53	14/686 (2.0%)
5	S	0.92	0/502	1.41	5/686 (0.7%)
5	V	0.96	0/502	1.47	11/686 (1.6%)
5	Y	0.93	0/502	1.45	9/686 (1.3%)
5	b	0.95	0/502	1.52	9/686 (1.3%)
5	e	0.93	0/502	1.48	7/686 (1.0%)
5	h	0.86	0/502	1.35	5/686 (0.7%)
5	k	1.01	0/502	1.49	11/686 (1.6%)
5	n	0.90	0/502	1.42	10/686 (1.5%)
5	q	0.93	0/502	1.44	11/686 (1.6%)
5	t	0.93	0/502	1.44	9/686 (1.3%)
5	w	0.95	0/502	1.45	8/686 (1.2%)
5	z	0.97	0/502	1.46	7/686 (1.0%)
6	1	1.03	0/451	1.38	4/621 (0.6%)
6	4	1.02	0/451	1.42	7/621 (1.1%)
6	7	0.92	0/451	1.31	5/621 (0.8%)
6	G	0.91	0/451	1.35	7/621 (1.1%)
6	N	0.94	0/451	1.40	4/621 (0.6%)
6	Q	0.98	0/451	1.38	6/621 (1.0%)
6	T	0.98	0/451	1.42	6/621 (1.0%)
6	W	1.04	1/451 (0.2%)	1.40	7/621 (1.1%)
6	Z	1.01	0/451	1.36	7/621 (1.1%)
6	c	0.95	0/451	1.44	9/621 (1.4%)
6	f	0.93	0/451	1.38	6/621 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	i	0.99	0/451	1.41	5/621 (0.8%)
6	l	0.94	0/451	1.32	4/621 (0.6%)
6	o	0.94	0/451	1.26	4/621 (0.6%)
6	r	0.92	0/451	1.34	5/621 (0.8%)
6	u	0.97	0/451	1.42	8/621 (1.3%)
6	x	1.04	0/451	1.47	9/621 (1.4%)
7	2	0.96	0/207	1.65	6/287 (2.1%)
7	5	0.73	0/207	1.39	4/287 (1.4%)
7	I	0.76	0/207	1.33	2/287 (0.7%)
7	O	0.86	0/207	1.54	5/287 (1.7%)
7	R	0.93	0/207	1.40	5/287 (1.7%)
7	U	0.85	0/207	1.47	5/287 (1.7%)
7	X	0.93	0/207	1.63	8/287 (2.8%)
7	a	0.77	0/207	1.40	3/287 (1.0%)
7	d	0.78	0/207	1.25	4/287 (1.4%)
7	g	0.73	0/207	1.34	4/287 (1.4%)
7	j	0.76	0/207	1.27	3/287 (1.0%)
7	m	0.83	0/207	1.58	6/287 (2.1%)
7	p	0.85	0/207	1.47	4/287 (1.4%)
7	s	0.84	0/207	1.46	7/287 (2.4%)
7	v	0.81	0/207	1.42	2/287 (0.7%)
7	y	0.90	0/207	1.52	6/287 (2.1%)
All	All	0.92	4/29155 (0.0%)	1.34	362/39974 (0.9%)

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	1	0	2
6	T	0	2
6	W	0	1
6	Z	0	1

Continued on next page...

Continued from previous page...

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	152	LEU	N-CA	8.13	1.54	1.46
2	L	266	TRP	N-CA	-5.17	1.39	1.46
6	W	15	ALA	N-CA	5.05	1.52	1.46
1	C	153	PRO	CA-CB	5.01	1.62	1.53

The worst 5 of 362 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	48	TRP	CB-CA-C	-11.49	97.11	111.82
5	e	48	TRP	CB-CA-C	-11.29	97.36	111.82
5	b	48	TRP	CB-CA-C	-10.69	96.55	111.73
2	L	164	TYR	N-CA-C	-10.30	93.58	110.17
6	G	47	ILE	N-CA-C	9.80	119.83	110.42

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2603	0	2587	86	0
2	L	2171	0	2098	85	0
3	M	2555	0	2452	55	0
4	H	2018	0	2020	56	0
5	3	487	0	506	43	0
5	6	487	0	506	72	0
5	F	487	0	506	50	0
5	K	487	0	506	36	0
5	P	487	0	506	37	0
5	S	487	0	506	40	0
5	V	487	0	506	27	0
5	Y	487	0	506	39	0
5	b	487	0	506	41	0
5	e	487	0	506	48	0
5	h	487	0	506	42	0
5	k	487	0	506	20	0
5	n	487	0	506	34	0
5	q	487	0	506	43	0
5	t	487	0	506	52	0
5	w	487	0	506	37	0
5	z	487	0	506	30	0
6	1	436	0	445	19	0
6	4	436	0	445	33	0
6	7	436	0	445	22	0
6	G	436	0	445	46	0
6	N	436	0	445	47	0
6	Q	436	0	445	39	0
6	T	436	0	445	52	0
6	W	436	0	445	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Z	436	0	445	28	0
6	c	436	0	445	34	0
6	f	436	0	445	34	0
6	i	436	0	445	49	0
6	l	436	0	445	34	0
6	o	436	0	445	35	0
6	r	436	0	445	45	0
6	u	436	0	445	57	0
6	x	436	0	445	38	0
7	2	199	0	202	18	0
7	5	199	0	202	16	0
7	I	199	0	202	18	0
7	O	199	0	202	15	0
7	R	199	0	202	20	0
7	U	199	0	202	11	0
7	X	199	0	202	25	0
7	a	199	0	202	16	0
7	d	199	0	202	5	0
7	g	199	0	202	13	0
7	j	199	0	202	17	0
7	m	199	0	202	23	0
7	p	199	0	202	12	0
7	s	199	0	202	20	0
7	v	199	0	202	10	0
7	y	199	0	202	12	0
8	C	172	0	128	39	0
9	1	66	0	72	15	0
9	3	66	0	72	9	0
9	4	66	0	72	19	0
9	6	66	0	72	16	0
9	7	66	0	71	16	0
9	F	66	0	72	9	0
9	G	66	0	72	13	0
9	K	66	0	72	10	0
9	L	132	0	144	20	0
9	M	132	0	144	16	0
9	N	66	0	72	16	0
9	P	66	0	72	7	0
9	Q	66	0	72	16	0
9	S	66	0	72	8	0
9	T	66	0	72	17	0
9	V	66	0	72	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	66	0	72	11	0
9	Y	66	0	72	12	0
9	Z	66	0	72	15	0
9	b	66	0	72	8	0
9	c	66	0	72	14	0
9	e	66	0	72	18	0
9	f	66	0	72	11	0
9	h	66	0	72	10	0
9	i	66	0	72	12	0
9	k	66	0	72	7	0
9	l	66	0	72	17	0
9	n	66	0	72	8	0
9	o	66	0	72	16	0
9	q	66	0	69	6	0
9	r	66	0	72	11	0
9	t	66	0	72	10	0
9	u	66	0	72	8	0
9	w	66	0	72	3	0
9	x	66	0	72	9	0
9	z	66	0	72	10	0
10	L	65	0	74	11	0
10	M	65	0	74	6	0
11	6	58	0	82	39	0
11	L	58	0	82	21	0
12	M	1	0	0	0	0
13	H	15	0	0	0	0
13	M	20	0	0	0	0
14	H	16	0	31	0	0
14	M	16	0	31	3	0
15	M	58	0	80	4	0
16	M	40	0	60	4	0
17	1	40	0	0	4	0
17	4	40	0	0	6	0
17	7	40	0	0	7	0
17	G	40	0	0	20	0
17	N	40	0	0	13	0
17	Q	40	0	0	10	0
17	T	40	0	0	11	0
17	W	40	0	0	10	0
17	Z	40	0	0	4	0
17	c	40	0	0	6	0
17	f	40	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	i	40	0	0	14	0
17	l	40	0	0	14	0
17	o	40	0	0	7	0
17	r	40	0	0	10	0
17	u	40	0	0	12	0
17	x	40	0	0	8	0
All	All	31994	0	31930	1816	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 1816 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:u:21:ILE:HG21	17:u:102:NS0:C8	1.22	1.63
6:o:47:ILE:CD1	7:m:17:LEU:HD22	1.30	1.57
6:u:47:ILE:CD1	7:s:17:LEU:HD22	1.30	1.57
6:r:21:ILE:CG2	17:r:102:NS0:C8	1.74	1.56
6:x:21:ILE:CG2	17:x:102:NS0:C8	1.77	1.56

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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%)	265 (94%)	16 (6%)	18 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	218/219 (100%)	207 (95%)	11 (5%)	22	51
3	M	249/249 (100%)	242 (97%)	7 (3%)	38	70
4	H	212/212 (100%)	191 (90%)	21 (10%)	7	22
5	3	50/51 (98%)	46 (92%)	4 (8%)	11	31
5	6	50/51 (98%)	46 (92%)	4 (8%)	11	31
5	F	50/51 (98%)	45 (90%)	5 (10%)	7	22
5	K	50/51 (98%)	46 (92%)	4 (8%)	11	31
5	P	50/51 (98%)	45 (90%)	5 (10%)	7	22
5	S	50/51 (98%)	46 (92%)	4 (8%)	11	31
5	V	50/51 (98%)	47 (94%)	3 (6%)	17	44
5	Y	50/51 (98%)	44 (88%)	6 (12%)	5	14
5	b	50/51 (98%)	46 (92%)	4 (8%)	11	31
5	e	50/51 (98%)	45 (90%)	5 (10%)	7	22
5	h	50/51 (98%)	47 (94%)	3 (6%)	17	44
5	k	50/51 (98%)	46 (92%)	4 (8%)	11	31
5	n	50/51 (98%)	45 (90%)	5 (10%)	7	22
5	q	50/51 (98%)	44 (88%)	6 (12%)	5	14
5	t	50/51 (98%)	46 (92%)	4 (8%)	11	31
5	w	50/51 (98%)	45 (90%)	5 (10%)	7	22
5	z	50/51 (98%)	45 (90%)	5 (10%)	7	22
6	1	46/47 (98%)	40 (87%)	6 (13%)	4	11
6	4	46/47 (98%)	43 (94%)	3 (6%)	15	41
6	7	46/47 (98%)	40 (87%)	6 (13%)	4	11
6	G	46/47 (98%)	42 (91%)	4 (9%)	9	27
6	N	46/47 (98%)	42 (91%)	4 (9%)	9	27
6	Q	46/47 (98%)	43 (94%)	3 (6%)	15	41
6	T	46/47 (98%)	40 (87%)	6 (13%)	4	11
6	W	46/47 (98%)	44 (96%)	2 (4%)	26	57
6	Z	46/47 (98%)	42 (91%)	4 (9%)	9	27
6	c	46/47 (98%)	41 (89%)	5 (11%)	6	18
6	f	46/47 (98%)	41 (89%)	5 (11%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	i	46/47 (98%)	39 (85%)	7 (15%)	3	8
6	l	46/47 (98%)	40 (87%)	6 (13%)	4	11
6	o	46/47 (98%)	40 (87%)	6 (13%)	4	11
6	r	46/47 (98%)	41 (89%)	5 (11%)	6	18
6	u	46/47 (98%)	43 (94%)	3 (6%)	15	41
6	x	46/47 (98%)	42 (91%)	4 (9%)	9	27
7	2	21/21 (100%)	20 (95%)	1 (5%)	23	53
7	5	21/21 (100%)	20 (95%)	1 (5%)	23	53
7	I	21/21 (100%)	20 (95%)	1 (5%)	23	53
7	O	21/21 (100%)	19 (90%)	2 (10%)	8	24
7	R	21/21 (100%)	19 (90%)	2 (10%)	8	24
7	U	21/21 (100%)	20 (95%)	1 (5%)	23	53
7	X	21/21 (100%)	20 (95%)	1 (5%)	23	53
7	a	21/21 (100%)	19 (90%)	2 (10%)	8	24
7	d	21/21 (100%)	19 (90%)	2 (10%)	8	24
7	g	21/21 (100%)	20 (95%)	1 (5%)	23	53
7	j	21/21 (100%)	21 (100%)	0	100	100
7	m	21/21 (100%)	17 (81%)	4 (19%)	1	4
7	p	21/21 (100%)	18 (86%)	3 (14%)	3	9
7	s	21/21 (100%)	18 (86%)	3 (14%)	3	9
7	v	21/21 (100%)	19 (90%)	2 (10%)	8	24
7	y	21/21 (100%)	19 (90%)	2 (10%)	8	24
All	All	2928/2963 (99%)	2690 (92%)	238 (8%)	13	30

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	q	21	LEU
7	d	28	THR
6	N	13	GLU
7	a	28	THR
7	y	31	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	45	GLN
4	H	92	GLN
7	j	16	ASN
7	2	16	ASN
2	L	144	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	0.55	0	8,9,11	1.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	5/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
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 oligosaccharides 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	$\# Z > 2$
10	BPB	L	303	-	57,70,70	2.56	14 (24%)	55,101,101	2.46	10 (18%)
13	SO4	H	303	-	4,4,4	0.46	0	6,6,6	0.07	0
9	BCB	r	101	-	60,74,74	2.93	21 (35%)	59,115,115	2.53	17 (28%)
13	SO4	M	403	-	4,4,4	0.43	0	6,6,6	0.11	0
9	BCB	n	101	-	60,74,74	2.97	18 (30%)	59,115,115	2.52	18 (30%)
8	HEC	C	403	1	46,50,50	1.74	10 (21%)	58,82,82	1.89	13 (22%)
17	NS0	1	102	-	39,39,39	3.78	19 (48%)	46,46,46	3.94	25 (54%)
9	BCB	c	101	-	60,74,74	2.93	22 (36%)	59,115,115	2.46	14 (23%)
9	BCB	6	102	-	60,74,74	3.18	18 (30%)	59,115,115	2.51	18 (30%)
16	NS5	M	411	-	39,39,39	0.74	0	46,46,46	2.00	12 (26%)
9	BCB	o	101	-	60,74,74	2.92	20 (33%)	59,115,115	2.61	16 (27%)
9	BCB	7	101	-	60,74,74	2.86	19 (31%)	59,115,115	2.54	17 (28%)
9	BCB	t	101	-	60,74,74	2.91	20 (33%)	59,115,115	2.55	18 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	SO4	H	302	-	4,4,4	0.48	0	6,6,6	0.26	0
9	BCB	u	101	-	60,74,74	2.91	19 (31%)	59,115,115	2.69	16 (27%)
9	BCB	S	101	-	60,74,74	2.92	20 (33%)	59,115,115	2.43	17 (28%)
8	HEC	C	402	1	46,50,50	1.96	14 (30%)	58,82,82	1.69	13 (22%)
11	UQ9	6	101	-	58,58,58	3.92	16 (27%)	72,73,73	2.46	24 (33%)
9	BCB	Q	101	-	60,74,74	2.86	19 (31%)	59,115,115	2.48	14 (23%)
9	BCB	b	101	-	60,74,74	2.97	20 (33%)	59,115,115	2.62	19 (32%)
17	NS0	r	102	-	39,39,39	3.83	19 (48%)	46,46,46	3.91	24 (52%)
9	BCB	P	101	-	60,74,74	2.95	20 (33%)	59,115,115	2.43	21 (35%)
17	NS0	i	102	-	39,39,39	3.79	19 (48%)	46,46,46	3.91	24 (52%)
9	BCB	e	101	-	60,74,74	2.98	21 (35%)	59,115,115	2.42	17 (28%)
9	BCB	z	101	-	60,74,74	2.95	19 (31%)	59,115,115	2.78	21 (35%)
9	BCB	T	101	-	60,74,74	2.95	19 (31%)	59,115,115	2.45	16 (27%)
9	BCB	L	302	-	60,74,74	2.96	19 (31%)	59,115,115	2.72	16 (27%)
14	LDA	M	409	-	13,15,15	1.98	1 (7%)	14,17,17	0.88	0
9	BCB	M	407	-	60,74,74	2.92	20 (33%)	59,115,115	2.45	21 (35%)
8	HEC	C	404	1	46,50,50	1.87	12 (26%)	58,82,82	1.66	9 (15%)
17	NS0	N	102	-	39,39,39	3.76	19 (48%)	46,46,46	3.98	24 (52%)
9	BCB	x	101	-	60,74,74	2.87	21 (35%)	59,115,115	2.58	14 (23%)
11	UQ9	L	304	-	58,58,58	3.94	17 (29%)	72,73,73	2.69	25 (34%)
9	BCB	w	101	-	60,74,74	3.14	19 (31%)	59,115,115	2.81	17 (28%)
9	BCB	K	101	-	60,74,74	2.93	21 (35%)	59,115,115	2.56	19 (32%)
17	NS0	T	102	-	39,39,39	3.85	19 (48%)	46,46,46	3.84	22 (47%)
17	NS0	G	102	-	39,39,39	3.90	19 (48%)	46,46,46	3.90	24 (52%)
17	NS0	o	102	-	39,39,39	3.81	19 (48%)	46,46,46	3.96	24 (52%)
17	NS0	W	102	-	39,39,39	3.79	19 (48%)	46,46,46	4.01	24 (52%)
17	NS0	4	102	-	39,39,39	3.80	19 (48%)	46,46,46	3.93	23 (50%)
9	BCB	f	101	-	60,74,74	2.86	19 (31%)	59,115,115	2.45	15 (25%)
9	BCB	W	101	-	60,74,74	2.90	20 (33%)	59,115,115	2.31	15 (25%)
8	HEC	C	401	1	46,50,50	1.98	13 (28%)	58,82,82	1.55	12 (20%)
13	SO4	M	402	-	4,4,4	0.48	0	6,6,6	0.47	0
9	BCB	G	101	-	60,74,74	2.88	20 (33%)	59,115,115	2.40	15 (25%)
17	NS0	Z	102	-	39,39,39	3.81	19 (48%)	46,46,46	3.87	23 (50%)
9	BCB	h	101	-	60,74,74	2.91	19 (31%)	59,115,115	2.43	17 (28%)
9	BCB	4	101	-	60,74,74	2.90	19 (31%)	59,115,115	2.30	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCB	1	101	-	60,74,74	3.06	20 (33%)	59,115,115	2.63	15 (25%)
9	BCB	l	101	-	60,74,74	2.82	21 (35%)	59,115,115	2.49	14 (23%)
13	SO4	H	304	-	4,4,4	0.48	0	6,6,6	0.18	0
17	NS0	7	102	-	39,39,39	4.16	19 (48%)	46,46,46	3.83	26 (56%)
17	NS0	u	102	-	39,39,39	3.79	19 (48%)	46,46,46	3.89	23 (50%)
13	SO4	M	404	-	4,4,4	0.53	0	6,6,6	0.21	0
9	BCB	Y	101	-	60,74,74	3.03	19 (31%)	59,115,115	2.68	21 (35%)
9	BCB	L	301	-	60,74,74	2.73	20 (33%)	59,115,115	2.39	25 (42%)
9	BCB	i	101	-	60,74,74	2.89	21 (35%)	59,115,115	2.55	12 (20%)
9	BCB	V	101	-	60,74,74	2.98	20 (33%)	59,115,115	2.53	19 (32%)
9	BCB	k	101	-	60,74,74	2.80	19 (31%)	59,115,115	2.40	17 (28%)
9	BCB	N	101	-	60,74,74	2.97	20 (33%)	59,115,115	2.37	14 (23%)
10	BPB	M	408	-	57,70,70	2.55	14 (24%)	55,101,101	2.55	17 (30%)
17	NS0	f	102	-	39,39,39	3.84	19 (48%)	46,46,46	3.91	25 (54%)
14	LDA	H	301	-	13,15,15	2.00	1 (7%)	14,17,17	0.48	0
9	BCB	F	101	-	60,74,74	2.96	18 (30%)	59,115,115	2.48	15 (25%)
13	SO4	M	405	-	4,4,4	0.41	0	6,6,6	0.12	0
15	MQ9	M	410	-	59,59,59	1.37	4 (6%)	73,75,75	2.12	26 (35%)
9	BCB	q	101	-	60,74,74	3.45	22 (36%)	59,115,115	2.69	19 (32%)
17	NS0	c	102	-	39,39,39	3.83	19 (48%)	46,46,46	3.85	24 (52%)
17	NS0	l	102	-	39,39,39	3.90	19 (48%)	46,46,46	3.87	24 (52%)
9	BCB	M	406	-	60,74,74	2.93	20 (33%)	59,115,115	2.45	15 (25%)
17	NS0	x	102	-	39,39,39	3.84	19 (48%)	46,46,46	3.89	23 (50%)
17	NS0	Q	102	-	39,39,39	3.83	19 (48%)	46,46,46	3.84	24 (52%)
9	BCB	3	101	-	60,74,74	2.98	17 (28%)	59,115,115	2.59	17 (28%)
9	BCB	Z	101	-	60,74,74	2.98	19 (31%)	59,115,115	2.42	15 (25%)

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
10	BPB	L	303	-	1/1/18/23	15/37/105/105	0/5/6/6
9	BCB	r	101	-	2/2/21/26	16/37/137/137	-
9	BCB	n	101	-	2/2/21/26	22/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEC	C	403	1	-	8/14/54/54	-
17	NS0	1	102	-	-	16/43/43/43	-
9	BCB	c	101	-	2/2/21/26	21/37/137/137	-
9	BCB	6	102	-	2/2/21/26	15/37/137/137	-
16	NS5	M	411	-	-	13/43/43/43	-
9	BCB	o	101	-	2/2/21/26	20/37/137/137	-
9	BCB	7	101	-	2/2/21/26	14/37/137/137	-
9	BCB	t	101	-	2/2/21/26	20/37/137/137	-
9	BCB	u	101	-	2/2/21/26	14/37/137/137	-
9	BCB	S	101	-	2/2/21/26	18/37/137/137	-
8	HEC	C	402	1	-	6/14/54/54	-
11	UQ9	6	101	-	-	19/57/81/81	0/1/1/1
9	BCB	Q	101	-	2/2/21/26	21/37/137/137	-
9	BCB	b	101	-	2/2/21/26	20/37/137/137	-
17	NS0	r	102	-	-	14/43/43/43	-
9	BCB	P	101	-	2/2/21/26	21/37/137/137	-
17	NS0	i	102	-	-	14/43/43/43	-
9	BCB	e	101	-	2/2/21/26	23/37/137/137	-
9	BCB	z	101	-	2/2/21/26	19/37/137/137	-
9	BCB	T	101	-	2/2/21/26	19/37/137/137	-
9	BCB	L	302	-	2/2/21/26	9/37/137/137	-
14	LDA	M	409	-	-	9/13/13/13	-
9	BCB	M	407	-	2/2/21/26	14/37/137/137	-
8	HEC	C	404	1	-	7/14/54/54	-
17	NS0	N	102	-	-	15/43/43/43	-
9	BCB	x	101	-	2/2/21/26	18/37/137/137	-
11	UQ9	L	304	-	-	16/57/81/81	0/1/1/1
9	BCB	w	101	-	2/2/21/26	15/37/137/137	-
9	BCB	K	101	-	2/2/21/26	19/37/137/137	-
17	NS0	T	102	-	-	15/43/43/43	-
17	NS0	G	102	-	-	13/43/43/43	-
17	NS0	o	102	-	-	14/43/43/43	-
17	NS0	W	102	-	-	13/43/43/43	-
17	NS0	4	102	-	-	14/43/43/43	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCB	f	101	-	2/2/21/26	15/37/137/137	-
9	BCB	W	101	-	2/2/21/26	16/37/137/137	-
8	HEC	C	401	1	-	7/14/54/54	-
9	BCB	G	101	-	2/2/21/26	15/37/137/137	-
17	NS0	Z	102	-	-	14/43/43/43	-
9	BCB	h	101	-	2/2/21/26	21/37/137/137	-
9	BCB	4	101	-	2/2/21/26	21/37/137/137	-
9	BCB	1	101	-	2/2/21/26	22/37/137/137	-
9	BCB	l	101	-	2/2/21/26	15/37/137/137	-
17	NS0	7	102	-	-	17/43/43/43	-
17	NS0	u	102	-	-	15/43/43/43	-
9	BCB	Y	101	-	2/2/21/26	19/37/137/137	-
9	BCB	L	301	-	3/3/21/26	10/37/137/137	-
9	BCB	i	101	-	2/2/21/26	16/37/137/137	-
9	BCB	V	101	-	2/2/21/26	24/37/137/137	-
9	BCB	k	101	-	2/2/21/26	19/37/137/137	-
9	BCB	N	101	-	2/2/21/26	20/37/137/137	-
10	BPB	M	408	-	1/1/18/23	15/37/105/105	0/5/6/6
17	NS0	f	102	-	-	14/43/43/43	-
14	LDA	H	301	-	-	9/13/13/13	-
9	BCB	F	101	-	2/2/21/26	18/37/137/137	-
15	MQ9	M	410	-	-	17/53/73/73	0/2/2/2
9	BCB	q	101	-	2/2/21/26	17/37/137/137	-
17	NS0	c	102	-	-	13/43/43/43	-
17	NS0	l	102	-	-	16/43/43/43	-
9	BCB	M	406	-	2/2/21/26	13/37/137/137	-
17	NS0	x	102	-	-	14/43/43/43	-
17	NS0	Q	102	-	-	14/43/43/43	-
9	BCB	3	101	-	2/2/21/26	15/37/137/137	-
9	BCB	Z	101	-	2/2/21/26	19/37/137/137	-

The worst 5 of 1187 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	q	101	BCB	CBB-CAB	-9.87	1.21	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	304	UQ9	C28-C29	9.03	1.53	1.33
11	6	101	UQ9	C23-C24	8.99	1.53	1.33
11	6	101	UQ9	C18-C19	8.95	1.53	1.33
11	L	304	UQ9	C13-C14	8.93	1.53	1.33

The worst 5 of 1209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	w	101	BCB	O2D-CGD-CBD	11.02	123.06	110.95
17	W	102	NS0	C20-C19-C17	-10.82	112.10	127.28
17	l	102	NS0	C20-C19-C17	-10.73	112.23	127.28
9	L	302	BCB	O2D-CGD-CBD	10.67	122.67	110.95
17	o	102	NS0	C20-C19-C17	-10.52	112.52	127.28

5 of 79 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	L	301	BCB	NA
9	L	301	BCB	NC
9	L	301	BCB	ND
9	L	302	BCB	NA
9	L	302	BCB	NC

5 of 1059 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	401	HEC	C2B-C3B-CAB-CBB
8	C	401	HEC	C4B-C3B-CAB-CBB
8	C	401	HEC	C2C-C3C-CAC-CBC
8	C	401	HEC	C4C-C3C-CAC-CBC
8	C	402	HEC	C2B-C3B-CAB-CBB

There are no ring outliers.

66 monomers are involved in 659 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	303	BPB	11	0
9	r	101	BCB	11	0
9	n	101	BCB	8	0
8	C	403	HEC	13	0
17	l	102	NS0	4	0

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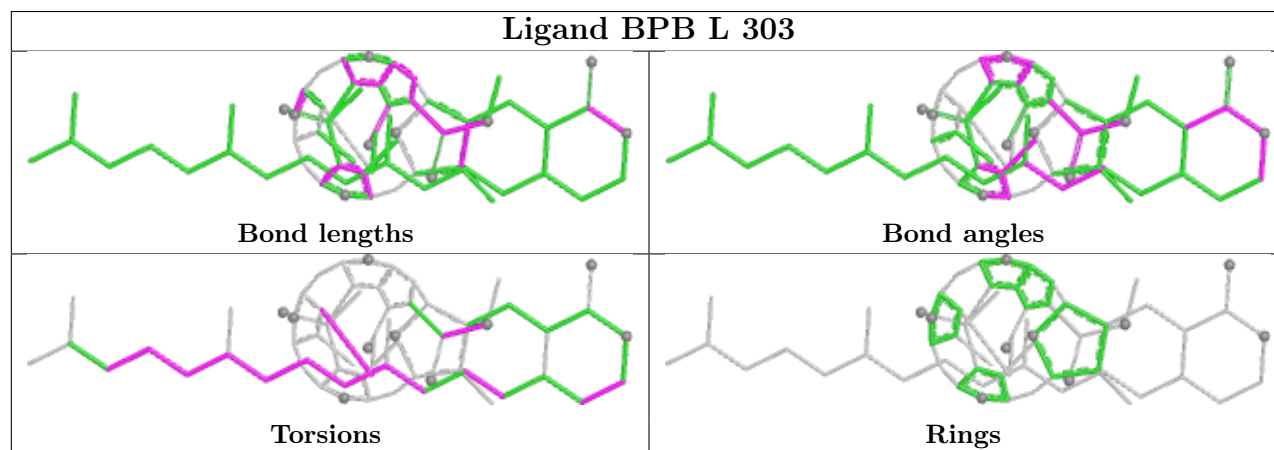
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	c	101	BCB	14	0
9	6	102	BCB	16	0
16	M	411	NS5	4	0
9	o	101	BCB	16	0
9	7	101	BCB	16	0
9	t	101	BCB	10	0
9	u	101	BCB	8	0
9	S	101	BCB	8	0
8	C	402	HEC	13	0
11	6	101	UQ9	39	0
9	Q	101	BCB	16	0
9	b	101	BCB	8	0
17	r	102	NS0	10	0
9	P	101	BCB	7	0
17	i	102	NS0	14	0
9	e	101	BCB	18	0
9	z	101	BCB	10	0
9	T	101	BCB	17	0
9	L	302	BCB	11	0
14	M	409	LDA	3	0
9	M	407	BCB	11	0
8	C	404	HEC	6	0
17	N	102	NS0	13	0
9	x	101	BCB	9	0
11	L	304	UQ9	21	0
9	w	101	BCB	3	0
9	K	101	BCB	10	0
17	T	102	NS0	11	0
17	G	102	NS0	20	0
17	o	102	NS0	7	0
17	W	102	NS0	10	0
17	4	102	NS0	6	0
9	f	101	BCB	11	0
9	W	101	BCB	11	0
8	C	401	HEC	7	0
9	G	101	BCB	13	0
17	Z	102	NS0	4	0
9	h	101	BCB	10	0
9	4	101	BCB	19	0
9	1	101	BCB	15	0
9	l	101	BCB	17	0
17	7	102	NS0	7	0

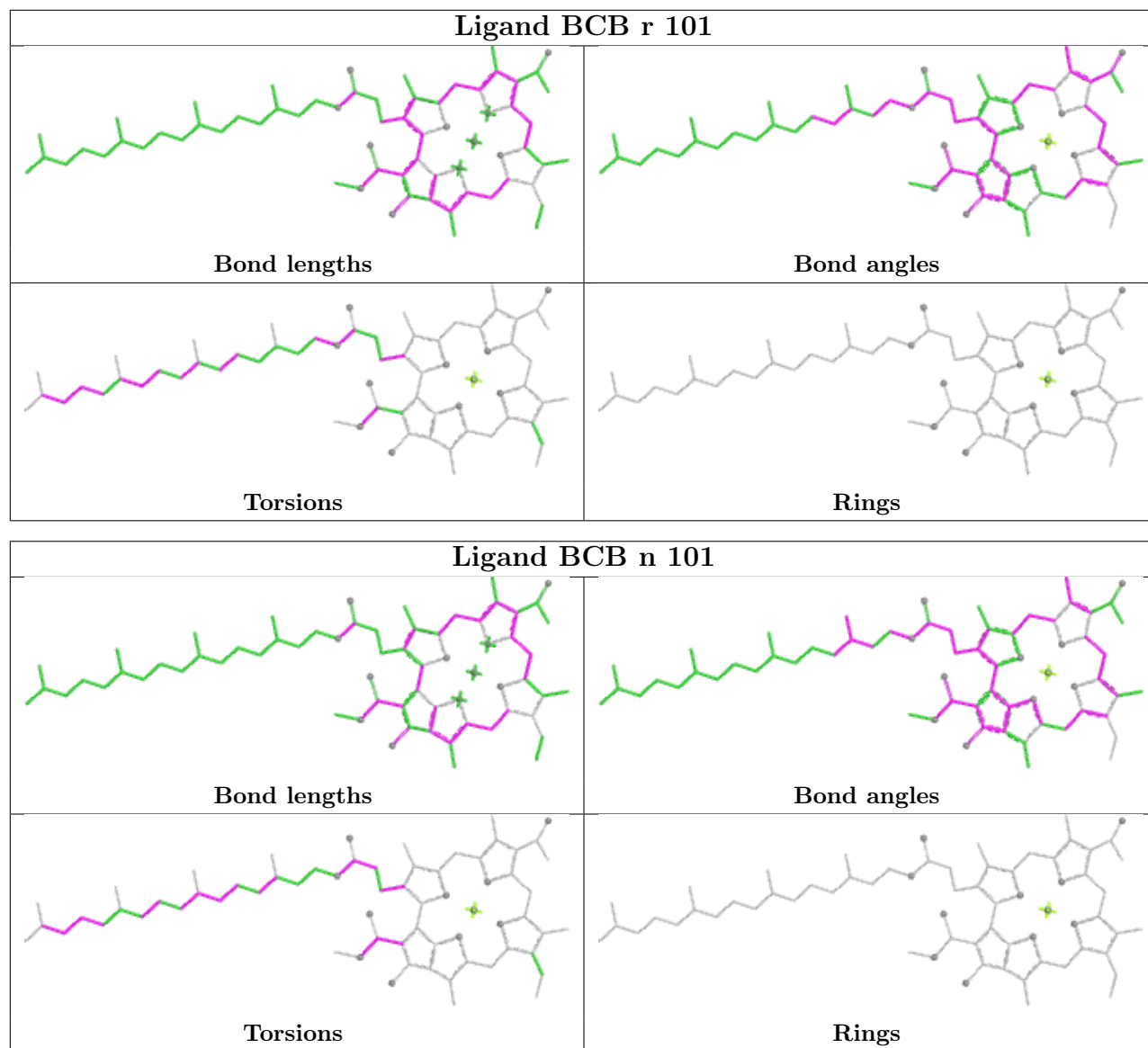
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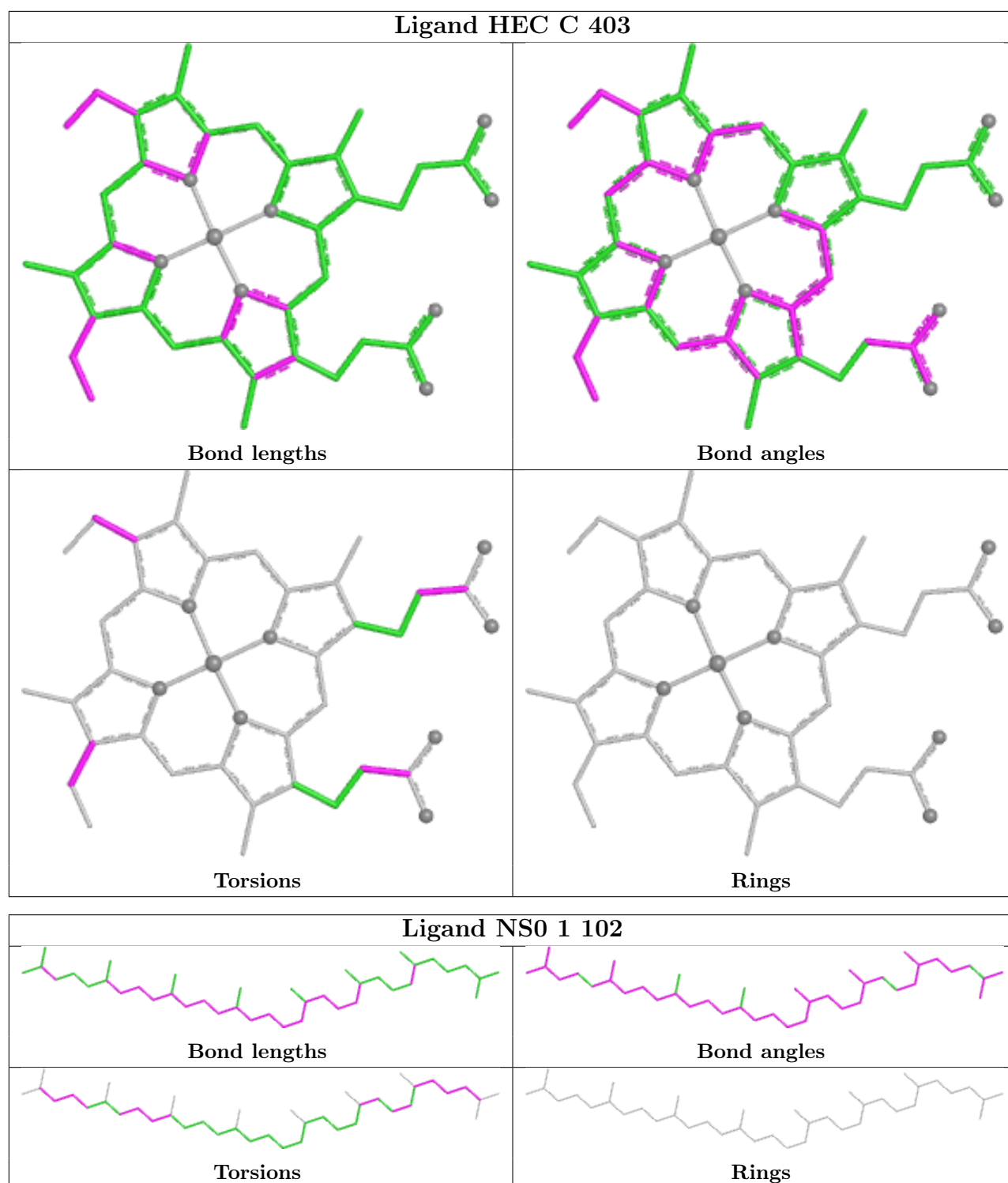
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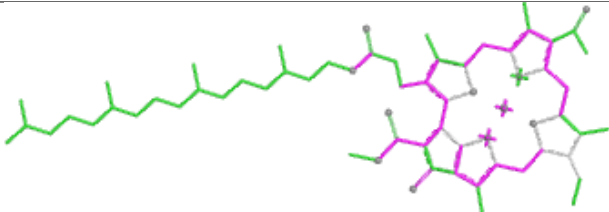
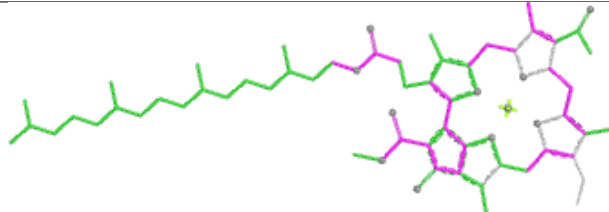
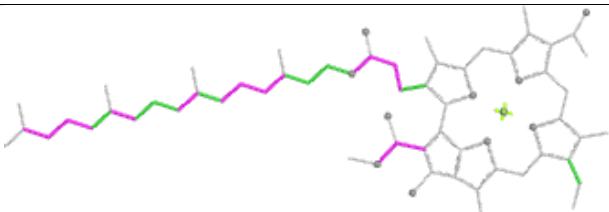
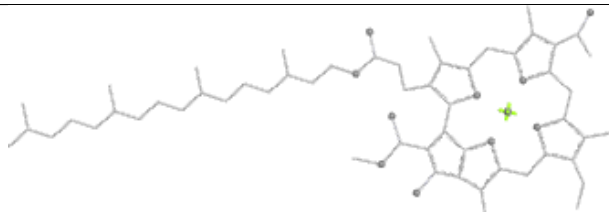
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	u	102	NS0	12	0
9	Y	101	BCB	12	0
9	L	301	BCB	12	0
9	i	101	BCB	12	0
9	V	101	BCB	8	0
9	k	101	BCB	7	0
9	N	101	BCB	16	0
10	M	408	BPB	6	0
17	f	102	NS0	11	0
9	F	101	BCB	9	0
15	M	410	MQ9	4	0
9	q	101	BCB	6	0
17	c	102	NS0	6	0
17	l	102	NS0	14	0
9	M	406	BCB	5	0
17	x	102	NS0	8	0
17	Q	102	NS0	10	0
9	3	101	BCB	9	0
9	Z	101	BCB	15	0

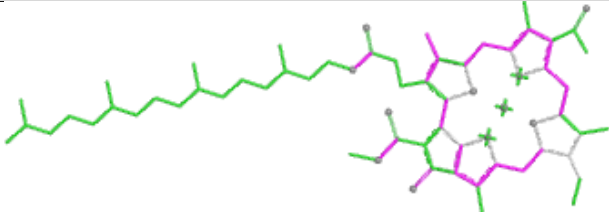
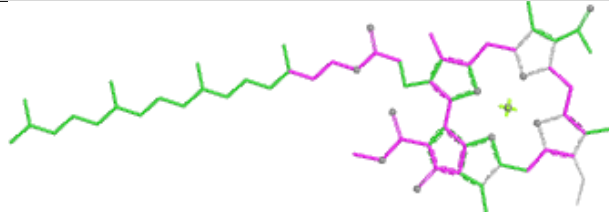
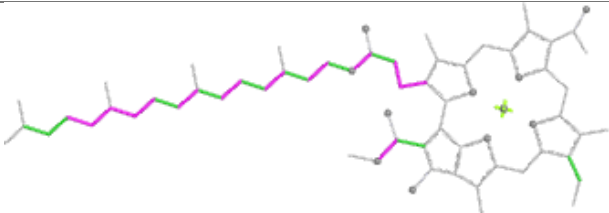
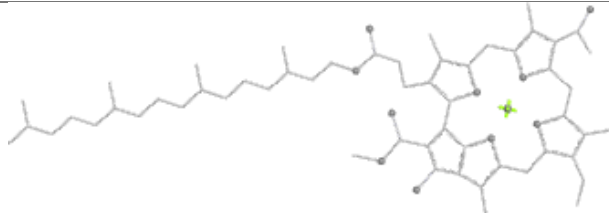
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

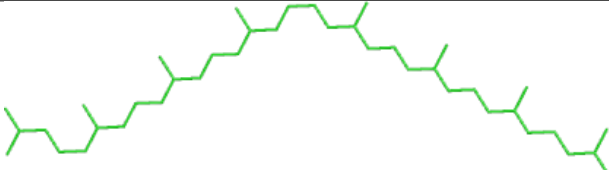
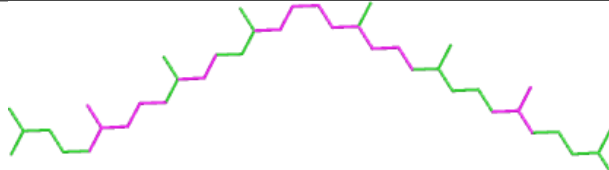
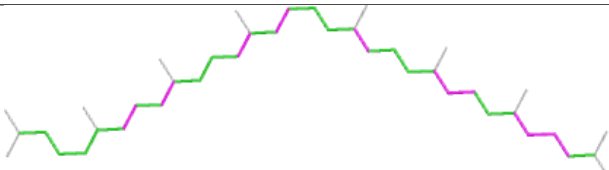
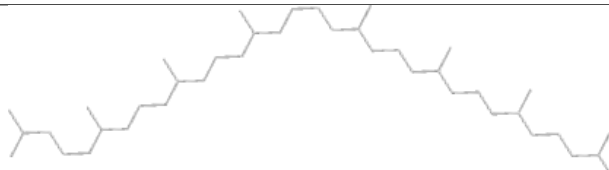


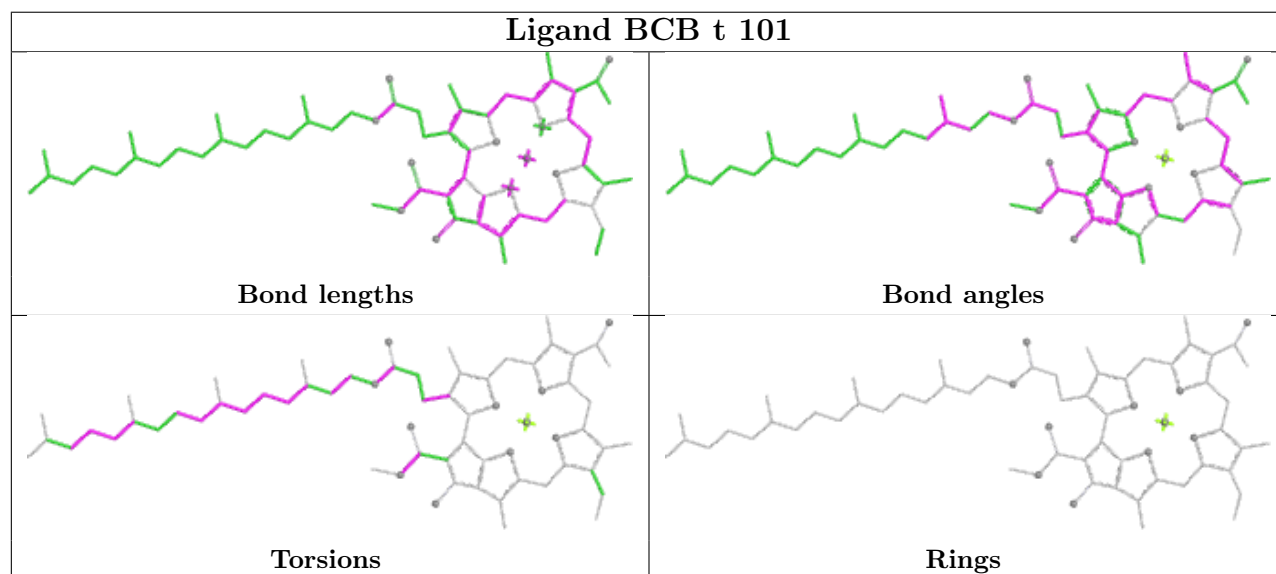
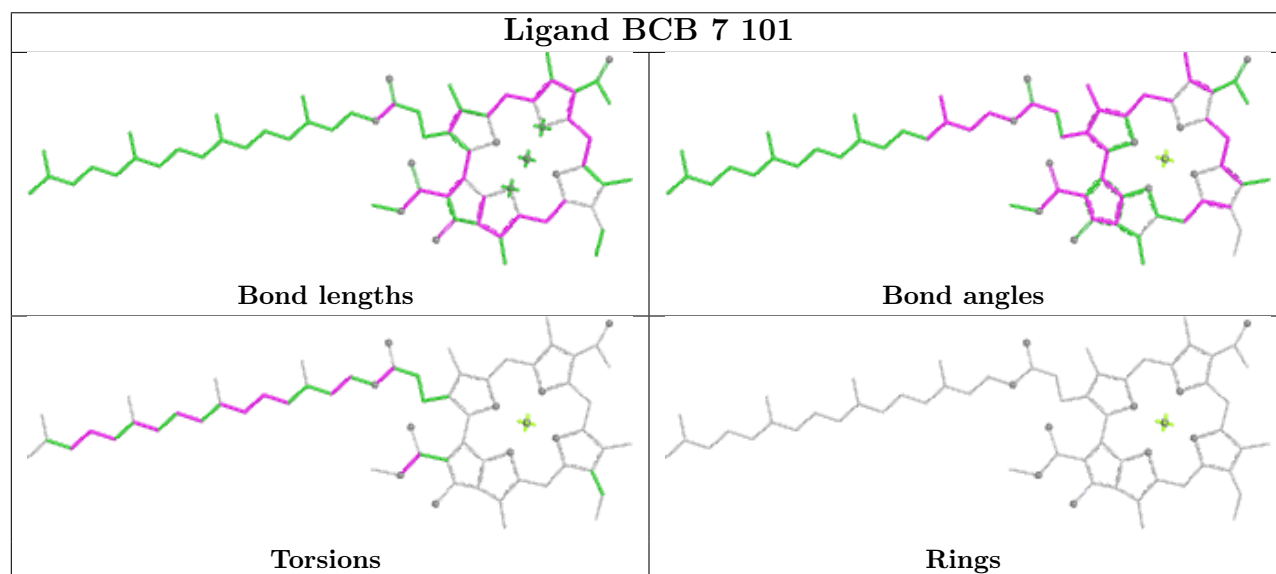
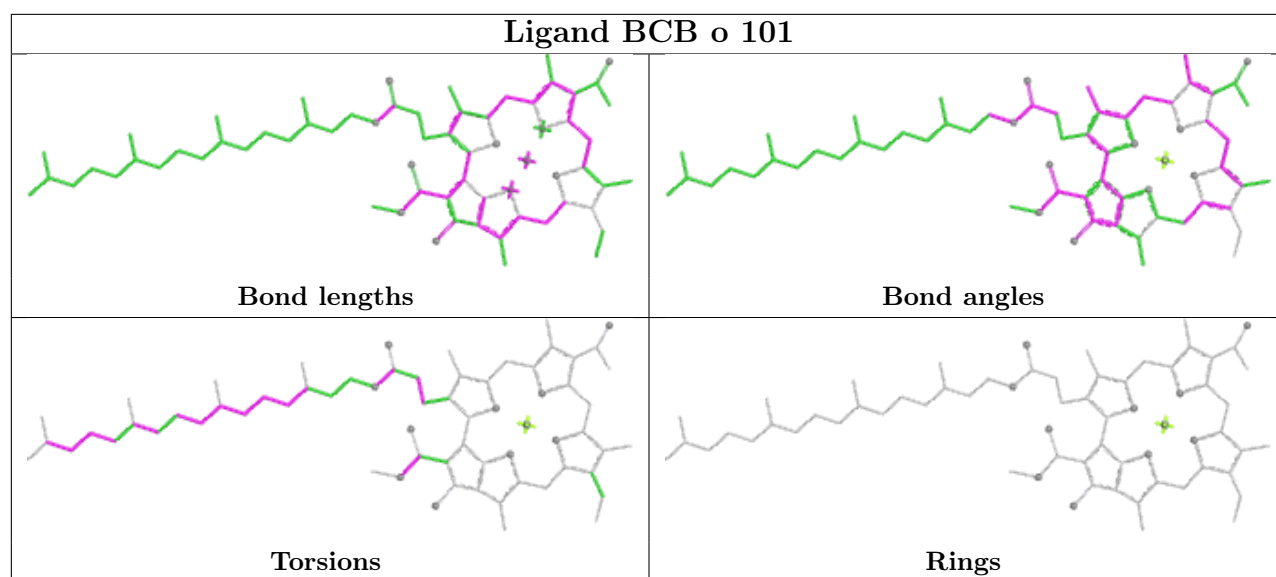


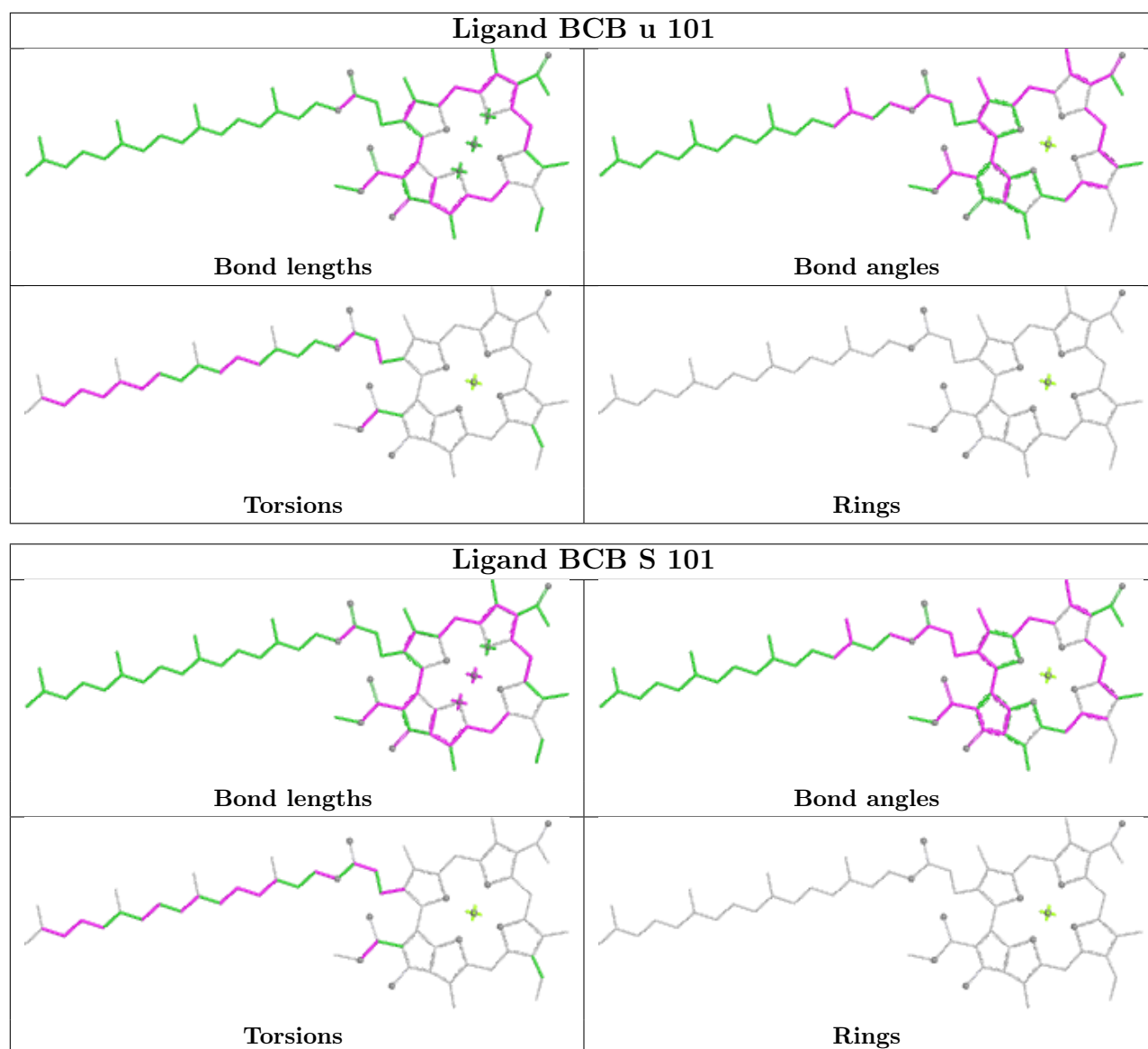


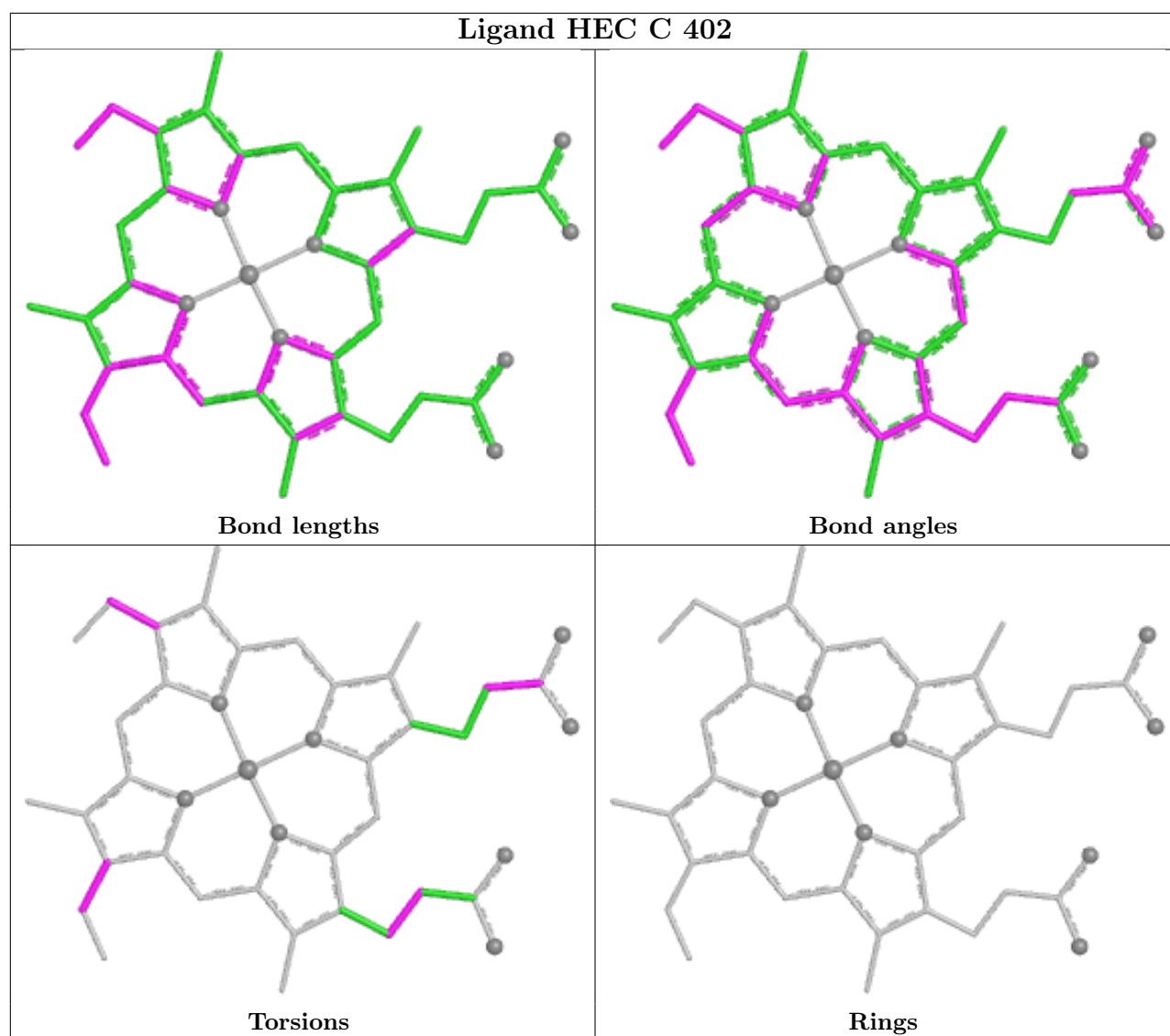
Ligand BCB c 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

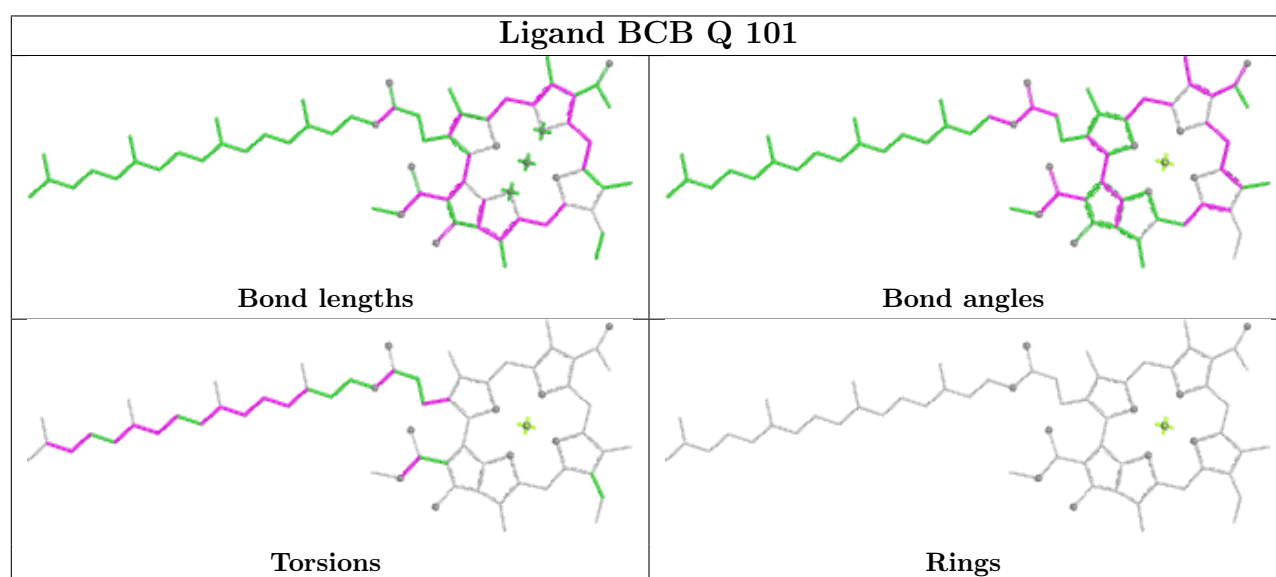
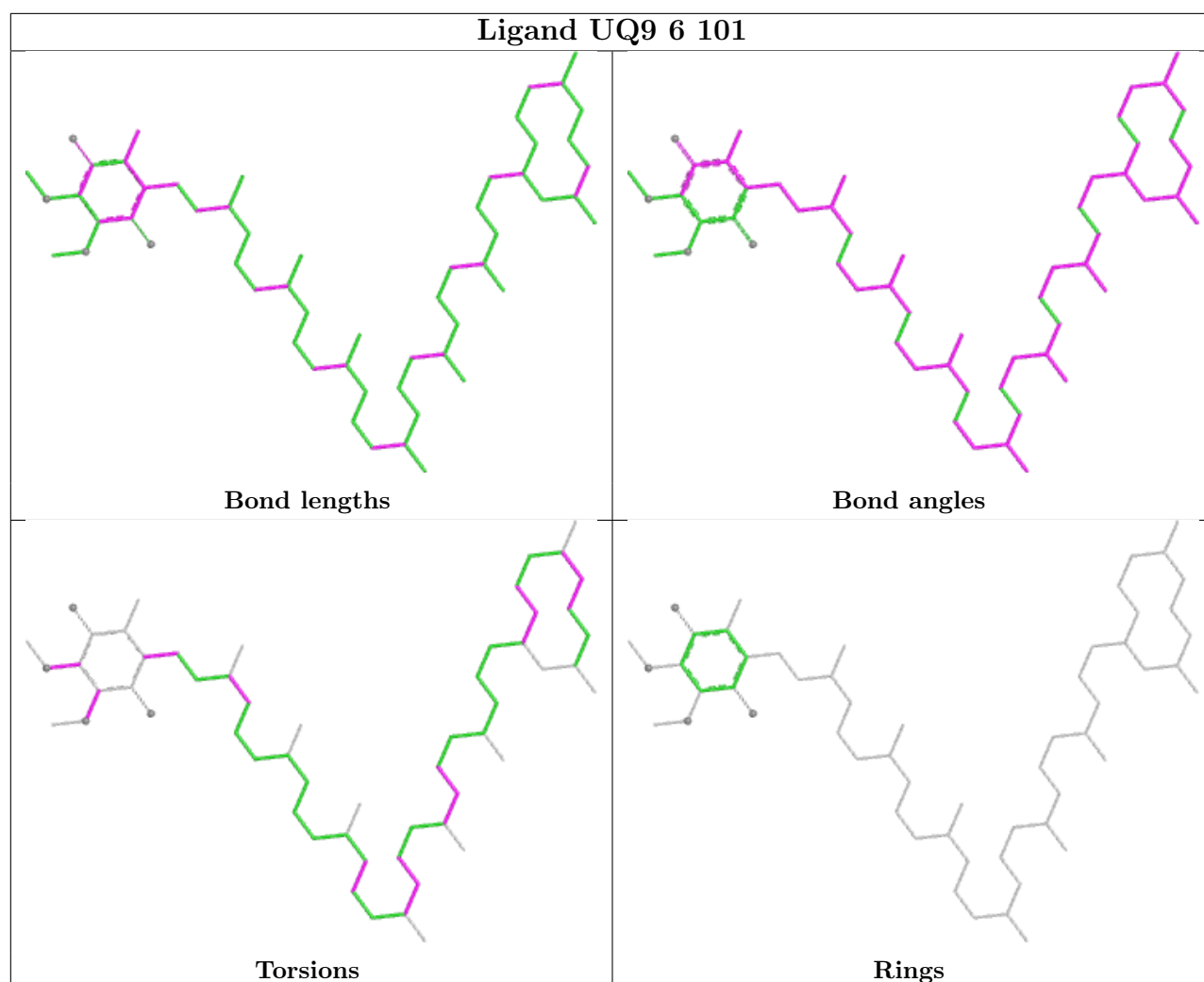
Ligand BCB 6 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

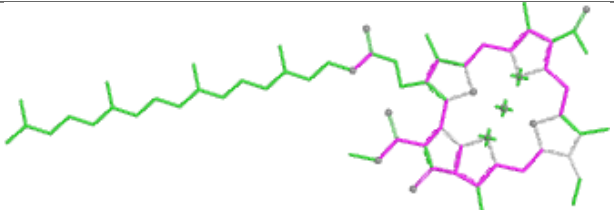
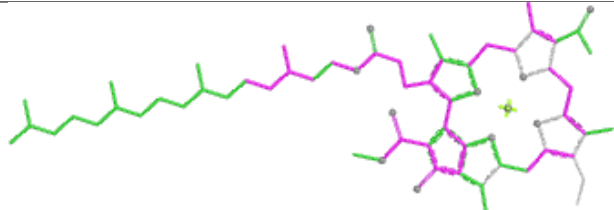
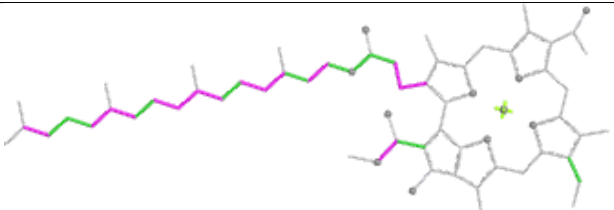
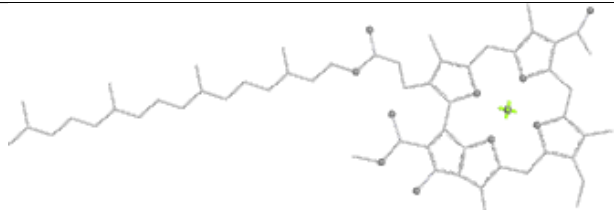
Ligand NS5 M 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

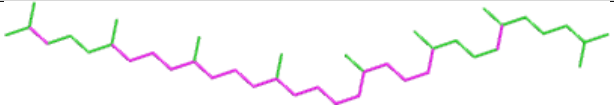
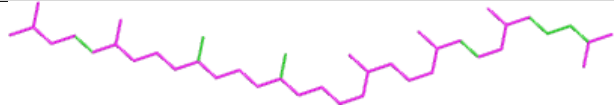
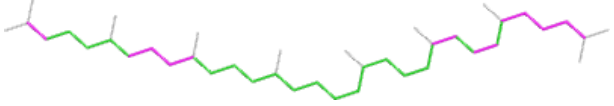
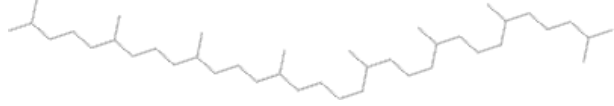


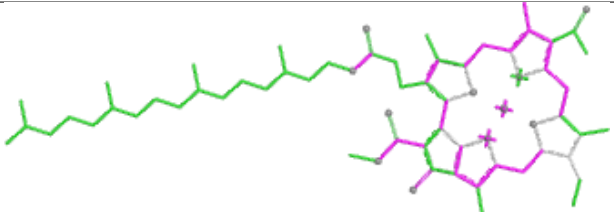
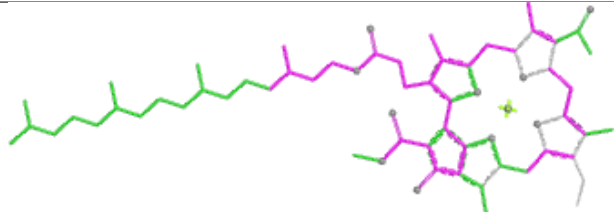
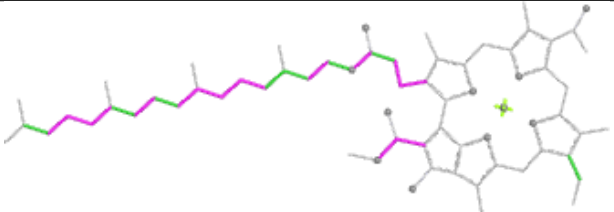
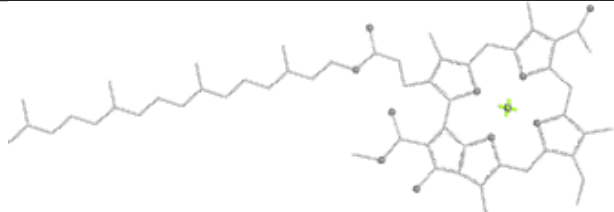


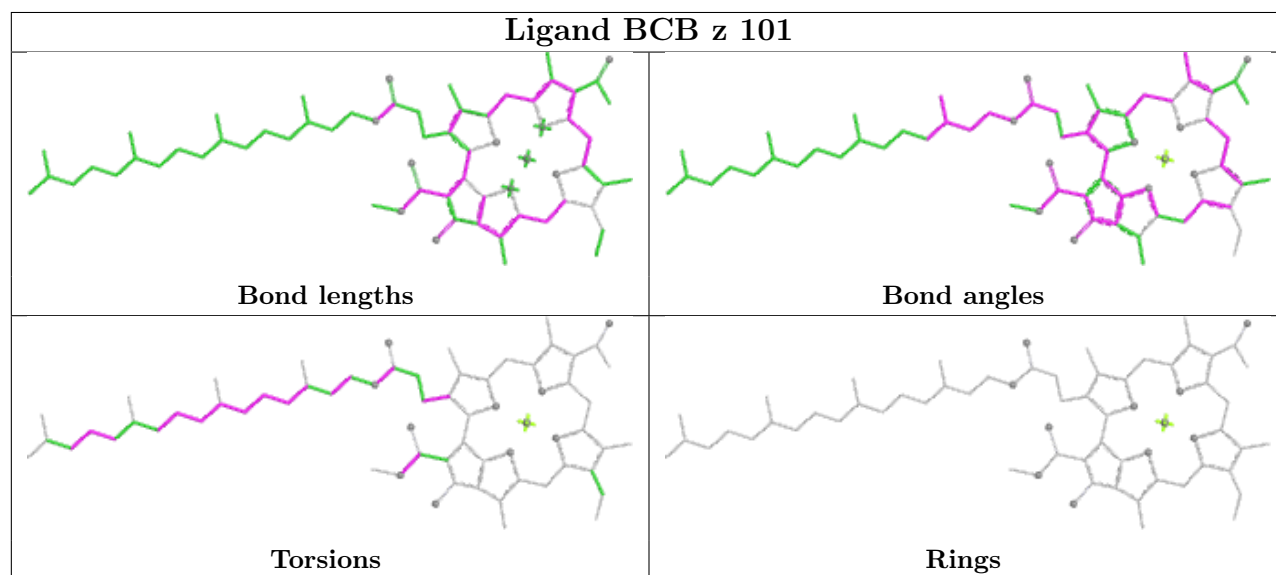
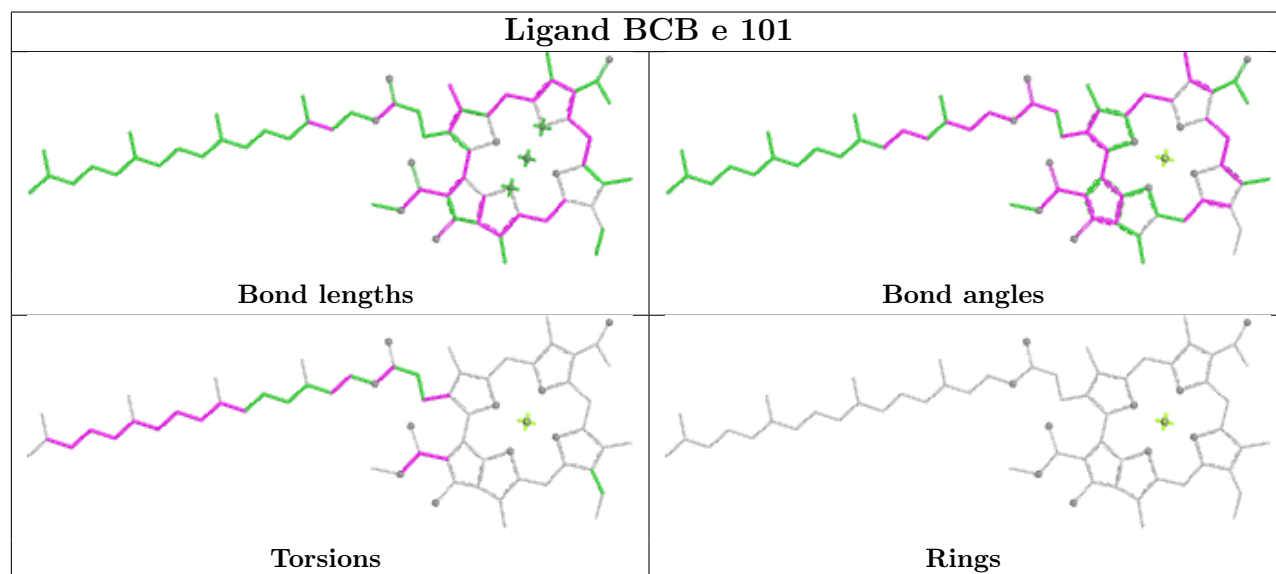
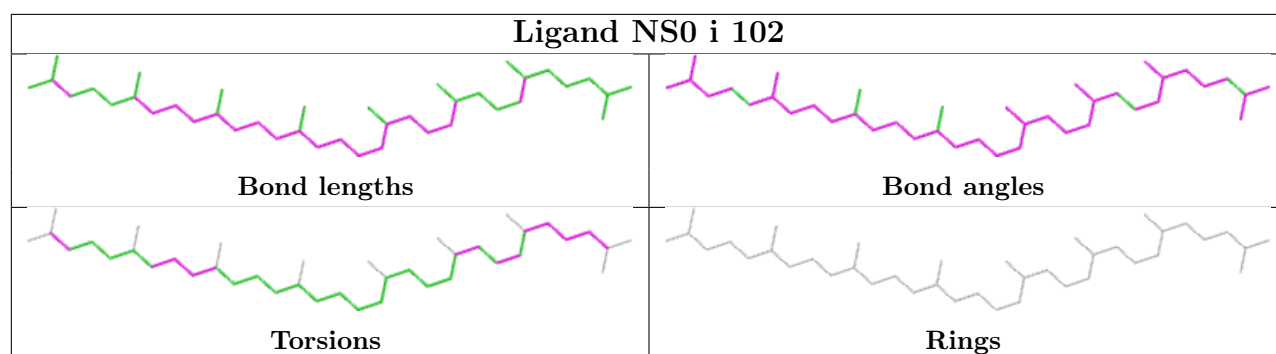


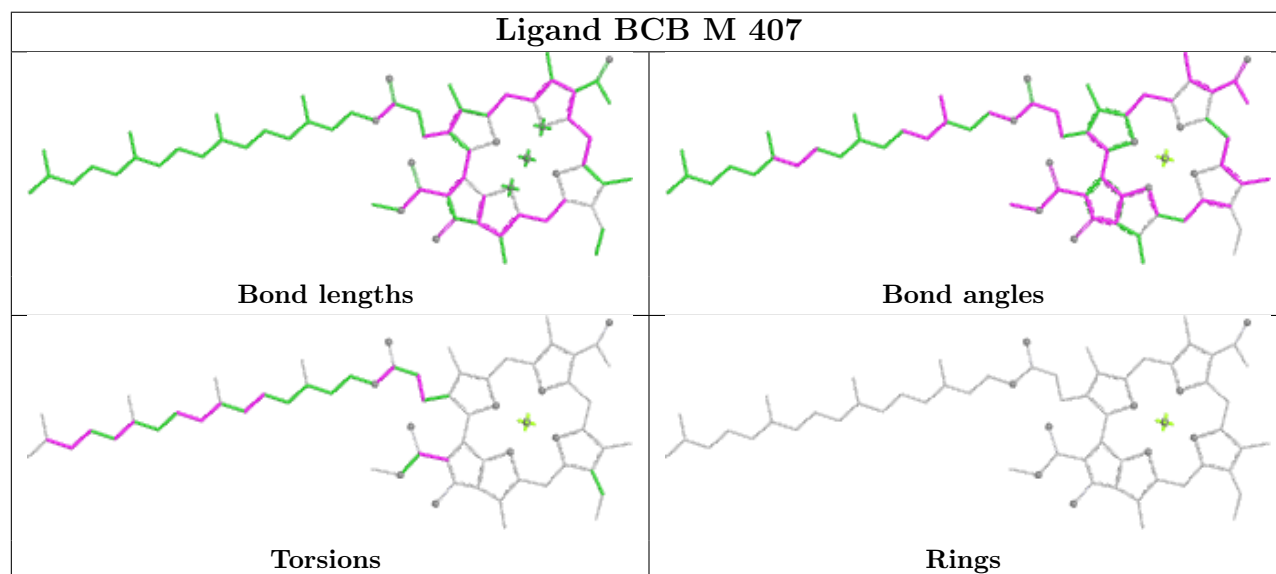
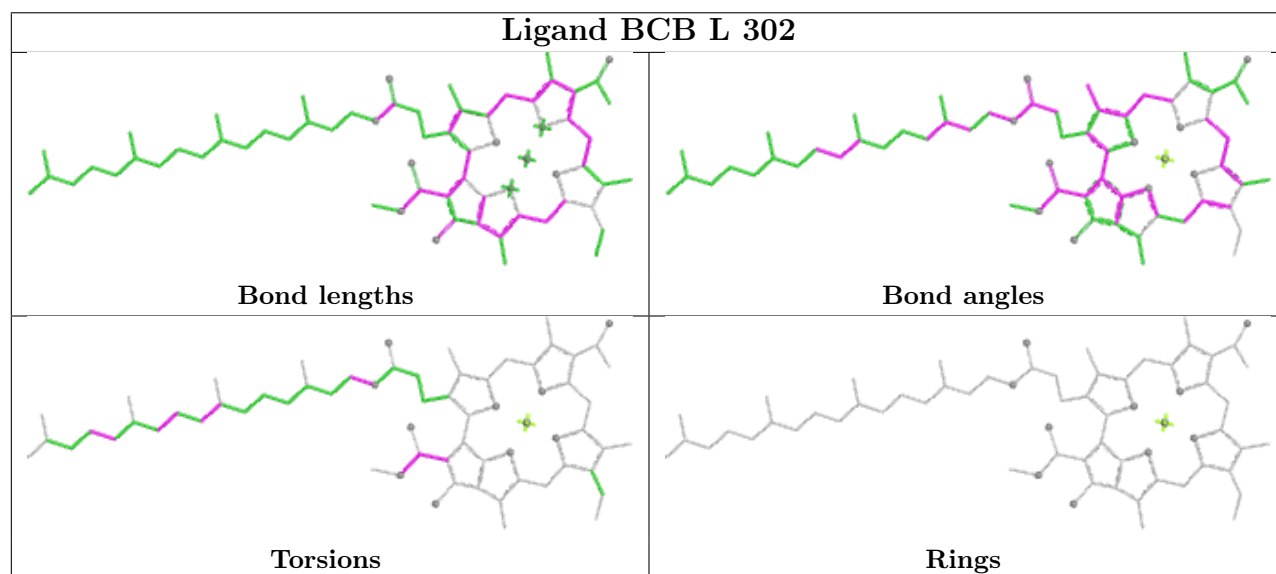
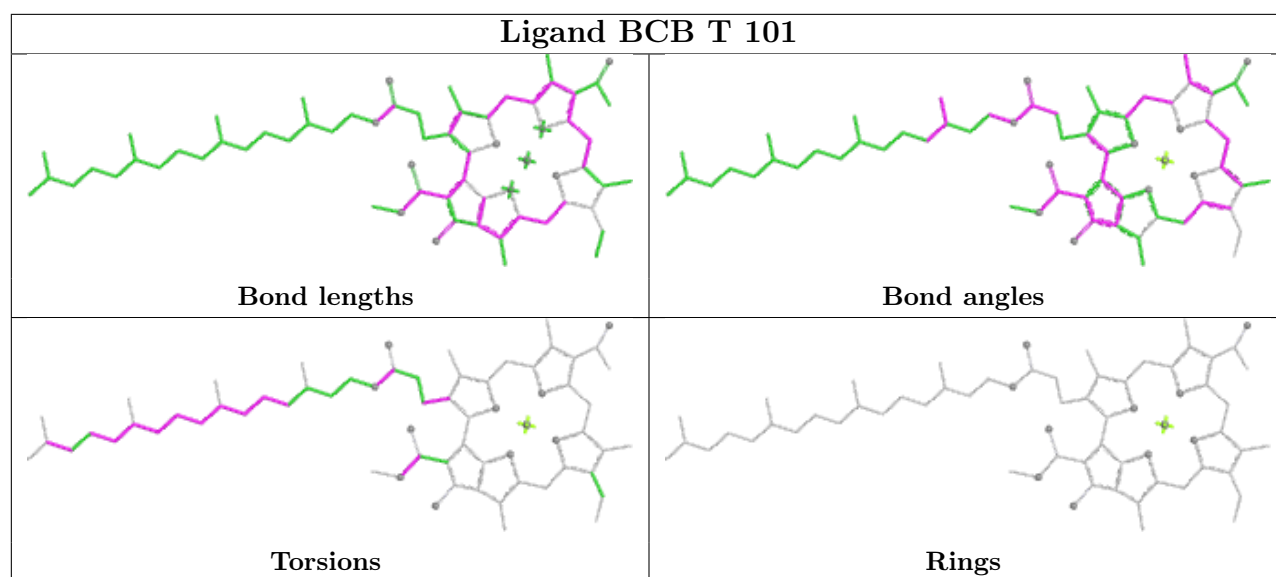


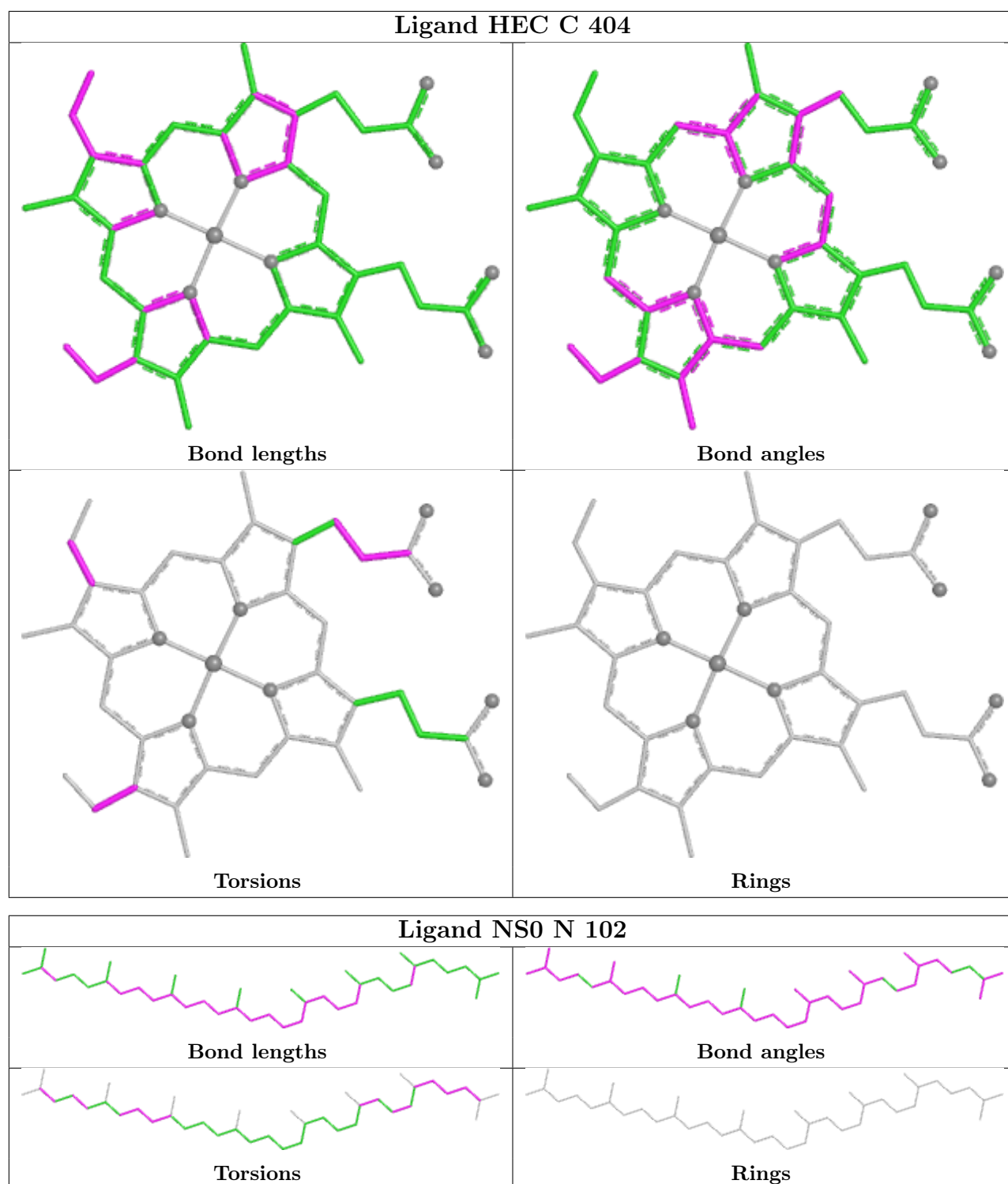
Ligand BCB b 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

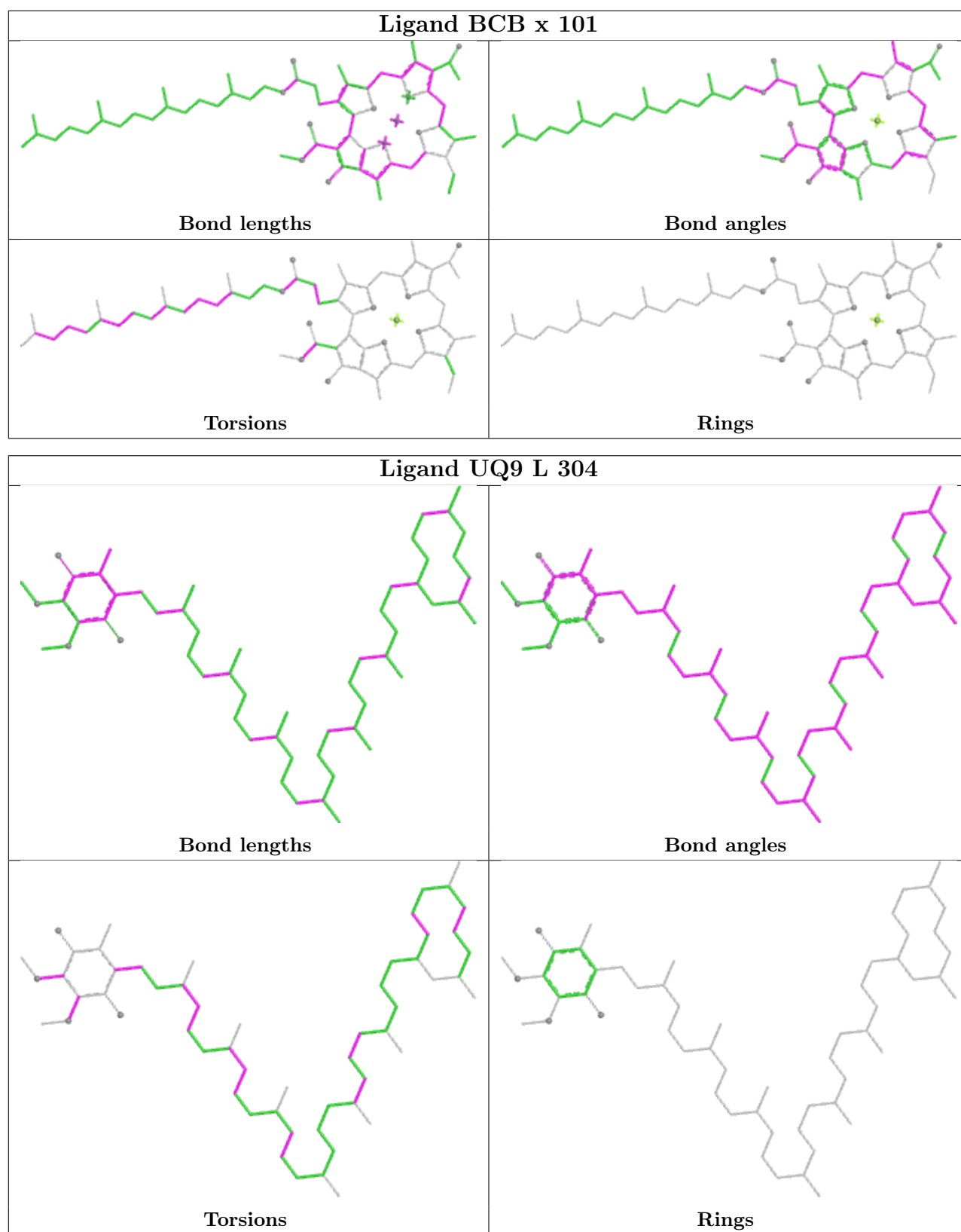
Ligand NS0 r 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

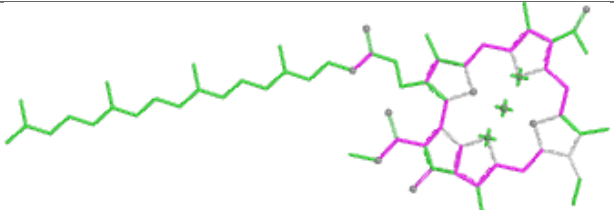
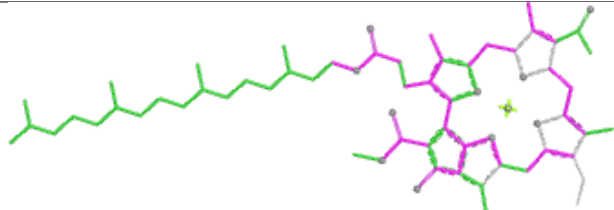
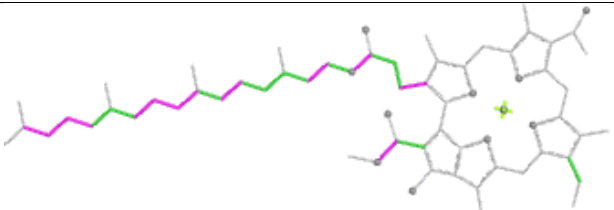
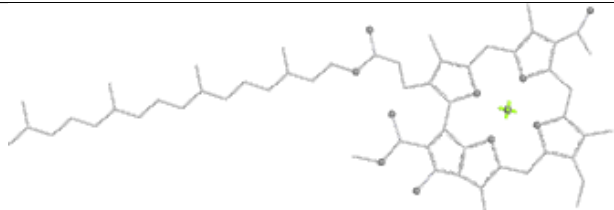
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Bond lengths	Bond angles
	
Torsions	Rings

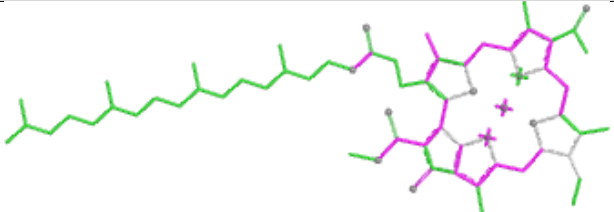
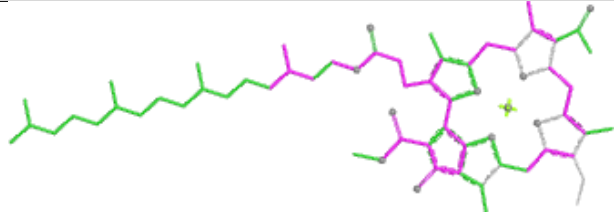
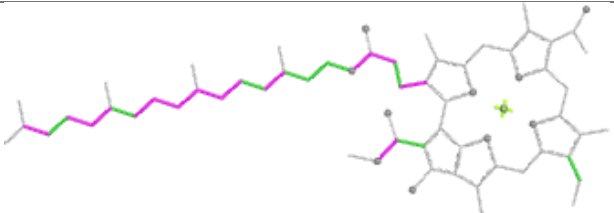
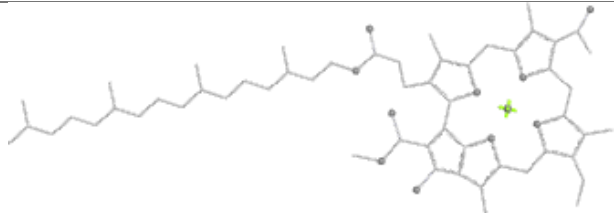


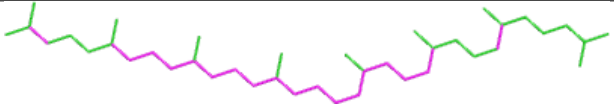
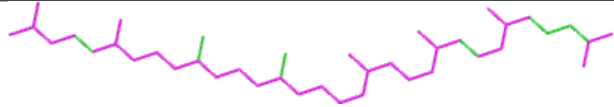
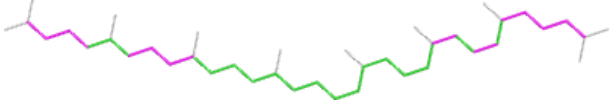
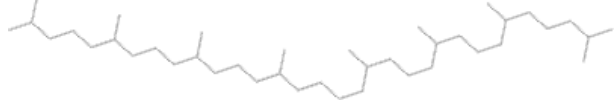


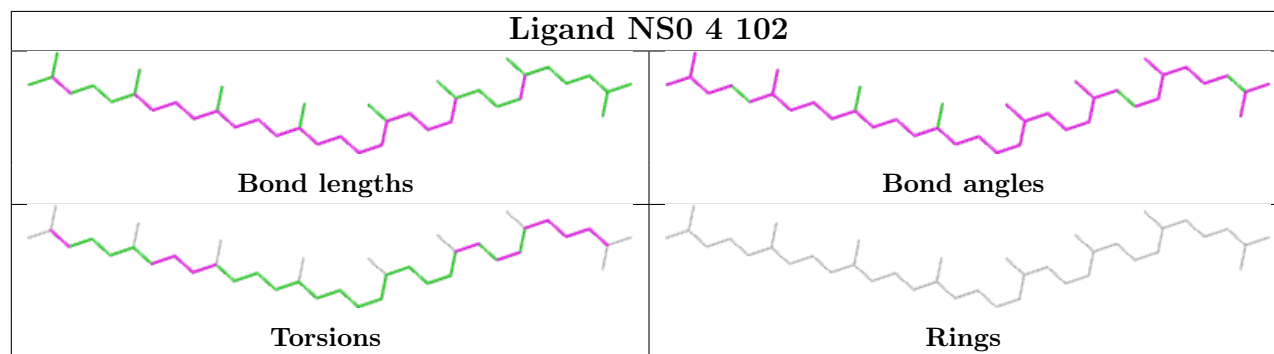
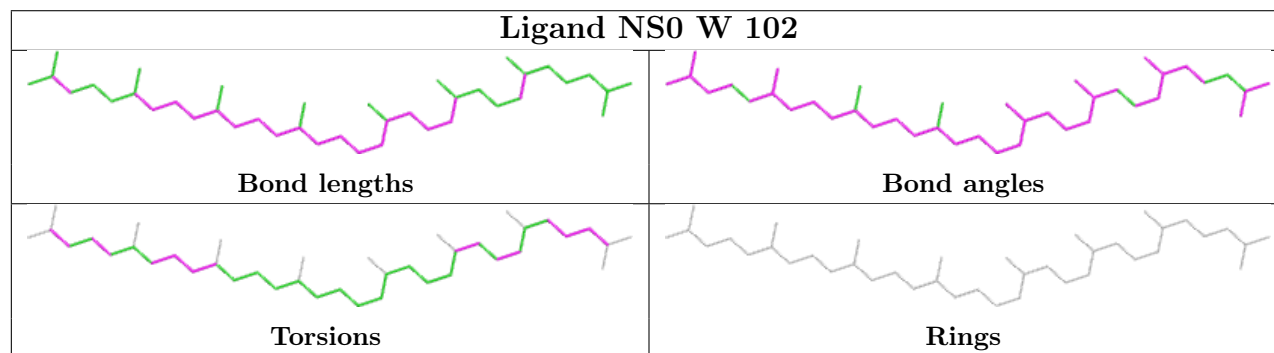
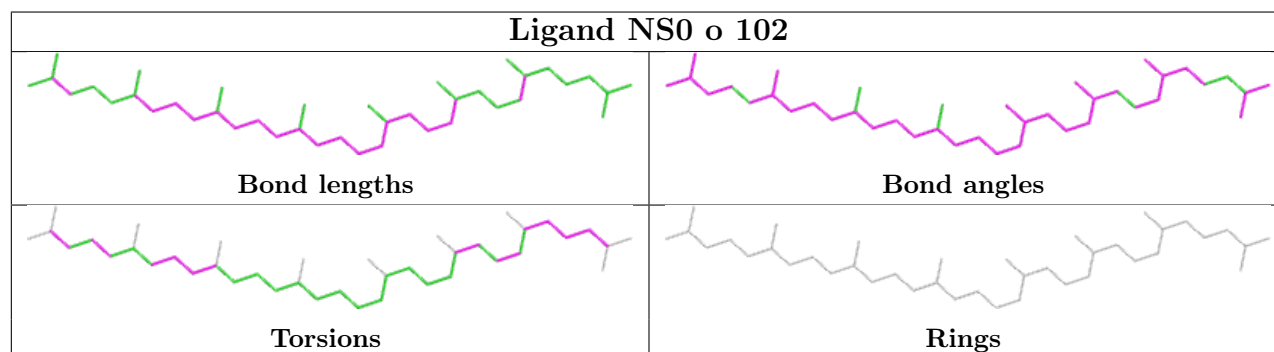
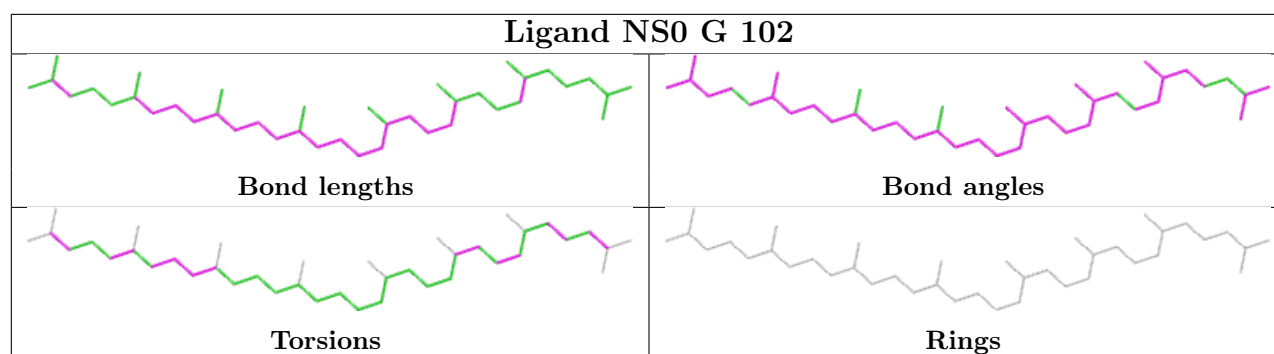


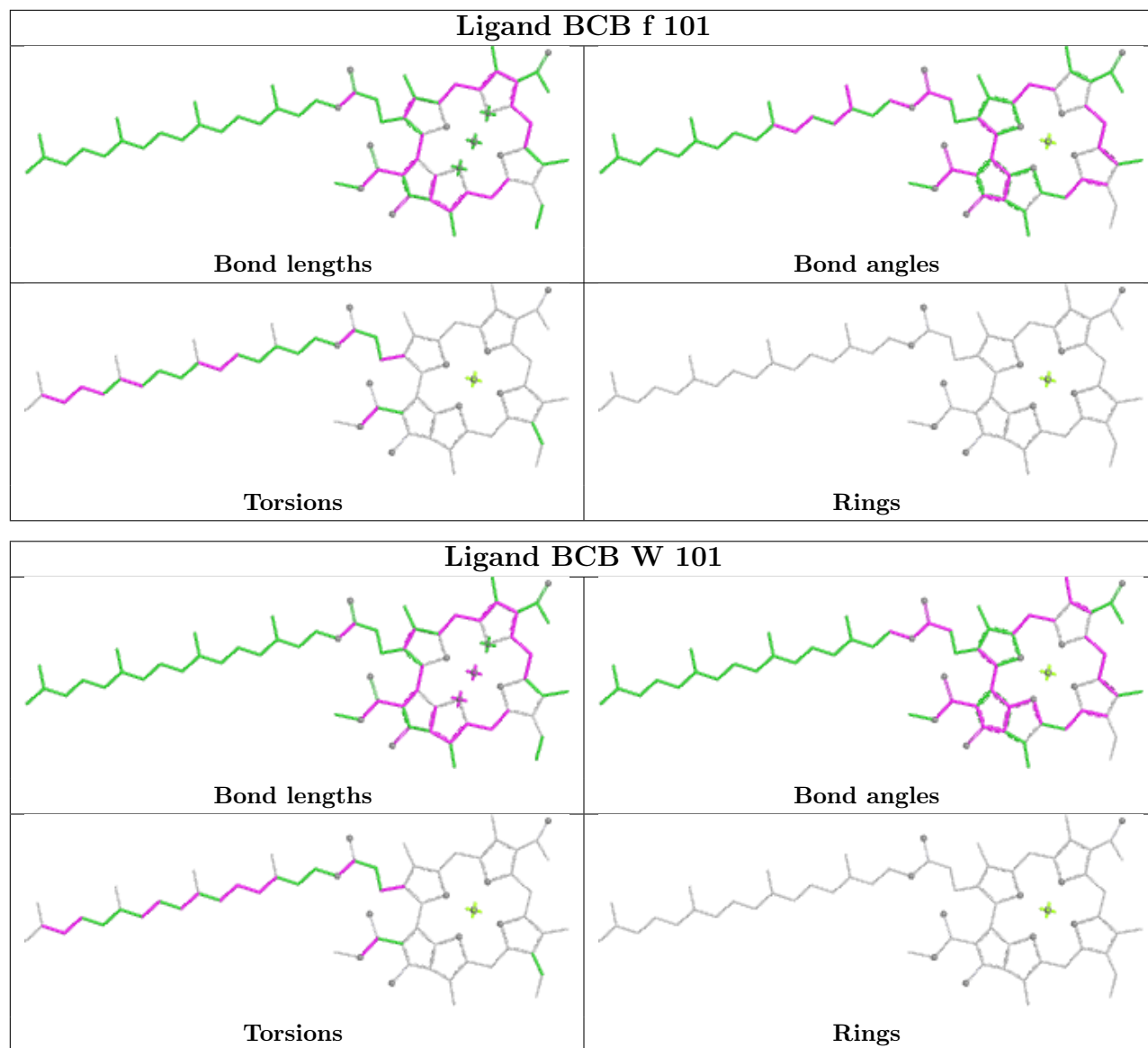


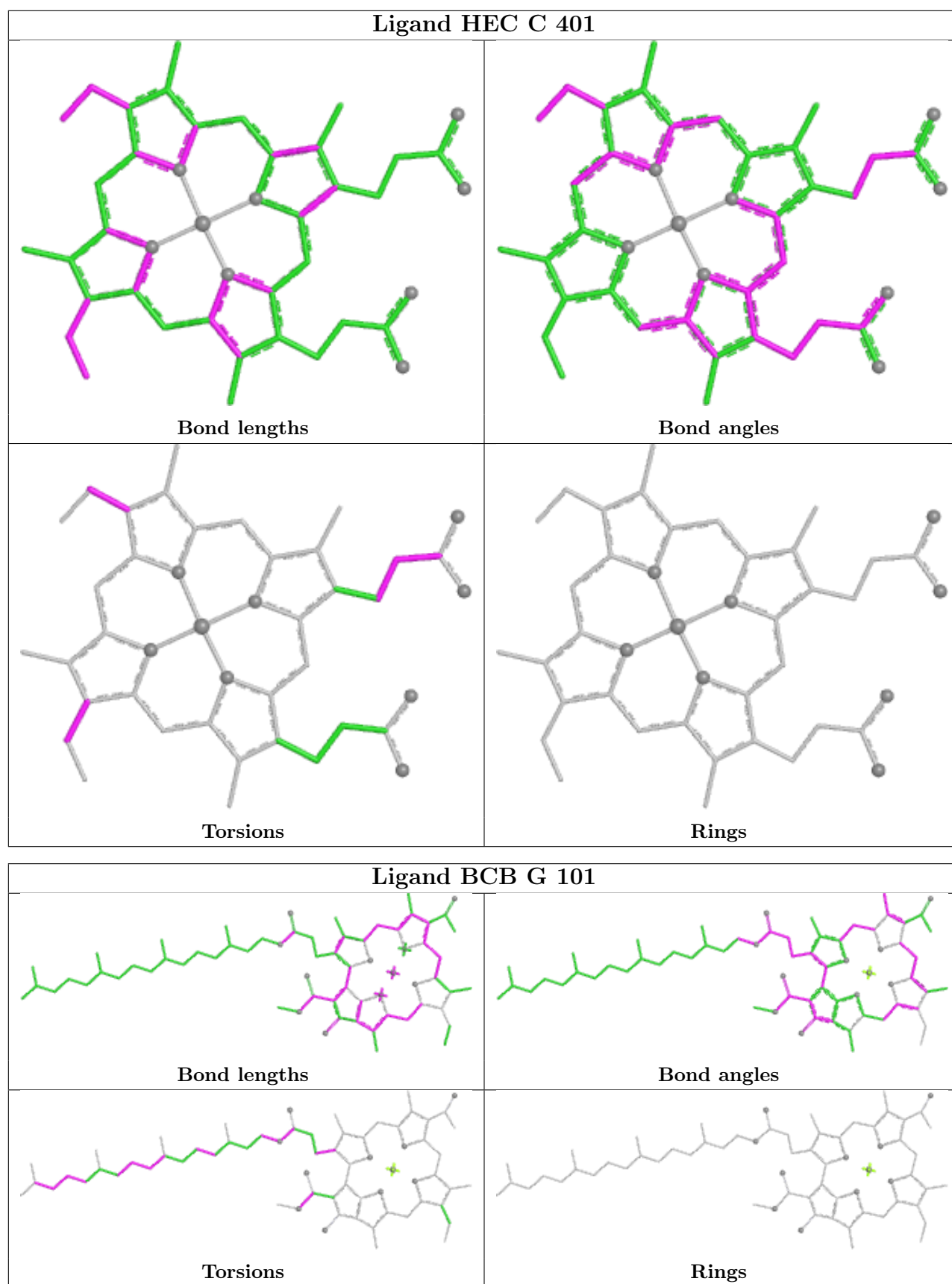
Ligand BCB w 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

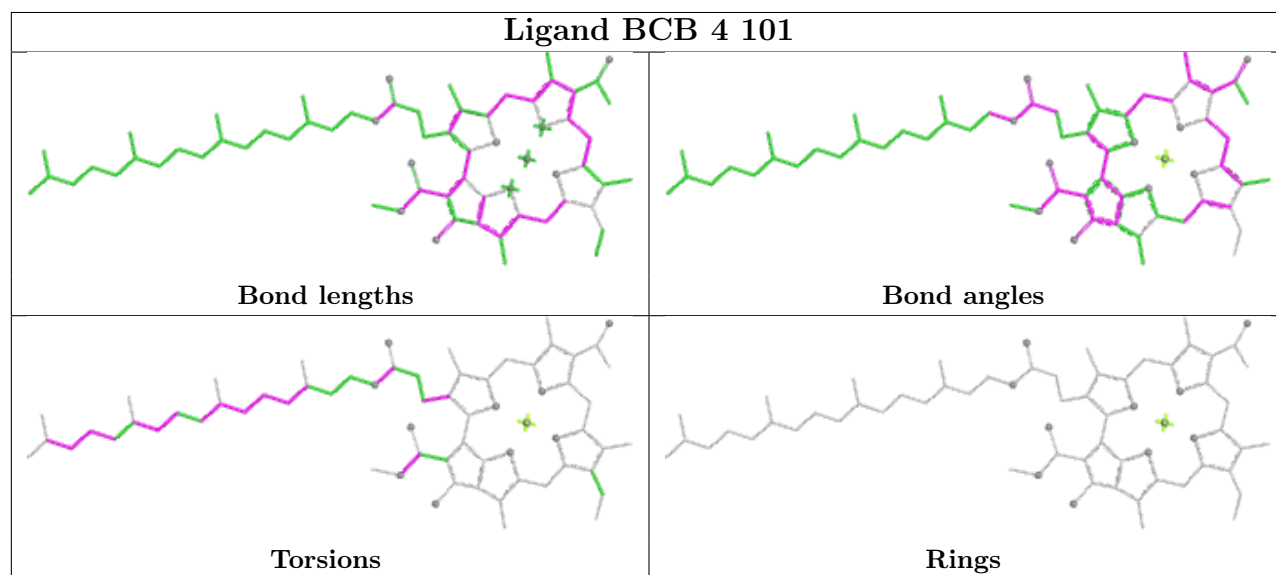
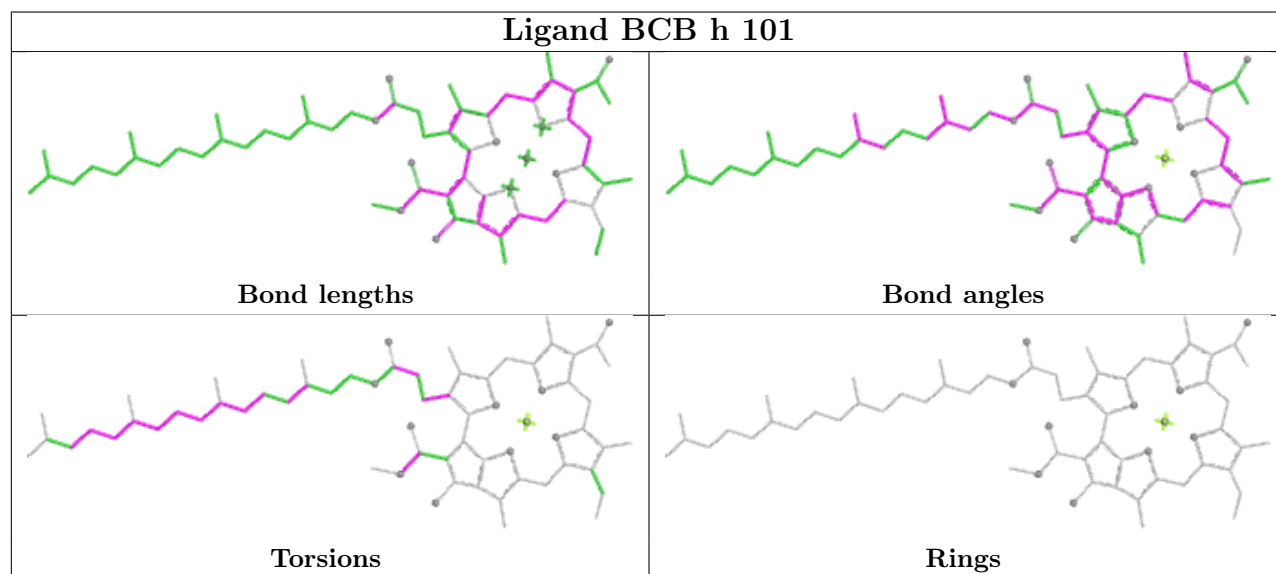
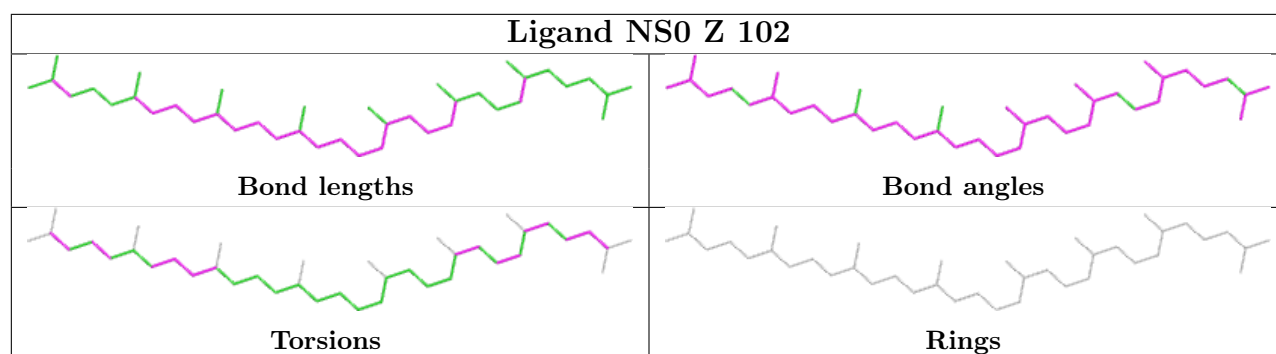
Ligand BCB K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

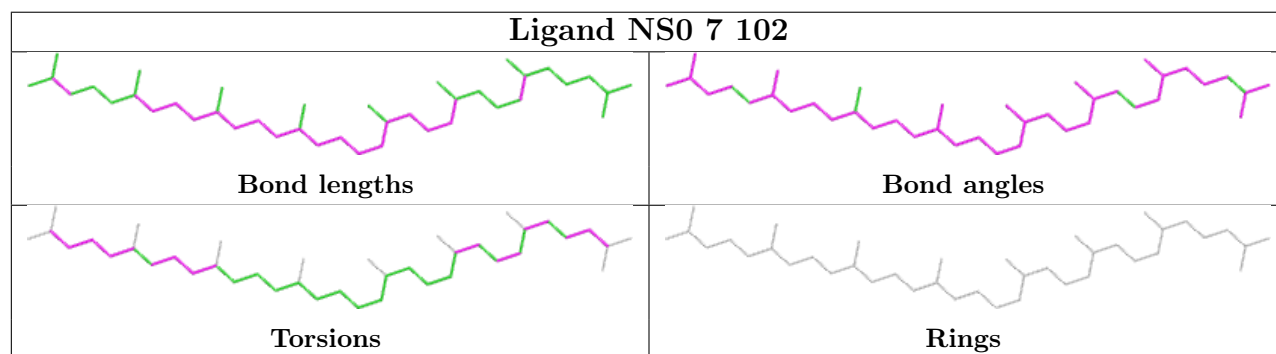
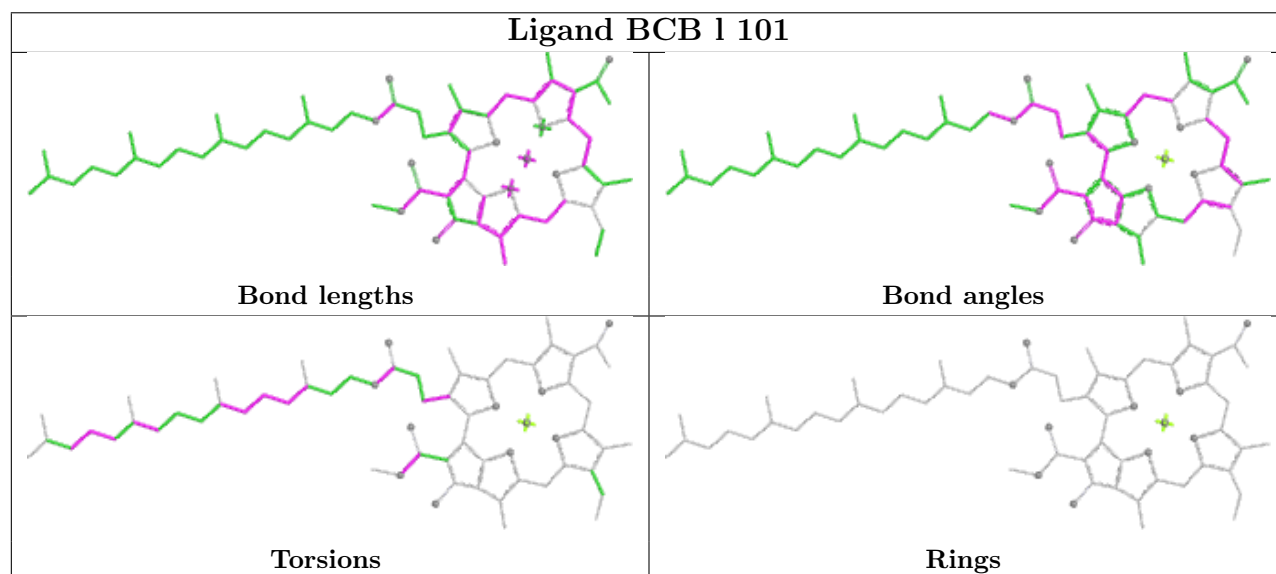
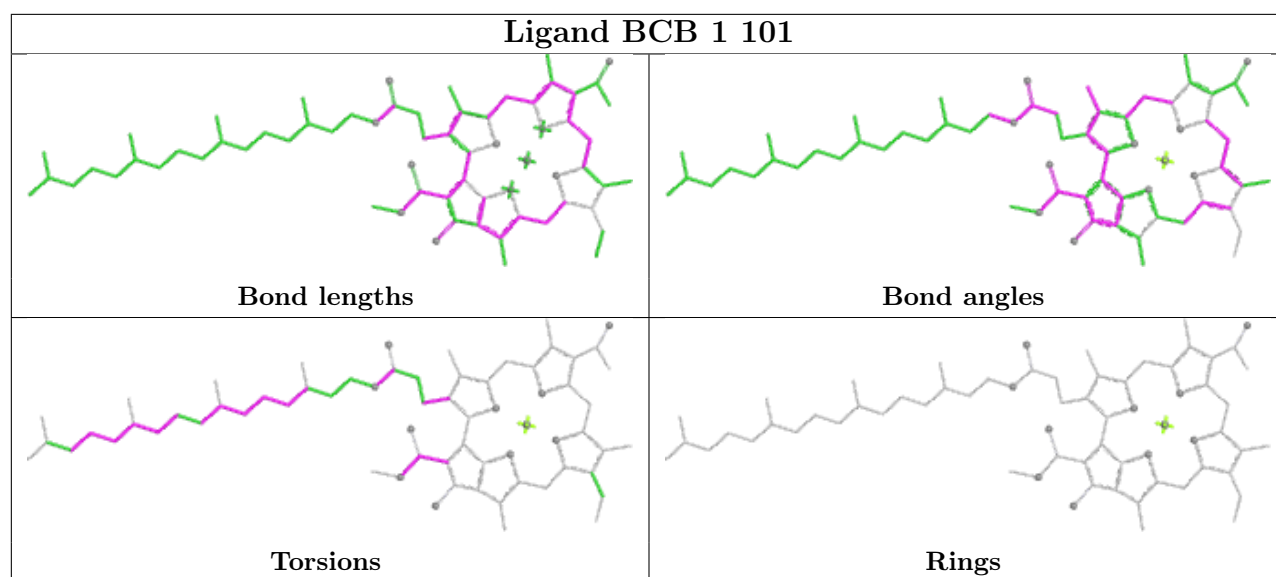
Ligand NS0 T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

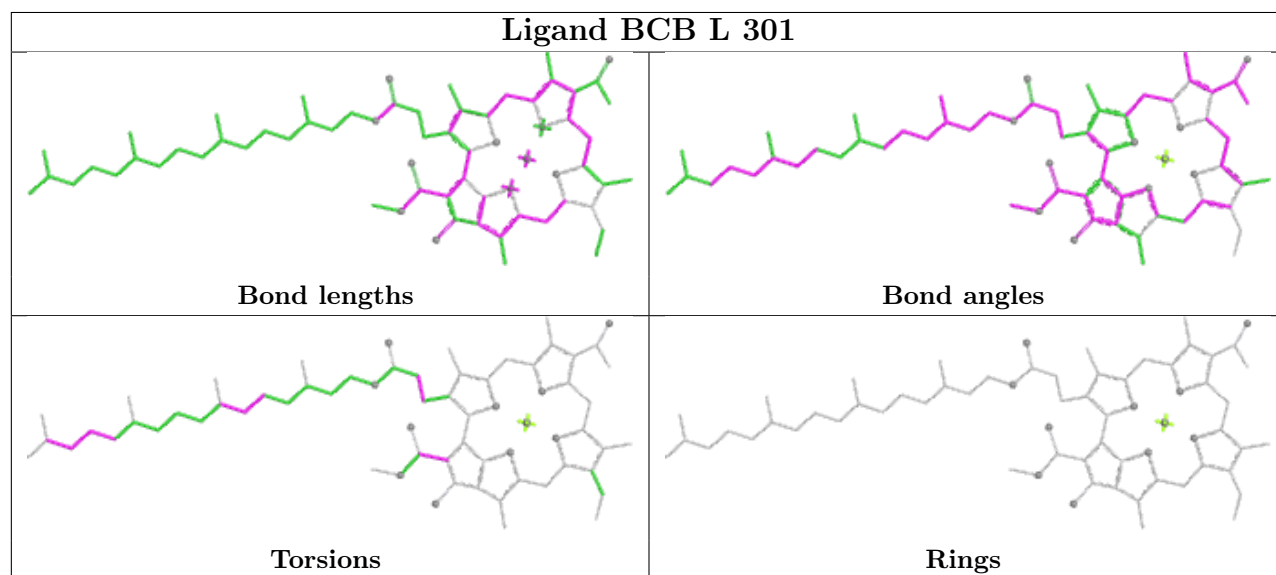
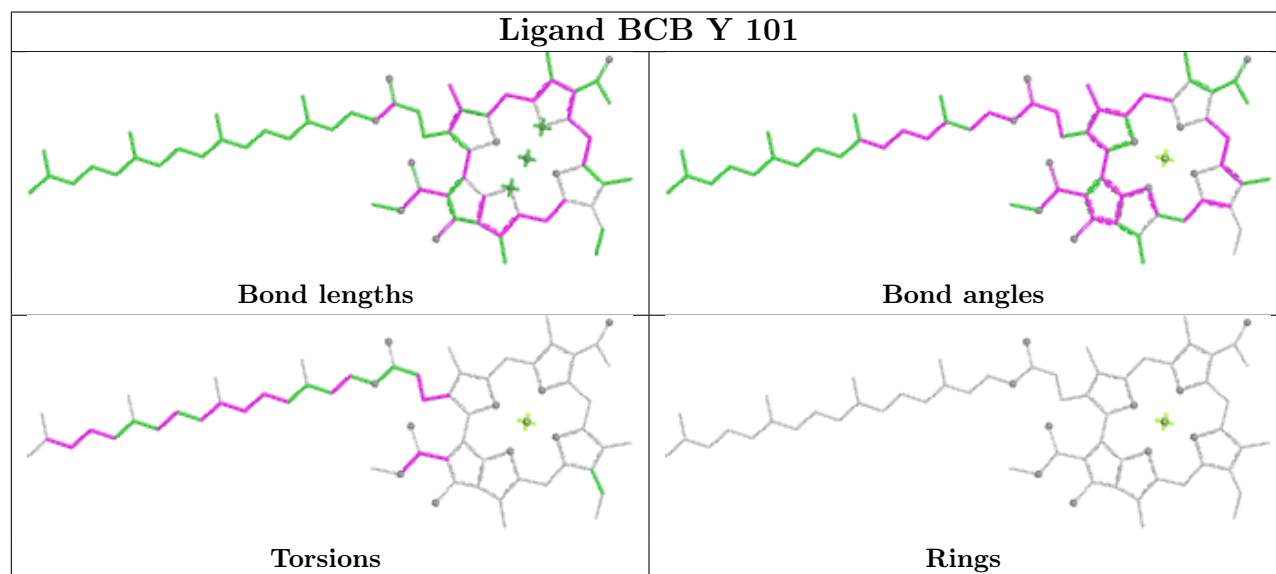
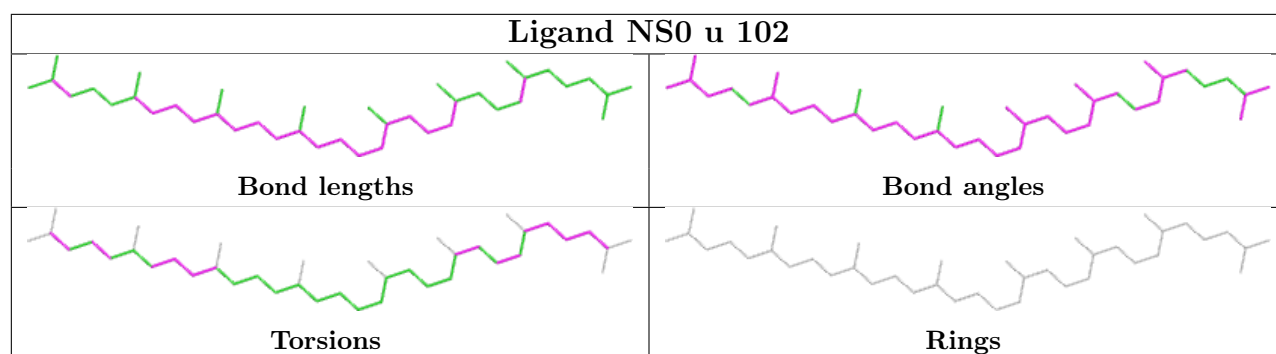


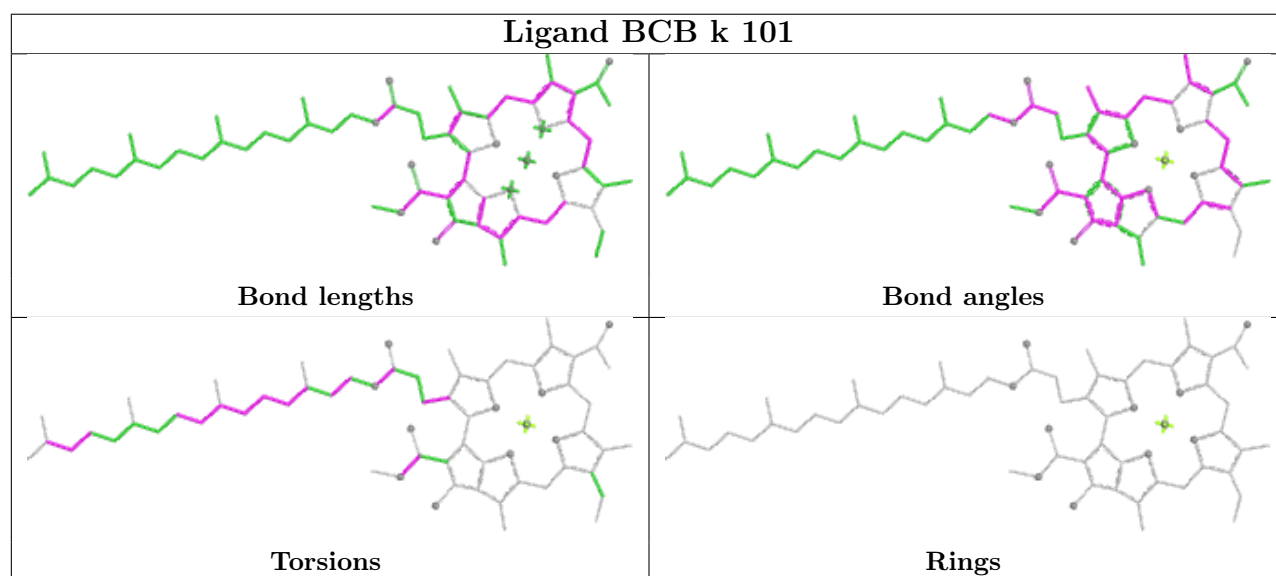
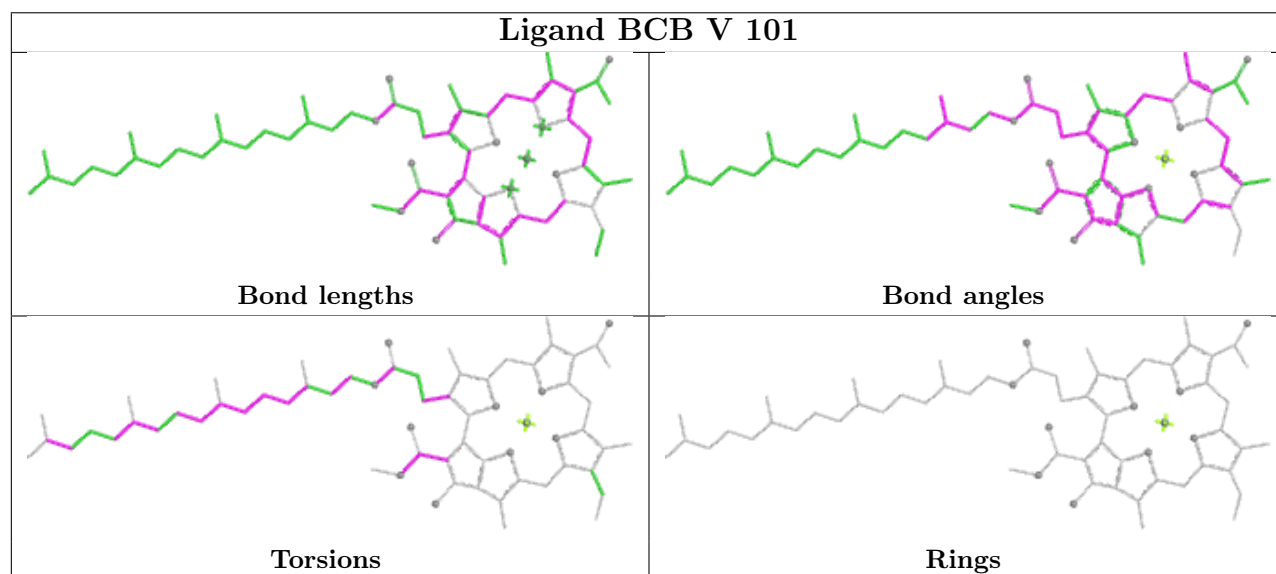
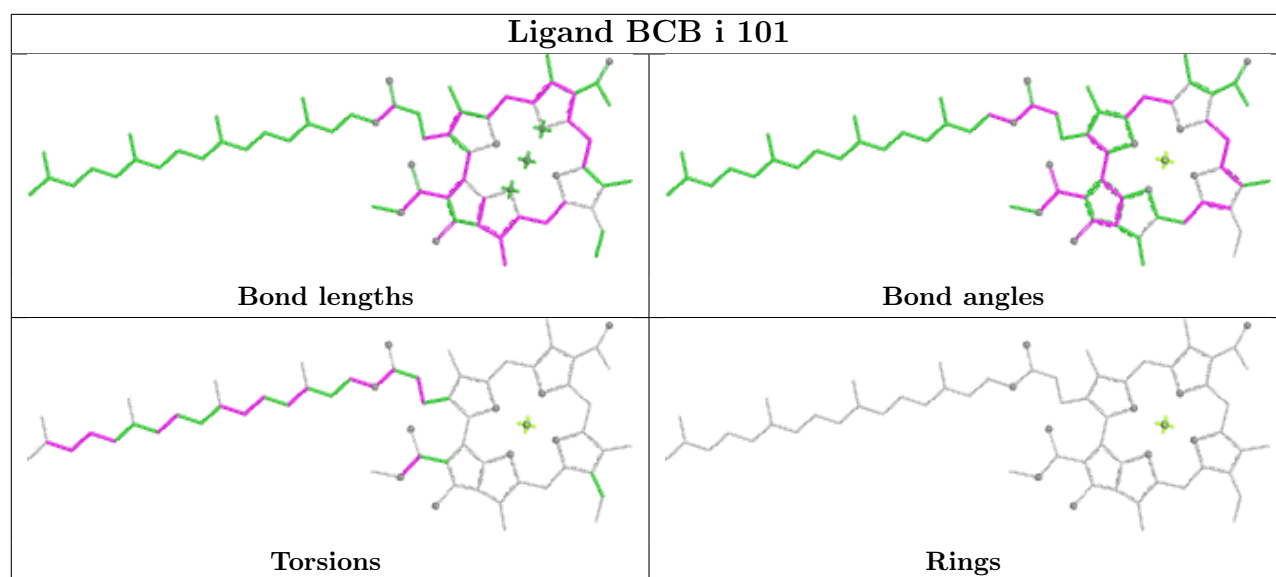


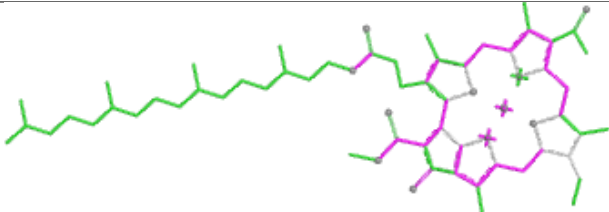
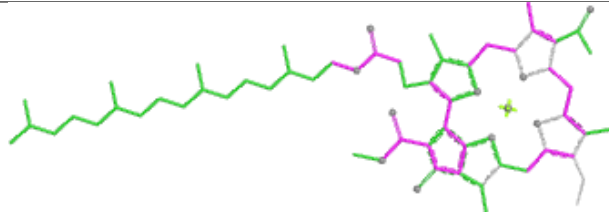
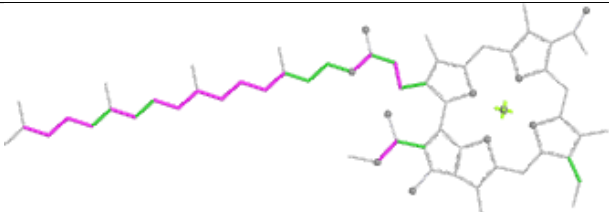
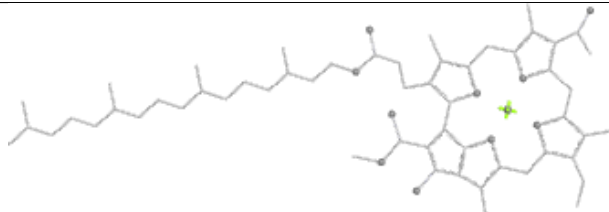


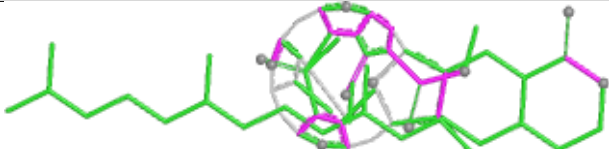
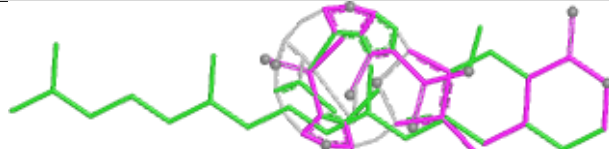
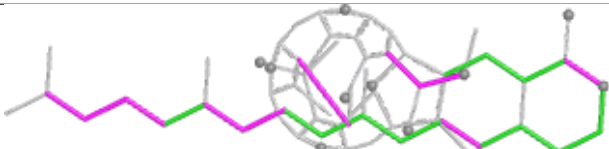
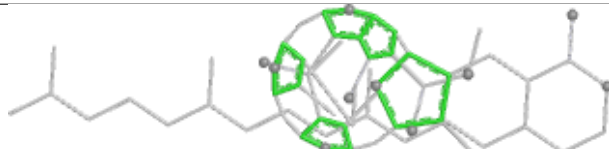


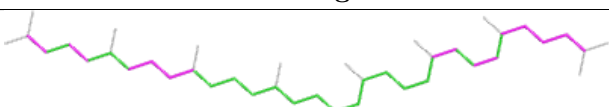
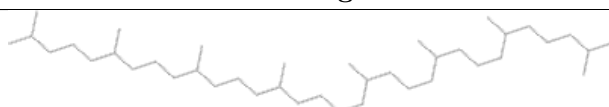


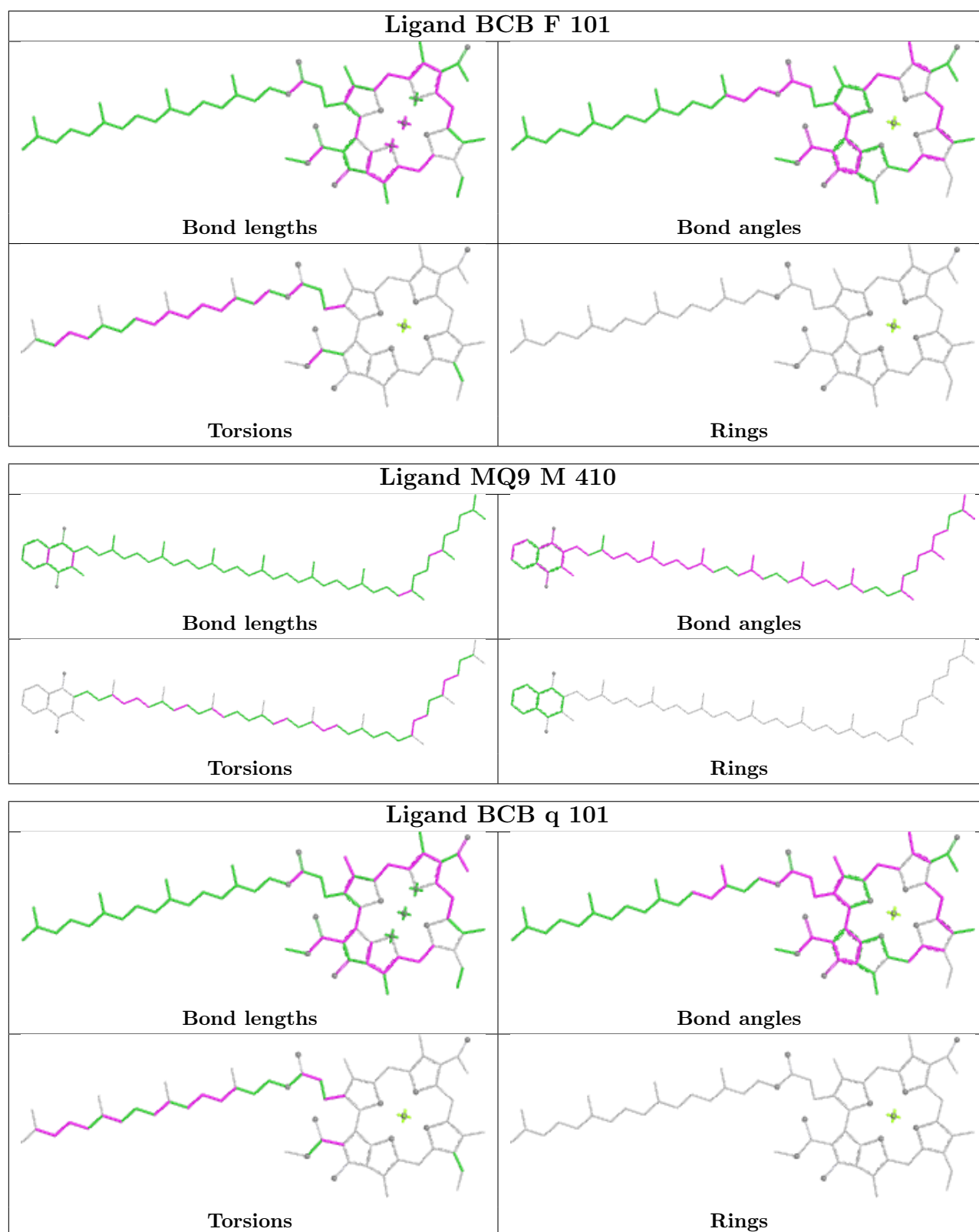


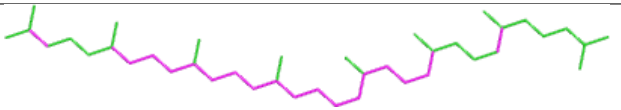
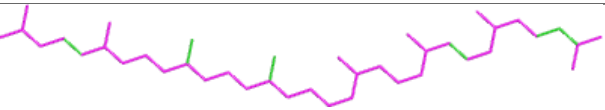
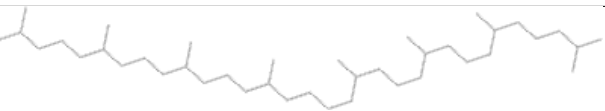


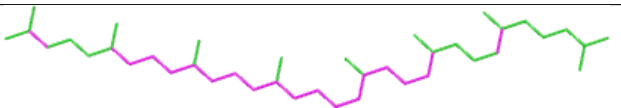
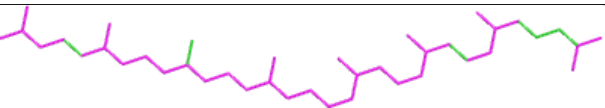
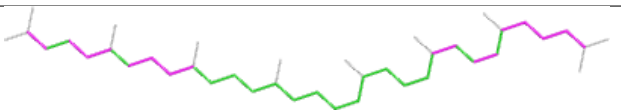
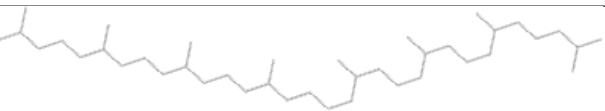
Ligand BCB N 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

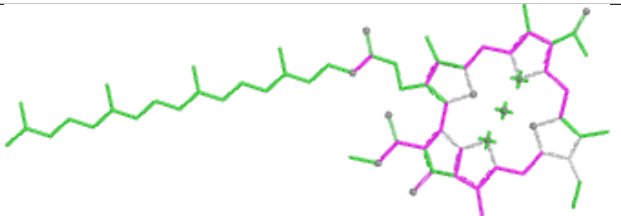
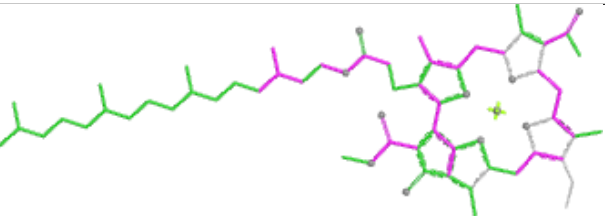
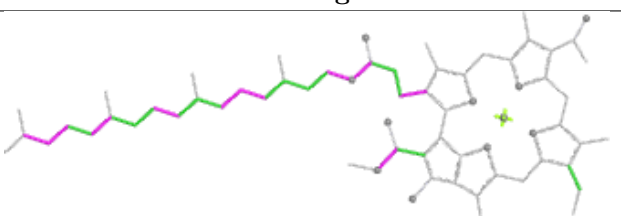
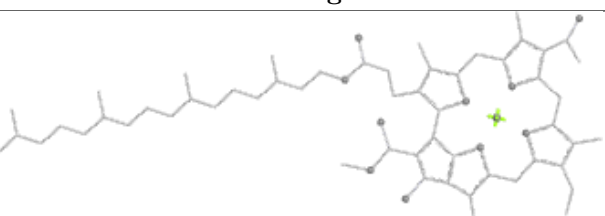
Ligand BPB M 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

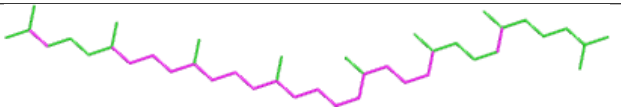
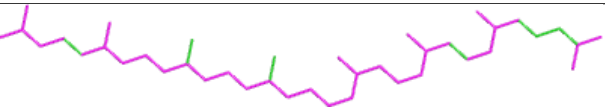
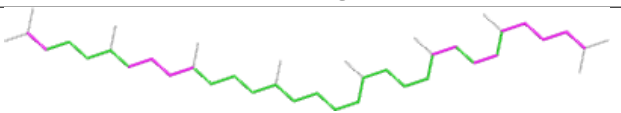
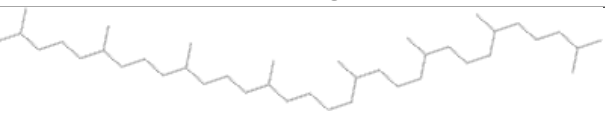
Ligand NS0 f 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

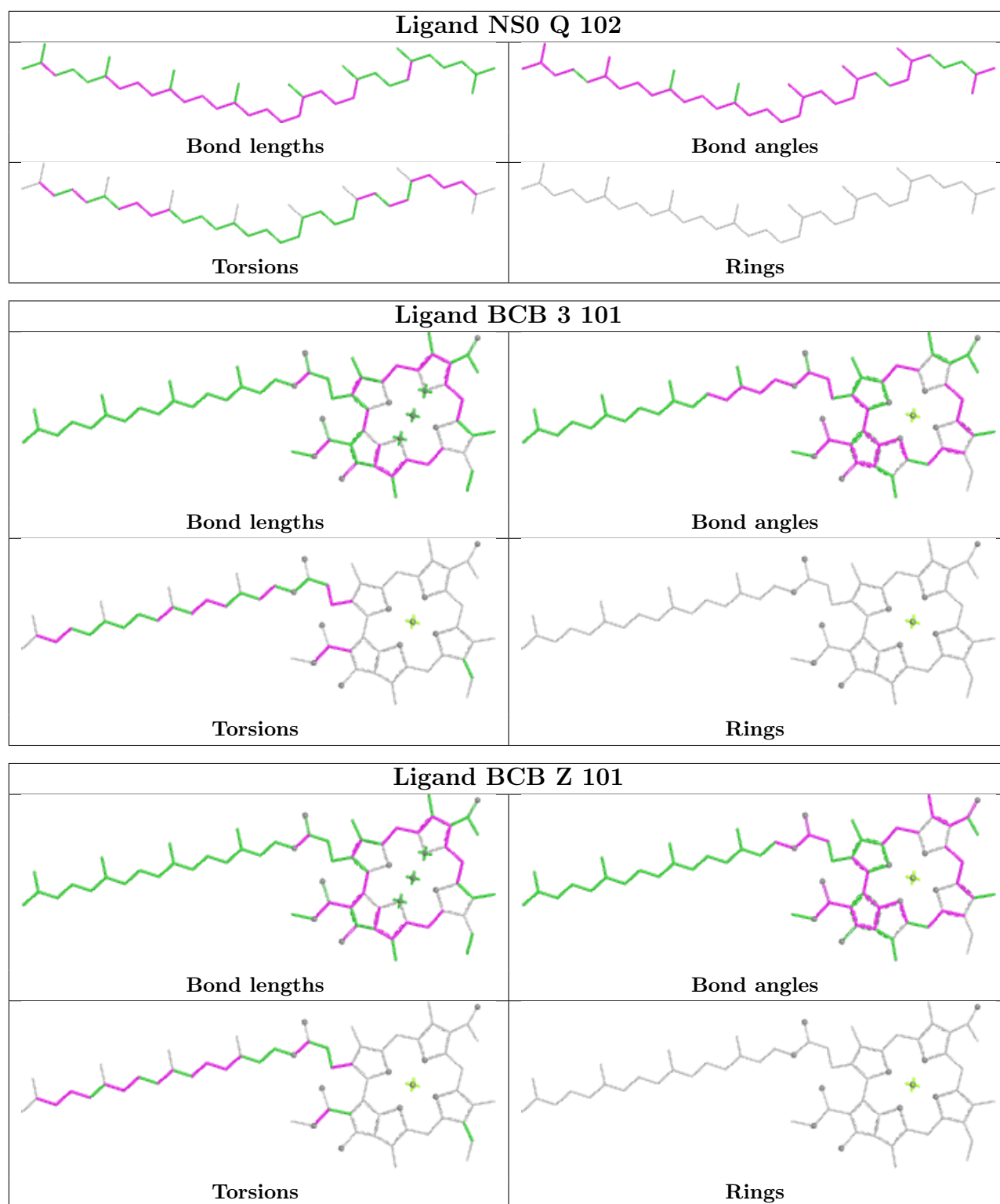


Ligand NS0 c 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 l 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCB M 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NS0 x 102	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage 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

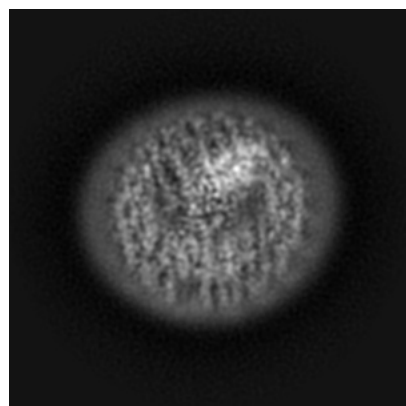
6 Map visualisation [i](#)

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.

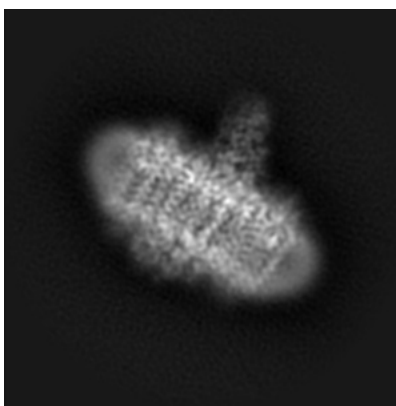
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

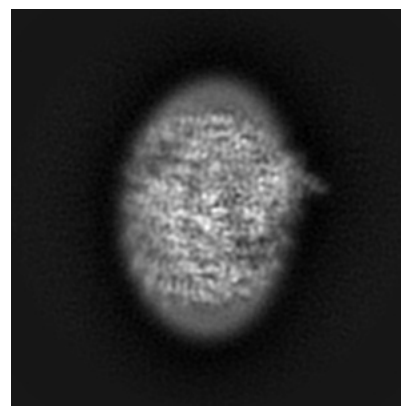
6.1.1 Primary map



X

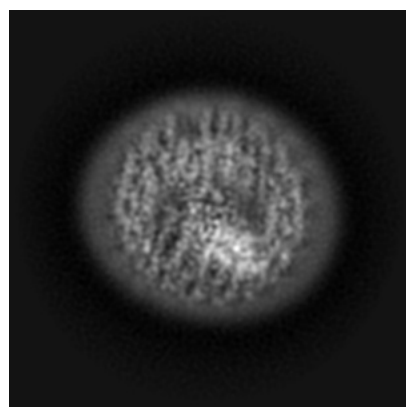


Y

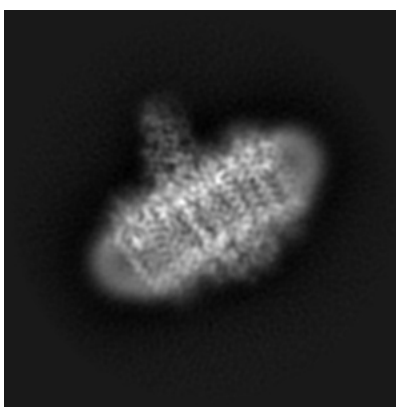


Z

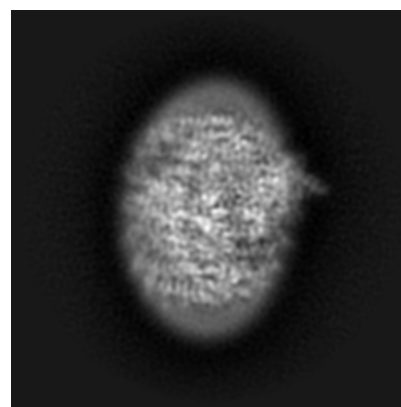
6.1.2 Raw map



X



Y

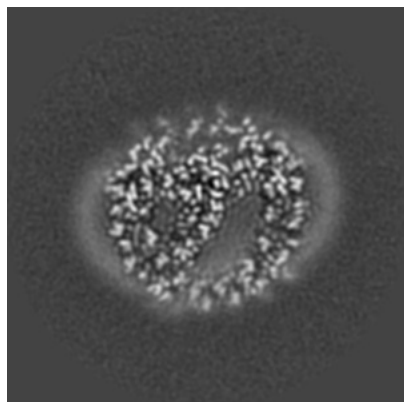


Z

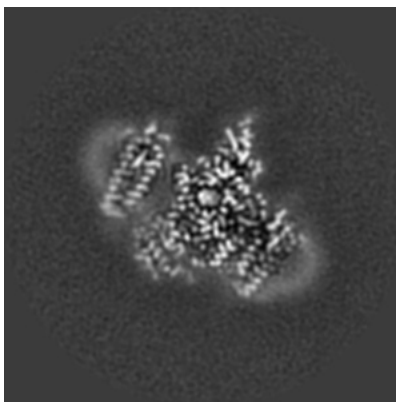
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

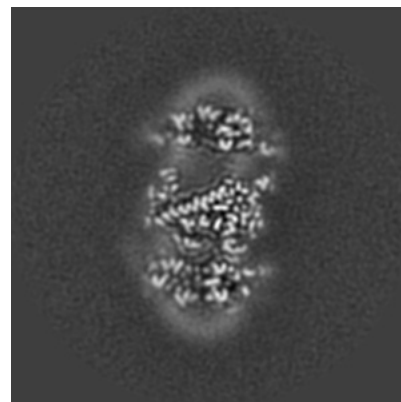
6.2.1 Primary map



X Index: 115

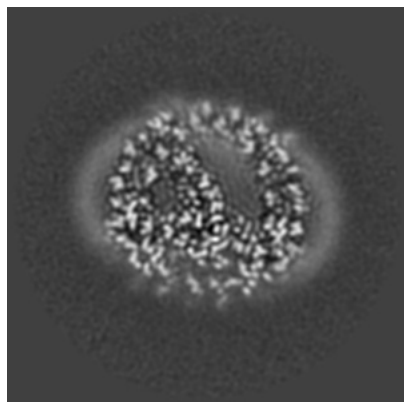


Y Index: 115

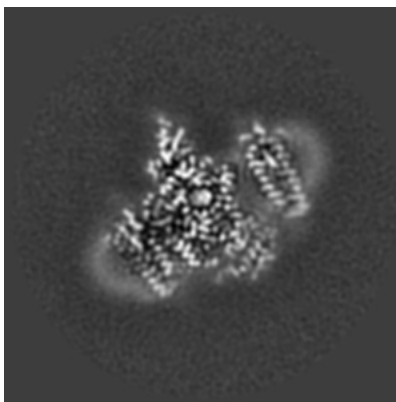


Z Index: 115

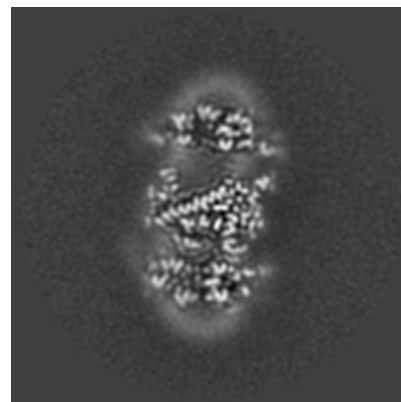
6.2.2 Raw map



X Index: 115



Y Index: 115

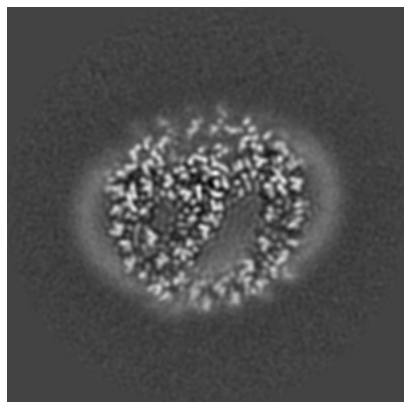


Z Index: 115

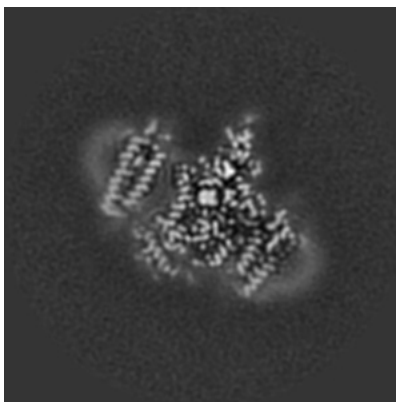
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

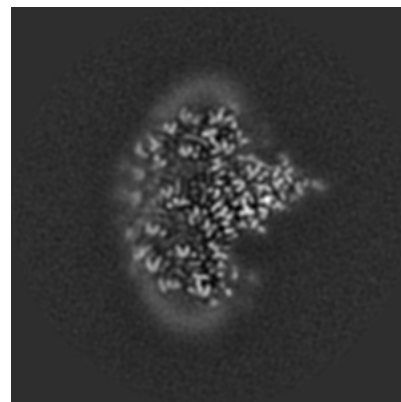
6.3.1 Primary map



X Index: 115

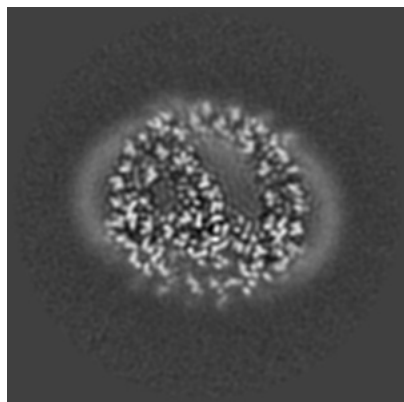


Y Index: 114

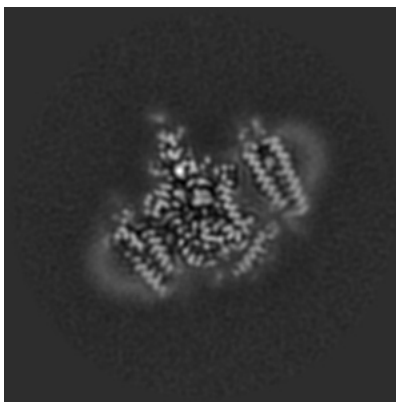


Z Index: 131

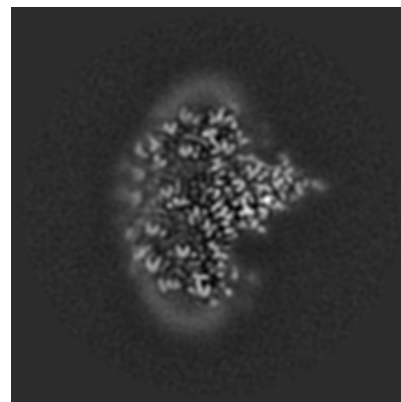
6.3.2 Raw map



X Index: 115



Y Index: 113

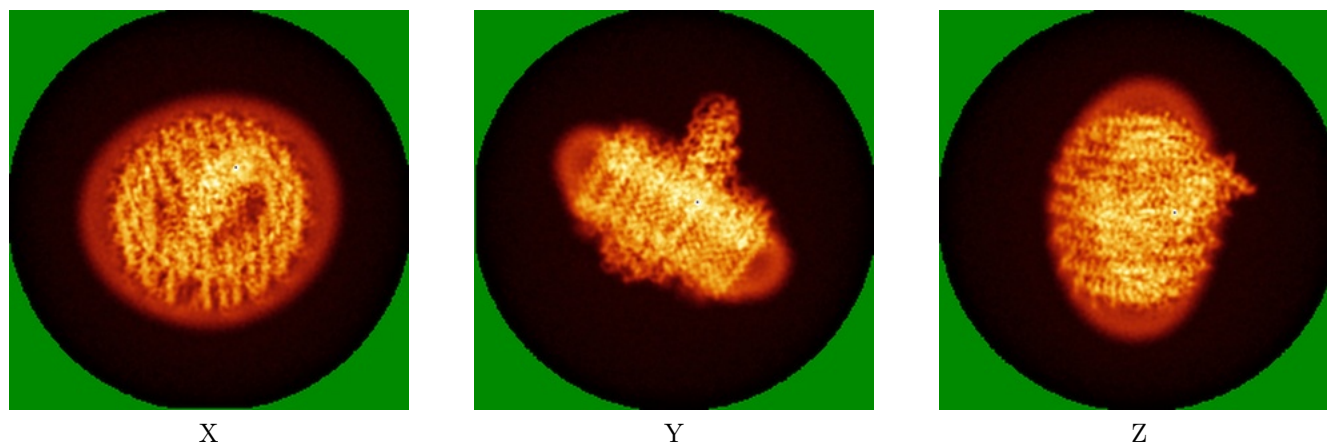


Z Index: 99

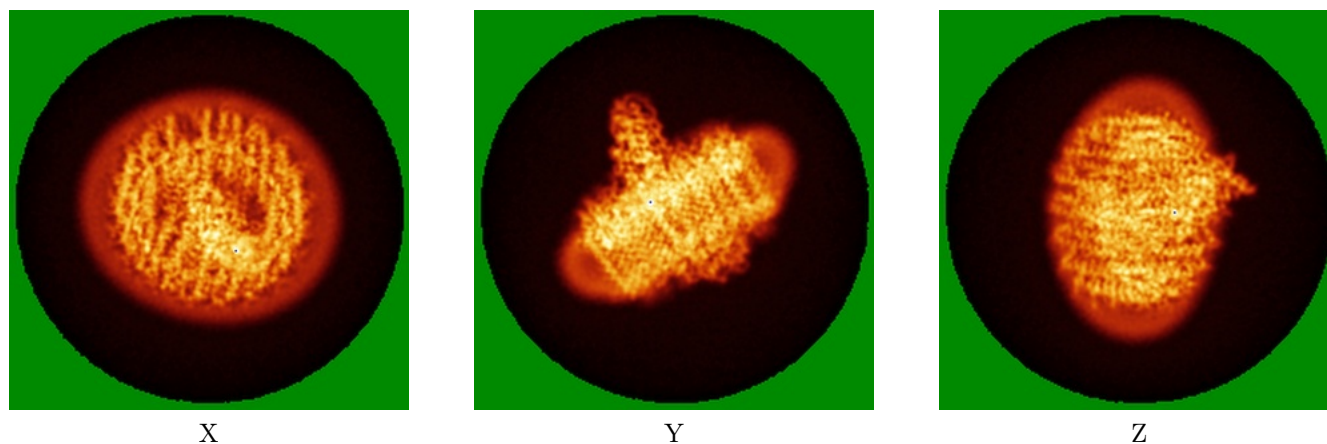
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

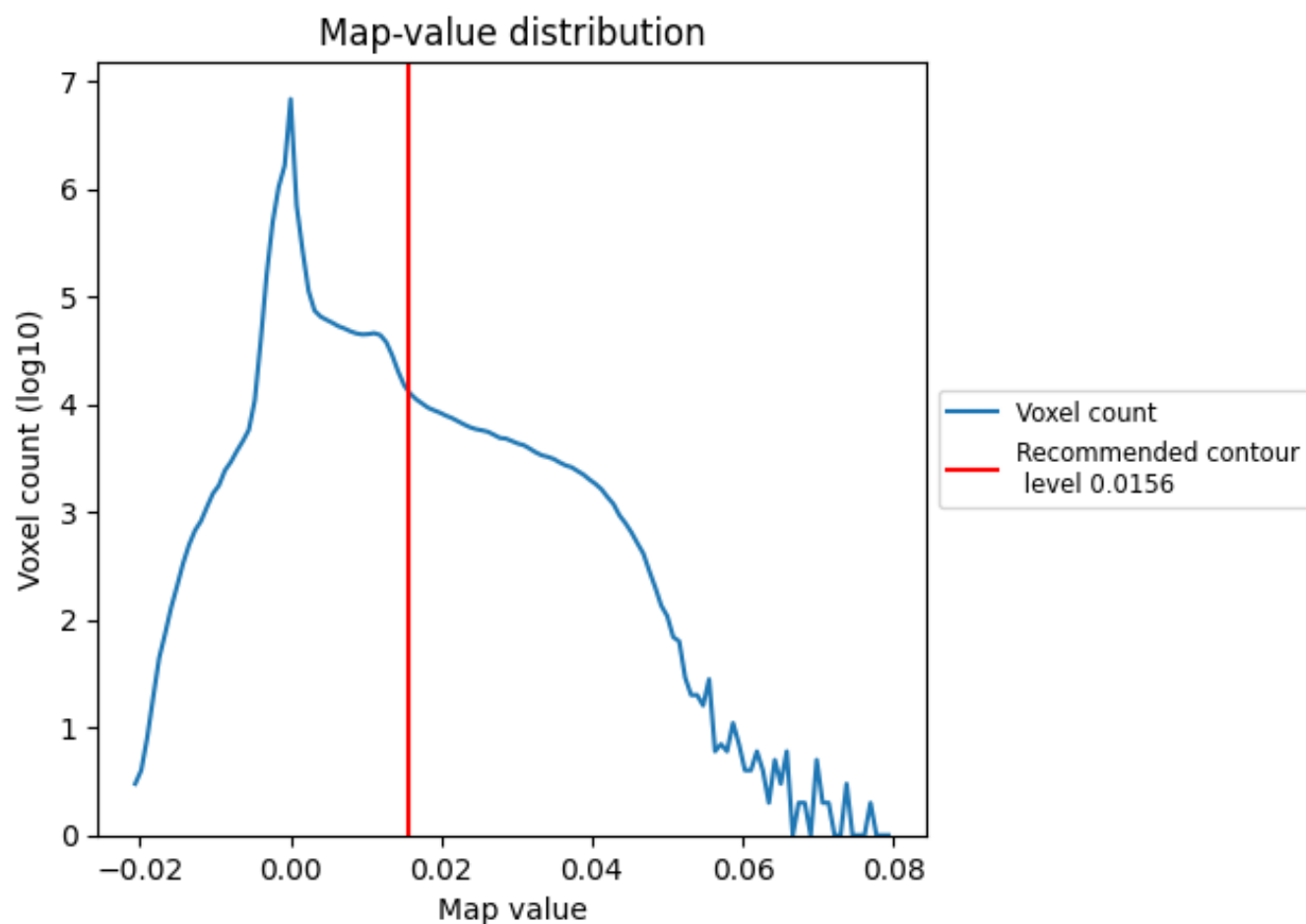
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

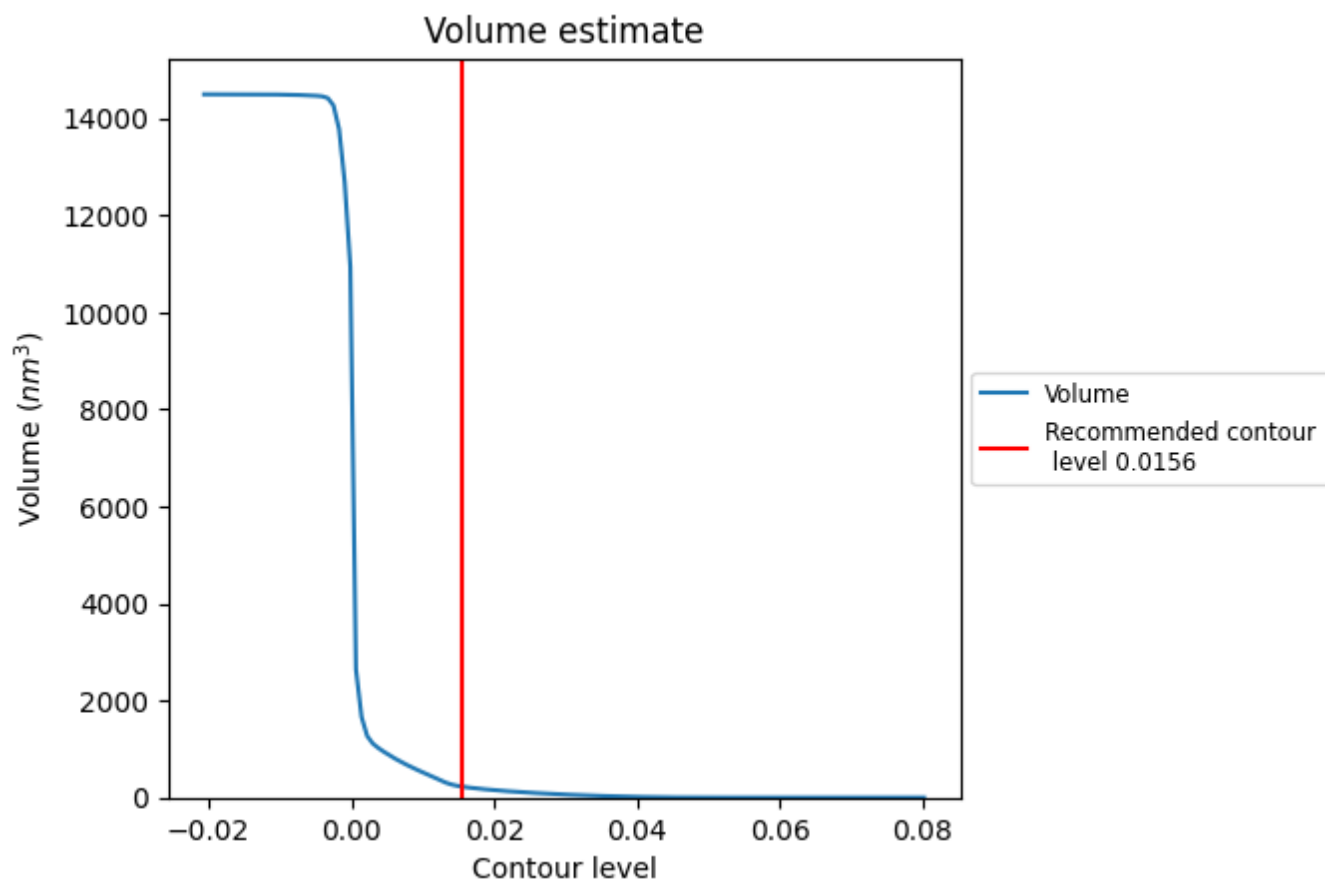
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

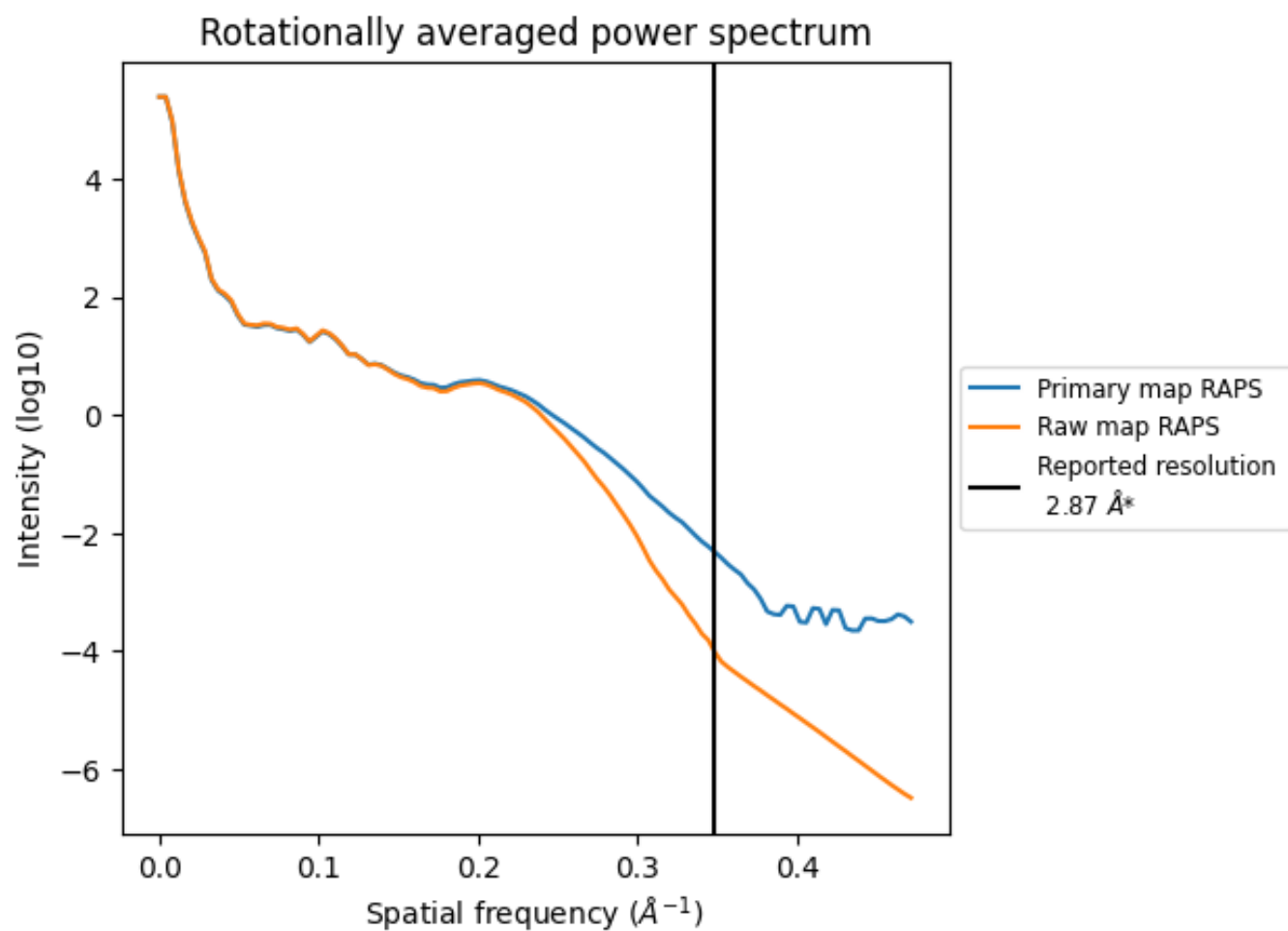
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

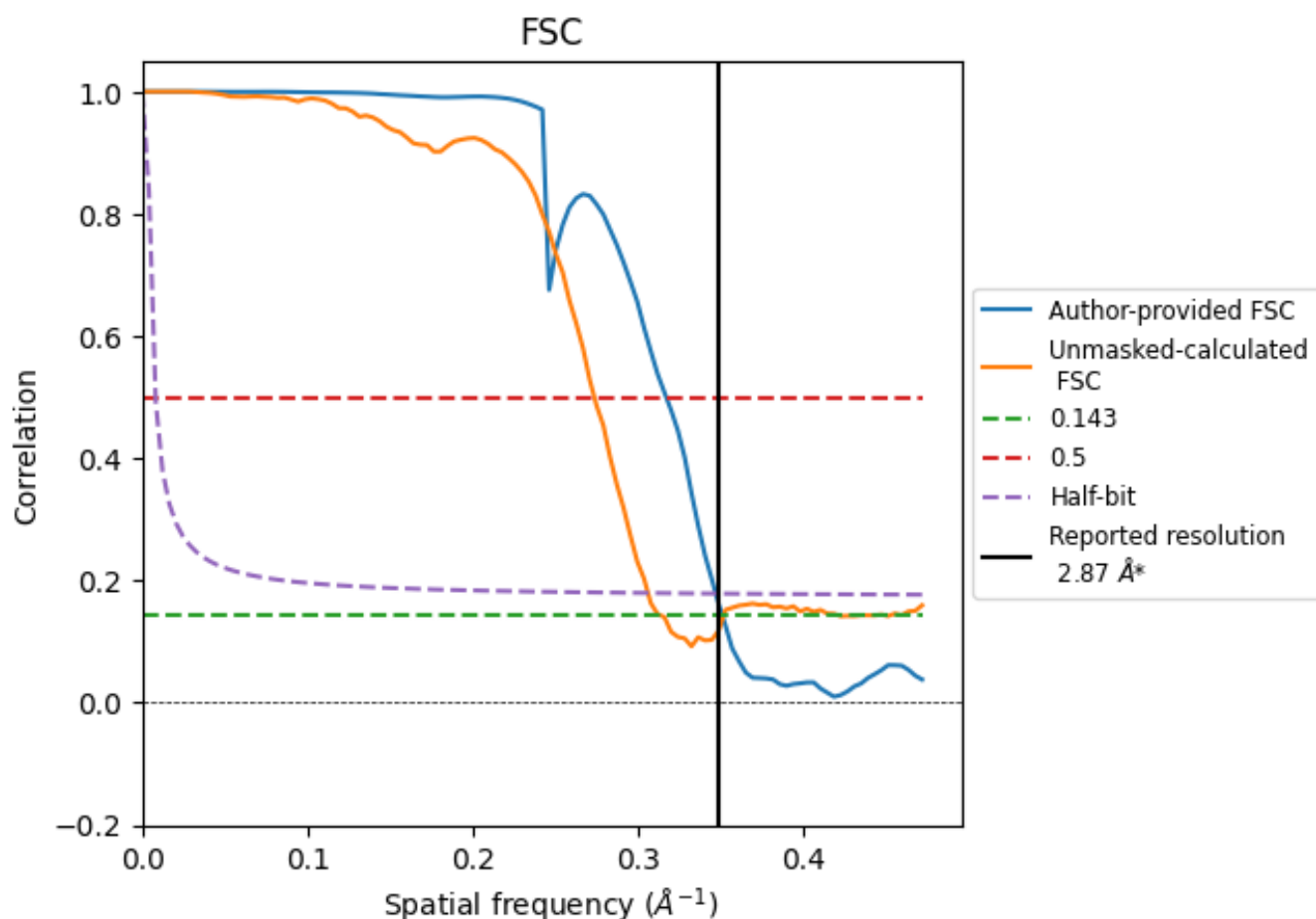


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

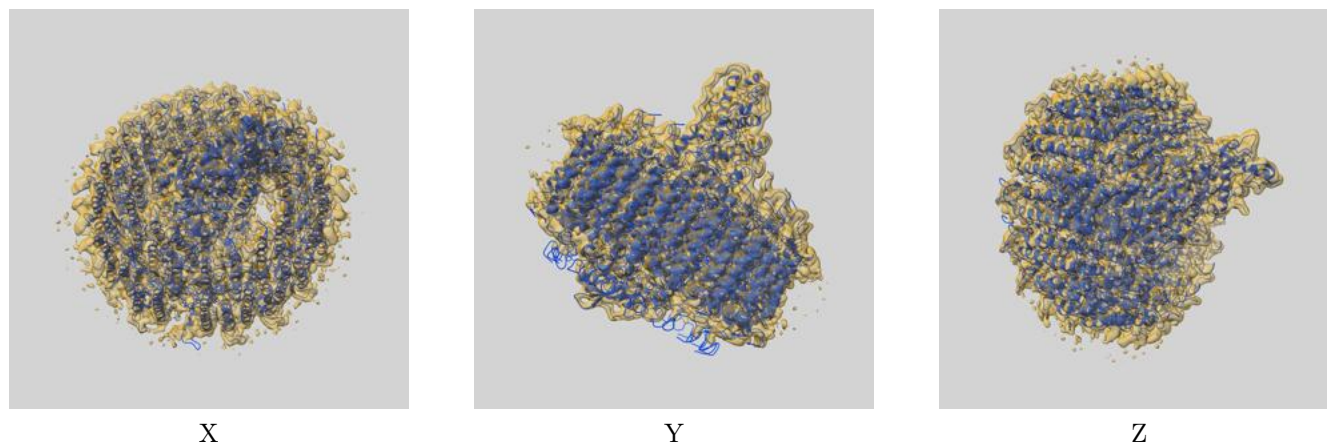
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.85	3.16	2.88
Unmasked-calculated*	3.19	3.66	3.27

*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](#)

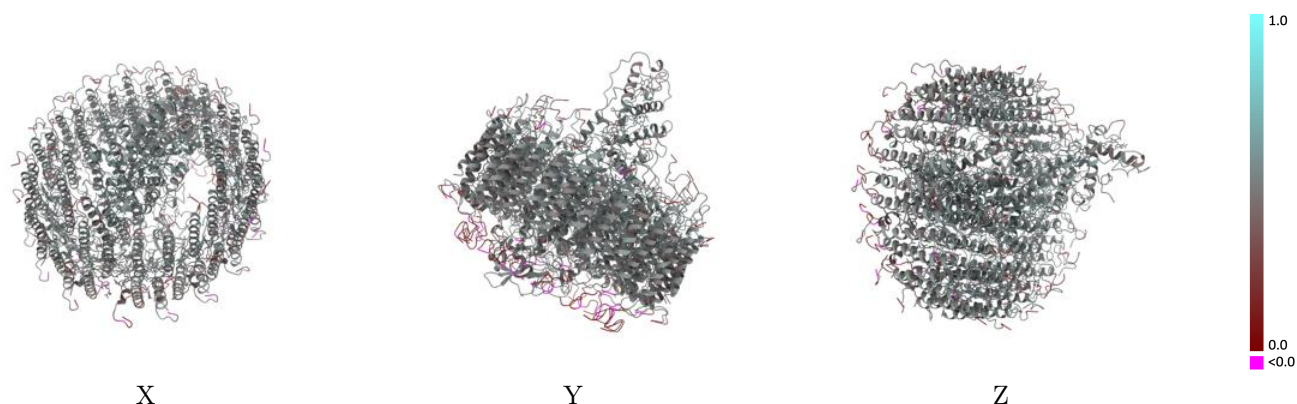
This section contains information regarding the fit between EMDB map EMD-3951 and PDB model 6ET5. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



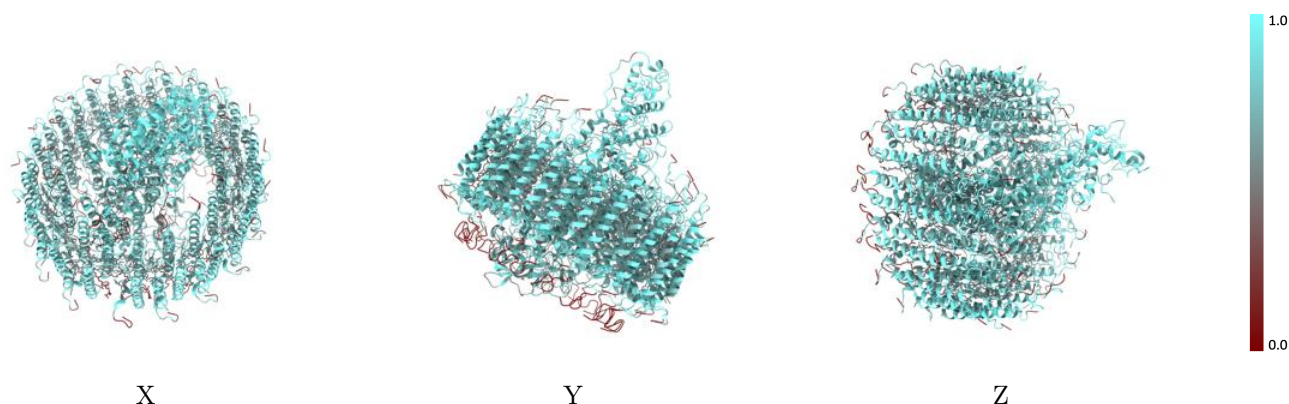
The images above show the 3D surface view of the map at the recommended contour level 0.0156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



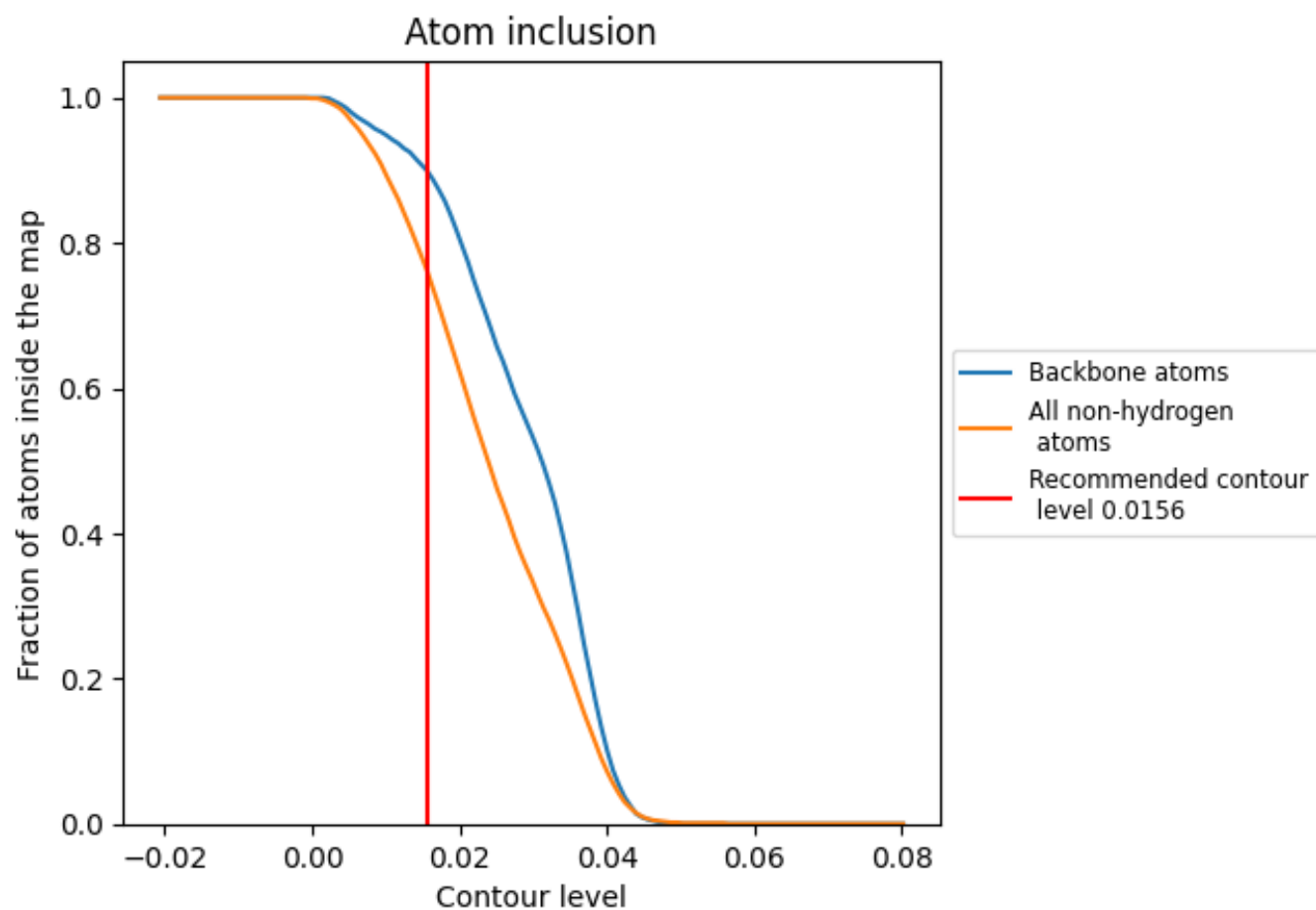
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.7610	 0.4690
1	 0.6930	 0.4460
2	 0.8080	 0.4560
3	 0.7880	 0.4780
4	 0.6890	 0.4410
5	 0.7310	 0.4390
6	 0.7020	 0.4620
7	 0.6530	 0.4290
C	 0.8860	 0.5100
F	 0.7130	 0.4330
G	 0.6440	 0.4030
H	 0.7060	 0.4740
I	 0.7930	 0.4380
K	 0.7640	 0.4710
L	 0.8380	 0.5230
M	 0.8380	 0.5190
N	 0.6910	 0.4340
O	 0.8190	 0.4540
P	 0.7770	 0.4740
Q	 0.6890	 0.4420
R	 0.7820	 0.4430
S	 0.7750	 0.4760
T	 0.7040	 0.4310
U	 0.8080	 0.4460
V	 0.7770	 0.4840
W	 0.6950	 0.4290
X	 0.7980	 0.4380
Y	 0.7840	 0.4810
Z	 0.6930	 0.4240
a	 0.6890	 0.4280
b	 0.7770	 0.4800
c	 0.6820	 0.4320
d	 0.7150	 0.4370
e	 0.7600	 0.4720
f	 0.7020	 0.4280



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Chain	Atom inclusion	Q-score
g	 0.7670	 0.4430
h	 0.7650	 0.4820
i	 0.6930	 0.4330
j	 0.6890	 0.4310
k	 0.7600	 0.4730
l	 0.6800	 0.4370
m	 0.7410	 0.4320
n	 0.7430	 0.4710
o	 0.6700	 0.4190
p	 0.7720	 0.4490
q	 0.7620	 0.4670
r	 0.6820	 0.4260
s	 0.8140	 0.4490
t	 0.7620	 0.4760
u	 0.6990	 0.4280
v	 0.7770	 0.4320
w	 0.7750	 0.4780
x	 0.7080	 0.4330
y	 0.8140	 0.4540
z	 0.7840	 0.4870