



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 10:39 PM EDT

PDB ID : 3WMM / pdb_00003wmm
Title : Crystal structure of the LH1-RC complex from Thermochromatium tepidum
in C2 form
Authors : Niwa, S.; Takeda, K.; Wang-Otomo, Z.-Y.; Miki, K.
Deposited on : 2013-11-22
Resolution : 3.01 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

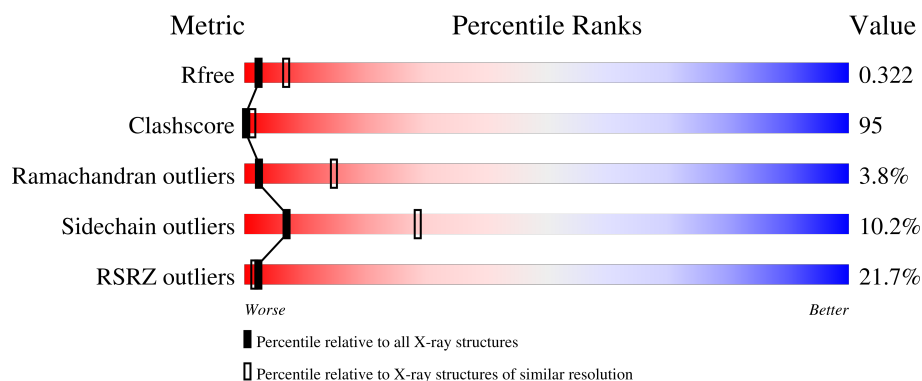
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	404	
2	L	281	
3	M	325	
4	H	259	
5	1	61	

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Mol	Chain	Length	Quality of chain
5	3	61	
5	5	61	
5	7	61	
5	9	61	
5	A	61	
5	D	61	
5	F	61	
5	I	61	
5	K	61	
5	O	61	
5	Q	61	
5	S	61	
5	U	61	
5	W	61	
5	Y	61	
6	0	47	
6	2	47	
6	4	47	
6	6	47	
6	8	47	
6	B	47	
6	E	47	
6	G	47	
6	J	47	
6	N	47	

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Mol	Chain	Length	Quality of chain
6	P	47	
6	R	47	
6	T	47	
6	V	47	
6	X	47	
6	Z	47	

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
12	PO4	H	304	-	-	X	-
15	CRT	2	102	-	-	X	X
15	CRT	4	102	-	-	X	-
15	CRT	8	101	-	-	X	-
15	CRT	A	101	-	-	X	-
15	CRT	A	103	-	-	X	X
15	CRT	B	102	-	-	X	-
15	CRT	G	102	-	-	X	-
15	CRT	J	101	-	-	X	-
15	CRT	N	102	-	-	X	-
15	CRT	P	102	-	-	X	-
15	CRT	R	102	-	-	X	-
15	CRT	T	102	-	-	X	-
15	CRT	V	102	-	-	X	-
15	CRT	W	103	-	-	X	-
15	CRT	X	102	-	-	X	-
17	PEF	H	301	-	X	-	-
9	BCL	0	101	-	-	X	-
9	BCL	3	102	-	-	X	-
9	BCL	4	101	-	-	X	-
9	BCL	5	102	-	-	X	-
9	BCL	7	103	-	-	X	-
9	BCL	9	102	-	-	X	-
9	BCL	A	102	-	-	X	-
9	BCL	B	101	-	-	X	-
9	BCL	D	102	-	-	X	-
9	BCL	E	101	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	BCL	F	102	-	-	X	-
9	BCL	G	101	-	-	X	-
9	BCL	I	102	-	-	X	-
9	BCL	I	103	-	-	X	-
9	BCL	K	102	-	-	X	-
9	BCL	M	401	-	-	X	-
9	BCL	N	101	-	-	X	-
9	BCL	O	102	-	-	X	-
9	BCL	P	101	-	-	X	-
9	BCL	Q	102	-	-	X	-
9	BCL	R	101	-	-	X	-
9	BCL	S	102	-	-	X	-
9	BCL	T	101	-	-	X	-
9	BCL	W	102	-	-	X	-
9	BCL	X	101	-	-	X	-
9	BCL	Y	102	-	-	X	-
9	BCL	Z	101	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 25819 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 C subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	317	Total	C	N	O	S	0	0	0
			2458	1551	430	460	17			

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	0	0
			2231	1501	359	361	10			

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	319	Total	C	N	O	S	0	0	0
			2551	1713	417	410	11			

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	258	Total	C	N	O	S	0	0	0
			1983	1275	339	364	5			

- Molecule 5 is a protein called LH1 alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	D	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	F	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			
5	I	60	Total	C	N	O	S	0	0	0
			473	313	77	81	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	O	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	Q	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	S	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	U	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	W	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	Y	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	1	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	3	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	5	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	7	60	Total 473	C 313	N 77	O 81	S 2	0	0	0
5	9	60	Total 473	C 313	N 77	O 81	S 2	0	0	0

- Molecule 6 is a protein called LH1 beta polypeptide.

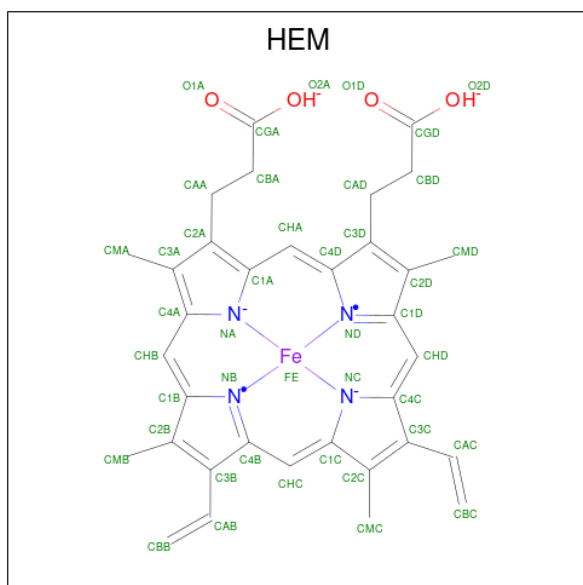
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	E	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	G	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	J	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	N	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	P	40	Total 337	C 228	N 52	O 55	S 2	0	0	0
6	R	40	Total 337	C 228	N 52	O 55	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	T	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	V	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	X	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	Z	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	2	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	4	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	6	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	8	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			
6	0	40	Total	C	N	O	S	0	0	0
			337	228	52	55	2			

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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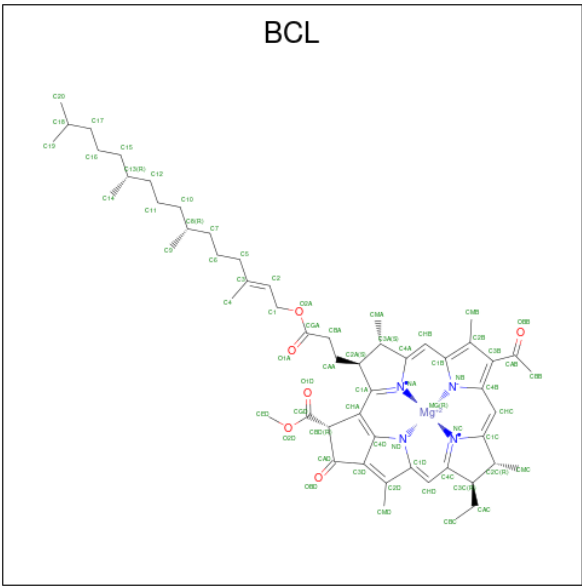
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total 1	Ca 1	0	0
8	A	1	Total 1	Ca 1	0	0
8	D	1	Total 1	Ca 1	0	0
8	F	1	Total 1	Ca 1	0	0
8	I	1	Total 1	Ca 1	0	0
8	K	1	Total 1	Ca 1	0	0
8	O	1	Total 1	Ca 1	0	0
8	Q	1	Total 1	Ca 1	0	0
8	S	1	Total 1	Ca 1	0	0
8	U	1	Total 1	Ca 1	0	0
8	W	1	Total 1	Ca 1	0	0
8	Y	1	Total 1	Ca 1	0	0
8	1	1	Total 1	Ca 1	0	0
8	3	1	Total 1	Ca 1	0	0
8	5	1	Total 1	Ca 1	0	0
8	7	1	Total 1	Ca 1	0	0
8	9	1	Total 1	Ca 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	K	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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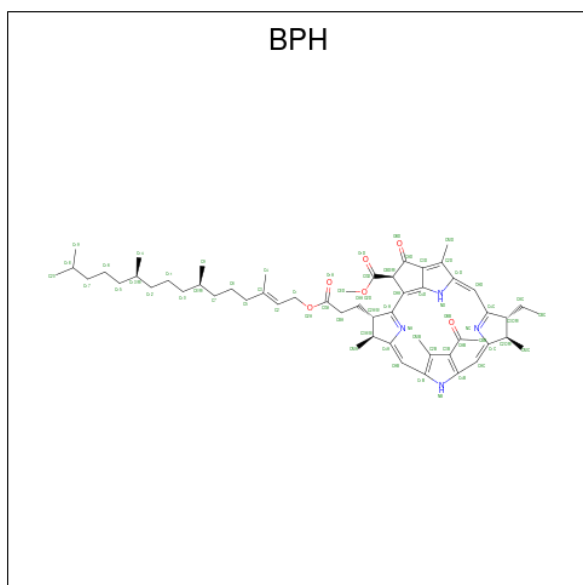
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	N	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	P	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	T	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	U	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	V	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	W	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	X	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	1	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	2	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	3	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	4	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	5	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	6	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	7	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	7	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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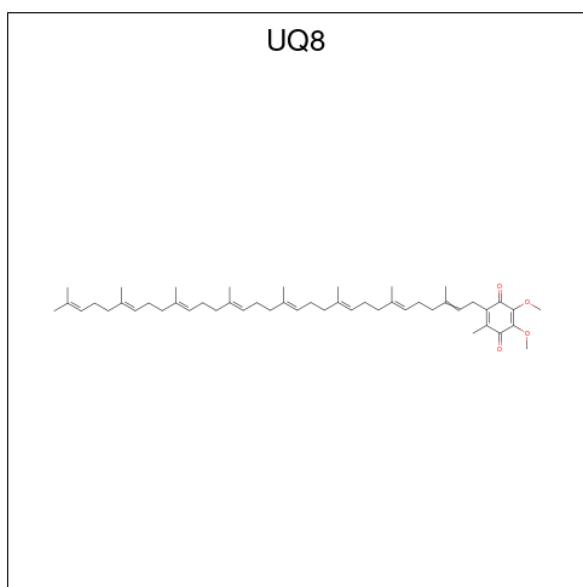
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	9	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	0	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



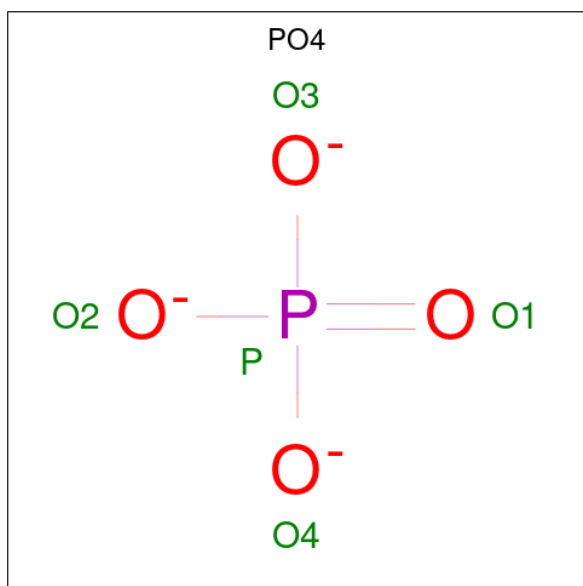
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			53	49	4		

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	O	P	0	0
			5	4	1		
12	M	1	Total	O	P	0	0
			5	4	1		
12	H	1	Total	O	P	0	0
			5	4	1		

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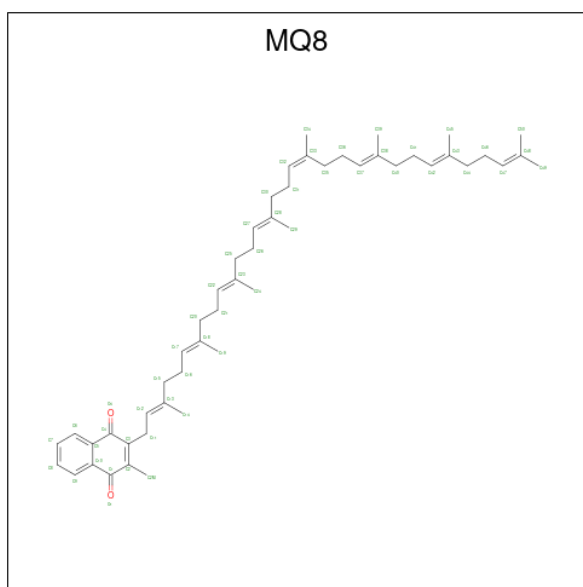
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe).

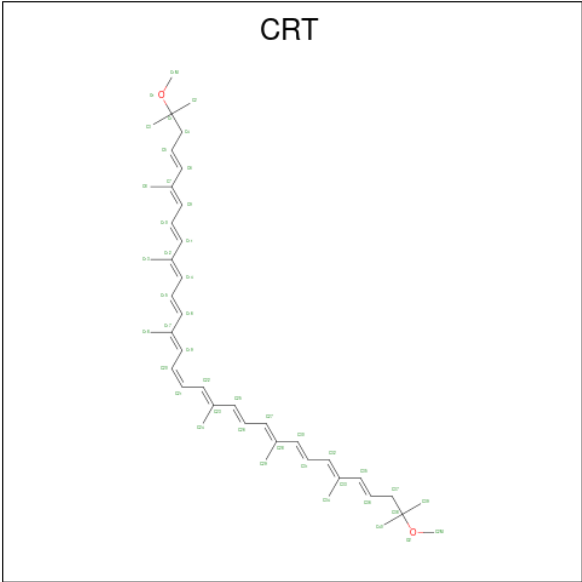
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	Fe	0	0
			1	1		

- Molecule 14 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C₅₁H₇₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			53	51	2		

- Molecule 15 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂).



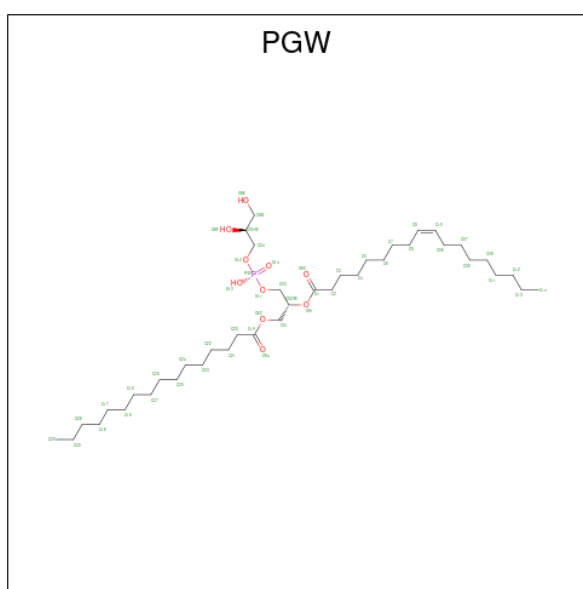
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			44	42	2		
15	A	1	Total	C	O	0	0
			44	42	2		
15	A	1	Total	C	O	0	0
			44	42	2		
15	B	1	Total	C	O	0	0
			44	42	2		
15	G	1	Total	C	O	0	0
			44	42	2		
15	J	1	Total	C	O	0	0
			44	42	2		
15	N	1	Total	C	O	0	0
			44	42	2		
15	P	1	Total	C	O	0	0
			44	42	2		
15	R	1	Total	C	O	0	0
			44	42	2		
15	T	1	Total	C	O	0	0
			44	42	2		
15	V	1	Total	C	O	0	0
			44	42	2		
15	W	1	Total	C	O	0	0
			44	42	2		
15	X	1	Total	C	O	0	0
			44	42	2		
15	2	1	Total	C	O	0	0
			44	42	2		

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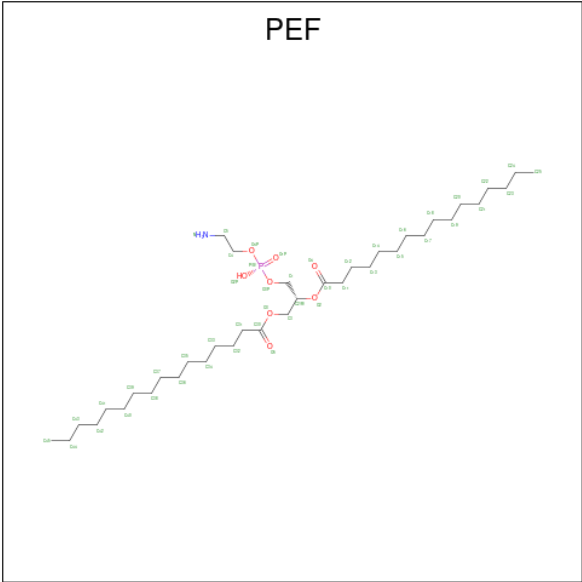
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	3	1	Total	C	O	0	0
			44	42	2		
15	4	1	Total	C	O	0	0
			44	42	2		
15	8	1	Total	C	O	0	0
			44	42	2		

- Molecule 16 is (1R)-2-[[[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	M	1	Total	C	O	P	0	0
			21	10	10	1		
16	H	1	Total	C	O	P	0	0
			21	10	10	1		

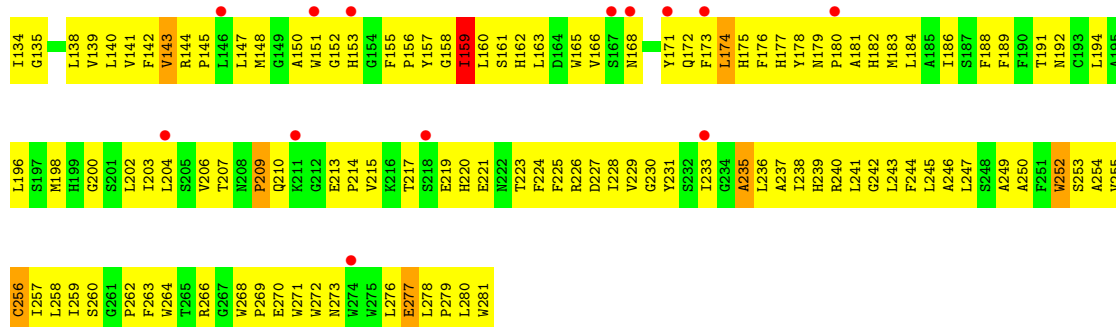
- Molecule 17 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C₃₇H₇₄NO₈P).



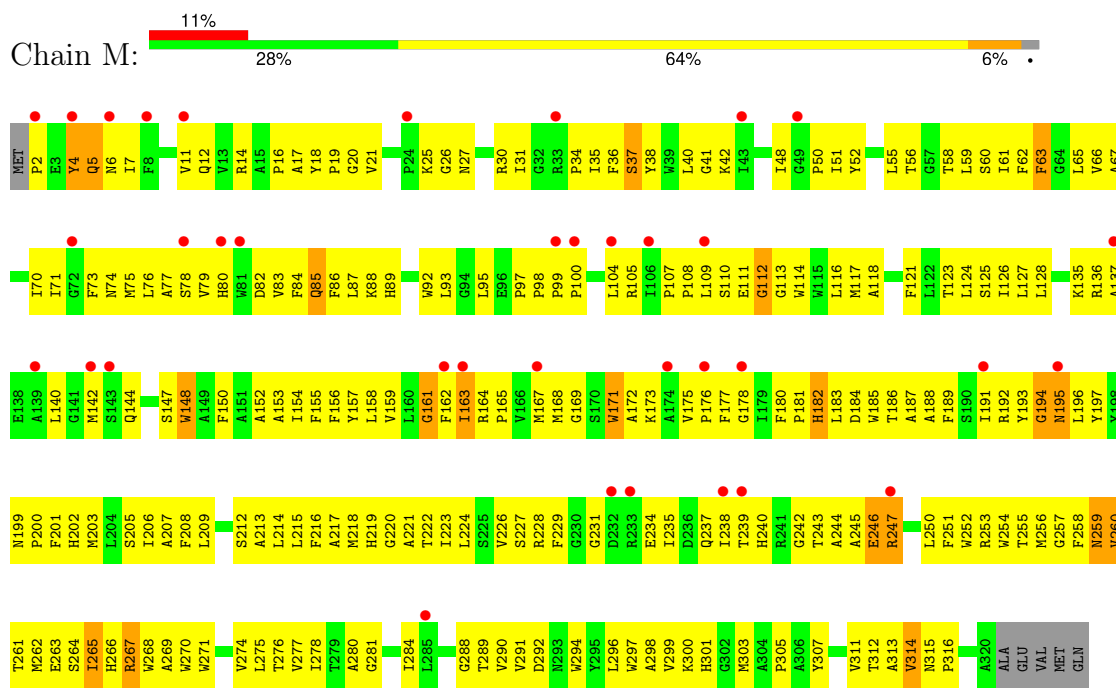
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

- Molecule 18 is water.

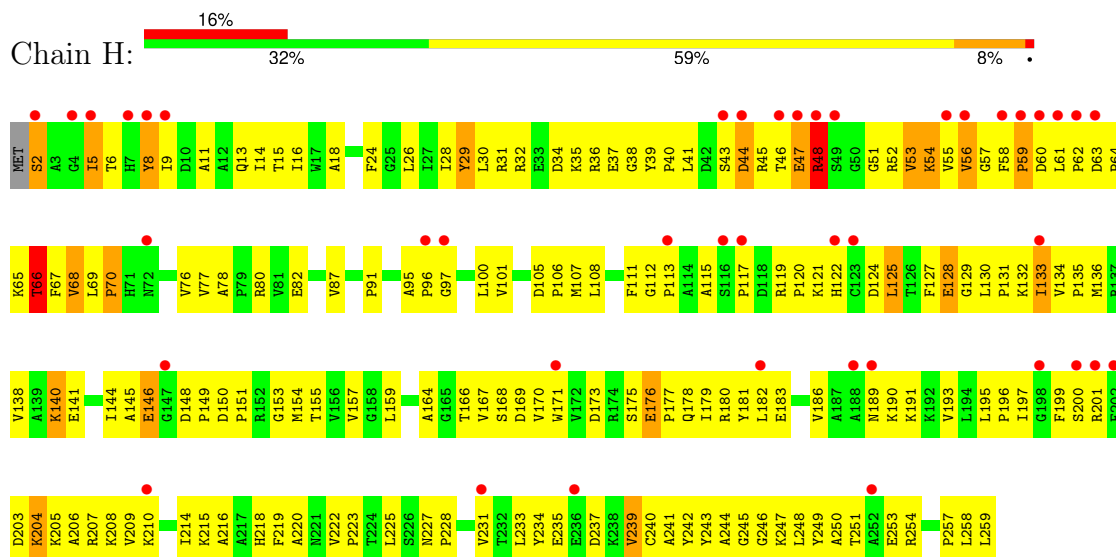
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	4	Total	O	0	0
			4	4		
18	H	1	Total	O	0	0
			1	1		



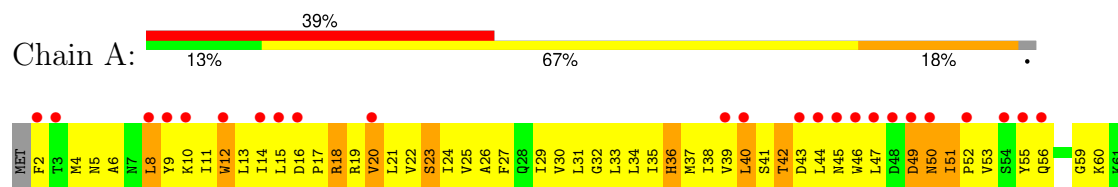
• Molecule 3: Photosynthetic reaction center M subunit



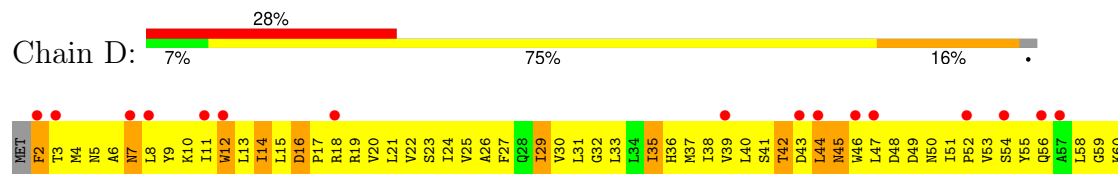
• Molecule 4: Photosynthetic reaction center H subunit



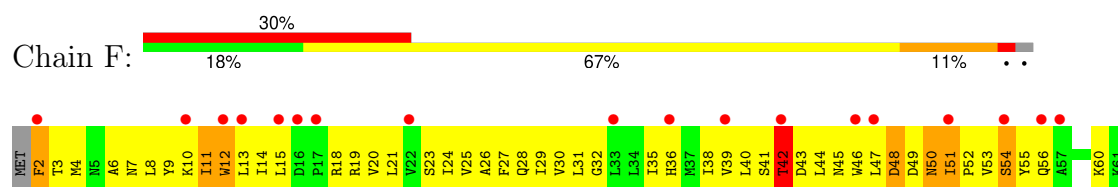
- Molecule 5: LH1 alpha polypeptide



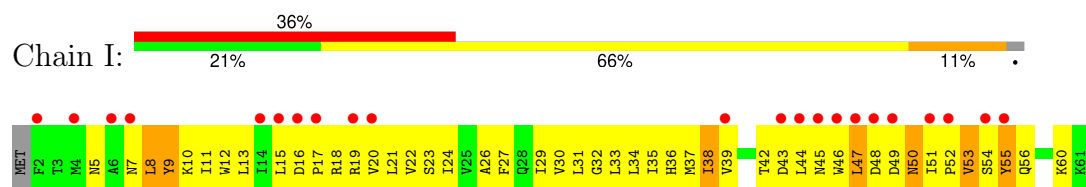
- Molecule 5: LH1 alpha polypeptide



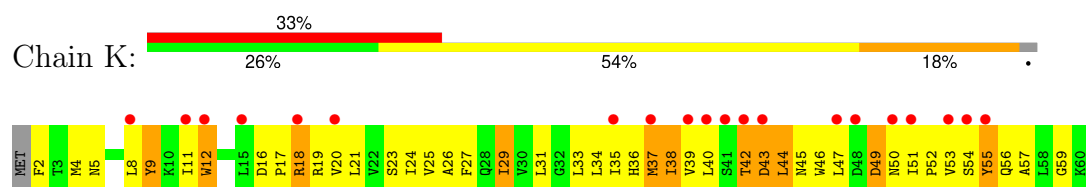
- Molecule 5: LH1 alpha polypeptide



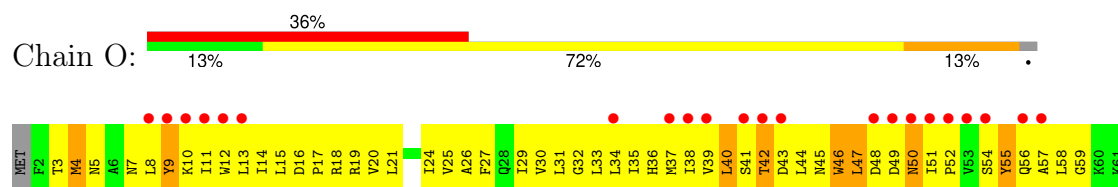
- Molecule 5: LH1 alpha polypeptide



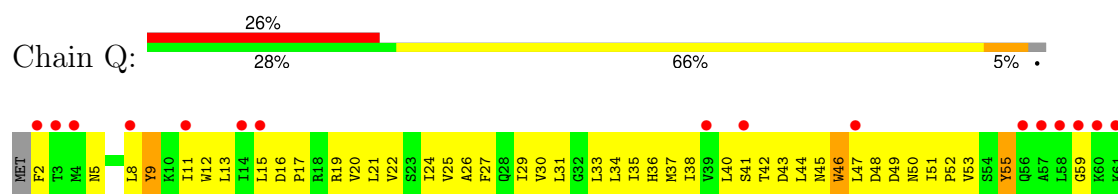
- Molecule 5: LH1 alpha polypeptide



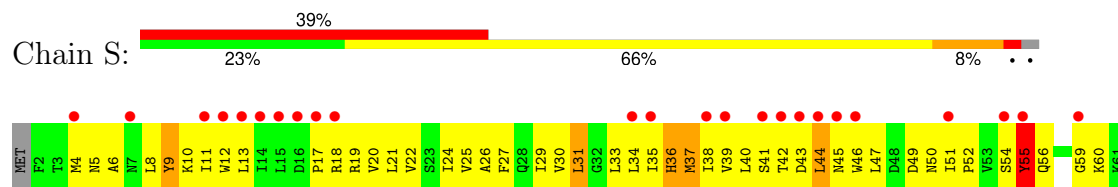
- Molecule 5: LH1 alpha polypeptide



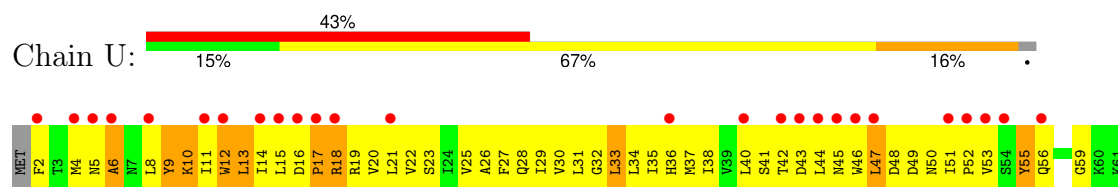
- Molecule 5: LH1 alpha polypeptide



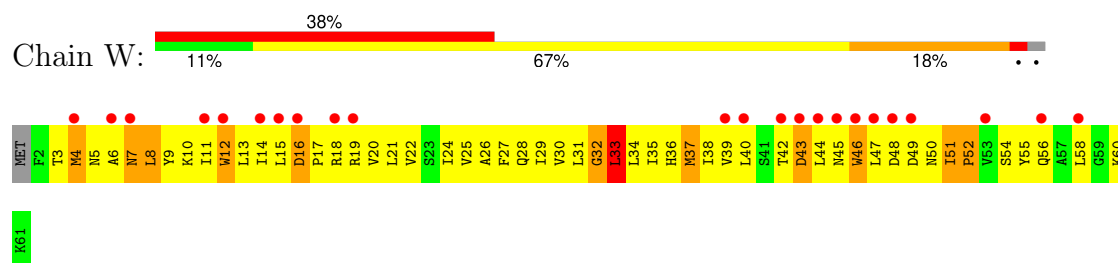
- Molecule 5: LH1 alpha polypeptide



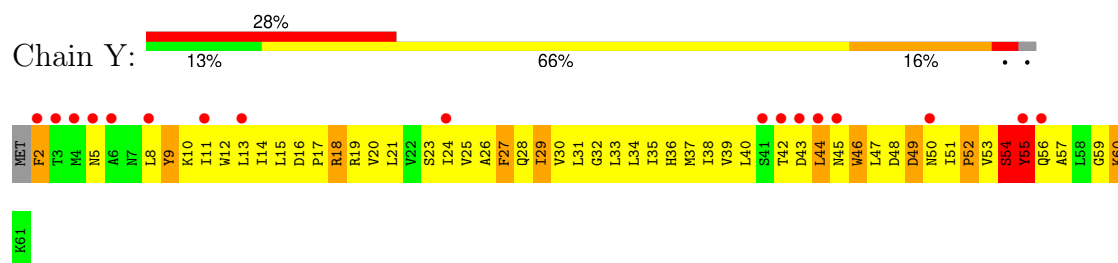
- Molecule 5: LH1 alpha polypeptide



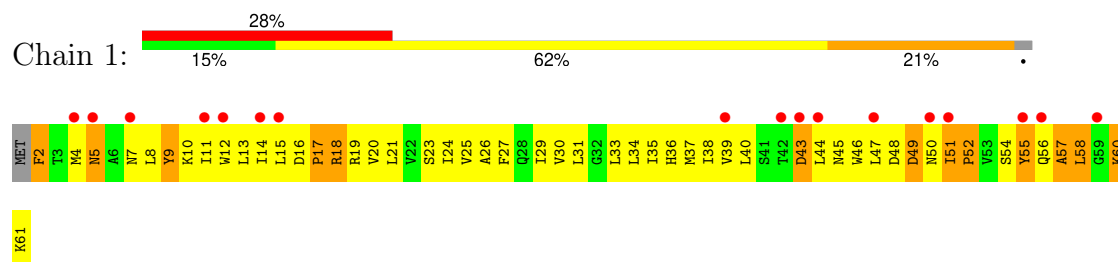
- Molecule 5: LH1 alpha polypeptide



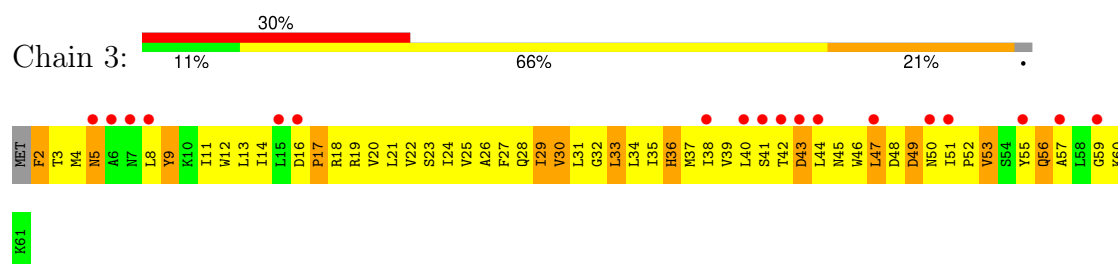
- Molecule 5: LH1 alpha polypeptide



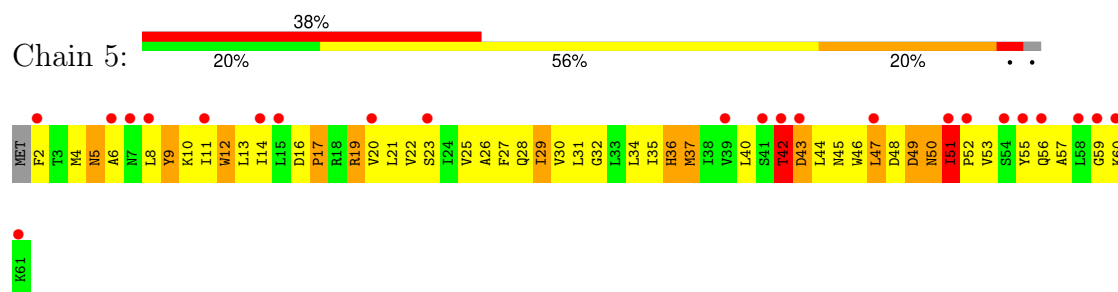
- Molecule 5: LH1 alpha polypeptide



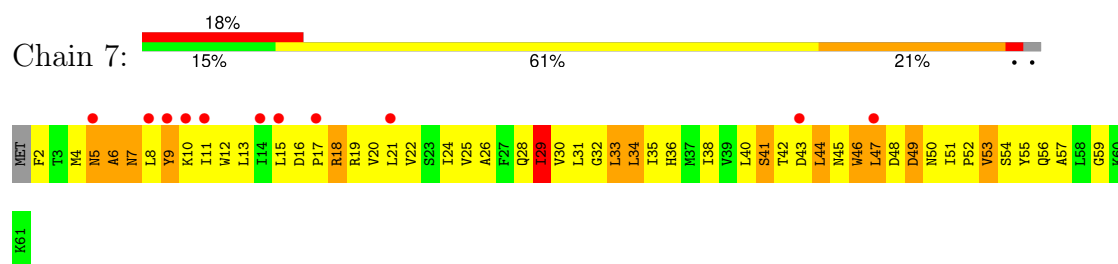
- Molecule 5: LH1 alpha polypeptide



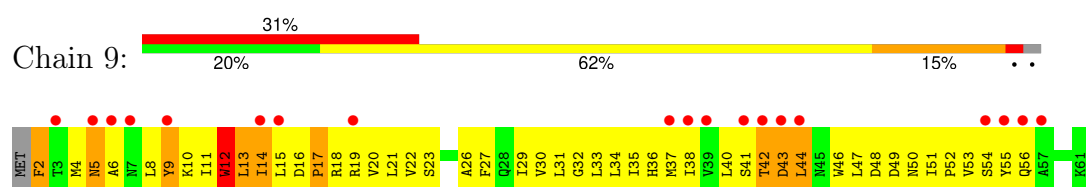
- Molecule 5: LH1 alpha polypeptide



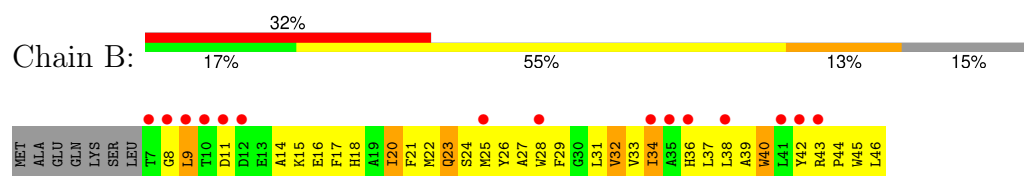
- Molecule 5: LH1 alpha polypeptide



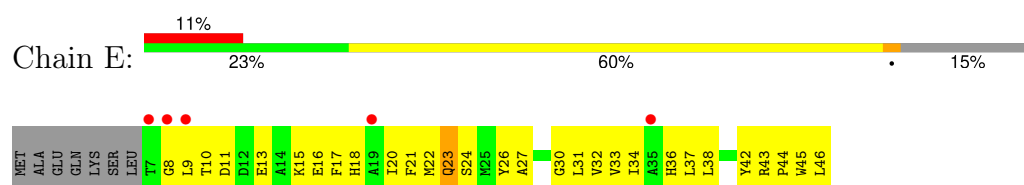
- Molecule 5: LH1 alpha polypeptide



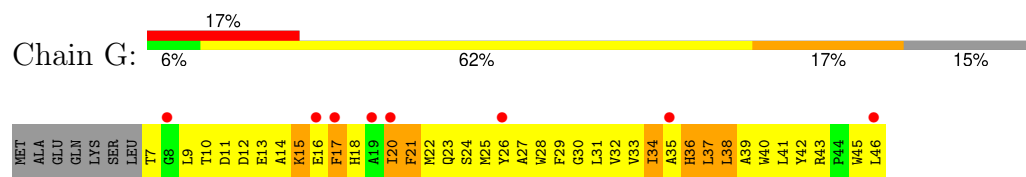
- Molecule 6: LH1 beta polypeptide



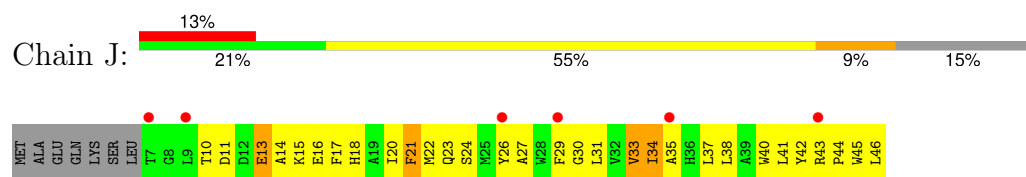
- Molecule 6: LH1 beta polypeptide



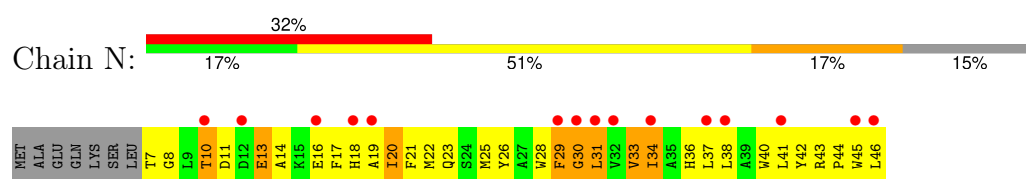
- Molecule 6: LH1 beta polypeptide



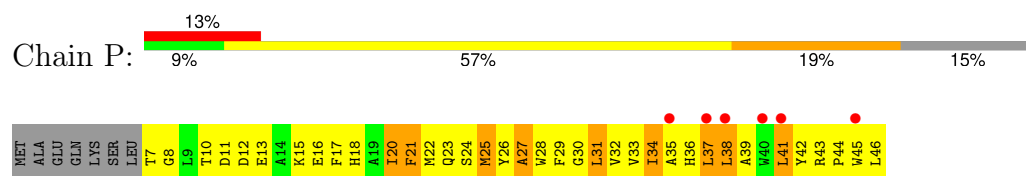
- Molecule 6: LH1 beta polypeptide



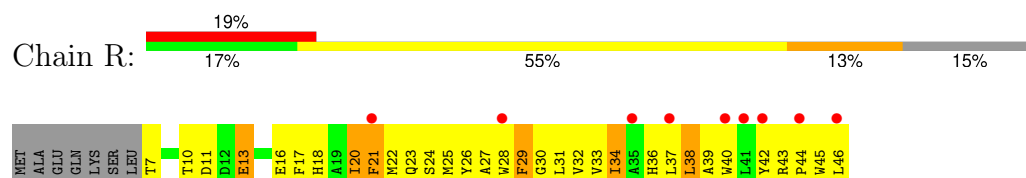
- Molecule 6: LH1 beta polypeptide



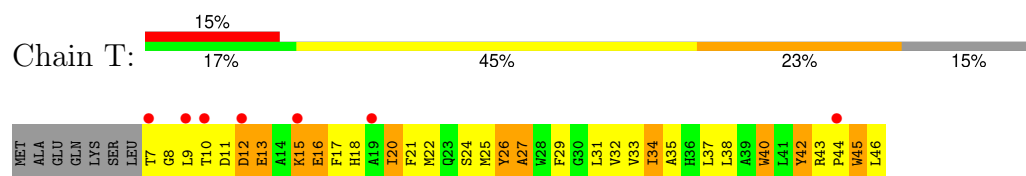
- Molecule 6: LH1 beta polypeptide



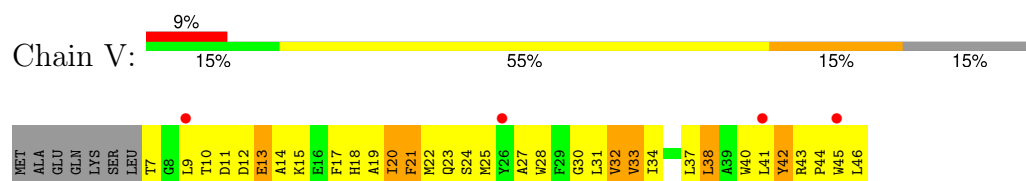
- Molecule 6: LH1 beta polypeptide



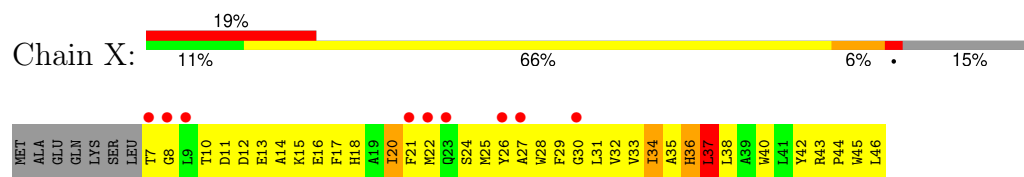
- Molecule 6: LH1 beta polypeptide



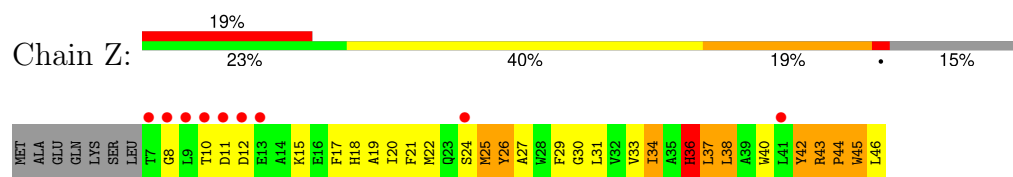
- Molecule 6: LH1 beta polypeptide



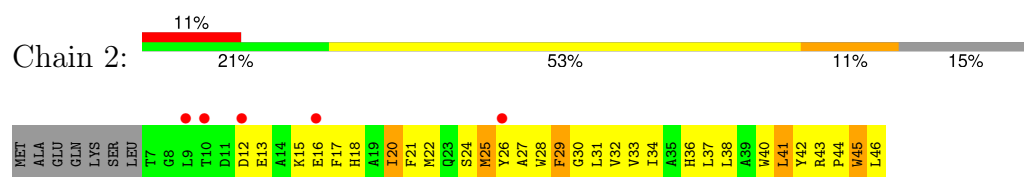
- Molecule 6: LH1 beta polypeptide



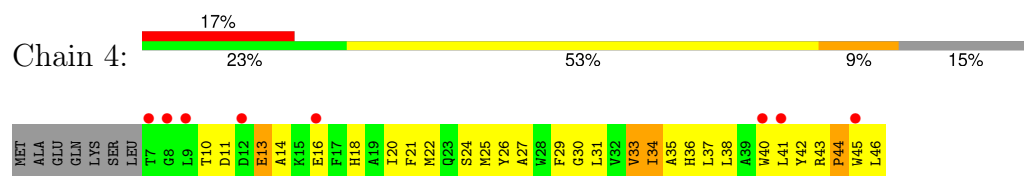
- Molecule 6: LH1 beta polypeptide



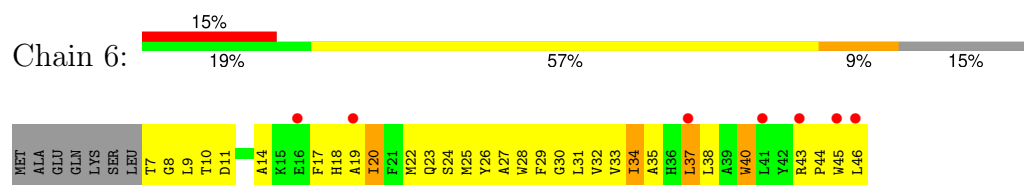
- Molecule 6: LH1 beta polypeptide



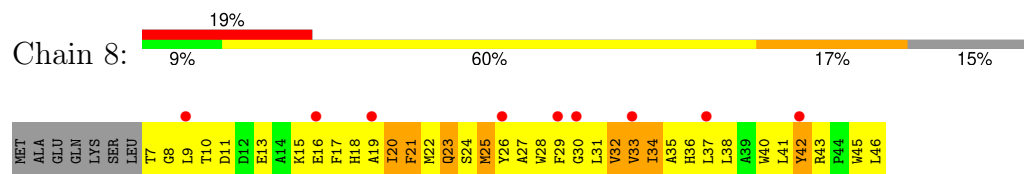
- Molecule 6: LH1 beta polypeptide



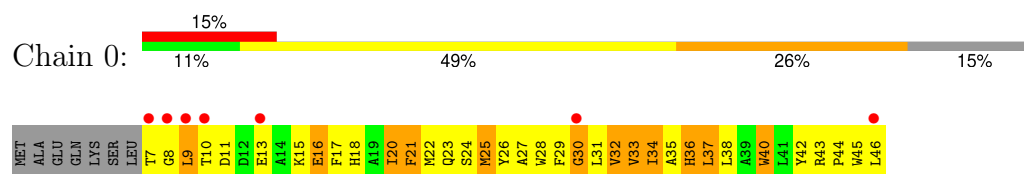
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.34Å 148.24Å 161.79Å 90.00° 117.59° 90.00°	Depositor
Resolution (Å)	47.99 – 3.01 47.99 – 3.01	Depositor EDS
% Data completeness (in resolution range)	83.0 (47.99-3.01) 83.0 (47.99-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.314 , 0.337 0.315 , 0.322	Depositor DCC
R_{free} test set	3884 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	25819	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CRT, PEF, CA, PO4, BCL, BPH, FE, PGW, MQ8, UQ8

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	0.48	0/2528	0.97	13/3451 (0.4%)
2	L	0.37	0/2318	0.86	5/3167 (0.2%)
3	M	0.34	0/2651	0.87	7/3628 (0.2%)
4	H	0.44	1/2038 (0.0%)	0.87	1/2776 (0.0%)
5	1	0.57	0/483	0.95	1/660 (0.2%)
5	3	0.50	0/483	0.99	2/660 (0.3%)
5	5	0.43	0/483	1.07	6/660 (0.9%)
5	7	0.49	0/483	1.04	3/660 (0.5%)
5	9	0.51	0/483	0.96	3/660 (0.5%)
5	A	0.57	0/483	1.13	4/660 (0.6%)
5	D	0.40	0/483	0.93	4/660 (0.6%)
5	F	0.55	0/483	0.96	2/660 (0.3%)
5	I	0.45	0/483	1.00	0/660
5	K	0.50	0/483	0.95	1/660 (0.2%)
5	O	0.46	0/483	1.08	5/660 (0.8%)
5	Q	0.38	0/483	0.94	0/660
5	S	0.40	0/483	0.97	2/660 (0.3%)
5	U	0.43	0/483	1.03	6/660 (0.9%)
5	W	0.49	0/483	0.93	2/660 (0.3%)
5	Y	0.52	1/483 (0.2%)	0.97	2/660 (0.3%)
6	0	0.55	0/350	0.86	1/476 (0.2%)
6	2	0.35	0/350	0.80	0/476
6	4	0.54	0/350	0.90	0/476
6	6	0.38	0/350	0.91	0/476
6	8	0.54	0/350	0.92	0/476
6	B	0.42	0/350	0.79	0/476
6	E	0.40	0/350	0.85	0/476
6	G	0.52	0/350	1.03	2/476 (0.4%)
6	J	0.47	0/350	0.83	0/476
6	N	0.46	0/350	0.95	1/476 (0.2%)
6	P	0.49	0/350	0.87	1/476 (0.2%)
6	R	0.43	0/350	0.85	0/476

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	T	0.40	0/350	0.95	2/476 (0.4%)
6	V	0.48	0/350	1.08	2/476 (0.4%)
6	X	0.44	0/350	0.86	0/476
6	Z	0.40	0/350	0.96	4/476 (0.8%)
All	All	0.45	2/22863 (0.0%)	0.93	82/31198 (0.3%)

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
6	X	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	66	THR	C-O	-5.33	1.18	1.24
5	Y	54	SER	C-N	-5.32	1.27	1.33

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	5	GLN	N-CA-C	-12.08	94.89	111.56
2	L	98	ILE	CB-CA-C	-8.19	101.39	111.88
6	N	30	GLY	N-CA-C	-7.91	103.33	112.50
5	K	42	THR	N-CA-C	7.80	119.48	110.97
3	M	163	ILE	N-CA-C	7.67	118.44	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	X	37	LEU	Mainchain

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	2458	0	2377	319	0
2	L	2231	0	2192	363	0
3	M	2551	0	2526	423	0
4	H	1983	0	1981	337	0
5	1	473	0	476	157	0
5	3	473	0	476	150	0
5	5	473	0	476	152	0
5	7	473	0	476	153	0
5	9	473	0	476	147	0
5	A	473	0	476	206	0
5	D	473	0	476	157	0
5	F	473	0	476	168	0
5	I	473	0	476	157	0
5	K	473	0	476	133	0
5	O	473	0	476	141	0
5	Q	473	0	476	122	0
5	S	473	0	476	125	0
5	U	473	0	476	147	0
5	W	473	0	476	191	0
5	Y	473	0	476	165	0
6	0	337	0	323	82	0
6	2	337	0	323	91	0
6	4	337	0	323	118	0
6	6	337	0	323	59	0
6	8	337	0	323	112	0
6	B	337	0	323	82	0
6	E	337	0	323	80	0
6	G	337	0	323	95	0
6	J	337	0	323	92	0
6	N	337	0	323	76	0
6	P	337	0	323	126	0
6	R	337	0	323	82	0
6	T	337	0	323	74	0
6	V	337	0	323	108	0
6	X	337	0	323	100	0
6	Z	337	0	323	77	0
7	C	172	0	120	17	0
8	1	1	0	0	0	0
8	3	1	0	0	0	0
8	5	1	0	0	0	0
8	7	1	0	0	0	0
8	9	1	0	0	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	S	1	0	0	0	0
8	U	1	0	0	0	0
8	W	1	0	0	0	0
8	Y	1	0	0	0	0
9	0	66	0	74	28	0
9	1	66	0	74	15	0
9	2	66	0	74	15	0
9	3	66	0	74	24	0
9	4	66	0	74	30	0
9	5	66	0	74	21	0
9	6	66	0	74	19	0
9	7	132	0	148	41	0
9	9	66	0	74	29	0
9	A	66	0	74	35	0
9	B	66	0	74	34	0
9	D	66	0	74	21	0
9	E	66	0	74	30	0
9	F	66	0	74	39	0
9	G	66	0	74	35	0
9	I	132	0	148	50	0
9	K	66	0	74	25	0
9	L	132	0	148	20	0
9	M	132	0	148	42	0
9	N	66	0	74	23	0
9	O	66	0	74	51	0
9	P	66	0	74	27	0
9	Q	66	0	74	22	0
9	R	66	0	74	27	0
9	S	66	0	74	24	0
9	T	66	0	74	22	0
9	U	66	0	74	18	0
9	V	66	0	74	8	0
9	W	66	0	74	33	0
9	X	66	0	74	36	0
9	Y	66	0	74	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Z	66	0	74	24	0
10	L	65	0	76	8	0
10	M	65	0	76	18	0
11	L	53	0	74	13	0
12	H	10	0	0	4	0
12	L	5	0	0	0	0
12	M	5	0	0	1	0
13	M	1	0	0	0	0
14	M	53	0	72	11	0
15	2	44	0	60	39	0
15	3	44	0	60	20	0
15	4	44	0	60	68	0
15	8	44	0	60	80	0
15	A	88	0	120	72	0
15	B	44	0	60	34	0
15	G	44	0	60	28	0
15	J	44	0	60	35	0
15	M	44	0	60	12	0
15	N	44	0	60	52	0
15	P	44	0	60	62	0
15	R	44	0	60	34	0
15	T	44	0	58	22	0
15	V	44	0	60	65	0
15	W	44	0	60	30	0
15	X	44	0	60	27	0
16	H	21	0	12	7	0
16	M	21	0	12	16	0
17	H	19	0	11	18	0
18	H	1	0	0	0	0
18	L	4	0	0	3	0
All	All	25819	0	25995	4917	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 95.

The worst 5 of 4917 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)
5:W:27:PHE:CE2	5:Y:29:ILE:HD11	1.30	1.64
5:U:27:PHE:CE2	5:W:29:ILE:HD11	1.30	1.63
6:V:21:PHE:CD2	15:V:102:CRT:H14	1.37	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:10:LYS:HD2	15:8:101:CRT:C2	1.27	1.58
6:P:17:PHE:CD1	15:P:102:CRT:H6	1.39	1.57

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	315/404 (78%)	230 (73%)	79 (25%)	6 (2%)	6	30
2	L	278/281 (99%)	219 (79%)	51 (18%)	8 (3%)	3	20
3	M	317/325 (98%)	254 (80%)	60 (19%)	3 (1%)	14	48
4	H	256/259 (99%)	204 (80%)	43 (17%)	9 (4%)	3	16
5	1	58/61 (95%)	34 (59%)	15 (26%)	9 (16%)	0	0
5	3	58/61 (95%)	38 (66%)	15 (26%)	5 (9%)	0	3
5	5	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	1
5	7	58/61 (95%)	37 (64%)	15 (26%)	6 (10%)	0	2
5	9	58/61 (95%)	39 (67%)	13 (22%)	6 (10%)	0	2
5	A	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	7	32
5	D	58/61 (95%)	40 (69%)	18 (31%)	0	100	100
5	F	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	1	9
5	I	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	1	9
5	K	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	1	9
5	O	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	7	32
5	Q	58/61 (95%)	42 (72%)	14 (24%)	2 (3%)	3	17
5	S	58/61 (95%)	38 (66%)	17 (29%)	3 (5%)	1	9
5	U	58/61 (95%)	34 (59%)	23 (40%)	1 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	W	58/61 (95%)	41 (71%)	12 (21%)	5 (9%)	0	3
5	Y	58/61 (95%)	39 (67%)	12 (21%)	7 (12%)	0	1
6	0	38/47 (81%)	29 (76%)	9 (24%)	0	100	100
6	2	38/47 (81%)	28 (74%)	8 (21%)	2 (5%)	1	9
6	4	38/47 (81%)	31 (82%)	6 (16%)	1 (3%)	4	23
6	6	38/47 (81%)	35 (92%)	3 (8%)	0	100	100
6	8	38/47 (81%)	27 (71%)	10 (26%)	1 (3%)	4	23
6	B	38/47 (81%)	33 (87%)	5 (13%)	0	100	100
6	E	38/47 (81%)	33 (87%)	5 (13%)	0	100	100
6	G	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	J	38/47 (81%)	29 (76%)	9 (24%)	0	100	100
6	N	38/47 (81%)	33 (87%)	4 (10%)	1 (3%)	4	23
6	P	38/47 (81%)	25 (66%)	12 (32%)	1 (3%)	4	23
6	R	38/47 (81%)	31 (82%)	7 (18%)	0	100	100
6	T	38/47 (81%)	30 (79%)	5 (13%)	3 (8%)	1	3
6	V	38/47 (81%)	35 (92%)	2 (5%)	1 (3%)	4	23
6	X	38/47 (81%)	32 (84%)	6 (16%)	0	100	100
6	Z	38/47 (81%)	28 (74%)	6 (16%)	4 (10%)	0	2
All	All	2702/2997 (90%)	2030 (75%)	570 (21%)	102 (4%)	2	15

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	235	ALA
4	H	53	VAL
5	I	50	ASN
5	I	53	VAL
5	Q	46	TRP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	265/317 (84%)	250 (94%)	15 (6%)	18	52
2	L	228/229 (100%)	222 (97%)	6 (3%)	40	72
3	M	256/261 (98%)	242 (94%)	14 (6%)	19	53
4	H	210/211 (100%)	195 (93%)	15 (7%)	13	43
5	1	50/56 (89%)	47 (94%)	3 (6%)	17	50
5	3	50/56 (89%)	42 (84%)	8 (16%)	2	12
5	5	50/56 (89%)	46 (92%)	4 (8%)	11	38
5	7	50/56 (89%)	42 (84%)	8 (16%)	2	12
5	9	50/56 (89%)	44 (88%)	6 (12%)	5	22
5	A	50/56 (89%)	43 (86%)	7 (14%)	3	16
5	D	50/56 (89%)	43 (86%)	7 (14%)	3	16
5	F	50/56 (89%)	46 (92%)	4 (8%)	11	38
5	I	50/56 (89%)	45 (90%)	5 (10%)	7	29
5	K	50/56 (89%)	42 (84%)	8 (16%)	2	12
5	O	50/56 (89%)	44 (88%)	6 (12%)	5	22
5	Q	50/56 (89%)	48 (96%)	2 (4%)	28	62
5	S	50/56 (89%)	45 (90%)	5 (10%)	7	29
5	U	50/56 (89%)	44 (88%)	6 (12%)	5	22
5	W	50/56 (89%)	43 (86%)	7 (14%)	3	16
5	Y	50/56 (89%)	44 (88%)	6 (12%)	5	22
6	0	33/39 (85%)	22 (67%)	11 (33%)	0	1
6	2	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	4	33/39 (85%)	30 (91%)	3 (9%)	9	33
6	6	33/39 (85%)	29 (88%)	4 (12%)	5	21
6	8	33/39 (85%)	25 (76%)	8 (24%)	1	4
6	B	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	E	33/39 (85%)	32 (97%)	1 (3%)	36	69
6	G	33/39 (85%)	25 (76%)	8 (24%)	1	4
6	J	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	N	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	P	33/39 (85%)	26 (79%)	7 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	R	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	T	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	V	33/39 (85%)	27 (82%)	6 (18%)	2	9
6	X	33/39 (85%)	28 (85%)	5 (15%)	3	14
6	Z	33/39 (85%)	29 (88%)	4 (12%)	5	21
All	All	2287/2538 (90%)	2054 (90%)	233 (10%)	7	29

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	P	25	MET
5	9	56	GLN
5	U	47	LEU
5	9	19	ARG
6	6	40	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
6	4	23	GLN
5	5	56	GLN
5	9	45	ASN
3	M	259	ASN
3	M	237	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 86 ligands modelled in this entry, 18 are monoatomic - leaving 68 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	BCL	F	102	5	69,74,74	1.41	10 (14%)	79,115,115	2.24	21 (26%)
15	CRT	N	102	-	43,43,43	1.51	9 (20%)	48,54,54	2.40	16 (33%)
9	BCL	S	102	5	69,74,74	1.40	14 (20%)	79,115,115	2.19	17 (21%)
9	BCL	R	101	6	69,74,74	1.50	12 (17%)	79,115,115	2.30	21 (26%)
9	BCL	E	101	6	69,74,74	1.53	12 (17%)	79,115,115	2.28	24 (30%)
9	BCL	I	103	6	69,74,74	1.48	12 (17%)	79,115,115	2.23	22 (27%)
15	CRT	B	102	-	43,43,43	1.42	5 (11%)	48,54,54	2.48	19 (39%)
15	CRT	W	103	-	43,43,43	1.69	8 (18%)	48,54,54	2.29	18 (37%)
9	BCL	L	303	2	69,74,74	1.31	9 (13%)	79,115,115	2.26	22 (27%)
9	BCL	L	301	2	69,74,74	1.34	9 (13%)	79,115,115	2.32	23 (29%)
17	PEF	H	301	-	18,18,46	3.18	7 (38%)	21,23,51	2.02	6 (28%)
9	BCL	6	101	6	69,74,74	1.38	11 (15%)	79,115,115	2.27	23 (29%)
15	CRT	8	101	-	43,43,43	1.40	4 (9%)	48,54,54	1.92	14 (29%)
16	PGW	H	302	-	20,20,50	0.93	1 (5%)	23,26,56	1.68	5 (21%)
10	BPH	M	403	-	59,70,70	1.62	4 (6%)	59,101,101	1.72	8 (13%)
9	BCL	4	101	6	69,74,74	1.45	12 (17%)	79,115,115	2.30	21 (26%)
9	BCL	D	102	5	69,74,74	1.40	11 (15%)	79,115,115	2.29	20 (25%)
9	BCL	U	102	5	69,74,74	1.47	11 (15%)	79,115,115	2.27	21 (26%)
9	BCL	G	101	6	69,74,74	1.37	9 (13%)	79,115,115	2.30	23 (29%)
9	BCL	I	102	5	69,74,74	1.40	11 (15%)	79,115,115	2.28	23 (29%)
9	BCL	Q	102	5	69,74,74	1.35	12 (17%)	79,115,115	2.25	19 (24%)
15	CRT	J	101	-	43,43,43	1.83	12 (27%)	48,54,54	2.89	21 (43%)
15	CRT	X	102	-	43,43,43	2.47	14 (32%)	48,54,54	2.66	17 (35%)
15	CRT	V	102	-	43,43,43	1.57	8 (18%)	48,54,54	2.77	19 (39%)
9	BCL	A	102	5	69,74,74	1.30	10 (14%)	79,115,115	2.23	19 (24%)
15	CRT	P	102	-	43,43,43	2.03	16 (37%)	48,54,54	2.78	17 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	W	102	5	69,74,74	1.32	9 (13%)	79,115,115	2.26	20 (25%)
15	CRT	M	406	-	43,43,43	1.38	3 (6%)	48,54,54	1.66	13 (27%)
9	BCL	1	102	5	69,74,74	1.39	11 (15%)	79,115,115	2.21	19 (24%)
9	BCL	P	101	6	69,74,74	1.40	11 (15%)	79,115,115	2.25	23 (29%)
9	BCL	9	102	5	69,74,74	1.36	11 (15%)	79,115,115	2.24	21 (26%)
9	BCL	5	102	5	69,74,74	1.38	10 (14%)	79,115,115	2.22	21 (26%)
9	BCL	T	101	6	69,74,74	1.42	11 (15%)	79,115,115	2.27	25 (31%)
9	BCL	M	401	3	69,74,74	1.46	11 (15%)	79,115,115	2.21	22 (27%)
15	CRT	3	103	-	43,43,43	1.72	13 (30%)	48,54,54	2.10	14 (29%)
7	HEM	C	503	1	50,50,50	1.92	13 (26%)	67,82,82	1.34	9 (13%)
9	BCL	M	402	3	69,74,74	1.40	10 (14%)	79,115,115	2.23	20 (25%)
9	BCL	X	101	6	69,74,74	1.46	12 (17%)	79,115,115	2.31	25 (31%)
9	BCL	Z	101	6	69,74,74	1.44	15 (21%)	79,115,115	2.26	21 (26%)
10	BPH	L	302	-	59,70,70	1.64	7 (11%)	59,101,101	1.80	8 (13%)
12	PO4	H	304	-	4,4,4	1.68	0	6,6,6	0.44	0
15	CRT	T	102	-	43,43,43	1.85	9 (20%)	48,54,54	3.37	18 (37%)
15	CRT	4	102	-	43,43,43	1.43	6 (13%)	48,54,54	1.99	17 (35%)
12	PO4	H	303	-	4,4,4	1.74	0	6,6,6	0.46	0
16	PGW	M	407	-	20,20,50	0.94	1 (5%)	23,26,56	1.68	5 (21%)
7	HEM	C	502	1	50,50,50	1.99	17 (34%)	67,82,82	1.39	8 (11%)
7	HEM	C	504	1	50,50,50	2.07	14 (28%)	67,82,82	1.33	8 (11%)
7	HEM	C	501	1	50,50,50	1.91	19 (38%)	67,82,82	1.39	8 (11%)
15	CRT	A	103	-	43,43,43	1.55	9 (20%)	48,54,54	1.89	13 (27%)
9	BCL	N	101	6	69,74,74	1.40	10 (14%)	79,115,115	2.29	23 (29%)
9	BCL	7	103	6	69,74,74	1.42	12 (17%)	79,115,115	2.40	26 (32%)
9	BCL	O	102	5	69,74,74	1.32	10 (14%)	79,115,115	2.19	23 (29%)
9	BCL	V	101	6	69,74,74	1.42	11 (15%)	79,115,115	2.23	24 (30%)
14	MQ8	M	405	-	54,54,54	0.94	2 (3%)	67,69,69	1.64	17 (25%)
12	PO4	L	305	-	4,4,4	1.73	0	6,6,6	0.46	0
15	CRT	A	101	-	43,43,43	2.00	13 (30%)	48,54,54	3.49	20 (41%)
15	CRT	2	102	-	43,43,43	1.33	7 (16%)	48,54,54	2.12	19 (39%)
9	BCL	K	102	5	69,74,74	1.39	12 (17%)	79,115,115	2.26	21 (26%)
9	BCL	B	101	6	69,74,74	1.37	10 (14%)	79,115,115	2.24	22 (27%)
9	BCL	Y	102	5	69,74,74	1.37	11 (15%)	79,115,115	2.18	20 (25%)
11	UQ8	L	304	-	53,53,53	1.48	4 (7%)	66,67,67	1.80	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCL	3	102	5	69,74,74	1.37	10 (14%)	79,115,115	2.29	21 (26%)
12	PO4	M	408	-	4,4,4	1.82	1 (25%)	6,6,6	0.47	0
9	BCL	2	101	6	69,74,74	1.52	14 (20%)	79,115,115	2.20	22 (27%)
9	BCL	0	101	6	69,74,74	1.40	11 (15%)	79,115,115	2.31	23 (29%)
9	BCL	7	102	5	69,74,74	1.33	9 (13%)	79,115,115	2.25	20 (25%)
15	CRT	R	102	-	43,43,43	1.49	7 (16%)	48,54,54	3.23	18 (37%)
15	CRT	G	102	-	43,43,43	1.39	7 (16%)	48,54,54	2.02	16 (33%)

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	BCL	F	102	5	-	18/41/137/137	-
15	CRT	N	102	-	-	2/51/51/51	-
9	BCL	S	102	5	-	18/41/137/137	-
9	BCL	R	101	6	-	12/41/137/137	-
9	BCL	E	101	6	-	8/41/137/137	-
9	BCL	I	103	6	-	11/41/137/137	-
15	CRT	B	102	-	-	5/51/51/51	-
15	CRT	W	103	-	-	1/51/51/51	-
9	BCL	L	303	2	-	12/41/137/137	-
9	BCL	L	301	2	-	14/41/137/137	-
17	PEF	H	301	-	-	15/20/20/50	-
9	BCL	6	101	6	-	18/41/137/137	-
15	CRT	8	101	-	-	2/51/51/51	-
16	PGW	H	302	-	-	10/23/23/55	-
10	BPH	M	403	-	-	9/37/105/105	0/5/6/6
9	BCL	4	101	6	-	11/41/137/137	-
9	BCL	D	102	5	-	18/41/137/137	-
9	BCL	U	102	5	-	14/41/137/137	-
9	BCL	G	101	6	-	8/41/137/137	-
9	BCL	I	102	5	-	19/41/137/137	-
9	BCL	Q	102	5	-	22/41/137/137	-
15	CRT	J	101	-	-	2/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	X	102	-	-	2/51/51/51	-
15	CRT	V	102	-	-	8/51/51/51	-
9	BCL	A	102	5	-	15/41/137/137	-
15	CRT	P	102	-	-	2/51/51/51	-
9	BCL	W	102	5	-	20/41/137/137	-
15	CRT	M	406	-	-	0/51/51/51	-
9	BCL	1	102	5	-	14/41/137/137	-
9	BCL	P	101	6	-	12/41/137/137	-
9	BCL	9	102	5	-	15/41/137/137	-
9	BCL	5	102	5	-	21/41/137/137	-
9	BCL	T	101	6	-	12/41/137/137	-
9	BCL	M	401	3	-	18/41/137/137	-
15	CRT	3	103	-	-	2/51/51/51	-
7	HEM	C	503	1	-	8/14/54/54	-
9	BCL	M	402	3	-	15/41/137/137	-
9	BCL	X	101	6	-	12/41/137/137	-
9	BCL	Z	101	6	-	10/41/137/137	-
10	BPH	L	302	-	-	12/37/105/105	0/5/6/6
15	CRT	T	102	-	-	5/51/51/51	-
15	CRT	4	102	-	-	2/51/51/51	-
16	PGW	M	407	-	-	10/23/23/55	-
7	HEM	C	502	1	-	9/14/54/54	-
7	HEM	C	504	1	-	7/14/54/54	-
7	HEM	C	501	1	-	9/14/54/54	-
15	CRT	A	103	-	-	1/51/51/51	-
9	BCL	N	101	6	-	11/41/137/137	-
9	BCL	7	103	6	-	10/41/137/137	-
9	BCL	O	102	5	-	20/41/137/137	-
9	BCL	V	101	6	-	14/41/137/137	-
14	MQ8	M	405	-	-	10/47/67/67	0/2/2/2
15	CRT	A	101	-	-	2/51/51/51	-
15	CRT	2	102	-	-	2/51/51/51	-
9	BCL	K	102	5	-	17/41/137/137	-
9	BCL	B	101	6	-	15/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	Y	102	5	-	14/41/137/137	-
11	UQ8	L	304	-	-	6/51/75/75	0/1/1/1
9	BCL	3	102	5	-	16/41/137/137	-
9	BCL	2	101	6	-	12/41/137/137	-
9	BCL	0	101	6	-	16/41/137/137	-
9	BCL	7	102	5	-	15/41/137/137	-
15	CRT	R	102	-	-	2/51/51/51	-
15	CRT	G	102	-	-	1/51/51/51	-

The worst 5 of 636 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302	BPH	C1D-C2D	8.74	1.49	1.39
10	M	403	BPH	C1D-C2D	8.71	1.49	1.39
15	X	102	CRT	C4-C5	7.77	1.61	1.50
11	L	304	UQ8	C43-C44	7.47	1.54	1.32
17	H	301	PEF	O4-C10	7.29	1.47	1.21

The worst 5 of 1170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	102	CRT	C1-C4-C5	15.74	153.86	112.98
15	R	102	CRT	C4-C5-C6	-12.53	107.31	124.91
15	T	102	CRT	C4-C5-C6	-11.57	108.66	124.91
15	A	101	CRT	C37-C36-C35	10.60	139.81	124.91
15	A	101	CRT	C36-C35-C33	-10.28	110.36	125.89

There are no chirality outliers.

5 of 673 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	501	HEM	C2B-C3B-CAB-CBB
7	C	501	HEM	C2C-C3C-CAC-CBC
7	C	501	HEM	C4C-C3C-CAC-CBC
7	C	502	HEM	C2B-C3B-CAB-CBB
7	C	502	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

67 monomers are involved in 1403 short contacts:

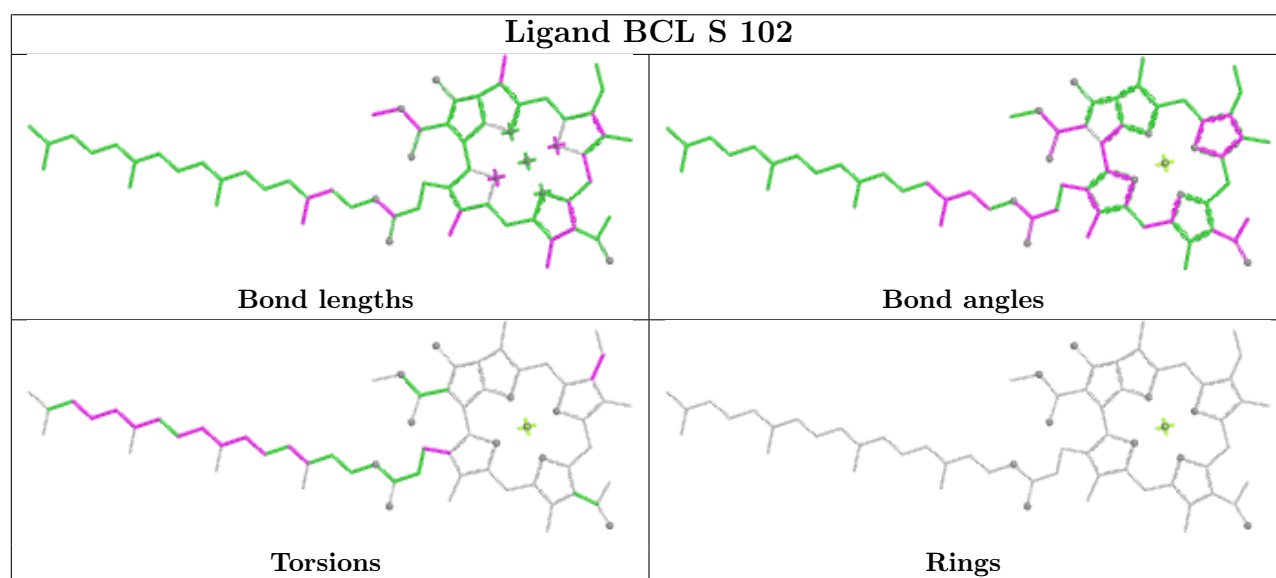
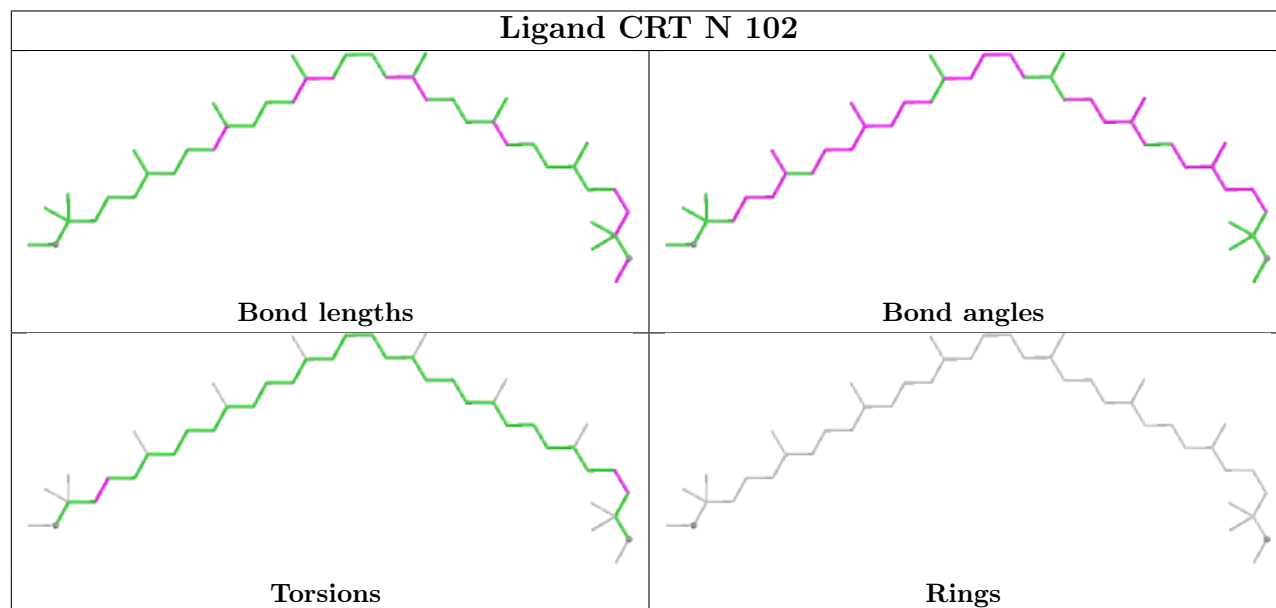
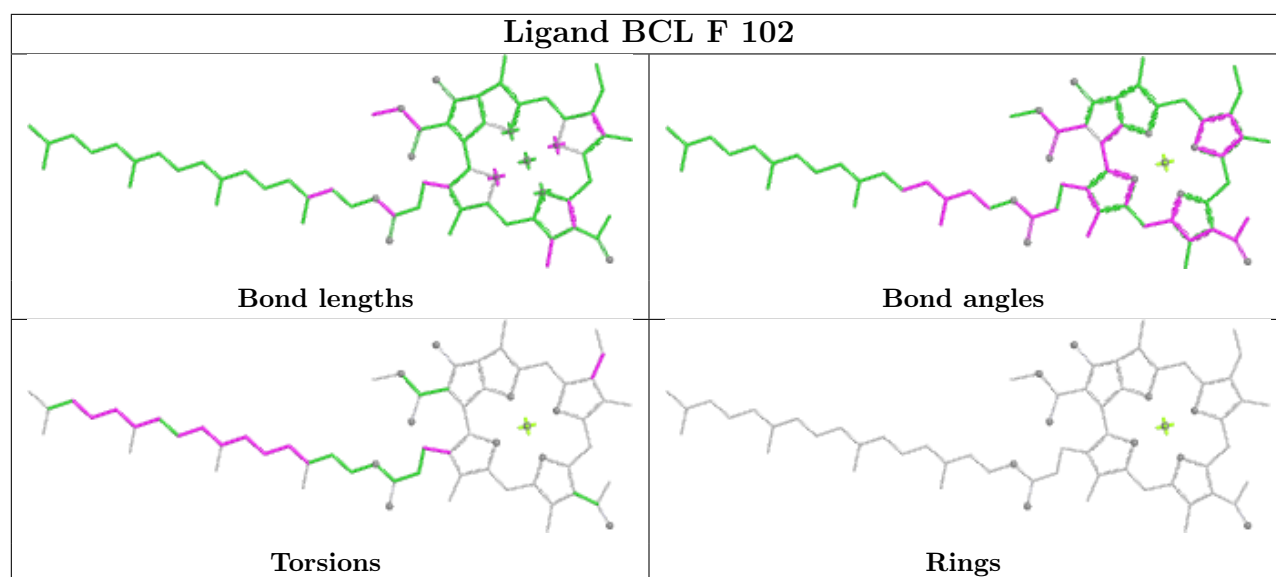
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	102	BCL	39	0
15	N	102	CRT	52	0
9	S	102	BCL	24	0
9	R	101	BCL	27	0
9	E	101	BCL	30	0
9	I	103	BCL	34	0
15	B	102	CRT	34	0
15	W	103	CRT	30	0
9	L	303	BCL	8	0
9	L	301	BCL	14	0
17	H	301	PEF	18	0
9	6	101	BCL	19	0
15	8	101	CRT	80	0
16	H	302	PGW	7	0
10	M	403	BPH	18	0
9	4	101	BCL	30	0
9	D	102	BCL	21	0
9	U	102	BCL	18	0
9	G	101	BCL	35	0
9	I	102	BCL	32	0
9	Q	102	BCL	22	0
15	J	101	CRT	35	0
15	X	102	CRT	27	0
15	V	102	CRT	65	0
9	A	102	BCL	35	0
15	P	102	CRT	62	0
9	W	102	BCL	33	0
15	M	406	CRT	12	0
9	1	102	BCL	15	0
9	P	101	BCL	27	0
9	9	102	BCL	29	0
9	5	102	BCL	21	0
9	T	101	BCL	22	0
9	M	401	BCL	31	0
15	3	103	CRT	20	0
7	C	503	HEM	9	0
9	M	402	BCL	12	0
9	X	101	BCL	36	0
9	Z	101	BCL	24	0
10	L	302	BPH	8	0
12	H	304	PO4	3	0
15	T	102	CRT	22	0
15	4	102	CRT	68	0

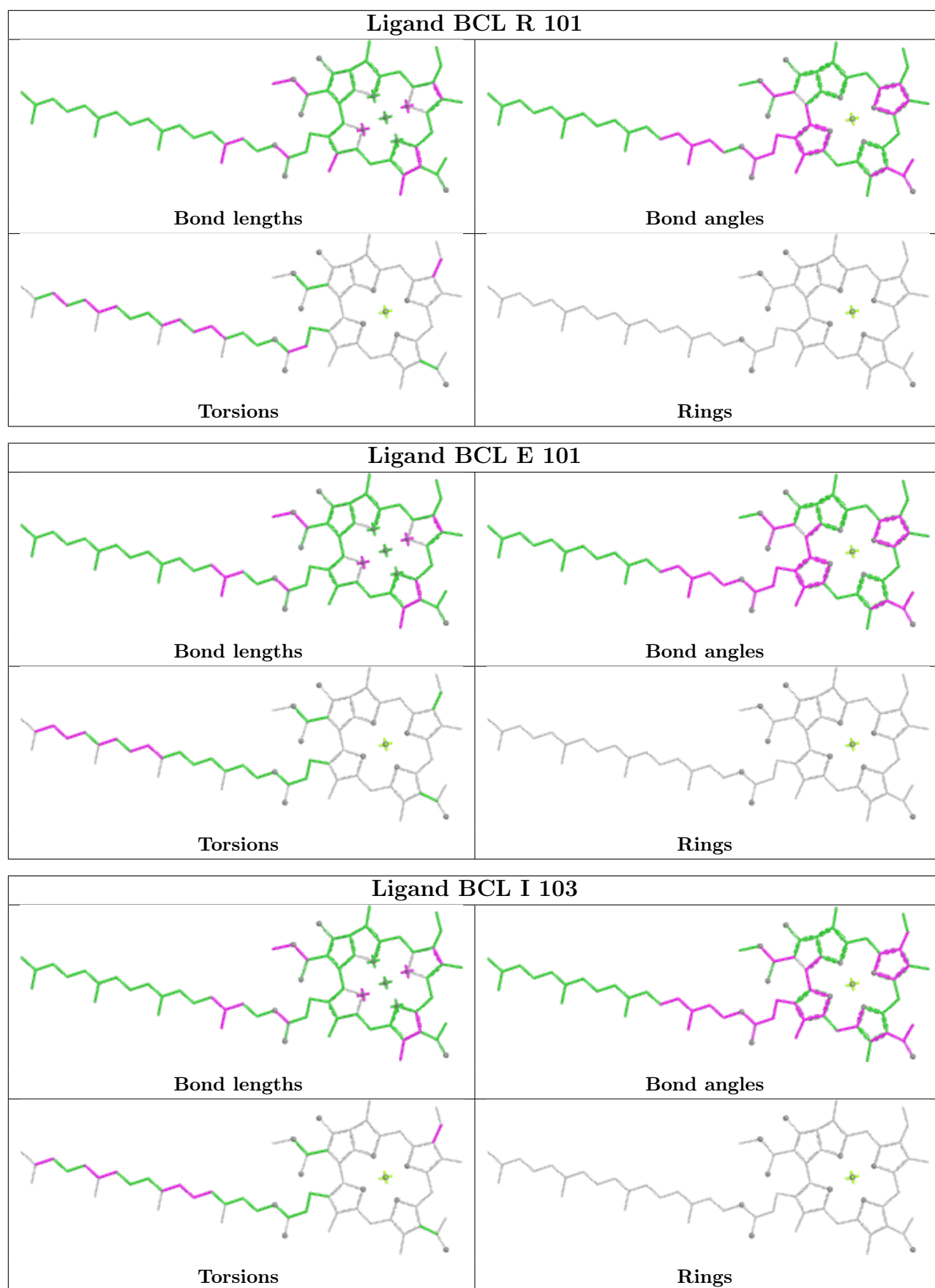
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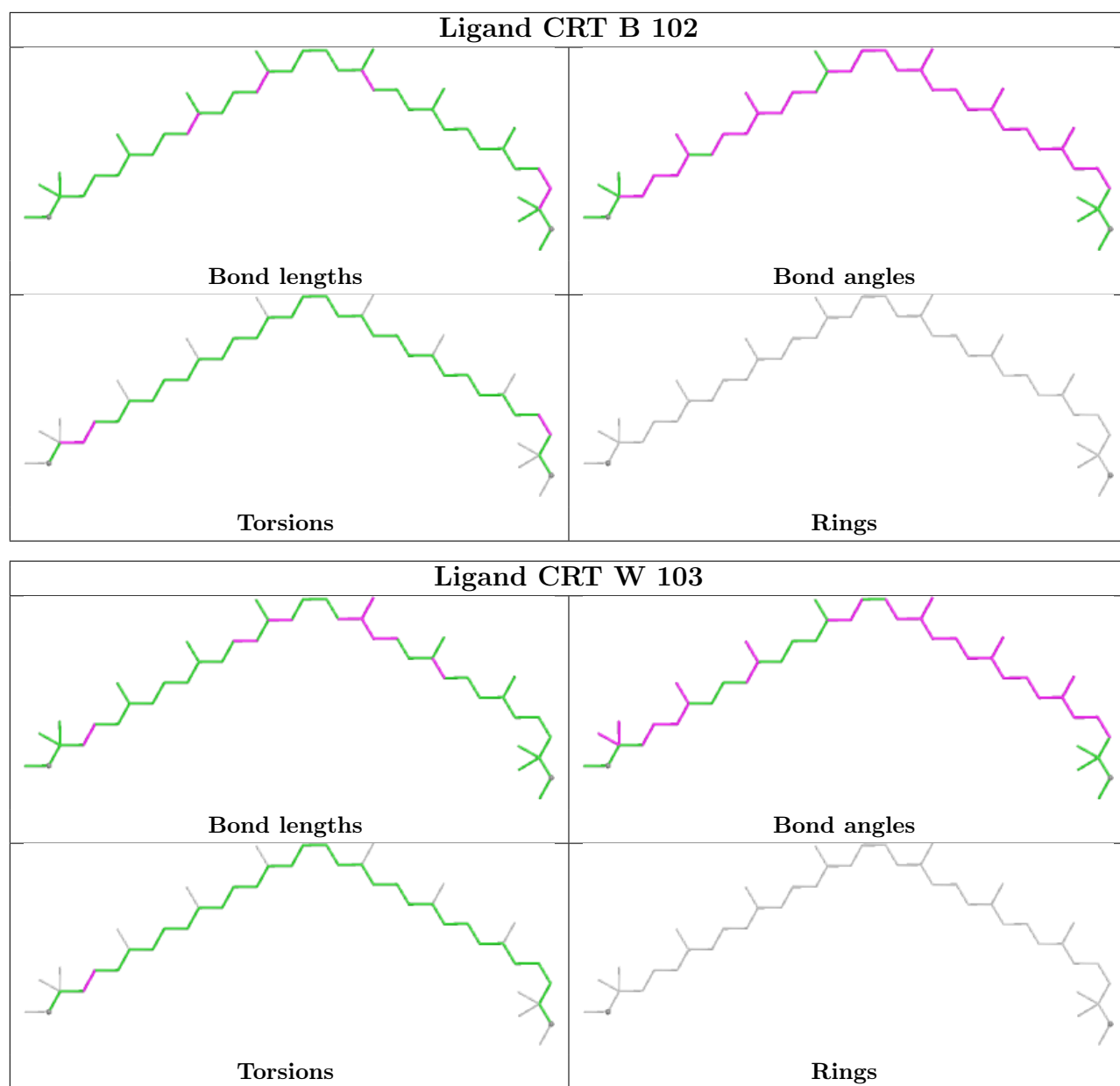
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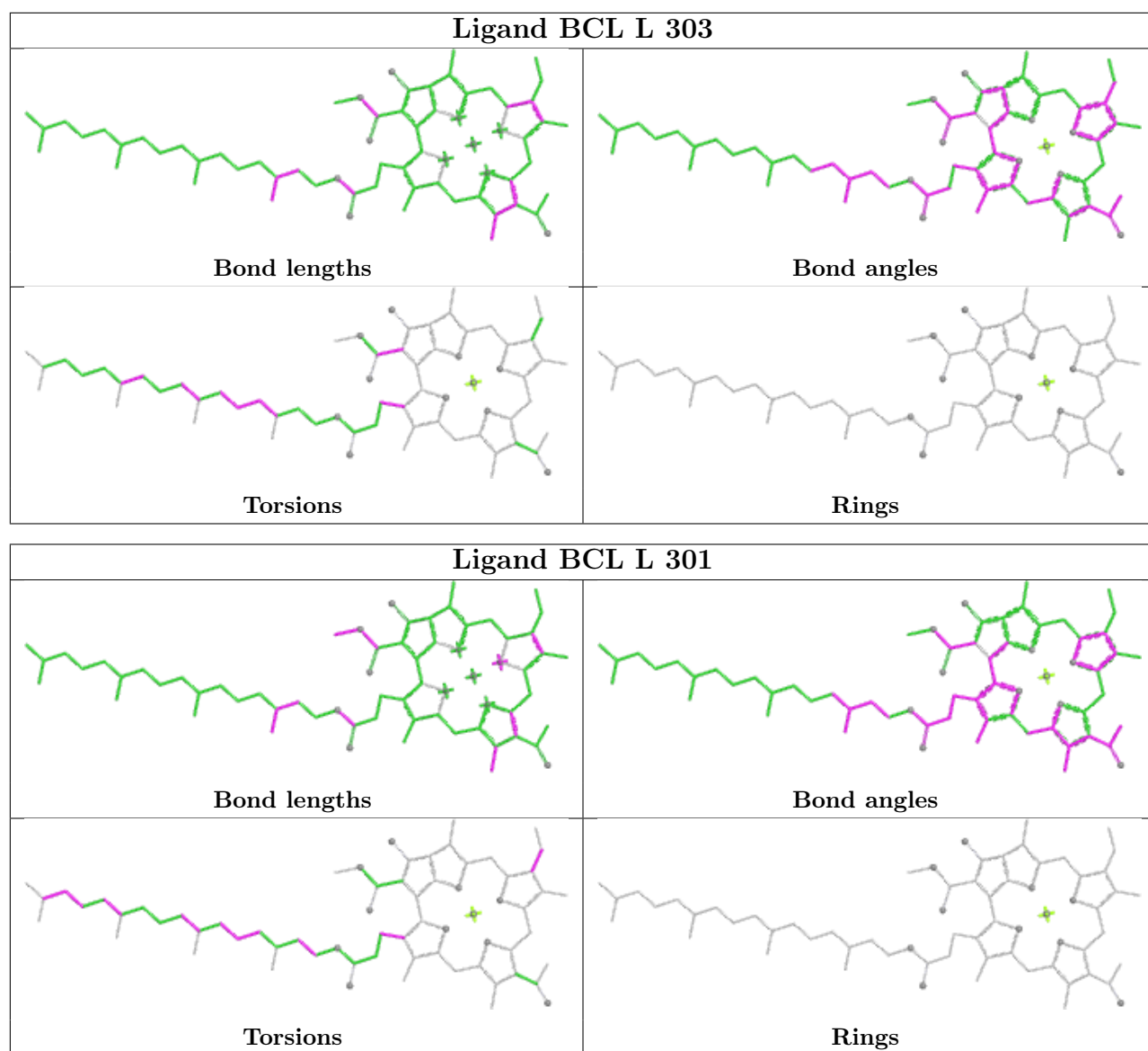
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	303	PO4	1	0
16	M	407	PGW	16	0
7	C	502	HEM	4	0
7	C	504	HEM	2	0
7	C	501	HEM	2	0
15	A	103	CRT	23	0
9	N	101	BCL	23	0
9	7	103	BCL	25	0
9	O	102	BCL	51	0
9	V	101	BCL	8	0
14	M	405	MQ8	11	0
15	A	101	CRT	49	0
15	2	102	CRT	39	0
9	K	102	BCL	25	0
9	B	101	BCL	34	0
9	Y	102	BCL	25	0
11	L	304	UQ8	13	0
9	3	102	BCL	24	0
12	M	408	PO4	1	0
9	2	101	BCL	15	0
9	0	101	BCL	28	0
9	7	102	BCL	16	0
15	R	102	CRT	34	0
15	G	102	CRT	28	0

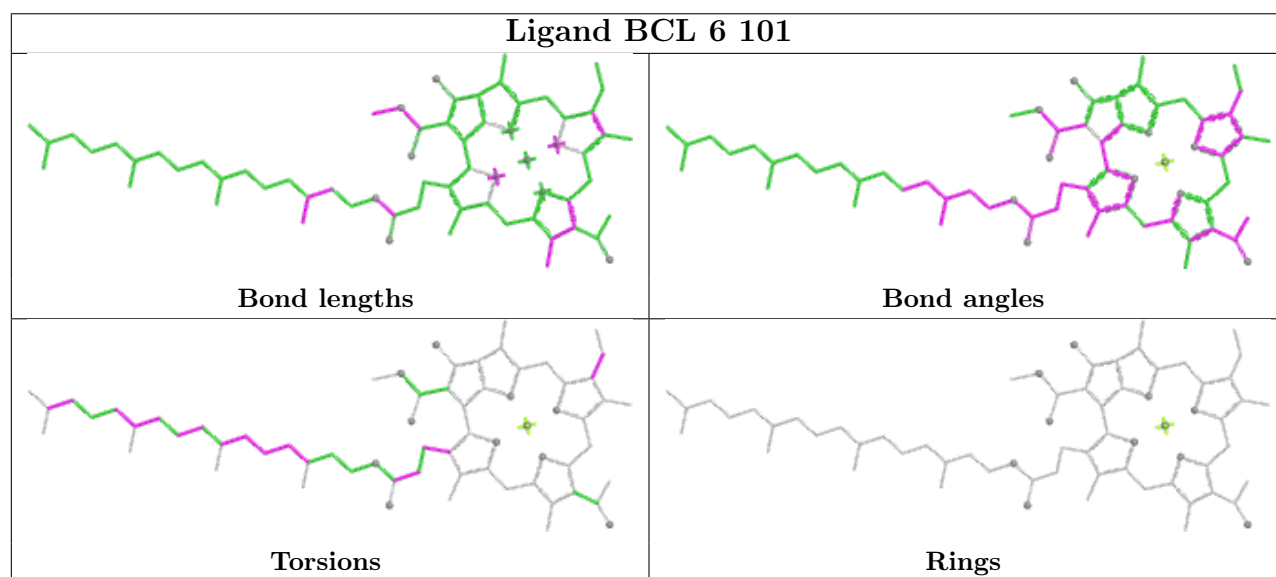
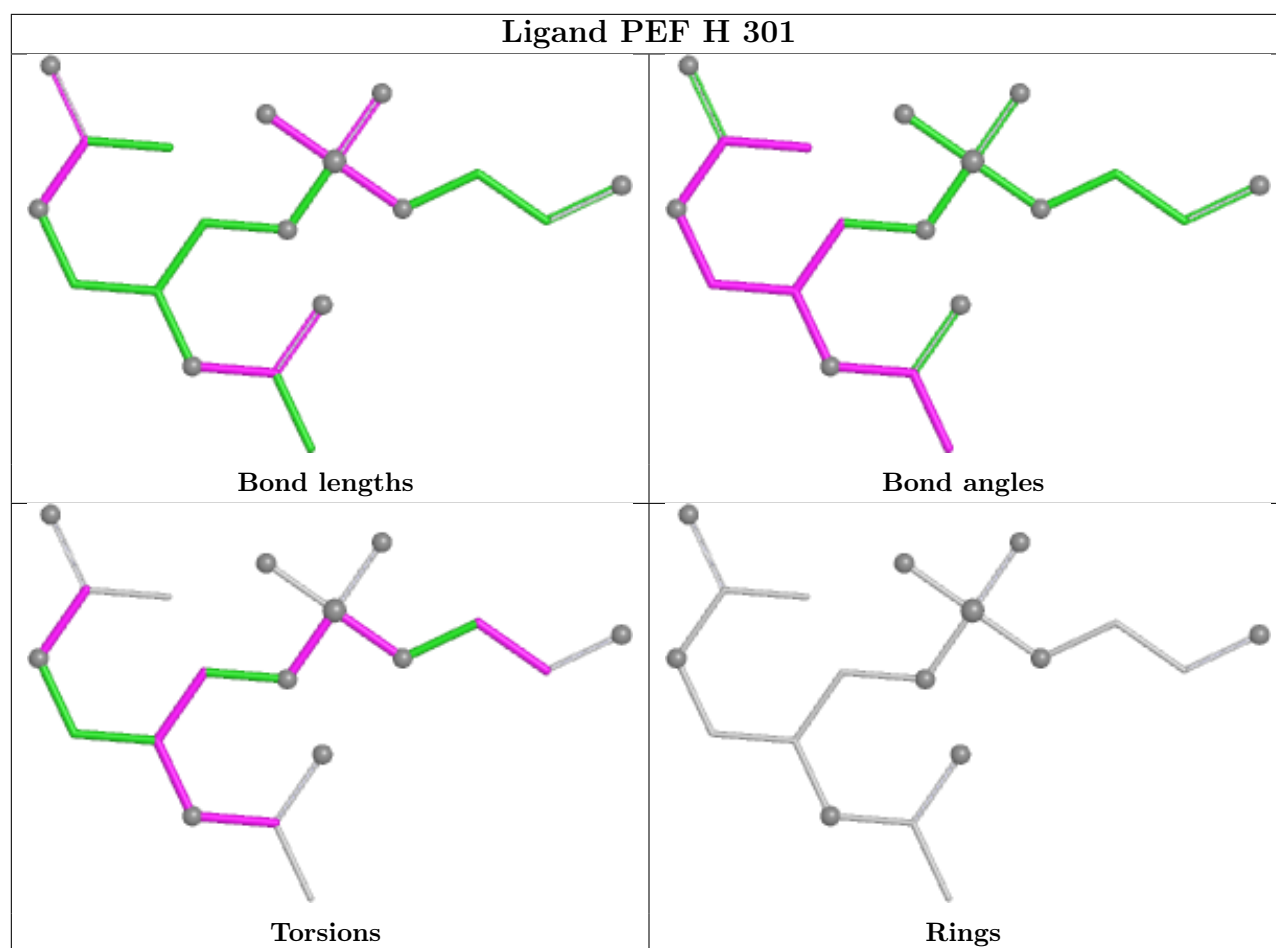
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

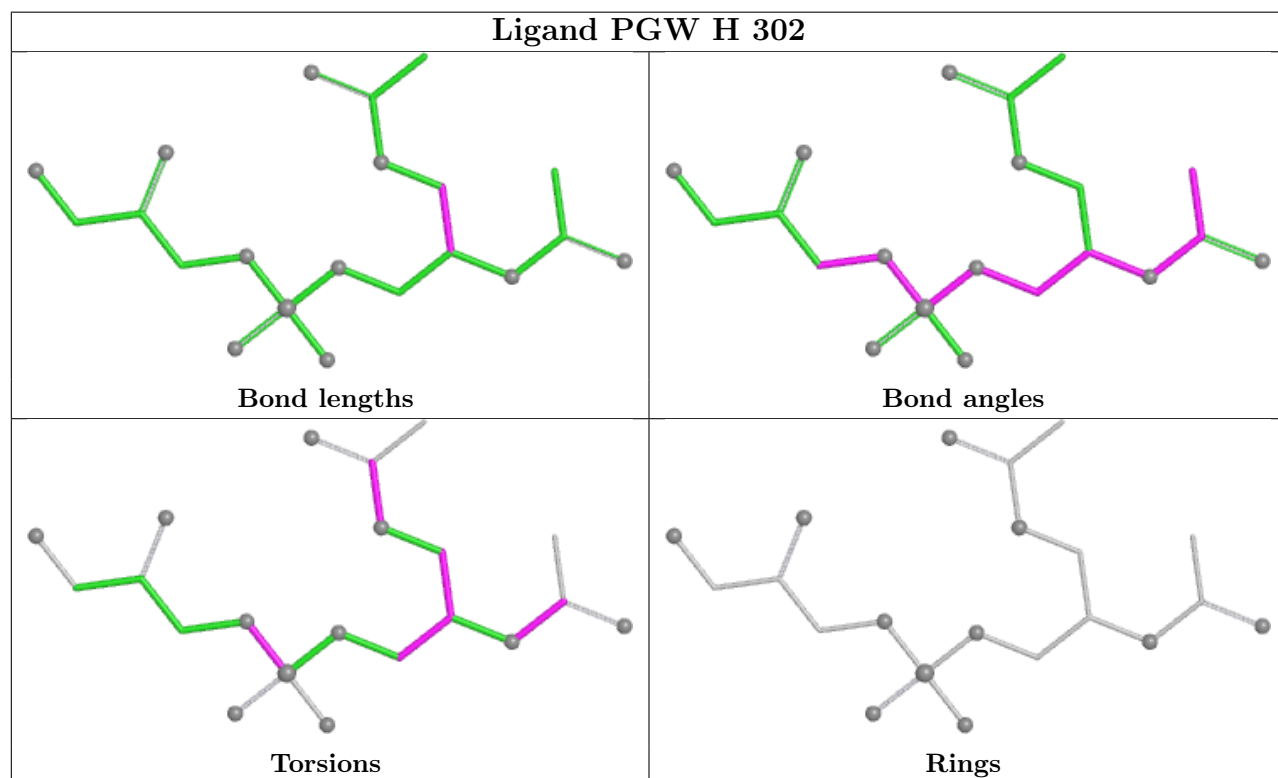
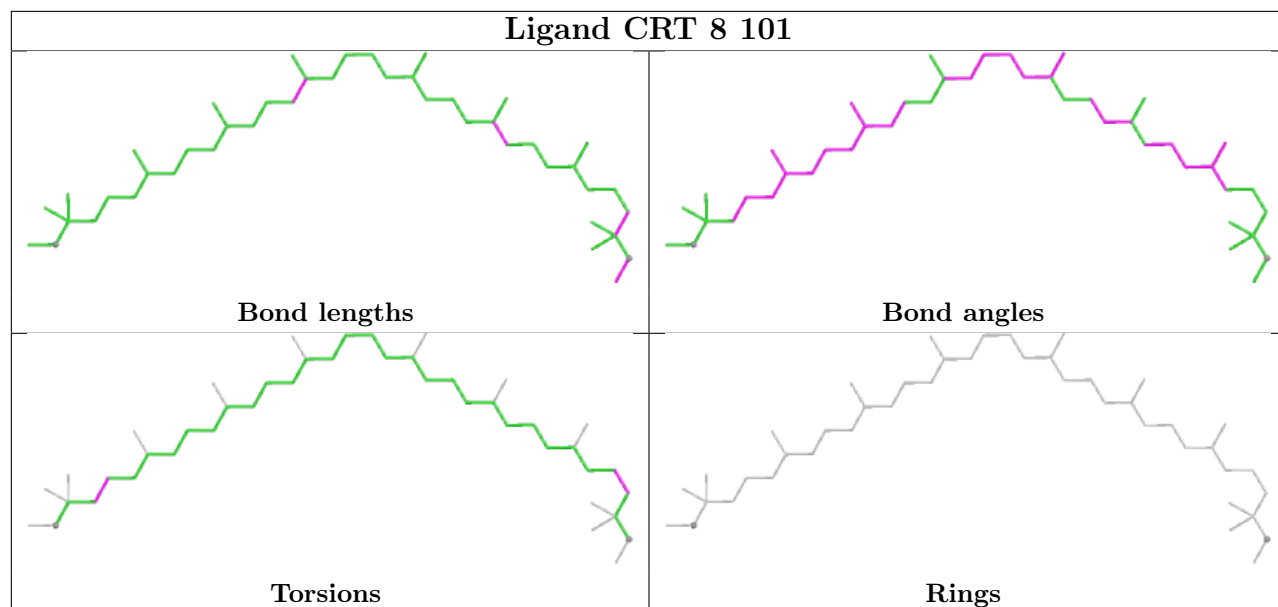


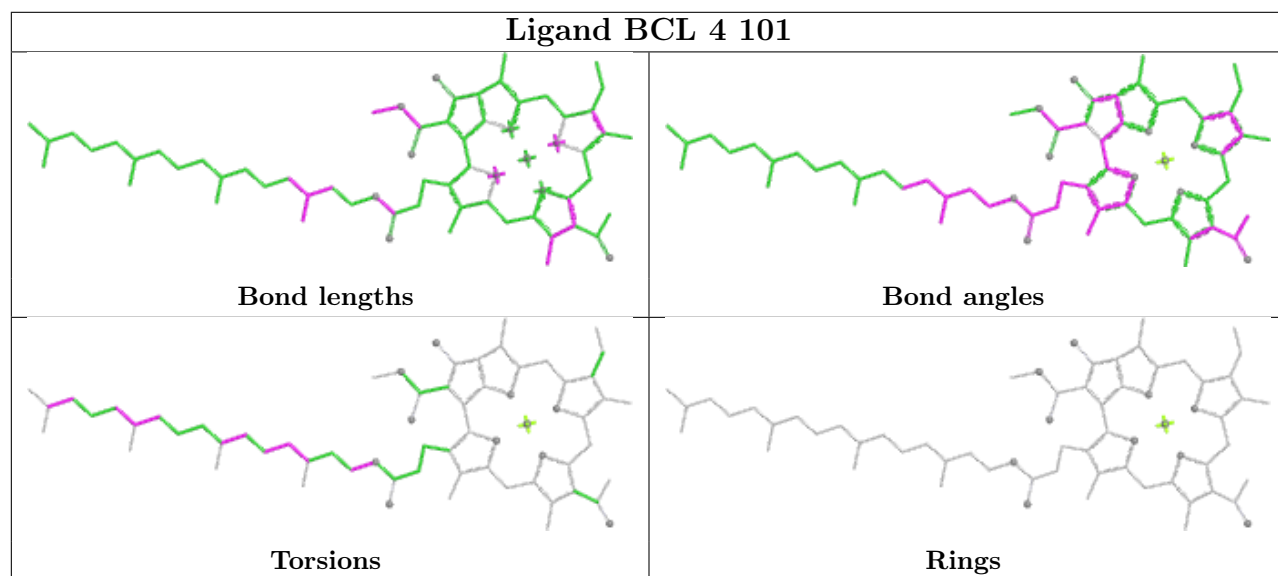
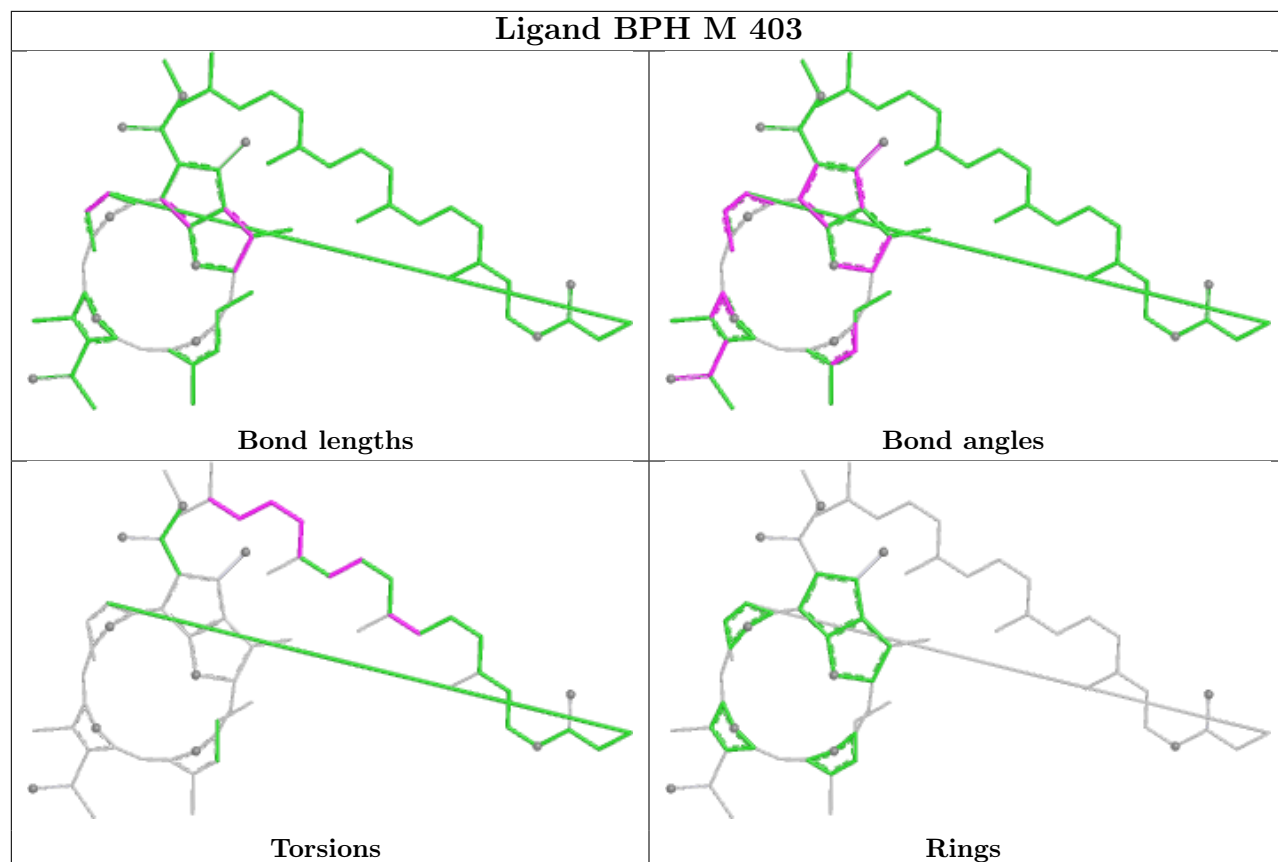


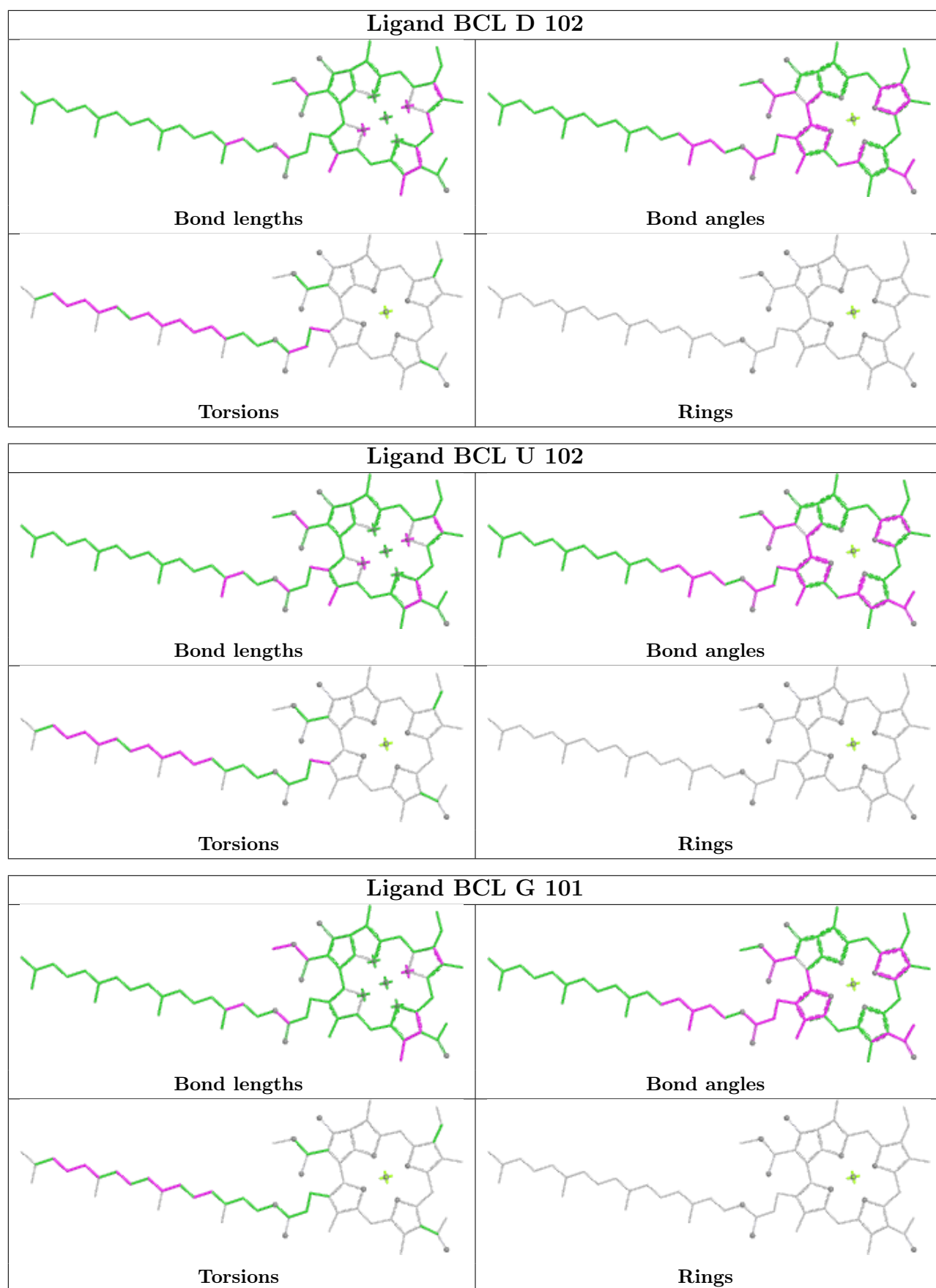


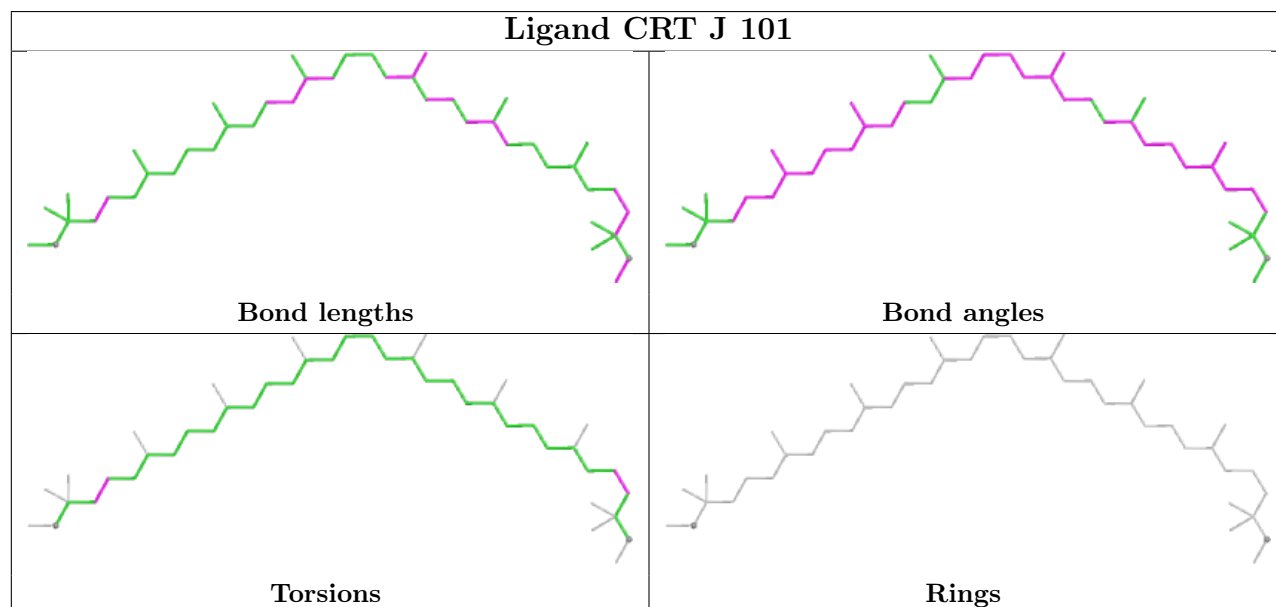
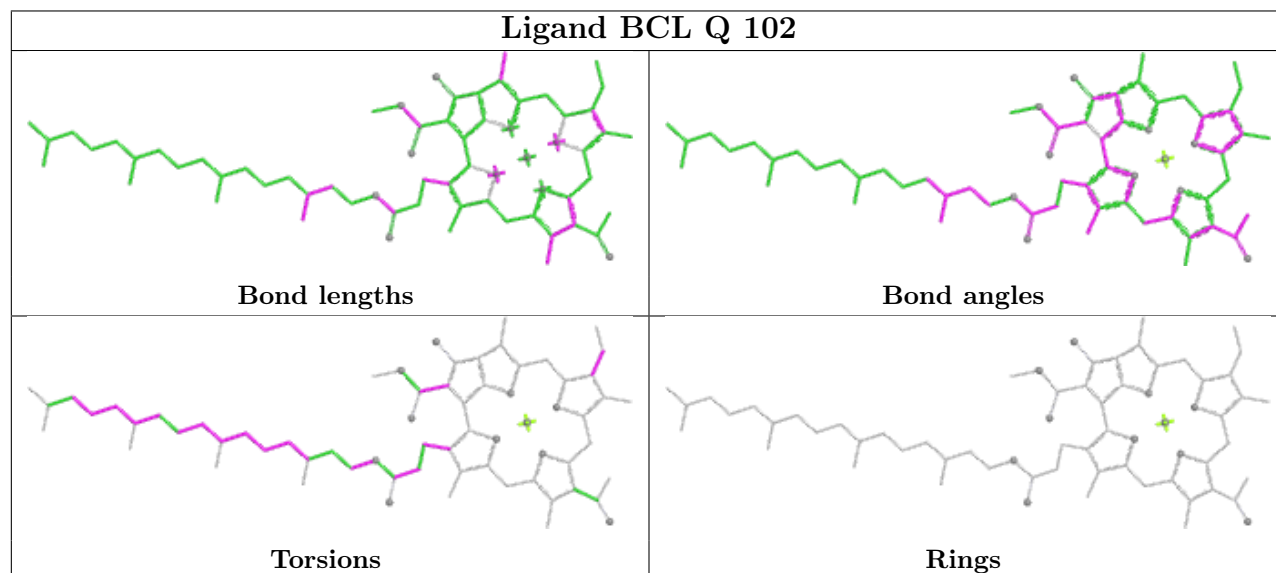
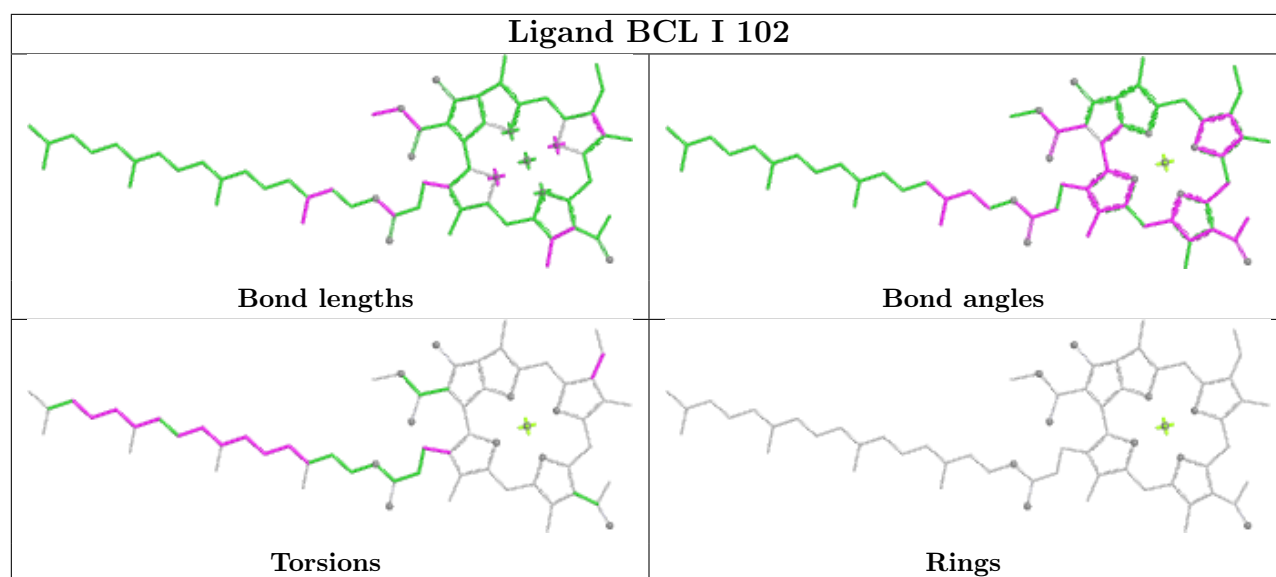


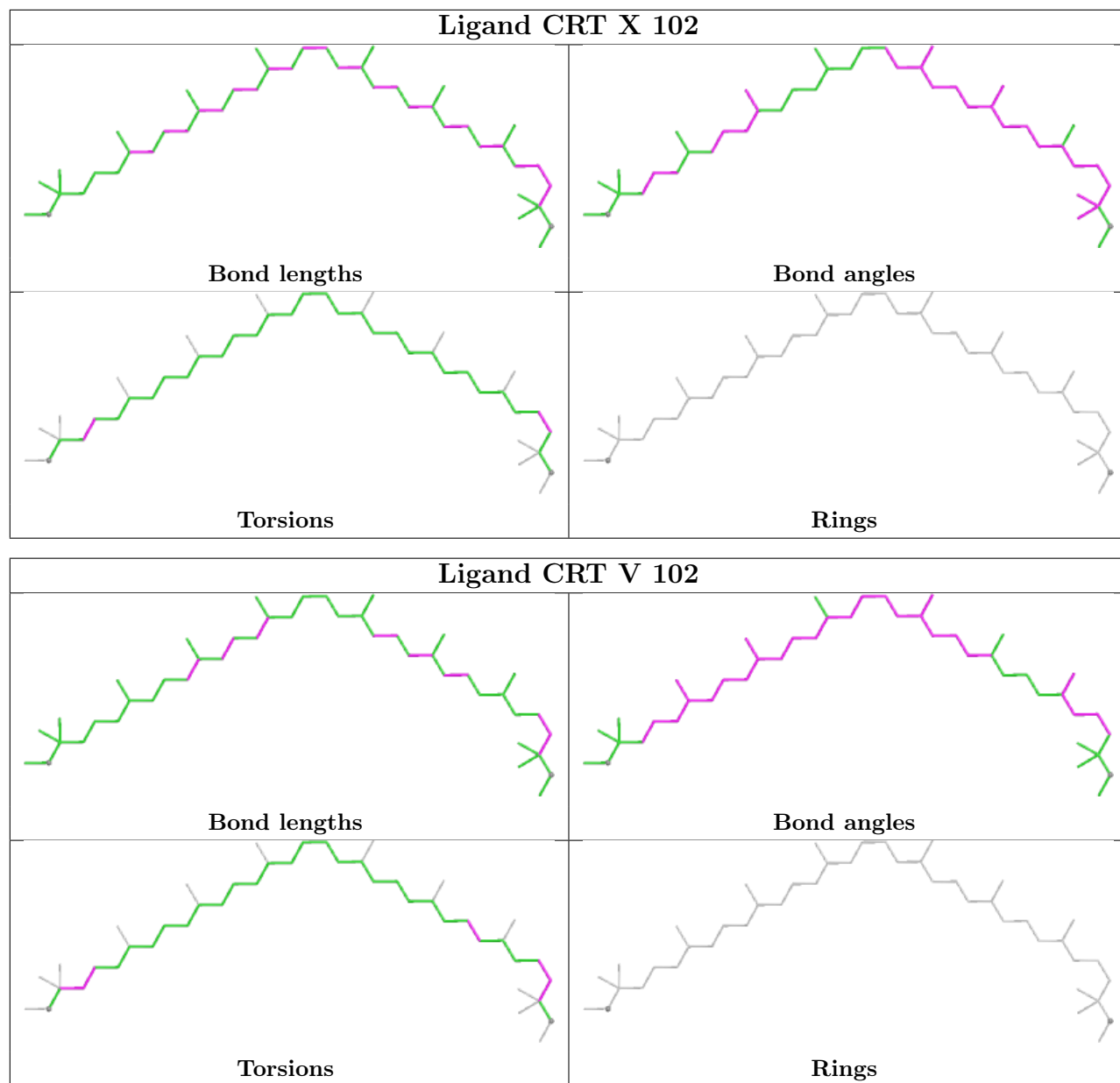


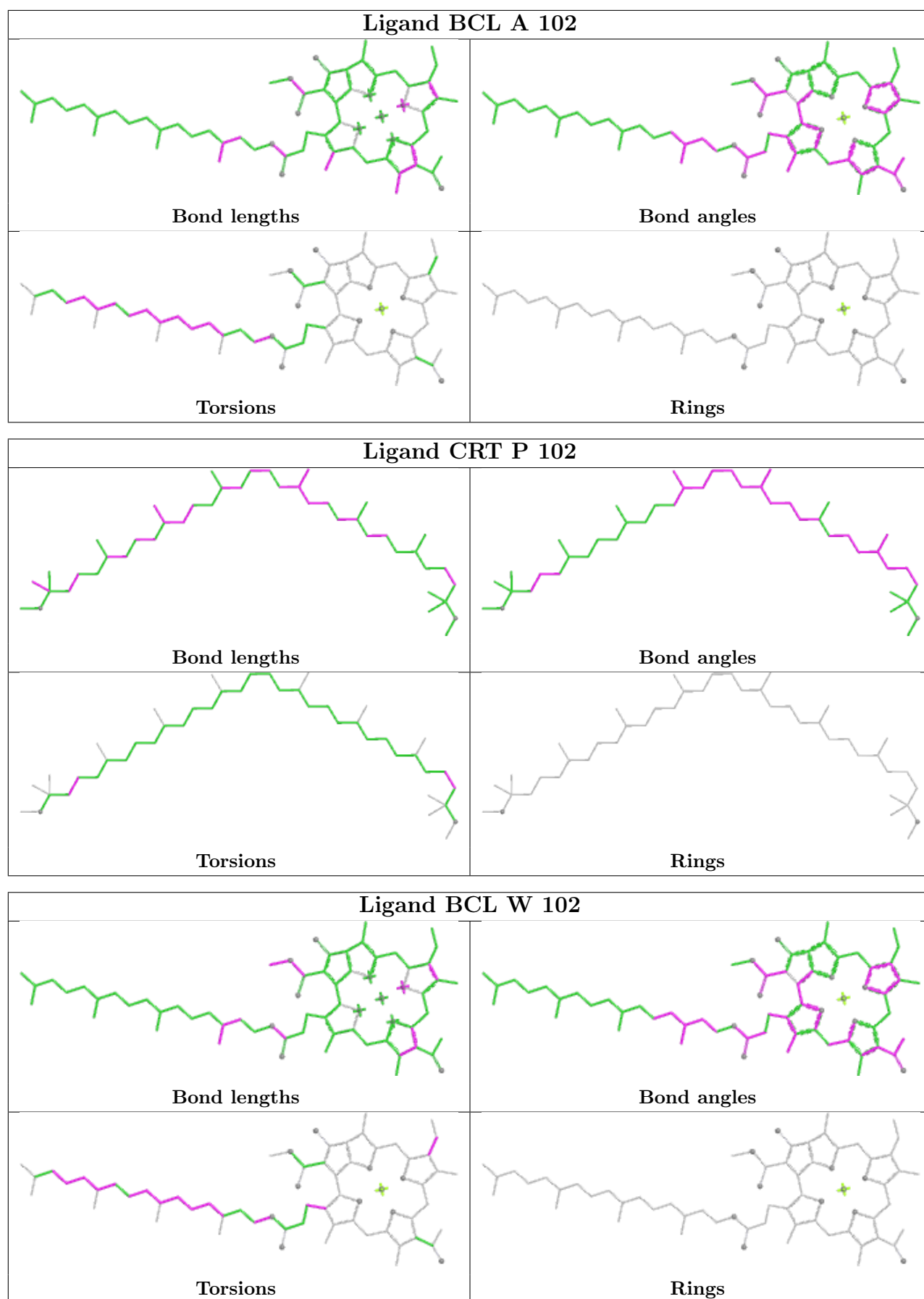


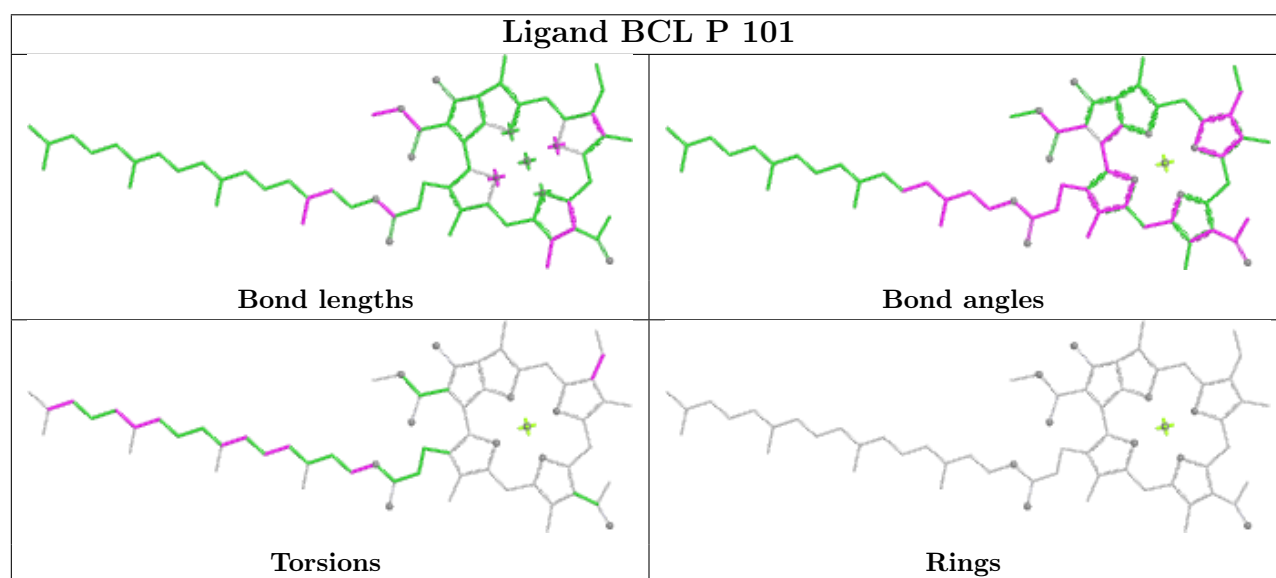
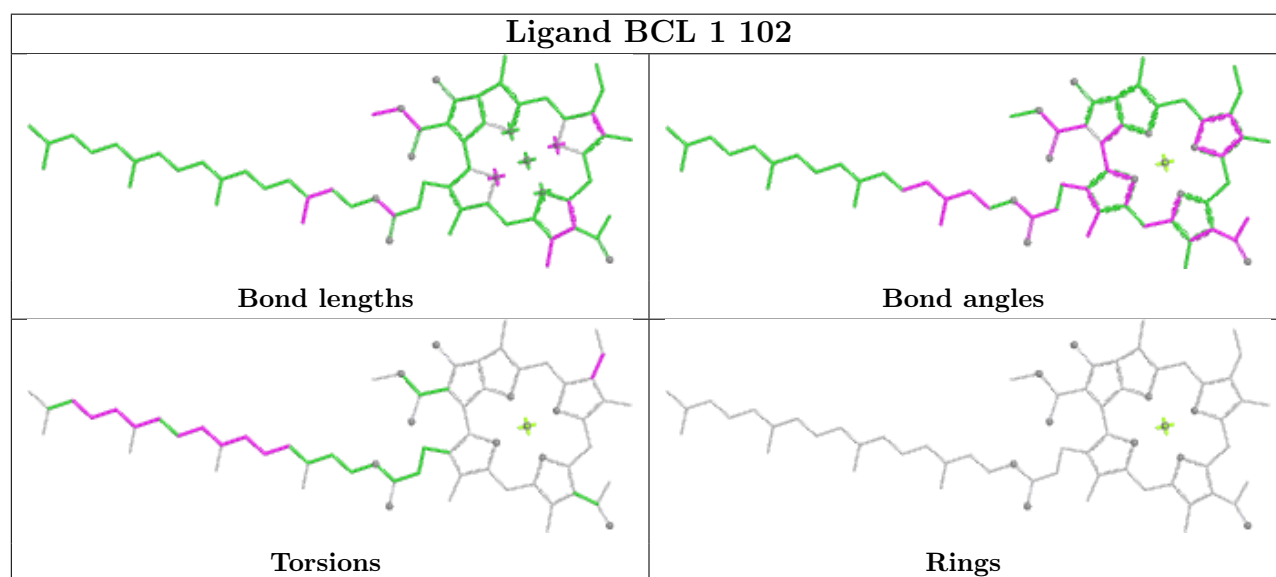
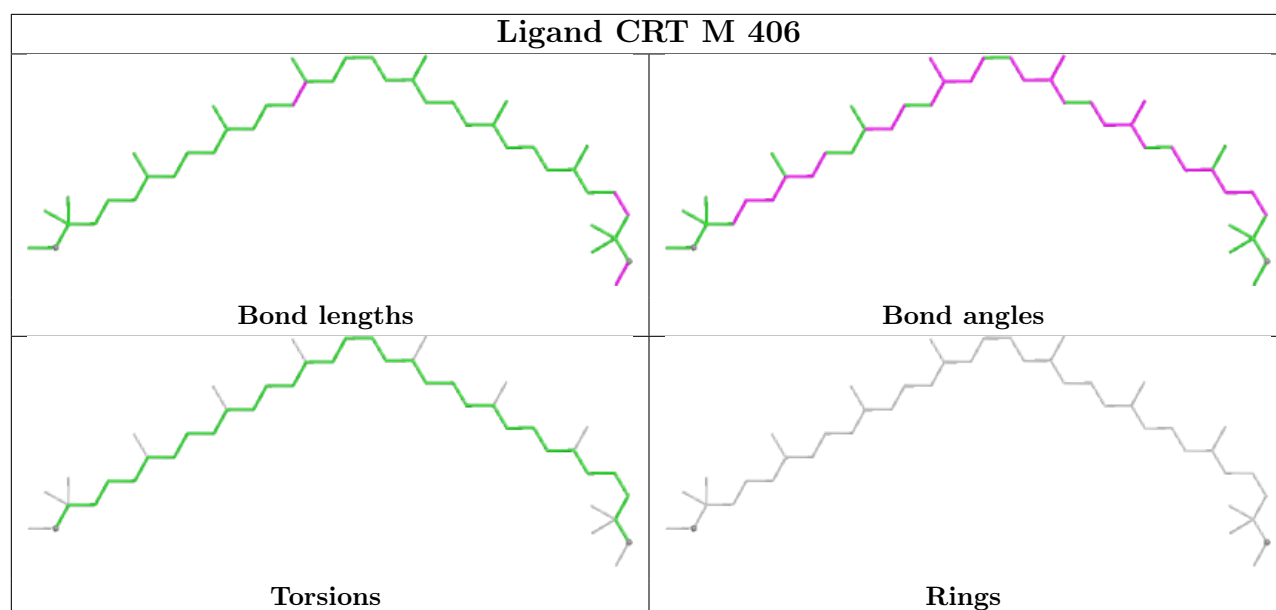


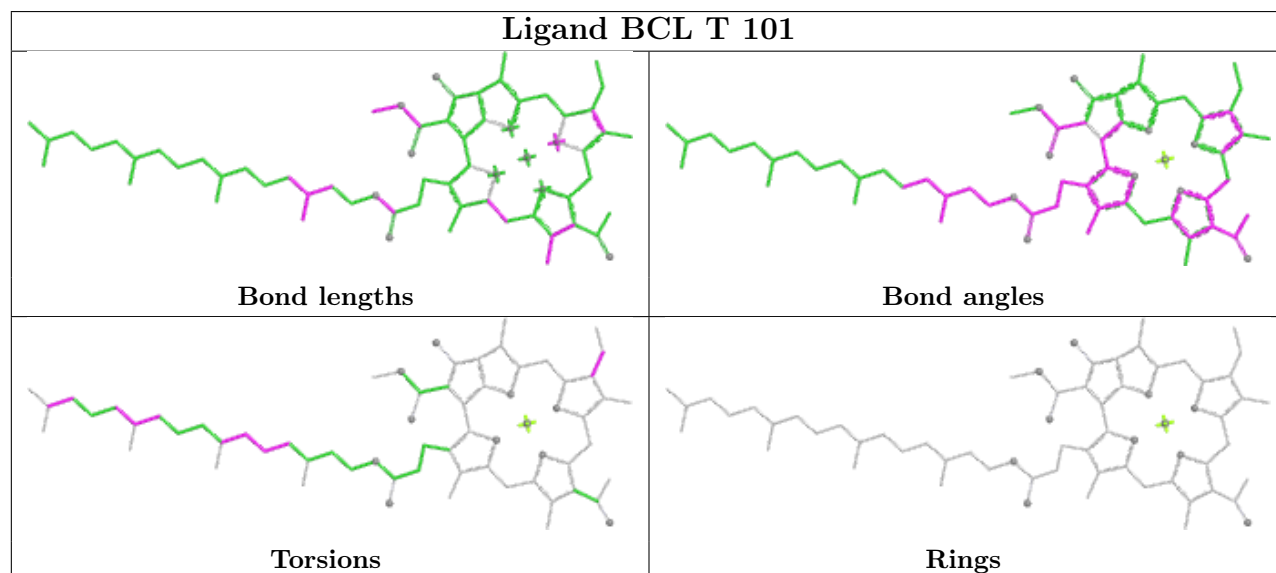
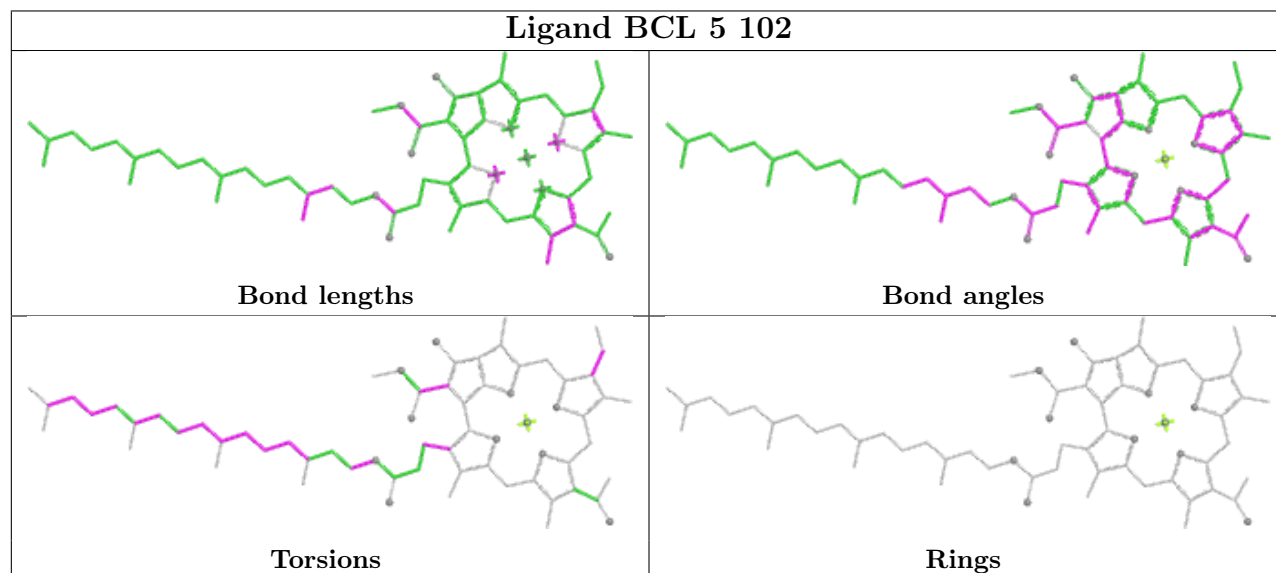
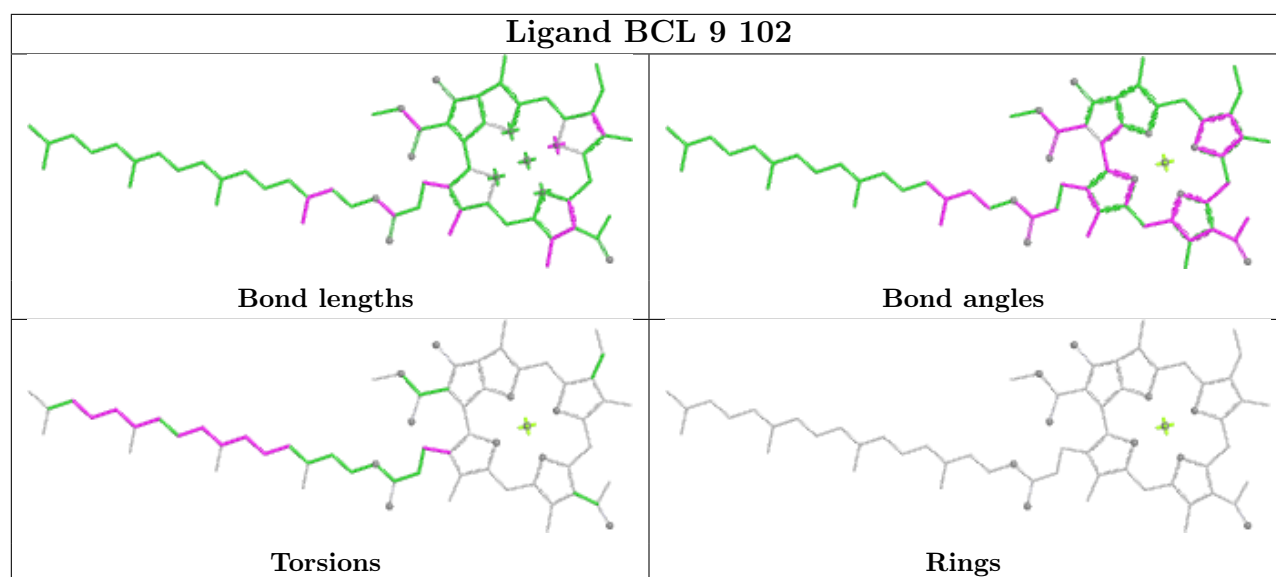


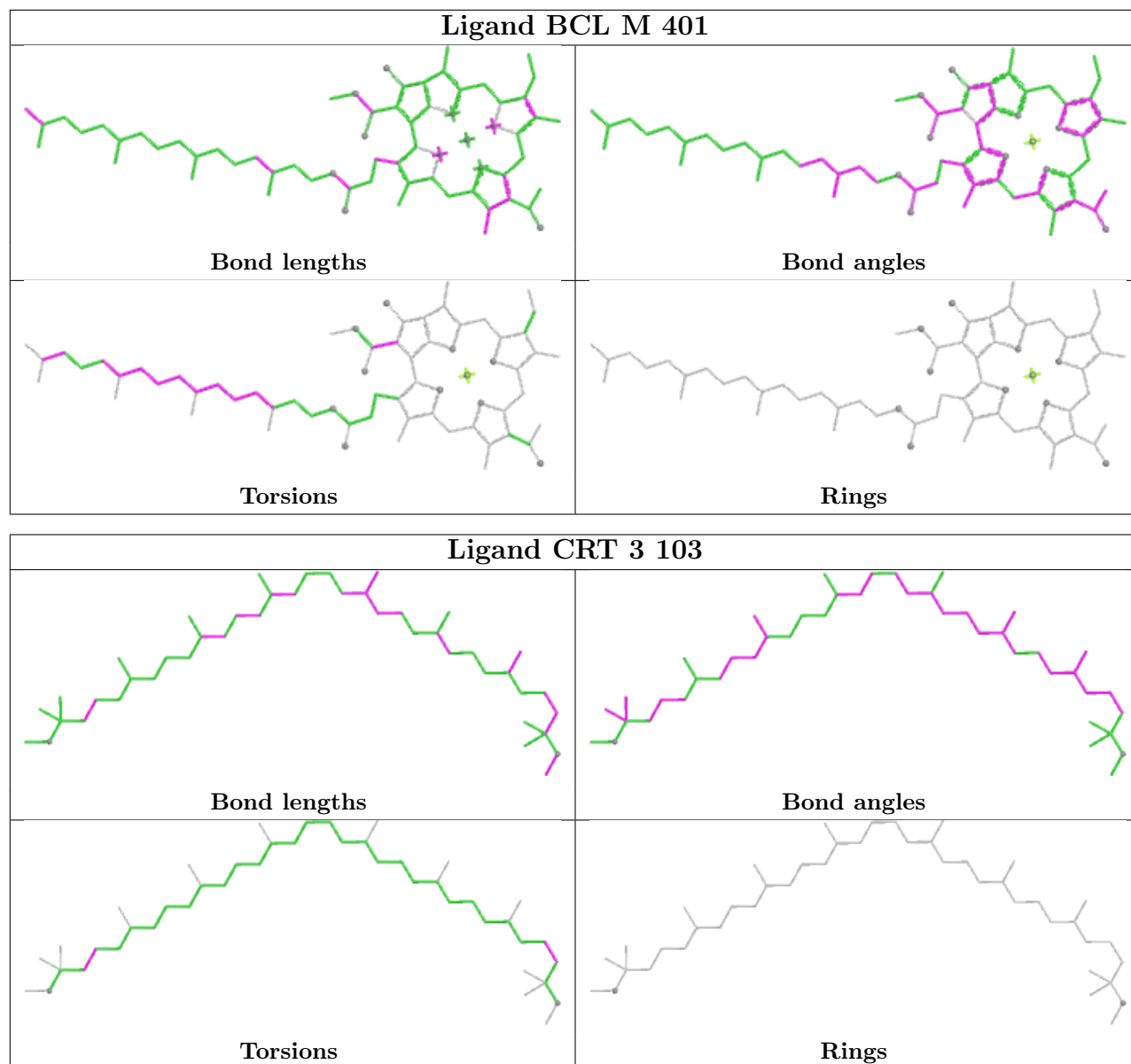


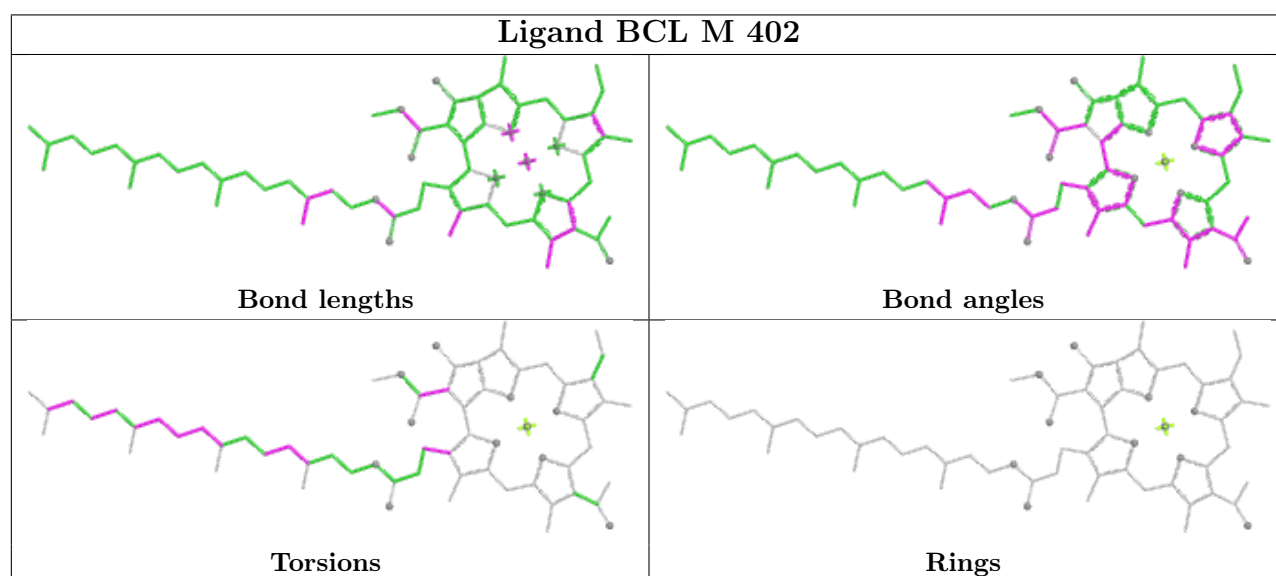
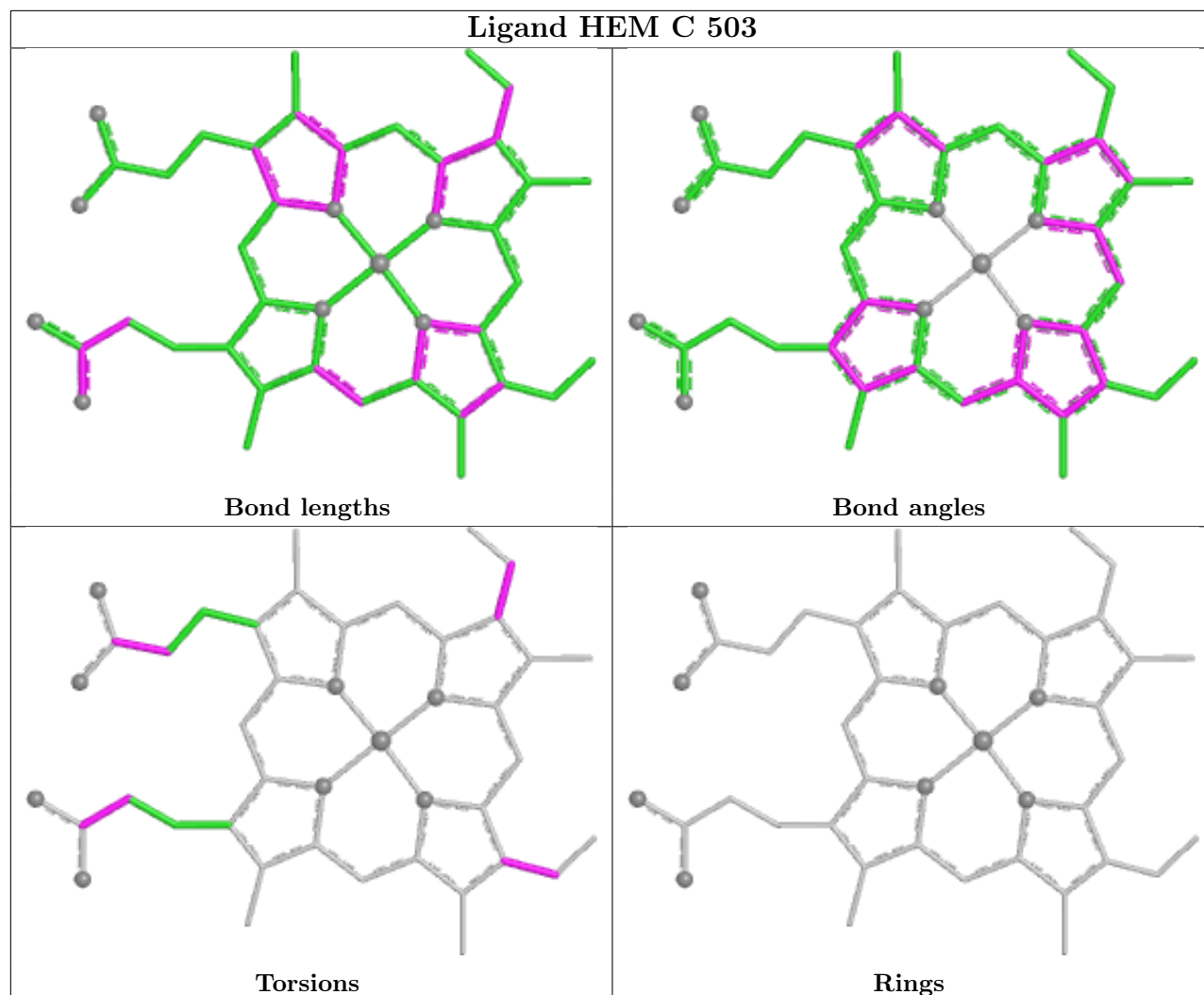


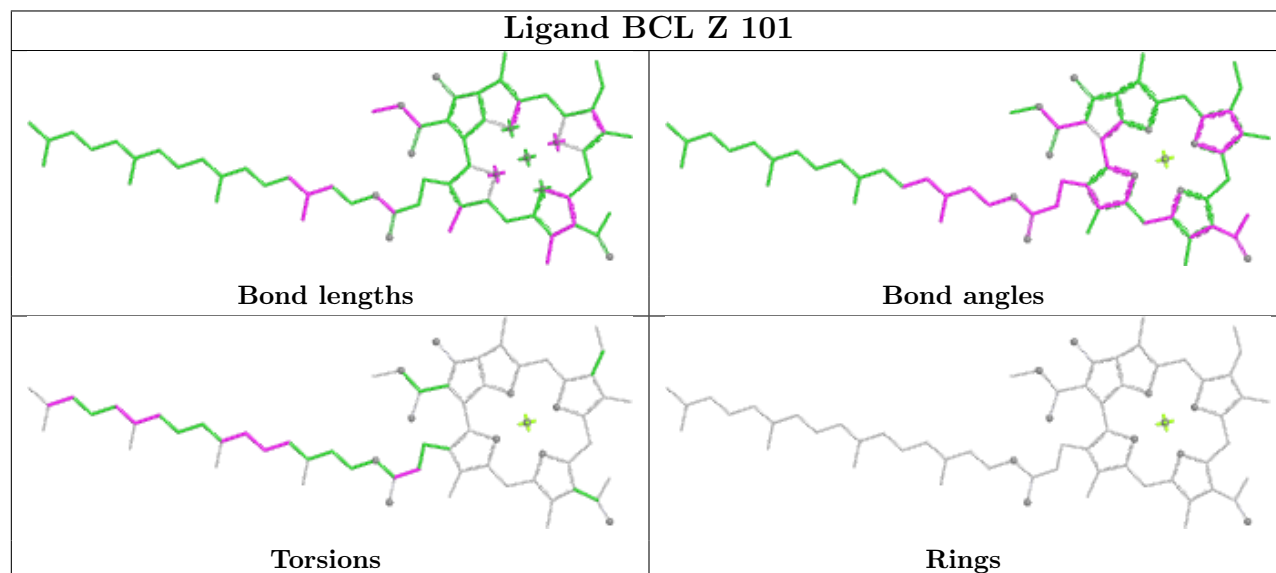
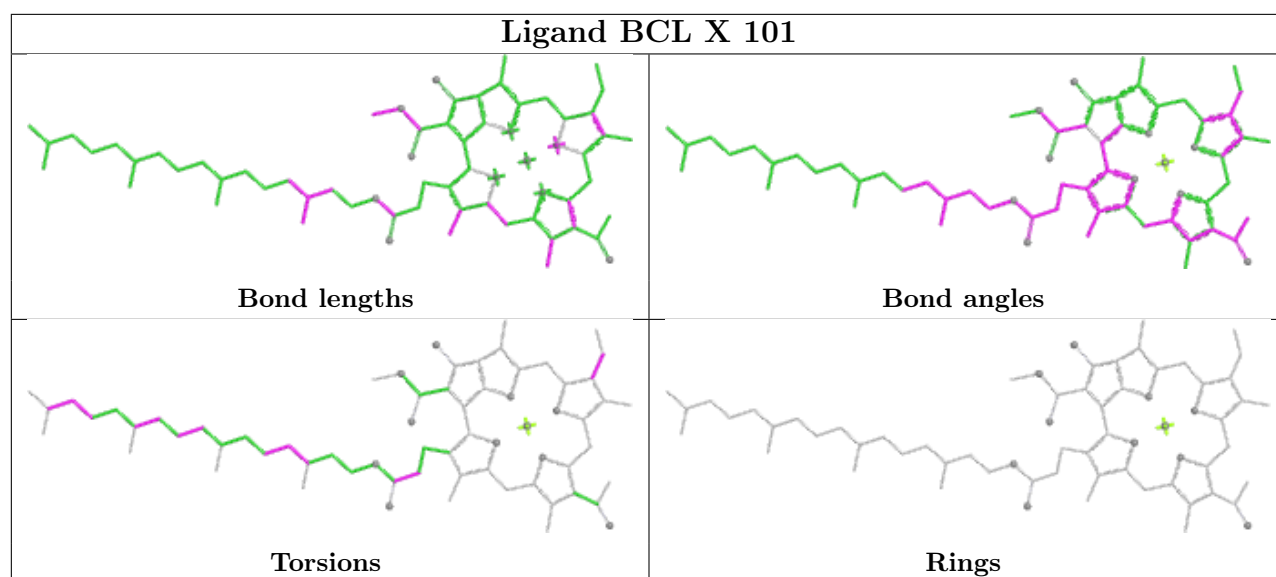


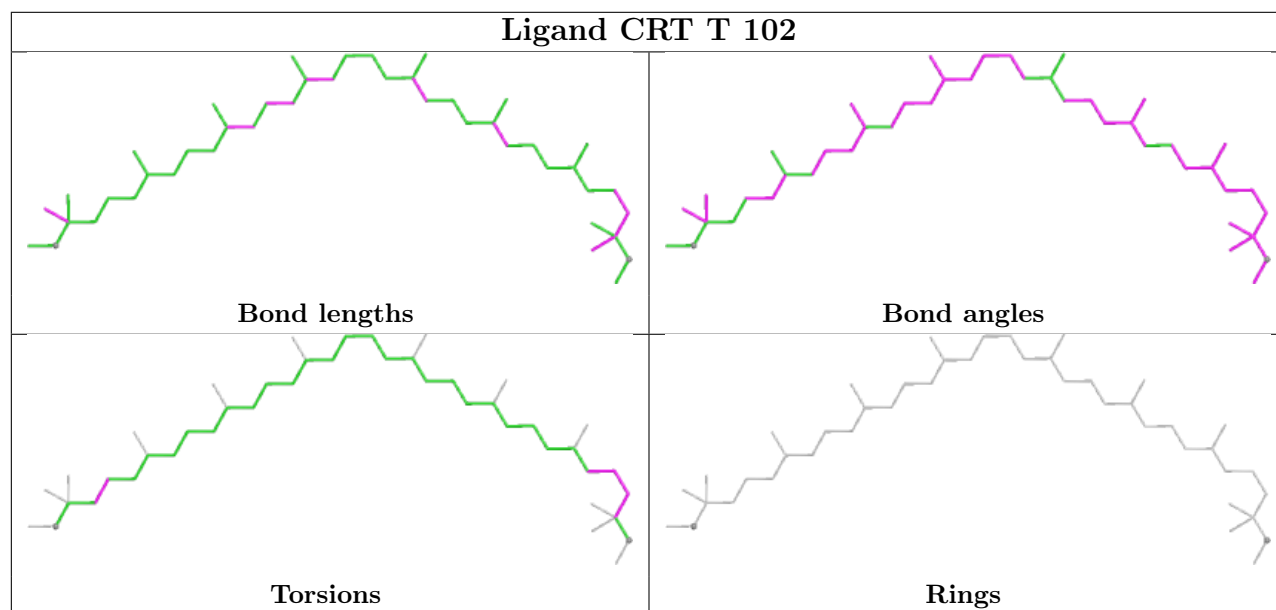
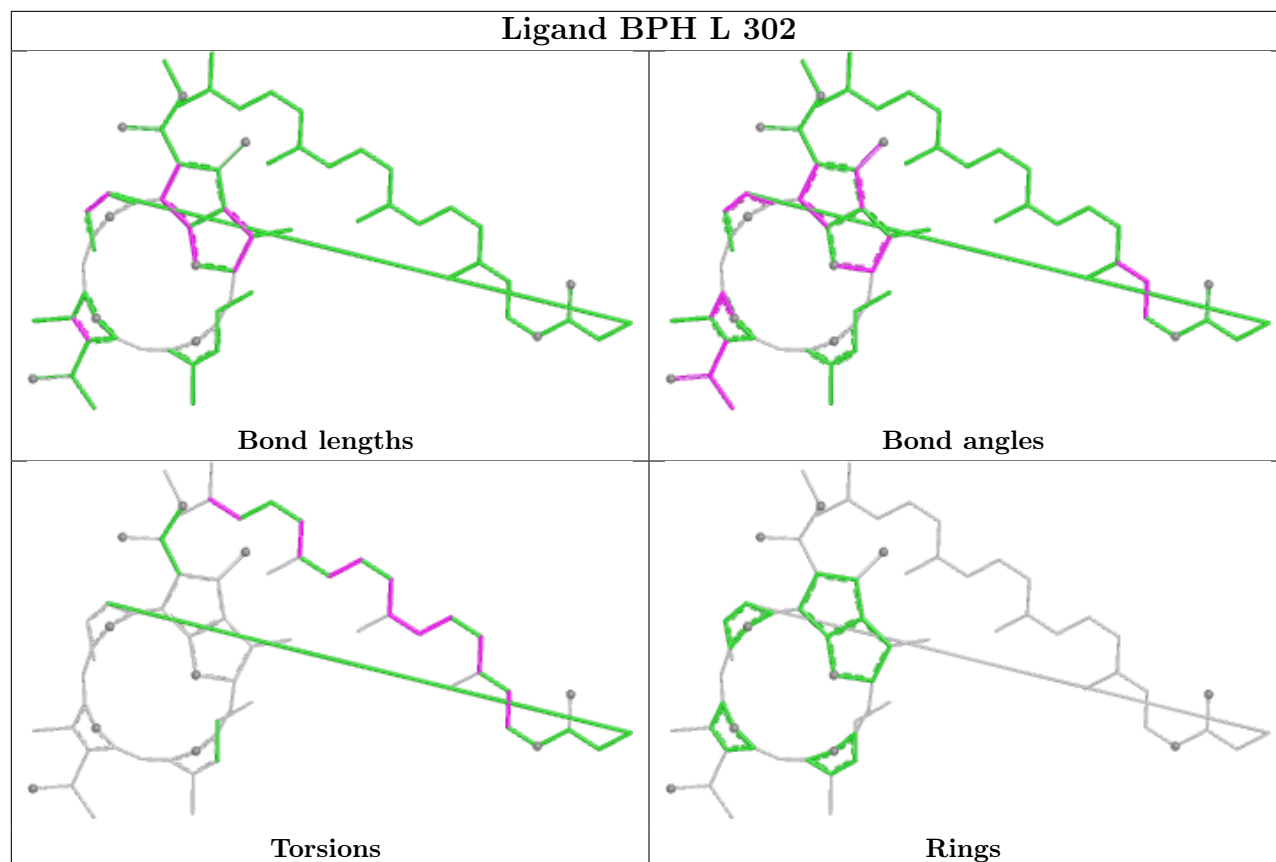


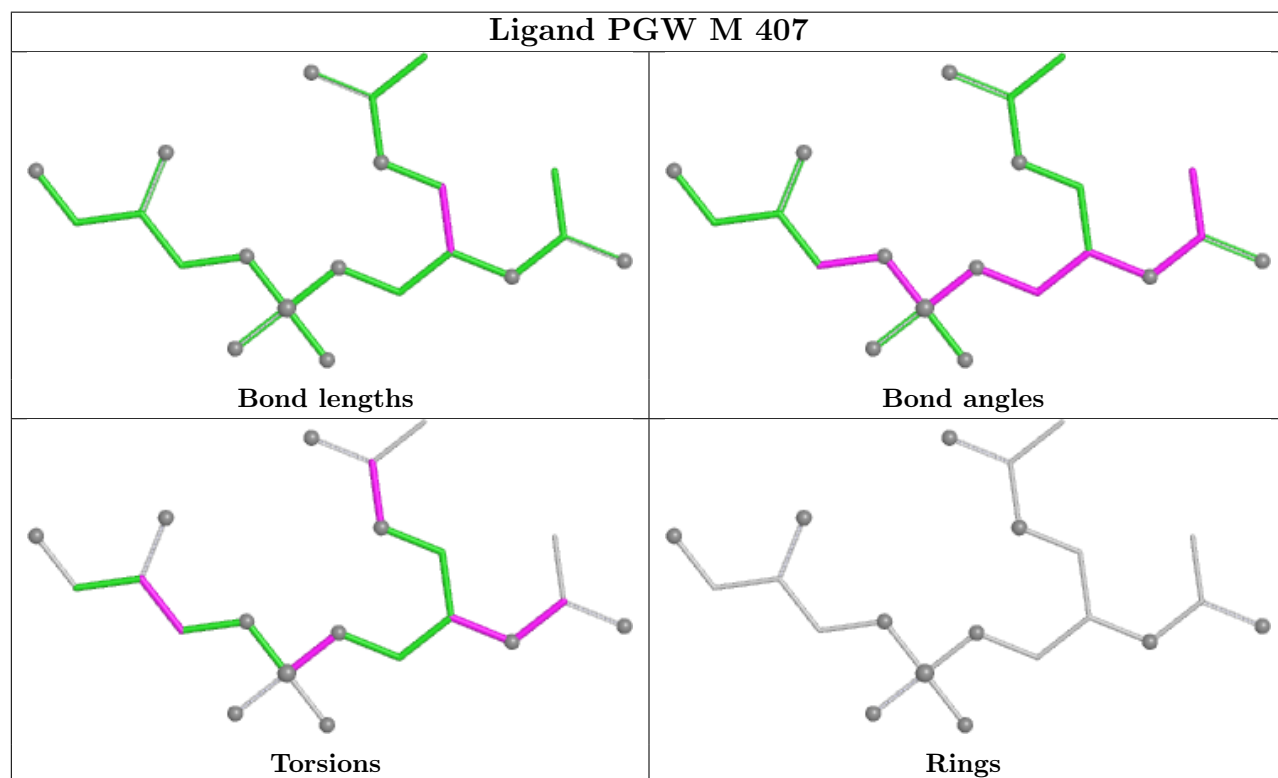
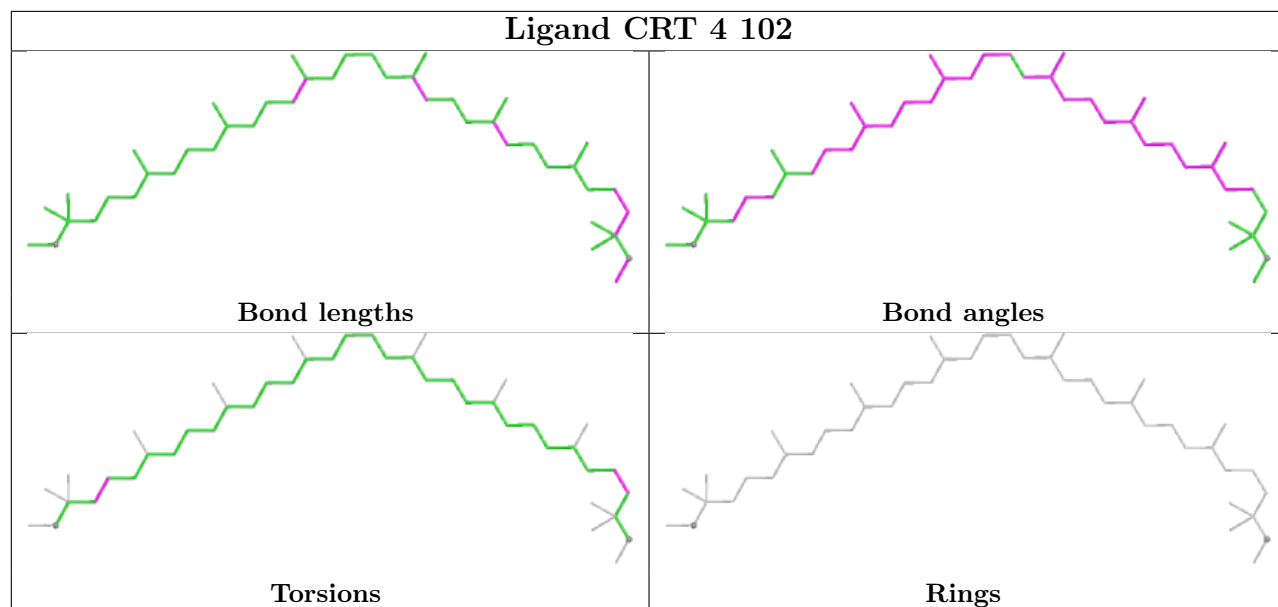


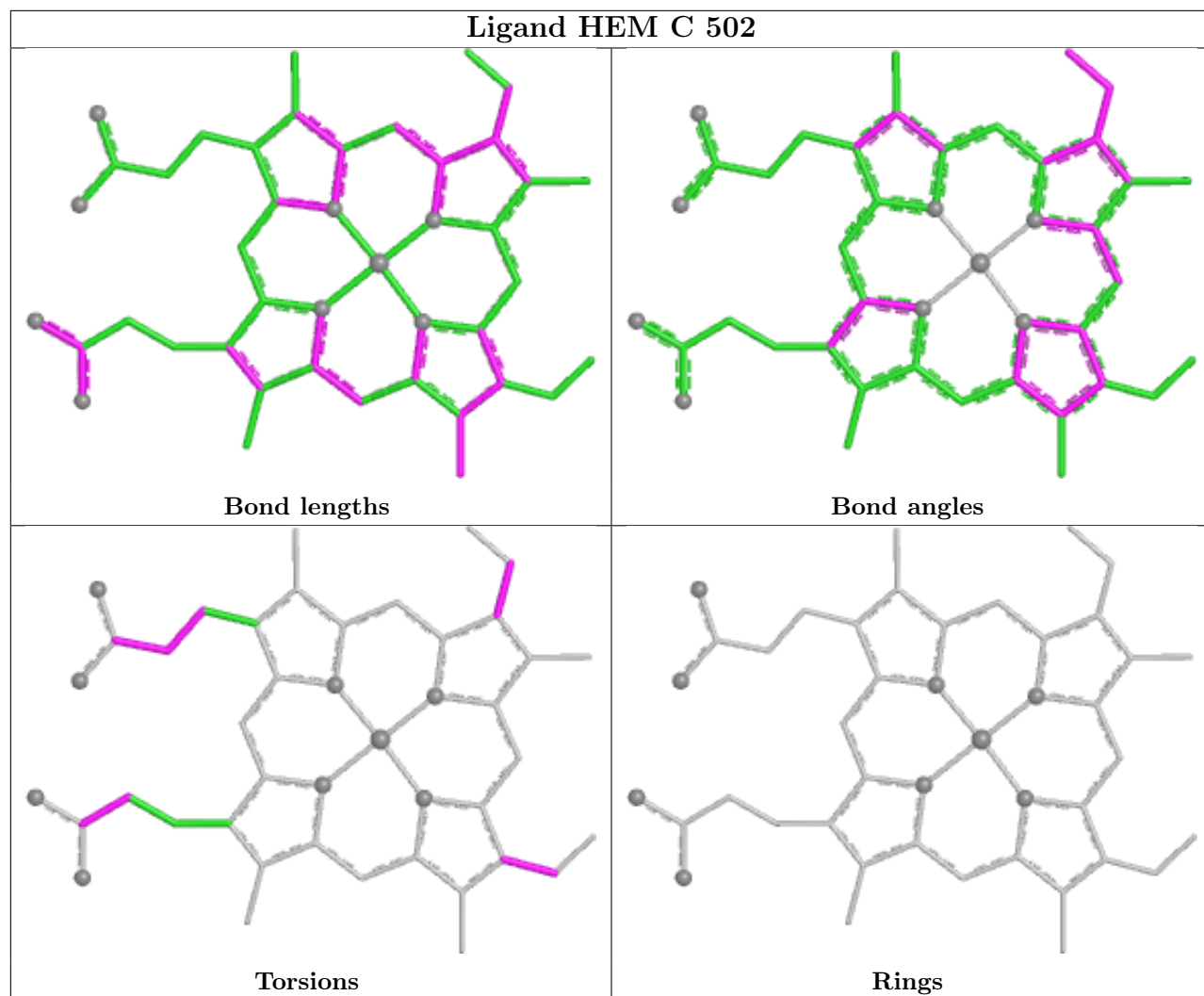


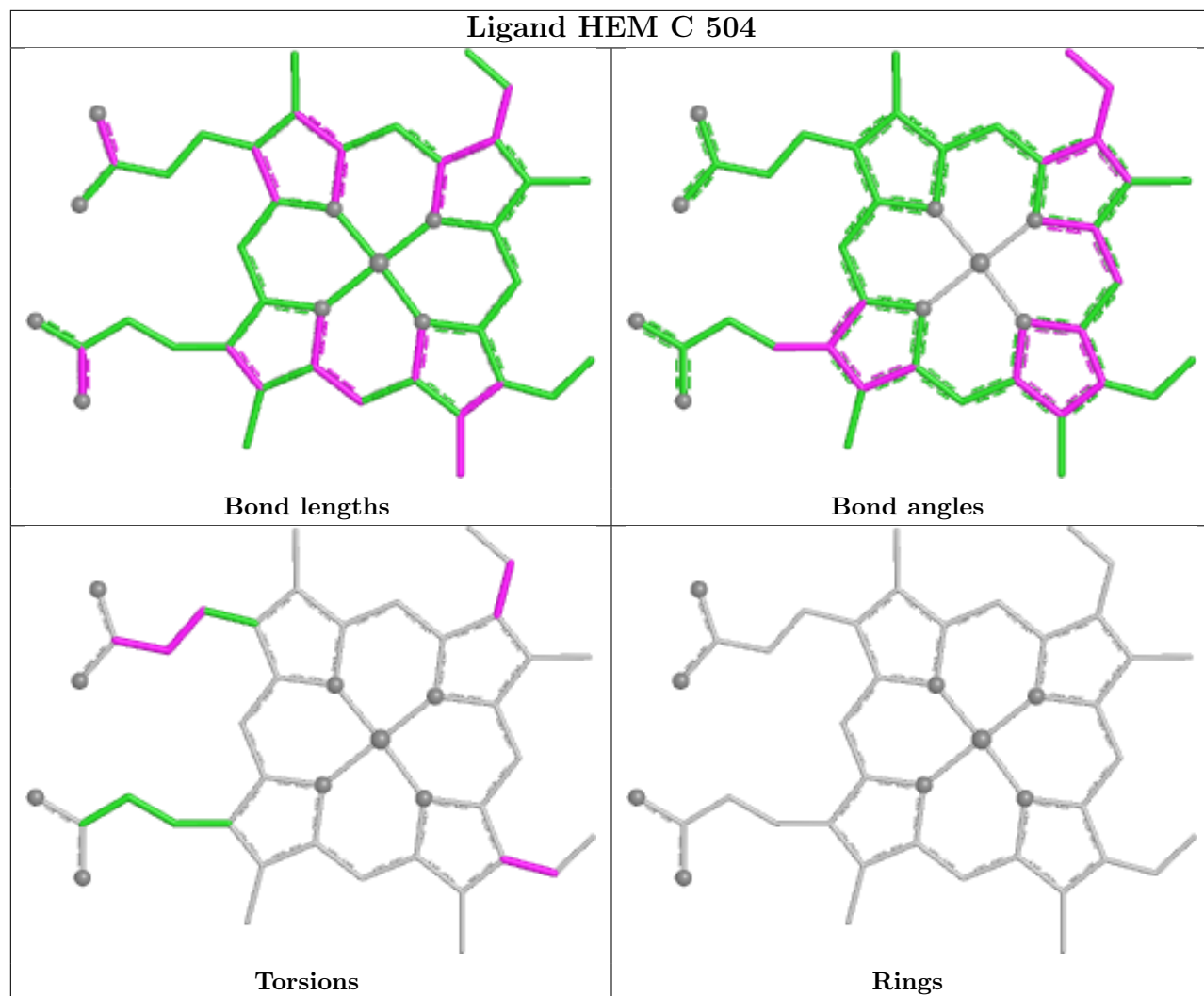


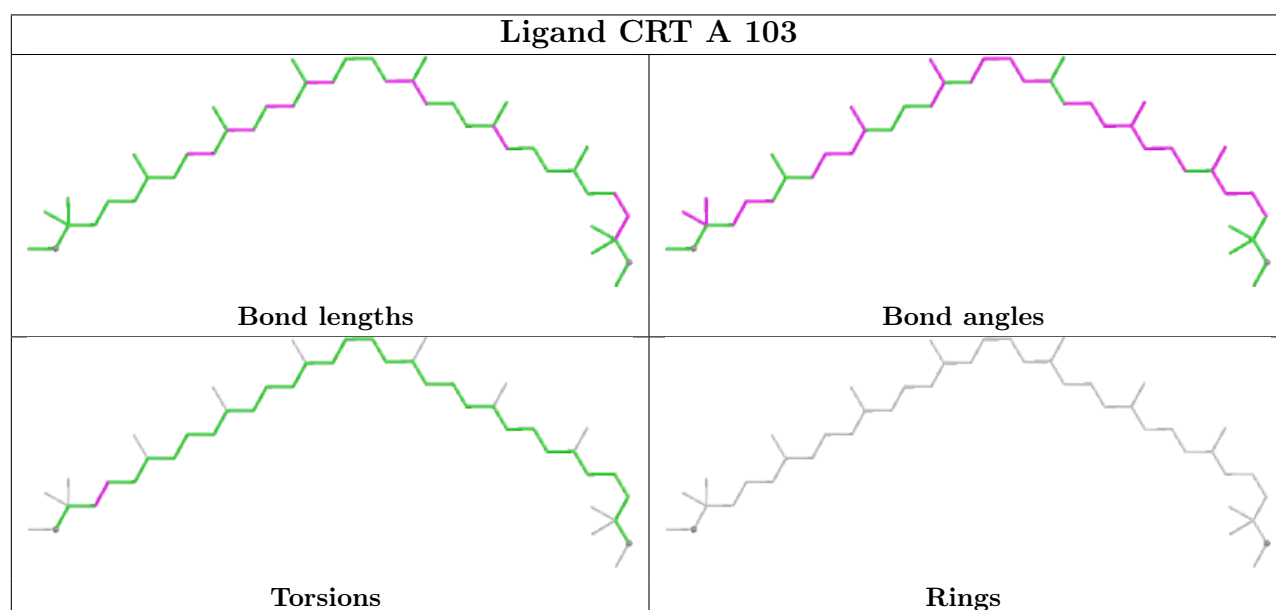
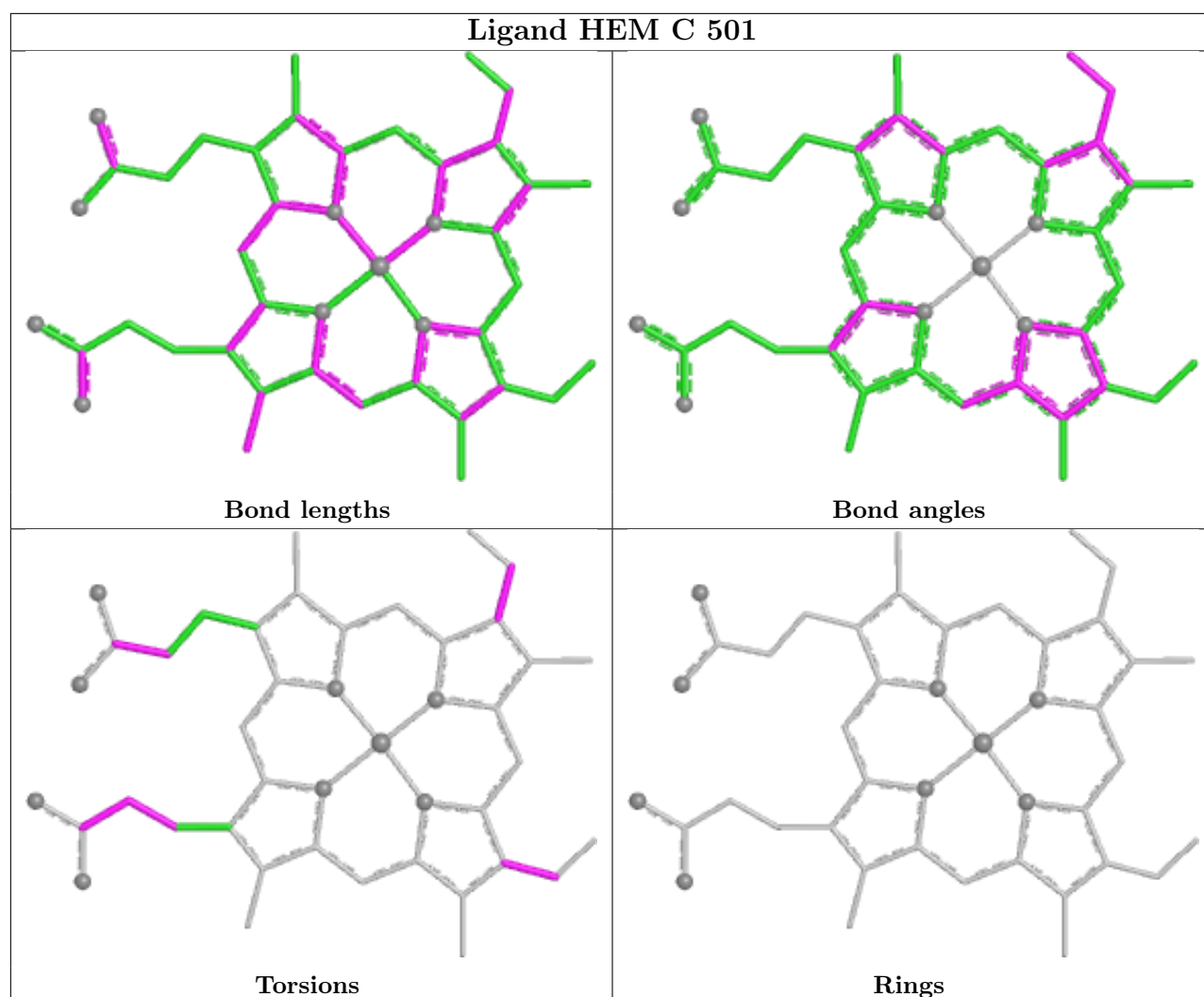


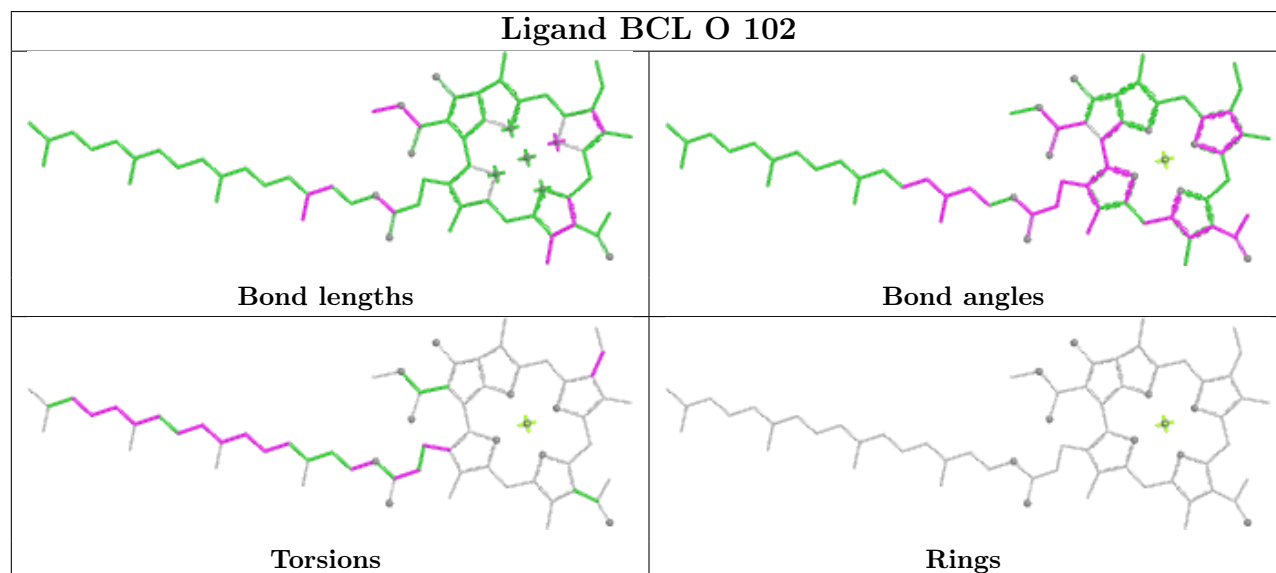
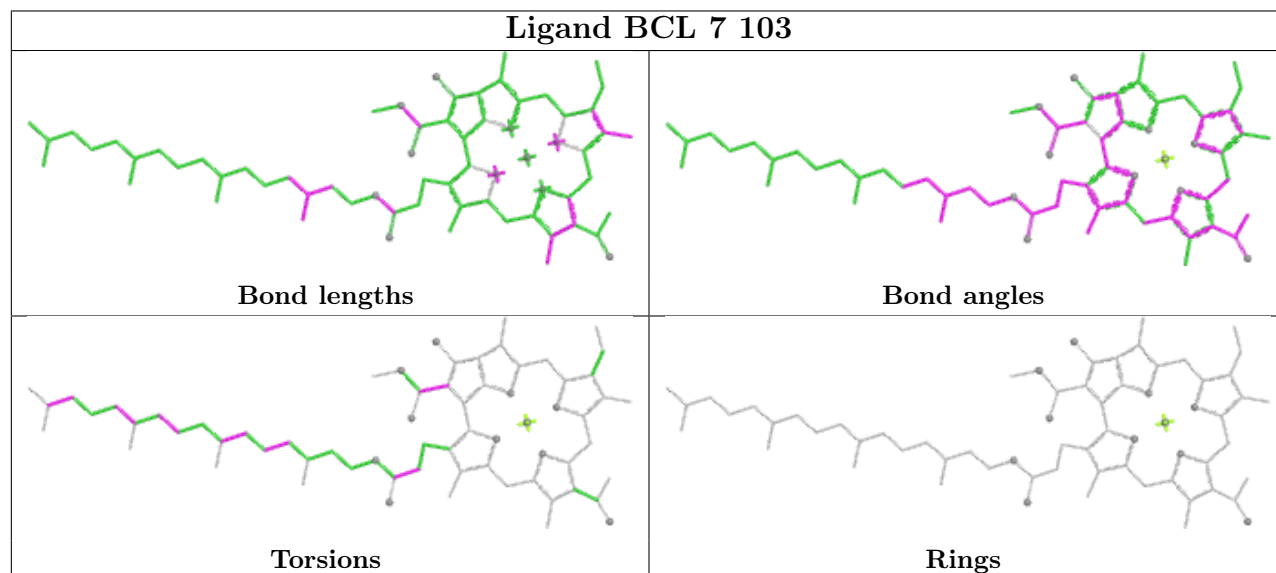
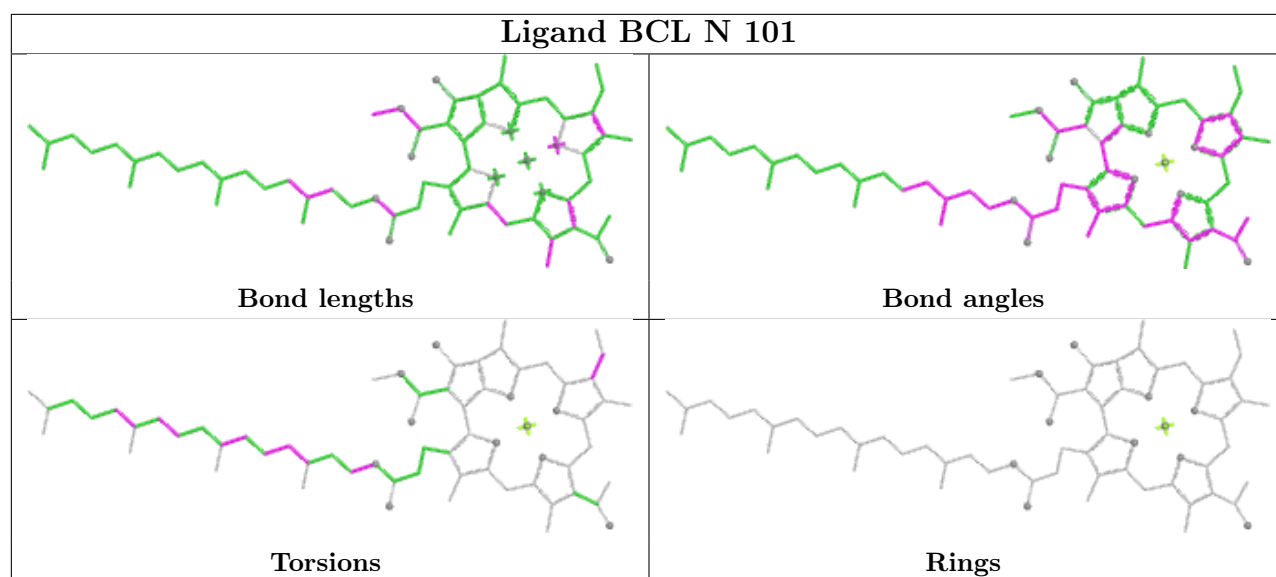


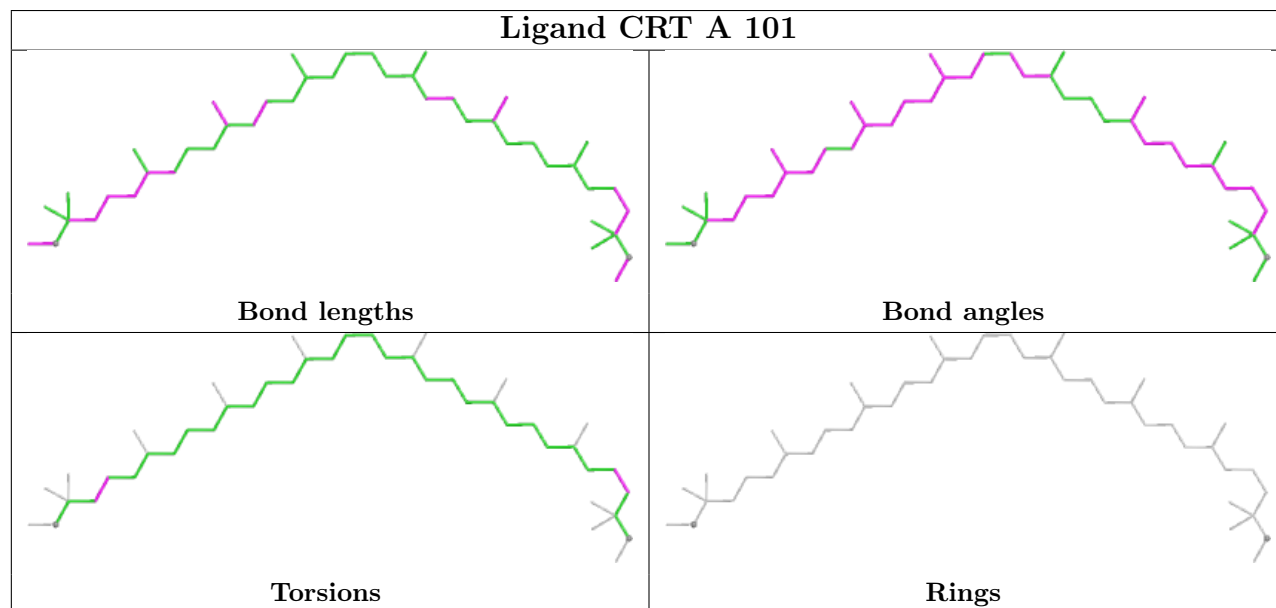
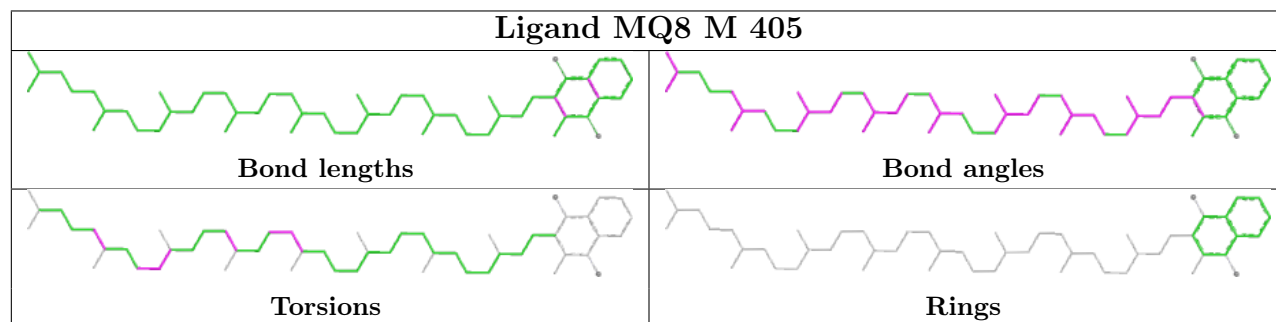
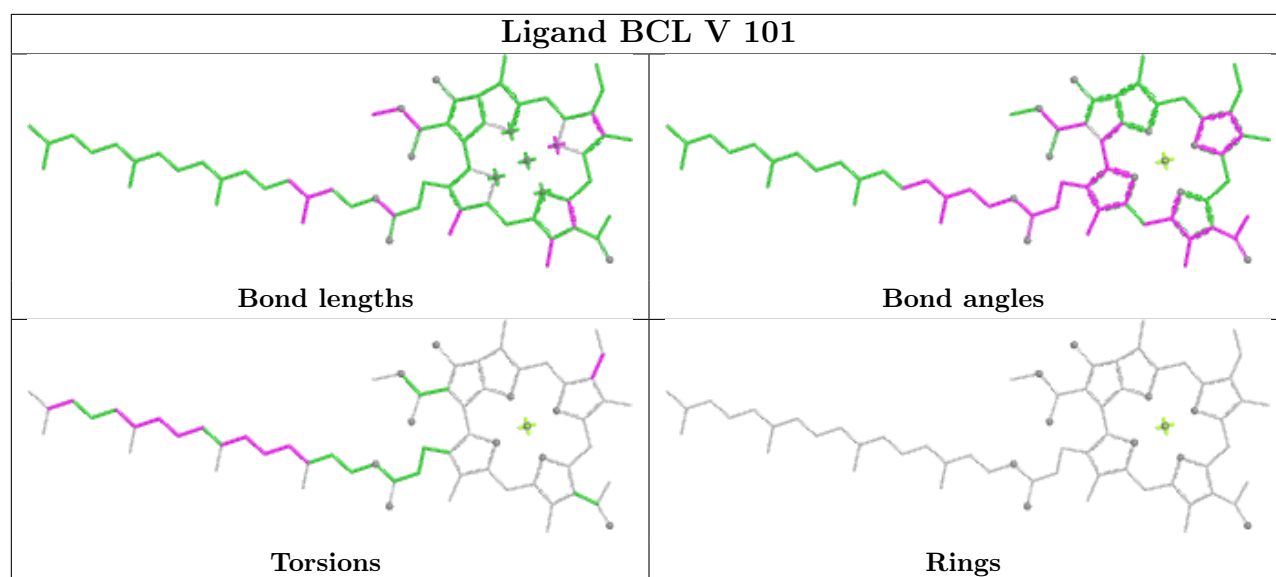


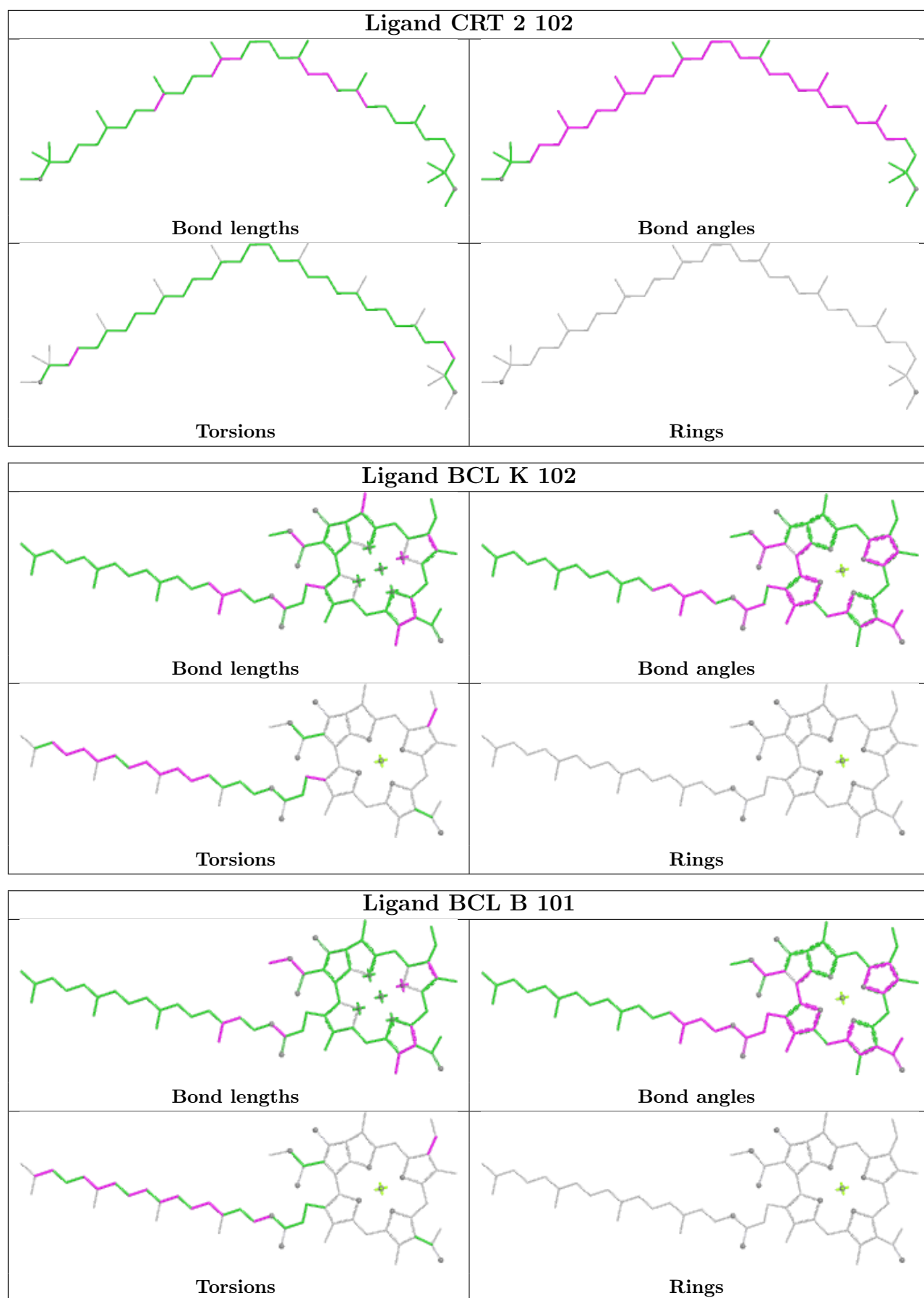


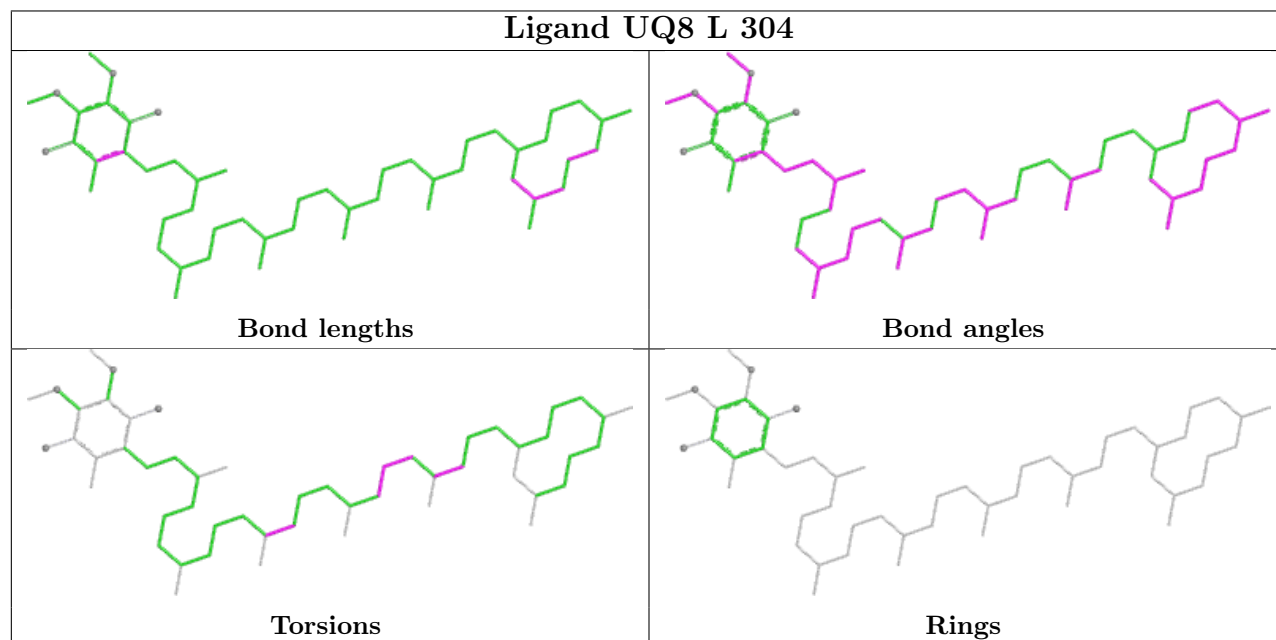
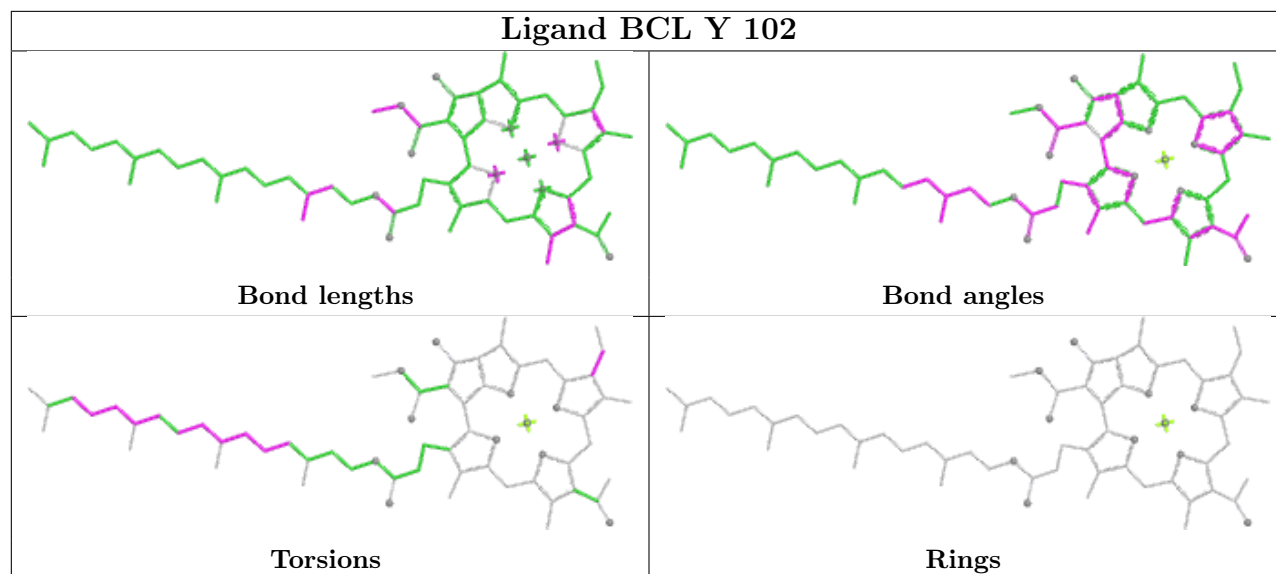


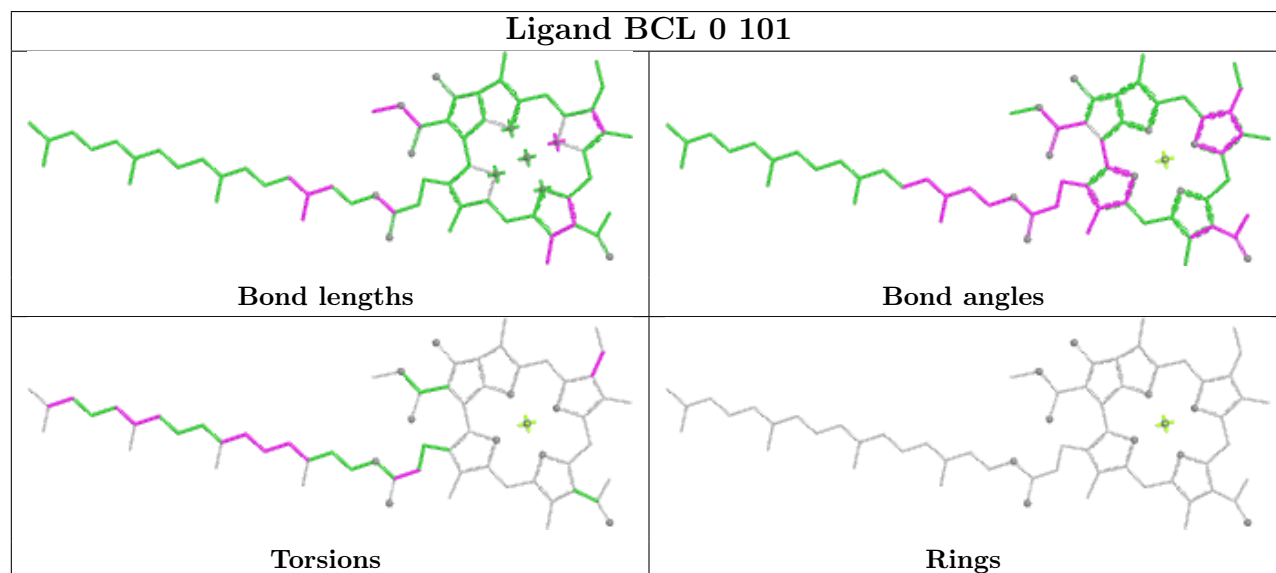
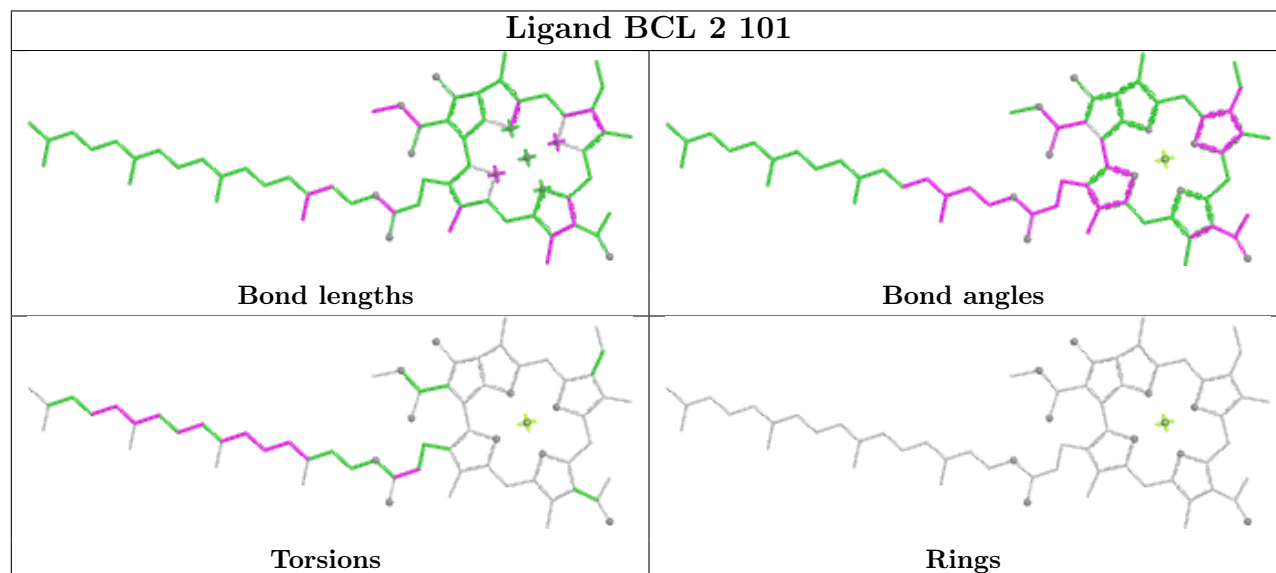
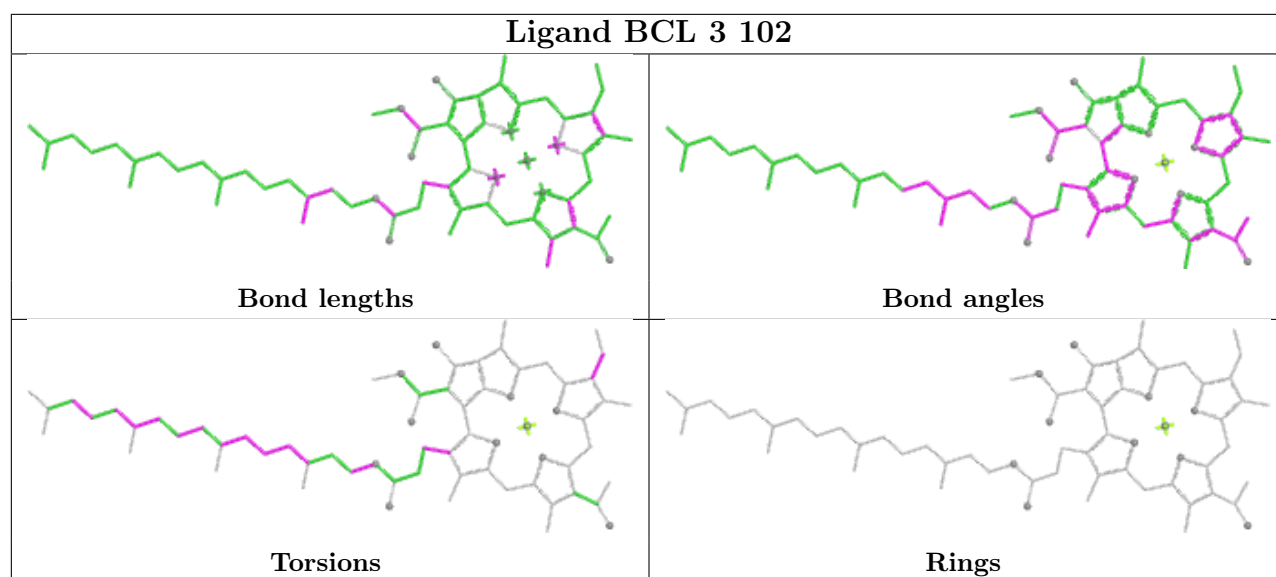


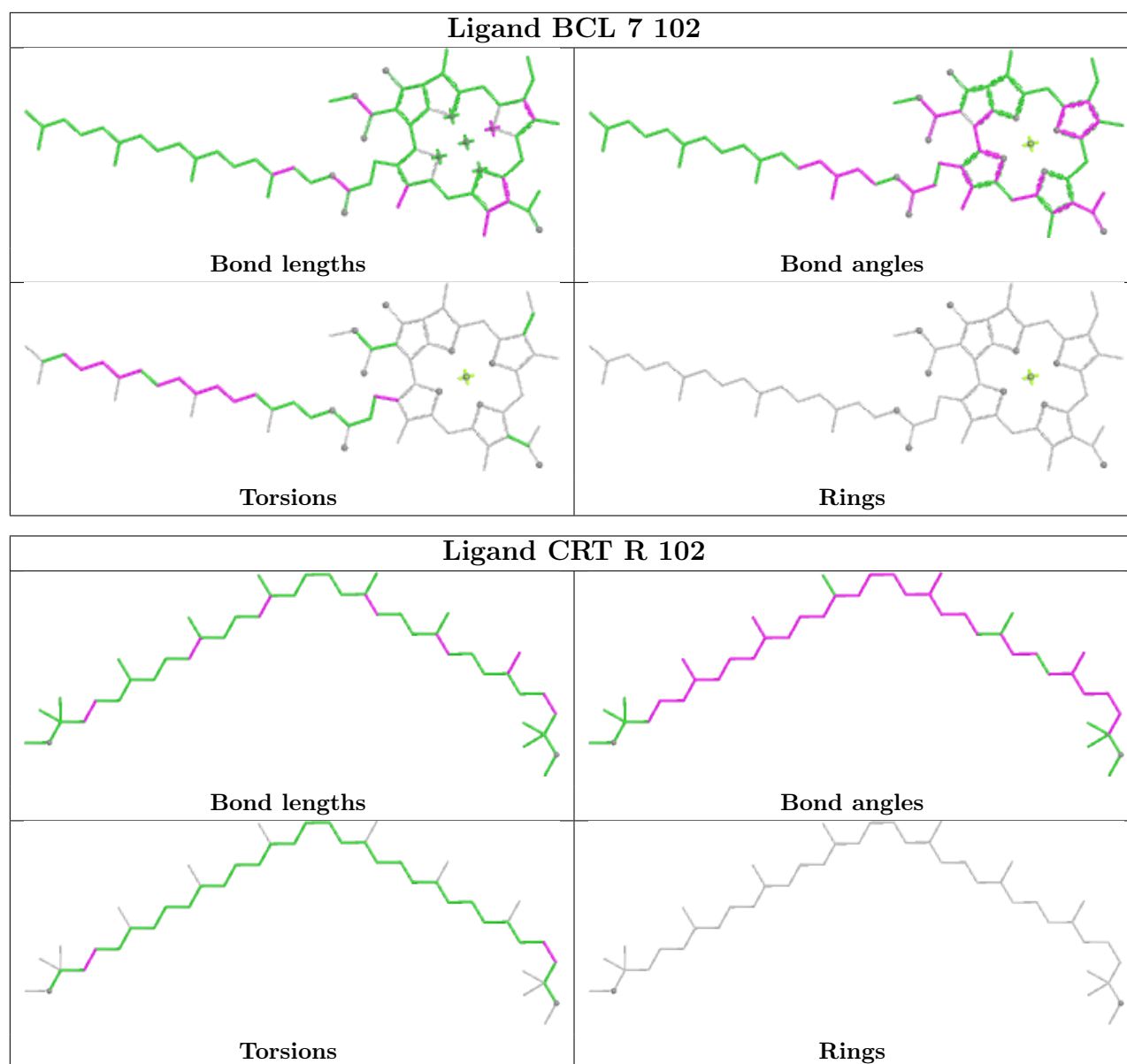


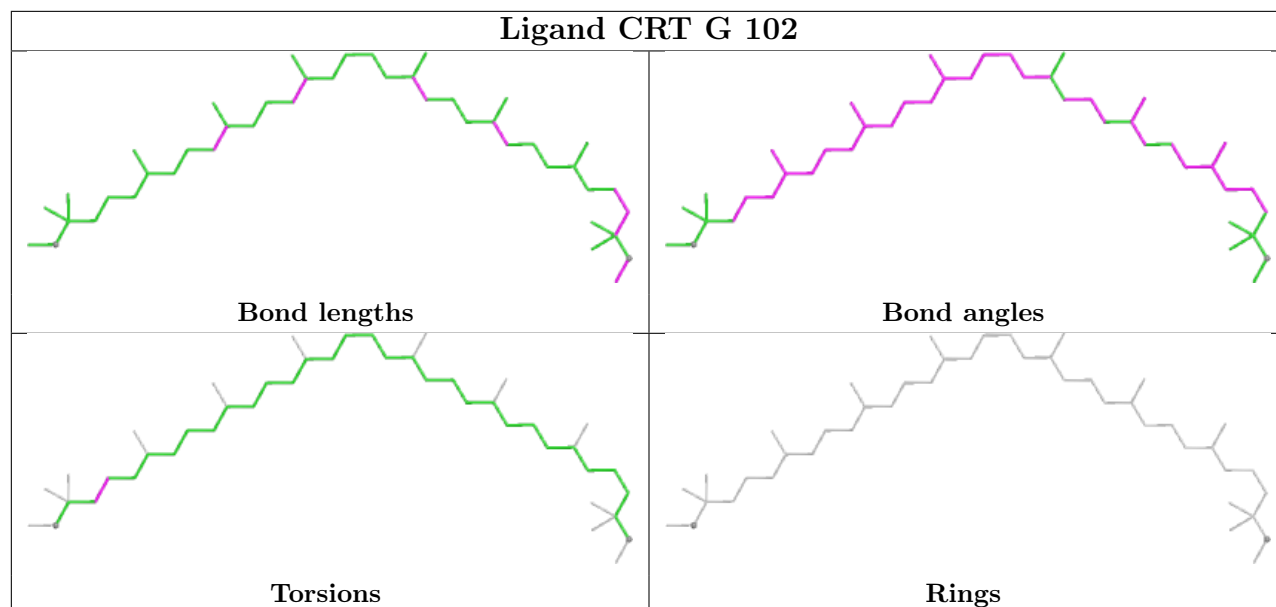












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	317/404 (78%)	0.84	46 (14%) 6 3	3, 67, 117, 142	1 (0%)
2	L	280/281 (99%)	0.64	31 (11%) 10 6	15, 66, 102, 123	0
3	M	319/325 (98%)	0.80	36 (11%) 10 6	32, 76, 115, 142	0
4	H	258/259 (99%)	1.03	42 (16%) 4 3	45, 89, 152, 198	0
5	1	60/61 (98%)	1.44	17 (28%) 1 1	62, 109, 257, 261	0
5	3	60/61 (98%)	1.38	18 (30%) 1 1	66, 137, 225, 231	0
5	5	60/61 (98%)	1.95	23 (38%) 1 1	82, 165, 250, 269	0
5	7	60/61 (98%)	1.23	11 (18%) 3 2	80, 149, 247, 254	0
5	9	60/61 (98%)	1.49	19 (31%) 1 1	74, 142, 282, 286	0
5	A	60/61 (98%)	1.96	24 (40%) 1 1	87, 147, 249, 250	0
5	D	60/61 (98%)	1.56	17 (28%) 1 1	86, 137, 260, 279	0
5	F	60/61 (98%)	1.59	18 (30%) 1 1	83, 178, 247, 256	0
5	I	60/61 (98%)	2.12	22 (36%) 1 1	81, 150, 244, 252	0
5	K	60/61 (98%)	1.48	20 (33%) 1 1	95, 155, 258, 259	0
5	O	60/61 (98%)	2.16	22 (36%) 1 1	84, 170, 249, 252	0
5	Q	60/61 (98%)	1.69	16 (26%) 1 1	105, 169, 257, 260	0
5	S	60/61 (98%)	2.50	24 (40%) 1 1	106, 167, 274, 278	0
5	U	60/61 (98%)	1.94	26 (43%) 0 1	80, 151, 265, 290	0
5	W	60/61 (98%)	1.83	23 (38%) 1 1	48, 114, 256, 264	0
5	Y	60/61 (98%)	1.53	17 (28%) 1 1	43, 105, 239, 258	0
6	0	40/47 (85%)	1.10	7 (17%) 4 3	112, 144, 199, 204	0
6	2	40/47 (85%)	0.87	5 (12%) 8 5	94, 117, 178, 181	0
6	4	40/47 (85%)	1.10	8 (20%) 3 2	100, 133, 177, 183	0
6	6	40/47 (85%)	0.81	7 (17%) 4 3	104, 144, 171, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
6	8	40/47 (85%)	1.10	9 (22%) 2 1	107, 140, 180, 182	0
6	B	40/47 (85%)	1.53	15 (37%) 1 1	106, 141, 220, 242	0
6	E	40/47 (85%)	0.85	5 (12%) 8 5	108, 131, 156, 162	0
6	G	40/47 (85%)	1.27	8 (20%) 3 2	125, 155, 169, 179	0
6	J	40/47 (85%)	0.99	6 (15%) 5 3	124, 152, 204, 205	0
6	N	40/47 (85%)	1.88	15 (37%) 1 1	143, 160, 187, 195	0
6	P	40/47 (85%)	1.25	6 (15%) 5 3	136, 158, 179, 183	0
6	R	40/47 (85%)	1.06	9 (22%) 2 1	137, 176, 194, 197	0
6	T	40/47 (85%)	1.26	7 (17%) 4 3	141, 164, 209, 210	0
6	V	40/47 (85%)	1.12	4 (10%) 12 7	107, 141, 157, 160	0
6	X	40/47 (85%)	1.04	9 (22%) 2 1	80, 109, 154, 166	0
6	Z	40/47 (85%)	1.13	9 (22%) 2 1	60, 100, 182, 189	0
All	All	2774/2997 (92%)	1.22	601 (21%) 2 1	3, 109, 237, 290	1 (0%)

The worst 5 of 601 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	Q	14	ILE	12.8
1	C	191	ALA	12.4
5	I	14	ILE	11.5
5	U	15	LEU	11.0
5	S	14	ILE	10.7

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	PGW	M	407	21/51	0.45	0.15	65,132,182,186	0
8	CA	5	101	1/1	0.59	0.23	141,141,141,141	0
15	CRT	A	101	44/44	0.65	0.35	100,120,180,182	0
15	CRT	N	102	44/44	0.71	0.32	151,161,169,169	0
15	CRT	R	102	44/44	0.73	0.29	89,127,136,137	0
15	CRT	2	102	44/44	0.73	0.42	110,160,199,221	0
15	CRT	8	101	44/44	0.73	0.34	138,179,215,216	0
15	CRT	M	406	44/44	0.73	0.24	71,78,104,107	0
15	CRT	J	101	44/44	0.75	0.33	133,168,197,198	0
15	CRT	V	102	44/44	0.76	0.28	76,133,176,179	0
8	CA	3	101	1/1	0.76	0.20	113,113,113,113	0
12	PO4	H	303	5/5	0.78	0.20	112,113,126,128	0
15	CRT	A	103	44/44	0.78	0.41	169,184,188,189	0
8	CA	O	101	1/1	0.78	0.22	167,167,167,167	0
12	PO4	M	408	5/5	0.79	0.11	106,119,123,135	0
15	CRT	W	103	44/44	0.80	0.30	77,126,154,155	0
15	CRT	B	102	44/44	0.80	0.34	125,143,171,171	0
9	BCL	6	101	66/66	0.81	0.24	105,119,198,199	0
11	UQ8	L	304	53/53	0.81	0.30	84,134,142,144	0
15	CRT	P	102	44/44	0.82	0.40	187,222,226,227	0
8	CA	C	505	1/1	0.82	0.24	93,93,93,93	0
15	CRT	T	102	44/44	0.82	0.33	136,158,177,178	0
12	PO4	H	304	5/5	0.82	0.15	130,131,142,148	0
15	CRT	3	103	44/44	0.83	0.31	116,145,185,187	0
15	CRT	4	102	44/44	0.83	0.26	107,121,188,189	0
12	PO4	L	305	5/5	0.83	0.12	84,104,111,116	0
9	BCL	N	101	66/66	0.83	0.22	101,123,189,191	0
15	CRT	G	102	44/44	0.84	0.30	138,158,216,217	0
9	BCL	9	102	66/66	0.84	0.18	122,129,145,154	0
15	CRT	X	102	44/44	0.84	0.33	131,163,207,207	0
9	BCL	I	102	66/66	0.84	0.19	79,89,147,149	0
9	BCL	I	103	66/66	0.85	0.27	96,117,201,205	0
9	BCL	D	102	66/66	0.85	0.23	120,130,197,203	0
8	CA	Q	101	1/1	0.85	0.11	159,159,159,159	0
9	BCL	2	101	66/66	0.86	0.24	81,102,191,196	0
9	BCL	4	101	66/66	0.86	0.21	72,101,222,225	0
9	BCL	G	101	66/66	0.86	0.25	110,123,217,218	0
8	CA	I	101	1/1	0.86	0.23	158,158,158,158	0
9	BCL	B	101	66/66	0.86	0.25	104,120,212,217	0
8	CA	A	104	1/1	0.86	0.21	185,185,185,185	0
9	BCL	P	101	66/66	0.86	0.18	69,83,204,210	0

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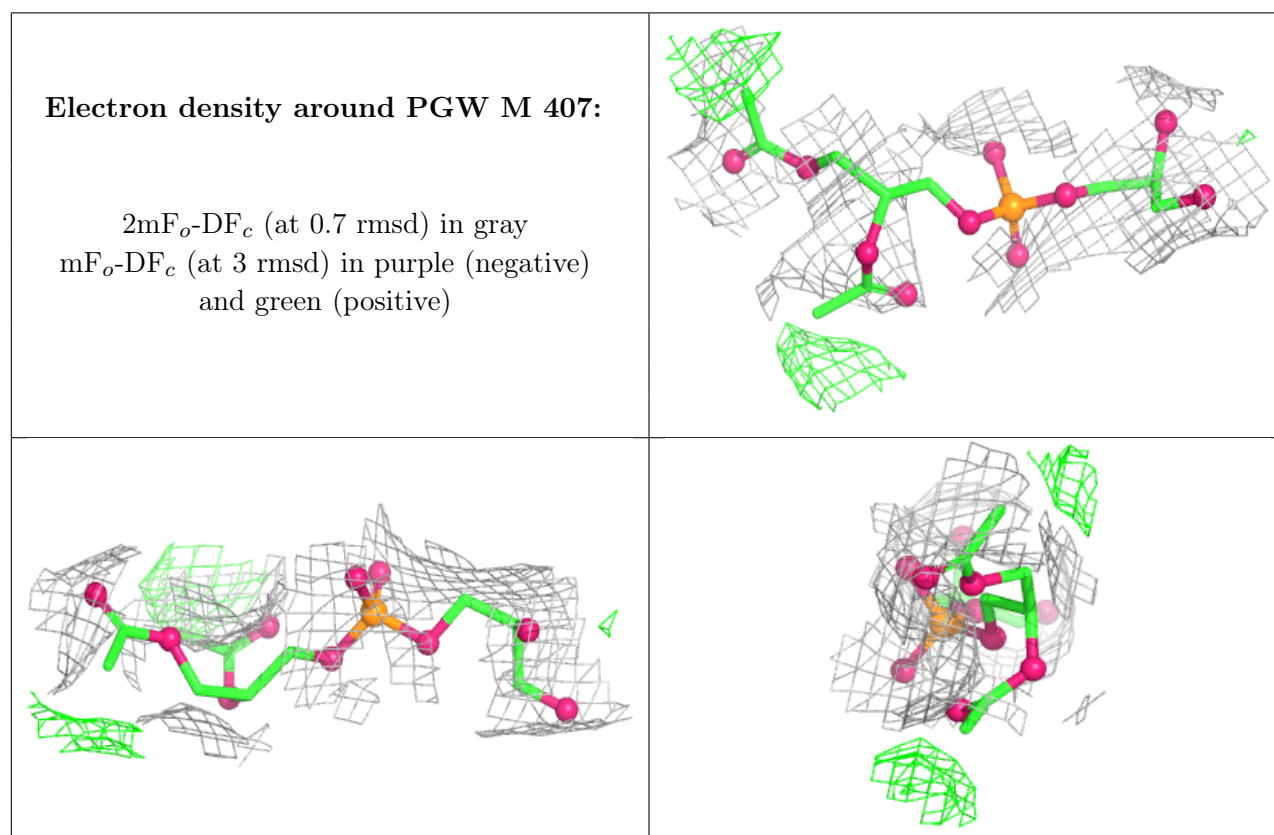
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	BCL	U	102	66/66	0.86	0.24	64,119,243,246	0
9	BCL	X	101	66/66	0.86	0.22	68,86,200,202	0
16	PGW	H	302	21/51	0.86	0.14	64,102,145,160	0
14	MQ8	M	405	53/53	0.87	0.25	27,87,158,160	0
9	BCL	O	101	66/66	0.87	0.16	76,101,202,207	0
9	BCL	F	102	66/66	0.87	0.18	102,112,154,155	0
8	CA	F	101	1/1	0.87	0.18	157,157,157,157	0
9	BCL	R	101	66/66	0.88	0.19	115,128,228,230	0
9	BCL	E	101	66/66	0.88	0.20	95,109,168,172	0
9	BCL	3	102	66/66	0.88	0.17	71,81,147,153	0
9	BCL	V	101	66/66	0.88	0.20	80,97,189,205	0
17	PEF	H	301	19/47	0.88	0.16	75,105,128,134	0
9	BCL	7	102	66/66	0.89	0.18	86,93,190,193	0
9	BCL	O	102	66/66	0.89	0.22	81,93,159,165	0
9	BCL	W	102	66/66	0.89	0.17	47,69,182,185	0
10	BPH	L	302	65/65	0.89	0.19	55,64,75,82	0
9	BCL	K	102	66/66	0.89	0.20	120,127,226,229	0
9	BCL	Z	101	66/66	0.89	0.23	59,71,165,167	0
8	CA	W	101	1/1	0.90	0.10	118,118,118,118	0
9	BCL	7	103	66/66	0.90	0.16	76,89,176,183	0
9	BCL	Q	102	66/66	0.90	0.20	108,115,183,188	0
9	BCL	A	102	66/66	0.90	0.23	123,129,202,205	0
9	BCL	T	101	66/66	0.90	0.21	53,88,229,234	0
10	BPH	M	403	65/65	0.90	0.14	43,59,137,144	0
9	BCL	5	102	66/66	0.90	0.27	124,134,210,214	0
9	BCL	Y	102	66/66	0.90	0.20	48,61,172,173	0
8	CA	D	101	1/1	0.91	0.13	142,142,142,142	0
9	BCL	L	303	66/66	0.91	0.15	20,53,66,82	0
9	BCL	1	102	66/66	0.91	0.18	62,74,153,162	0
9	BCL	S	102	66/66	0.91	0.20	98,112,174,177	0
9	BCL	M	401	66/66	0.91	0.15	40,55,106,109	0
8	CA	K	101	1/1	0.92	0.13	152,152,152,152	0
8	CA	1	101	1/1	0.92	0.13	92,92,92,92	0
8	CA	S	101	1/1	0.93	0.07	154,154,154,154	0
8	CA	7	101	1/1	0.94	0.06	161,161,161,161	0
9	BCL	L	301	66/66	0.94	0.13	10,45,66,69	0
9	BCL	M	402	66/66	0.94	0.12	28,43,60,64	0
8	CA	U	101	1/1	0.95	0.07	125,125,125,125	0
8	CA	Y	101	1/1	0.95	0.14	79,79,79,79	0
7	HEM	C	501	43/43	0.96	0.11	54,64,73,75	0
7	HEM	C	502	43/43	0.96	0.12	41,49,59,64	0
7	HEM	C	503	43/43	0.96	0.13	56,67,85,91	0

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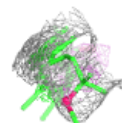
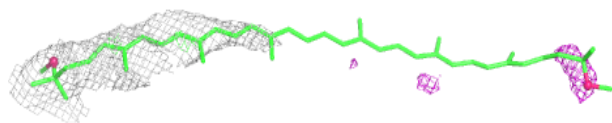
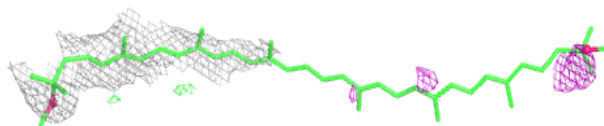
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	FE	M	404	1/1	0.96	0.14	127,127,127,127	0
7	HEM	C	504	43/43	0.96	0.14	43,52,64,74	0
8	CA	9	101	1/1	0.97	0.06	124,124,124,124	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

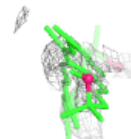
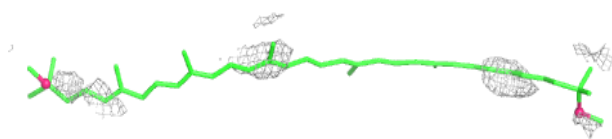
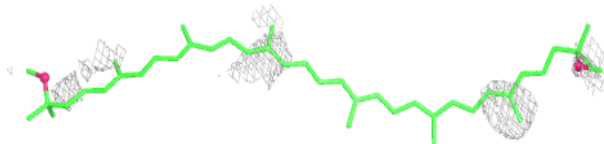


Electron density around CRT A 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

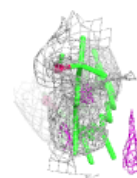
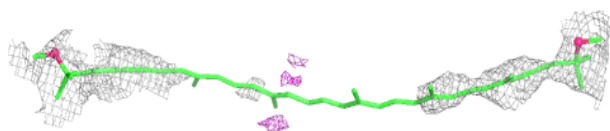
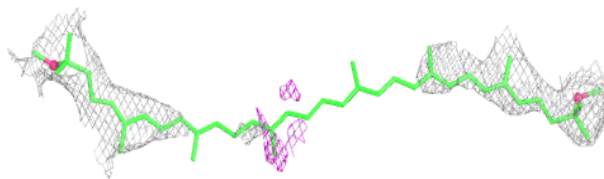
**Electron density around CRT N 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

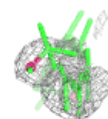
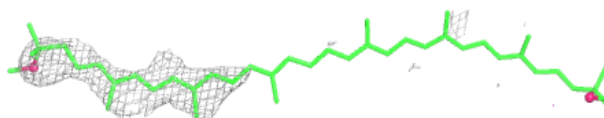


Electron density around CRT R 102:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

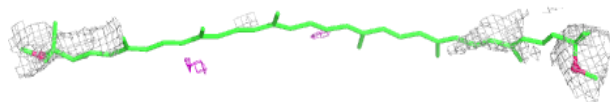
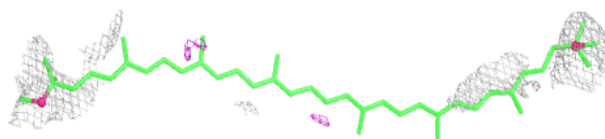
**Electron density around CRT 2 102:**

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and green (positive)

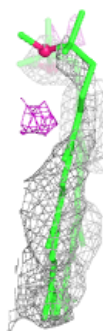
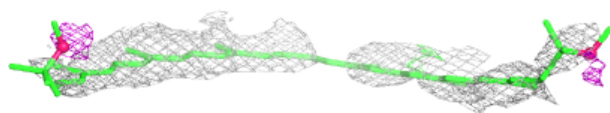
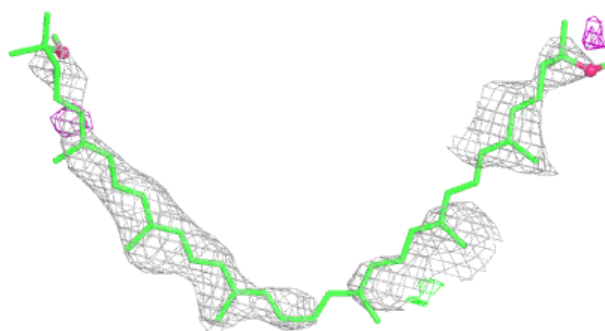


Electron density around CRT 8 101:

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and green (positive)

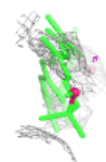
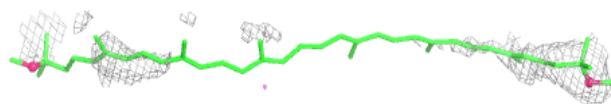
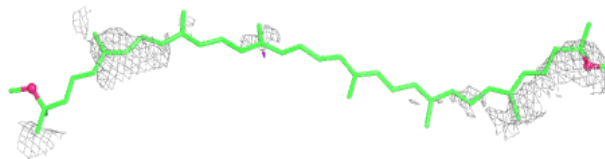
**Electron density around CRT M 406:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

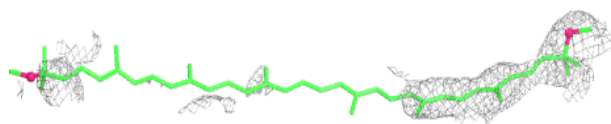
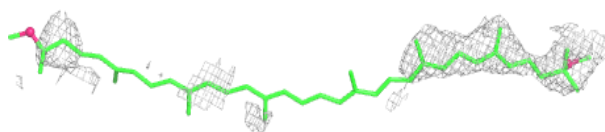


Electron density around CRT J 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

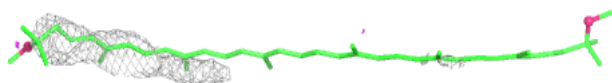
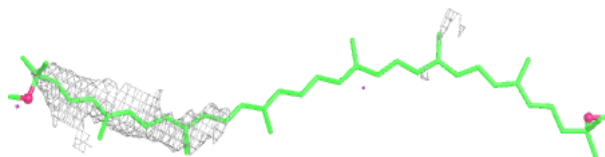
**Electron density around CRT V 102:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

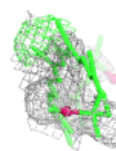
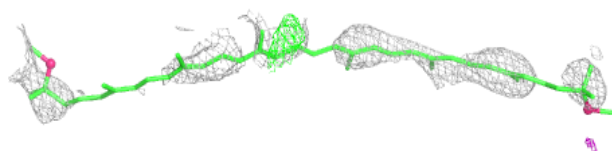
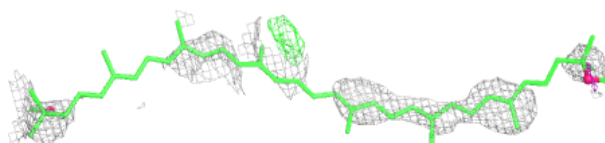


Electron density around CRT A 103:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

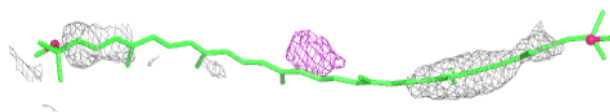
**Electron density around CRT W 103:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



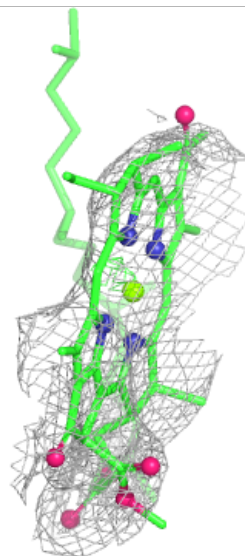
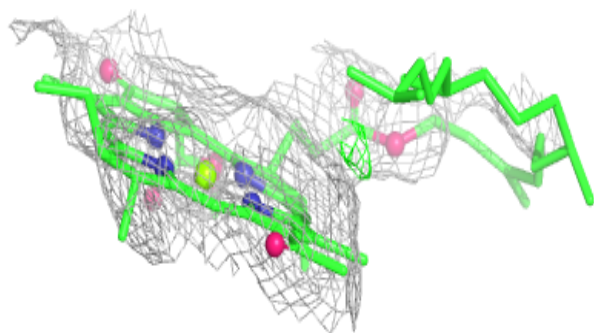
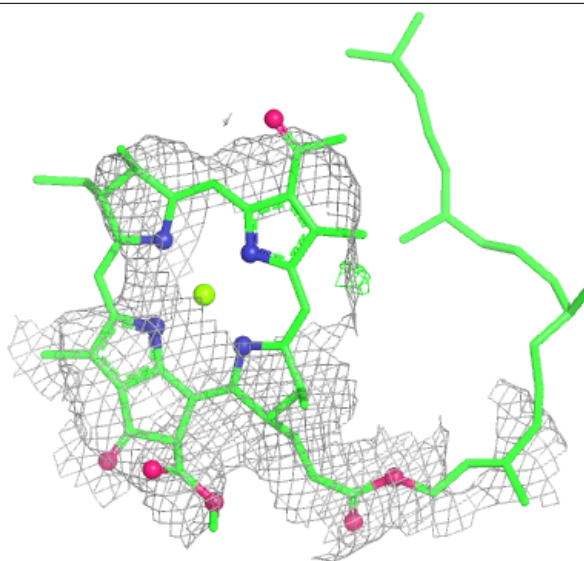
Electron density around CRT B 102:

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and green (positive)



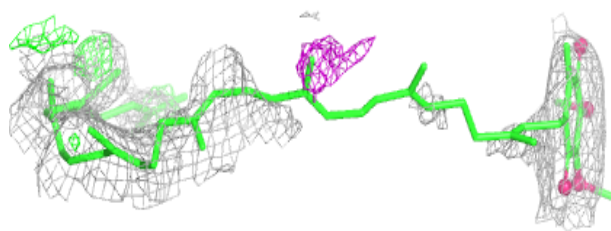
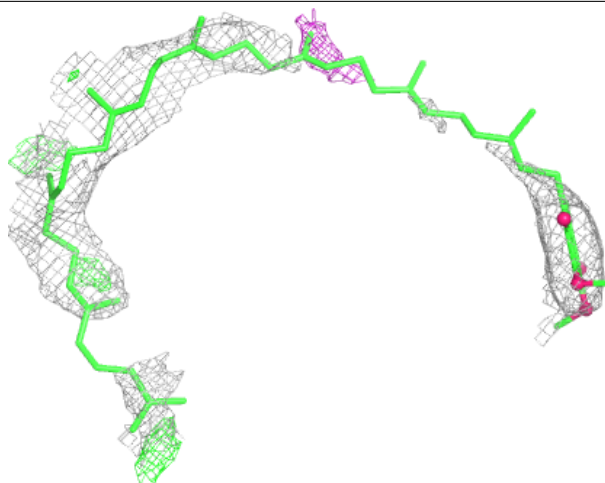
Electron density around BCL 6 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



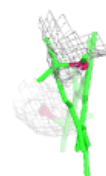
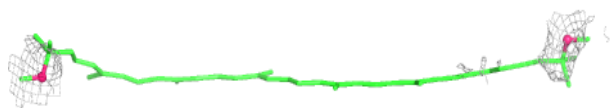
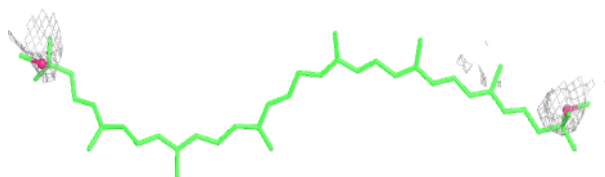
Electron density around UQ8 L 304:

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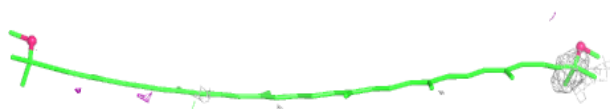
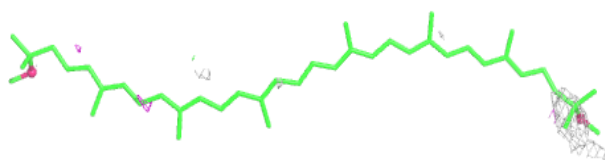


Electron density around CRT P 102:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

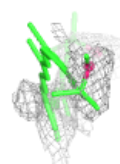
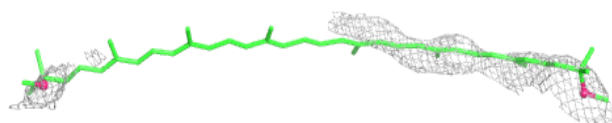
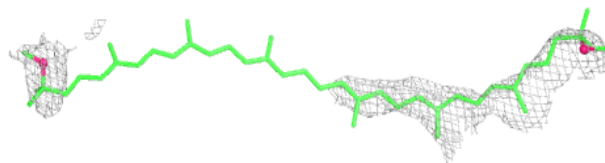
**Electron density around CRT T 102:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

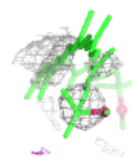
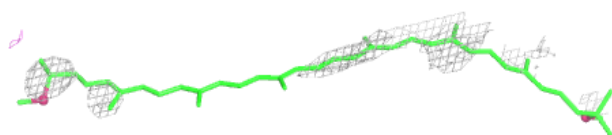
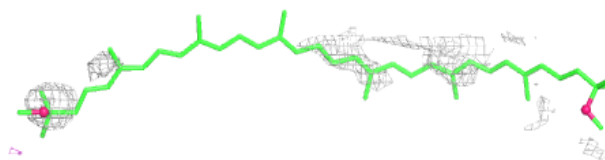


Electron density around CRT 3 103:

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and green (positive)

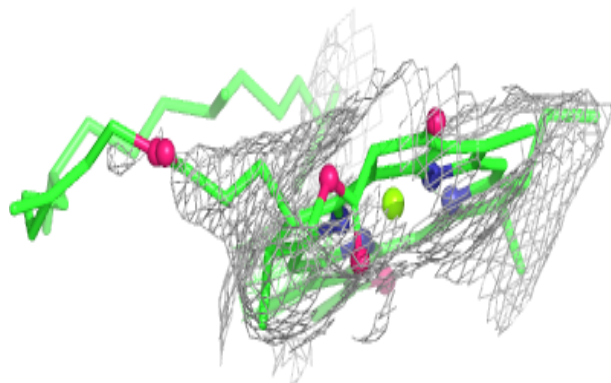
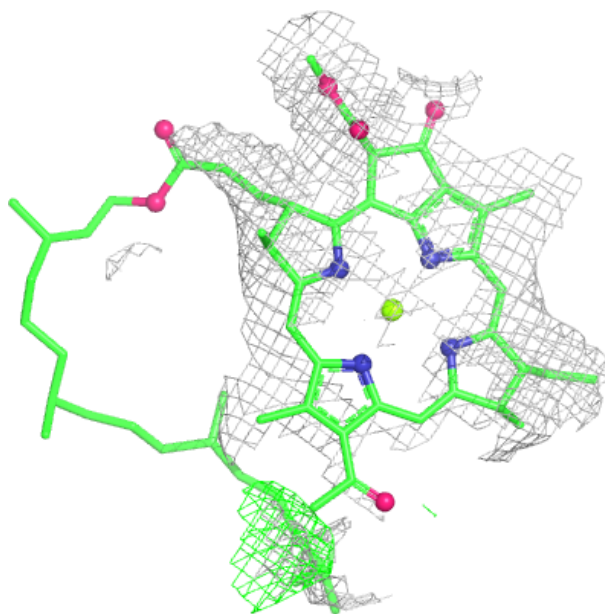
**Electron density around CRT 4 102:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



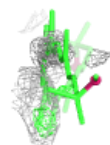
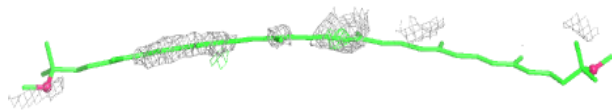
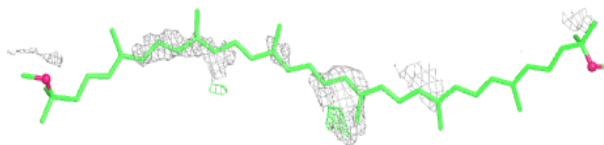
Electron density around BCL N 101:

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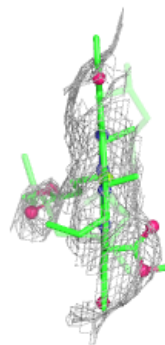
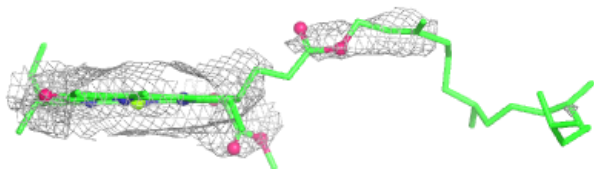
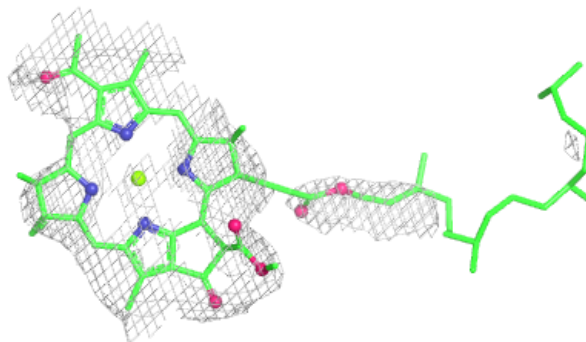


Electron density around CRT G 102:

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and green (positive)

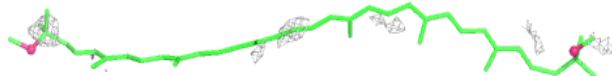
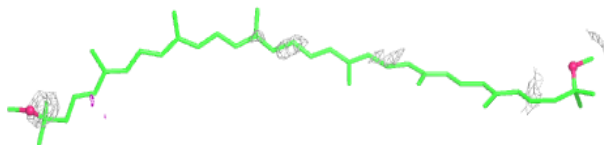
**Electron density around BCL 9 102:**

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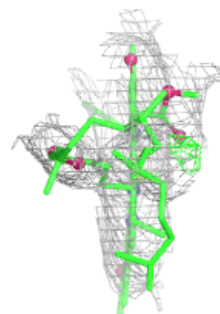
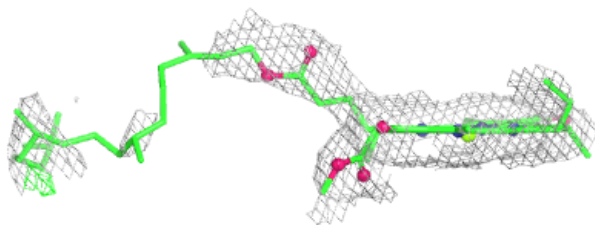
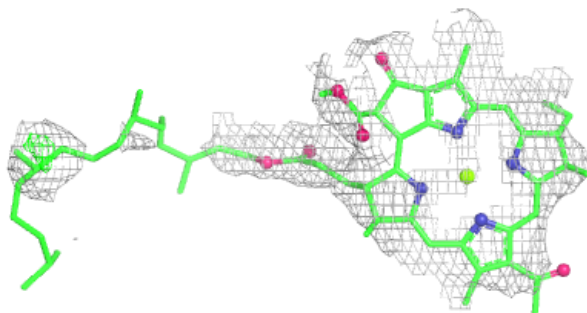


Electron density around CRT X 102:

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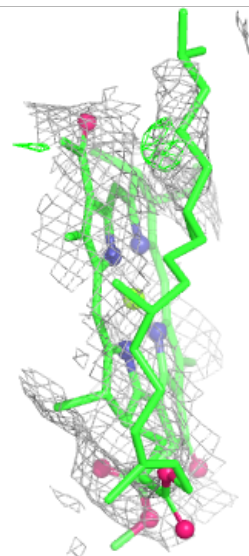
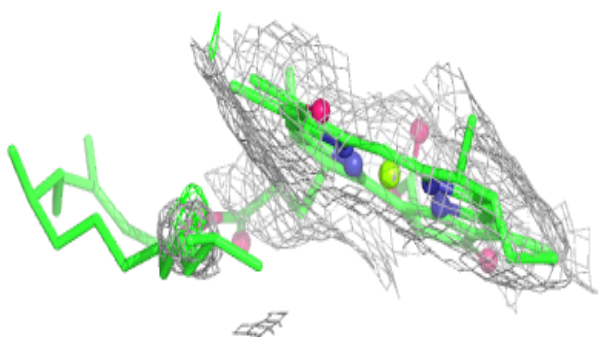
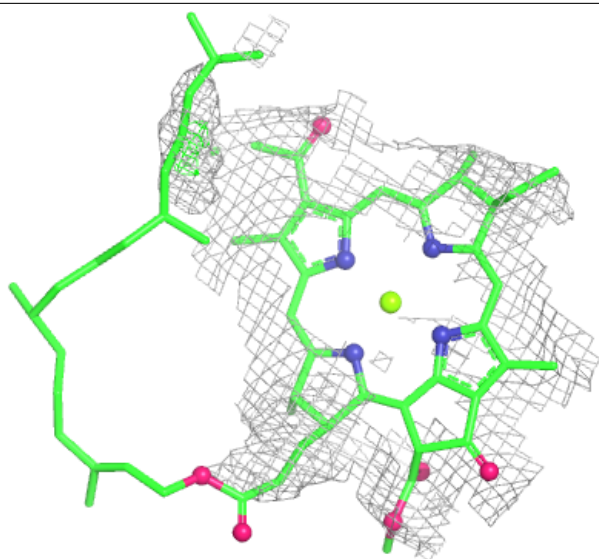
**Electron density around BCL I 102:**

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and green (positive)



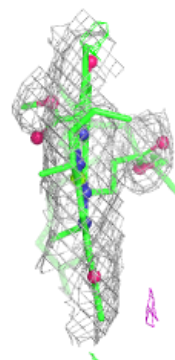
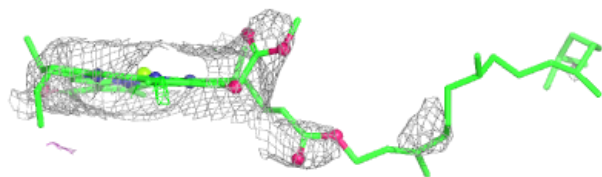
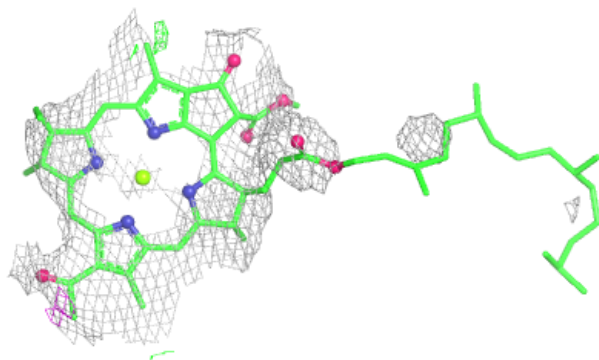
Electron density around BCL I 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



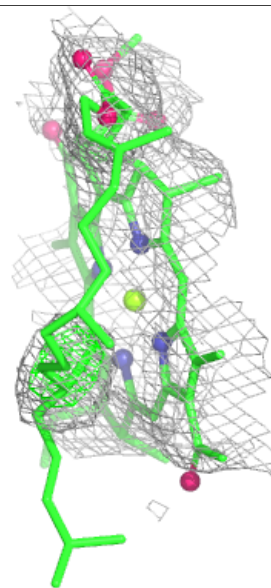
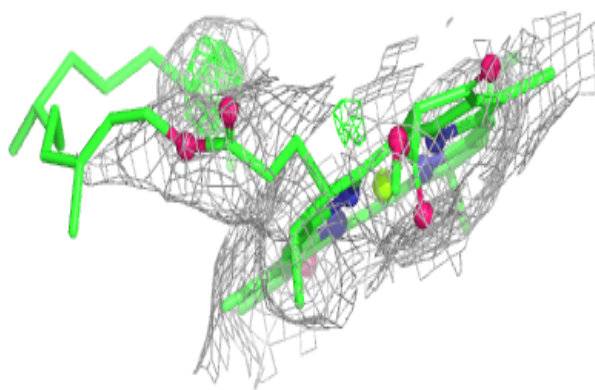
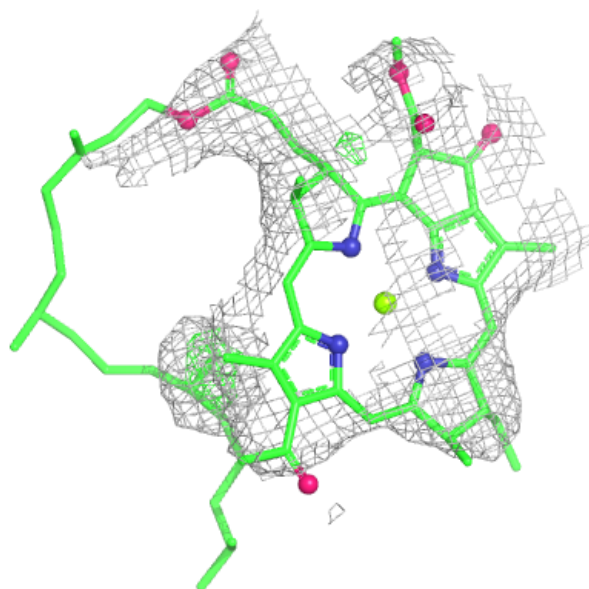
Electron density around BCL D 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



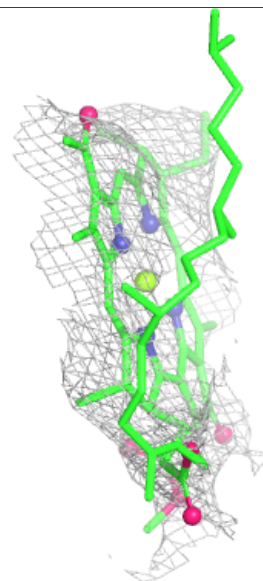
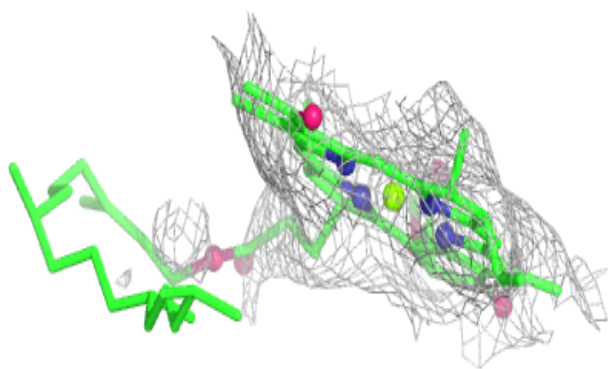
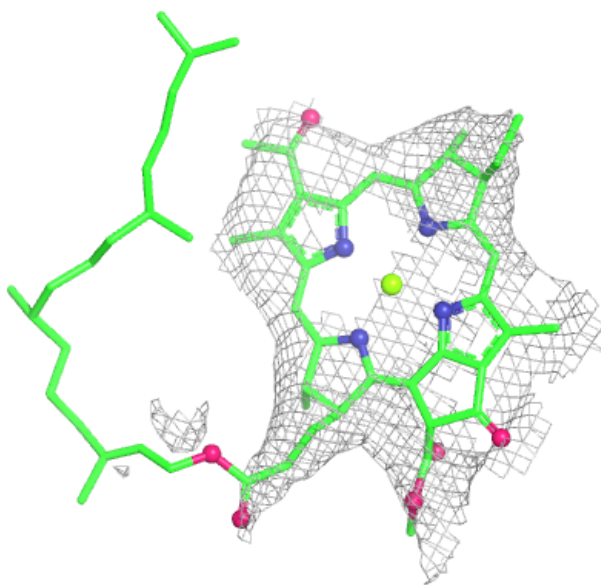
Electron density around BCL 2 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



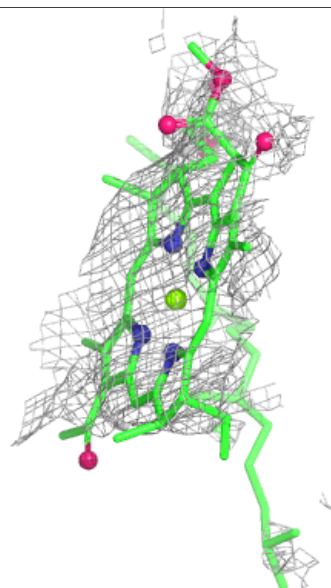
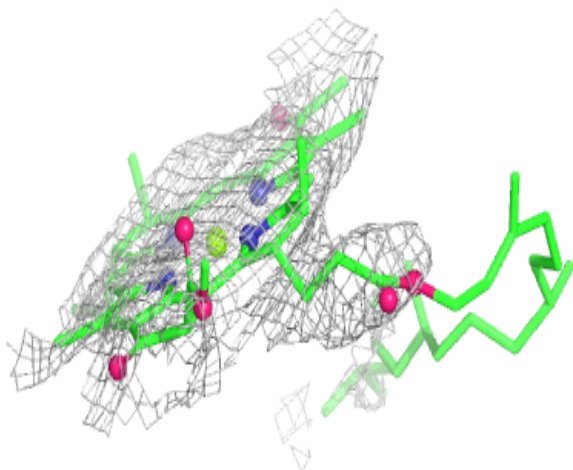
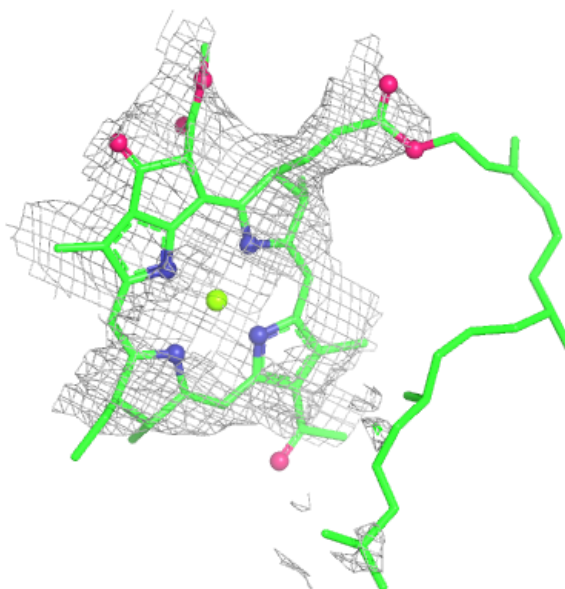
Electron density around BCL 4 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



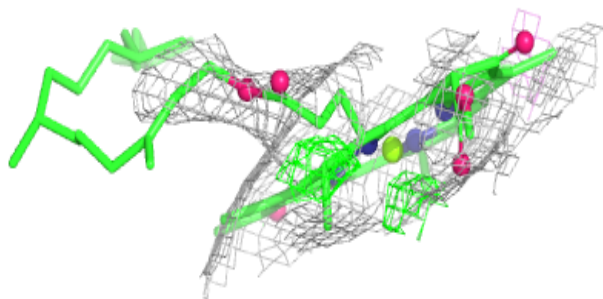
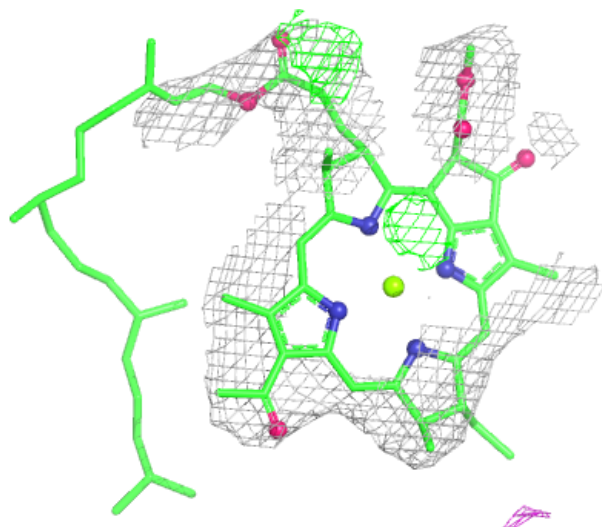
Electron density around BCL G 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



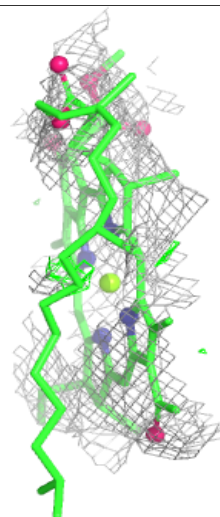
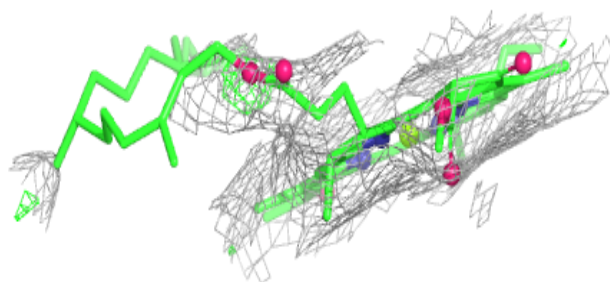
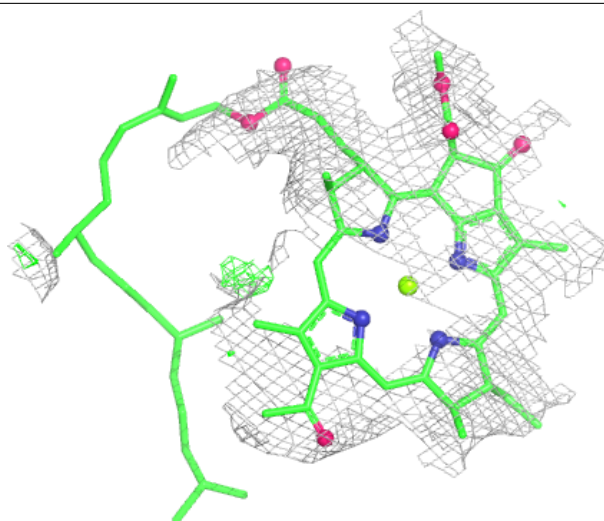
Electron density around BCL B 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



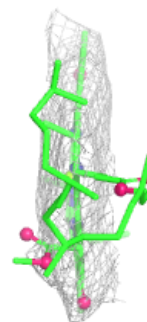
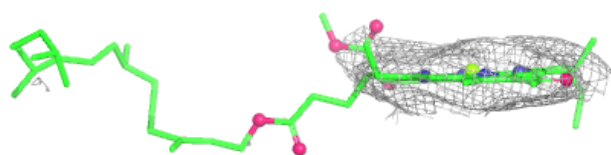
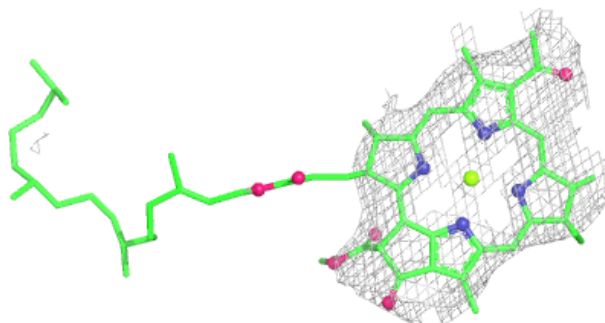
Electron density around BCL P 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



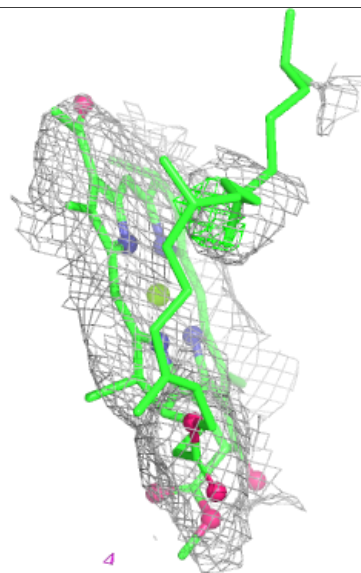
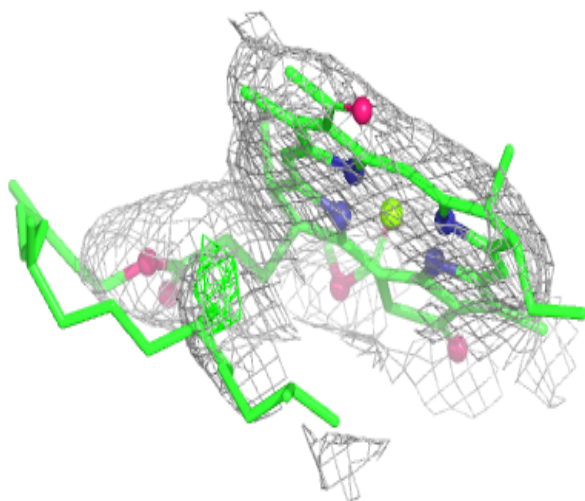
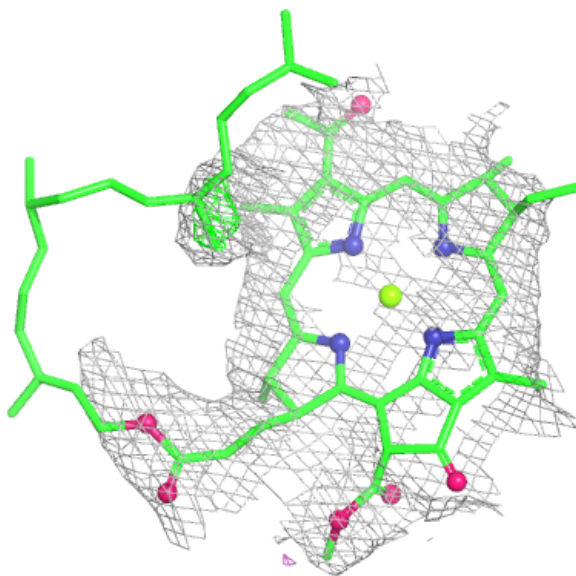
Electron density around BCL U 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



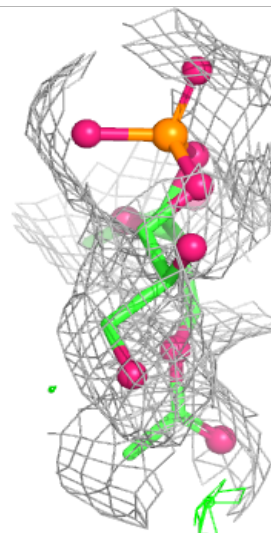
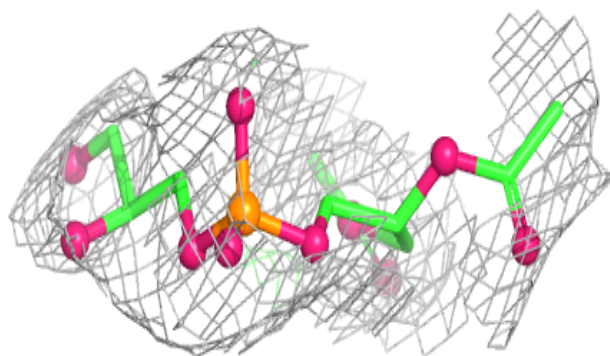
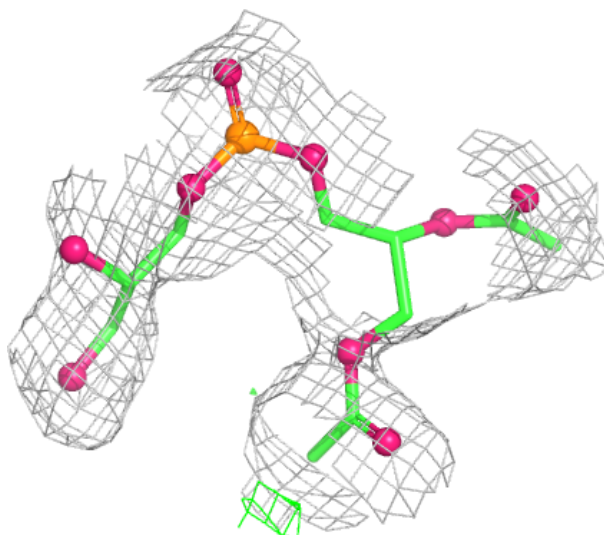
Electron density around BCL X 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



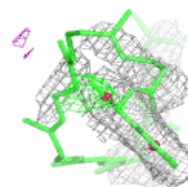
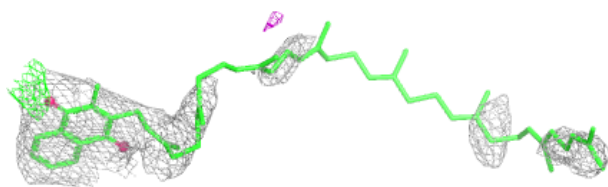
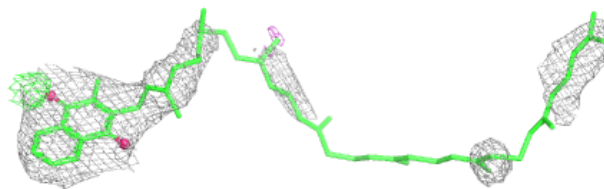
Electron density around PGW H 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



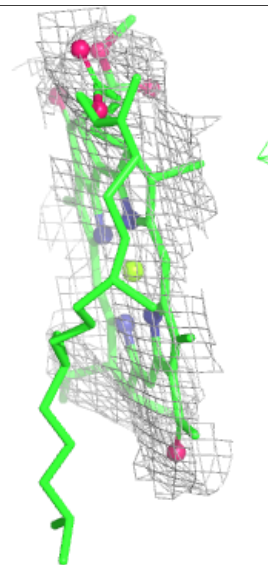
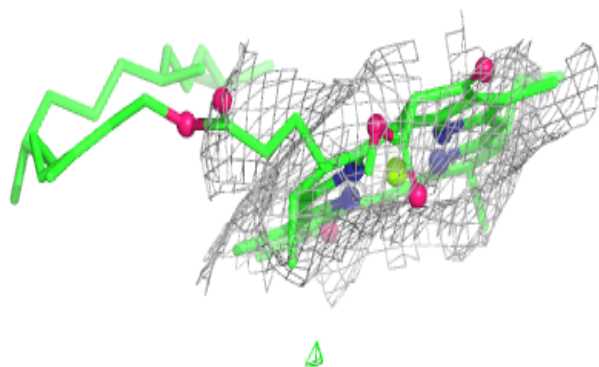
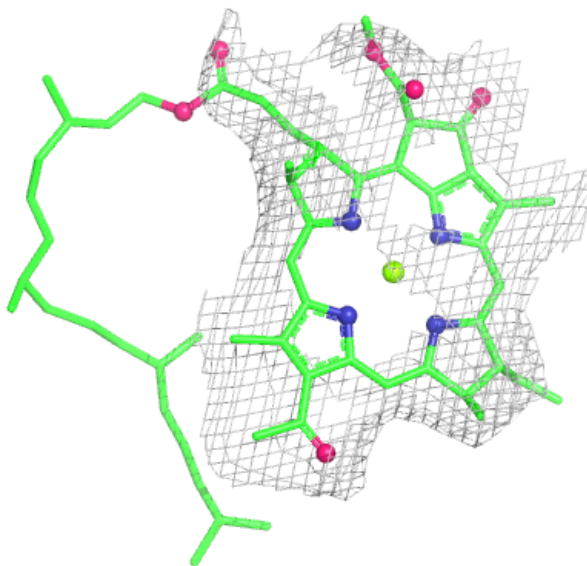
Electron density around MQ8 M 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



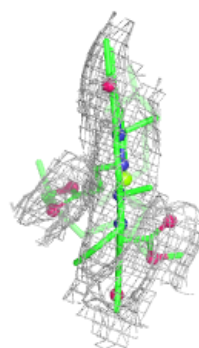
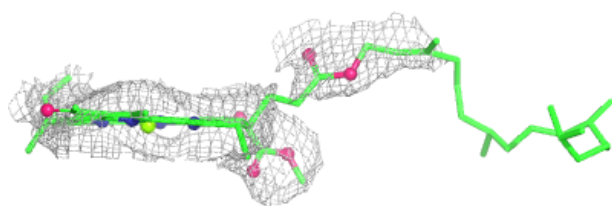
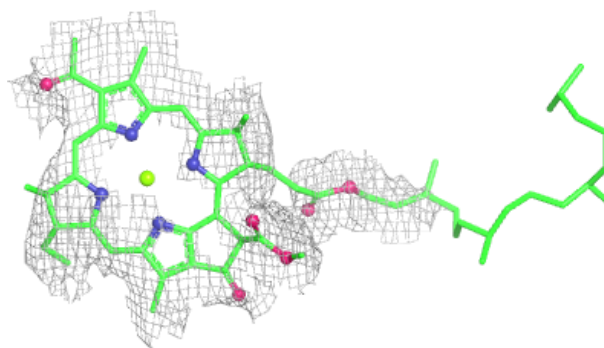
Electron density around BCL 0 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



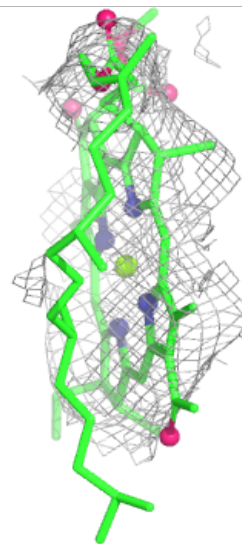
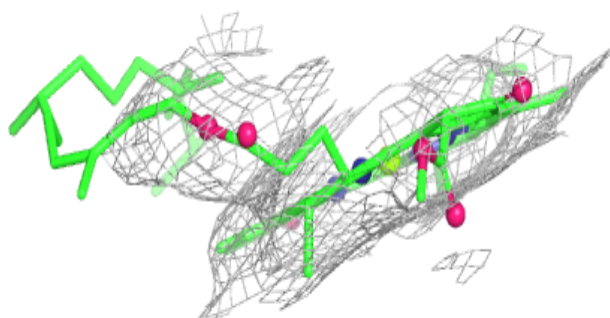
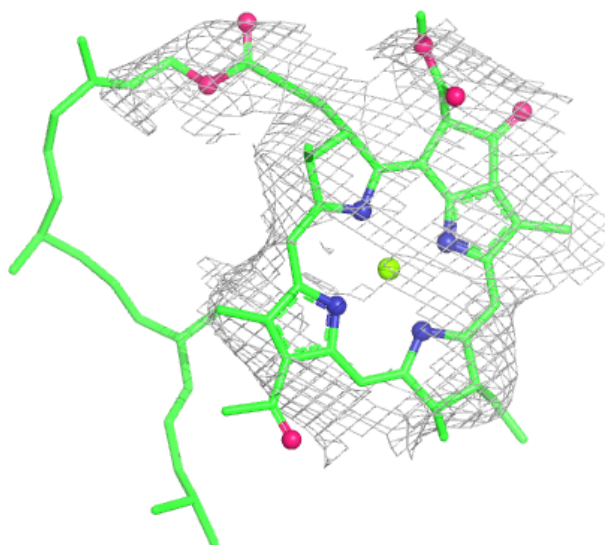
Electron density around BCL F 102:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



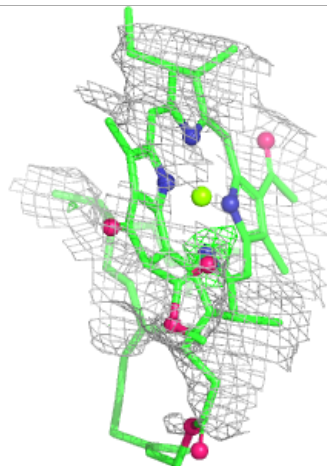
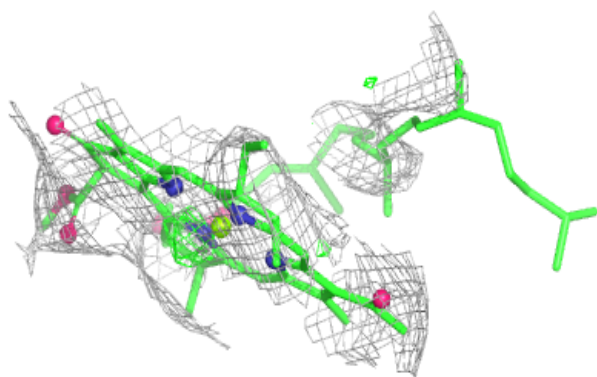
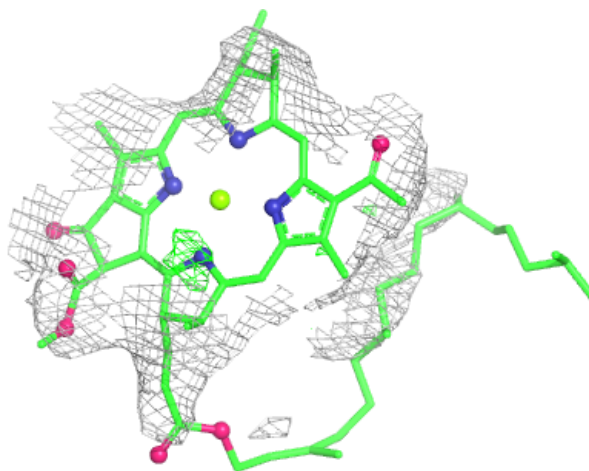
Electron density around BCL R 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



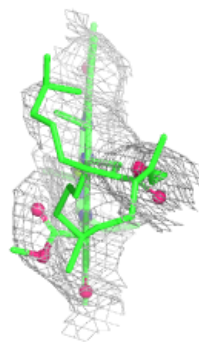
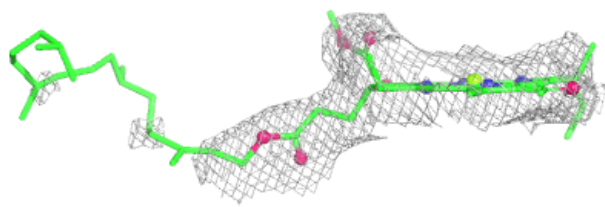
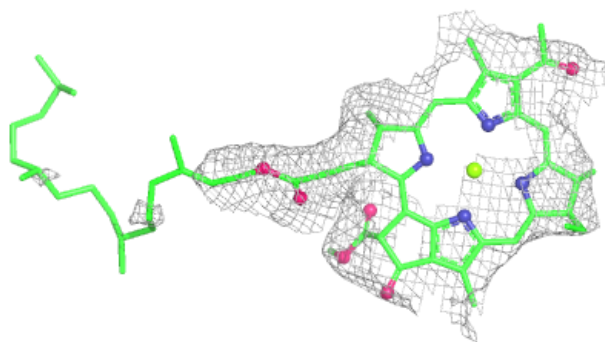
Electron density around BCL E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



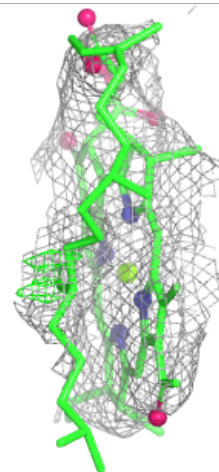
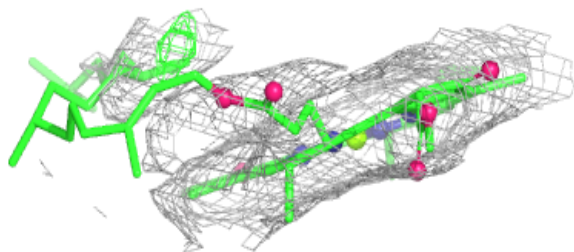
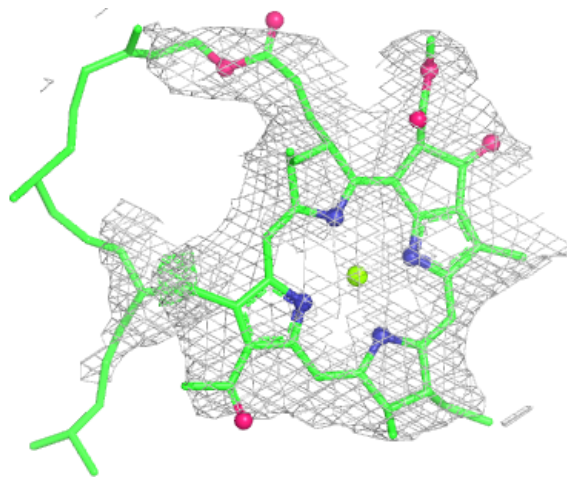
Electron density around BCL 3 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



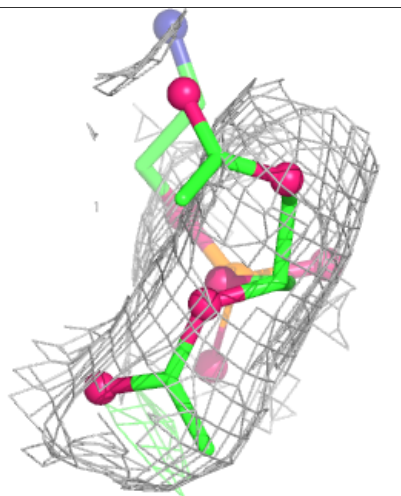
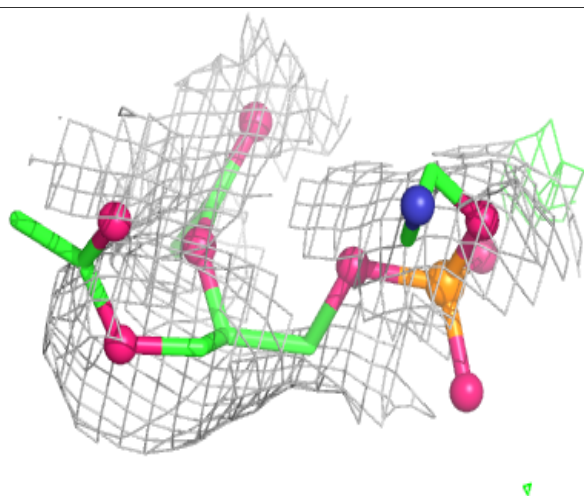
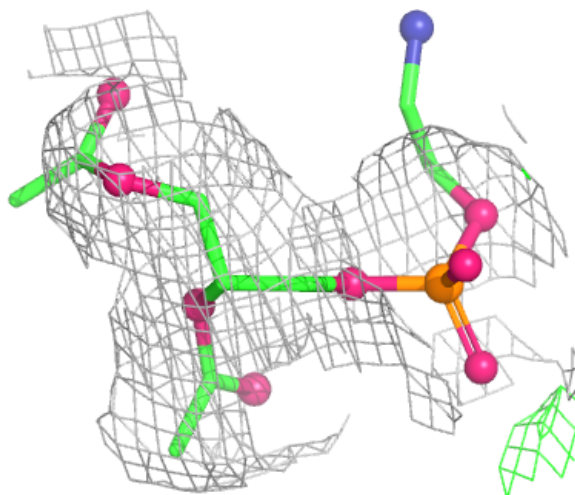
Electron density around BCL V 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



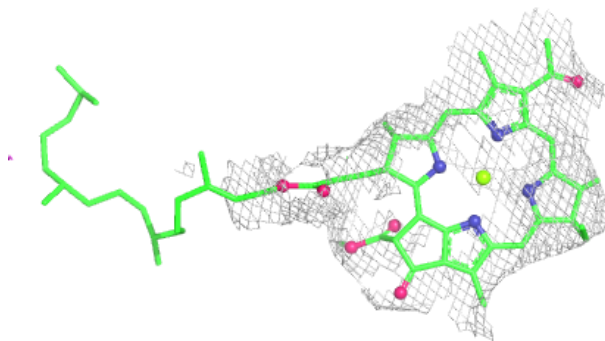
Electron density around PEF H 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

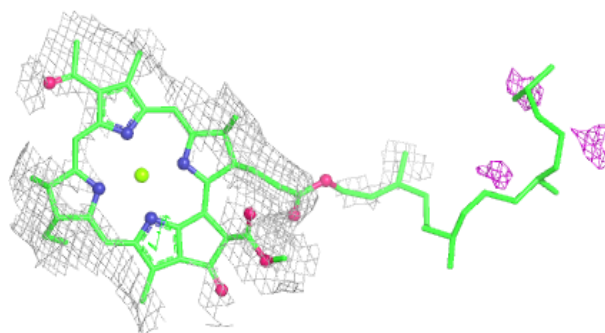


Electron density around BCL 7 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

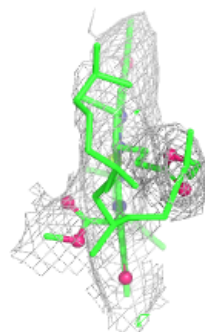
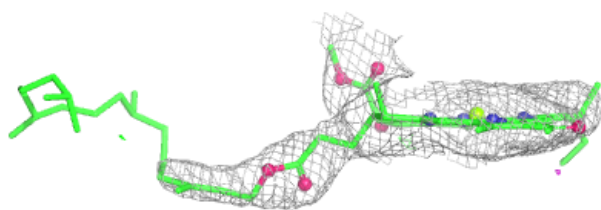
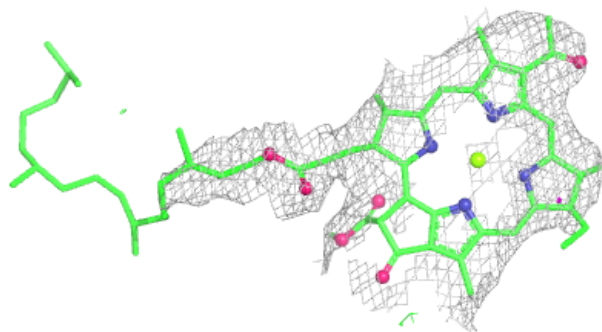
**Electron density around BCL O 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



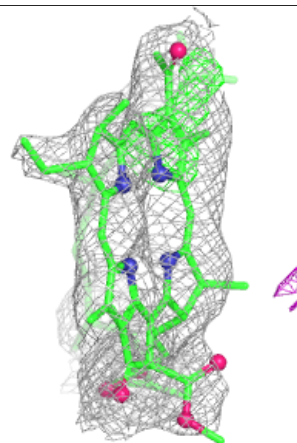
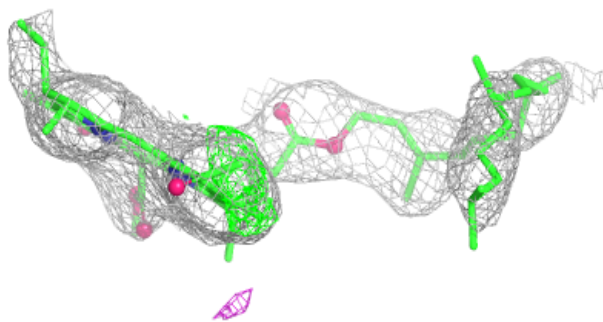
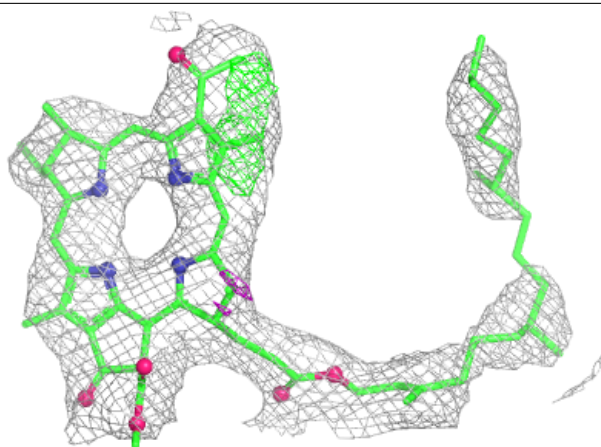
Electron density around BCL W 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



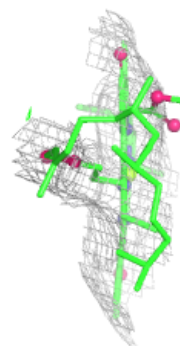
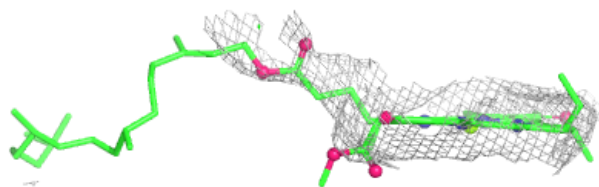
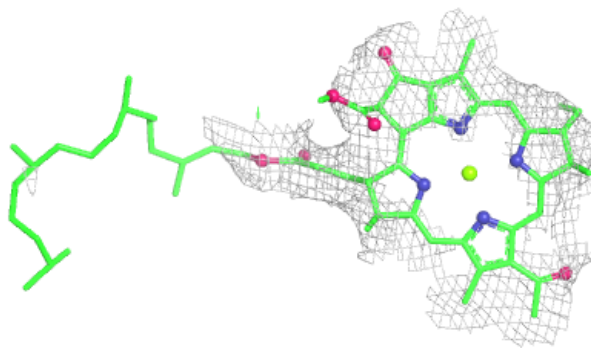
Electron density around BPH L 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



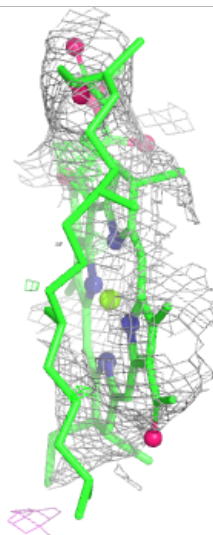
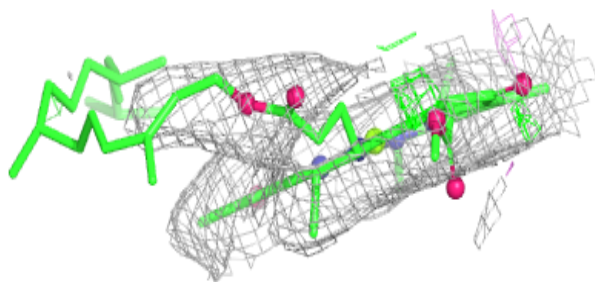
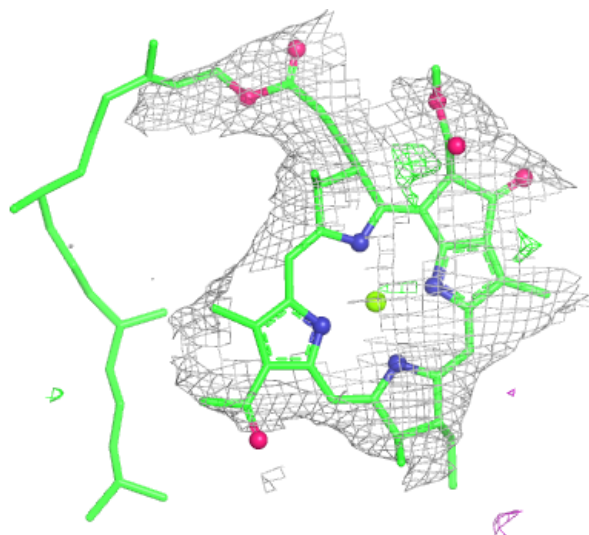
Electron density around BCL K 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



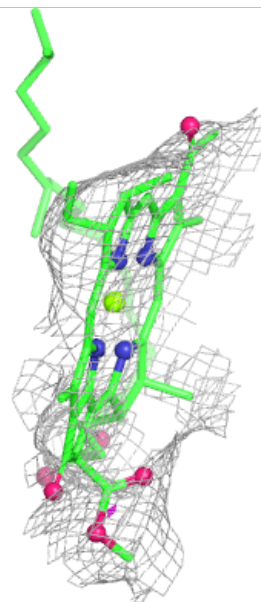
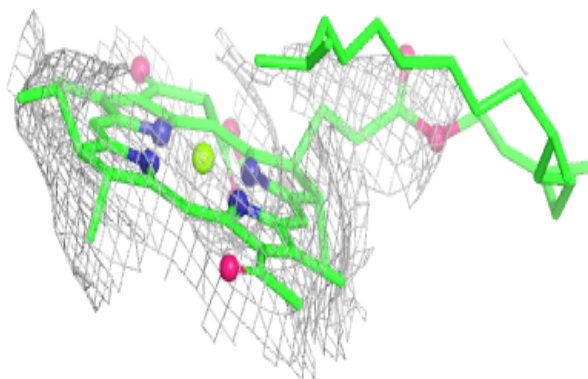
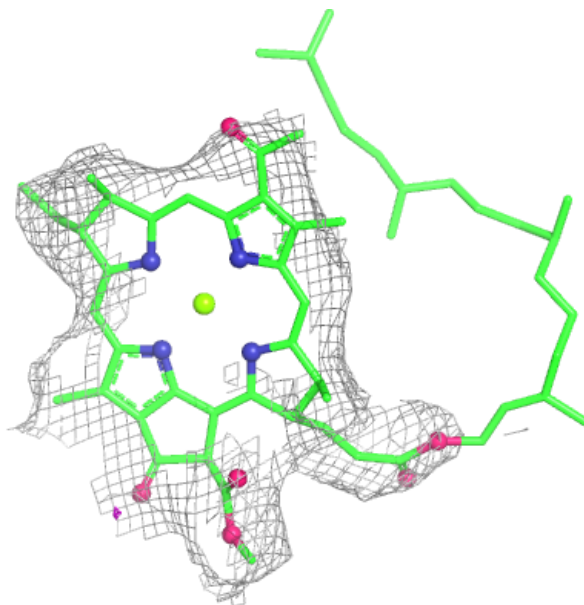
Electron density around BCL Z 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



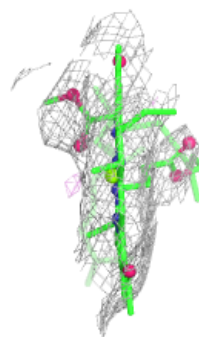
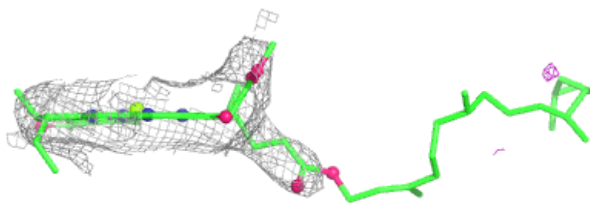
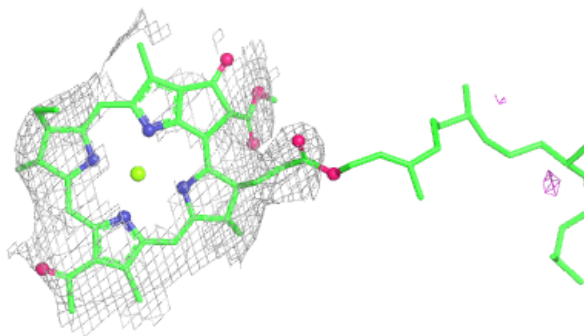
Electron density around BCL 7 103:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

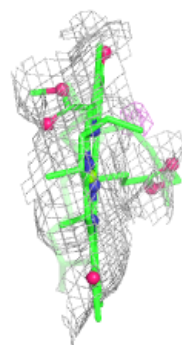
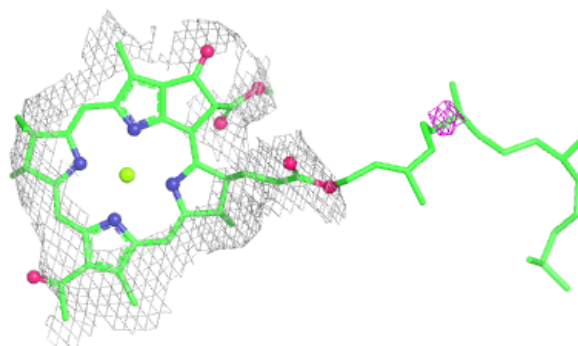


Electron density around BCL Q 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

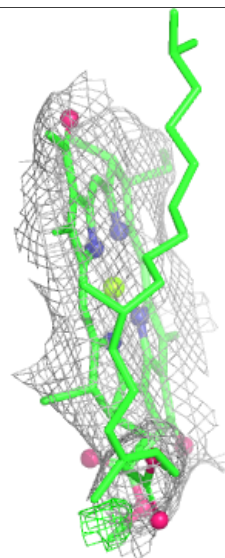
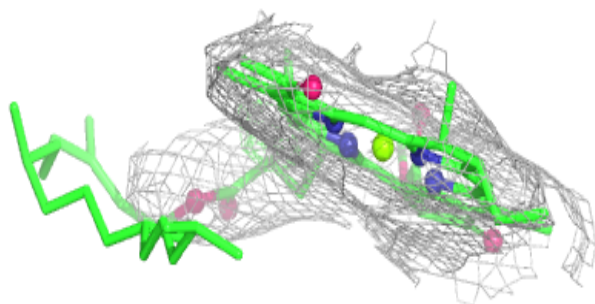
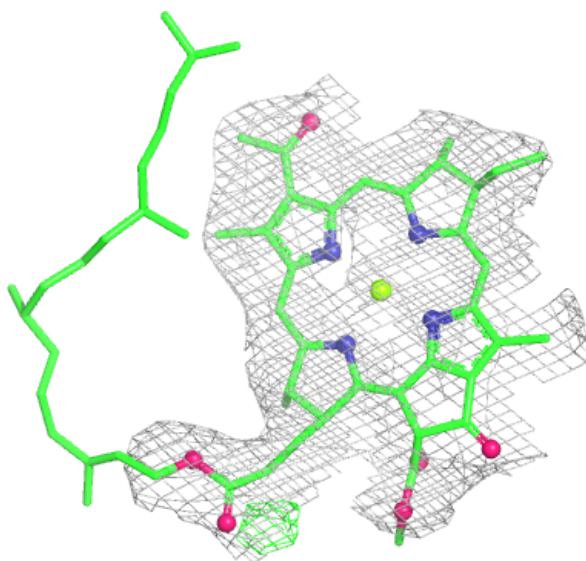
**Electron density around BCL A 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



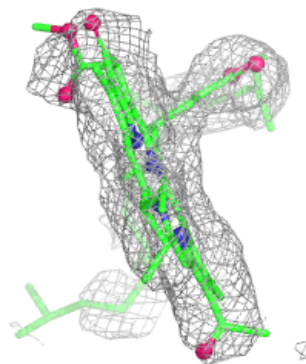
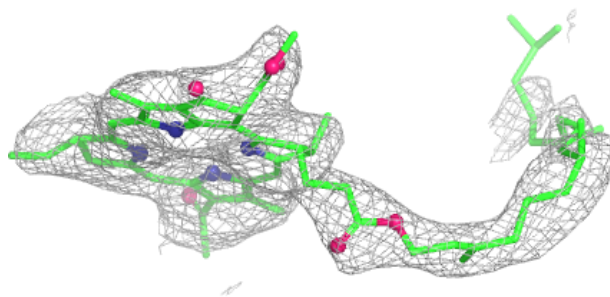
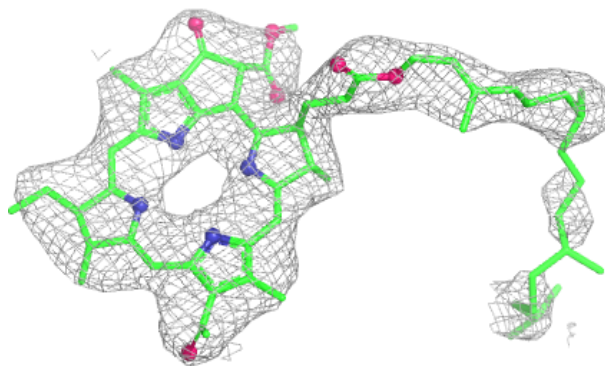
Electron density around BCL T 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

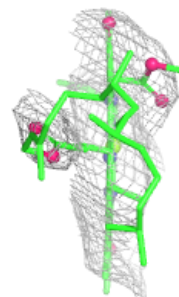
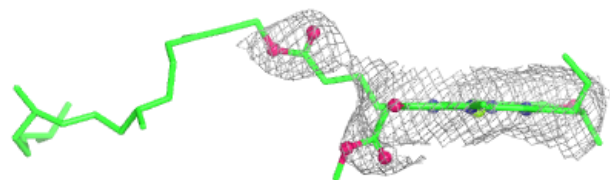
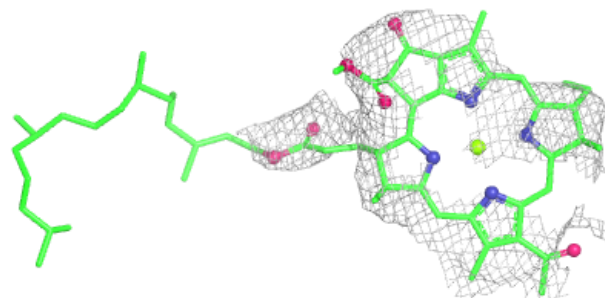


Electron density around BPH M 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

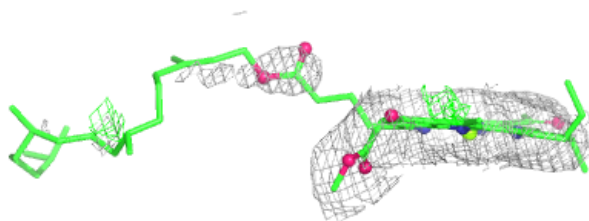
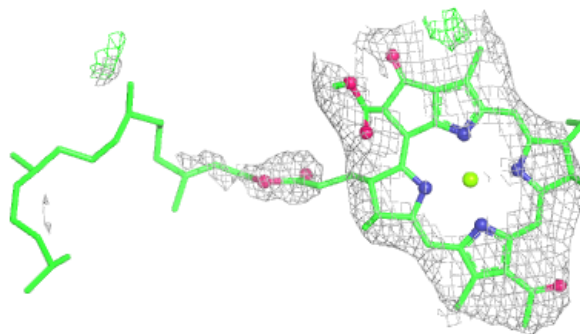
**Electron density around BCL 5 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



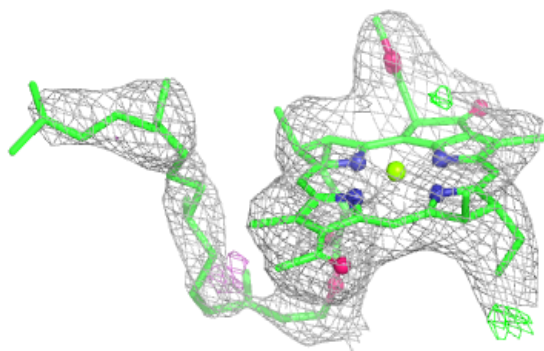
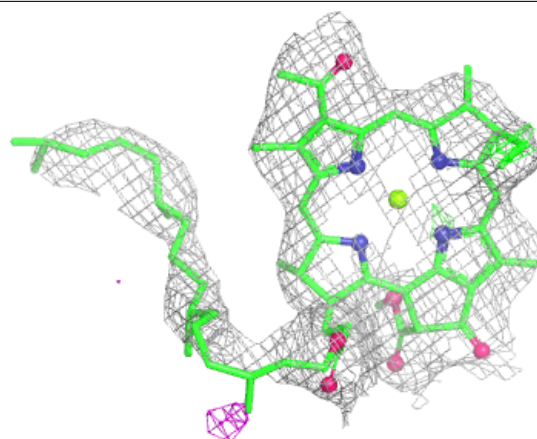
Electron density around BCL Y 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

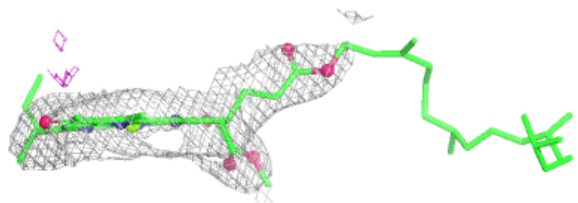
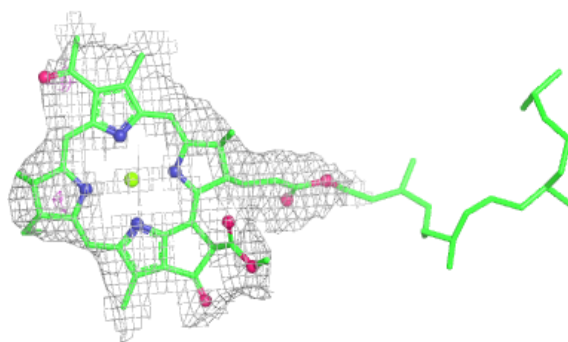


Electron density around BCL L 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

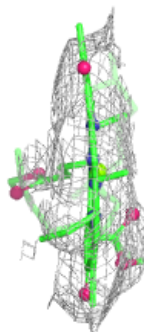
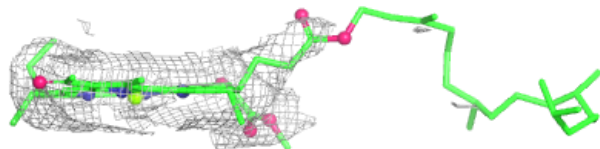
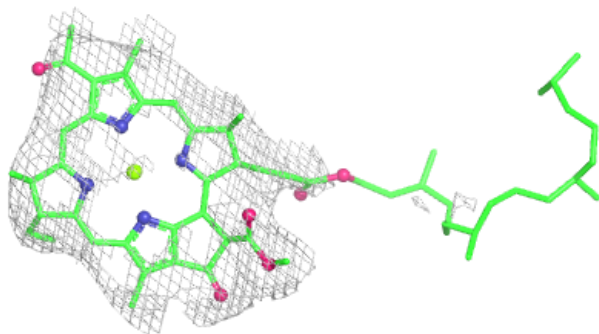
**Electron density around BCL 1 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

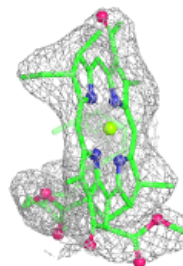
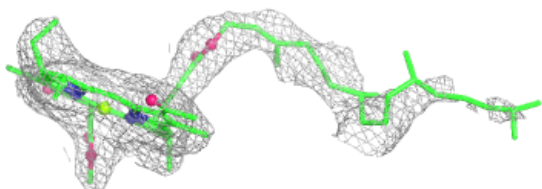
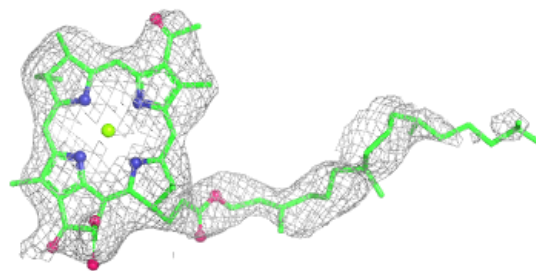


Electron density around BCL S 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

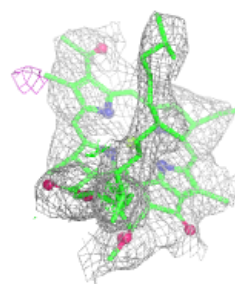
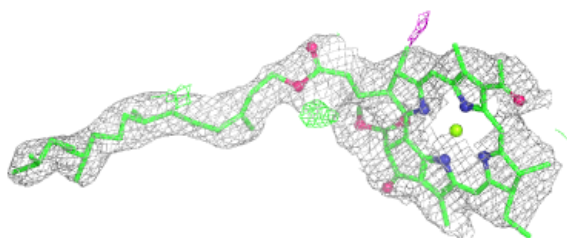
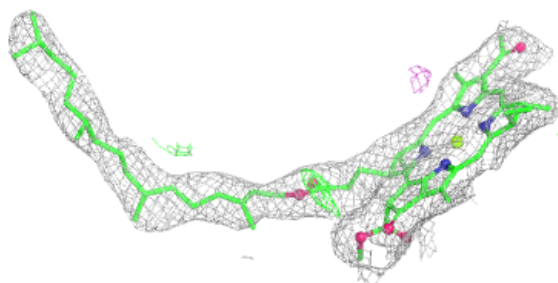
**Electron density around BCL M 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

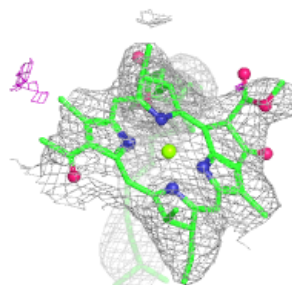
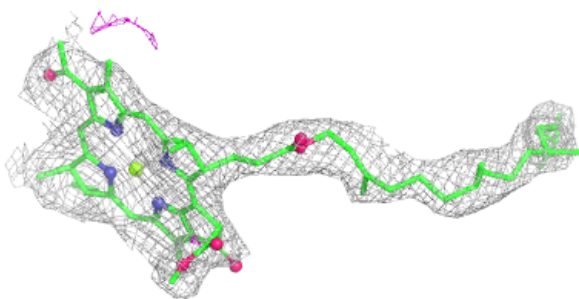
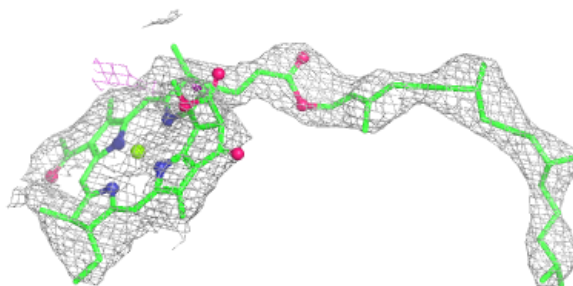


Electron density around BCL L 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

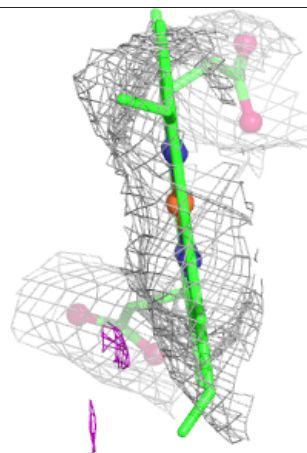
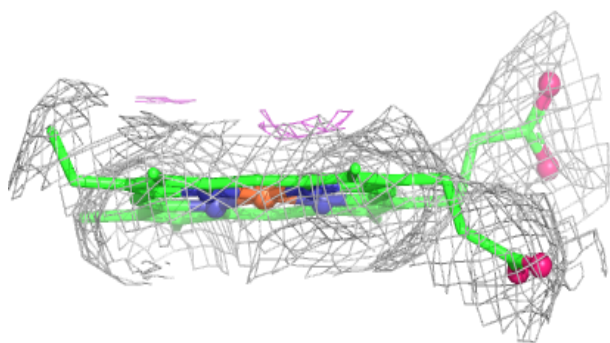
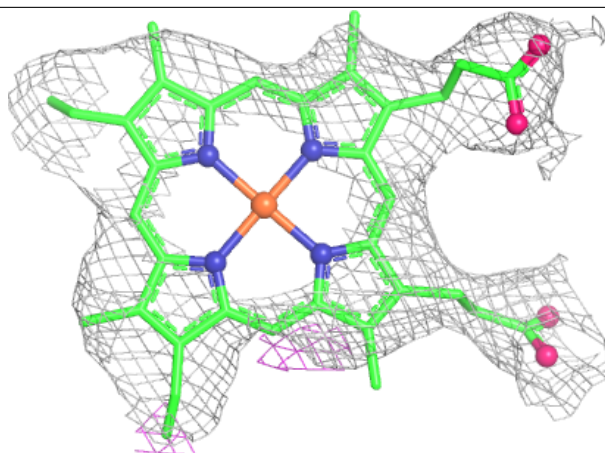
**Electron density around BCL M 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



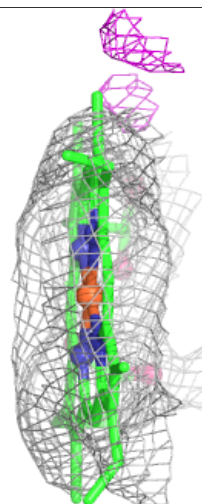
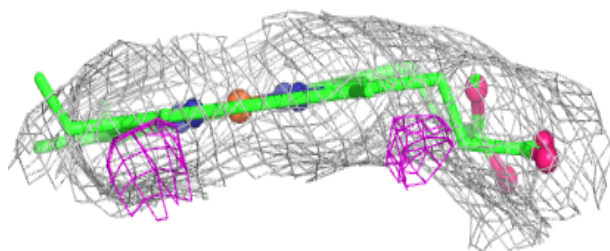
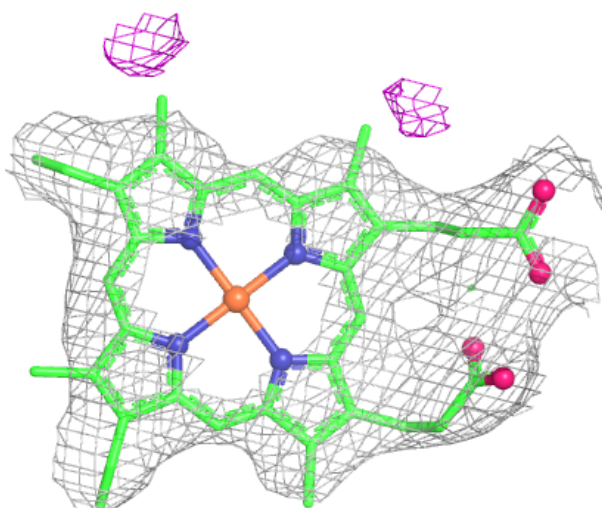
Electron density around HEM C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



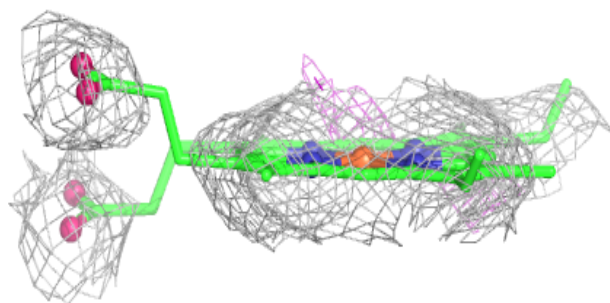
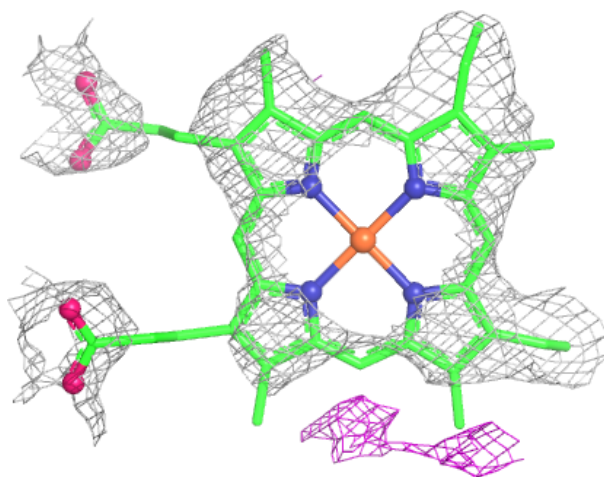
Electron density around HEM C 502:

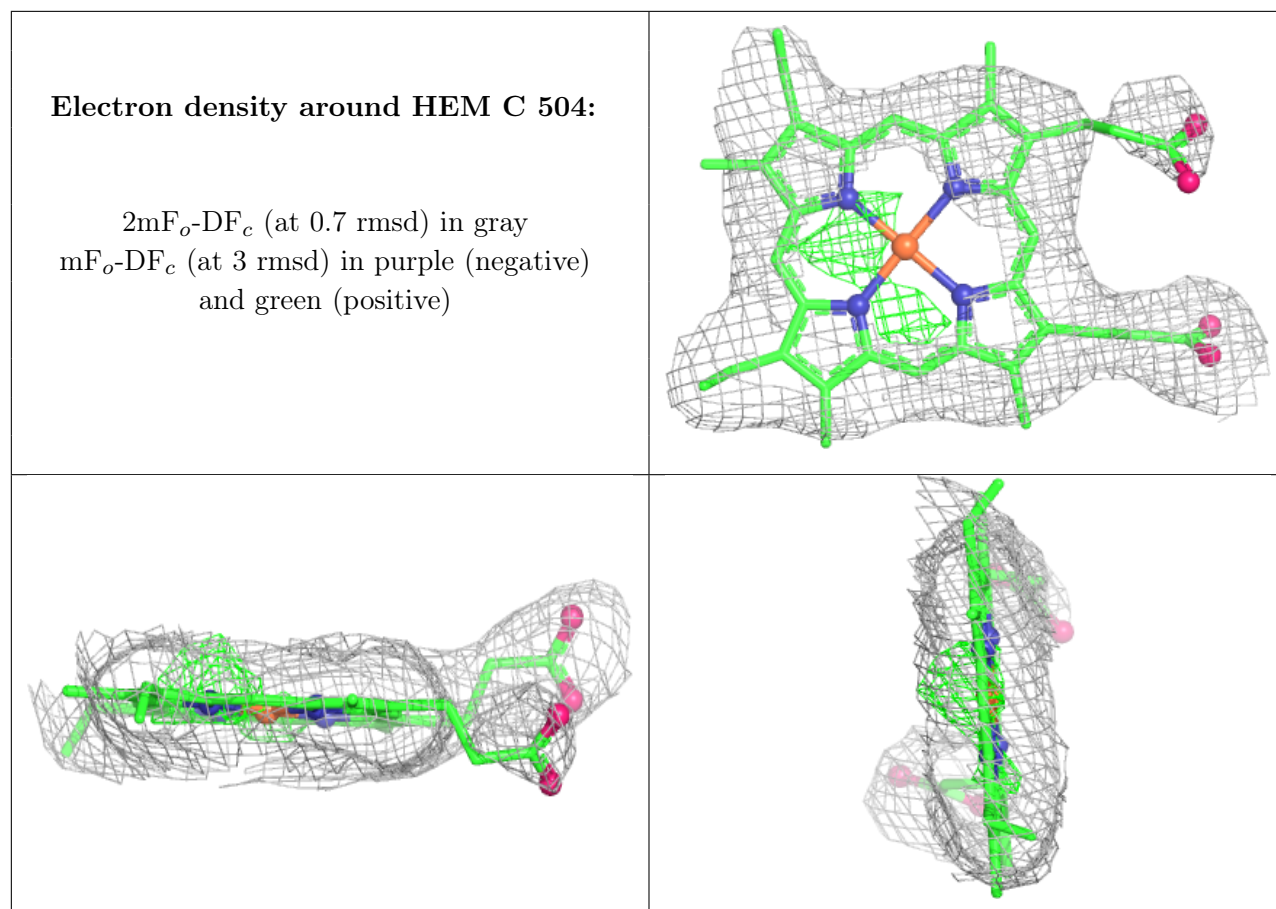
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.