



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2023 – 05:03 AM EDT

PDB ID : 2FKW  
Title : Structure of LH2 from Rps. acidophila crystallized in lipidic mesophases  
Authors : Papiz, M.Z.; Cherezov, V.; Clogston, J.; Caffrey, M.  
Deposited on : 2006-01-05  
Resolution : 2.45 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

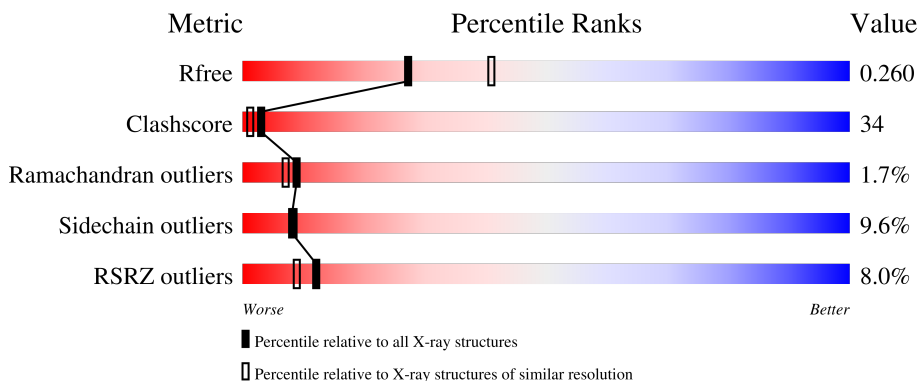
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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.



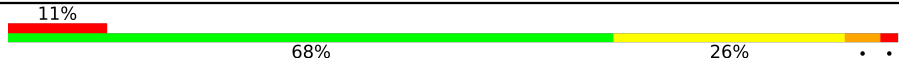

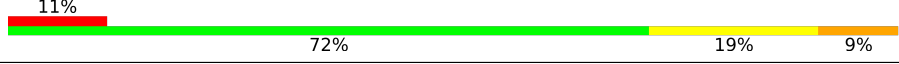
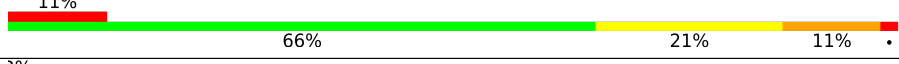

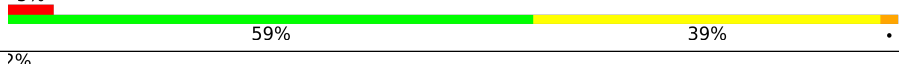


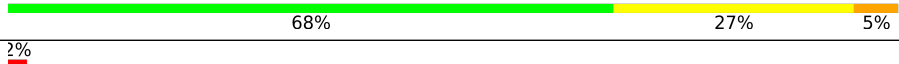


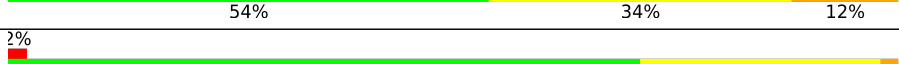

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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	A	53	 11% 58% 32% 9%
1	C	53	 13% 58% 32% 6% .
1	E	53	 13% 66% 21% 11% .
1	G	53	 11% 68% 25% 8%
1	I	53	 11% 64% 30% . .

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Mol	Chain	Length	Quality of chain
1	K	53	
1	M	53	
1	O	53	
1	R	53	
2	B	41	
2	D	41	
2	F	41	
2	H	41	
2	J	41	
2	L	41	
2	N	41	
2	P	41	
2	S	41	

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
3	BCL	A	1501	X	-	-	-
3	BCL	A	1701	X	-	-	-
3	BCL	B	1601	X	-	-	-
3	BCL	C	1502	X	-	-	-
3	BCL	C	1702	X	-	-	-
3	BCL	G	1704	X	-	X	-
3	BCL	H	1604	X	-	-	-
3	BCL	I	1705	-	-	X	-
3	BCL	J	1605	X	-	-	-
3	BCL	K	1506	X	-	-	-
3	BCL	K	1706	X	-	-	-
3	BCL	L	1606	X	-	X	-
3	BCL	M	1707	X	-	X	-
3	BCL	N	1607	X	-	-	-
3	BCL	O	1508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BCL	O	1708	X	-	-	-
3	BCL	P	1608	X	-	-	-
3	BCL	R	1509	X	-	-	-
3	BCL	R	1709	X	-	X	-
3	BCL	S	1609	X	-	-	-
4	LDA	A	1816	-	-	-	X
4	LDA	C	1815	-	-	-	X
4	LDA	E	1823	-	-	-	X
4	LDA	G	1824	-	-	X	-
4	LDA	I	1812	-	-	-	X
4	LDA	I	1825	-	-	-	X
4	LDA	K	1810	-	-	-	X
4	LDA	M	1827	-	-	-	X
4	LDA	R	1818	-	-	X	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9829 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 Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	C	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	E	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	G	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	I	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	K	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	M	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	O	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	R	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			

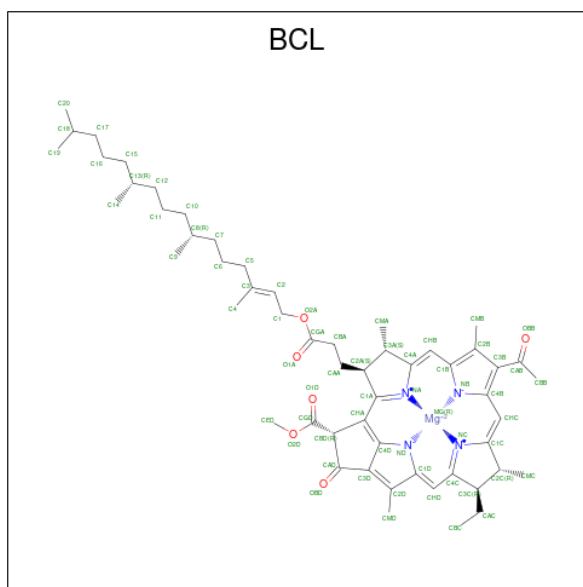
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	modified residue	UNP P26789
C	1	CXM	MET	modified residue	UNP P26789
E	1	CXM	MET	modified residue	UNP P26789
G	1	CXM	MET	modified residue	UNP P26789
I	1	CXM	MET	modified residue	UNP P26789
K	1	CXM	MET	modified residue	UNP P26789
M	1	CXM	MET	modified residue	UNP P26789
O	1	CXM	MET	modified residue	UNP P26789
R	1	CXM	MET	modified residue	UNP P26789

- Molecule 2 is a protein called Light-harvesting protein B-800/850, beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	D	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	F	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	H	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	J	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	L	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	N	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	P	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	S	41	Total	C	N	O	0	0	0
			323	213	53	57			

- Molecule 3 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



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

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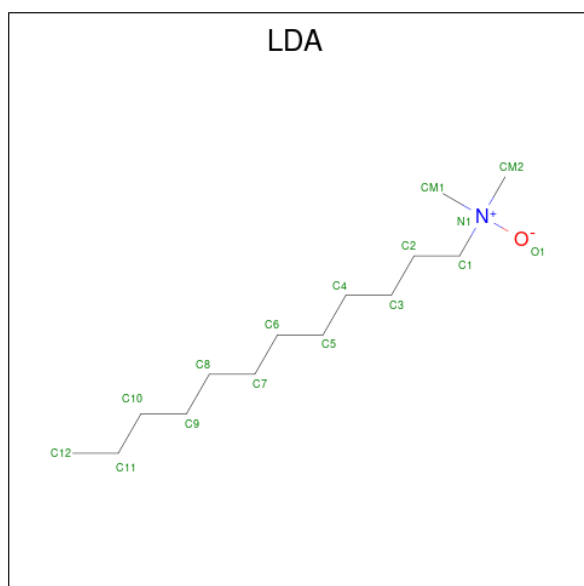
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	K	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	K	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	O	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	O	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	P	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	D	1	Total	C	N	O	0	0
			16	14	1	1		
4	E	1	Total	C	N	O	0	0
			16	14	1	1		
4	E	1	Total	C	N	O	0	0
			16	14	1	1		

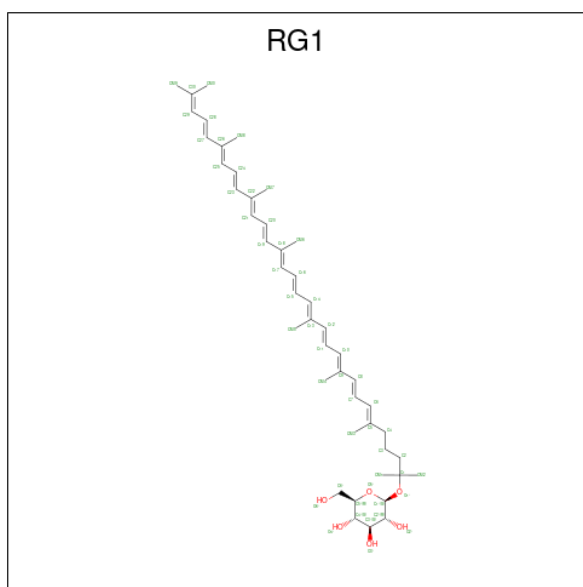
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			16	14	1	1		
4	G	1	Total	C	N	O	0	0
			16	14	1	1		
4	G	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	I	1	Total	C	N	O	0	0
			16	14	1	1		
4	I	1	Total	C	N	O	0	0
			16	14	1	1		
4	I	1	Total	C	N	O	0	0
			16	14	1	1		
4	J	1	Total	C	N	O	0	0
			16	14	1	1		
4	K	1	Total	C	N	O	0	0
			16	14	1	1		
4	K	1	Total	C	N	O	0	0
			16	14	1	1		
4	L	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	N	1	Total	C	N	O	0	0
			16	14	1	1		
4	O	1	Total	C	N	O	0	0
			16	14	1	1		
4	P	1	Total	C	N	O	0	0
			16	14	1	1		
4	R	1	Total	C	N	O	0	0
			16	14	1	1		
4	R	1	Total	C	N	O	0	0
			16	14	1	1		
4	R	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is Rhodopin b-D-glucoside (three-letter code: RG1) (formula: C<sub>46</sub>H<sub>66</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	C O	0	0
			52	46 6		
5	F	1	Total	C O	0	0
			52	46 6		
5	H	1	Total	C O	0	0
			52	46 6		
5	J	1	Total	C O	0	0
			52	46 6		
5	L	1	Total	C O	0	0
			52	46 6		
5	N	1	Total	C O	0	0
			52	46 6		
5	P	1	Total	C O	0	0
			52	46 6		
5	R	1	Total	C O	0	0
			52	46 6		
5	S	1	Total	C O	0	0
			52	46 6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total	O	0	0
			33	33		
6	B	26	Total	O	0	0
			26	26		
6	C	24	Total	O	0	0
			24	24		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	27	Total 27	O 27	0	0
6	E	40	Total 40	O 40	0	0
6	F	28	Total 28	O 28	0	0
6	G	41	Total 41	O 41	0	0
6	H	37	Total 37	O 37	2	0
6	I	38	Total 38	O 38	0	0
6	J	39	Total 39	O 39	1	0
6	K	47	Total 47	O 47	0	0
6	L	29	Total 29	O 29	0	0
6	M	36	Total 36	O 36	0	0
6	N	30	Total 30	O 30	0	0
6	O	33	Total 33	O 33	1	0
6	P	32	Total 32	O 32	0	0
6	R	39	Total 39	O 39	0	0
6	S	34	Total 34	O 34	0	0

### 3 Residue-property plots [i](#)

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

- Molecule 1: Light-harvesting protein B-800/850, alpha chain



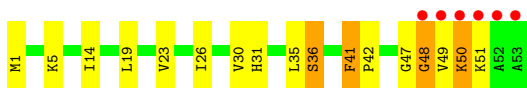
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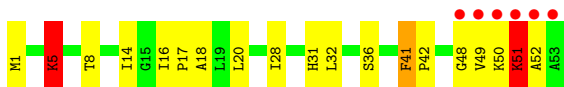
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



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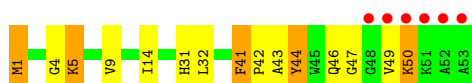
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



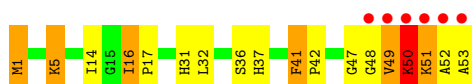
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



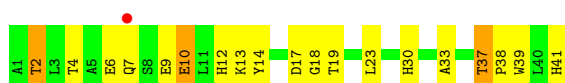
- Molecule 2: Light-harvesting protein B-800/850, beta chain



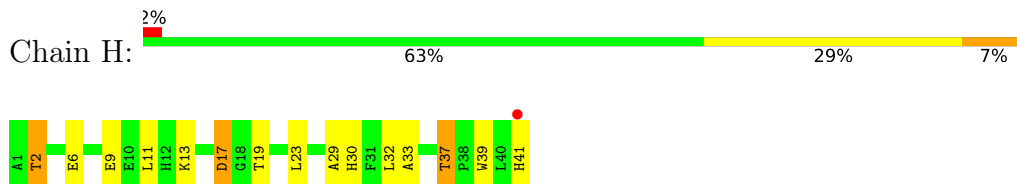
- Molecule 2: Light-harvesting protein B-800/850, beta chain



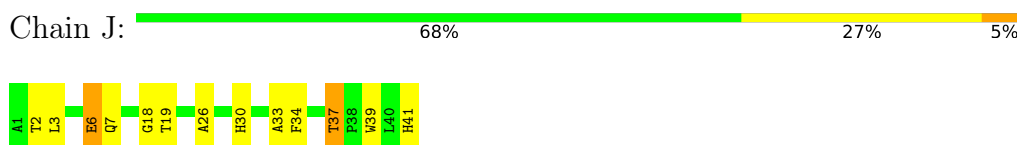
- Molecule 2: Light-harvesting protein B-800/850, beta chain



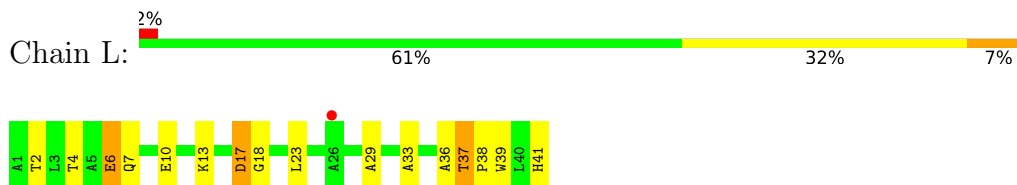
- Molecule 2: Light-harvesting protein B-800/850, beta chain



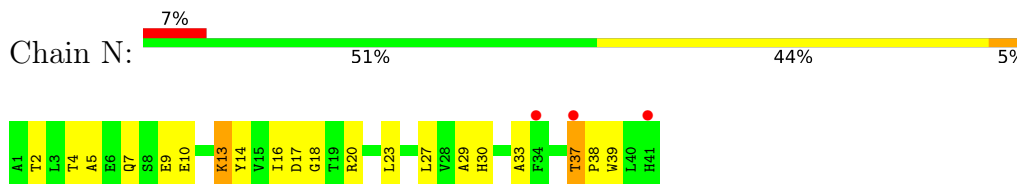
- Molecule 2: Light-harvesting protein B-800/850, beta chain



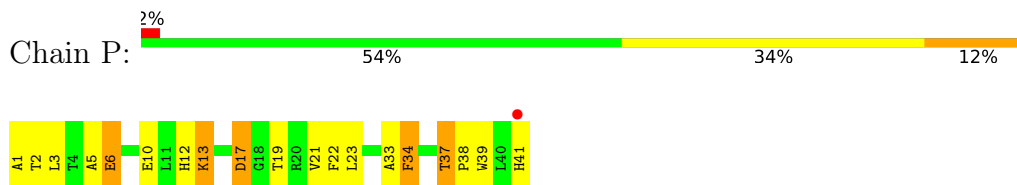
- Molecule 2: Light-harvesting protein B-800/850, beta chain



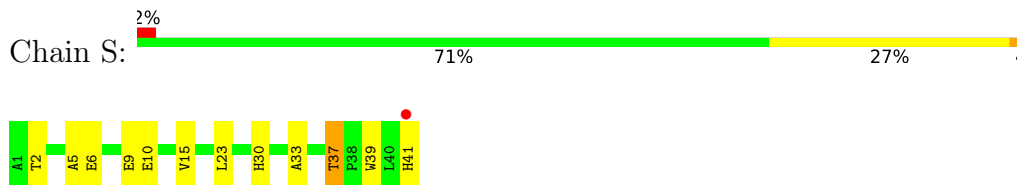
- Molecule 2: Light-harvesting protein B-800/850, beta chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.44Å 126.38Å 129.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 38.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-2.45) 99.7 (38.85-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.183 , 0.254 0.203 , 0.260	Depositor DCC
$R_{free}$ test set	2531 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtrriage
Anisotropy	0.620	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 73.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CXM, LDA, BCL, RG1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.27	1/404 (0.2%)	0.51	0/556
1	C	1.51	4/404 (1.0%)	0.51	0/556
1	E	1.35	1/404 (0.2%)	0.53	0/556
1	G	1.34	2/404 (0.5%)	0.50	0/556
1	I	1.38	1/404 (0.2%)	0.53	0/556
1	K	1.47	2/404 (0.5%)	0.55	0/556
1	M	1.35	1/404 (0.2%)	0.57	0/556
1	O	1.36	2/404 (0.5%)	0.51	0/556
1	R	1.35	3/404 (0.7%)	0.53	0/556
2	B	1.40	1/332 (0.3%)	0.49	0/453
2	D	1.25	1/332 (0.3%)	0.45	0/453
2	F	1.48	2/332 (0.6%)	0.42	0/453
2	H	1.40	2/332 (0.6%)	0.45	0/453
2	J	1.29	2/332 (0.6%)	0.44	0/453
2	L	1.62	5/332 (1.5%)	0.47	0/453
2	N	1.38	2/332 (0.6%)	0.44	0/453
2	P	1.60	3/332 (0.9%)	0.49	0/453
2	S	1.21	1/332 (0.3%)	0.45	0/453
All	All	1.39	36/6624 (0.5%)	0.50	0/9081

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
1	A	0	2
1	C	2	1
1	E	1	0
1	G	1	0
1	I	2	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	1	1
1	M	3	1
1	O	0	1
1	R	2	0
All	All	12	7

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	6	GLU	CG-CD	11.70	1.69	1.51
2	L	10	GLU	CG-CD	11.28	1.68	1.51
2	F	10	GLU	CG-CD	9.26	1.65	1.51
2	L	17	ASP	CB-CG	7.49	1.67	1.51
1	A	49	VAL	CA-CB	7.42	1.70	1.54

There are no bond angle outliers.

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	52	ALA	CA
1	C	53	ALA	CA
1	E	51	LYS	CA
1	G	50	LYS	CA
1	I	49	VAL	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	LYS	Peptide
1	A	51	LYS	Peptide
1	C	52	ALA	Peptide
1	I	51	LYS	Peptide
1	K	50	LYS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	403	0	422	25	0
1	C	403	0	422	27	0
1	E	403	0	422	27	0
1	G	403	0	422	21	0
1	I	403	0	422	21	0
1	K	403	0	422	27	0
1	M	403	0	422	32	0
1	O	403	0	422	17	0
1	R	403	0	422	22	0
2	B	323	0	321	25	0
2	D	323	0	321	22	0
2	F	323	0	321	24	0
2	H	323	0	321	19	0
2	J	323	0	321	23	0
2	L	323	0	321	22	0
2	N	323	0	321	29	0
2	P	323	0	321	30	0
2	S	323	0	321	11	0
3	A	132	0	146	25	0
3	B	66	0	74	11	0
3	C	132	0	148	15	0
3	D	66	0	74	8	0
3	E	132	0	147	12	0
3	F	66	0	74	12	0
3	G	132	0	147	27	0
3	H	66	0	73	12	0
3	I	132	0	148	33	0
3	J	66	0	73	17	0
3	K	132	0	146	14	0
3	L	66	0	74	25	0
3	M	132	0	147	28	0
3	N	66	0	74	16	0
3	O	132	0	147	21	0
3	P	66	0	73	10	0
3	R	132	0	147	28	0
3	S	66	0	74	13	0
4	A	32	0	62	11	0
4	B	16	0	31	2	0
4	C	32	0	62	6	0
4	D	16	0	31	3	0
4	E	32	0	62	14	0
4	F	16	0	31	7	0
4	G	32	0	62	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	16	0	31	3	0
4	I	48	0	93	15	0
4	J	16	0	31	1	0
4	K	32	0	62	12	0
4	L	16	0	31	5	0
4	M	32	0	62	6	0
4	N	16	0	31	2	0
4	O	16	0	31	7	0
4	P	16	0	31	3	0
4	R	48	0	93	12	0
5	D	52	0	66	5	0
5	F	52	0	66	5	0
5	H	52	0	66	5	0
5	J	52	0	66	1	0
5	L	52	0	66	4	0
5	N	52	0	66	4	0
5	P	52	0	66	4	0
5	R	52	0	66	4	0
5	S	52	0	66	5	0
6	A	33	0	0	9	0
6	B	26	0	0	6	0
6	C	24	0	0	3	0
6	D	27	0	0	8	0
6	E	40	0	0	20	0
6	F	28	0	0	7	0
6	G	41	0	0	22	0
6	H	37	0	0	5	0
6	I	38	0	0	11	0
6	J	39	0	0	14	0
6	K	47	0	0	28	0
6	L	29	0	0	2	0
6	M	36	0	0	10	0
6	N	30	0	0	8	0
6	O	33	0	0	11	0
6	P	32	0	0	8	0
6	R	39	0	0	24	0
6	S	34	0	0	4	0
All	All	9829	0	10104	659	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 34.

The worst 5 of 659 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)
1:M:1:CXM:SD	1:M:1:CXM:CE	2.21	1.28
1:G:48:GLY:HA2	6:G:1839:HOH:O	1.32	1.24
4:I:1825:LDA:HM22	6:I:1845:HOH:O	1.06	1.24
4:H:1804:LDA:H92	6:H:1825:HOH:O	1.38	1.22
1:E:49:VAL:HG11	6:E:1850:HOH:O	1.45	1.15

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	A	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
1	C	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	1	0
1	E	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	1	0
1	G	51/53 (96%)	51 (100%)	0	0	100	100
1	I	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	K	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	7	5
1	M	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	1	0
1	O	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	7	5
1	R	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	1	0
2	B	39/41 (95%)	39 (100%)	0	0	100	100
2	D	39/41 (95%)	39 (100%)	0	0	100	100
2	F	39/41 (95%)	39 (100%)	0	0	100	100
2	H	39/41 (95%)	39 (100%)	0	0	100	100
2	J	39/41 (95%)	39 (100%)	0	0	100	100
2	L	39/41 (95%)	39 (100%)	0	0	100	100
2	N	39/41 (95%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
2	S	39/41 (95%)	39 (100%)	0	0	100	100
All	All	810/846 (96%)	775 (96%)	21 (3%)	14 (2%)	9	7

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	LYS
1	E	51	LYS
1	E	52	ALA
1	K	50	LYS
1	M	50	LYS

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	40/40 (100%)	37 (92%)	3 (8%)	13	16
1	C	40/40 (100%)	37 (92%)	3 (8%)	13	16
1	E	40/40 (100%)	34 (85%)	6 (15%)	3	2
1	G	40/40 (100%)	36 (90%)	4 (10%)	7	7
1	I	40/40 (100%)	35 (88%)	5 (12%)	4	3
1	K	40/40 (100%)	39 (98%)	1 (2%)	47	60
1	M	40/40 (100%)	38 (95%)	2 (5%)	24	32
1	O	40/40 (100%)	38 (95%)	2 (5%)	24	32
1	R	40/40 (100%)	36 (90%)	4 (10%)	7	7
2	B	33/33 (100%)	30 (91%)	3 (9%)	9	10
2	D	33/33 (100%)	30 (91%)	3 (9%)	9	10
2	F	33/33 (100%)	29 (88%)	4 (12%)	5	4
2	H	33/33 (100%)	29 (88%)	4 (12%)	5	4
2	J	33/33 (100%)	31 (94%)	2 (6%)	18	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	33/33 (100%)	28 (85%)	5 (15%)	3	2
2	N	33/33 (100%)	30 (91%)	3 (9%)	9	10
2	P	33/33 (100%)	28 (85%)	5 (15%)	3	2
2	S	33/33 (100%)	29 (88%)	4 (12%)	5	4
All	All	657/657 (100%)	594 (90%)	63 (10%)	8	8

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	17	ASP
1	R	16	ILE
2	J	2	THR
2	P	37	THR
2	S	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	7	GLN
1	R	37	HIS
2	S	7	GLN
2	H	7	GLN
1	I	37	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CXM	E	1	3,1	8,10,11	1.42	2 (25%)	7,11,13	1.55	1 (14%)
1	CXM	R	1	3,1	8,10,11	1.74	1 (12%)	7,11,13	1.51	1 (14%)
1	CXM	I	1	3,1	8,10,11	1.44	2 (25%)	7,11,13	1.69	1 (14%)
1	CXM	M	1	3,1	8,10,11	3.04	2 (25%)	7,11,13	1.29	2 (28%)
1	CXM	G	1	3,1	8,10,11	1.86	2 (25%)	7,11,13	1.33	2 (28%)
1	CXM	A	1	3,1	8,10,11	1.63	2 (25%)	7,11,13	1.56	2 (28%)
1	CXM	O	1	3,1	8,10,11	1.65	2 (25%)	7,11,13	1.56	1 (14%)
1	CXM	K	1	3,1	8,10,11	1.67	3 (37%)	7,11,13	1.85	1 (14%)
1	CXM	C	1	3,1	8,10,11	2.41	2 (25%)	7,11,13	1.50	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	E	1	3,1	-	1/9/10/12	-
1	CXM	R	1	3,1	-	3/9/10/12	-
1	CXM	I	1	3,1	-	2/9/10/12	-
1	CXM	M	1	3,1	-	2/9/10/12	-
1	CXM	G	1	3,1	-	2/9/10/12	-
1	CXM	A	1	3,1	-	2/9/10/12	-
1	CXM	O	1	3,1	-	4/9/10/12	-
1	CXM	K	1	3,1	-	2/9/10/12	-
1	CXM	C	1	3,1	-	0/9/10/12	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	1	CXM	CE-SD	7.14	2.21	1.78
1	C	1	CXM	ON1-CN	5.22	1.31	1.21
1	M	1	CXM	ON1-CN	4.52	1.30	1.21
1	R	1	CXM	ON1-CN	3.96	1.29	1.21
1	G	1	CXM	CE-SD	3.60	2.00	1.78

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	K	1	CXM	ON1-CN-N	-3.92	118.42	124.85
1	I	1	CXM	ON1-CN-N	-3.75	118.70	124.85
1	R	1	CXM	ON1-CN-N	-3.65	118.86	124.85
1	C	1	CXM	ON1-CN-N	-3.51	119.09	124.85
1	O	1	CXM	ON1-CN-N	-3.47	119.16	124.85

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	C-CA-CB-CG
1	G	1	CXM	O-C-CA-CB
1	K	1	CXM	O-C-CA-CB
1	R	1	CXM	O-C-CA-CB
1	O	1	CXM	CB-CG-SD-CE

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1	CXM	2	0
1	R	1	CXM	1	0
1	M	1	CXM	4	0
1	O	1	CXM	1	0
1	K	1	CXM	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

63 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	LDA	B	1801	-	12,15,15	2.13	1 (8%)	14,17,17	0.43	0
3	BCL	M	1507	1	58,74,74	2.21	14 (24%)	69,115,115	2.58	22 (31%)
3	BCL	R	1709	1	58,74,74	2.52	22 (37%)	69,115,115	2.28	22 (31%)
4	LDA	M	1811	-	12,15,15	1.94	1 (8%)	14,17,17	0.50	0
3	BCL	K	1506	1	58,74,74	2.54	18 (31%)	69,115,115	2.54	25 (36%)
3	BCL	O	1708	1	58,74,74	2.35	15 (25%)	69,115,115	2.21	20 (28%)
4	LDA	D	1802	-	12,15,15	2.08	1 (8%)	14,17,17	0.61	0
4	LDA	L	1806	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
3	BCL	D	1602	2	58,74,74	2.37	19 (32%)	69,115,115	2.49	22 (31%)
3	BCL	O	1508	1	58,74,74	2.18	13 (22%)	69,115,115	2.39	25 (36%)
4	LDA	P	1808	-	12,15,15	1.94	1 (8%)	14,17,17	0.58	0
4	LDA	F	1803	-	12,15,15	2.25	1 (8%)	14,17,17	0.57	0
4	LDA	I	1812	-	12,15,15	2.39	1 (8%)	14,17,17	0.37	0
4	LDA	K	1810	-	12,15,15	2.15	1 (8%)	14,17,17	0.49	0
3	BCL	I	1705	1	58,74,74	2.20	18 (31%)	69,115,115	2.29	16 (23%)
5	RG1	N	1407	-	52,52,52	1.22	4 (7%)	64,67,67	1.55	13 (20%)
3	BCL	H	1604	2	58,74,74	2.12	18 (31%)	69,115,115	2.52	29 (42%)
4	LDA	R	1809	-	12,15,15	1.97	1 (8%)	14,17,17	0.52	0
4	LDA	A	1817	-	12,15,15	2.01	1 (8%)	14,17,17	0.44	0
4	LDA	C	1815	-	12,15,15	2.11	1 (8%)	14,17,17	0.35	0
5	RG1	S	1409	-	52,52,52	1.38	8 (15%)	64,67,67	1.57	16 (25%)
3	BCL	G	1504	1	58,74,74	2.36	12 (20%)	69,115,115	2.25	25 (36%)
3	BCL	J	1605	2	58,74,74	2.26	18 (31%)	69,115,115	2.64	23 (33%)
3	BCL	K	1706	1	58,74,74	2.17	14 (24%)	69,115,115	2.37	19 (27%)
4	LDA	H	1804	-	12,15,15	1.90	1 (8%)	14,17,17	0.57	0
5	RG1	J	1405	-	52,52,52	1.28	6 (11%)	64,67,67	1.61	14 (21%)
5	RG1	L	1406	-	52,52,52	1.37	7 (13%)	64,67,67	1.50	13 (20%)
4	LDA	R	1818	-	12,15,15	2.00	1 (8%)	14,17,17	0.46	0
4	LDA	I	1813	-	12,15,15	2.05	1 (8%)	14,17,17	0.40	0
3	BCL	C	1702	1	58,74,74	2.37	15 (25%)	69,115,115	2.27	21 (30%)
4	LDA	G	1824	-	12,15,15	2.08	1 (8%)	14,17,17	0.35	0
3	BCL	F	1603	2	58,74,74	2.10	14 (24%)	69,115,115	2.31	22 (31%)
3	BCL	E	1703	1	58,74,74	2.12	10 (17%)	69,115,115	2.13	21 (30%)
4	LDA	I	1825	-	12,15,15	2.06	1 (8%)	14,17,17	0.51	0
4	LDA	A	1816	-	12,15,15	2.00	1 (8%)	14,17,17	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	LDA	E	1822	-	12,15,15	1.89	1 (8%)	14,17,17	0.51	0
3	BCL	A	1701	1	58,74,74	2.78	22 (37%)	69,115,115	2.46	23 (33%)
3	BCL	B	1601	2	58,74,74	2.05	15 (25%)	69,115,115	2.70	21 (30%)
3	BCL	M	1707	1	58,74,74	2.33	15 (25%)	69,115,115	2.13	18 (26%)
4	LDA	R	1819	-	12,15,15	1.92	1 (8%)	14,17,17	0.42	0
5	RG1	D	1402	-	52,52,52	1.29	7 (13%)	64,67,67	1.63	16 (25%)
4	LDA	M	1827	-	12,15,15	2.01	1 (8%)	14,17,17	0.42	0
3	BCL	L	1606	2	58,74,74	2.37	20 (34%)	69,115,115	3.04	24 (34%)
3	BCL	N	1607	2	58,74,74	2.15	14 (24%)	69,115,115	2.52	21 (30%)
4	LDA	O	1820	-	12,15,15	2.14	1 (8%)	14,17,17	0.43	0
4	LDA	C	1821	-	12,15,15	1.92	1 (8%)	14,17,17	0.41	0
3	BCL	P	1608	2	58,74,74	2.27	19 (32%)	69,115,115	2.47	23 (33%)
5	RG1	P	1408	-	52,52,52	1.38	10 (19%)	64,67,67	1.60	12 (18%)
4	LDA	G	1814	-	12,15,15	2.08	1 (8%)	14,17,17	0.44	0
3	BCL	R	1509	1	58,74,74	2.39	15 (25%)	69,115,115	2.60	25 (36%)
3	BCL	C	1502	1	58,74,74	1.95	16 (27%)	69,115,115	2.36	23 (33%)
4	LDA	J	1805	-	12,15,15	1.90	1 (8%)	14,17,17	0.31	0
4	LDA	E	1823	-	12,15,15	1.87	1 (8%)	14,17,17	0.46	0
3	BCL	S	1609	2	58,74,74	2.06	13 (22%)	69,115,115	2.47	23 (33%)
4	LDA	K	1826	-	12,15,15	1.89	1 (8%)	14,17,17	0.53	0
5	RG1	R	1401	-	52,52,52	1.26	5 (9%)	64,67,67	1.69	12 (18%)
3	BCL	A	1501	1	58,74,74	2.32	16 (27%)	69,115,115	2.44	23 (33%)
3	BCL	E	1503	1	58,74,74	2.07	13 (22%)	69,115,115	2.42	21 (30%)
5	RG1	F	1403	-	52,52,52	1.34	5 (9%)	64,67,67	1.64	17 (26%)
3	BCL	G	1704	1	58,74,74	2.23	16 (27%)	69,115,115	2.43	24 (34%)
3	BCL	I	1505	1	58,74,74	2.03	15 (25%)	69,115,115	2.20	19 (27%)
5	RG1	H	1404	-	52,52,52	1.34	5 (9%)	64,67,67	1.66	13 (20%)
4	LDA	N	1807	-	12,15,15	1.92	1 (8%)	14,17,17	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	B	1801	-	-	8/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BCL	R	1709	1	1/1/21/25	16/37/137/137	-
3	BCL	M	1507	1	-	5/37/137/137	-
4	LDA	M	1811	-	-	7/13/13/13	-
3	BCL	K	1506	1	1/1/21/25	8/37/137/137	-
3	BCL	O	1708	1	1/1/21/25	11/37/137/137	-
4	LDA	D	1802	-	-	8/13/13/13	-
4	LDA	L	1806	-	-	10/13/13/13	-
3	BCL	D	1602	2	-	9/37/137/137	-
3	BCL	O	1508	1	2/2/21/25	11/37/137/137	-
4	LDA	P	1808	-	-	8/13/13/13	-
4	LDA	F	1803	-	-	9/13/13/13	-
4	LDA	I	1812	-	-	7/13/13/13	-
4	LDA	K	1810	-	-	7/13/13/13	-
3	BCL	I	1705	1	-	8/37/137/137	-
5	RG1	N	1407	-	-	3/51/71/71	0/1/1/1
3	BCL	H	1604	2	1/1/21/25	15/37/137/137	-
4	LDA	R	1809	-	-	10/13/13/13	-
4	LDA	A	1817	-	-	9/13/13/13	-
4	LDA	C	1815	-	-	6/13/13/13	-
5	RG1	S	1409	-	-	3/51/71/71	0/1/1/1
3	BCL	G	1504	1	-	7/37/137/137	-
3	BCL	J	1605	2	1/1/21/25	11/37/137/137	-
3	BCL	K	1706	1	1/1/21/25	6/37/137/137	-
4	LDA	H	1804	-	-	6/13/13/13	-
5	RG1	J	1405	-	-	6/51/71/71	0/1/1/1
5	RG1	L	1406	-	-	5/51/71/71	0/1/1/1
4	LDA	R	1818	-	-	5/13/13/13	-
4	LDA	I	1813	-	-	5/13/13/13	-
3	BCL	C	1702	1	1/1/21/25	16/37/137/137	-
4	LDA	G	1824	-	-	4/13/13/13	-
3	BCL	F	1603	2	-	12/37/137/137	-
3	BCL	E	1703	1	-	14/37/137/137	-
4	LDA	I	1825	-	-	8/13/13/13	-
4	LDA	A	1816	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	E	1822	-	-	7/13/13/13	-
3	BCL	A	1701	1	1/1/21/25	11/37/137/137	-
3	BCL	B	1601	2	1/1/21/25	10/37/137/137	-
3	BCL	M	1707	1	1/1/21/25	13/37/137/137	-
4	LDA	R	1819	-	-	8/13/13/13	-
5	RG1	D	1402	-	-	4/51/71/71	0/1/1/1
4	LDA	M	1827	-	-	4/13/13/13	-
3	BCL	L	1606	2	3/3/21/25	9/37/137/137	-
3	BCL	N	1607	2	1/1/21/25	18/37/137/137	-
4	LDA	O	1820	-	-	5/13/13/13	-
4	LDA	C	1821	-	-	5/13/13/13	-
3	BCL	P	1608	2	2/2/21/25	16/37/137/137	-
5	RG1	P	1408	-	-	7/51/71/71	0/1/1/1
4	LDA	G	1814	-	-	8/13/13/13	-
3	BCL	R	1509	1	1/1/21/25	10/37/137/137	-
3	BCL	C	1502	1	1/1/21/25	6/37/137/137	-
4	LDA	J	1805	-	-	9/13/13/13	-
4	LDA	E	1823	-	-	5/13/13/13	-
3	BCL	S	1609	2	1/1/21/25	15/37/137/137	-
4	LDA	K	1826	-	-	6/13/13/13	-
5	RG1	R	1401	-	-	3/51/71/71	0/1/1/1
3	BCL	A	1501	1	1/1/21/25	5/37/137/137	-
3	BCL	E	1503	1	-	7/37/137/137	-
5	RG1	F	1403	-	-	4/51/71/71	0/1/1/1
3	BCL	G	1704	1	1/1/21/25	8/37/137/137	-
3	BCL	I	1505	1	-	6/37/137/137	-
5	RG1	H	1404	-	-	9/51/71/71	0/1/1/1
4	LDA	N	1807	-	-	6/13/13/13	-

The worst 5 of 513 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1702	BCL	C2-C3	8.30	1.52	1.33
3	K	1506	BCL	CAC-C3C	-7.93	1.38	1.54
3	G	1504	BCL	C4B-NB	7.91	1.42	1.35
4	I	1812	LDA	O1-N1	-7.79	1.23	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1509	BCL	C4B-NB	7.41	1.41	1.35

The worst 5 of 726 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1606	BCL	C4A-NA-C1A	-14.72	100.09	106.71
3	B	1601	BCL	C4A-NA-C1A	-13.70	100.55	106.71
3	R	1509	BCL	C4A-NA-C1A	-12.45	101.11	106.71
3	M	1507	BCL	C4A-NA-C1A	-12.02	101.30	106.71
3	D	1602	BCL	C4A-NA-C1A	-11.87	101.37	106.71

5 of 23 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1501	BCL	CBD
3	A	1701	BCL	C3C
3	B	1601	BCL	C8
3	C	1502	BCL	C13
3	C	1702	BCL	C13

5 of 513 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1701	BCL	C4C-C3C-CAC-CBC
3	C	1702	BCL	C1-C2-C3-C4
3	C	1702	BCL	C1-C2-C3-C5
3	E	1503	BCL	C2C-C3C-CAC-CBC
3	F	1603	BCL	C11-C10-C8-C7

There are no ring outliers.

60 monomers are involved in 432 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1801	LDA	2	0
3	M	1507	BCL	7	0
3	R	1709	BCL	21	0
4	M	1811	LDA	4	0
3	K	1506	BCL	9	0
3	O	1708	BCL	10	0
4	D	1802	LDA	3	0
4	L	1806	LDA	5	0

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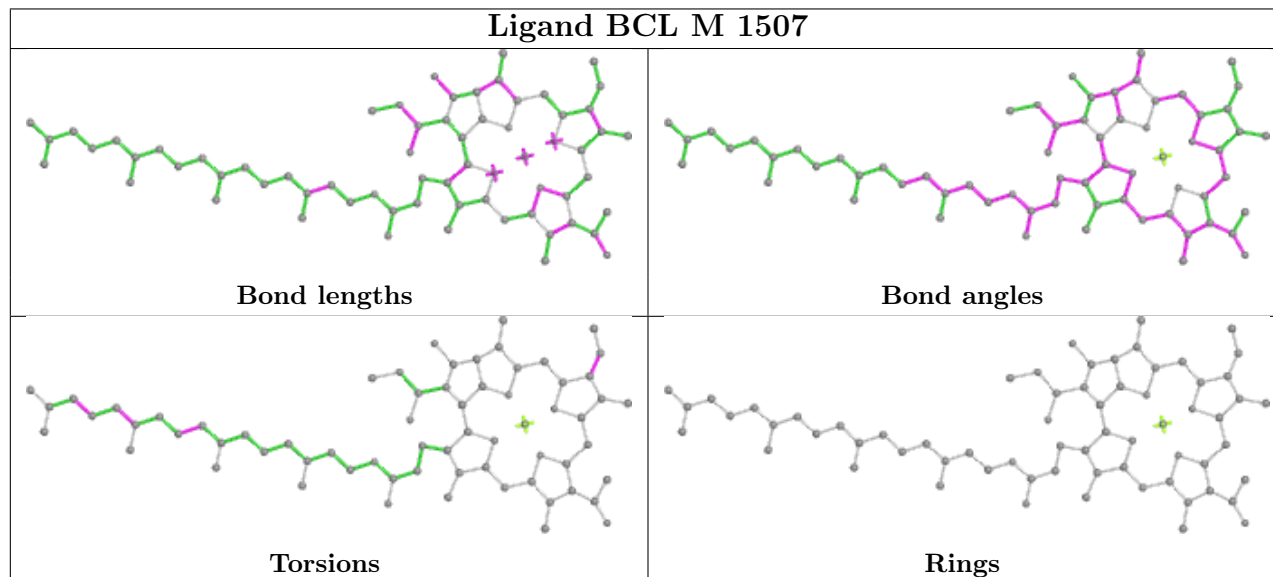
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1602	BCL	8	0
3	O	1508	BCL	11	0
4	P	1808	LDA	3	0
4	F	1803	LDA	7	0
4	I	1812	LDA	7	0
4	K	1810	LDA	8	0
3	I	1705	BCL	21	0
5	N	1407	RG1	4	0
3	H	1604	BCL	12	0
4	A	1817	LDA	3	0
4	C	1815	LDA	6	0
5	S	1409	RG1	5	0
3	G	1504	BCL	6	0
3	J	1605	BCL	17	0
3	K	1706	BCL	5	0
4	H	1804	LDA	3	0
5	J	1405	RG1	1	0
5	L	1406	RG1	4	0
4	R	1818	LDA	12	0
4	I	1813	LDA	2	0
3	C	1702	BCL	8	0
4	G	1824	LDA	14	0
3	F	1603	BCL	12	0
3	E	1703	BCL	7	0
4	I	1825	LDA	6	0
4	A	1816	LDA	8	0
4	E	1822	LDA	8	0
3	A	1701	BCL	8	0
3	B	1601	BCL	11	0
3	M	1707	BCL	21	0
5	D	1402	RG1	5	0
4	M	1827	LDA	2	0
3	L	1606	BCL	25	0
3	N	1607	BCL	16	0
4	O	1820	LDA	7	0
3	P	1608	BCL	10	0
5	P	1408	RG1	4	0
4	G	1814	LDA	3	0
3	R	1509	BCL	7	0
3	C	1502	BCL	7	0
4	J	1805	LDA	1	0
4	E	1823	LDA	6	0

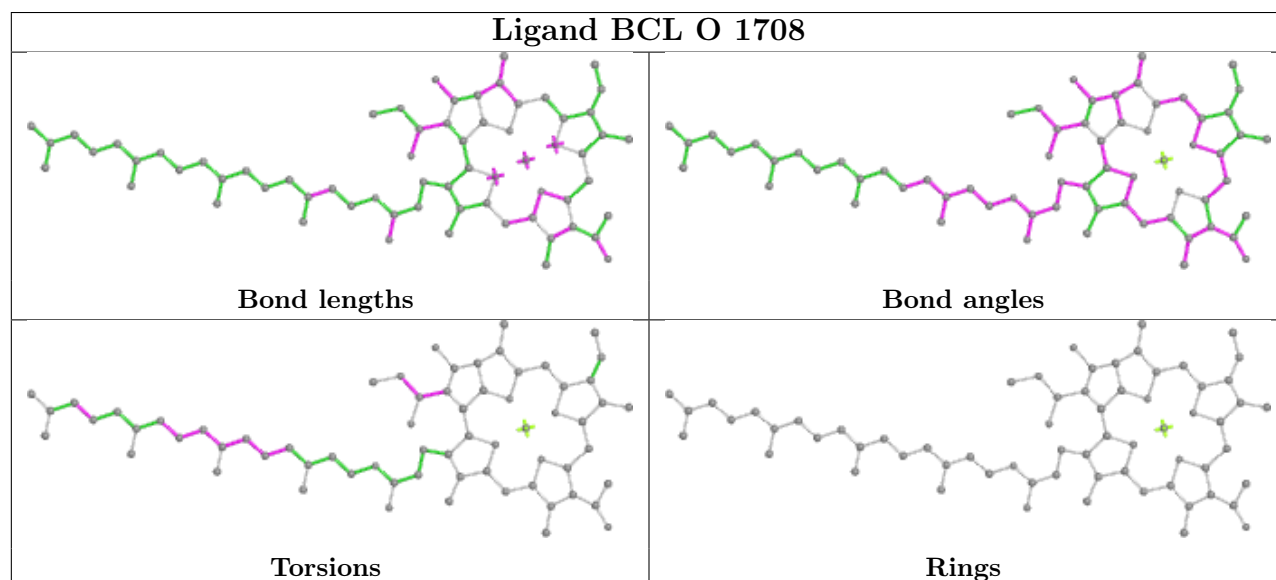
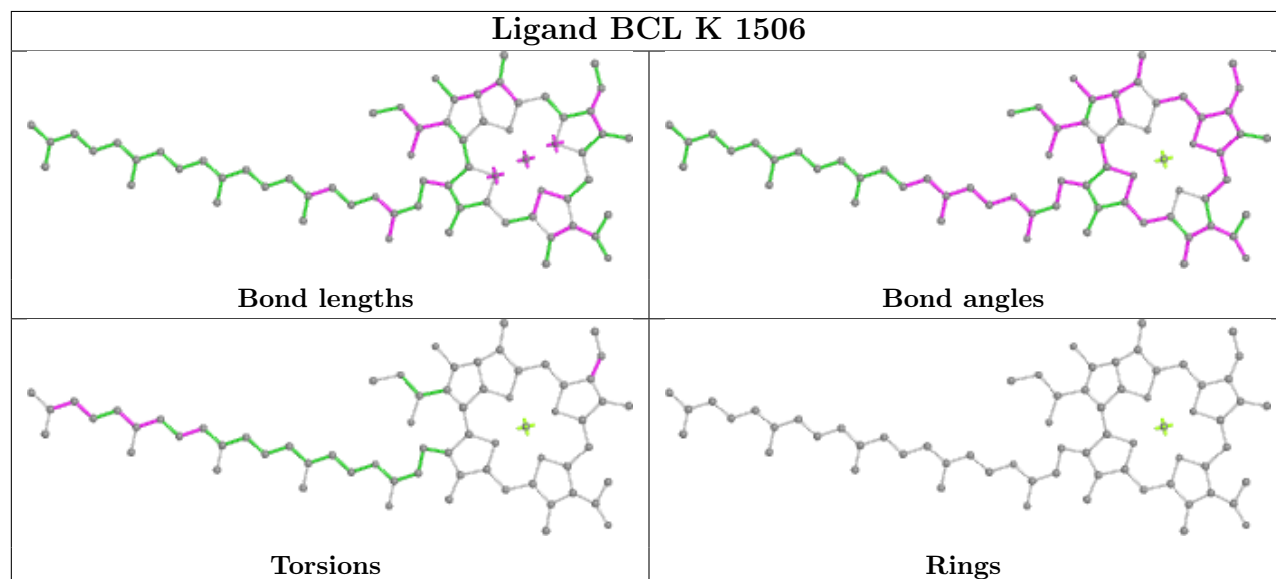
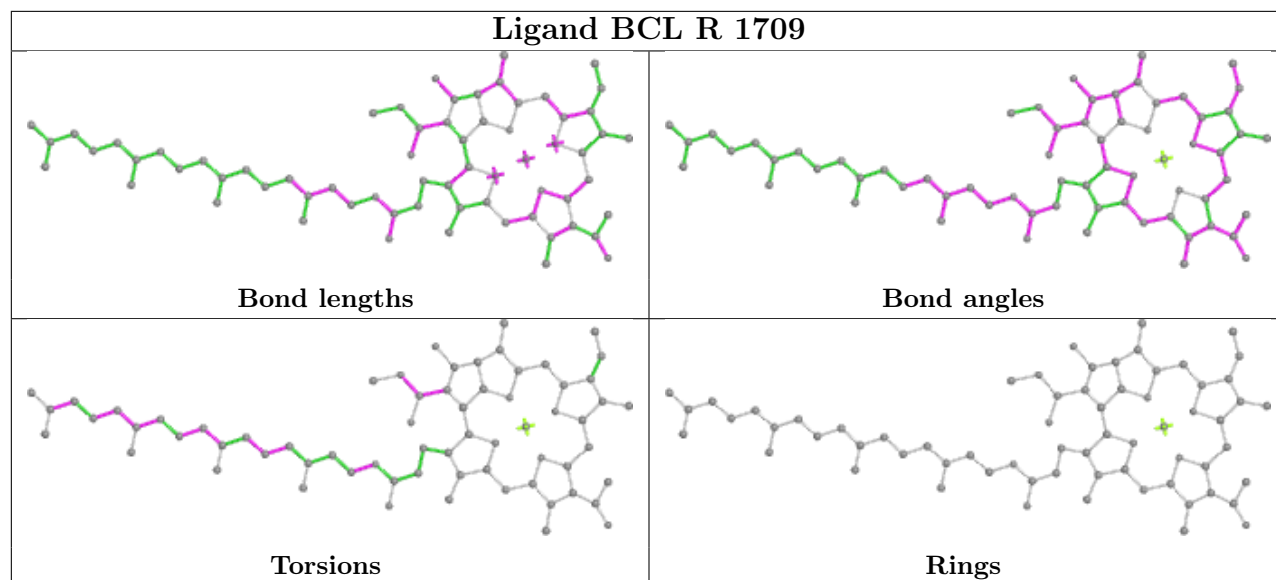
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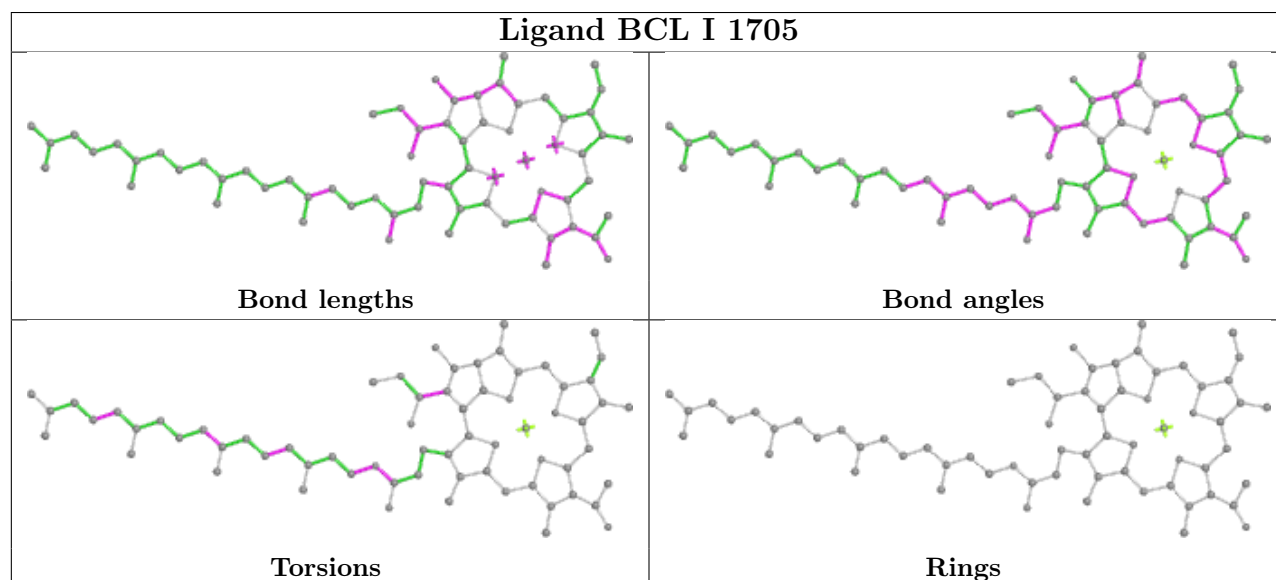
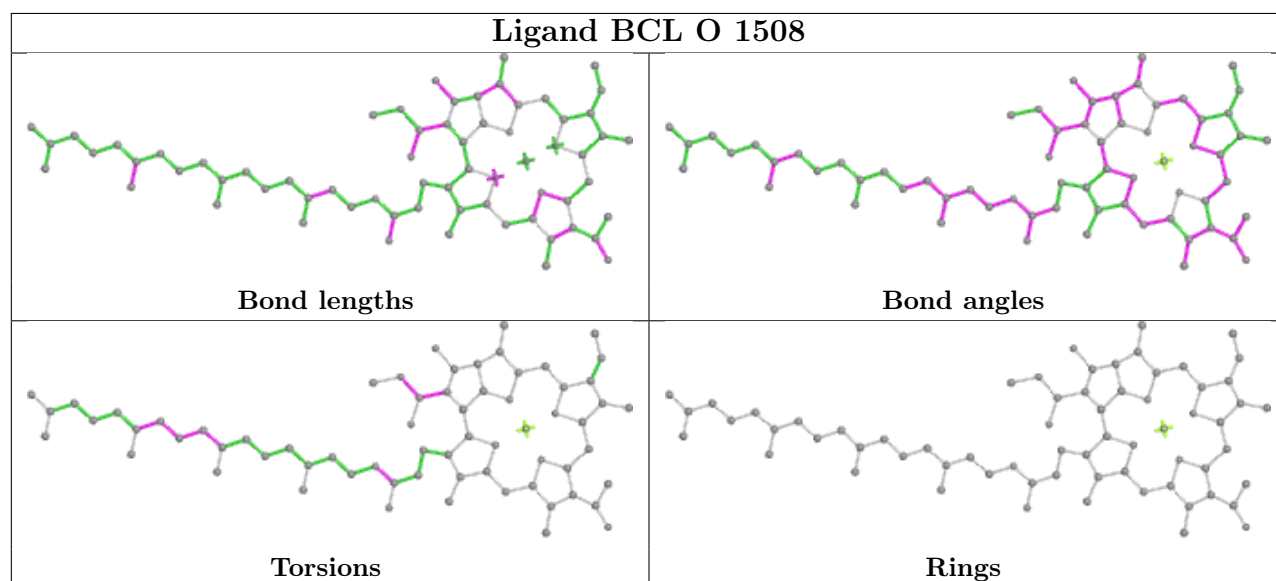
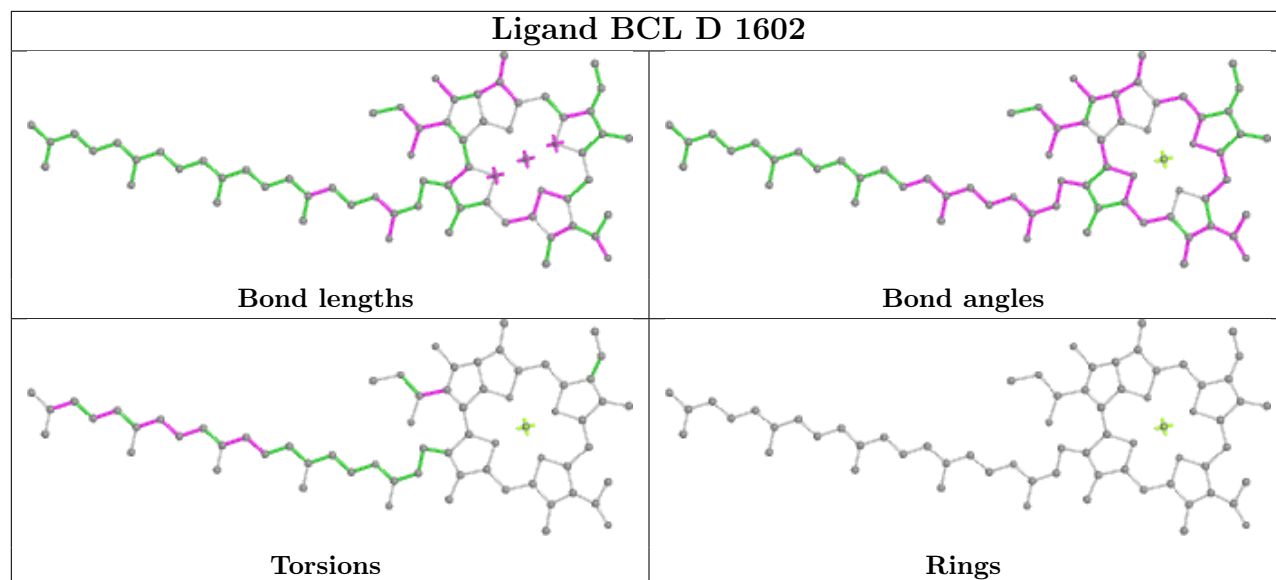
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	1609	BCL	13	0
4	K	1826	LDA	4	0
5	R	1401	RG1	4	0
3	A	1501	BCL	17	0
3	E	1503	BCL	5	0
5	F	1403	RG1	5	0
3	G	1704	BCL	21	0
3	I	1505	BCL	12	0
5	H	1404	RG1	5	0
4	N	1807	LDA	2	0

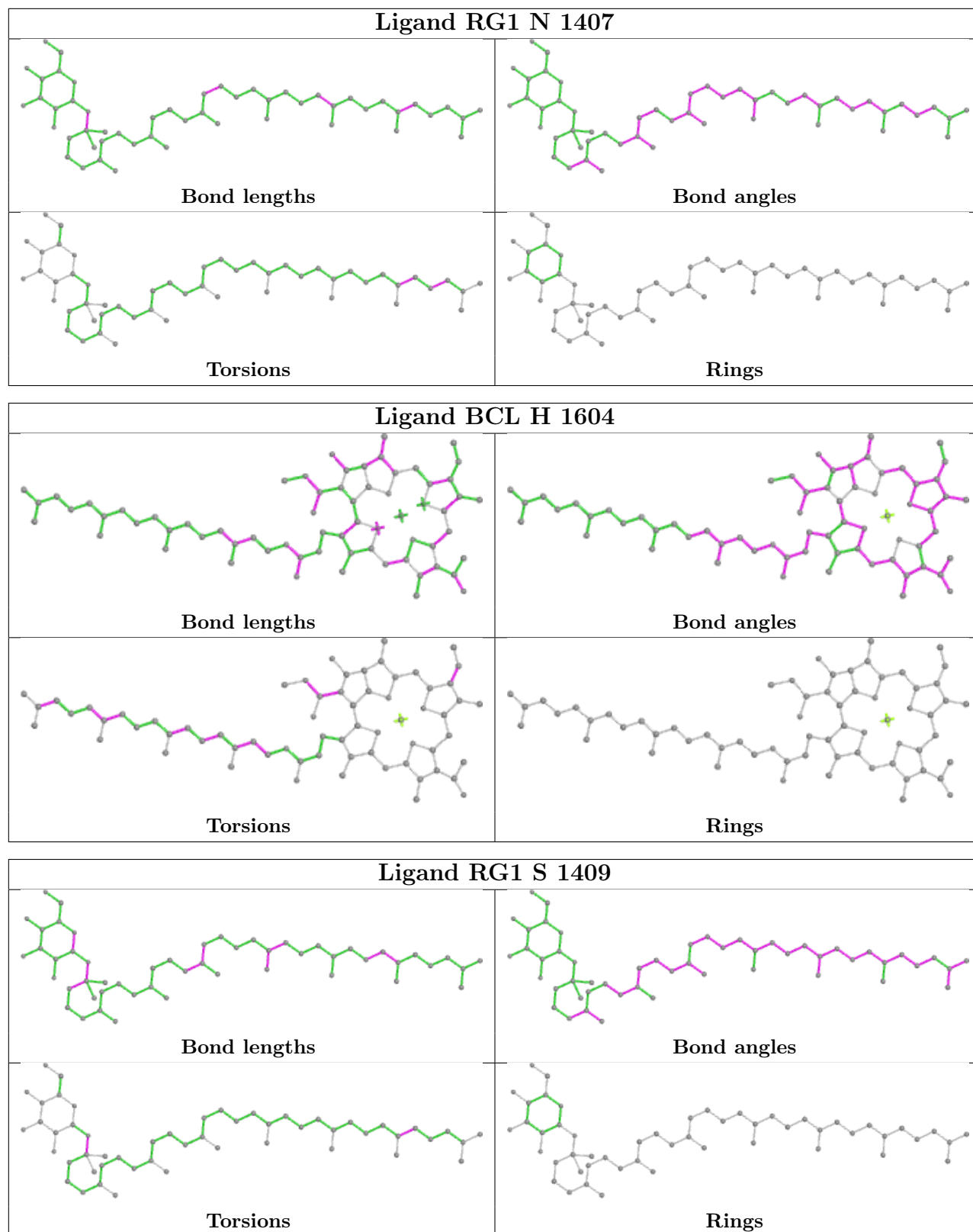
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

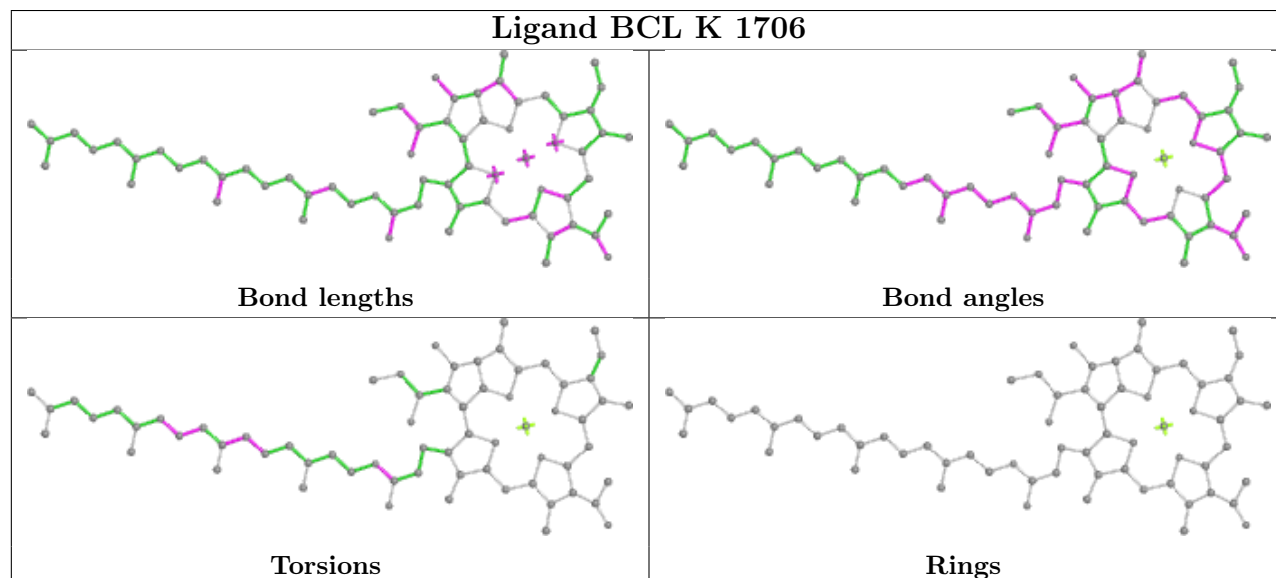
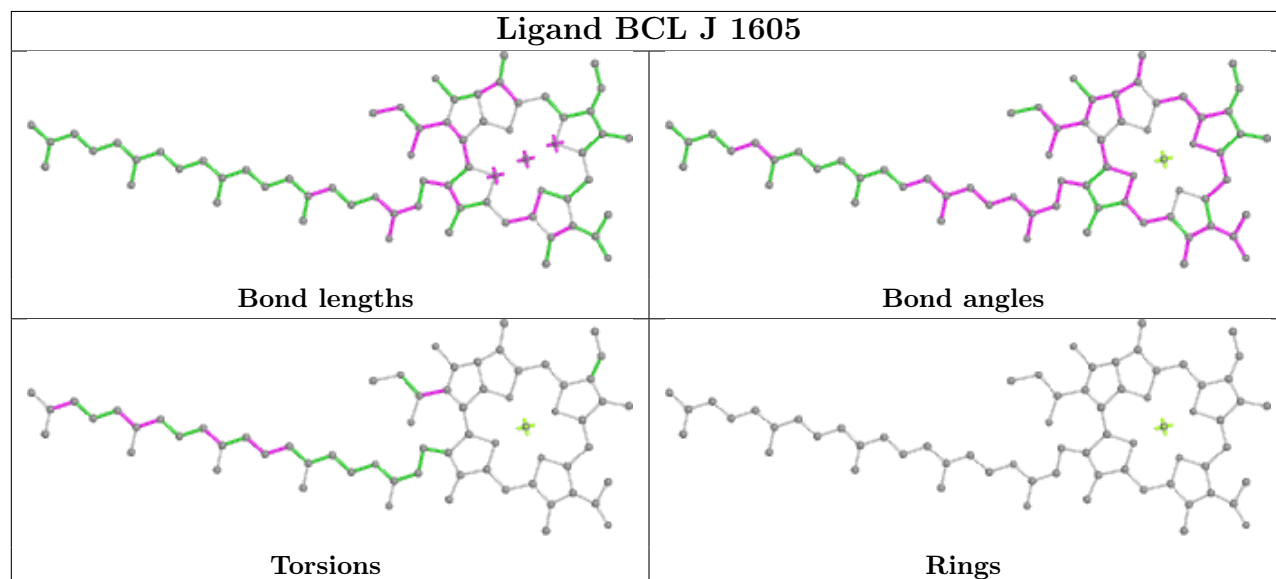
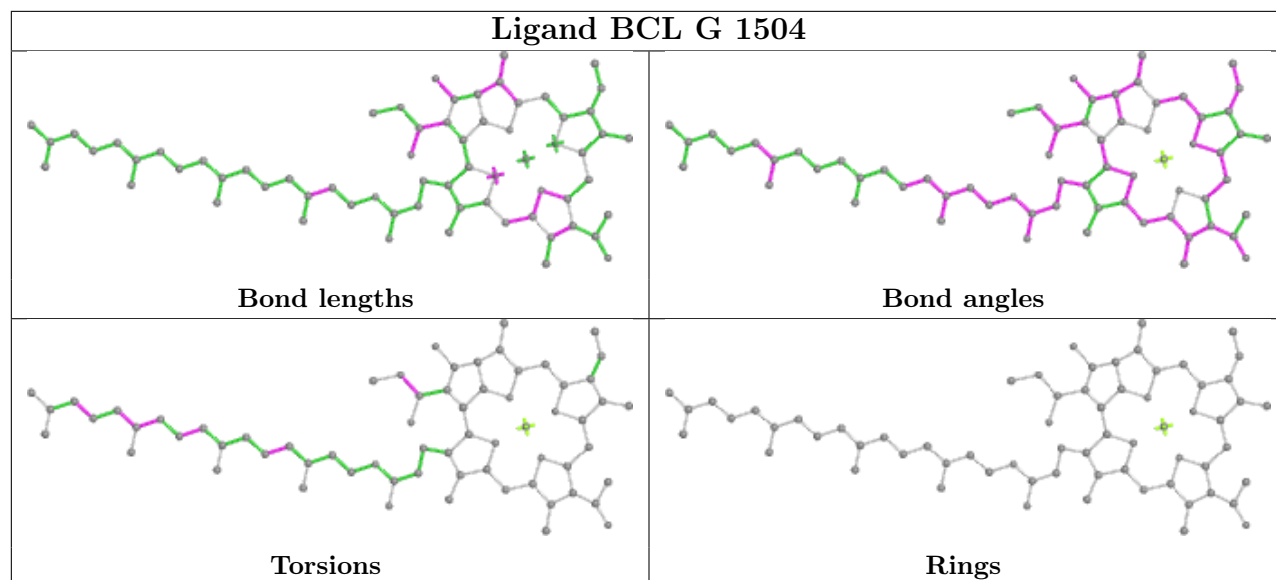


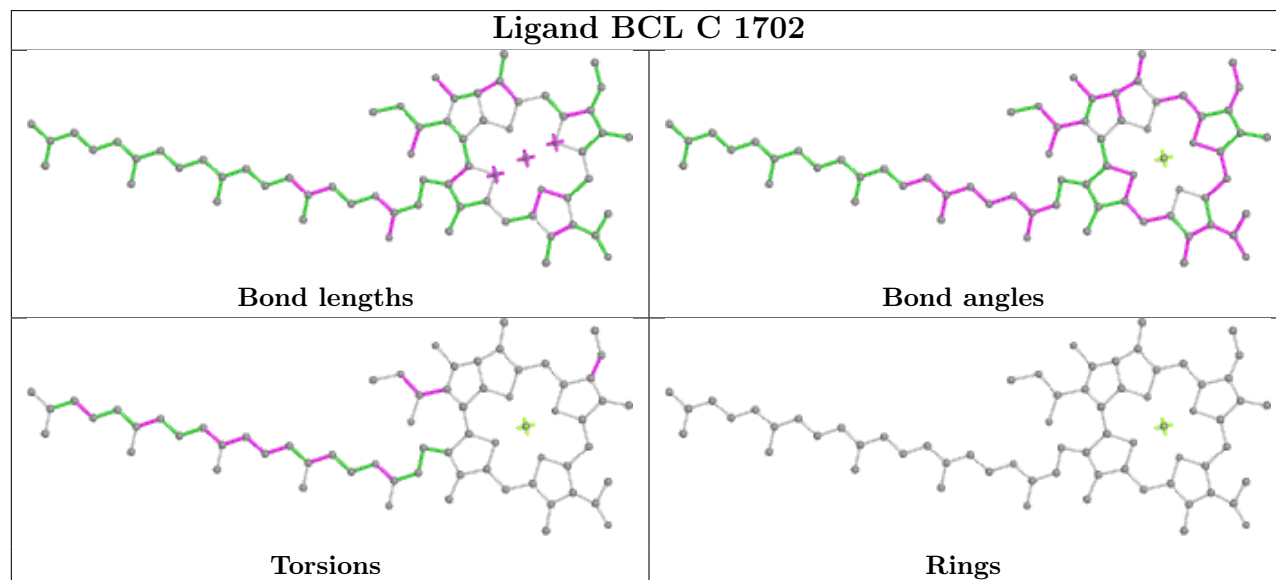
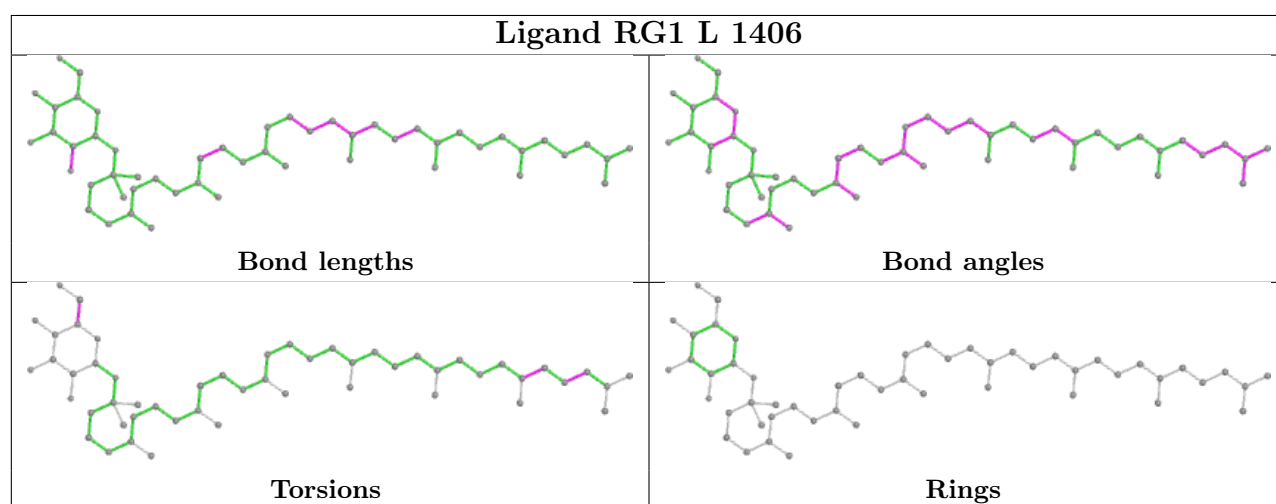
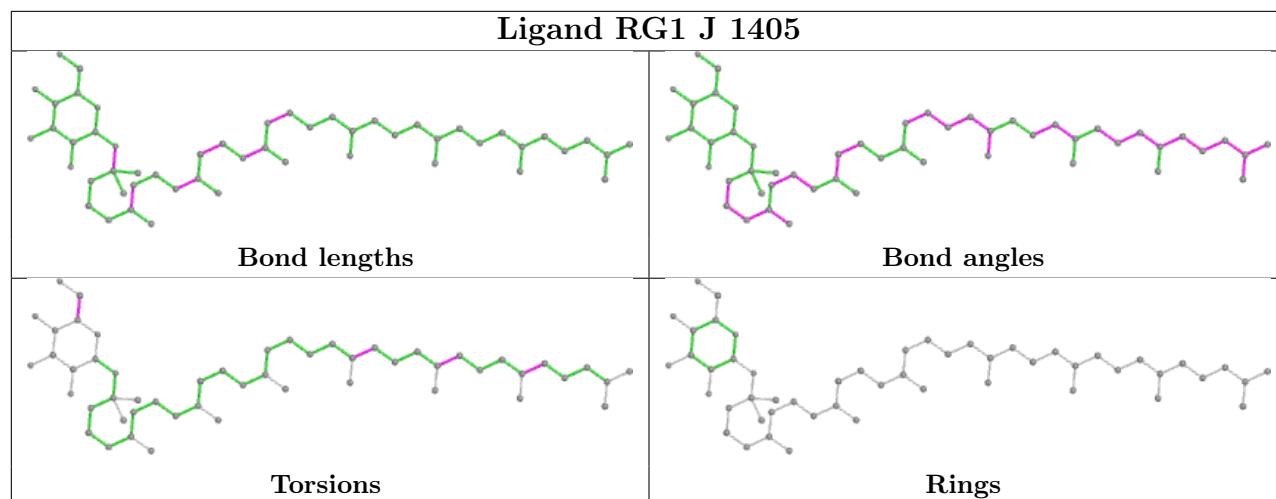


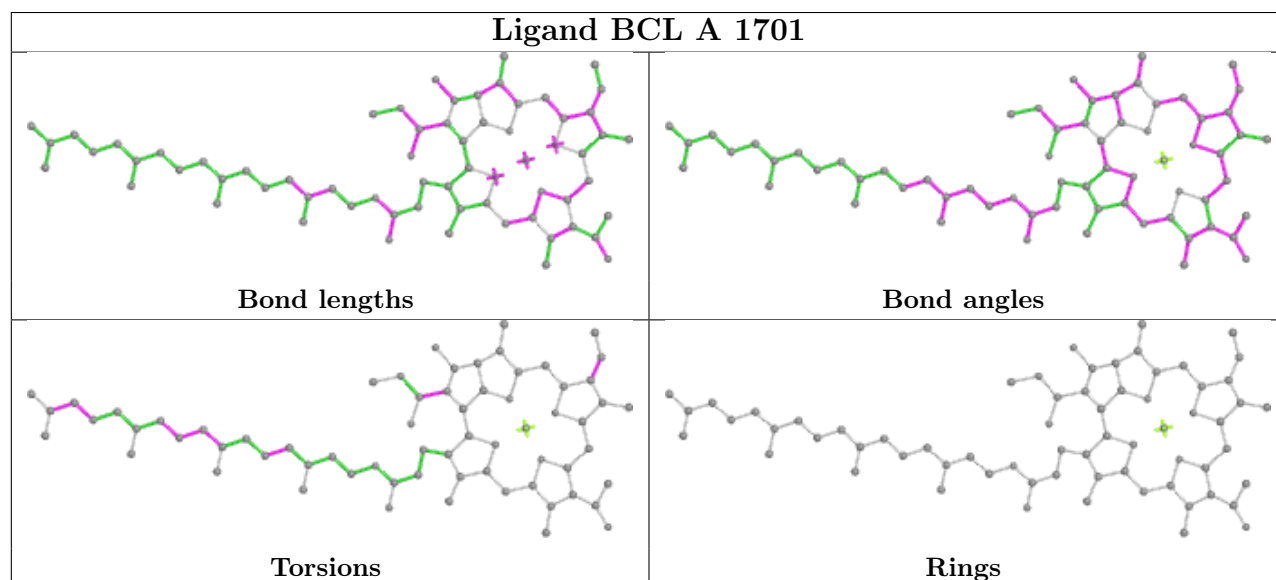
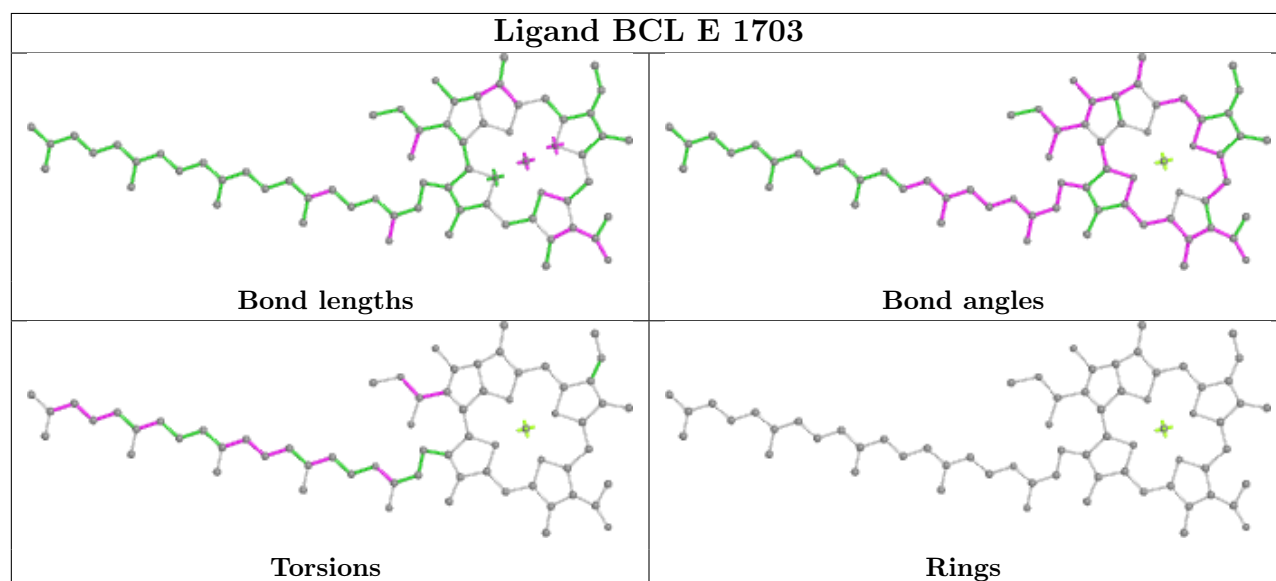
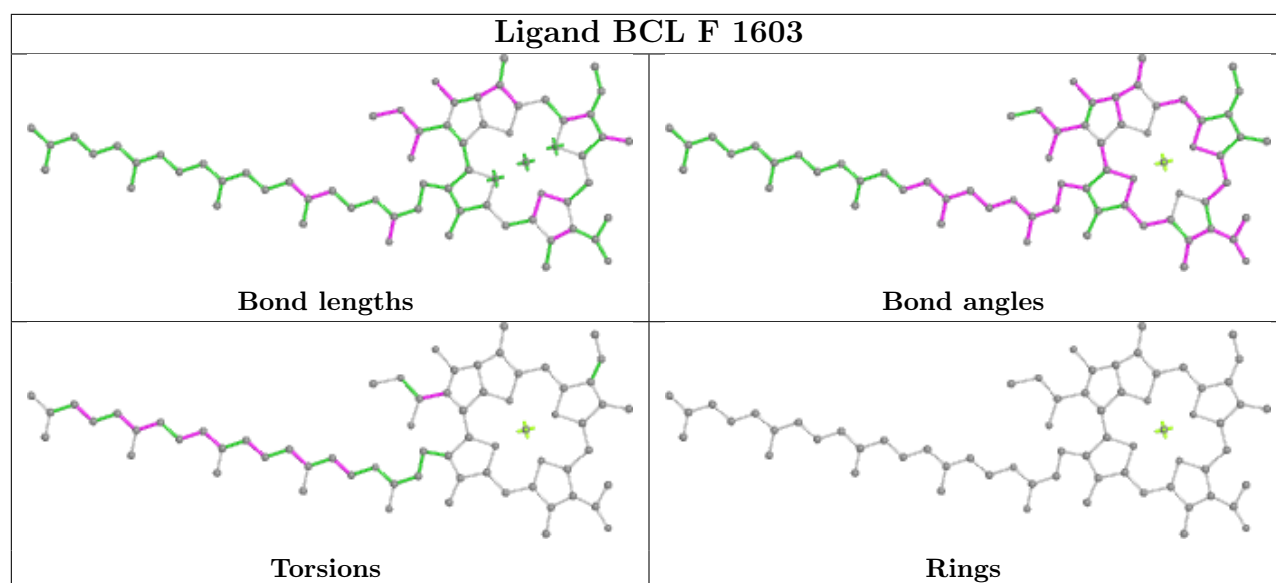


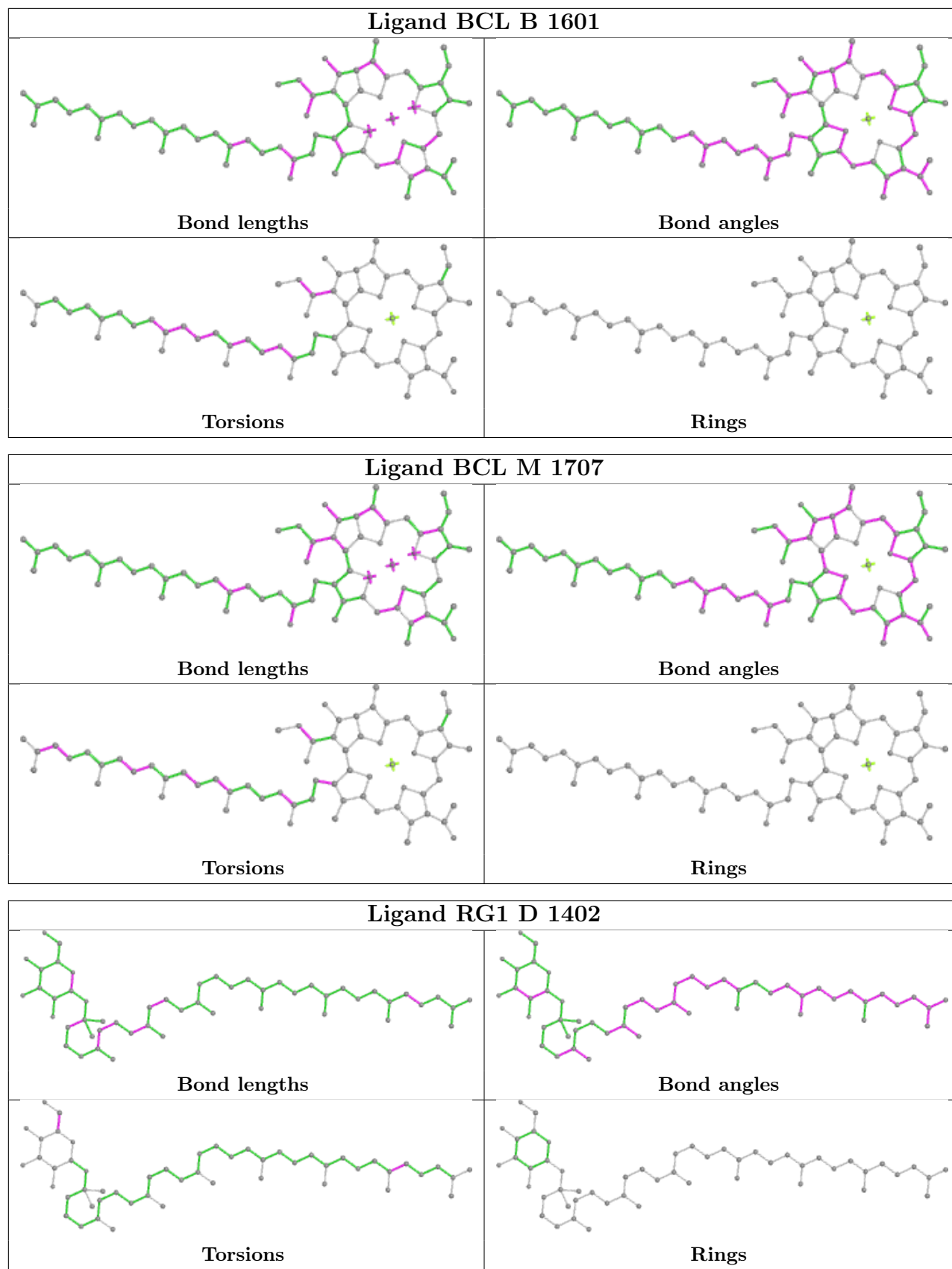


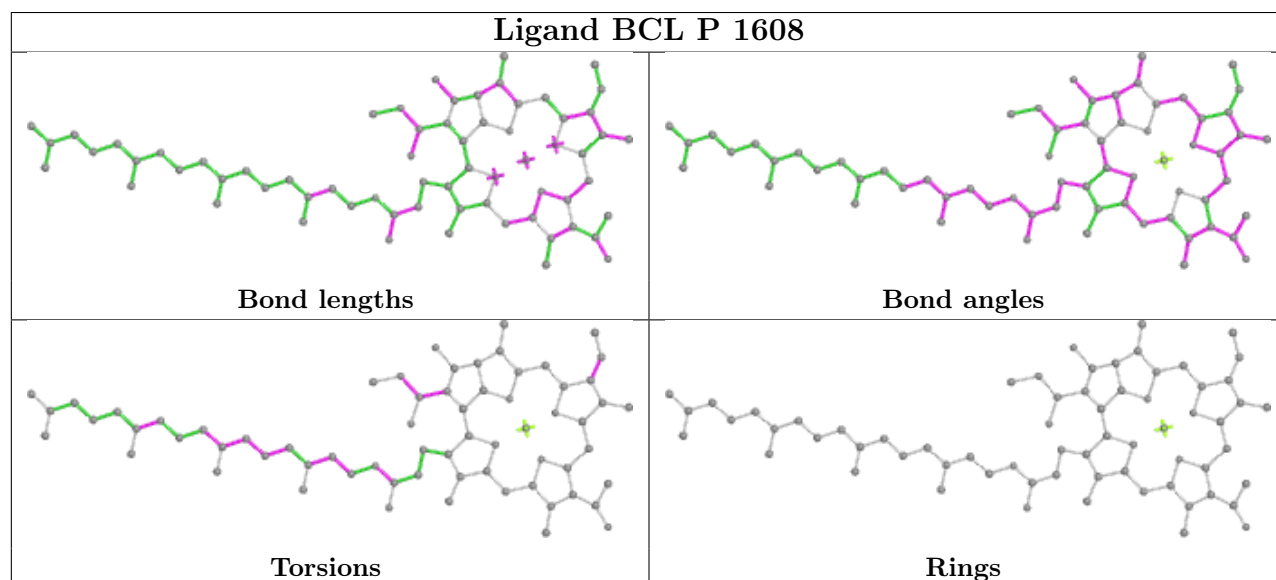
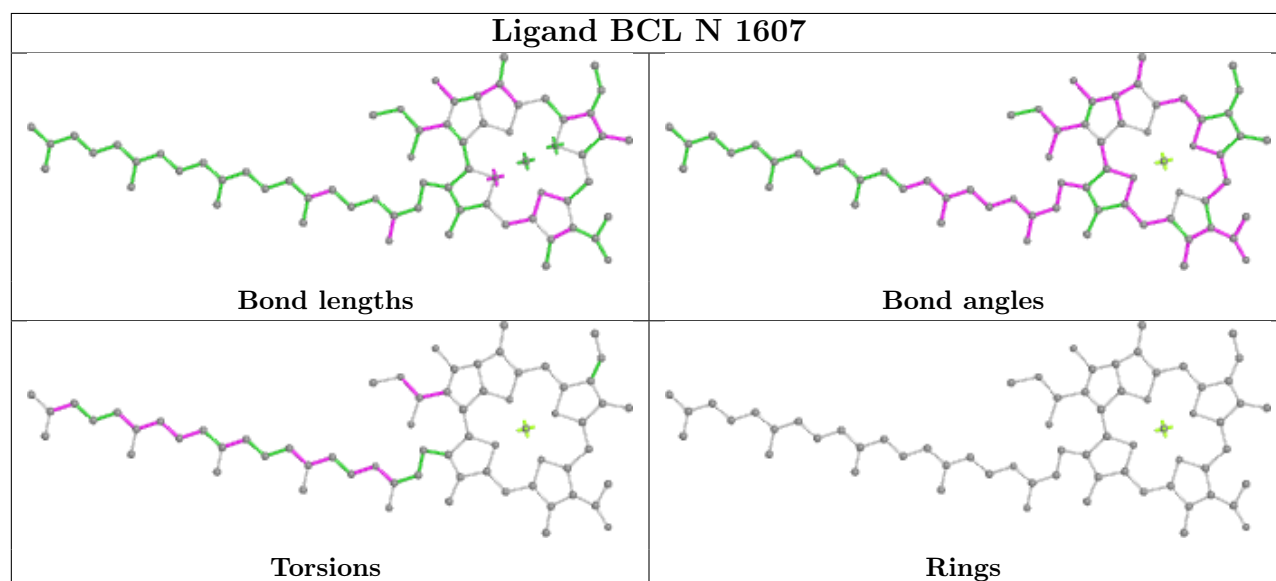
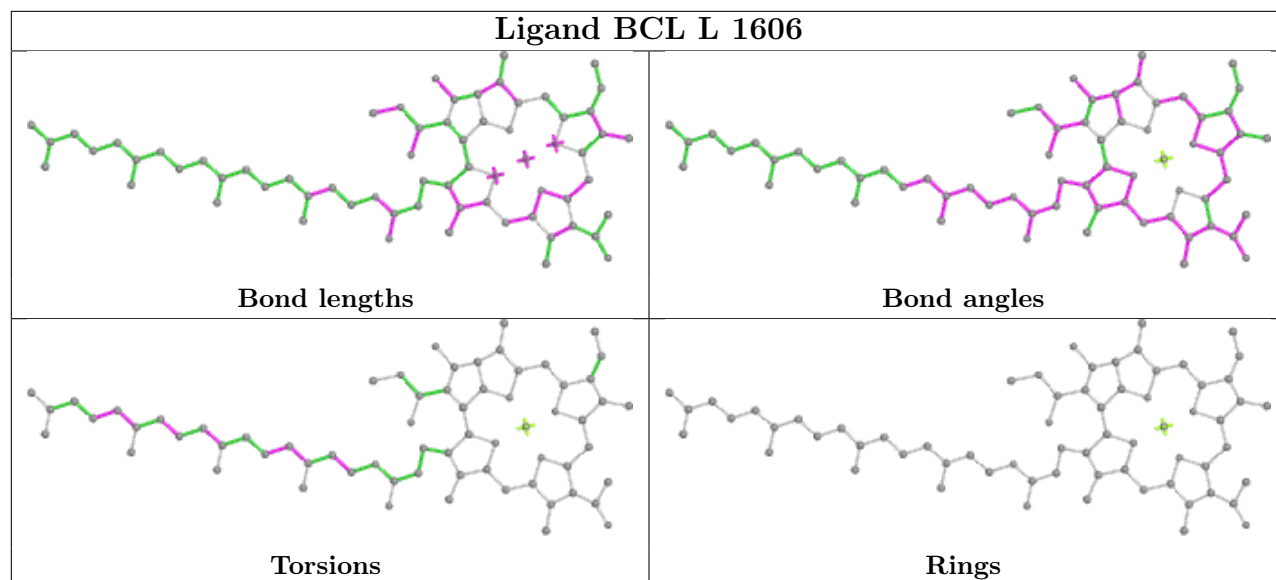


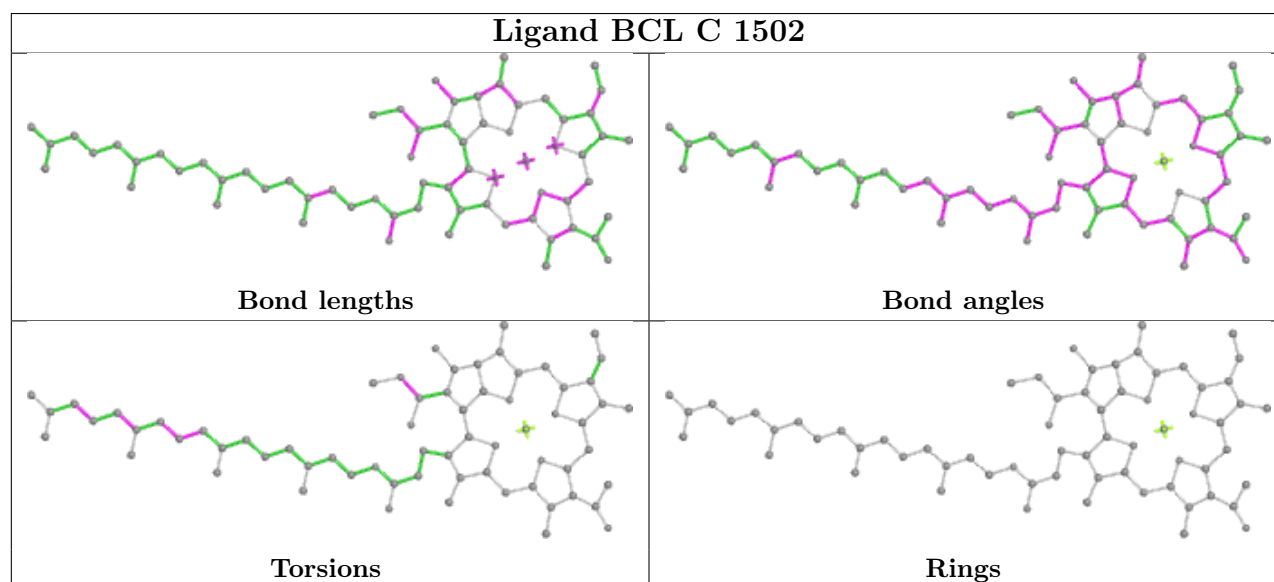
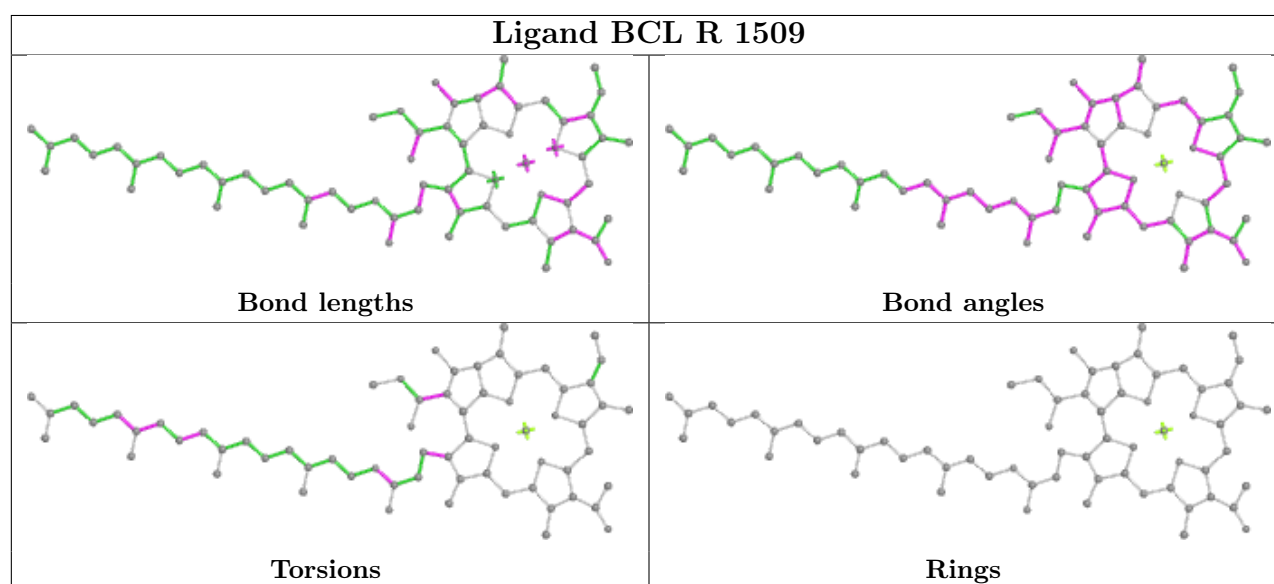
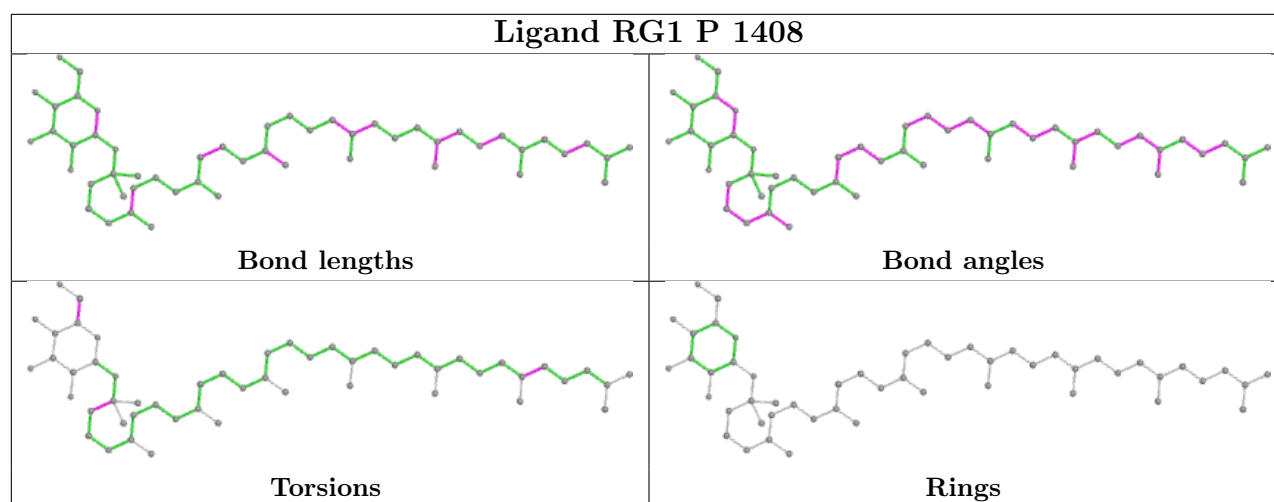




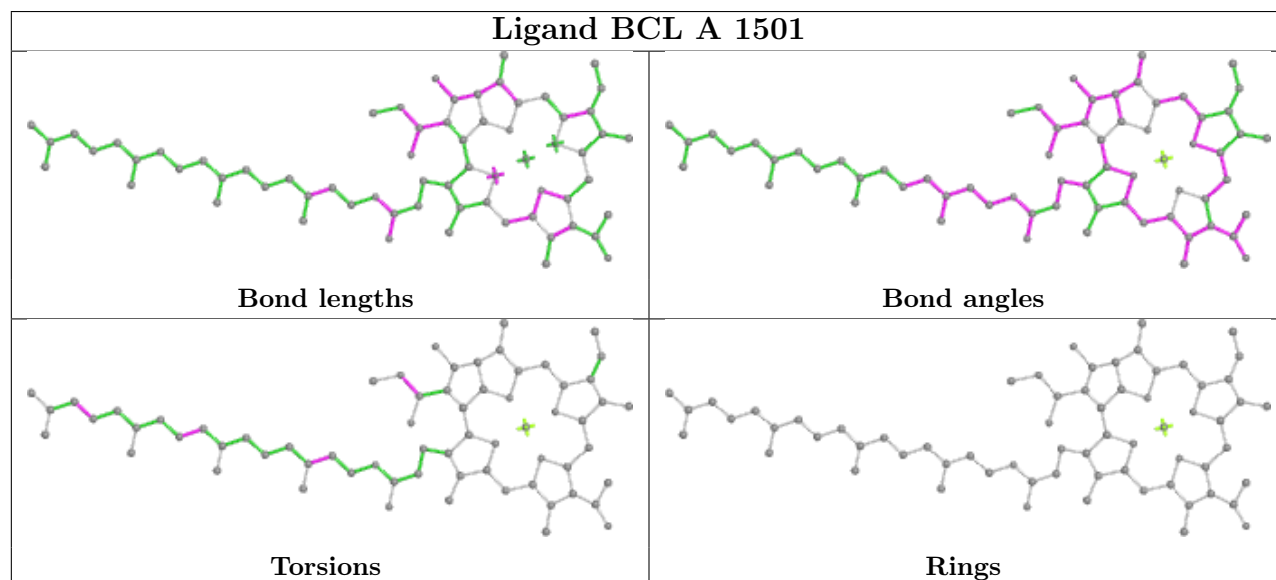
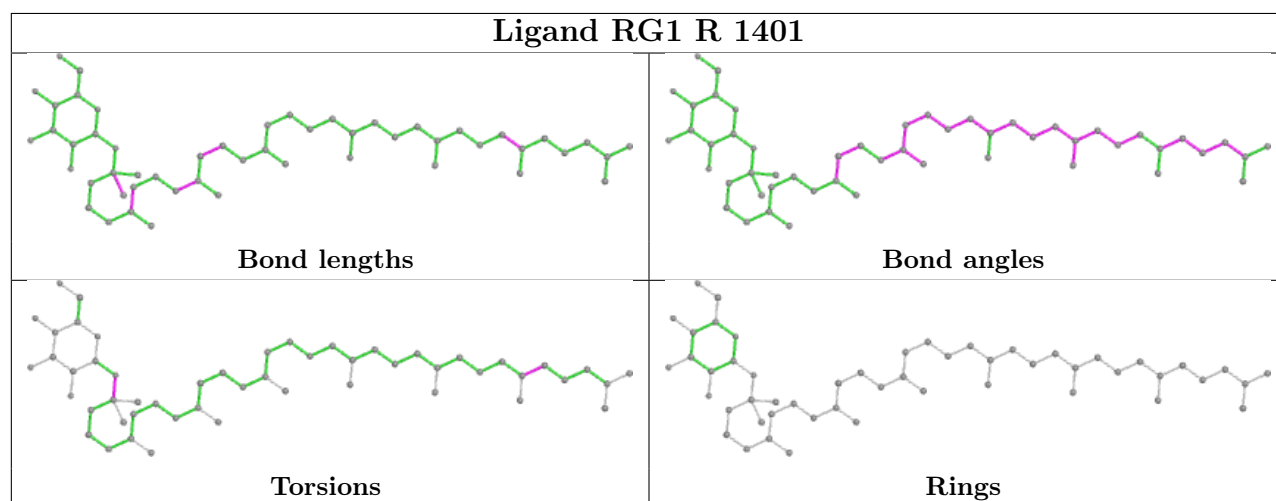
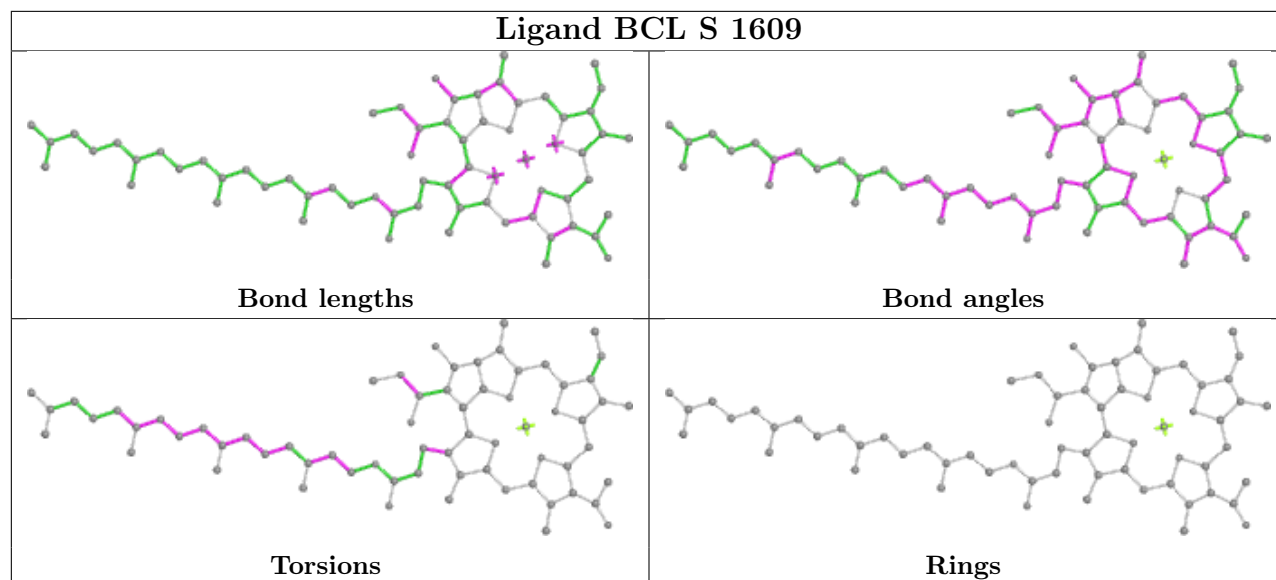


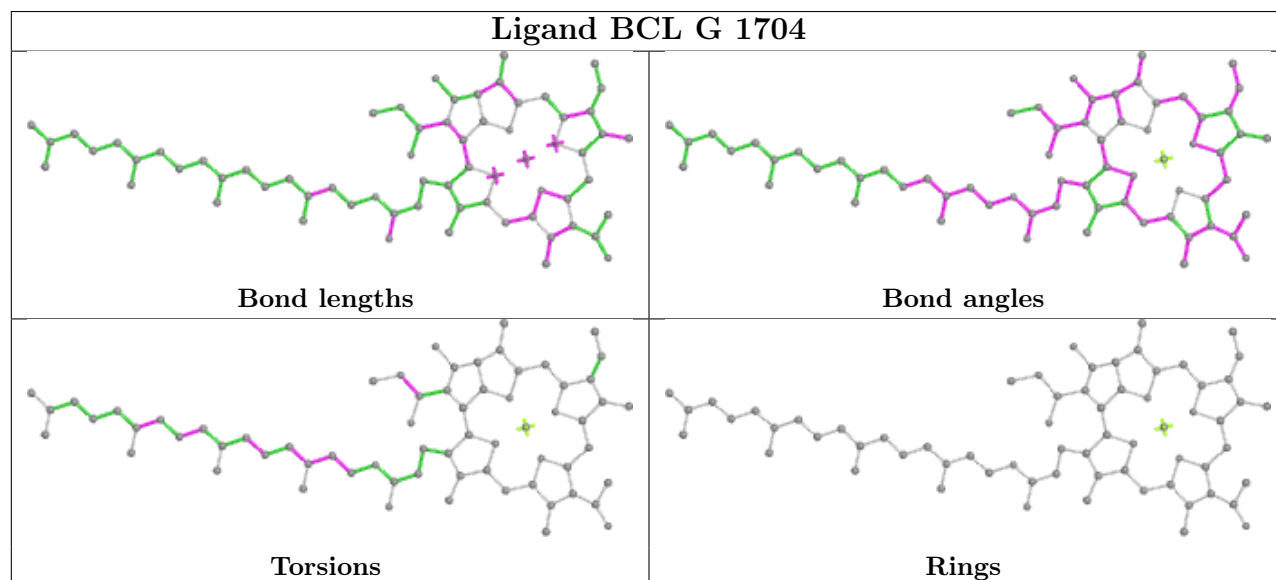
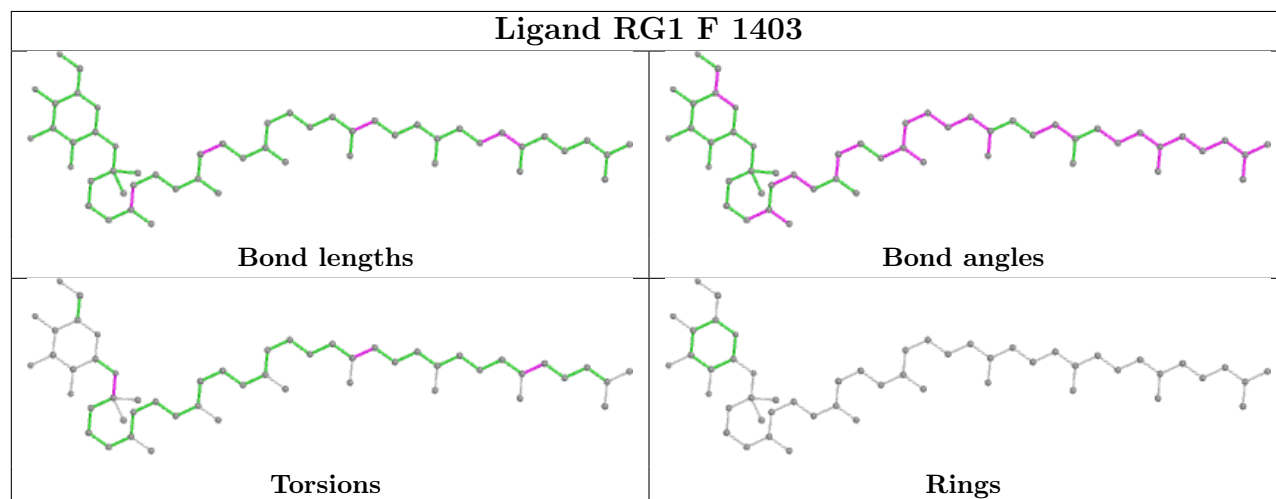
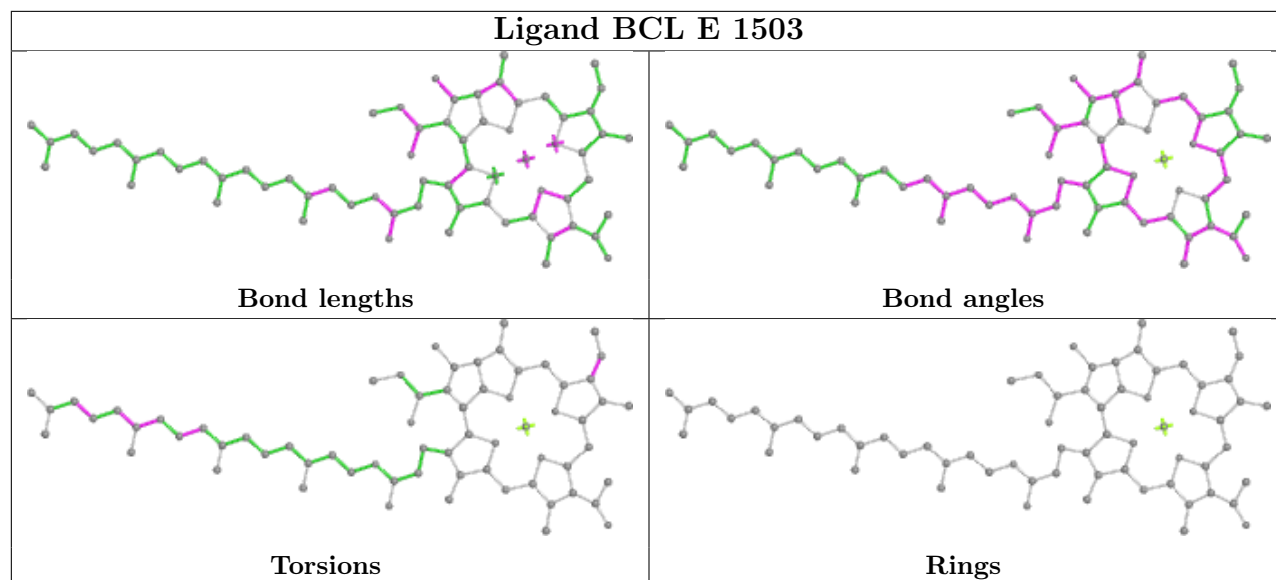


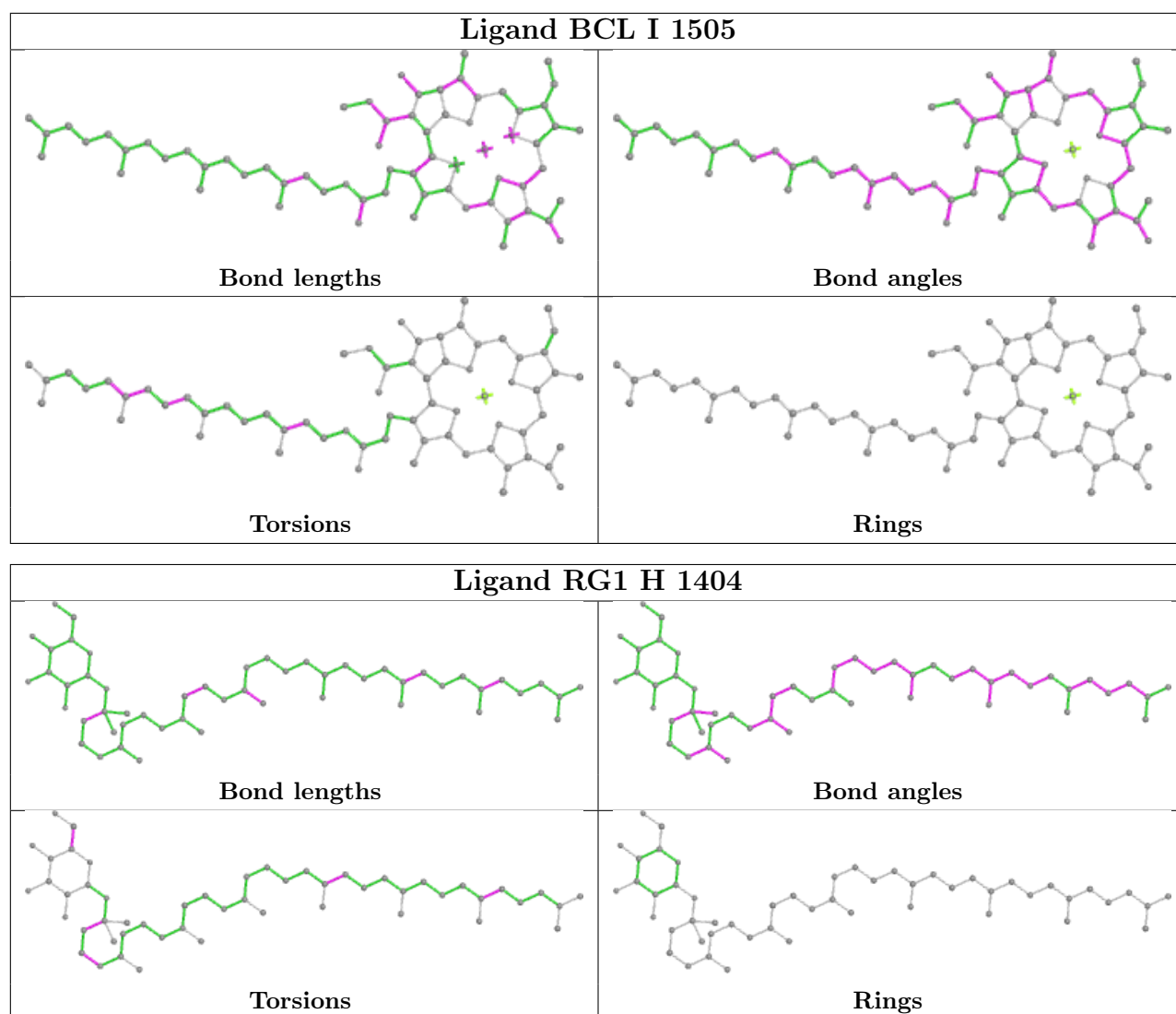












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	52/53 (98%)	0.42	6 (11%) 4 3	35, 41, 88, 98	0
1	C	52/53 (98%)	0.99	7 (13%) 3 2	34, 41, 88, 102	0
1	E	52/53 (98%)	1.42	7 (13%) 3 2	35, 40, 88, 101	0
1	G	52/53 (98%)	0.77	6 (11%) 4 3	33, 40, 87, 99	0
1	I	52/53 (98%)	0.96	6 (11%) 4 3	34, 39, 88, 100	0
1	K	52/53 (98%)	0.68	6 (11%) 4 3	33, 40, 88, 100	0
1	M	52/53 (98%)	0.60	6 (11%) 4 3	35, 40, 88, 101	0
1	O	52/53 (98%)	0.91	6 (11%) 4 3	34, 41, 87, 100	0
1	R	52/53 (98%)	0.74	6 (11%) 4 3	35, 41, 87, 97	0
2	B	41/41 (100%)	-0.23	1 (2%) 59 54	42, 46, 54, 67	0
2	D	41/41 (100%)	0.02	2 (4%) 29 27	41, 46, 55, 64	0
2	F	41/41 (100%)	0.01	1 (2%) 59 54	38, 45, 52, 65	0
2	H	41/41 (100%)	-0.21	1 (2%) 59 54	37, 45, 52, 64	0
2	J	41/41 (100%)	-0.24	0 100 100	40, 45, 53, 65	0
2	L	41/41 (100%)	0.43	1 (2%) 59 54	39, 43, 52, 65	0
2	N	41/41 (100%)	0.21	3 (7%) 15 11	41, 45, 52, 69	0
2	P	41/41 (100%)	-0.02	1 (2%) 59 54	40, 46, 53, 68	0
2	S	41/41 (100%)	-0.35	1 (2%) 59 54	41, 46, 54, 67	0
All	All	837/846 (98%)	0.45	67 (8%) 12 9	33, 43, 79, 102	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	ALA	23.9
1	E	52	ALA	20.1
1	E	49	VAL	17.1

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Mol	Chain	Res	Type	RSRZ
1	M	49	VAL	16.6
1	C	52	ALA	16.2

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CXM	K	1	11/12	0.94	0.12	40,46,54,54	0
1	CXM	C	1	11/12	0.95	0.28	45,47,55,58	0
1	CXM	I	1	11/12	0.95	0.15	38,45,51,52	0
1	CXM	A	1	11/12	0.95	0.12	45,48,60,62	0
1	CXM	R	1	11/12	0.95	0.21	45,48,54,59	0
1	CXM	G	1	11/12	0.96	0.16	45,46,52,58	0
1	CXM	M	1	11/12	0.96	0.13	40,45,51,52	0
1	CXM	O	1	11/12	0.96	0.14	45,47,54,58	0
1	CXM	E	1	11/12	0.96	0.15	41,46,48,50	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	LDA	E	1823	16/16	0.18	0.65	89,99,122,123	0
4	LDA	C	1815	16/16	0.46	0.53	79,96,103,103	0
4	LDA	M	1827	16/16	0.48	0.40	96,101,105,107	0
4	LDA	N	1807	16/16	0.52	0.32	61,66,76,78	0
4	LDA	I	1812	16/16	0.56	0.46	87,106,111,111	0
4	LDA	E	1822	16/16	0.57	0.34	69,91,107,108	0
4	LDA	K	1810	16/16	0.57	0.56	107,110,116,116	0

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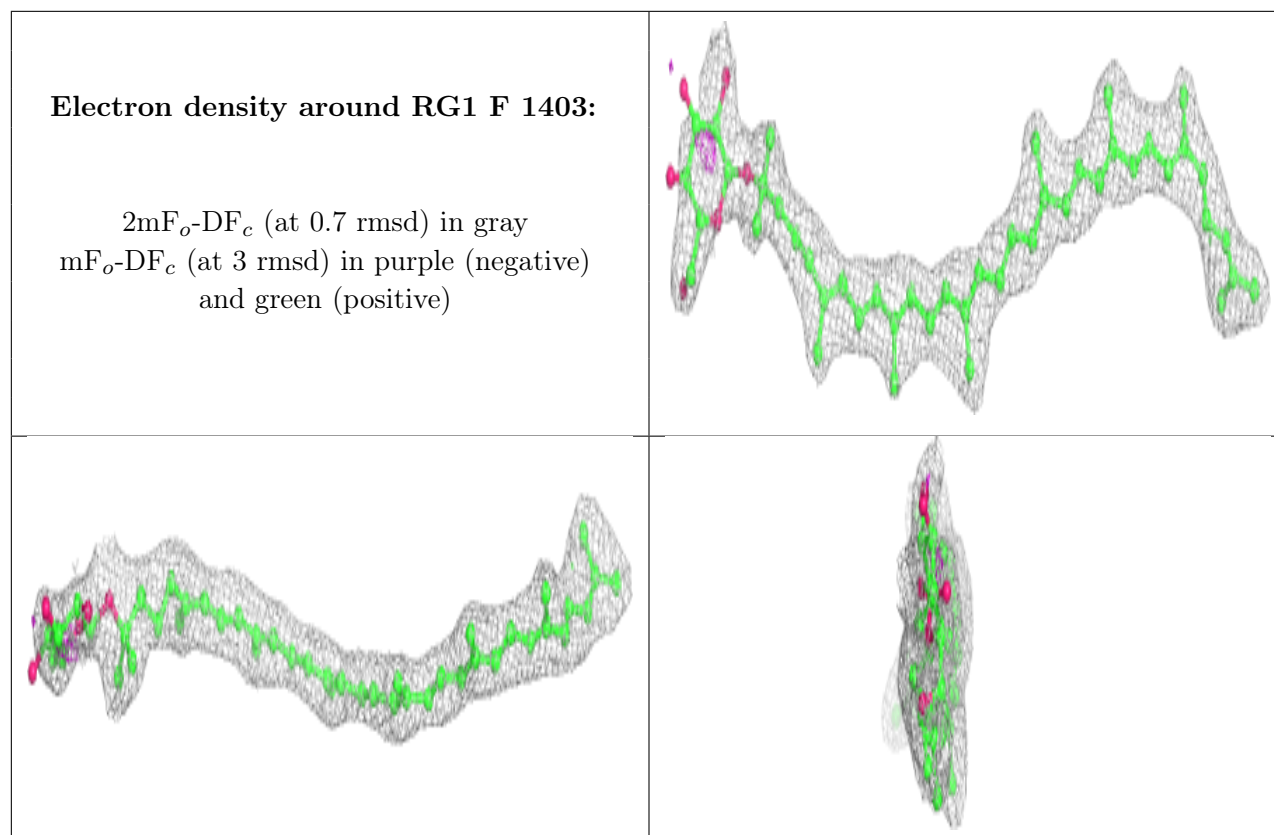
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	LDA	R	1818	16/16	0.58	0.41	85,90,95,96	0
4	LDA	M	1811	16/16	0.60	0.36	75,77,84,84	0
4	LDA	A	1816	16/16	0.61	0.42	86,87,91,93	0
4	LDA	G	1824	16/16	0.61	0.37	89,105,120,121	0
4	LDA	G	1814	16/16	0.63	0.29	70,74,83,84	0
4	LDA	C	1821	16/16	0.63	0.34	82,90,101,103	0
4	LDA	P	1808	16/16	0.64	0.38	53,61,84,86	0
4	LDA	I	1825	16/16	0.65	0.40	95,101,108,108	0
4	LDA	L	1806	16/16	0.70	0.30	44,52,74,75	0
4	LDA	B	1801	16/16	0.70	0.29	49,62,76,78	0
4	LDA	D	1802	16/16	0.71	0.34	53,57,75,77	0
4	LDA	R	1809	16/16	0.71	0.26	57,63,71,73	0
4	LDA	O	1820	16/16	0.71	0.29	71,80,92,95	0
4	LDA	F	1803	16/16	0.73	0.24	50,56,67,67	0
4	LDA	J	1805	16/16	0.75	0.21	44,54,67,68	0
4	LDA	I	1813	16/16	0.76	0.19	50,54,76,76	0
4	LDA	R	1819	16/16	0.76	0.33	80,83,85,87	0
5	RG1	F	1403	52/52	0.77	0.25	28,38,77,82	0
4	LDA	K	1826	16/16	0.80	0.24	83,88,103,104	0
5	RG1	J	1405	52/52	0.81	0.24	28,37,76,80	0
4	LDA	A	1817	16/16	0.82	0.21	67,69,87,87	0
5	RG1	D	1402	52/52	0.83	0.19	30,44,77,81	0
4	LDA	H	1804	16/16	0.84	0.26	49,57,66,67	0
5	RG1	N	1407	52/52	0.85	0.20	29,37,69,73	0
5	RG1	S	1409	52/52	0.85	0.20	29,40,77,78	0
5	RG1	R	1401	52/52	0.87	0.23	30,40,74,77	0
3	BCL	C	1702	66/66	0.88	0.19	41,48,78,80	0
5	RG1	P	1408	52/52	0.88	0.22	32,42,75,78	0
5	RG1	H	1404	52/52	0.89	0.21	27,37,78,80	0
3	BCL	R	1709	66/66	0.89	0.19	43,53,78,82	0
3	BCL	N	1607	66/66	0.89	0.15	31,41,63,65	0
3	BCL	J	1605	66/66	0.90	0.16	31,39,64,66	0
3	BCL	G	1704	66/66	0.90	0.20	32,45,73,76	0
3	BCL	A	1701	66/66	0.91	0.17	42,49,80,83	0
5	RG1	L	1406	52/52	0.91	0.18	26,35,74,77	0
3	BCL	M	1707	66/66	0.92	0.17	29,44,74,76	0
3	BCL	I	1705	66/66	0.92	0.17	34,41,73,75	0
3	BCL	O	1708	66/66	0.92	0.16	42,50,79,81	0
3	BCL	A	1501	66/66	0.92	0.17	33,42,51,65	0
3	BCL	E	1703	66/66	0.93	0.17	29,37,69,72	0
3	BCL	R	1509	66/66	0.93	0.17	31,38,49,57	0
3	BCL	I	1505	66/66	0.93	0.15	28,36,42,48	0

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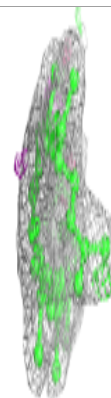
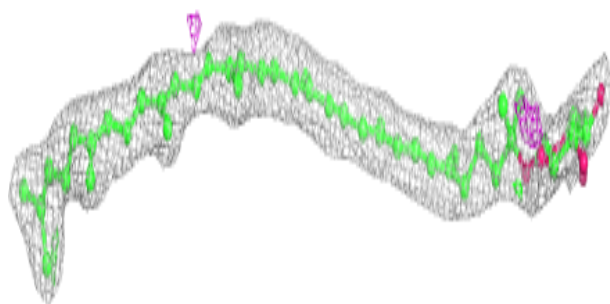
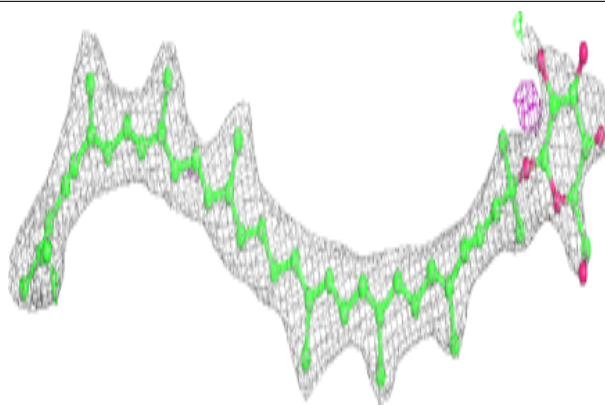
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BCL	S	1609	66/66	0.93	0.15	31,41,69,72	0
3	BCL	O	1508	66/66	0.93	0.14	30,37,46,54	0
3	BCL	K	1506	66/66	0.94	0.18	28,35,47,51	0
3	BCL	K	1706	66/66	0.94	0.15	27,36,78,82	0
3	BCL	P	1608	66/66	0.94	0.16	34,42,66,68	0
3	BCL	L	1606	66/66	0.94	0.16	27,36,66,69	0
3	BCL	H	1604	66/66	0.94	0.15	29,39,63,64	0
3	BCL	F	1603	66/66	0.94	0.17	26,35,62,64	0
3	BCL	D	1602	66/66	0.95	0.13	30,37,64,67	0
3	BCL	G	1504	66/66	0.95	0.15	26,34,44,49	0
3	BCL	B	1601	66/66	0.95	0.15	33,42,67,68	0
3	BCL	C	1502	66/66	0.96	0.12	33,38,50,57	0
3	BCL	M	1507	66/66	0.96	0.12	27,35,41,48	0
3	BCL	E	1503	66/66	0.97	0.11	28,35,46,49	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.

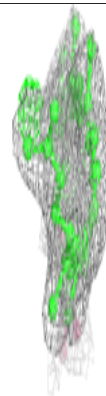
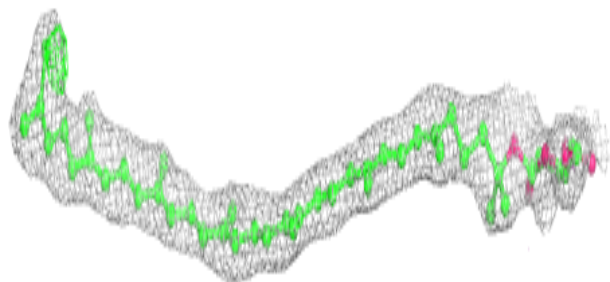
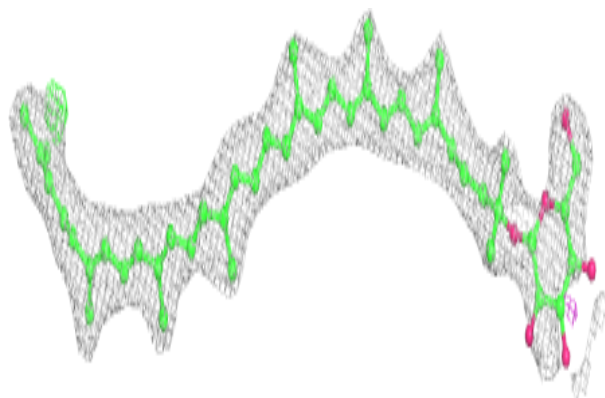


**Electron density around RG1 J 1405:**

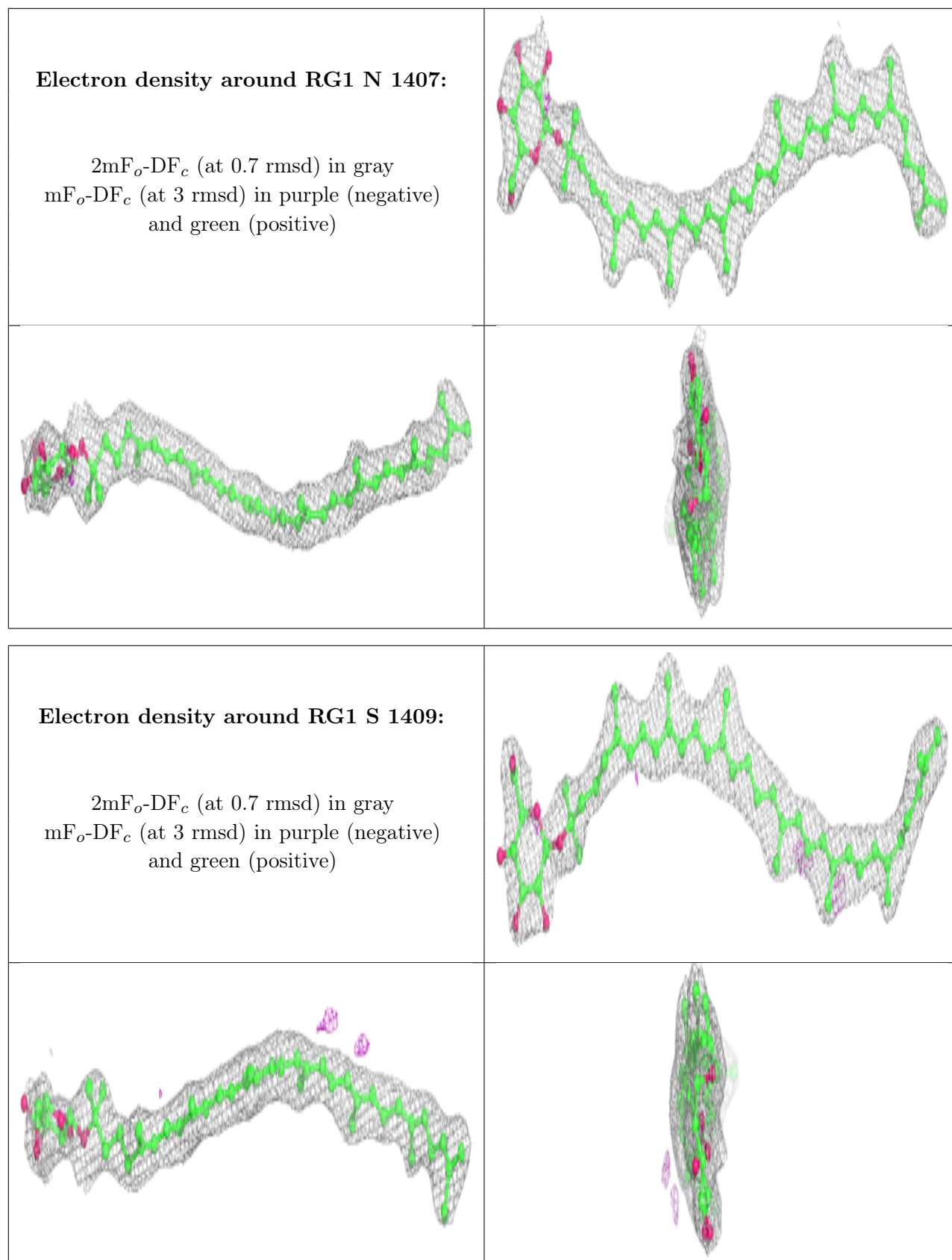
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around RG1 D 1402:**

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

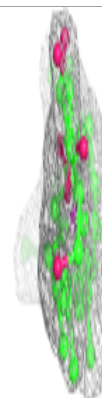
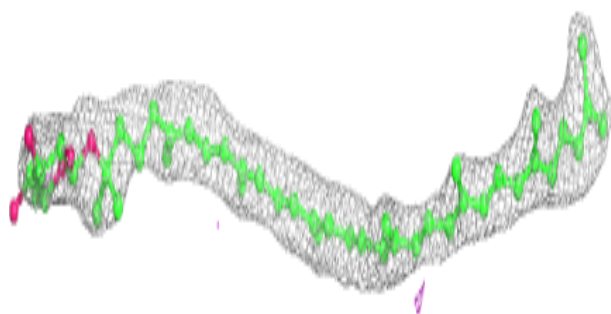
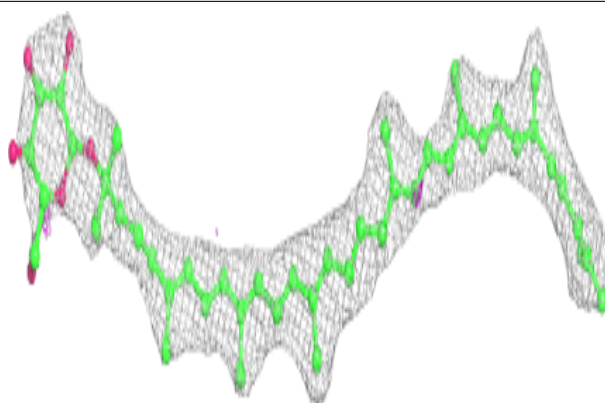




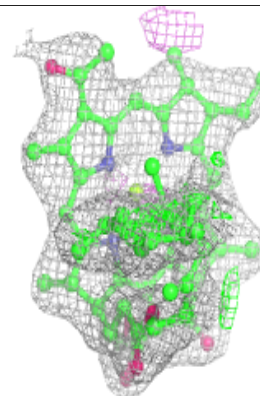
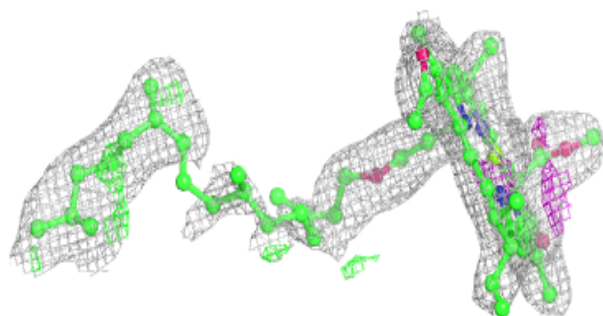
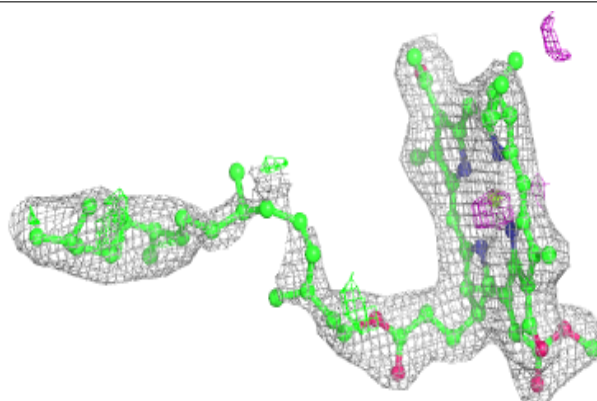


**Electron density around RG1 R 1401:**

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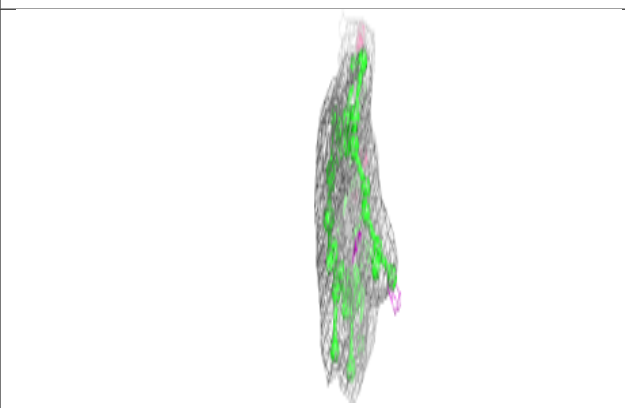
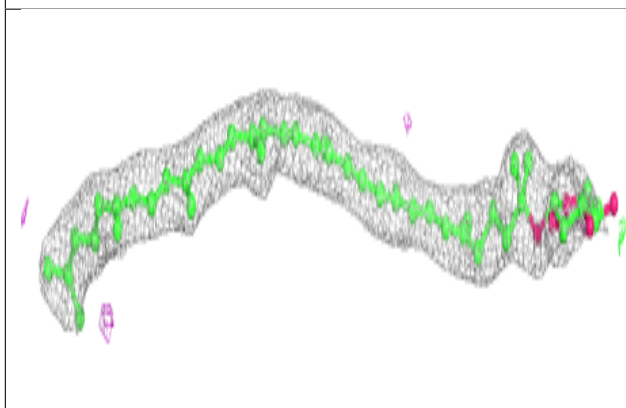
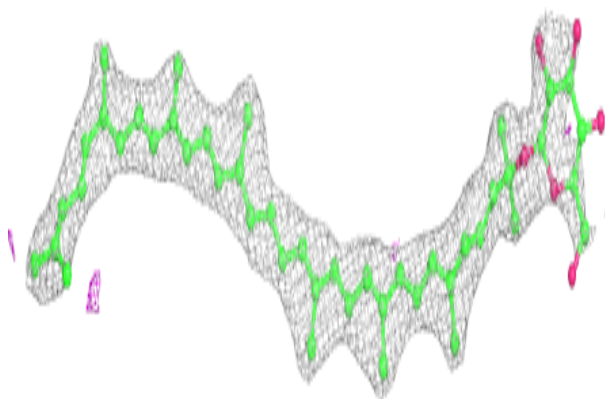
**Electron density around BCL C 1702:**

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and green (positive)

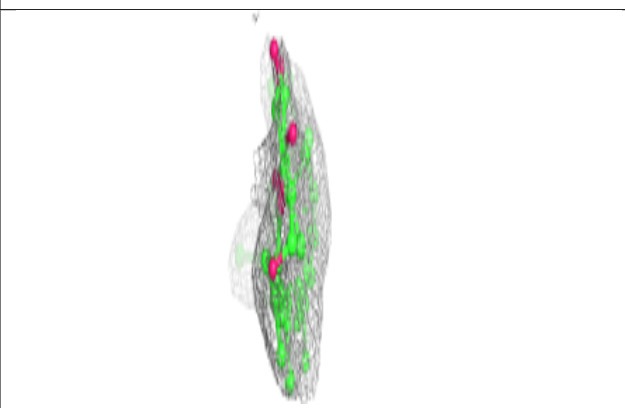
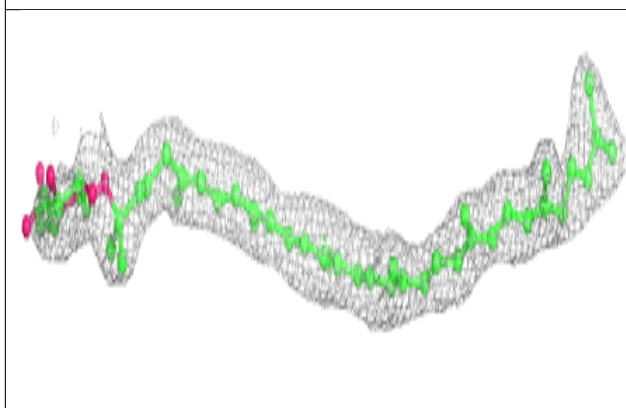
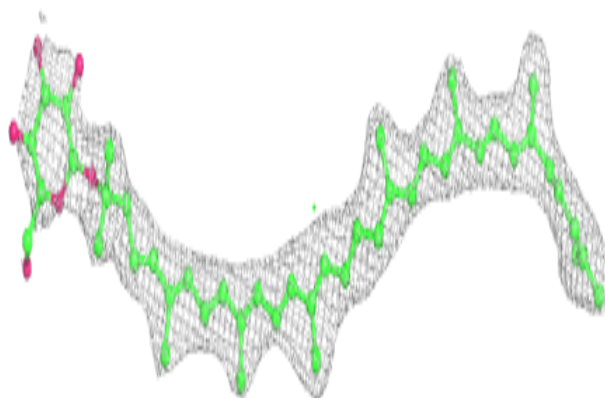


**Electron density around RG1 P 1408:**

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

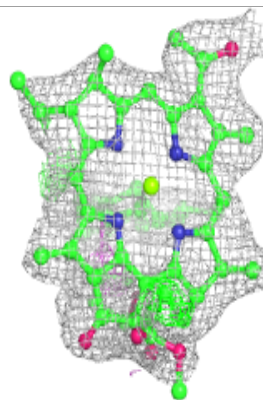
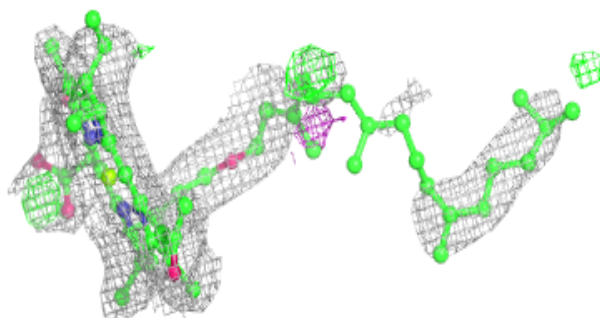
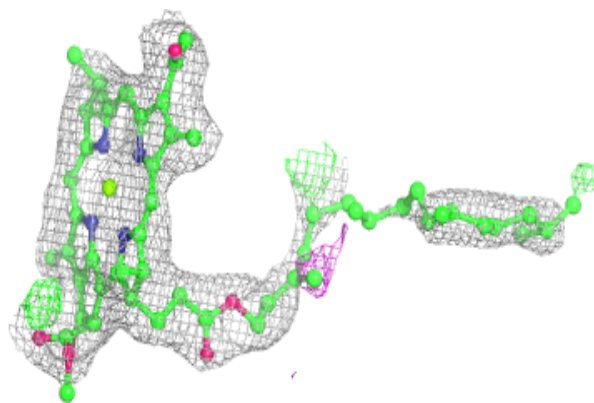
**Electron density around RG1 H 1404:**

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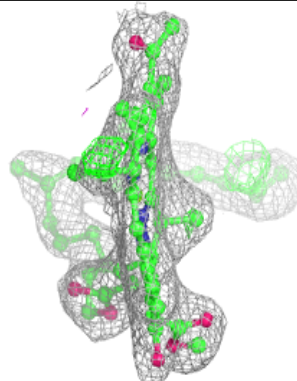
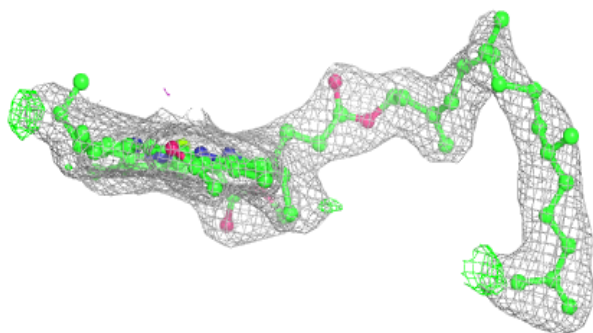
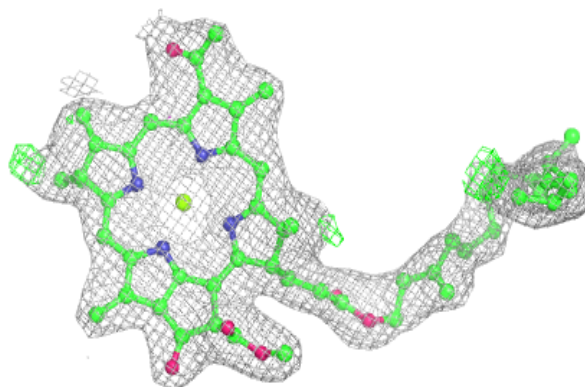


**Electron density around BCL R 1709:**

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

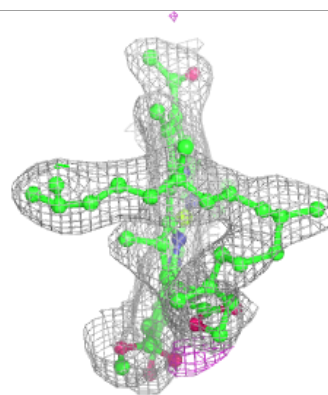
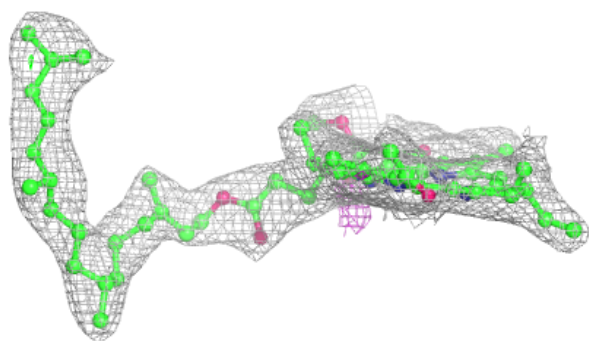
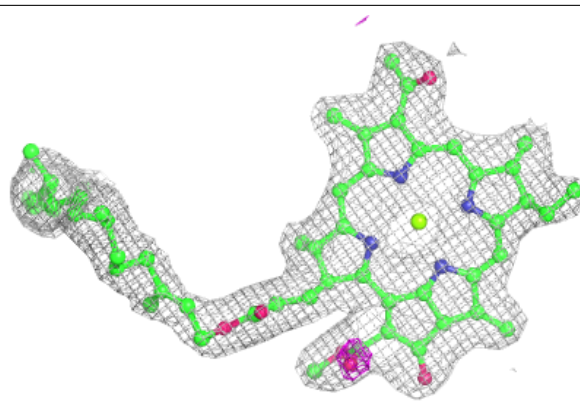
**Electron density around BCL N 1607:**

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and green (positive)

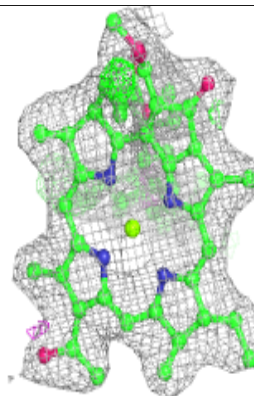
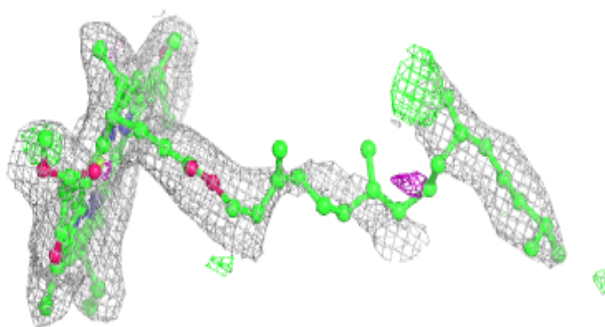
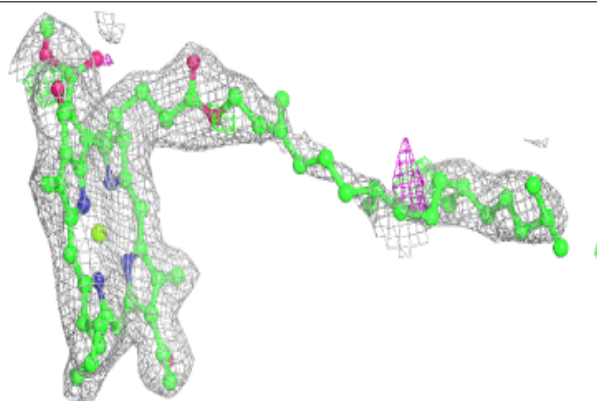


**Electron density around BCL J 1605:**

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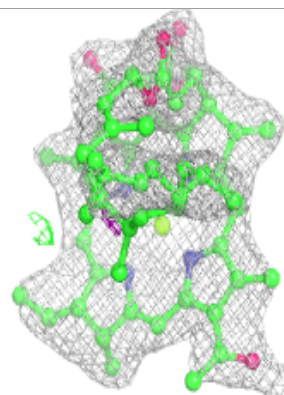
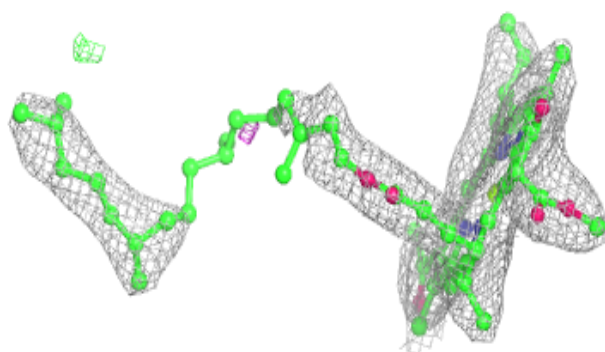
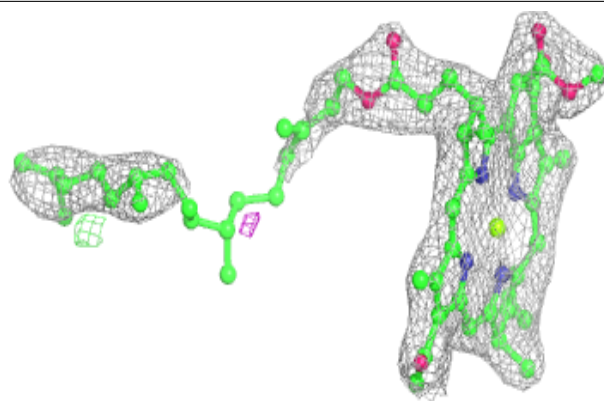
**Electron density around BCL G 1704:**

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and green (positive)

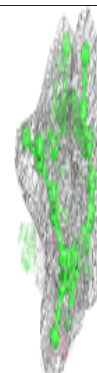
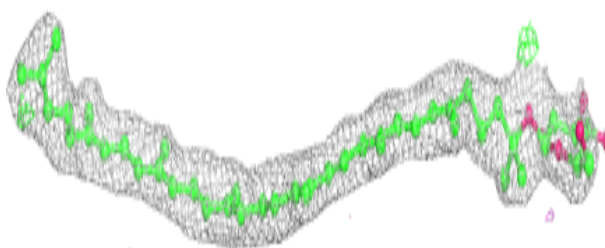
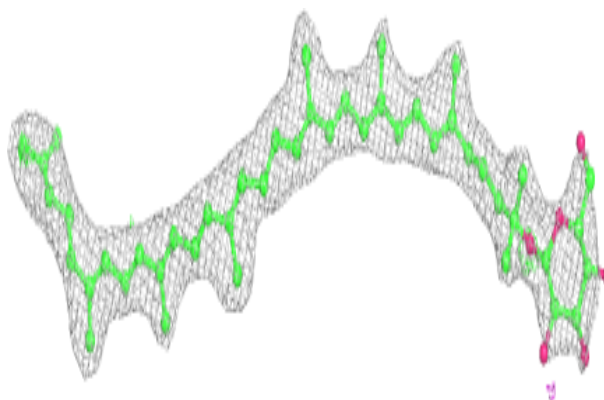


**Electron density around BCL A 1701:**

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and green (positive)

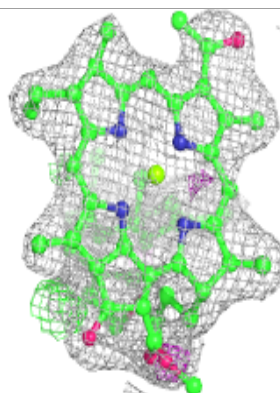
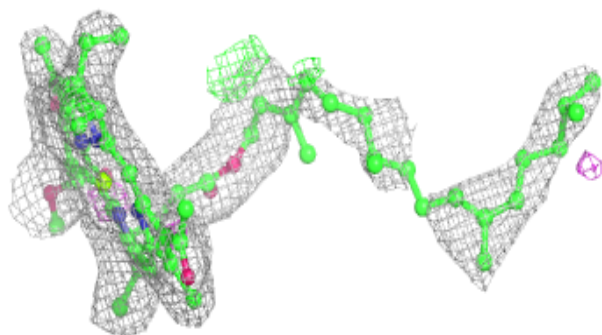
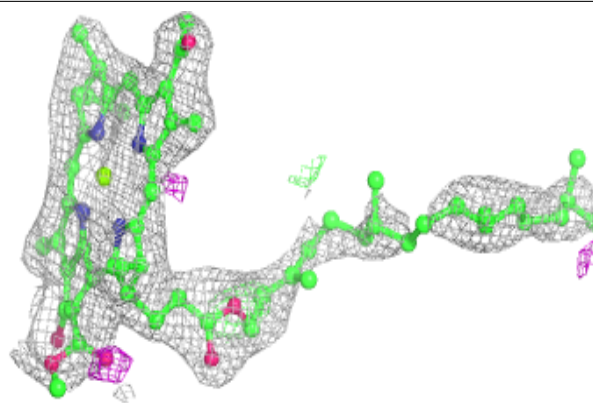
**Electron density around RG1 L 1406:**

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and green (positive)

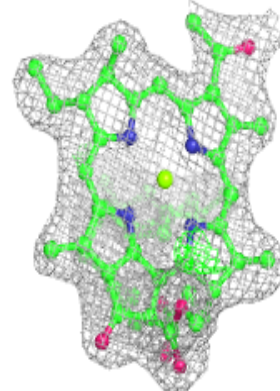
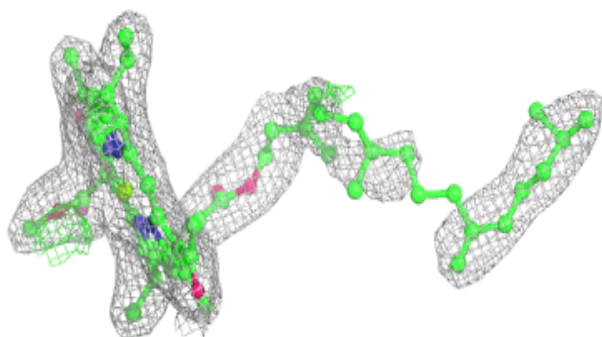
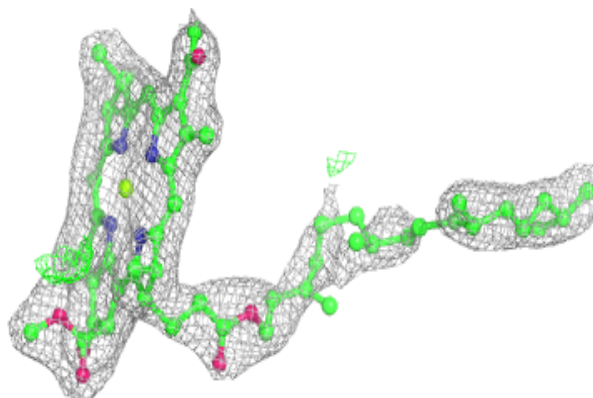


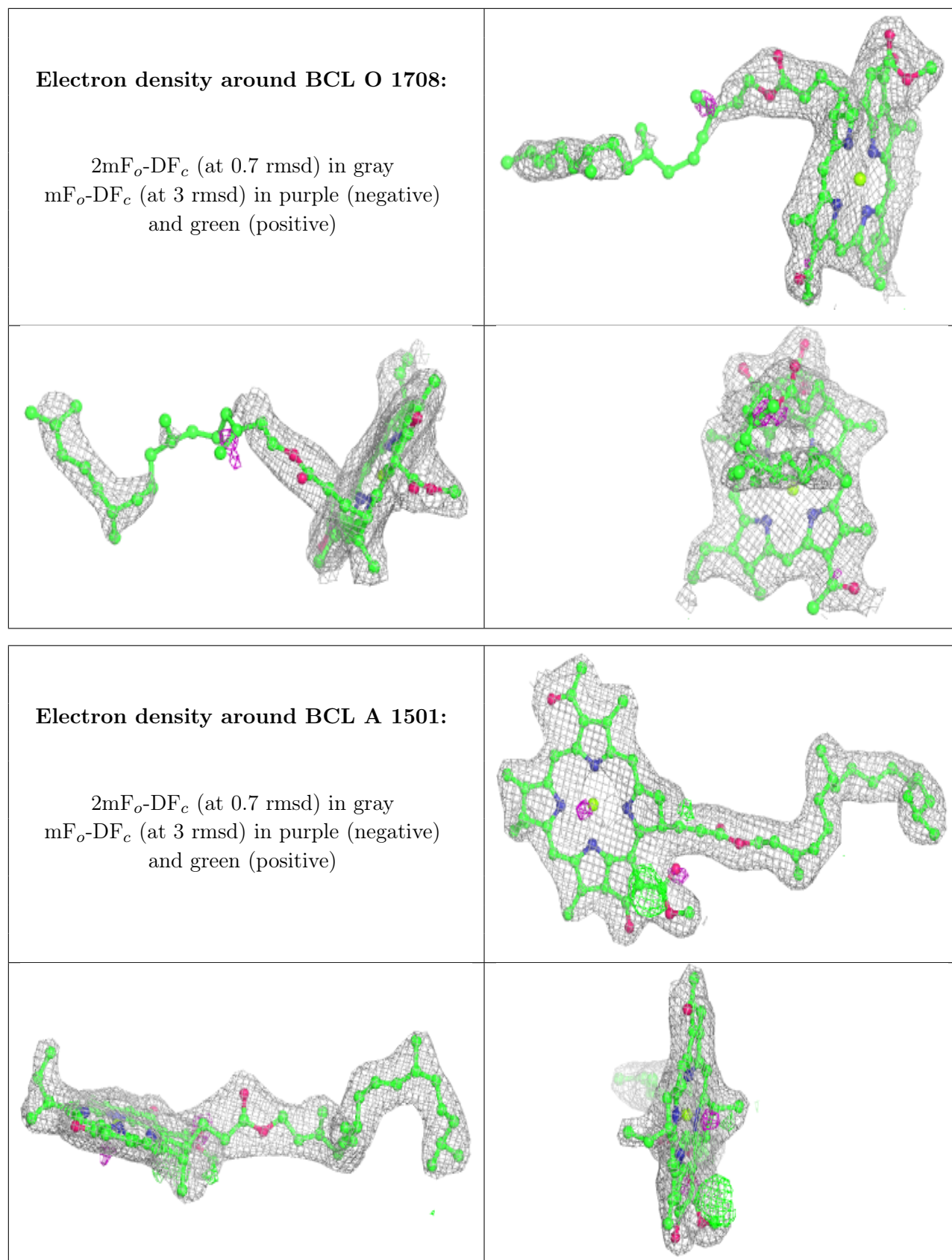
**Electron density around BCL M 1707:**

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

**Electron density around BCL I 1705:**

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

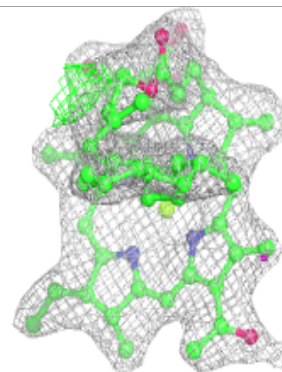
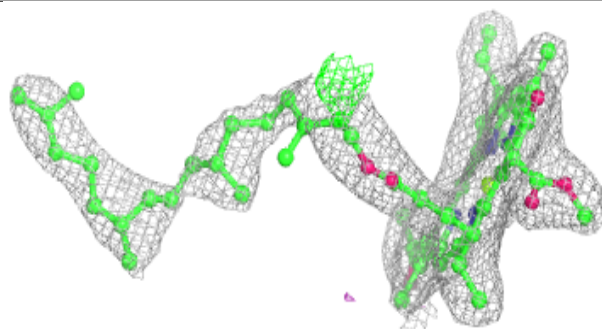
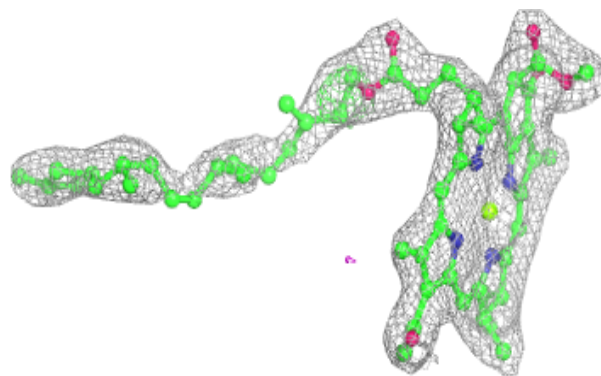




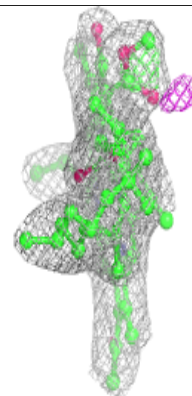
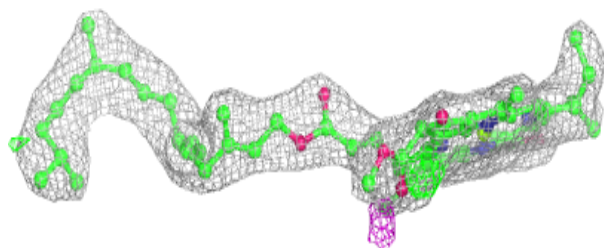
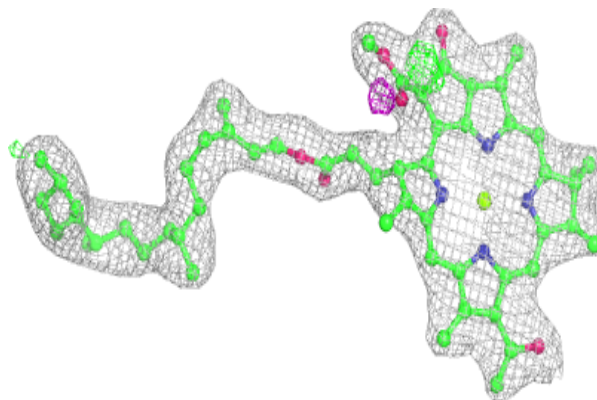


**Electron density around BCL E 1703:**

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

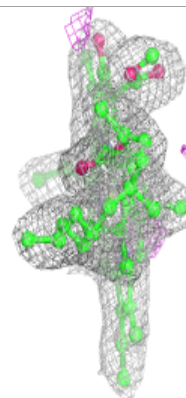
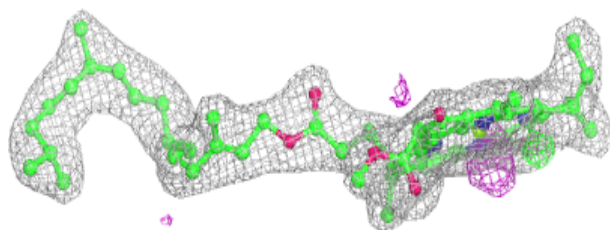
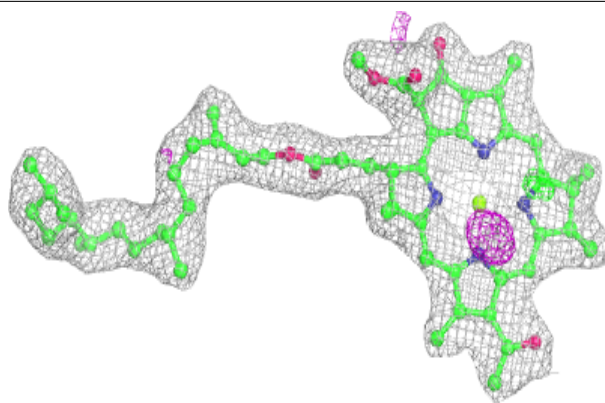
**Electron density around BCL R 1509:**

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

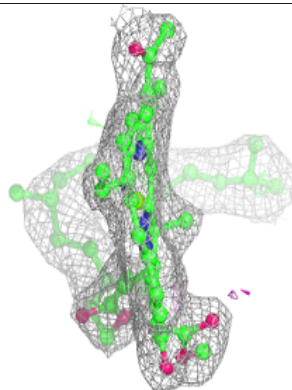
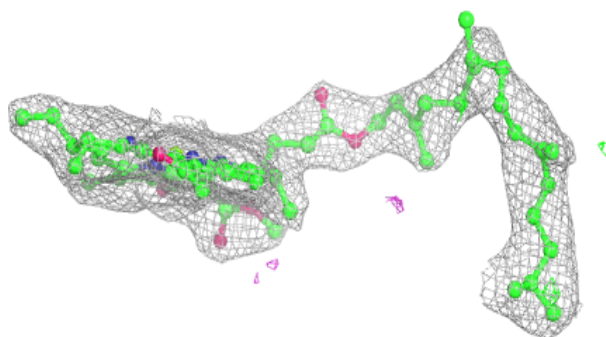
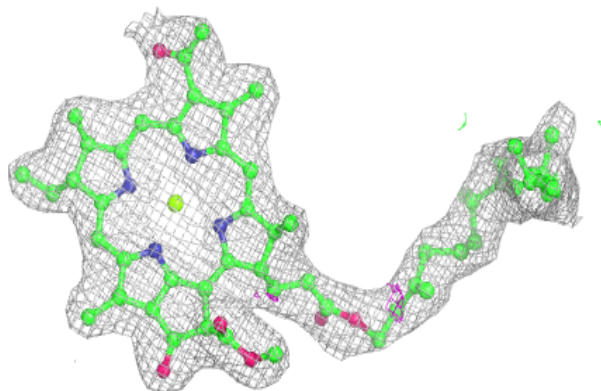


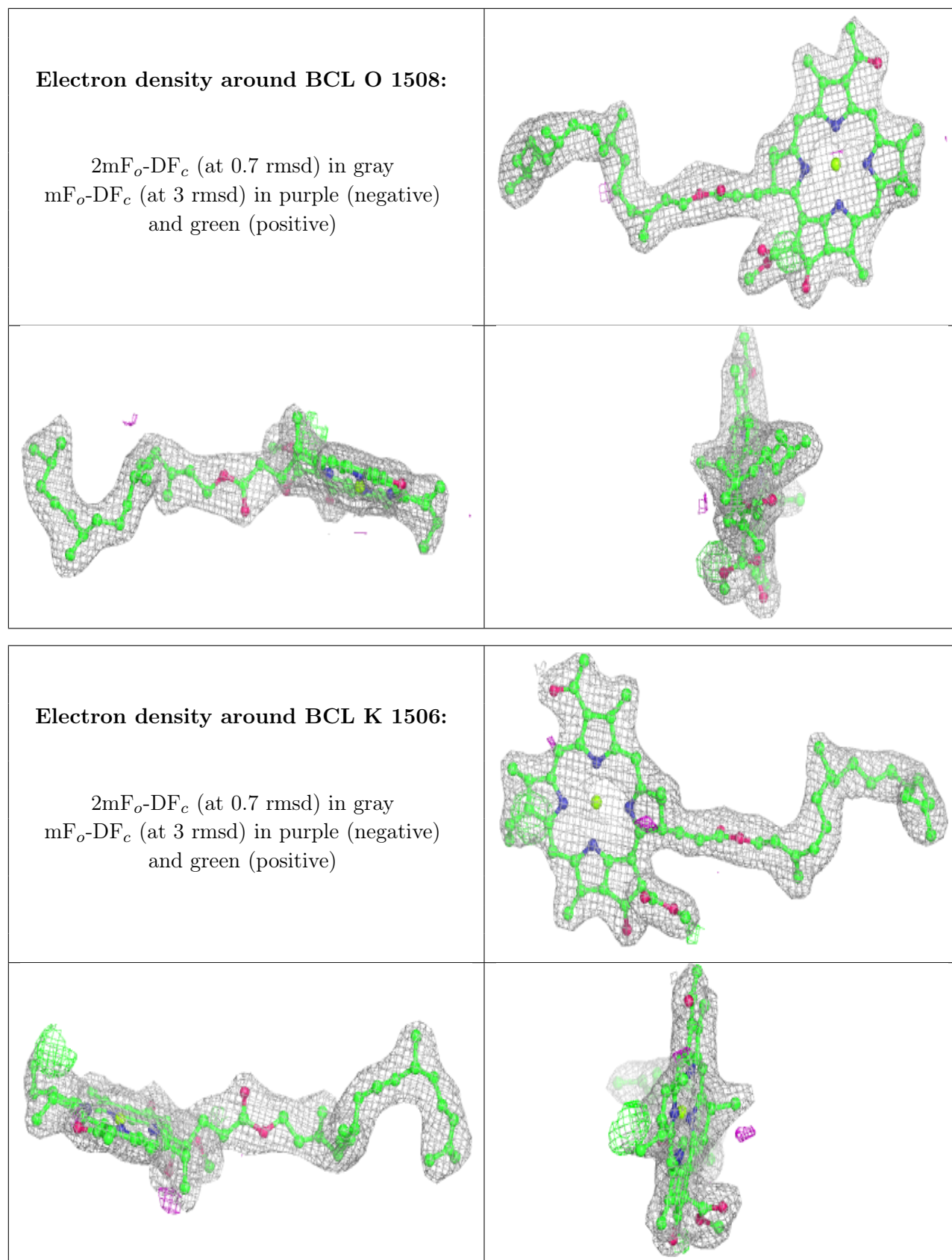
**Electron density around BCL I 1505:**

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

**Electron density around BCL S 1609:**

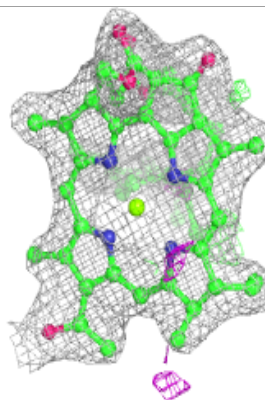
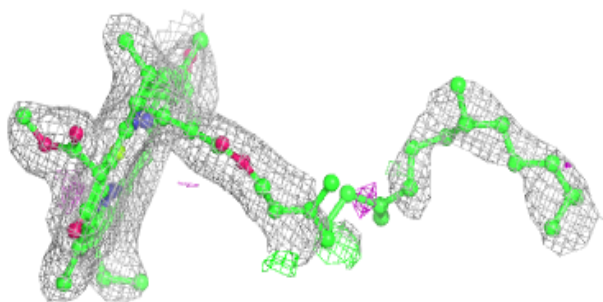
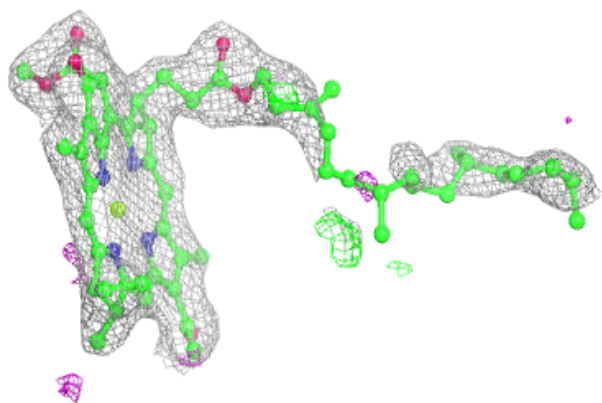
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



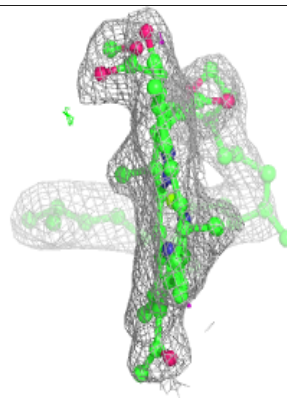
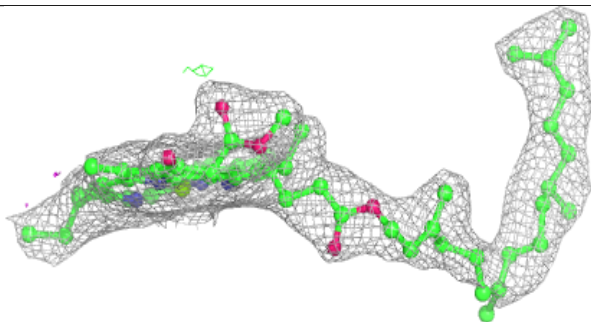
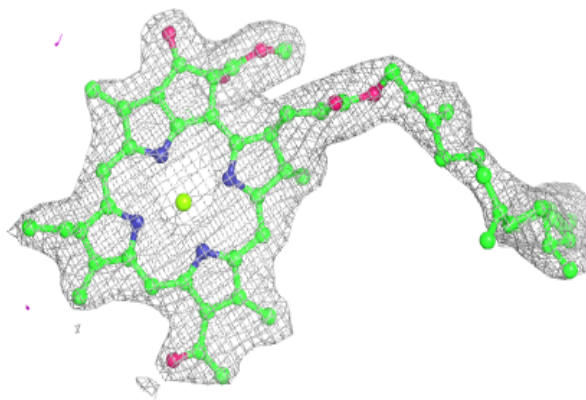


**Electron density around BCL K 1706:**

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

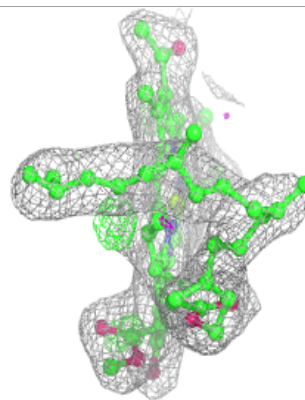
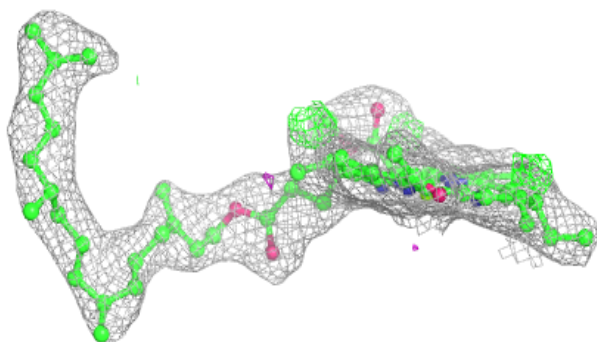
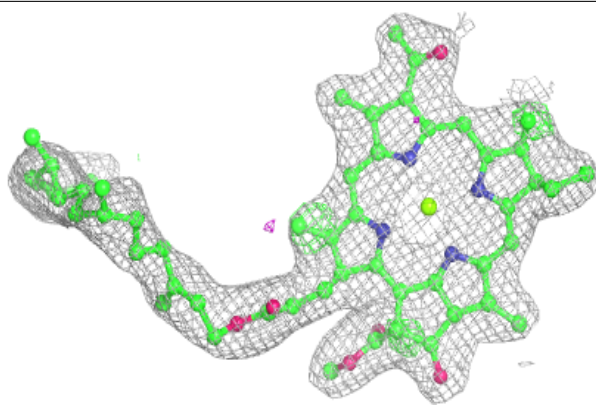
**Electron density around BCL P 1608:**

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

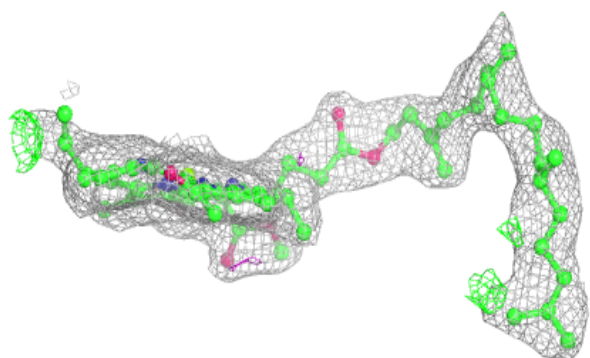
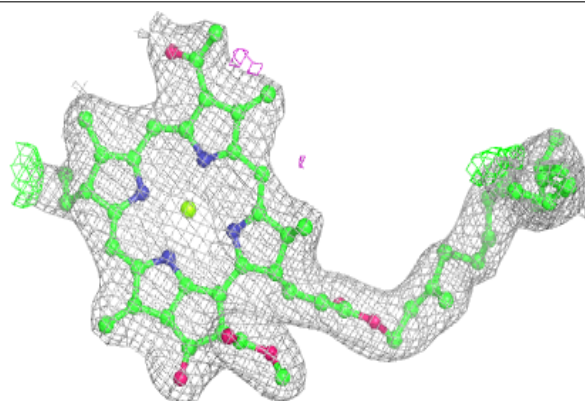


**Electron density around BCL L 1606:**

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

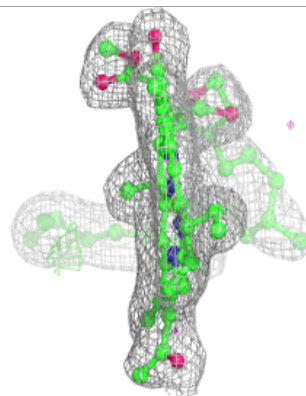
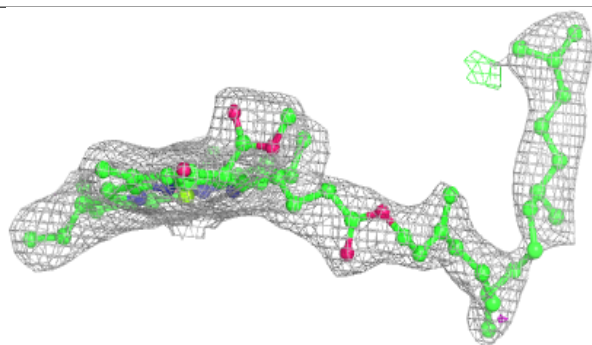
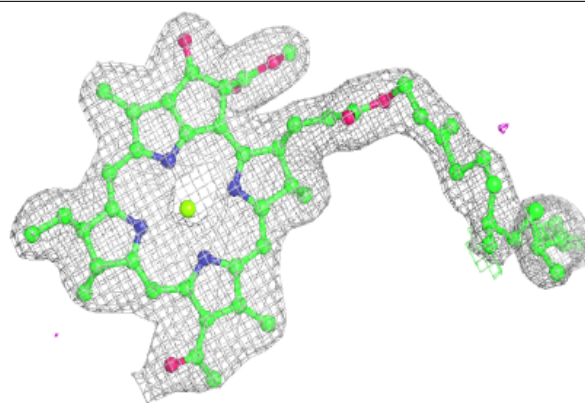
**Electron density around BCL H 1604:**

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

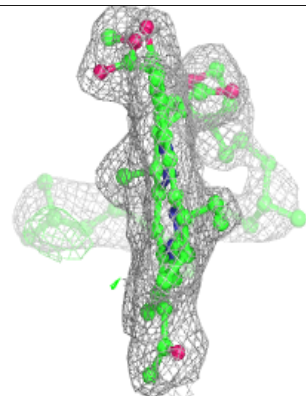
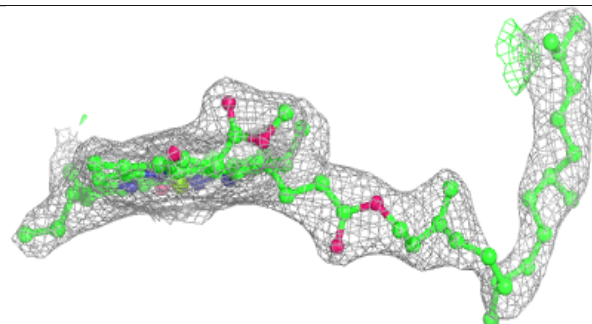
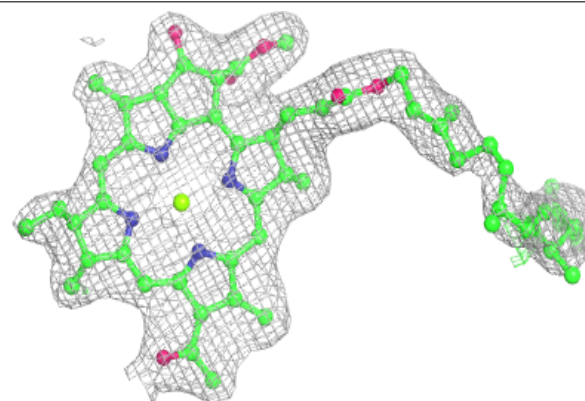


**Electron density around BCL F 1603:**

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

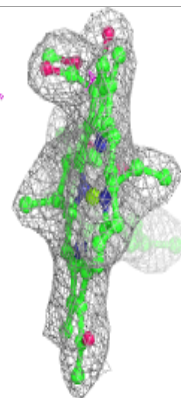
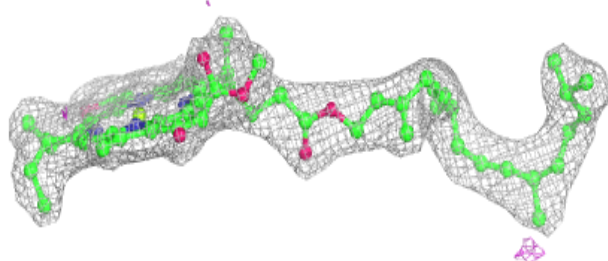
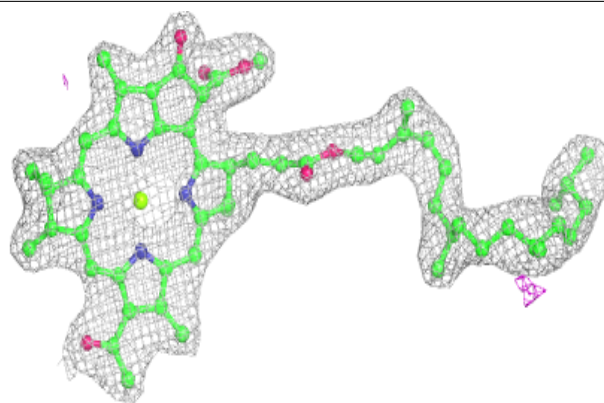
**Electron density around BCL D 1602:**

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

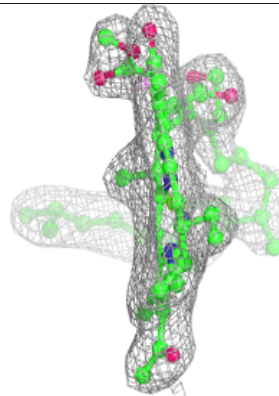
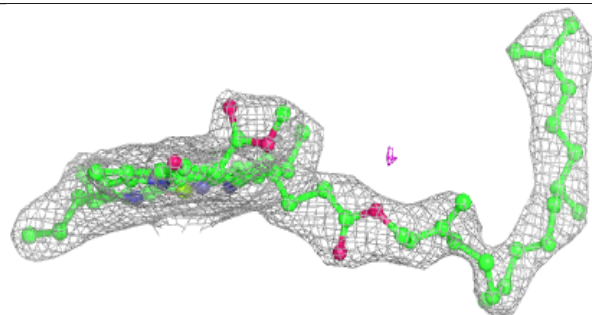
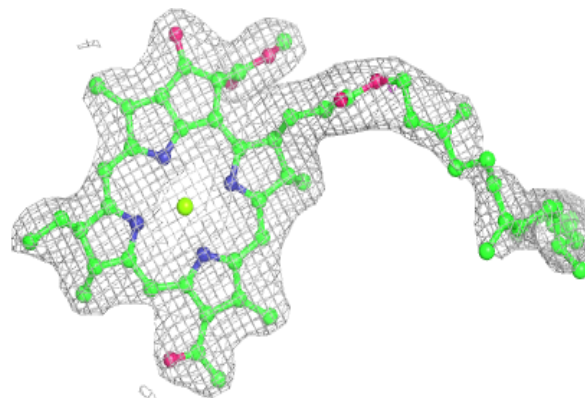


**Electron density around BCL G 1504:**

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

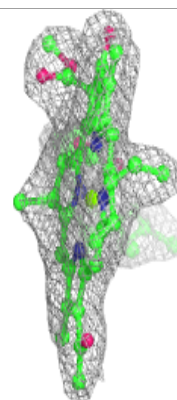
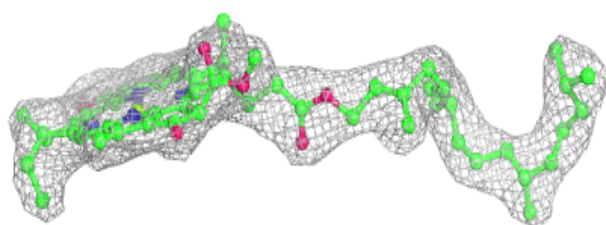
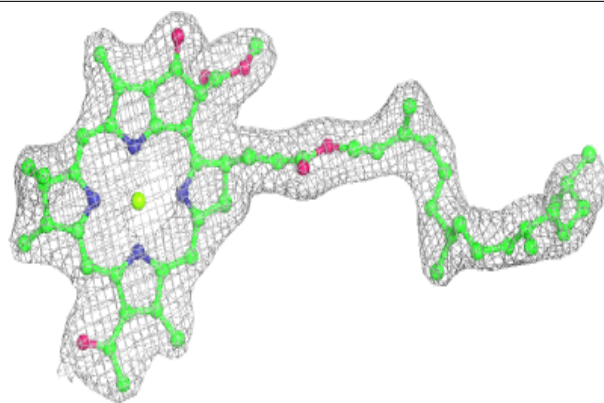
**Electron density around BCL B 1601:**

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

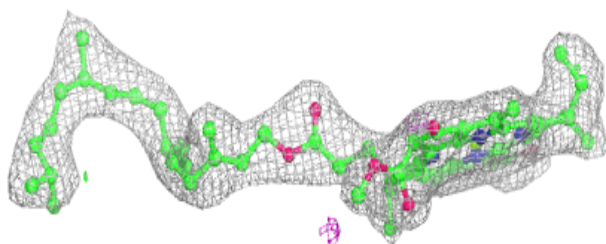
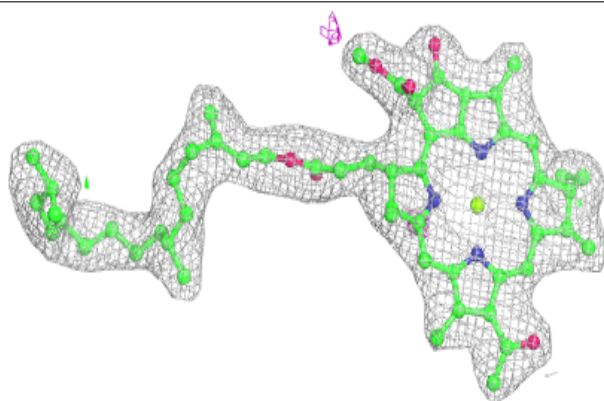


**Electron density around BCL C 1502:**

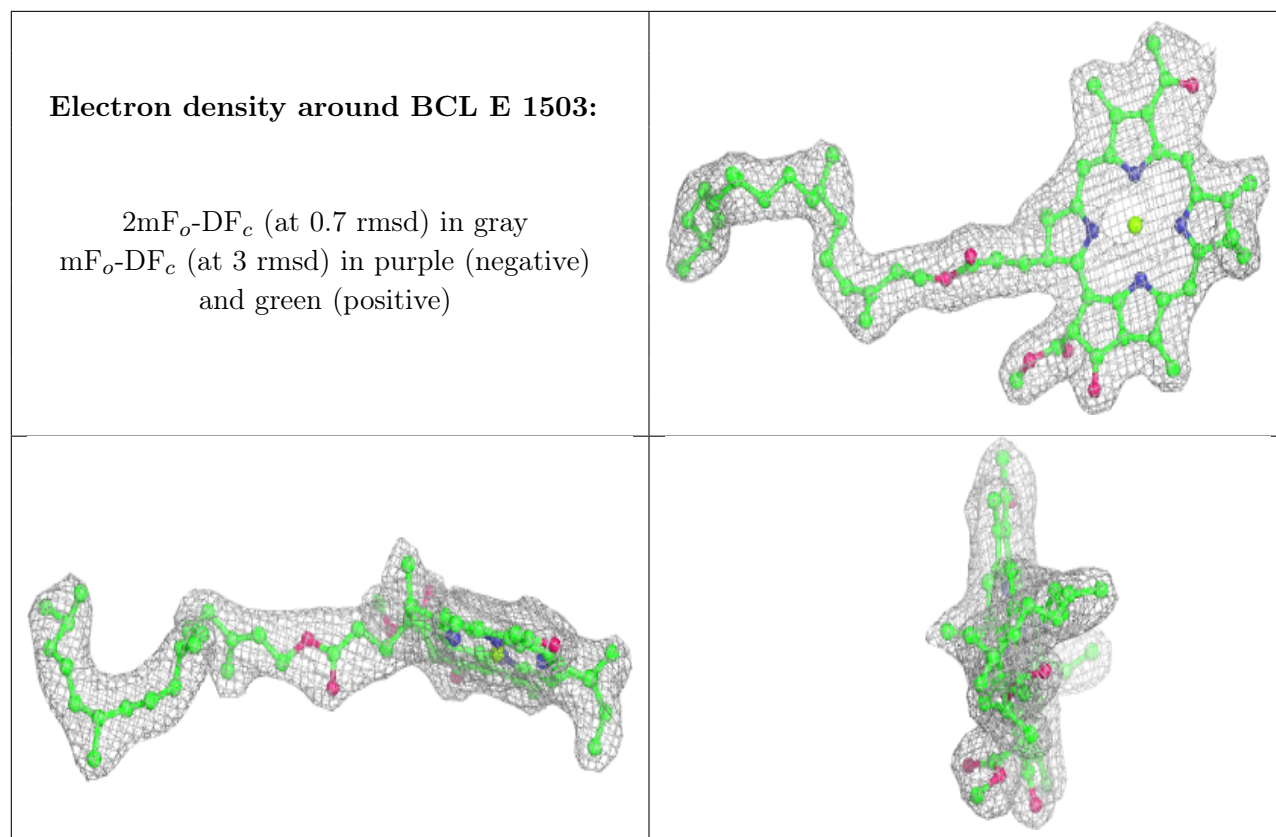
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around BCL M 1507:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.