



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 09:27 am BST

PDB ID : 6R7D  
Title : Crystal structure of LTC4S in complex with AZ13690257  
Authors : Kack, H.; Ek, M.  
Deposited on : 2019-03-28  
Resolution : 2.35 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.

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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 : 2.11  
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) : 2.11

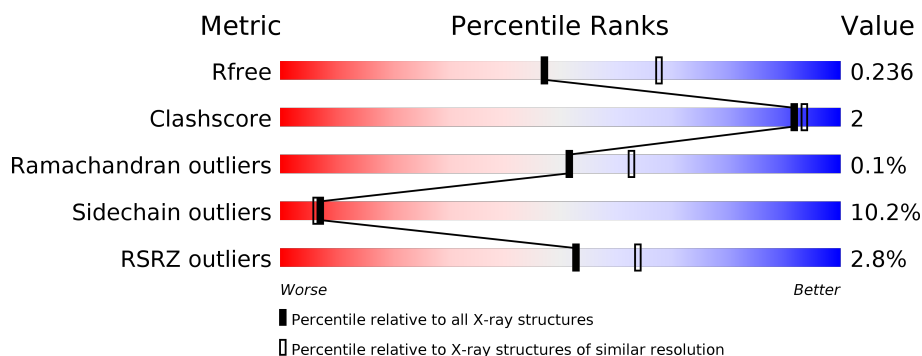
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	157	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>.. 5%</div> </div> </div>
1	B	157	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	C	157	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 6%</div> </div> </div>
1	D	157	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• •</div> </div> </div>
1	E	157	<div> <div></div> <div> <div></div> <div>79%</div> <div>13%</div> <div>.. 5%</div> </div> </div>
1	F	157	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>.. •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	157	
1	H	157	
1	I	157	
1	J	157	
1	K	157	
1	L	157	

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
4	PLM	F	204	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15151 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 Leukotriene C4 synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1178	779	213	184	2			
1	B	149	Total	C	N	O	S	0	0	0
			1178	779	213	184	2			
1	C	148	Total	C	N	O	S	0	0	0
			1167	773	209	183	2			
1	D	150	Total	C	N	O	S	0	0	0
			1177	779	211	185	2			
1	E	149	Total	C	N	O	S	0	0	0
			1178	779	213	184	2			
1	F	150	Total	C	N	O	S	0	0	0
			1185	783	214	186	2			
1	G	149	Total	C	N	O	S	0	0	0
			1178	779	213	184	2			
1	H	151	Total	C	N	O	S	0	0	0
			1188	785	215	186	2			
1	I	148	Total	C	N	O	S	0	0	0
			1167	773	209	183	2			
1	J	149	Total	C	N	O	S	0	0	0
			1178	779	213	184	2			
1	K	150	Total	C	N	O	S	0	0	0
			1185	783	214	186	2			
1	L	148	Total	C	N	O	S	0	0	0
			1167	773	209	183	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q16873
A	-5	ALA	-	expression tag	UNP Q16873
A	-4	HIS	-	expression tag	UNP Q16873
A	-3	HIS	-	expression tag	UNP Q16873
A	-2	HIS	-	expression tag	UNP Q16873

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP Q16873
A	0	HIS	-	expression tag	UNP Q16873
A	1	HIS	-	expression tag	UNP Q16873
B	-6	MET	-	initiating methionine	UNP Q16873
B	-5	ALA	-	expression tag	UNP Q16873
B	-4	HIS	-	expression tag	UNP Q16873
B	-3	HIS	-	expression tag	UNP Q16873
B	-2	HIS	-	expression tag	UNP Q16873
B	-1	HIS	-	expression tag	UNP Q16873
B	0	HIS	-	expression tag	UNP Q16873
B	1	HIS	-	expression tag	UNP Q16873
C	-6	MET	-	initiating methionine	UNP Q16873
C	-5	ALA	-	expression tag	UNP Q16873
C	-4	HIS	-	expression tag	UNP Q16873
C	-3	HIS	-	expression tag	UNP Q16873
C	-2	HIS	-	expression tag	UNP Q16873
C	-1	HIS	-	expression tag	UNP Q16873
C	0	HIS	-	expression tag	UNP Q16873
C	1	HIS	-	expression tag	UNP Q16873
D	-6	MET	-	initiating methionine	UNP Q16873
D	-5	ALA	-	expression tag	UNP Q16873
D	-4	HIS	-	expression tag	UNP Q16873
D	-3	HIS	-	expression tag	UNP Q16873
D	-2	HIS	-	expression tag	UNP Q16873
D	-1	HIS	-	expression tag	UNP Q16873
D	0	HIS	-	expression tag	UNP Q16873
D	1	HIS	-	expression tag	UNP Q16873
E	-6	MET	-	initiating methionine	UNP Q16873
E	-5	ALA	-	expression tag	UNP Q16873
E	-4	HIS	-	expression tag	UNP Q16873
E	-3	HIS	-	expression tag	UNP Q16873
E	-2	HIS	-	expression tag	UNP Q16873
E	-1	HIS	-	expression tag	UNP Q16873
E	0	HIS	-	expression tag	UNP Q16873
E	1	HIS	-	expression tag	UNP Q16873
F	-6	MET	-	initiating methionine	UNP Q16873
F	-5	ALA	-	expression tag	UNP Q16873
F	-4	HIS	-	expression tag	UNP Q16873
F	-3	HIS	-	expression tag	UNP Q16873
F	-2	HIS	-	expression tag	UNP Q16873
F	-1	HIS	-	expression tag	UNP Q16873
F	0	HIS	-	expression tag	UNP Q16873

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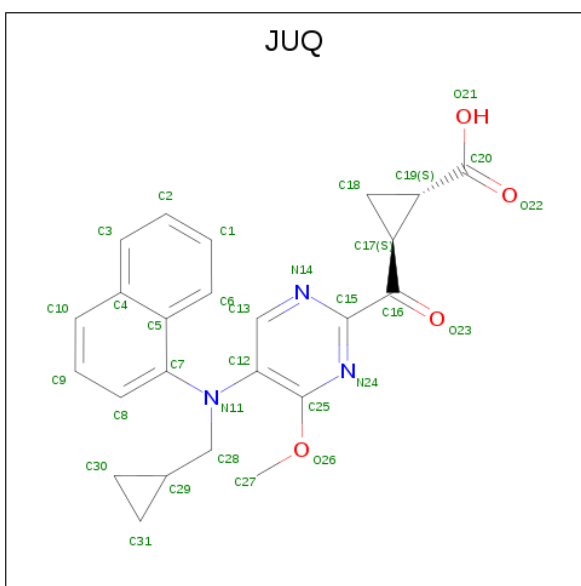
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	expression tag	UNP Q16873
G	-6	MET	-	initiating methionine	UNP Q16873
G	-5	ALA	-	expression tag	UNP Q16873
G	-4	HIS	-	expression tag	UNP Q16873
G	-3	HIS	-	expression tag	UNP Q16873
G	-2	HIS	-	expression tag	UNP Q16873
G	-1	HIS	-	expression tag	UNP Q16873
G	0	HIS	-	expression tag	UNP Q16873
G	1	HIS	-	expression tag	UNP Q16873
H	-6	MET	-	initiating methionine	UNP Q16873
H	-5	ALA	-	expression tag	UNP Q16873
H	-4	HIS	-	expression tag	UNP Q16873
H	-3	HIS	-	expression tag	UNP Q16873
H	-2	HIS	-	expression tag	UNP Q16873
H	-1	HIS	-	expression tag	UNP Q16873
H	0	HIS	-	expression tag	UNP Q16873
H	1	HIS	-	expression tag	UNP Q16873
I	-6	MET	-	initiating methionine	UNP Q16873
I	-5	ALA	-	expression tag	UNP Q16873
I	-4	HIS	-	expression tag	UNP Q16873
I	-3	HIS	-	expression tag	UNP Q16873
I	-2	HIS	-	expression tag	UNP Q16873
I	-1	HIS	-	expression tag	UNP Q16873
I	0	HIS	-	expression tag	UNP Q16873
I	1	HIS	-	expression tag	UNP Q16873
J	-6	MET	-	initiating methionine	UNP Q16873
J	-5	ALA	-	expression tag	UNP Q16873
J	-4	HIS	-	expression tag	UNP Q16873
J	-3	HIS	-	expression tag	UNP Q16873
J	-2	HIS	-	expression tag	UNP Q16873
J	-1	HIS	-	expression tag	UNP Q16873
J	0	HIS	-	expression tag	UNP Q16873
J	1	HIS	-	expression tag	UNP Q16873
K	-6	MET	-	initiating methionine	UNP Q16873
K	-5	ALA	-	expression tag	UNP Q16873
K	-4	HIS	-	expression tag	UNP Q16873
K	-3	HIS	-	expression tag	UNP Q16873
K	-2	HIS	-	expression tag	UNP Q16873
K	-1	HIS	-	expression tag	UNP Q16873
K	0	HIS	-	expression tag	UNP Q16873
K	1	HIS	-	expression tag	UNP Q16873
L	-6	MET	-	initiating methionine	UNP Q16873

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	ALA	-	expression tag	UNP Q16873
L	-4	HIS	-	expression tag	UNP Q16873
L	-3	HIS	-	expression tag	UNP Q16873
L	-2	HIS	-	expression tag	UNP Q16873
L	-1	HIS	-	expression tag	UNP Q16873
L	0	HIS	-	expression tag	UNP Q16873
L	1	HIS	-	expression tag	UNP Q16873

- Molecule 2 is (1 {S},2 {S})-2-[5-[cyclopropylmethyl(naphthalen-1-yl)amino]-4-methoxypyrimidin-2-yl]carbonylcyclopropane-1-carboxylic acid (three-letter code: JUQ) (formula: C<sub>24</sub>H<sub>23</sub>N<sub>3</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	24	3	4		
2	B	1	Total	C	N	O	0	0
			31	24	3	4		
2	C	1	Total	C	N	O	0	0
			31	24	3	4		
2	D	1	Total	C	N	O	0	0
			31	24	3	4		
2	E	1	Total	C	N	O	0	0
			31	24	3	4		
2	F	1	Total	C	N	O	0	0
			31	24	3	4		
2	G	1	Total	C	N	O	0	0
			31	24	3	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			31	24	3	4		
2	I	1	Total	C	N	O	0	0
			31	24	3	4		
2	J	1	Total	C	N	O	0	0
			31	24	3	4		
2	K	1	Total	C	N	O	0	0
			31	24	3	4		
2	L	1	Total	C	N	O	0	0
			31	24	3	4		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Ni	0	0
			1	1		
3	J	1	Total	Ni	0	0
			1	1		
3	D	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		
3	I	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		
3	L	1	Total	Ni	0	0
			1	1		

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 10 10	0	0
4	A	1	Total C O 18 16 2	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C O 18 16 2	0	0
4	A	1	Total C O 15 13 2	0	0
4	B	1	Total C 12 12	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C O 18 16 2	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	C	1	Total C O 10 8 2	0	0
4	C	1	Total C O 18 16 2	0	0
4	C	1	Total C 10 10	0	0

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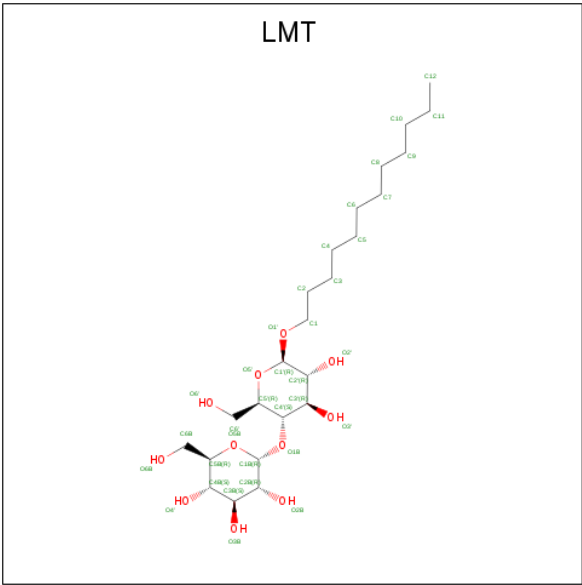
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0
4	D	1	Total C 10 10	0	0
4	D	1	Total C 10 10	0	0
4	D	1	Total C O 18 16 2	0	0
4	D	1	Total C O 15 13 2	0	0
4	E	1	Total C 10 10	0	0
4	E	1	Total C 7 7	0	0
4	E	1	Total C 10 10	0	0
4	F	1	Total C 8 8	0	0
4	F	1	Total C 10 10	0	0
4	F	1	Total C 10 10	0	0
4	F	1	Total C 10 10	0	0
4	G	1	Total C 10 10	0	0
4	G	1	Total C 10 10	0	0
4	G	1	Total C O 15 13 2	0	0
4	H	1	Total C 12 12	0	0
4	H	1	Total C 10 10	0	0
4	I	1	Total C 10 10	0	0
4	I	1	Total C O 18 16 2	0	0
4	J	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total C 8 8	0	0
4	J	1	Total C 10 10	0	0
4	J	1	Total C O 18 16 2	0	0
4	J	1	Total C O 15 13 2	0	0
4	L	1	Total C O 18 16 2	0	0
4	L	1	Total C 8 8	0	0
4	L	1	Total C O 14 12 2	0	0
4	L	1	Total C 10 10	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 35 24 11	0	0

- Molecule 6 is water.

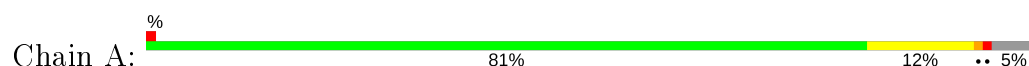
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	11	Total O 11 11	0	0
6	C	6	Total O 6 6	0	0
6	D	8	Total O 8 8	0	0
6	E	10	Total O 10 10	0	0
6	F	11	Total O 11 11	0	0
6	G	8	Total O 8 8	0	0
6	H	5	Total O 5 5	0	0
6	I	11	Total O 11 11	0	0
6	J	6	Total O 6 6	0	0
6	K	11	Total O 11 11	0	0
6	L	3	Total O 3 3	0	0



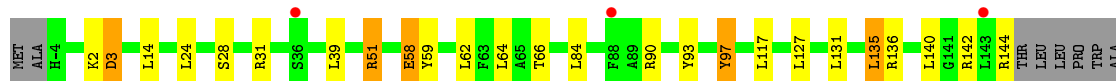
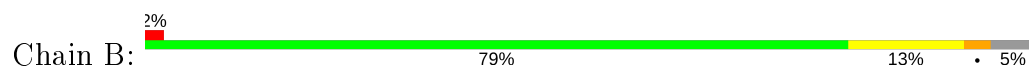
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

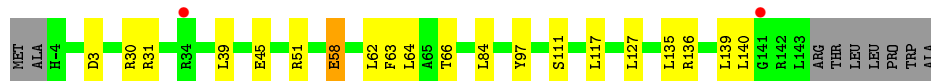
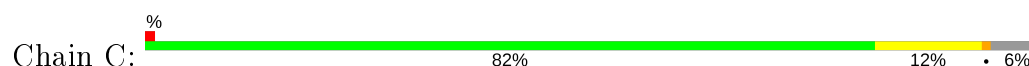
- Molecule 1: Leukotriene C4 synthase



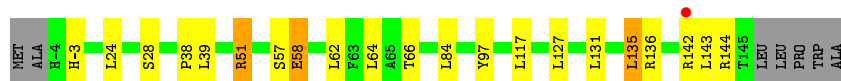
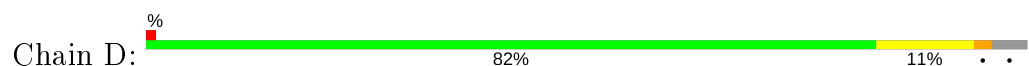
- Molecule 1: Leukotriene C4 synthase



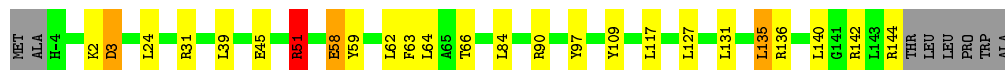
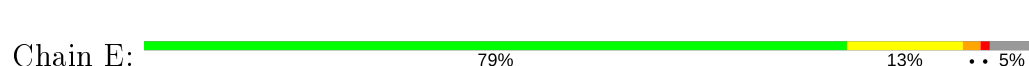
- Molecule 1: Leukotriene C4 synthase



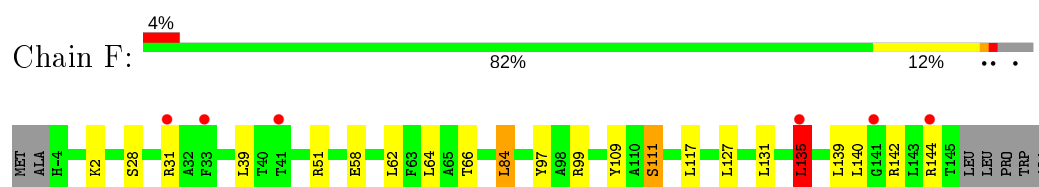
- Molecule 1: Leukotriene C4 synthase



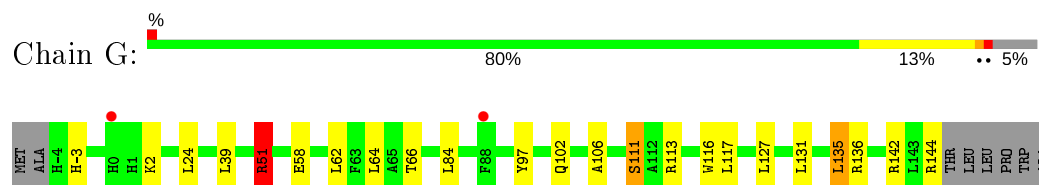
- Molecule 1: Leukotriene C4 synthase



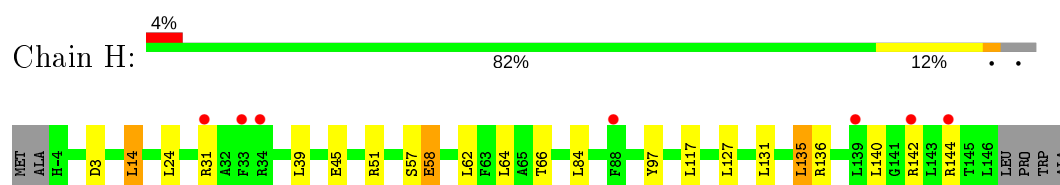
- Molecule 1: Leukotriene C4 synthase



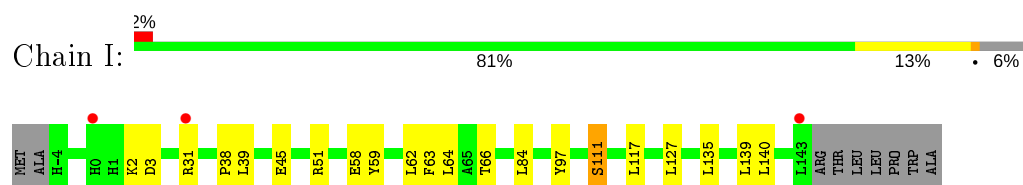
- Molecule 1: Leukotriene C4 synthase



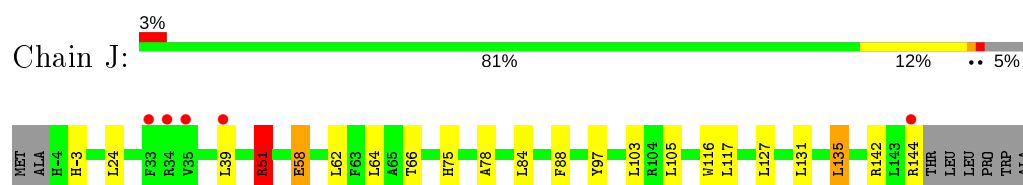
- Molecule 1: Leukotriene C4 synthase



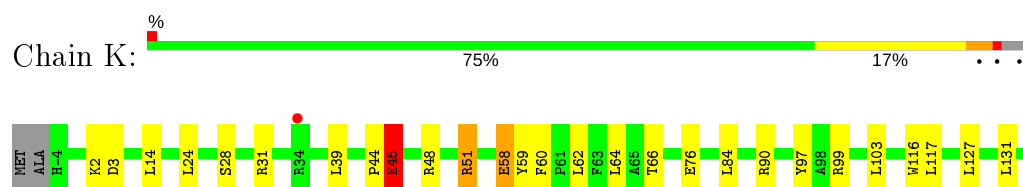
- Molecule 1: Leukotriene C4 synthase



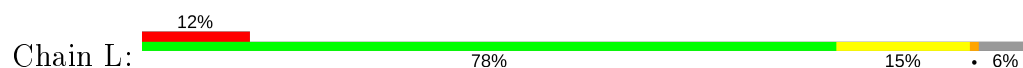
- Molecule 1: Leukotriene C4 synthase

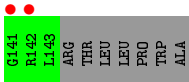
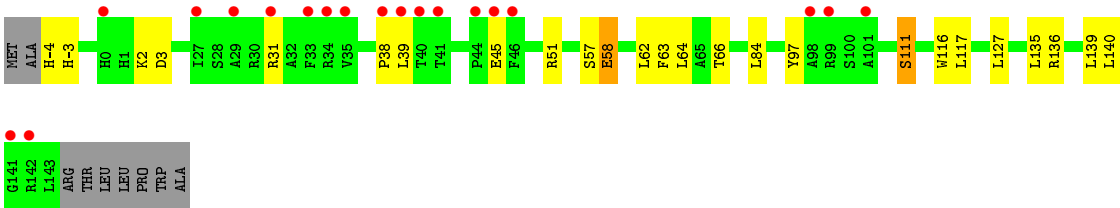


- Molecule 1: Leukotriene C4 synthase



- Molecule 1: Leukotriene C4 synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.59Å 169.38Å 174.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.53 – 2.35 85.96 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (121.53-2.35) 100.0 (85.96-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0135 2015/10/01	Depositor
R, $R_{free}$	0.208 , 0.230 0.214 , 0.236	Depositor DCC
$R_{free}$ test set	7340 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15151	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI, PLM, JUQ, LMT

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	1.34	1/1213 (0.1%)	1.29	5/1653 (0.3%)
1	B	1.41	8/1213 (0.7%)	1.33	12/1653 (0.7%)
1	C	1.26	3/1202 (0.2%)	1.25	10/1639 (0.6%)
1	D	1.19	3/1212 (0.2%)	1.23	7/1653 (0.4%)
1	E	1.28	5/1213 (0.4%)	1.28	12/1653 (0.7%)
1	F	1.27	4/1220 (0.3%)	1.26	13/1663 (0.8%)
1	G	1.22	3/1213 (0.2%)	1.21	6/1653 (0.4%)
1	H	1.09	2/1223 (0.2%)	1.20	8/1667 (0.5%)
1	I	1.26	3/1202 (0.2%)	1.22	11/1639 (0.7%)
1	J	1.25	3/1213 (0.2%)	1.21	4/1653 (0.2%)
1	K	1.33	8/1220 (0.7%)	1.28	12/1663 (0.7%)
1	L	1.26	8/1202 (0.7%)	1.26	11/1639 (0.7%)
All	All	1.27	51/14546 (0.4%)	1.25	111/19828 (0.6%)

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	111	SER	CB-OG	-10.23	1.28	1.42
1	I	111	SER	CB-OG	-9.70	1.29	1.42
1	B	58	GLU	CD-OE1	8.83	1.35	1.25
1	D	144	ARG	N-CA	8.27	1.62	1.46
1	L	-3	HIS	C-O	8.26	1.39	1.23

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ARG	NE-CZ-NH1	19.16	129.88	120.30
1	A	51	ARG	NE-CZ-NH1	18.37	129.48	120.30
1	D	51	ARG	NE-CZ-NH1	17.92	129.26	120.30
1	I	51	ARG	NE-CZ-NH1	-17.05	111.78	120.30
1	C	51	ARG	NE-CZ-NH1	-16.87	111.86	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1178	0	1211	6	0
1	B	1178	0	1211	3	0
1	C	1167	0	1198	1	0
1	D	1177	0	1202	4	0
1	E	1178	0	1211	4	0
1	F	1185	0	1218	3	0
1	G	1178	0	1211	13	0
1	H	1188	0	1215	3	0
1	I	1167	0	1198	3	0
1	J	1178	0	1211	14	0
1	K	1185	0	1218	7	0
1	L	1167	0	1198	2	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	0	0
2	D	31	0	0	0	0
2	E	31	0	0	0	0
2	F	31	0	0	0	0
2	G	31	0	0	0	0
2	H	31	0	0	0	0
2	I	31	0	0	0	0
2	J	31	0	0	1	0
2	K	31	0	0	0	0
2	L	31	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	A	71	0	122	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	70	0	130	0	0
4	C	58	0	100	0	0
4	D	53	0	91	0	0
4	E	27	0	48	0	0
4	F	38	0	69	1	0
4	G	35	0	60	1	0
4	H	22	0	42	0	0
4	I	28	0	50	0	0
4	J	61	0	103	0	0
4	L	50	0	82	0	0
5	B	35	0	46	0	0
6	A	7	0	0	0	0
6	B	11	0	0	0	0
6	C	6	0	0	0	0
6	D	8	0	0	0	0
6	E	10	0	0	0	0
6	F	11	0	0	0	0
6	G	8	0	0	1	0
6	H	5	0	0	0	0
6	I	11	0	0	1	0
6	J	6	0	0	0	0
6	K	11	0	0	2	0
6	L	3	0	0	0	0
All	All	15151	0	15445	48	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 2.

The worst 5 of 48 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:G:102:GLN:OE1	1:J:105:LEU:CD1	1.72	1.36
1:G:102:GLN:OE1	1:J:105:LEU:HD13	1.41	1.18
1:K:45:GLU:OE1	6:K:301:HOH:O	1.82	0.97
1:G:102:GLN:OE1	1:J:105:LEU:HD11	1.80	0.80
1:G:106:ALA:HB1	1:J:103:LEU:HD23	1.62	0.79

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	147/157 (94%)	143 (97%)	3 (2%)	1 (1%)	22	23
1	B	147/157 (94%)	144 (98%)	3 (2%)	0	100	100
1	C	146/157 (93%)	144 (99%)	2 (1%)	0	100	100
1	D	148/157 (94%)	145 (98%)	3 (2%)	0	100	100
1	E	147/157 (94%)	145 (99%)	2 (1%)	0	100	100
1	F	148/157 (94%)	144 (97%)	4 (3%)	0	100	100
1	G	147/157 (94%)	144 (98%)	3 (2%)	0	100	100
1	H	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
1	I	146/157 (93%)	143 (98%)	3 (2%)	0	100	100
1	J	147/157 (94%)	146 (99%)	1 (1%)	0	100	100
1	K	148/157 (94%)	146 (99%)	2 (1%)	0	100	100
1	L	146/157 (93%)	143 (98%)	3 (2%)	0	100	100
All	All	1766/1884 (94%)	1732 (98%)	33 (2%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS

### 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	A	114/120 (95%)	101 (89%)	13 (11%)	5	5
1	B	114/120 (95%)	102 (90%)	12 (10%)	7	6
1	C	113/120 (94%)	103 (91%)	10 (9%)	10	8
1	D	113/120 (94%)	103 (91%)	10 (9%)	10	8
1	E	114/120 (95%)	101 (89%)	13 (11%)	5	5
1	F	115/120 (96%)	104 (90%)	11 (10%)	8	7
1	G	114/120 (95%)	103 (90%)	11 (10%)	8	7
1	H	114/120 (95%)	101 (89%)	13 (11%)	5	5
1	I	113/120 (94%)	103 (91%)	10 (9%)	10	8
1	J	114/120 (95%)	103 (90%)	11 (10%)	8	7
1	K	115/120 (96%)	101 (88%)	14 (12%)	5	4
1	L	113/120 (94%)	102 (90%)	11 (10%)	8	7
All	All	1366/1440 (95%)	1227 (90%)	139 (10%)	7	6

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	111	SER
1	G	127	LEU
1	L	39	LEU
1	F	127	LEU
1	G	39	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	55	ASN
1	G	-3	HIS
1	J	55	ASN
1	D	55	ASN
1	J	-3	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 8 are monoatomic - leaving 56 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$
2	JUQ	I	201	-	32,35,35	1.25	3 (9%)	38,51,51	1.71	10 (26%)
4	PLM	A	203	-	9,9,17	0.53	0	8,8,17	0.27	0
4	PLM	C	204	-	14,17,17	0.41	0	13,17,17	0.49	0
4	PLM	F	203	-	9,9,17	0.59	0	8,8,17	0.20	0
4	PLM	E	203	-	6,6,17	0.54	0	5,5,17	0.18	0
4	PLM	G	203	-	9,9,17	0.54	0	8,8,17	0.88	1 (12%)
4	PLM	E	204	-	9,9,17	0.47	0	8,8,17	0.23	0
4	PLM	D	206	-	11,14,17	0.45	0	10,14,17	0.59	0
4	PLM	L	203	-	14,17,17	0.44	0	13,17,17	0.42	0
4	PLM	I	203	-	9,9,17	0.61	0	8,8,17	0.38	0
2	JUQ	C	201	-	32,35,35	1.32	4 (12%)	38,51,51	2.15	13 (34%)
2	JUQ	A	201	-	32,35,35	1.20	1 (3%)	38,51,51	1.61	8 (21%)
4	PLM	F	205	-	9,9,17	0.53	0	8,8,17	0.35	0
4	PLM	A	205	-	9,9,17	0.48	0	8,8,17	0.38	0
4	PLM	F	204	-	9,9,17	0.56	0	8,8,17	0.15	0
4	PLM	D	203	-	9,9,17	0.56	0	8,8,17	0.46	0
2	JUQ	F	201	-	32,35,35	1.39	3 (9%)	38,51,51	1.81	8 (21%)
4	PLM	J	207	-	11,14,17	0.48	0	10,14,17	0.55	0
2	JUQ	J	201	-	32,35,35	1.12	2 (6%)	38,51,51	1.80	6 (15%)
4	PLM	L	206	-	9,9,17	0.57	0	8,8,17	0.59	0
4	PLM	B	207	-	9,9,17	0.45	0	8,8,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PLM	A	207	-	11,14,17	0.43	0	10,14,17	0.59	0
4	PLM	C	207	-	9,9,17	0.69	0	8,8,17	0.43	0
4	PLM	G	204	-	9,9,17	0.39	0	8,8,17	0.32	0
4	PLM	F	202	-	7,7,17	0.45	0	6,6,17	0.39	0
4	PLM	G	205	-	11,14,17	0.45	0	10,14,17	0.62	0
4	PLM	L	204	-	7,7,17	0.45	0	6,6,17	0.46	0
4	PLM	J	204	-	7,7,17	0.52	0	6,6,17	0.65	0
2	JUQ	E	201	-	32,35,35	1.34	4 (12%)	38,51,51	2.43	15 (39%)
4	PLM	D	204	-	9,9,17	0.74	0	8,8,17	0.55	0
4	PLM	B	204	-	9,9,17	0.46	0	8,8,17	0.24	0
4	PLM	H	203	-	9,9,17	0.68	0	8,8,17	0.34	0
4	PLM	H	202	-	11,11,17	0.61	0	10,10,17	0.52	0
4	PLM	J	205	-	9,9,17	0.47	0	8,8,17	0.46	0
5	LMT	B	209	-	36,36,36	0.69	1 (2%)	47,47,47	1.05	1 (2%)
4	PLM	B	205	-	9,9,17	0.68	0	8,8,17	0.40	0
4	PLM	A	204	-	14,17,17	0.41	0	13,17,17	0.69	0
4	PLM	B	206	-	14,17,17	0.42	0	13,17,17	0.29	0
4	PLM	B	208	-	9,9,17	0.48	0	8,8,17	0.46	0
4	PLM	E	202	-	9,9,17	0.53	0	8,8,17	0.45	0
2	JUQ	D	201	-	32,35,35	1.03	1 (3%)	38,51,51	1.57	5 (13%)
4	PLM	C	206	-	9,9,17	0.46	0	8,8,17	0.32	0
2	JUQ	L	201	-	32,35,35	1.33	3 (9%)	38,51,51	2.38	15 (39%)
4	PLM	B	203	-	11,11,17	0.54	0	10,10,17	0.72	0
4	PLM	C	203	-	6,9,17	0.35	0	5,9,17	0.38	0
4	PLM	I	204	-	14,17,17	0.30	0	13,17,17	0.84	0
4	PLM	J	206	-	14,17,17	0.36	0	13,17,17	0.69	0
4	PLM	J	203	-	9,9,17	0.62	0	8,8,17	0.68	0
4	PLM	D	205	-	14,17,17	0.45	0	13,17,17	0.64	0
4	PLM	A	206	-	14,17,17	0.42	0	13,17,17	0.57	0
2	JUQ	G	201	-	32,35,35	1.29	2 (6%)	38,51,51	1.95	14 (36%)
4	PLM	C	205	-	9,9,17	0.62	0	8,8,17	0.36	0
4	PLM	L	205	-	10,13,17	0.60	0	9,13,17	0.62	0
2	JUQ	B	201	-	32,35,35	1.41	5 (15%)	38,51,51	2.02	15 (39%)
2	JUQ	K	201	-	32,35,35	1.21	2 (6%)	38,51,51	1.98	10 (26%)
2	JUQ	H	201	-	32,35,35	1.28	4 (12%)	38,51,51	1.93	8 (21%)

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
2	JUQ	I	201	-	-	4/18/33/33	0/5/5/5
4	PLM	A	203	-	-	4/7/7/15	-
4	PLM	C	204	-	-	6/13/15/15	-
4	PLM	F	203	-	-	3/7/7/15	-
4	PLM	E	203	-	-	1/4/4/15	-
4	PLM	G	203	-	-	2/7/7/15	-
4	PLM	E	204	-	-	1/7/7/15	-
4	PLM	D	206	-	-	4/10/12/15	-
4	PLM	L	203	-	-	7/13/15/15	-
4	PLM	I	203	-	-	4/7/7/15	-
2	JUQ	C	201	-	-	5/18/33/33	0/5/5/5
2	JUQ	A	201	-	-	4/18/33/33	0/5/5/5
4	PLM	F	205	-	-	7/7/7/15	-
4	PLM	A	205	-	-	5/7/7/15	-
4	PLM	F	204	-	-	1/7/7/15	-
4	PLM	D	203	-	-	4/7/7/15	-
2	JUQ	F	201	-	-	3/18/33/33	0/5/5/5
4	PLM	J	207	-	-	6/10/12/15	-
2	JUQ	J	201	-	-	5/18/33/33	0/5/5/5
4	PLM	L	206	-	-	2/7/7/15	-
4	PLM	B	207	-	-	2/7/7/15	-
4	PLM	A	207	-	-	6/10/12/15	-
4	PLM	C	207	-	-	2/7/7/15	-
4	PLM	G	204	-	-	3/7/7/15	-
4	PLM	F	202	-	-	2/5/5/15	-
4	PLM	G	205	-	-	4/10/12/15	-
4	PLM	L	204	-	-	1/5/5/15	-
4	PLM	J	204	-	-	1/5/5/15	-
2	JUQ	E	201	-	-	7/18/33/33	0/5/5/5
4	PLM	D	204	-	-	2/7/7/15	-
4	PLM	B	204	-	-	3/7/7/15	-
4	PLM	H	203	-	-	4/7/7/15	-
4	PLM	H	202	-	-	0/9/9/15	-
4	PLM	J	205	-	-	2/7/7/15	-
5	LMT	B	209	-	-	1/21/61/61	0/2/2/2
4	PLM	B	205	-	-	1/7/7/15	-
4	PLM	A	204	-	-	1/13/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLM	B	206	-	-	8/13/15/15	-
4	PLM	B	208	-	-	3/7/7/15	-
4	PLM	E	202	-	-	3/7/7/15	-
2	JUQ	D	201	-	-	5/18/33/33	0/5/5/5
4	PLM	C	206	-	-	4/7/7/15	-
2	JUQ	L	201	-	-	7/18/33/33	0/5/5/5
4	PLM	B	203	-	-	7/9/9/15	-
4	PLM	C	203	-	-	2/5/7/15	-
4	PLM	I	204	-	-	6/13/15/15	-
4	PLM	J	206	-	-	2/13/15/15	-
4	PLM	J	203	-	-	0/7/7/15	-
4	PLM	D	205	-	-	2/13/15/15	-
4	PLM	A	206	-	-	4/13/15/15	-
2	JUQ	G	201	-	-	3/18/33/33	0/5/5/5
4	PLM	C	205	-	-	3/7/7/15	-
4	PLM	L	205	-	-	6/9/11/15	-
2	JUQ	B	201	-	-	4/18/33/33	0/5/5/5
2	JUQ	K	201	-	-	3/18/33/33	0/5/5/5
2	JUQ	H	201	-	-	7/18/33/33	0/5/5/5

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	JUQ	C7-N11	4.26	1.49	1.43
2	F	201	JUQ	C15-C16	-4.22	1.44	1.52
2	G	201	JUQ	C15-C16	-4.05	1.45	1.52
2	I	201	JUQ	C17-C16	-3.86	1.47	1.52
2	C	201	JUQ	C28-N11	3.69	1.51	1.46

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	JUQ	C27-O26-C25	-6.96	110.32	117.21
2	K	201	JUQ	C25-C12-N11	6.95	127.12	119.99
2	J	201	JUQ	C25-C12-N11	6.59	126.75	119.99
2	H	201	JUQ	C25-C12-N11	5.87	126.01	119.99
2	E	201	JUQ	C8-C7-N11	5.84	126.54	120.58

There are no chirality outliers.

5 of 199 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	201	JUQ	C29-C28-N11-C12
4	C	204	PLM	C1-C2-C3-C4
4	L	203	PLM	C1-C2-C3-C4
2	C	201	JUQ	C15-C16-C17-C18
2	C	201	JUQ	O23-C16-C17-C18

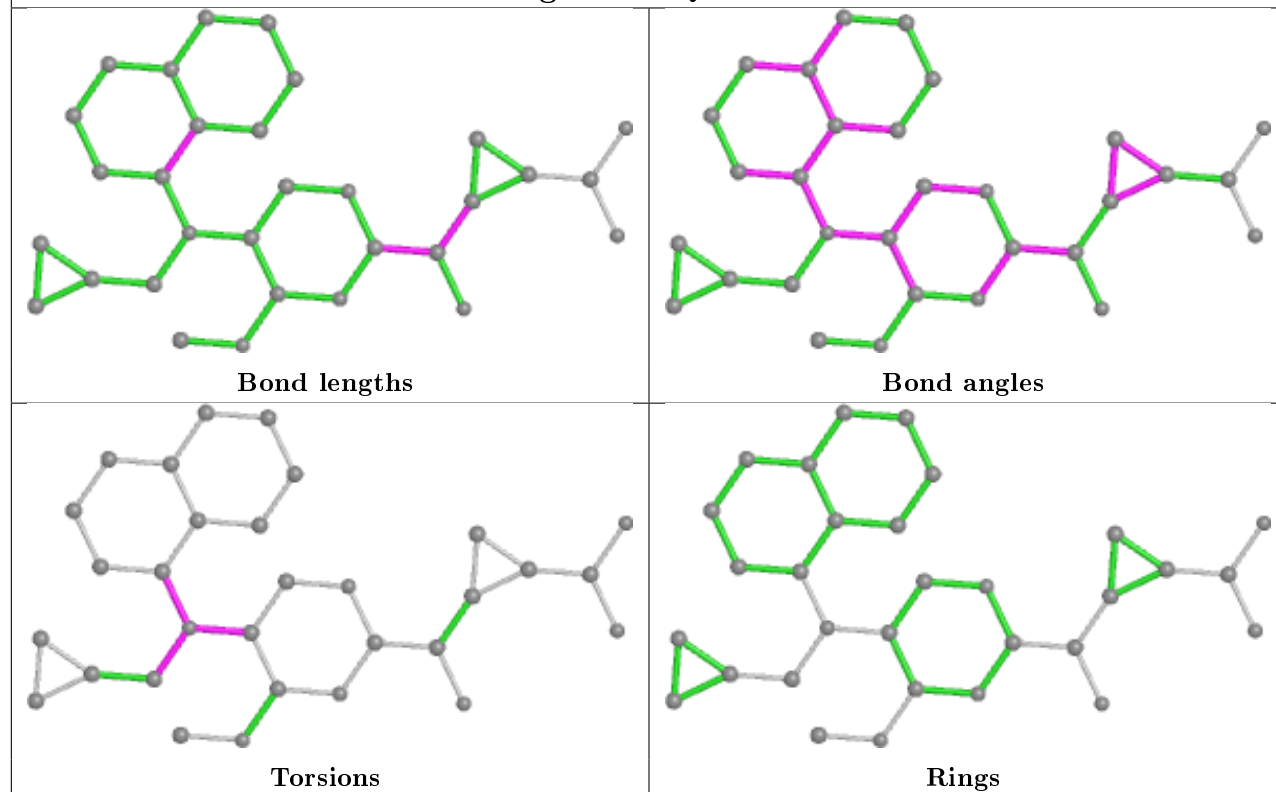
There are no ring outliers.

4 monomers are involved in 4 short contacts:

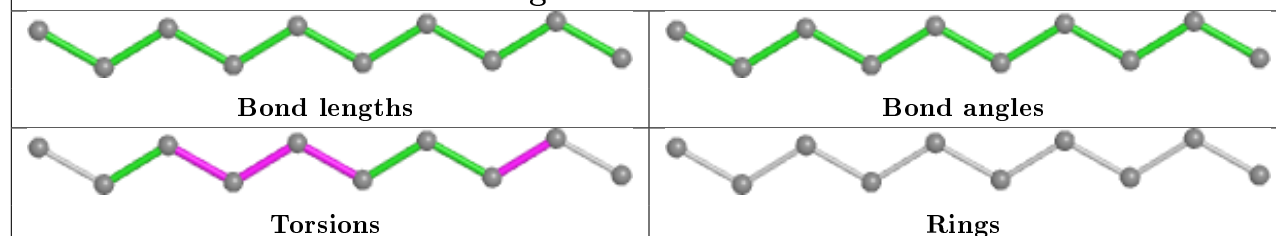
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	201	JUQ	1	0
4	G	204	PLM	1	0
4	F	202	PLM	1	0
4	A	206	PLM	1	0

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

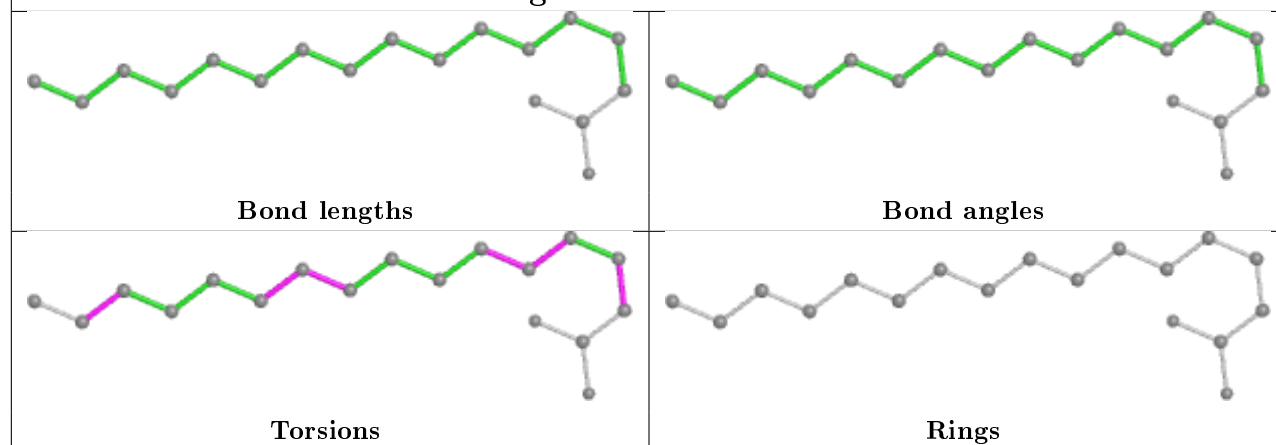
## Ligand JUQ I 201

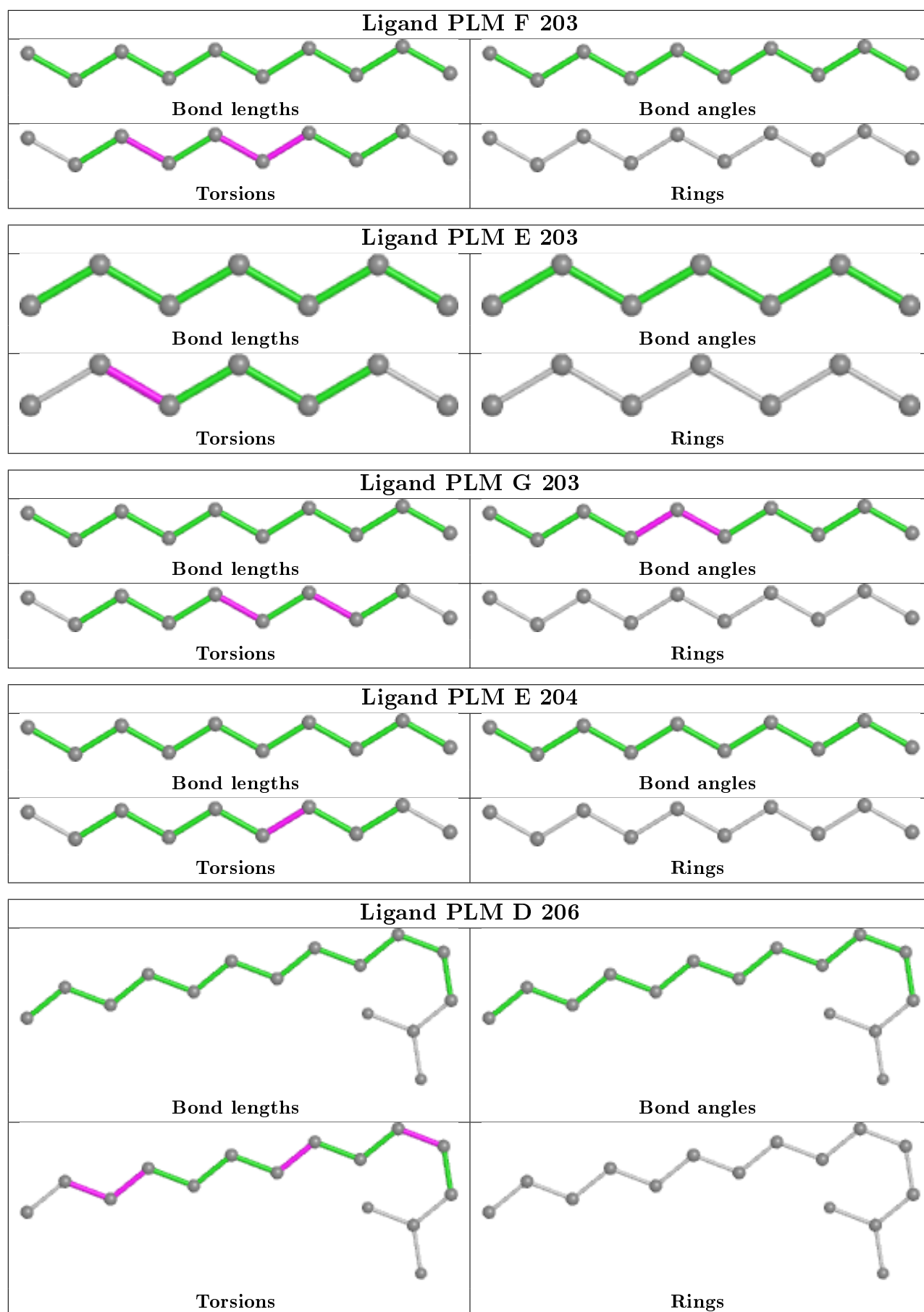


## Ligand PLM A 203

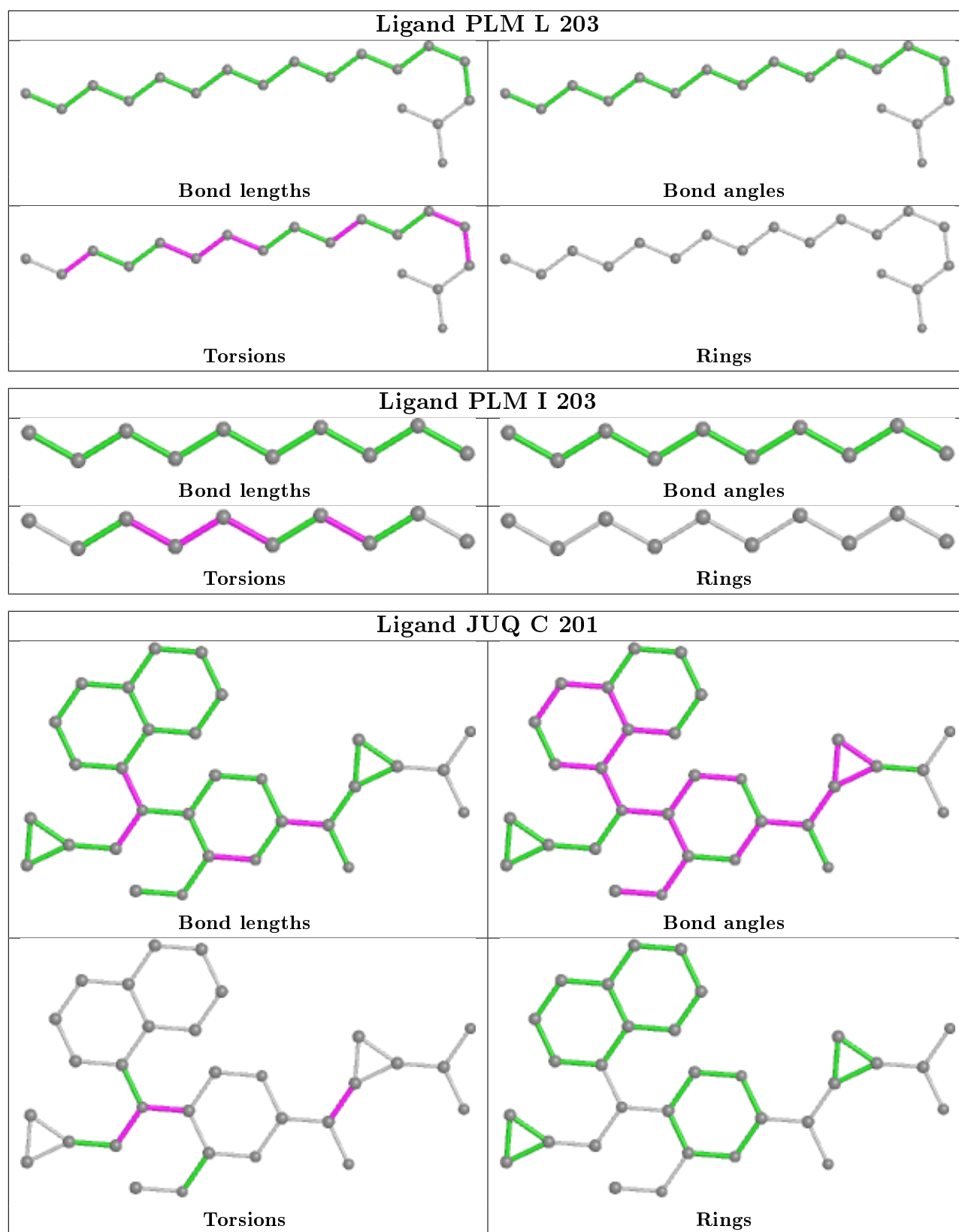


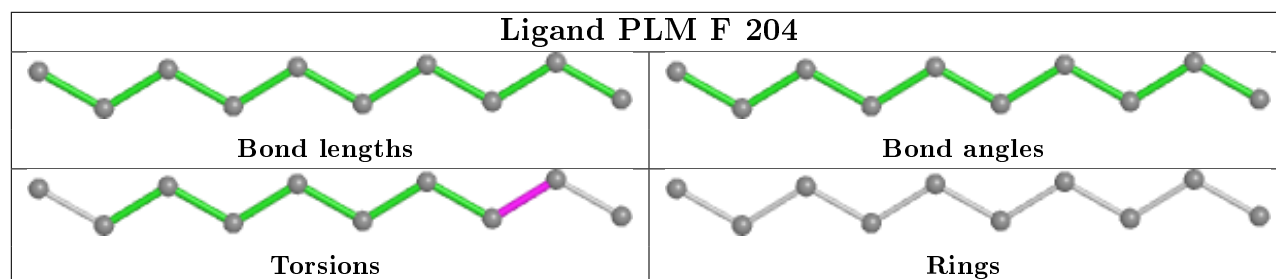
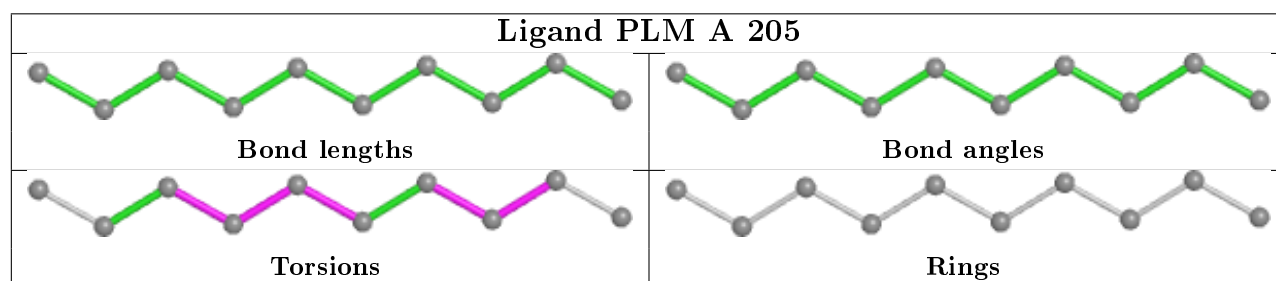
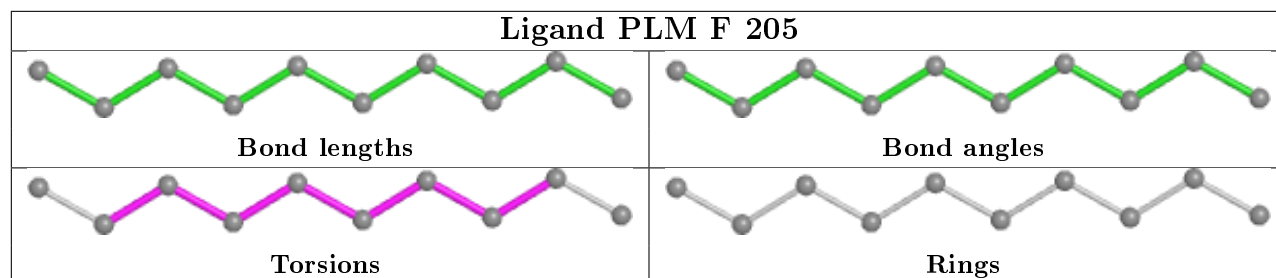
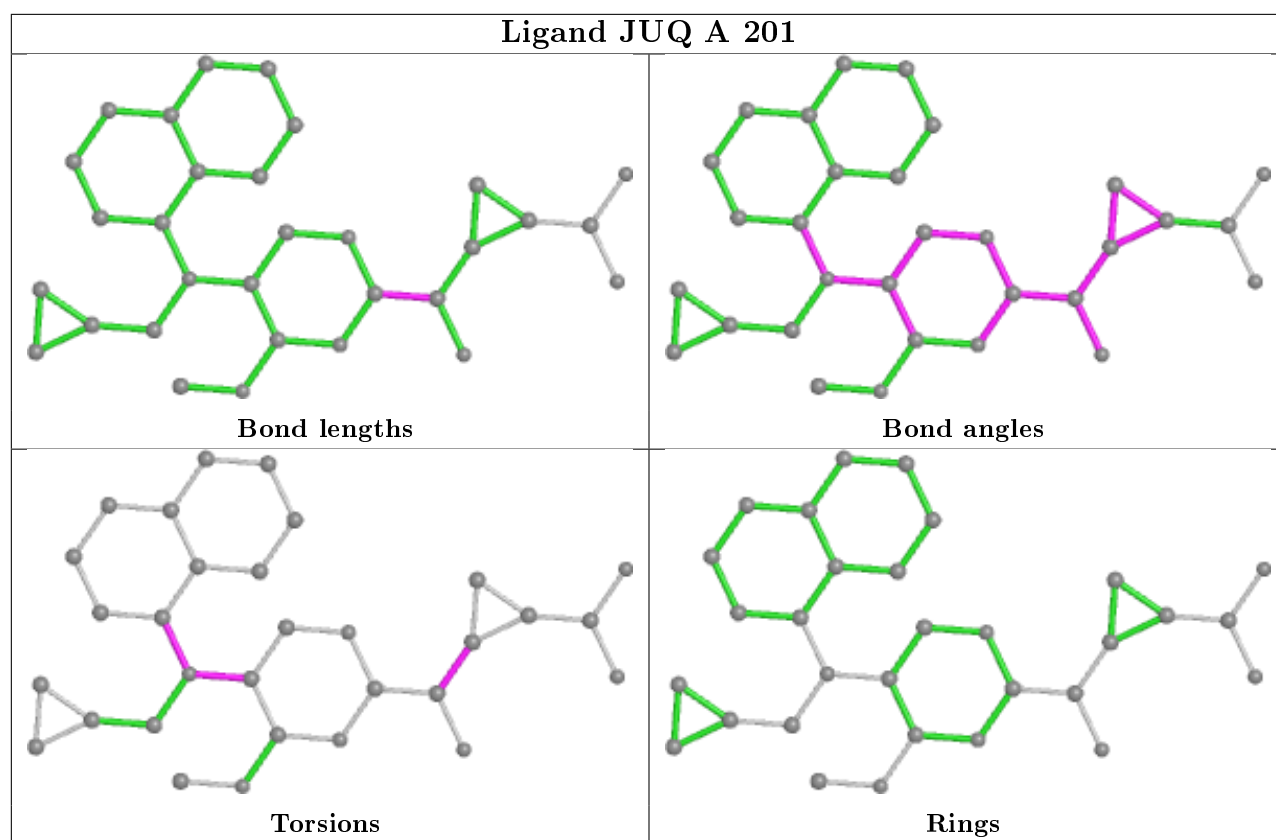
## Ligand PLM C 204

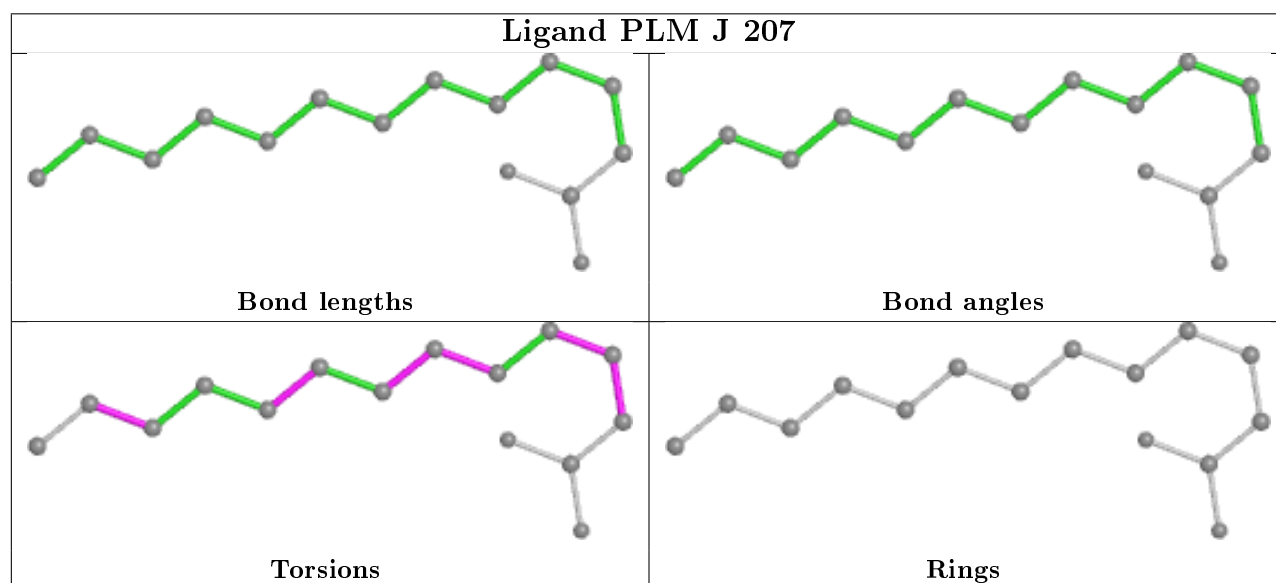
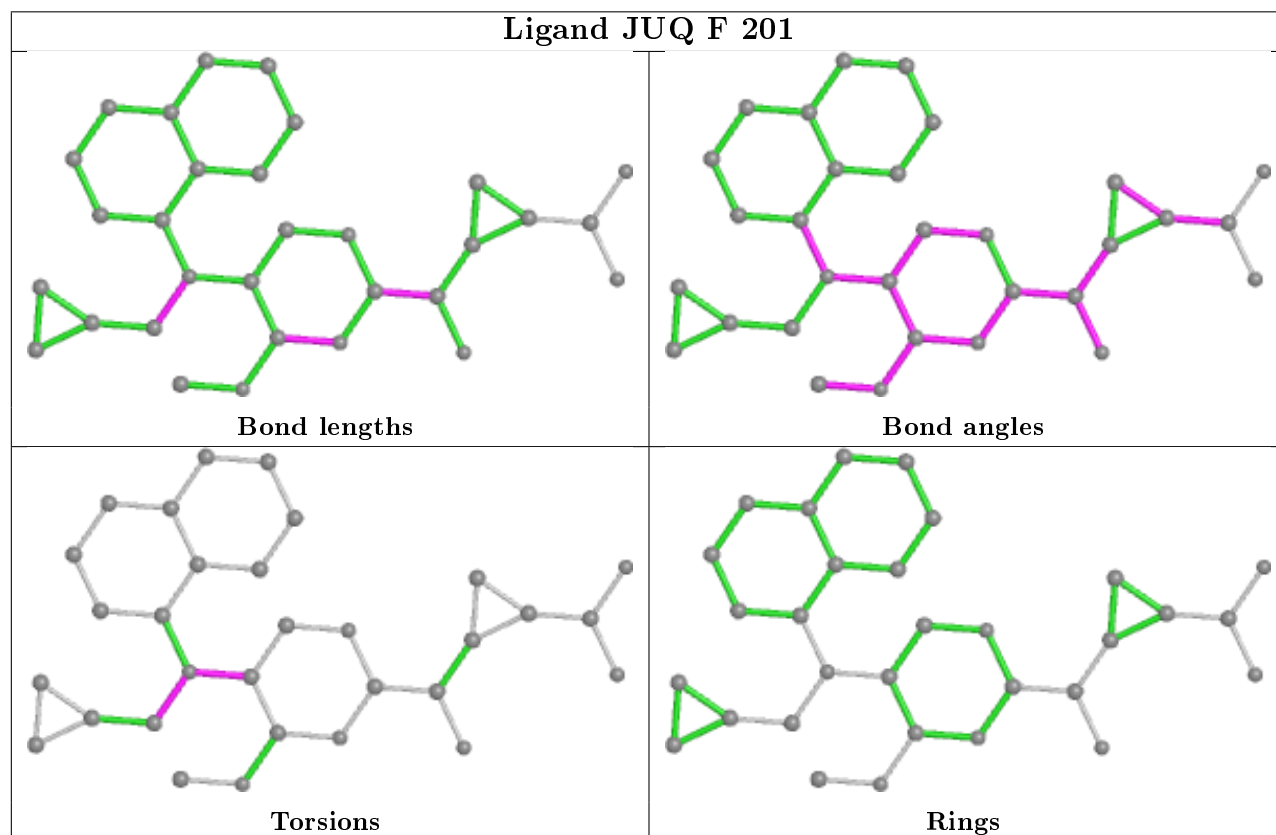
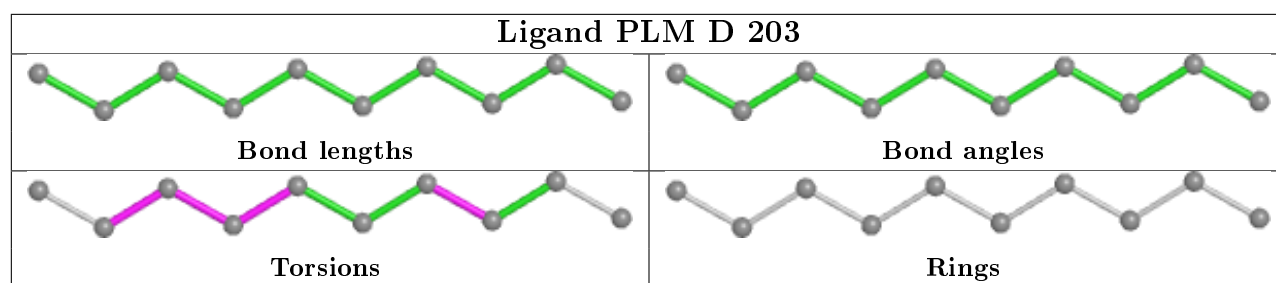




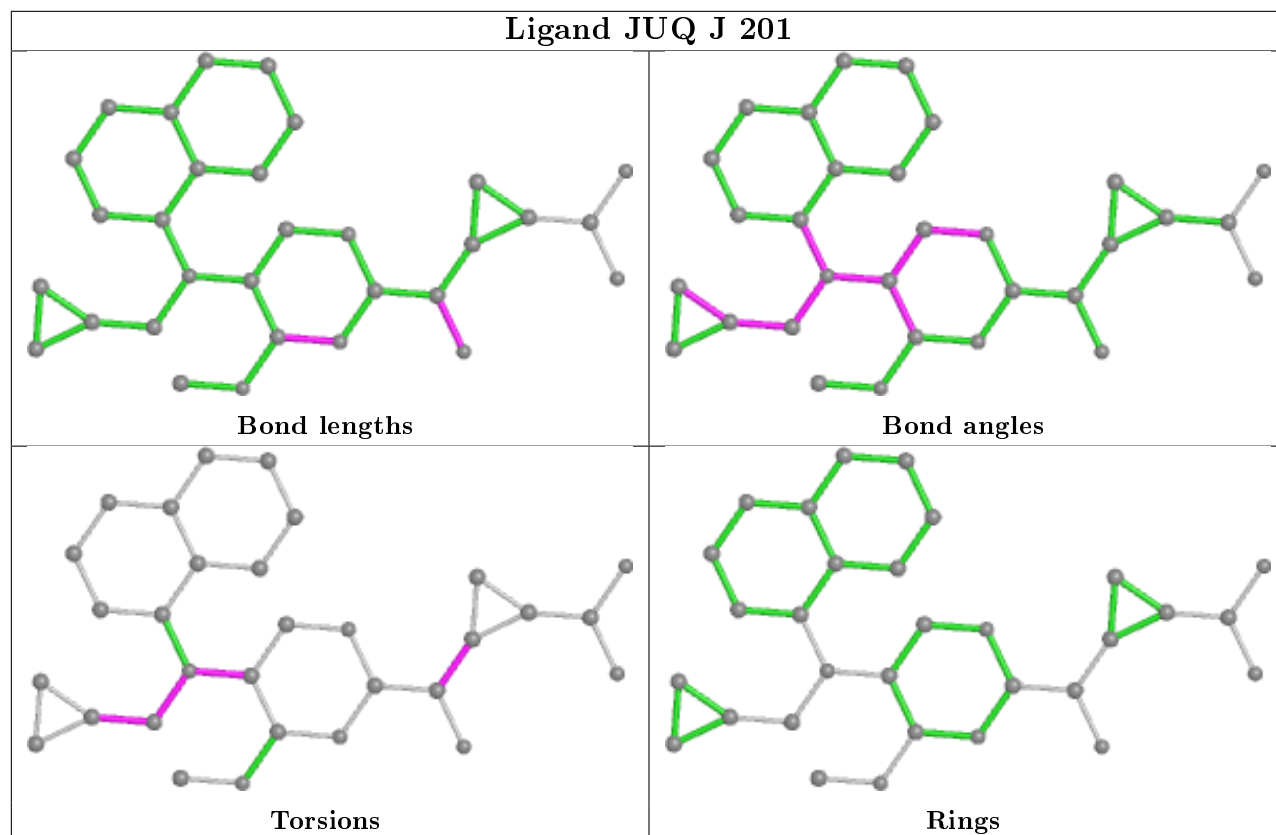




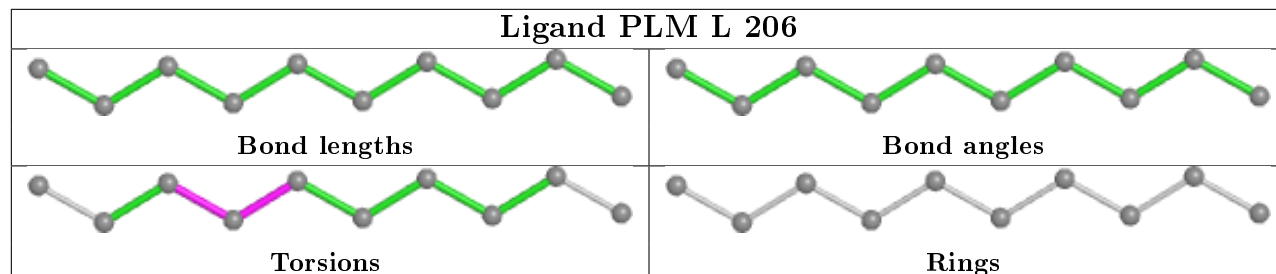




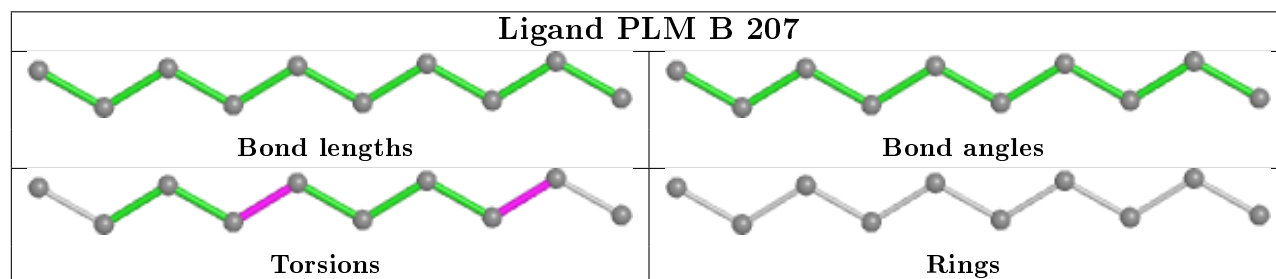
## Ligand JUQ J 201

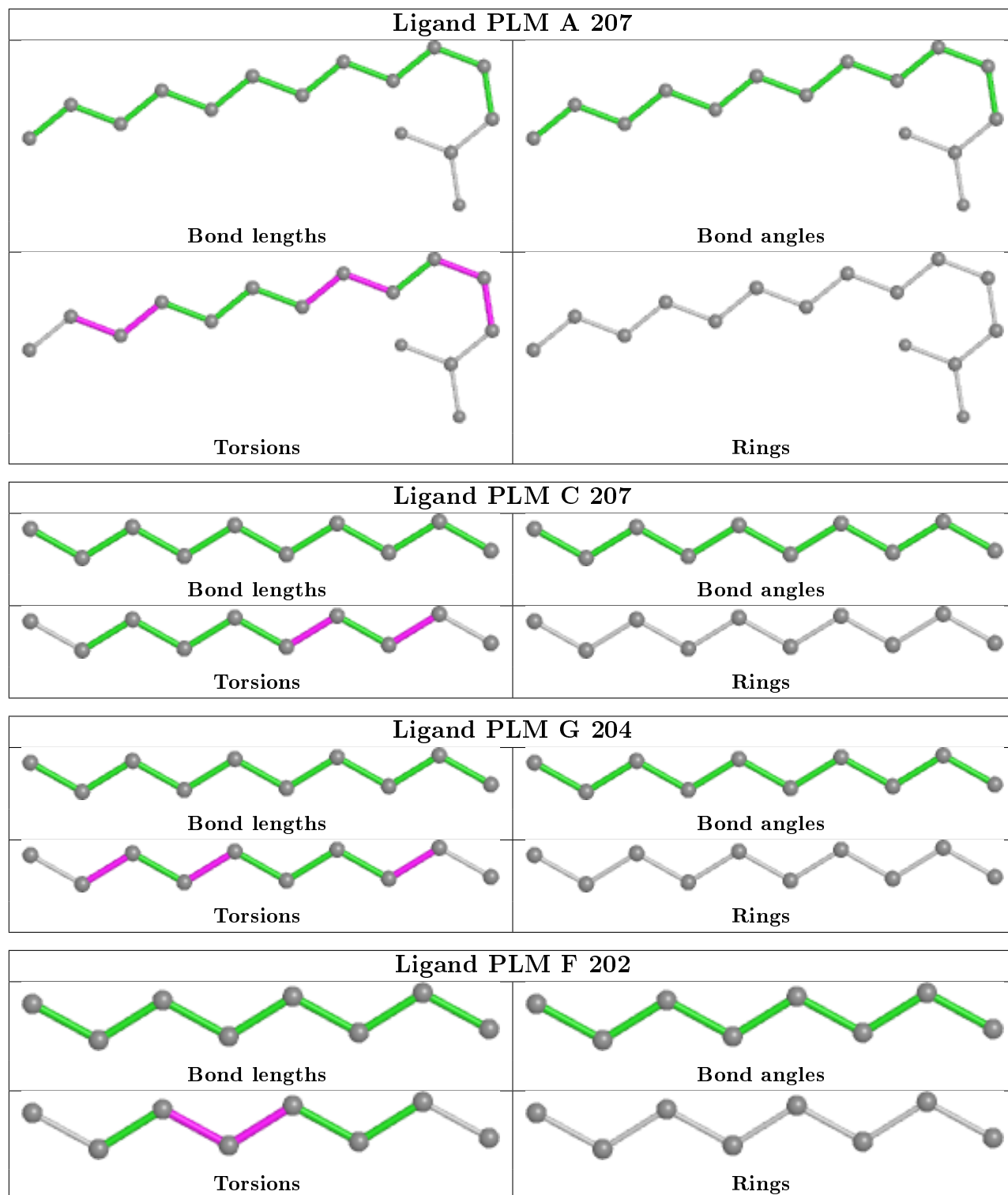


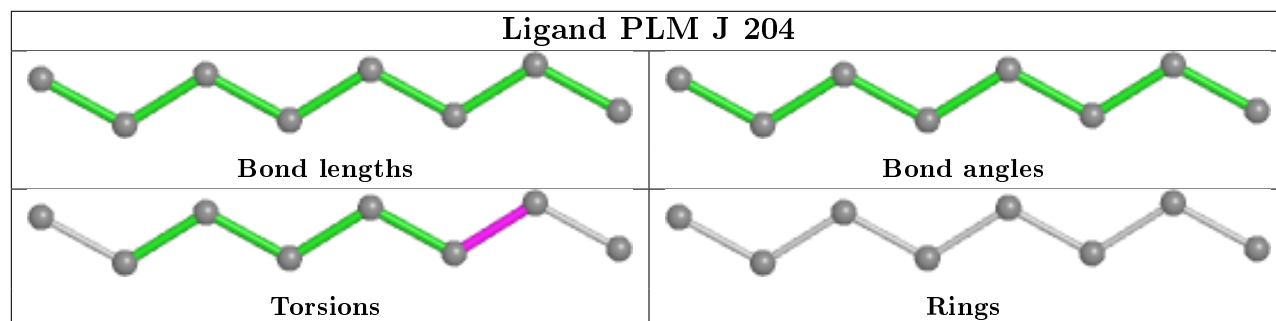
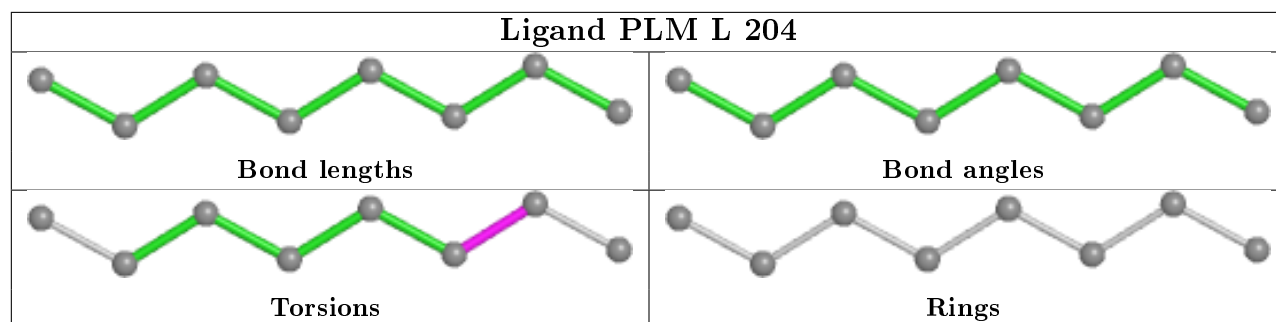
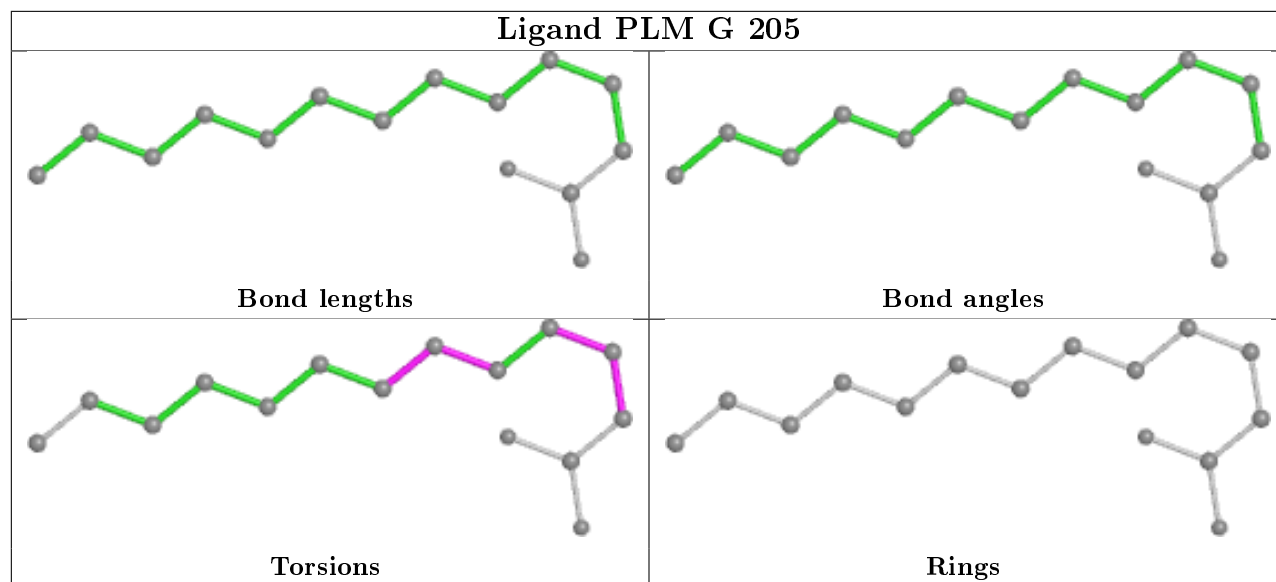
## Ligand PLM L 206

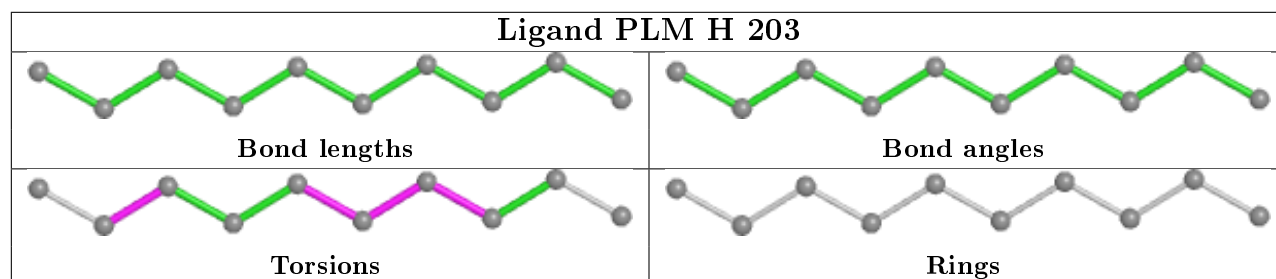
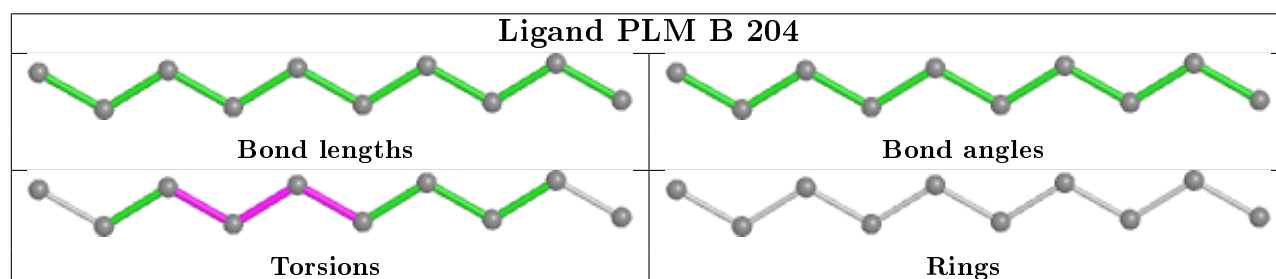
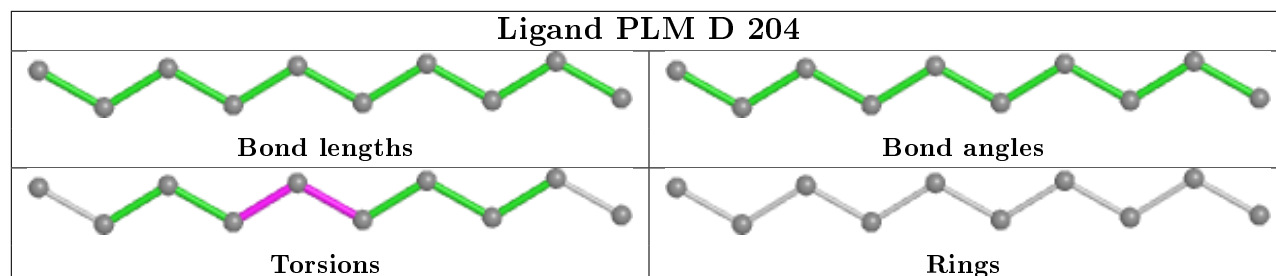
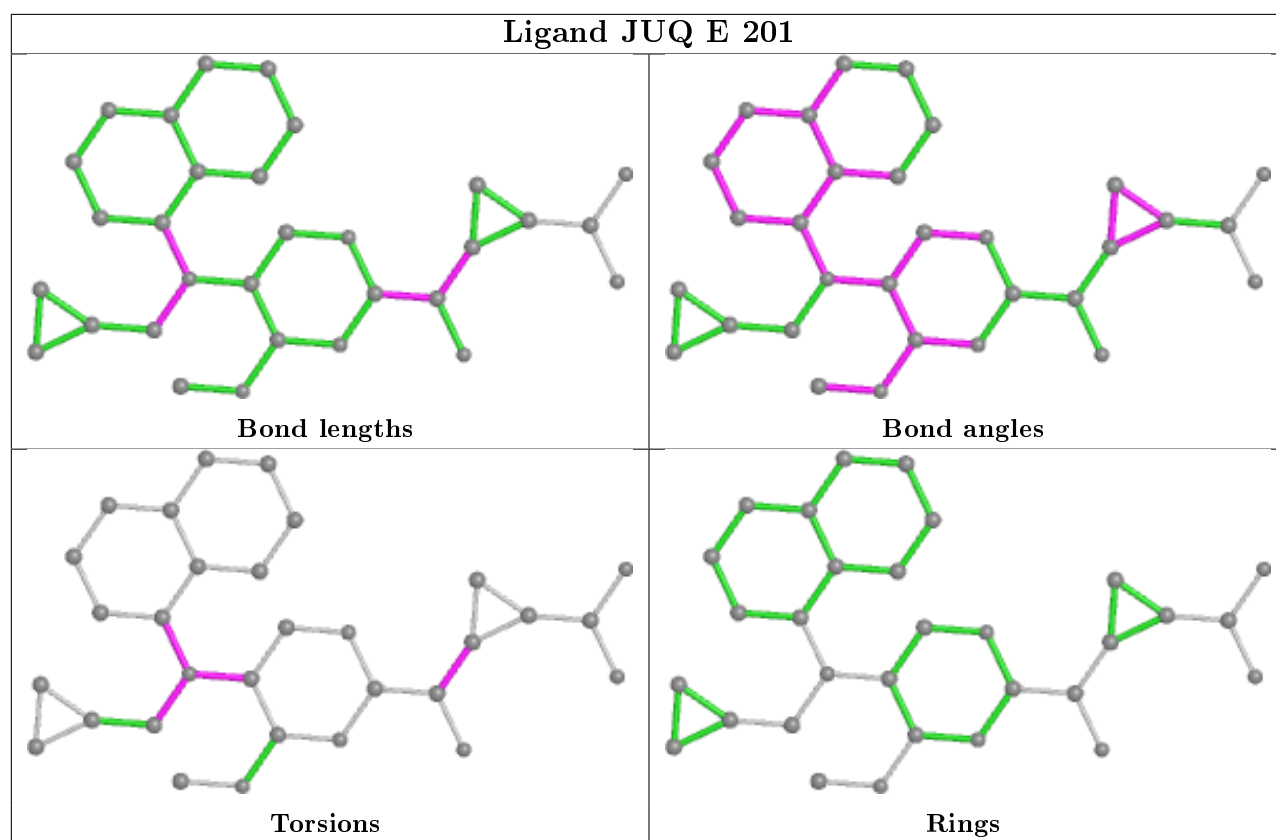


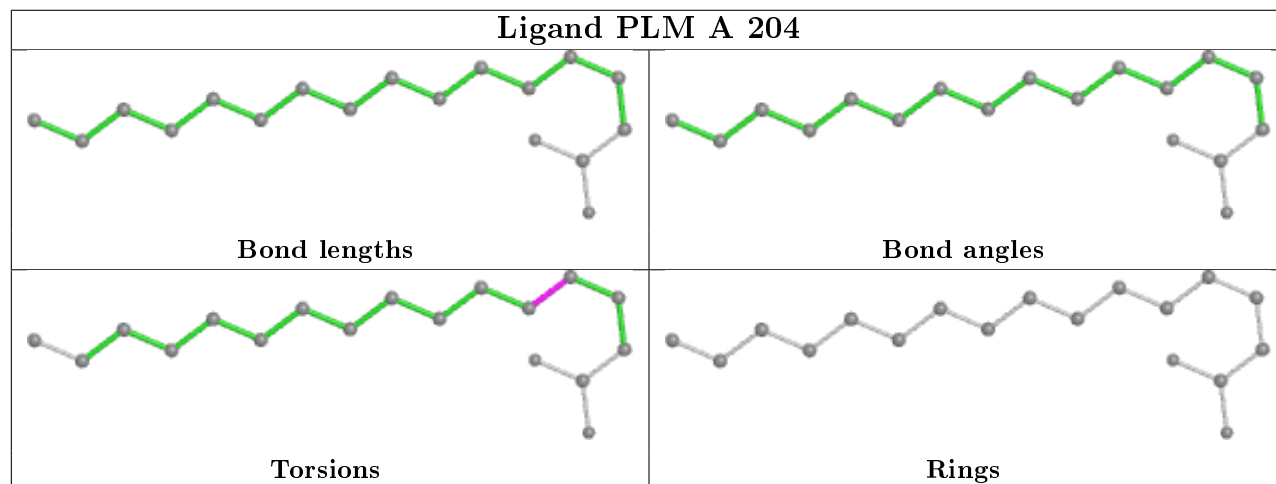
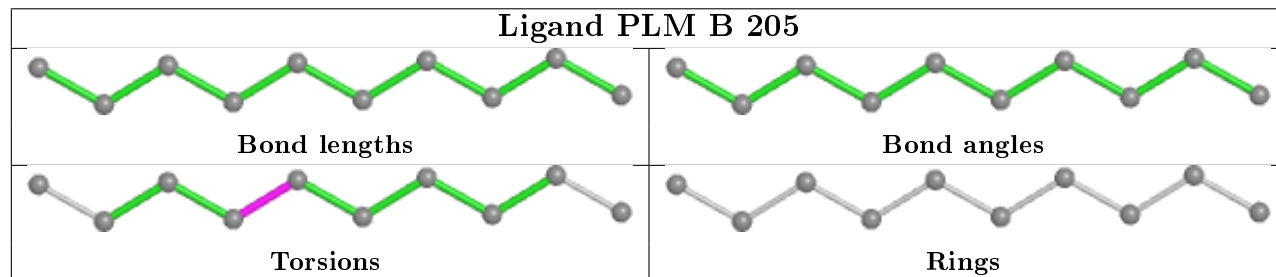
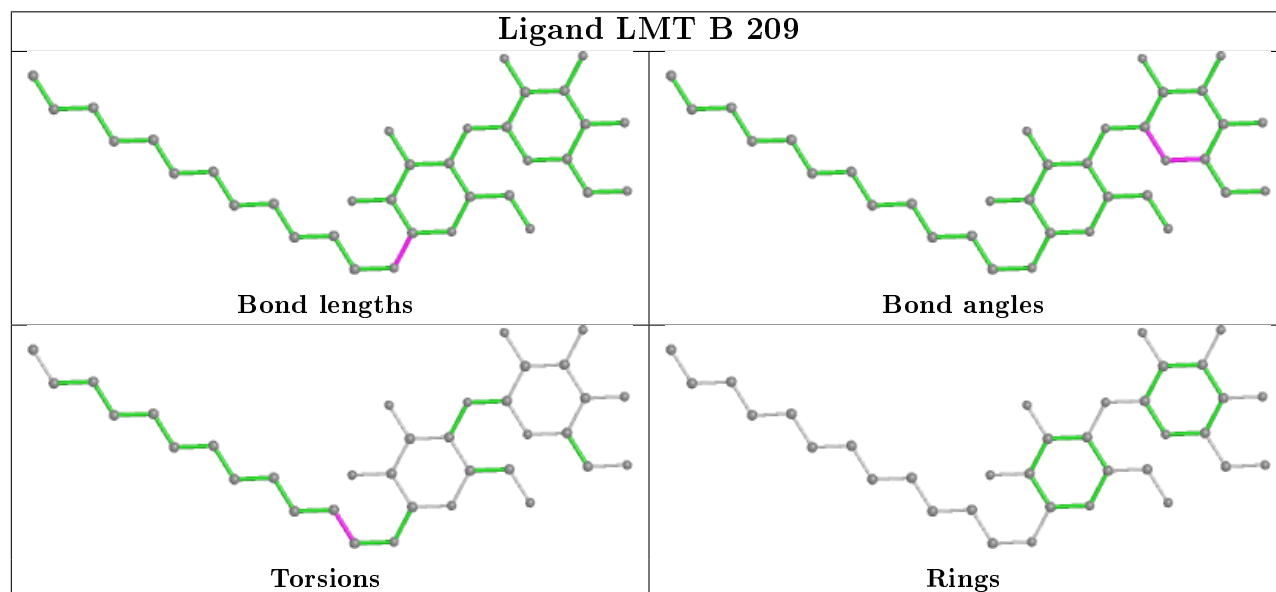
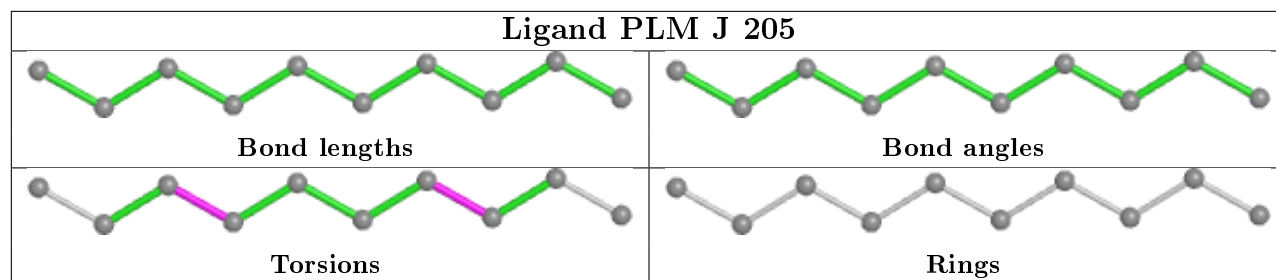
## Ligand PLM B 207



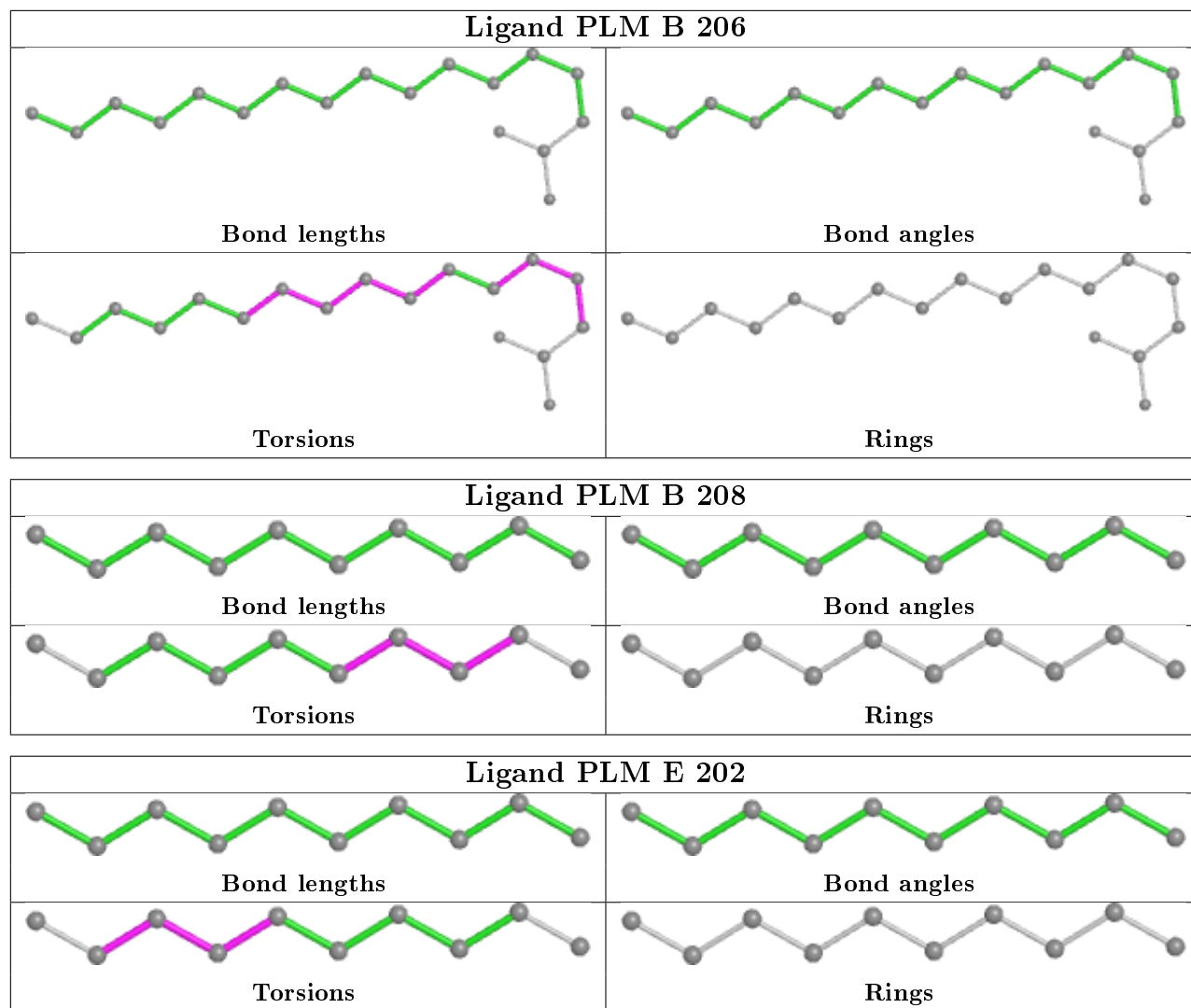




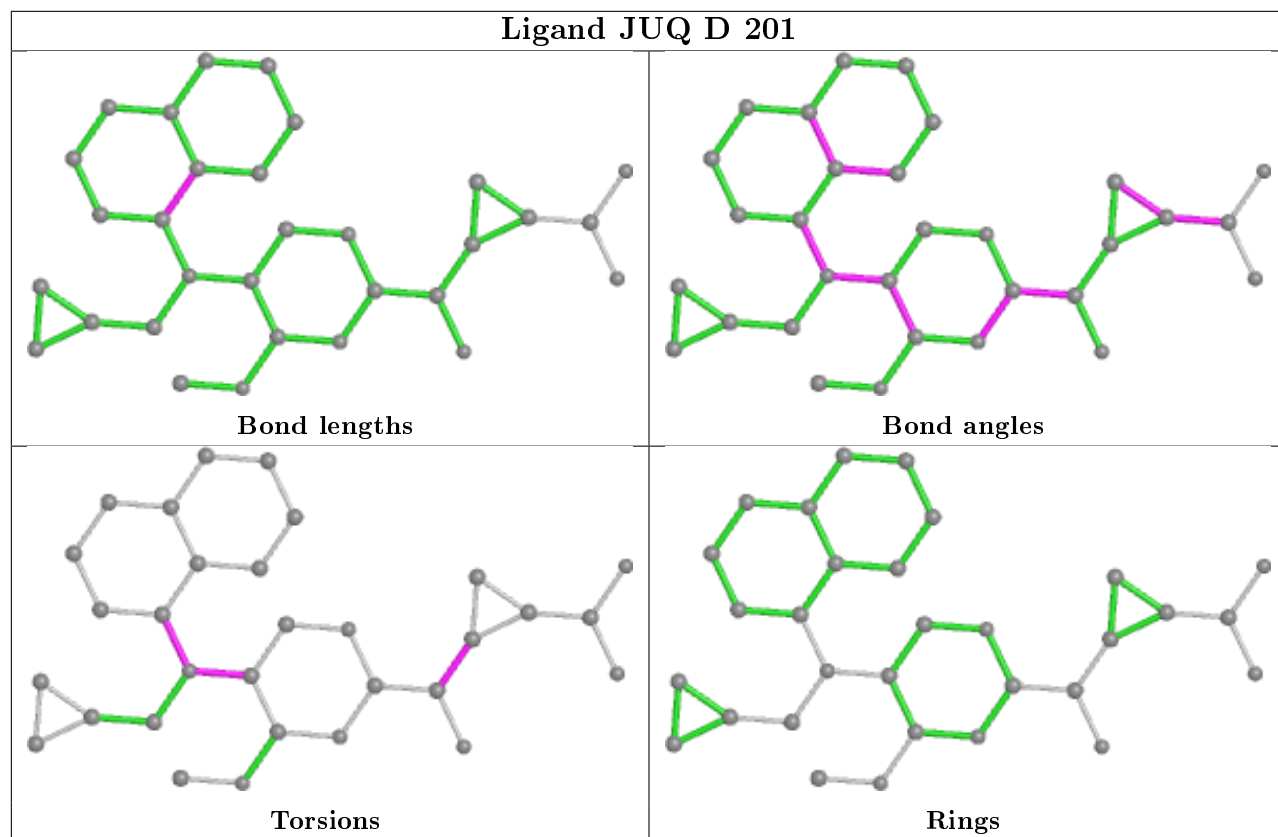




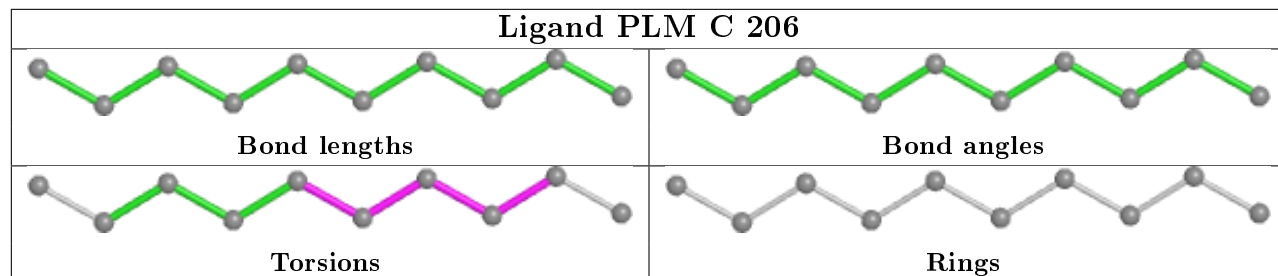


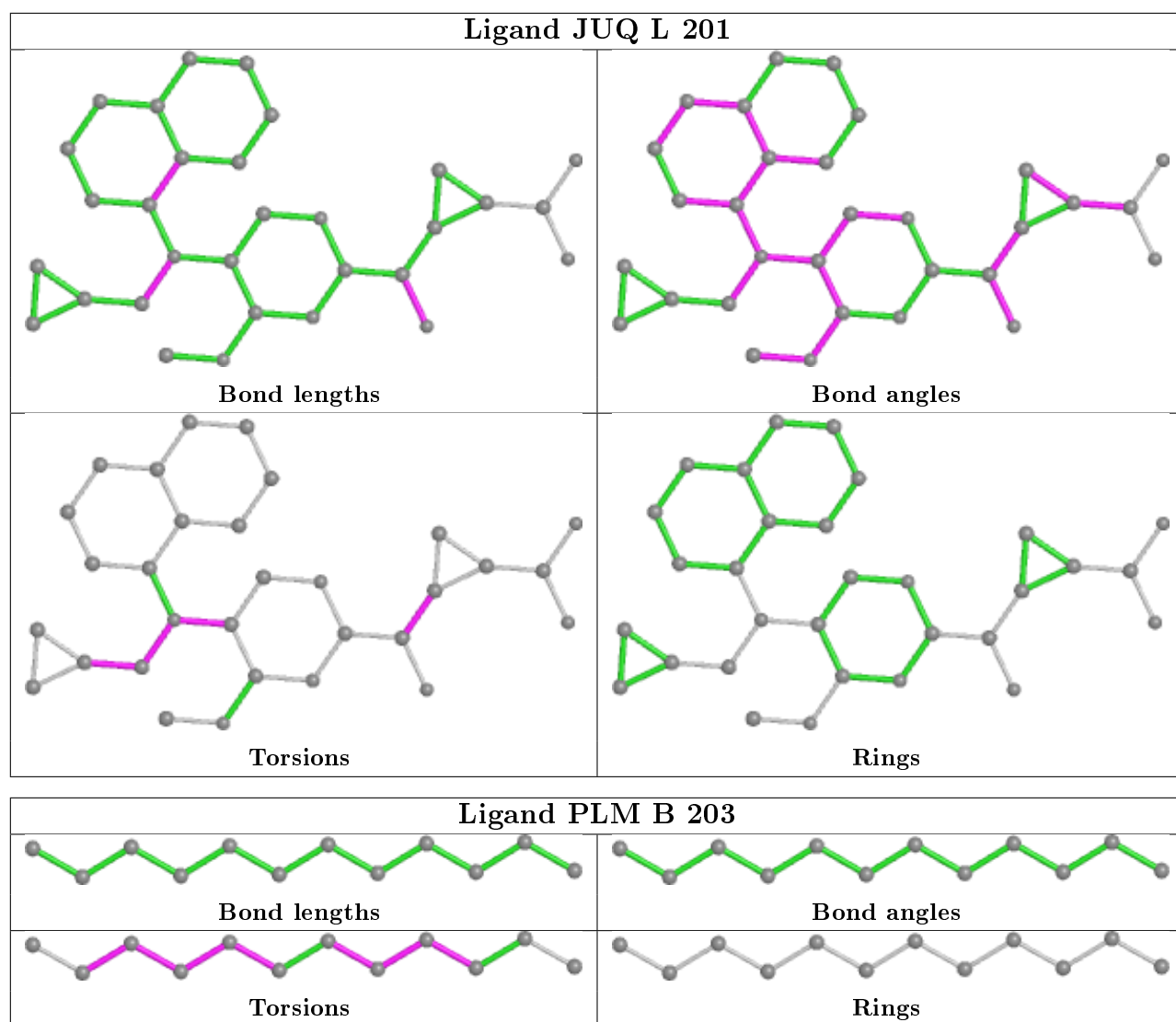


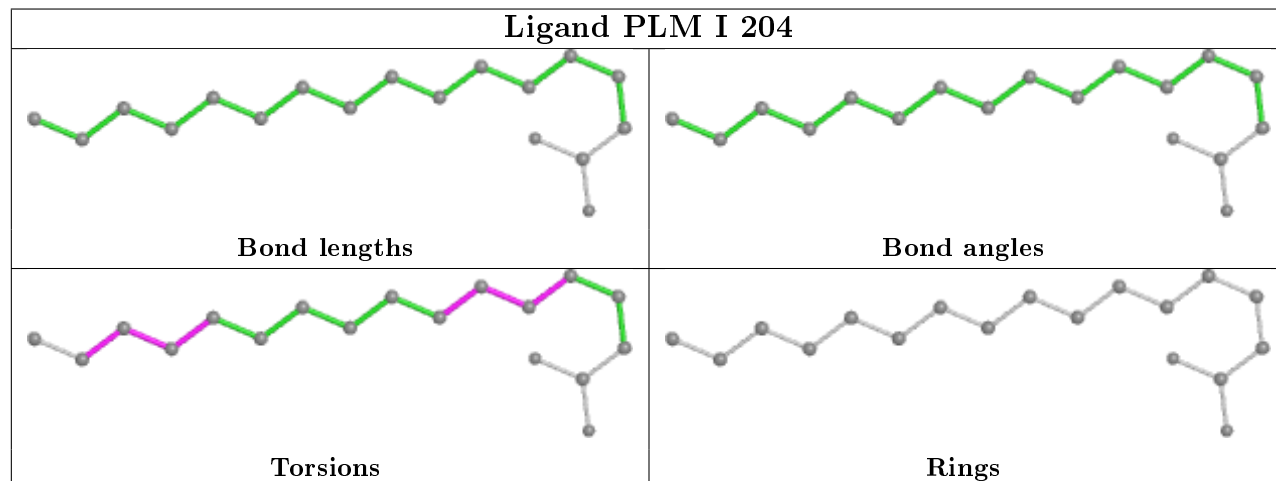
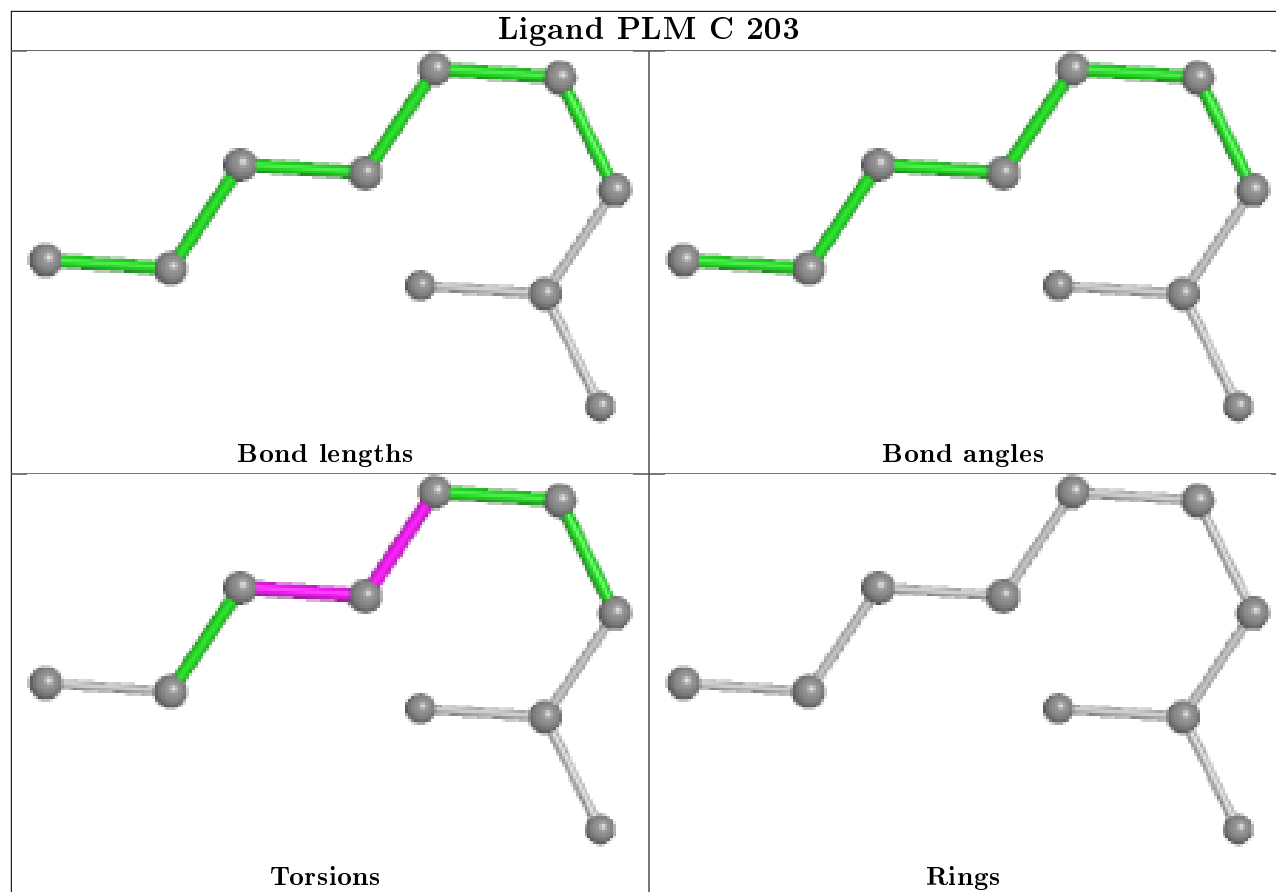
## Ligand JUQ D 201

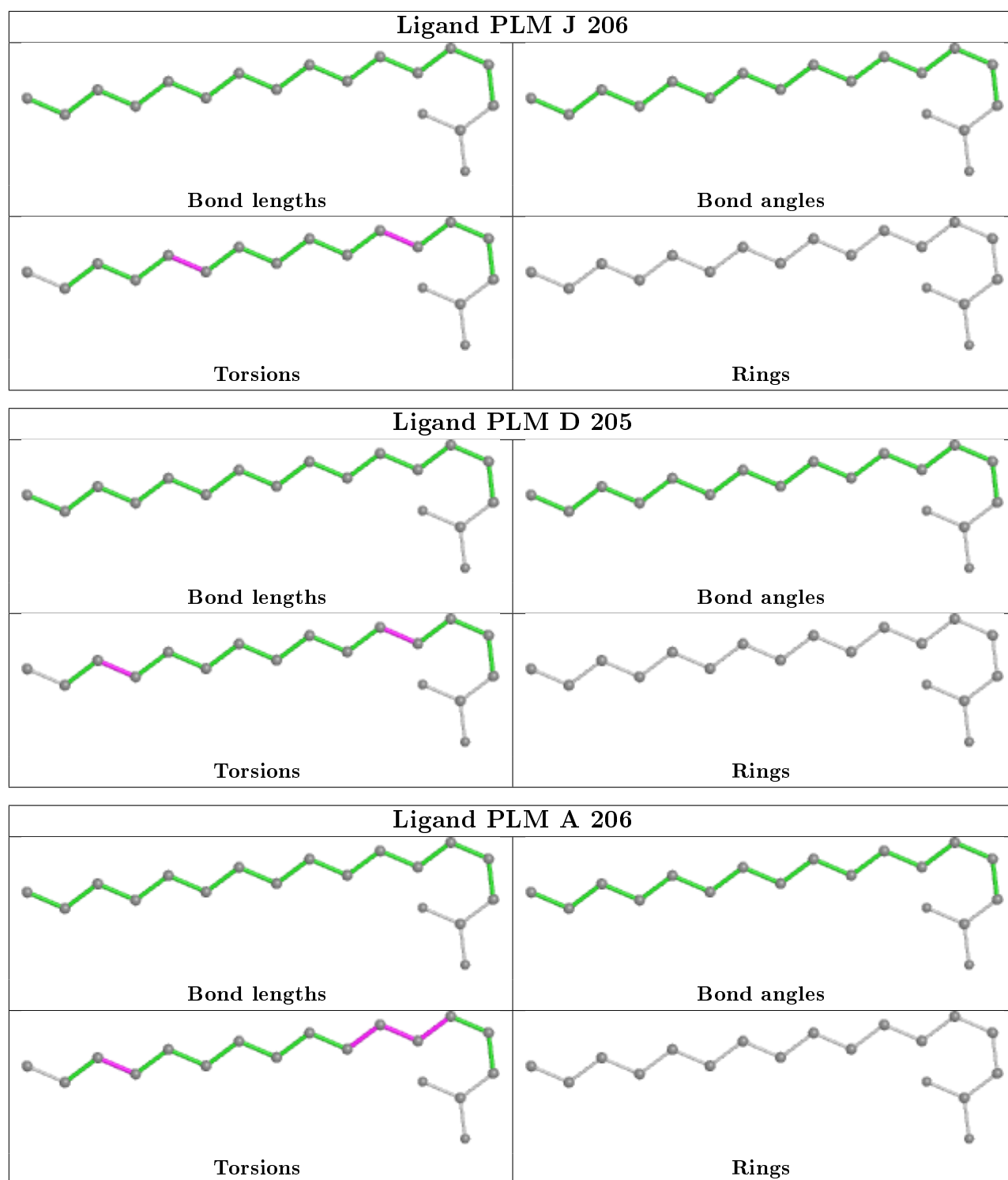


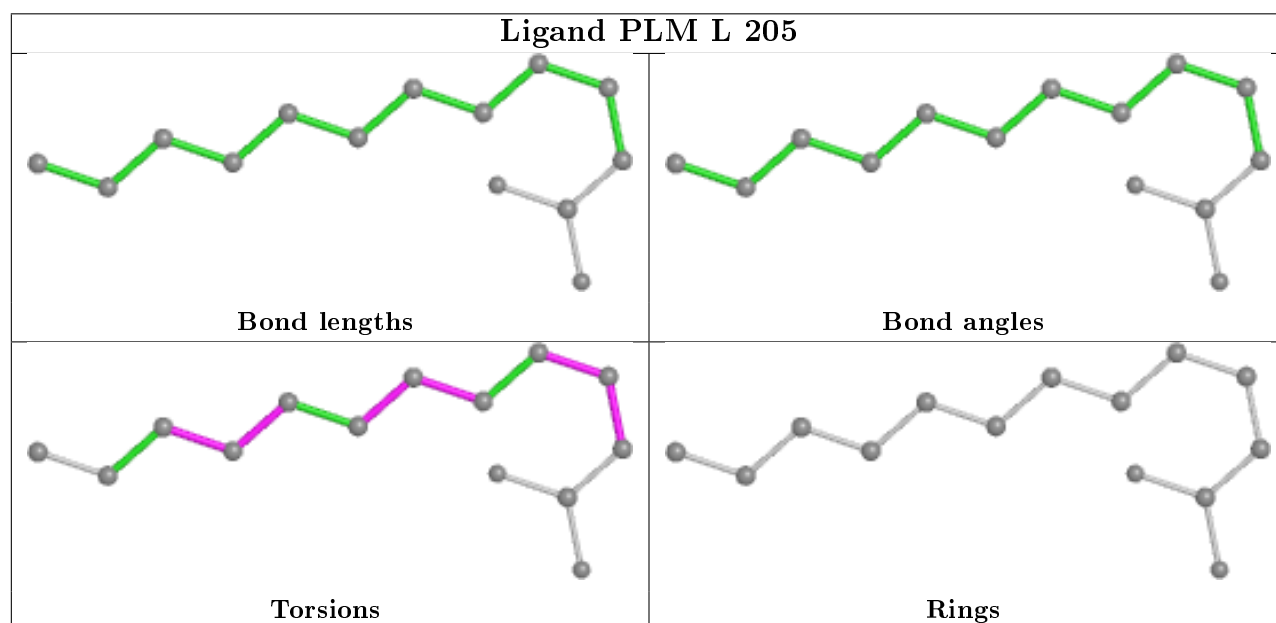
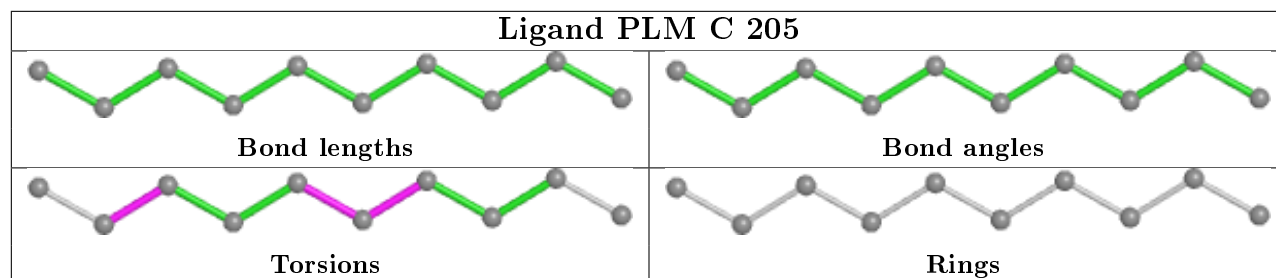
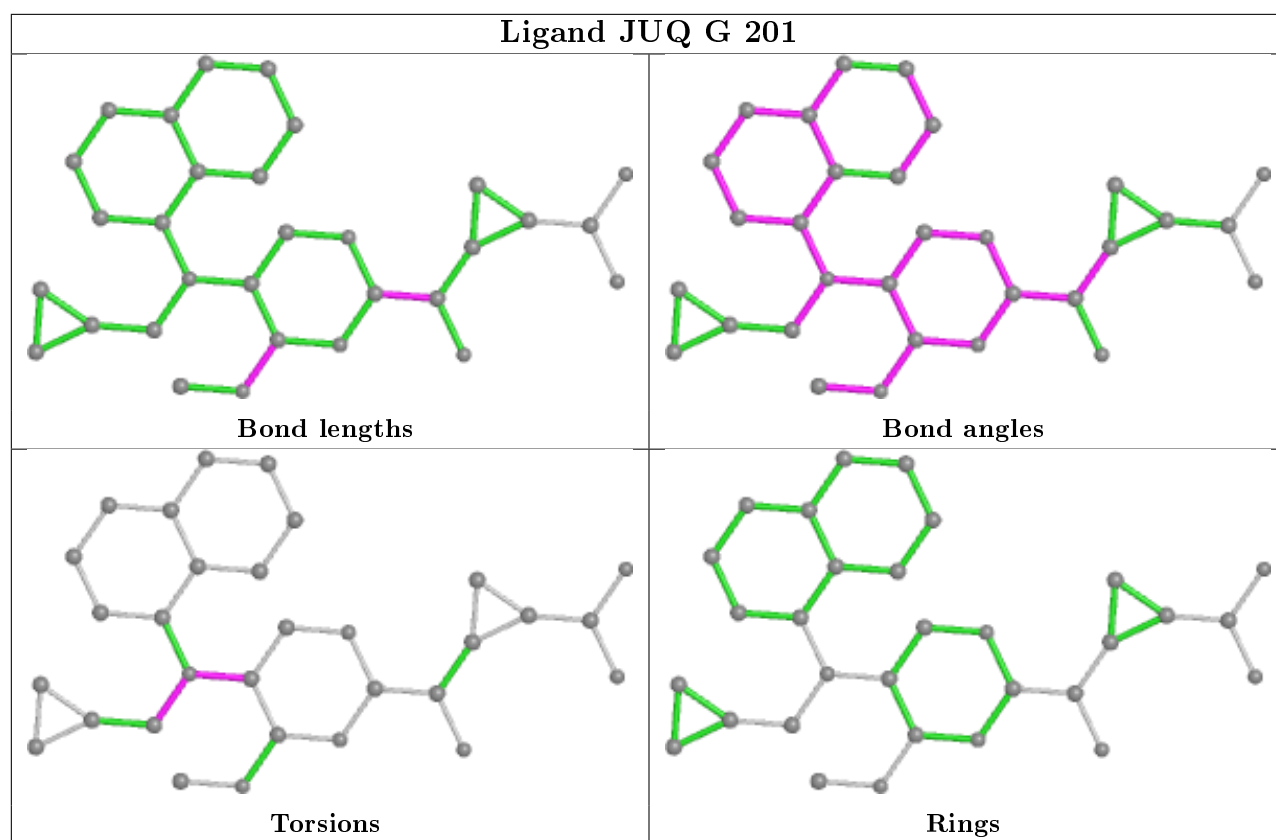
## Ligand PLM C 206



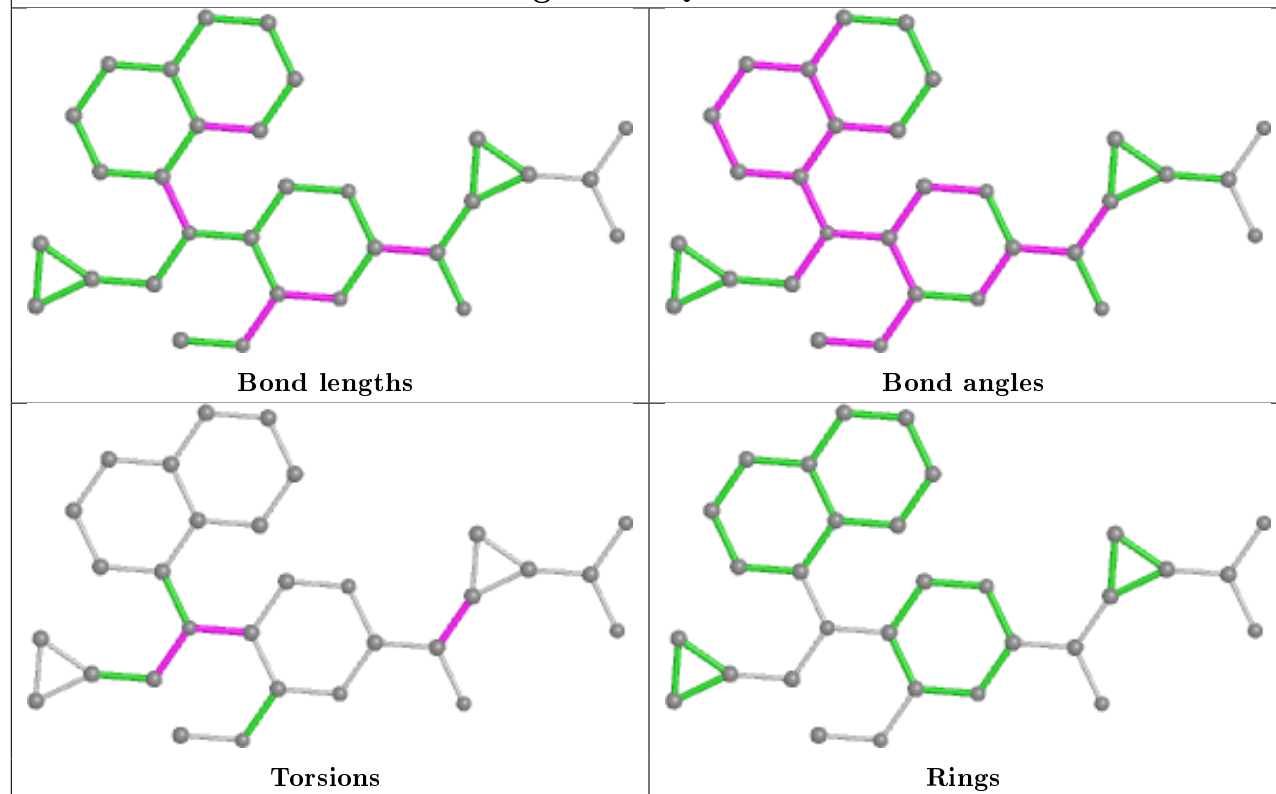




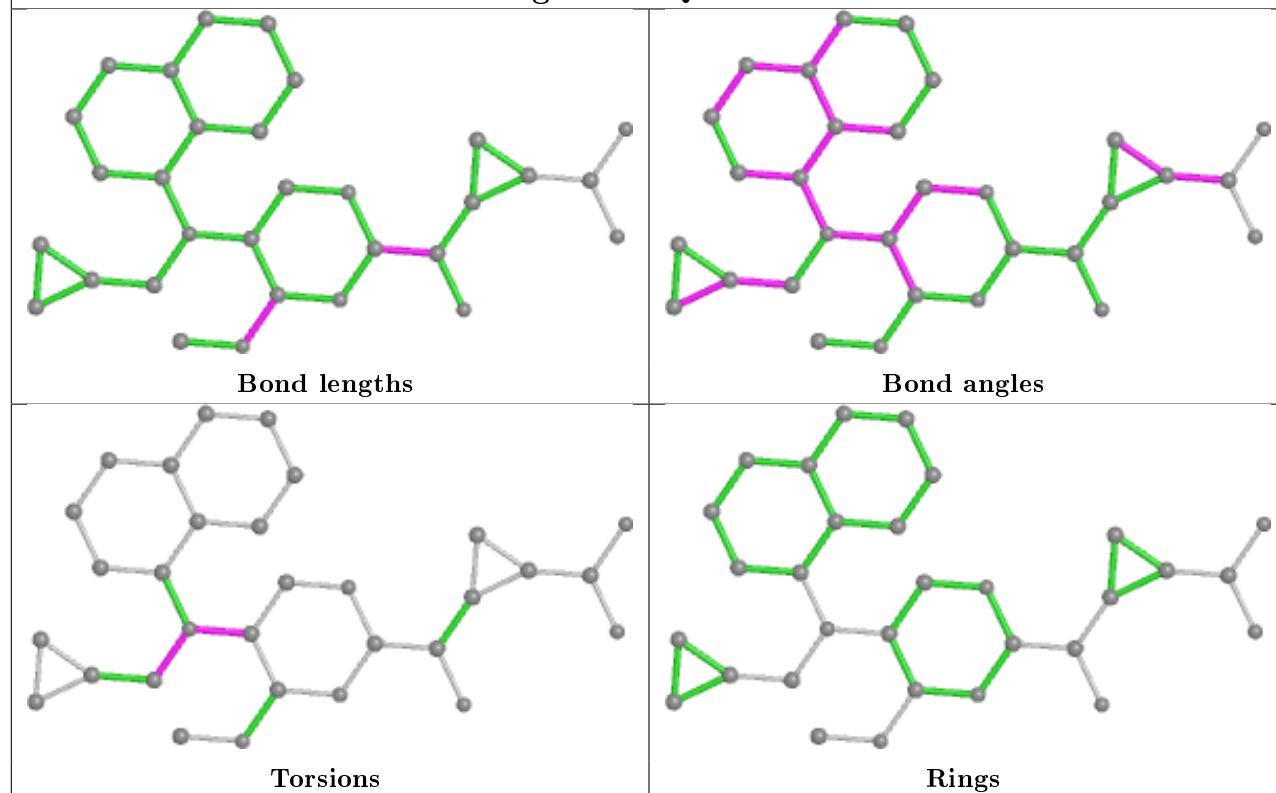


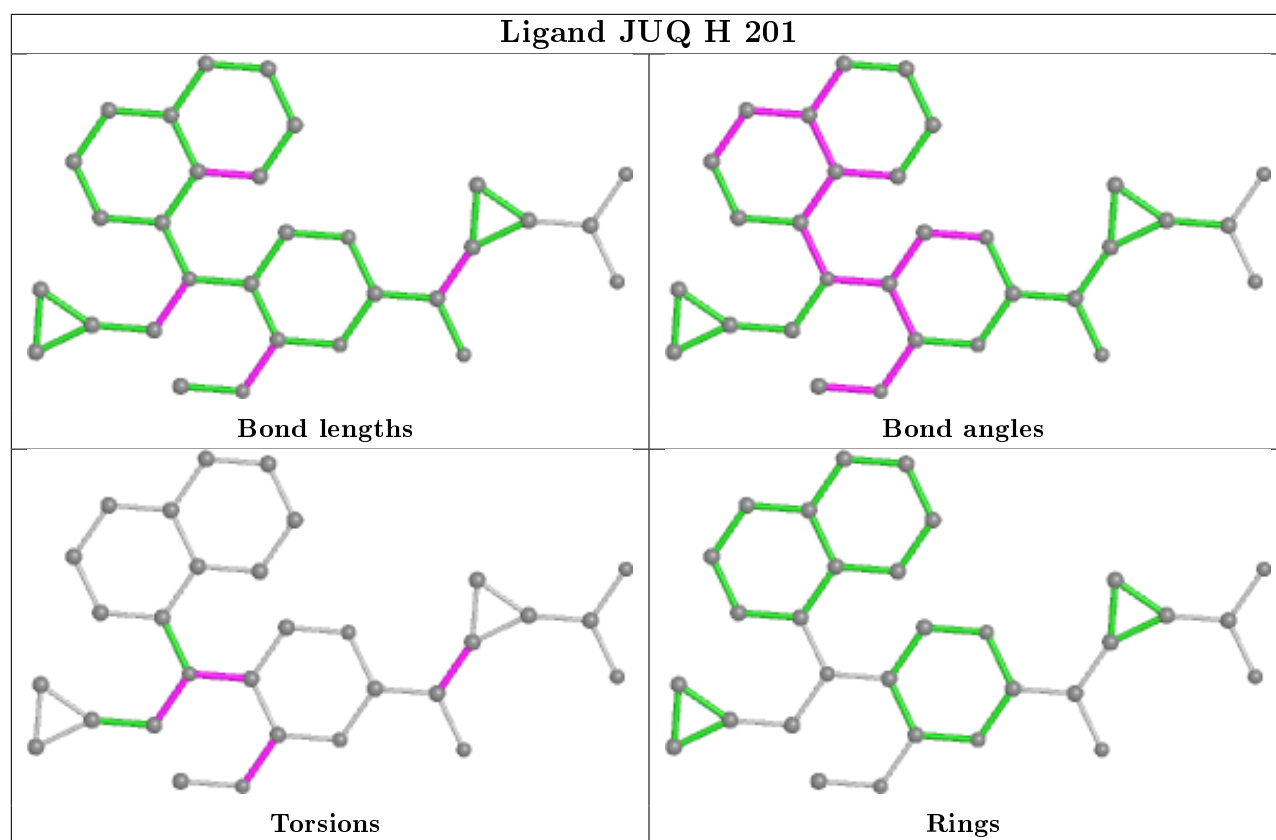


## Ligand JUQ B 201



## Ligand JUQ K 201





## 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	149/157 (94%)	0.54	1 (0%) 87 92	39, 51, 75, 111	0
1	B	149/157 (94%)	0.56	3 (2%) 65 75	37, 49, 77, 113	0
1	C	148/157 (94%)	0.50	2 (1%) 75 83	38, 52, 78, 110	0
1	D	150/157 (95%)	0.40	1 (0%) 87 92	40, 55, 86, 108	0
1	E	149/157 (94%)	0.43	0 100 100	37, 47, 74, 106	0
1	F	150/157 (95%)	0.49	6 (4%) 38 51	38, 52, 85, 129	0
1	G	149/157 (94%)	0.42	2 (1%) 77 84	39, 52, 87, 122	0
1	H	151/157 (96%)	0.58	7 (4%) 32 45	40, 60, 92, 111	0
1	I	148/157 (94%)	0.50	3 (2%) 65 75	38, 50, 73, 104	0
1	J	149/157 (94%)	0.66	5 (3%) 45 57	37, 52, 83, 114	0
1	K	150/157 (95%)	0.50	1 (0%) 87 92	37, 50, 80, 114	0
1	L	148/157 (94%)	0.87	19 (12%) 3 6	40, 58, 90, 116	0
All	All	1790/1884 (95%)	0.54	50 (2%) 53 64	37, 52, 86, 129	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	39	LEU	5.3
1	L	35	VAL	4.5
1	J	34	ARG	4.4
1	L	98	ALA	4.0
1	L	34	ARG	3.8

### 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 carbohydrates 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, 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	PLM	C	207	10/18	0.65	0.26	64,69,85,88	0
4	PLM	F	204	10/18	0.71	0.59	85,98,112,115	0
4	PLM	L	205	14/18	0.75	0.22	55,81,94,95	0
4	PLM	D	204	10/18	0.76	0.24	70,73,80,80	0
4	PLM	B	205	10/18	0.76	0.27	66,73,93,101	0
4	PLM	H	203	10/18	0.78	0.25	66,74,78,82	0
4	PLM	L	203	18/18	0.78	0.23	70,86,105,106	0
4	PLM	A	207	15/18	0.78	0.20	62,70,94,94	0
4	PLM	J	206	18/18	0.78	0.23	58,80,104,106	0
4	PLM	A	206	18/18	0.78	0.22	68,80,95,100	0
4	PLM	C	205	10/18	0.78	0.24	78,88,92,93	0
4	PLM	B	206	18/18	0.79	0.26	67,85,113,116	0
5	LMT	B	209	35/35	0.79	0.30	62,99,131,146	0
4	PLM	J	204	8/18	0.80	0.25	71,81,84,85	0
4	PLM	C	204	18/18	0.81	0.21	63,81,94,101	0
4	PLM	G	203	10/18	0.81	0.19	53,60,79,83	0
4	PLM	D	203	10/18	0.81	0.21	60,63,78,82	0
4	PLM	I	203	10/18	0.82	0.25	65,74,80,86	0
4	PLM	G	204	10/18	0.82	0.21	69,84,91,92	0
4	PLM	D	206	15/18	0.82	0.19	68,78,101,103	0
4	PLM	A	205	10/18	0.83	0.25	72,76,90,93	0
4	PLM	H	202	12/18	0.83	0.23	68,73,90,95	0
4	PLM	F	205	10/18	0.83	0.32	66,75,79,79	0
4	PLM	B	203	12/18	0.84	0.24	60,68,93,94	0
4	PLM	I	204	18/18	0.84	0.23	69,81,104,108	0
4	PLM	L	206	10/18	0.84	0.22	59,74,81,83	0
4	PLM	J	205	10/18	0.84	0.23	55,67,72,78	0
4	PLM	B	207	10/18	0.84	0.22	69,88,96,100	0
4	PLM	F	203	10/18	0.85	0.15	72,86,98,100	0
4	PLM	E	202	10/18	0.85	0.19	71,76,85,89	0
4	PLM	J	207	15/18	0.86	0.21	60,74,85,88	0
4	PLM	J	203	10/18	0.86	0.24	67,69,75,77	0

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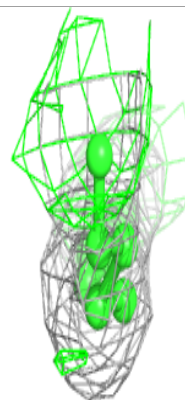
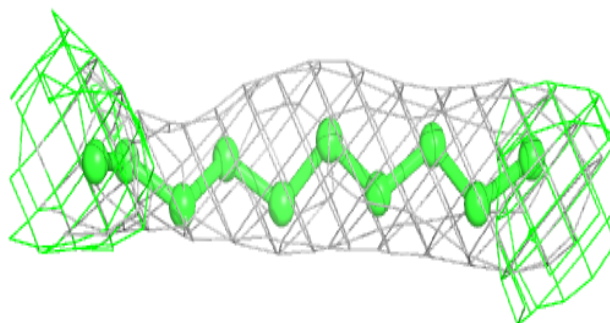
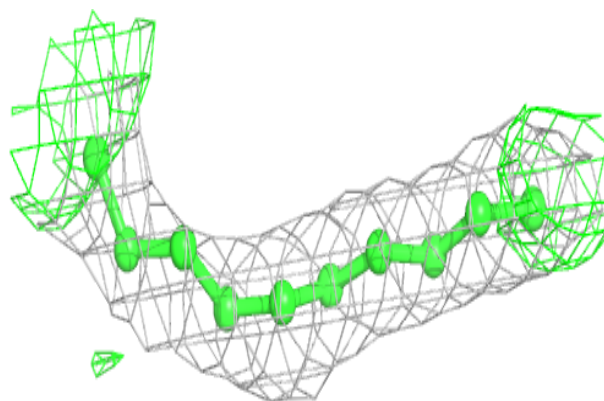
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PLM	A	204	18/18	0.87	0.17	57,78,95,102	0
4	PLM	A	203	10/18	0.87	0.18	61,66,69,73	0
4	PLM	E	203	7/18	0.87	0.21	68,73,78,79	0
4	PLM	G	205	15/18	0.88	0.21	62,80,103,104	0
4	PLM	F	202	8/18	0.89	0.27	66,69,93,105	0
4	PLM	D	205	18/18	0.89	0.19	65,81,95,95	0
4	PLM	L	204	8/18	0.90	0.22	52,64,77,81	0
4	PLM	B	204	10/18	0.90	0.27	77,84,106,108	0
4	PLM	C	206	10/18	0.90	0.20	62,69,76,79	0
4	PLM	B	208	10/18	0.91	0.20	64,72,74,80	0
4	PLM	E	204	10/18	0.91	0.21	62,72,92,93	0
4	PLM	C	203	10/18	0.91	0.20	63,77,89,91	0
2	JUQ	C	201	31/31	0.94	0.17	39,50,57,60	0
2	JUQ	A	201	31/31	0.95	0.17	40,49,61,62	0
2	JUQ	D	201	31/31	0.95	0.15	43,57,64,67	0
2	JUQ	J	201	31/31	0.95	0.16	39,57,65,69	0
2	JUQ	B	201	31/31	0.95	0.16	35,46,53,56	0
2	JUQ	H	201	31/31	0.95	0.17	47,61,67,71	0
2	JUQ	L	201	31/31	0.96	0.15	47,57,67,70	0
2	JUQ	F	201	31/31	0.96	0.15	43,47,54,61	0
2	JUQ	K	201	31/31	0.96	0.16	44,50,62,63	0
2	JUQ	G	201	31/31	0.96	0.16	38,46,53,55	0
2	JUQ	I	201	31/31	0.97	0.16	46,51,57,63	0
2	JUQ	E	201	31/31	0.97	0.16	37,45,52,56	0
3	NI	B	202	1/1	0.99	0.17	56,56,56,56	0
3	NI	A	202	1/1	0.99	0.20	54,54,54,54	0
3	NI	C	202	1/1	0.99	0.20	58,58,58,58	0
3	NI	L	202	1/1	0.99	0.15	60,60,60,60	0
3	NI	J	202	1/1	0.99	0.21	53,53,53,53	0
3	NI	D	202	1/1	0.99	0.20	54,54,54,54	0
3	NI	I	202	1/1	0.99	0.17	61,61,61,61	0
3	NI	G	202	1/1	1.00	0.20	51,51,51,51	0

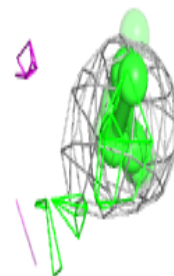
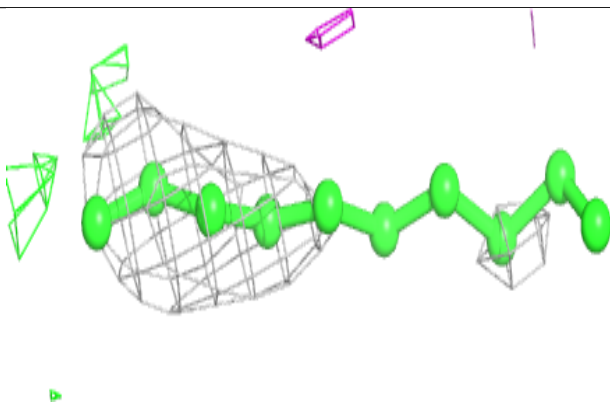
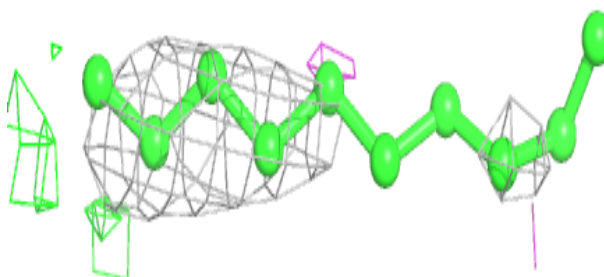
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PLM C 207:**

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

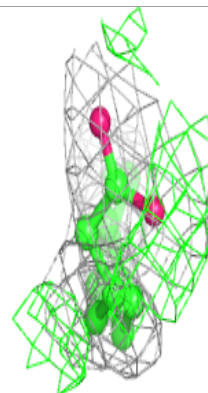
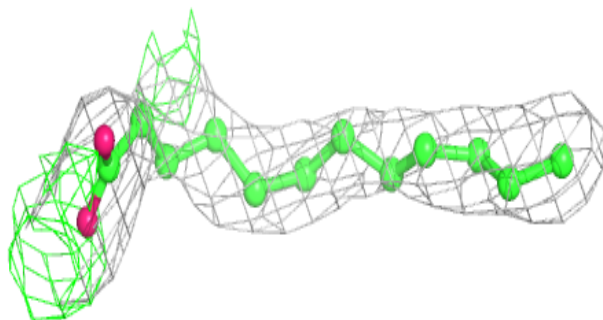
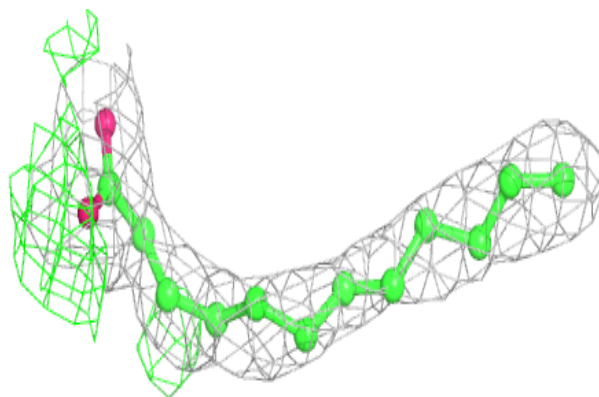
**Electron density around PLM F 204:**

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

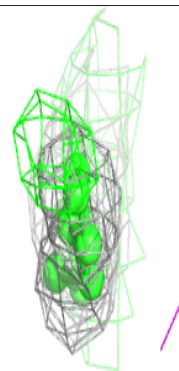
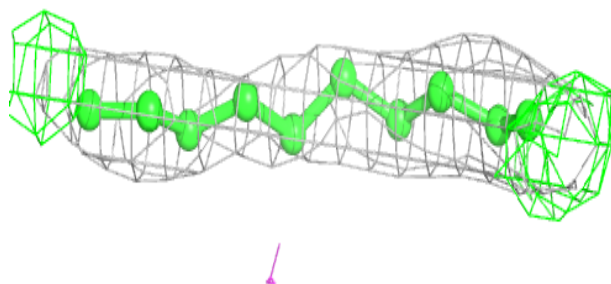
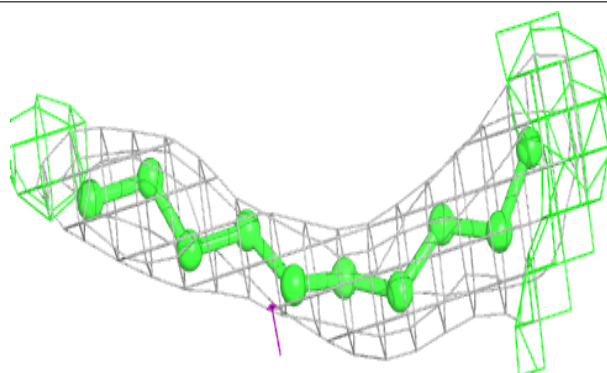


**Electron density around PLM L 205:**

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

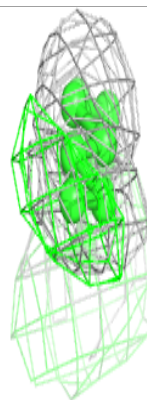
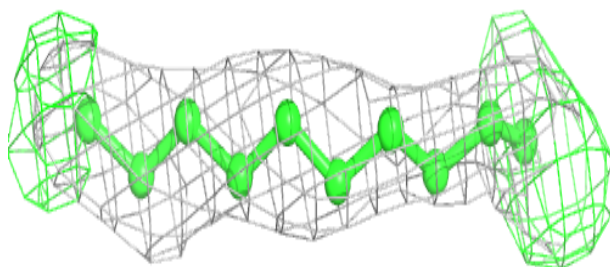
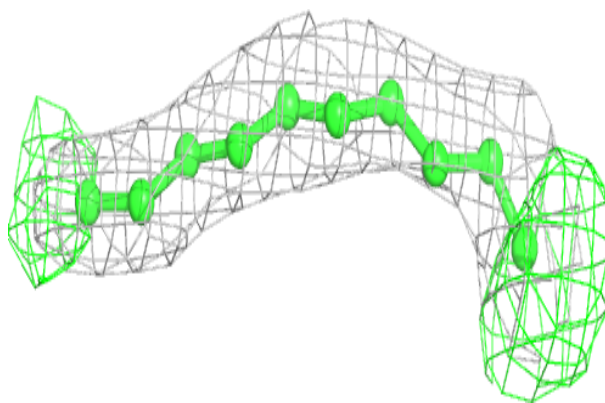
**Electron density around PLM D 204:**

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

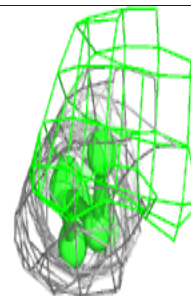
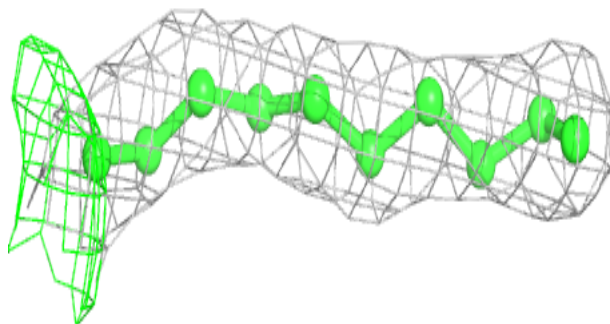
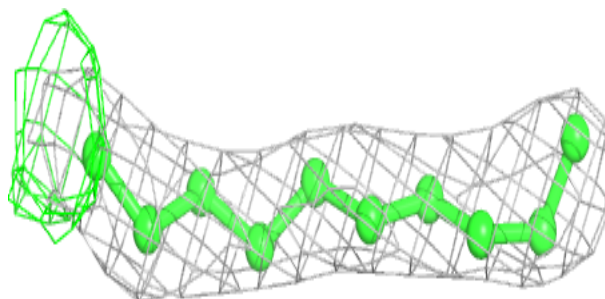


**Electron density around PLM B 205:**

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

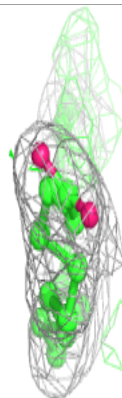
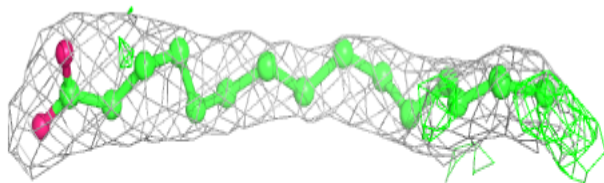
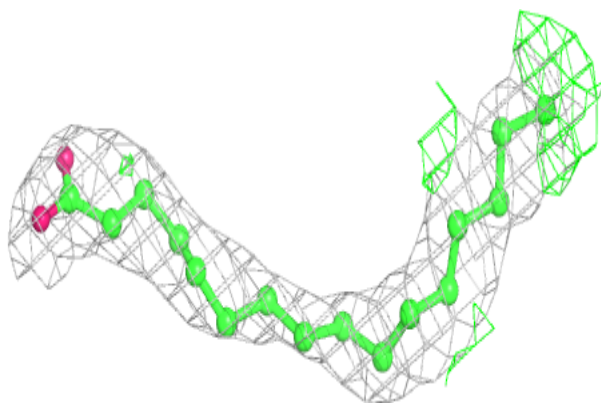
**Electron density around PLM H 203:**

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

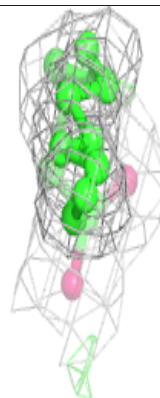
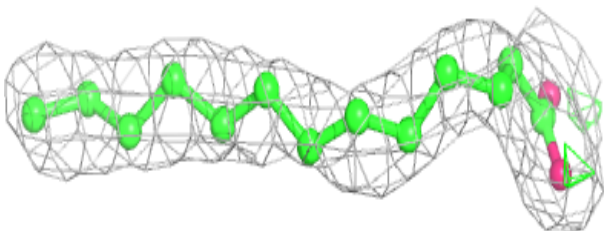
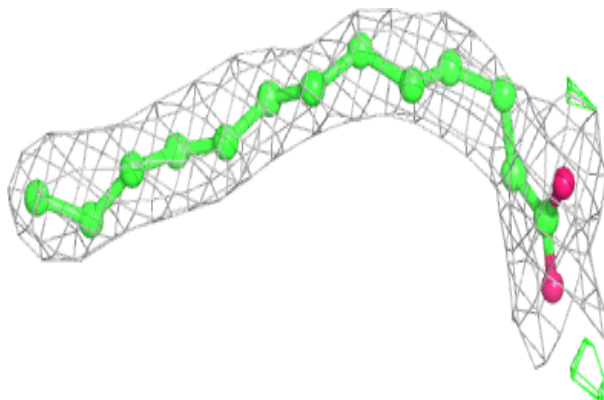


**Electron density around PLM L 203:**

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

**Electron density around PLM A 207:**

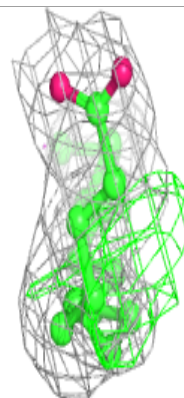
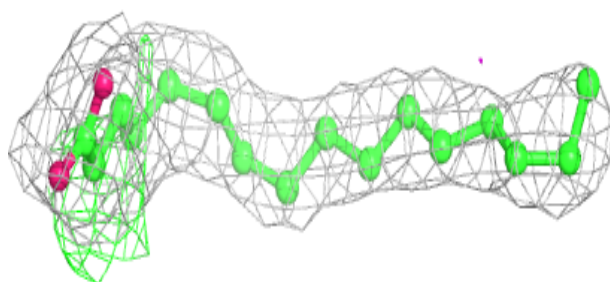
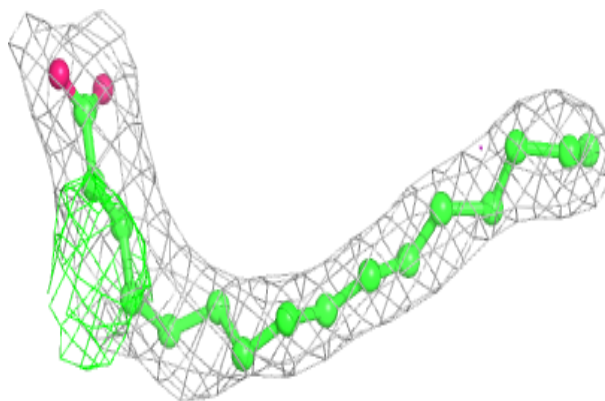
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



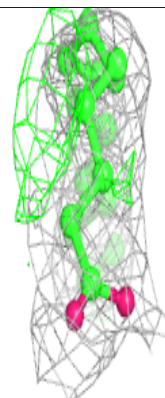
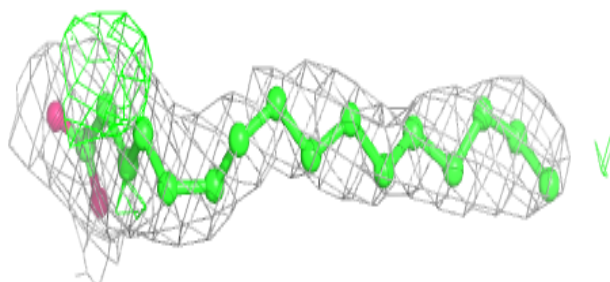
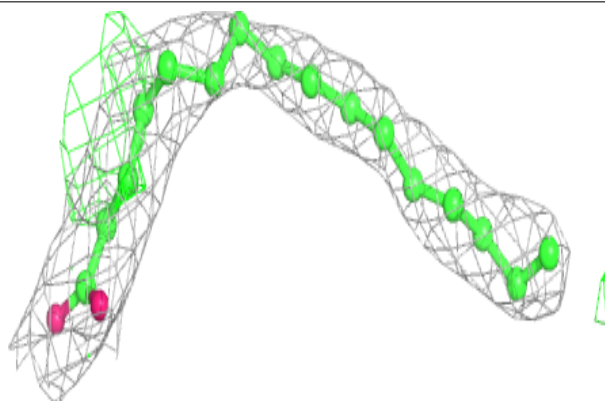


**Electron density around PLM J 206:**

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

**Electron density around PLM A 206:**

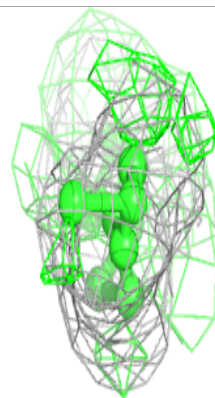
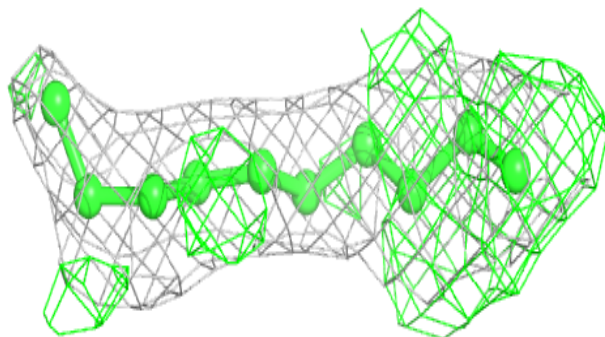
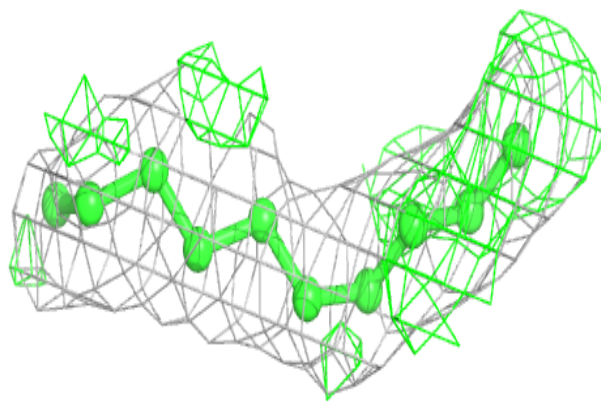
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



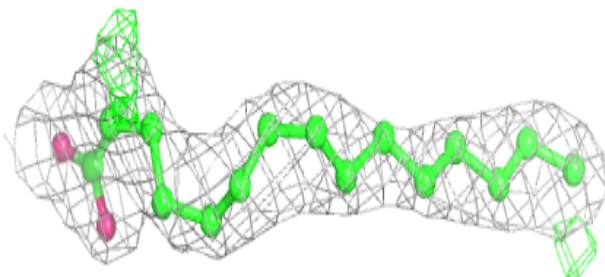
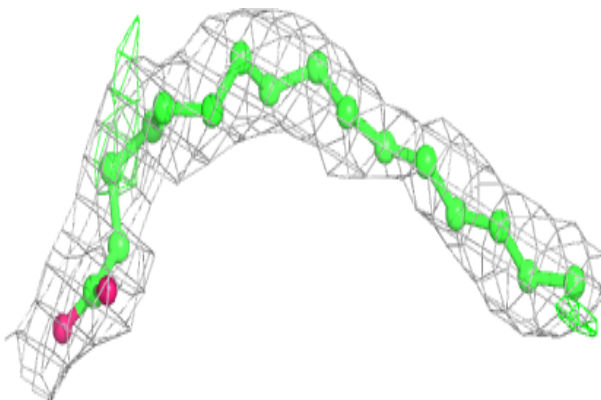


**Electron density around PLM C 205:**

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

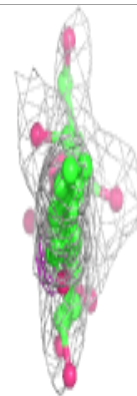
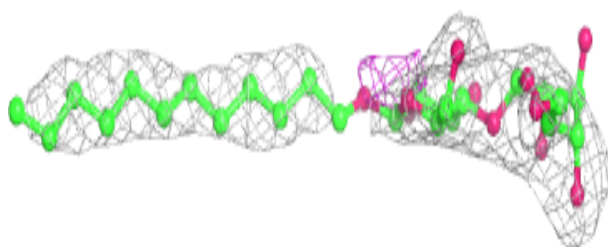
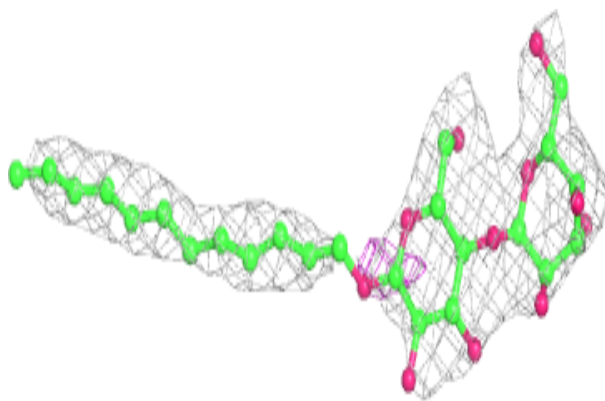
**Electron density around PLM B 206:**

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

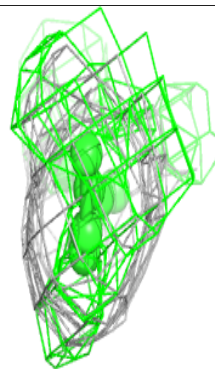
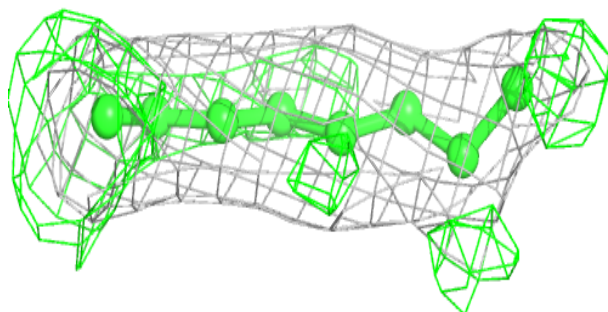
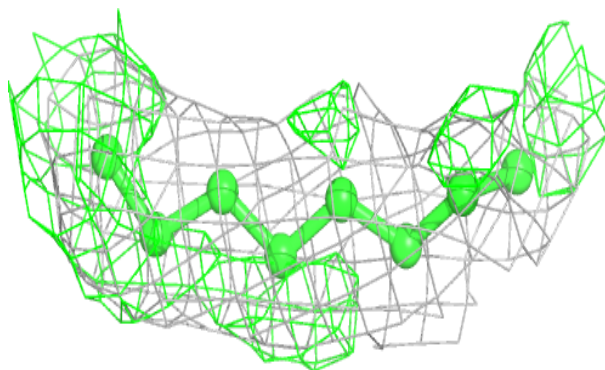


**Electron density around LMT B 209:**

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

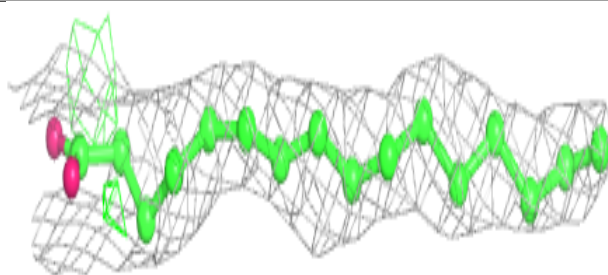
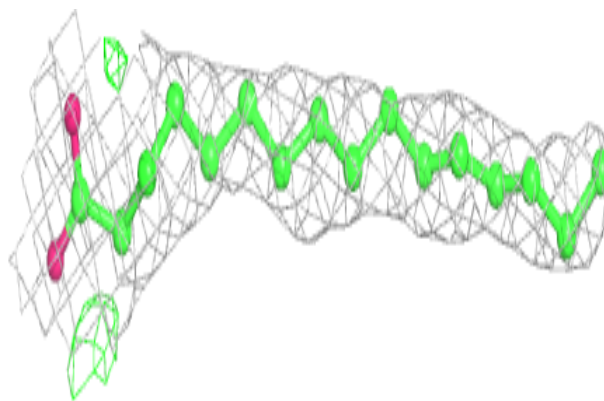
**Electron density around PLM J 204:**

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

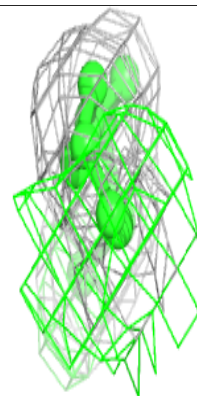
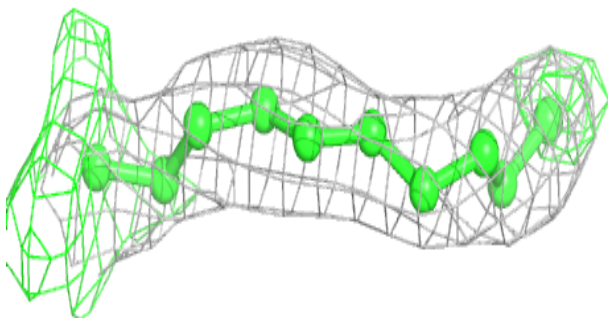
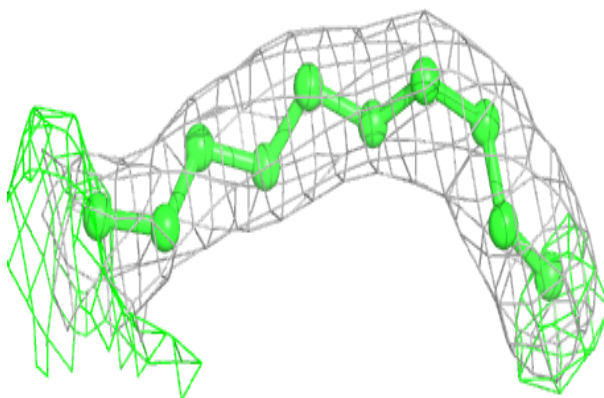


**Electron density around PLM C 204:**

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

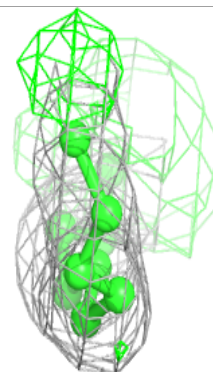
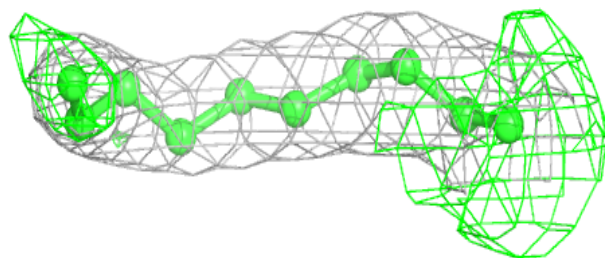
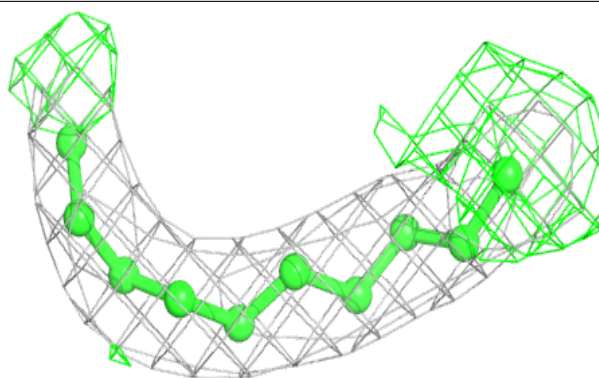
**Electron density around PLM G 203:**

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

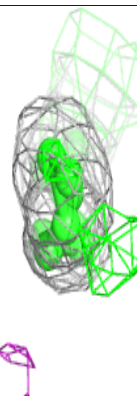
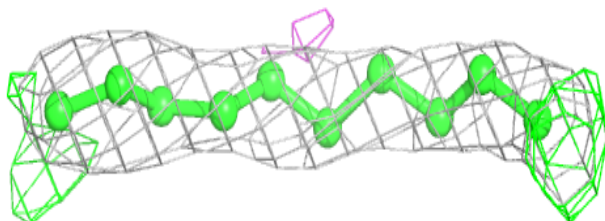
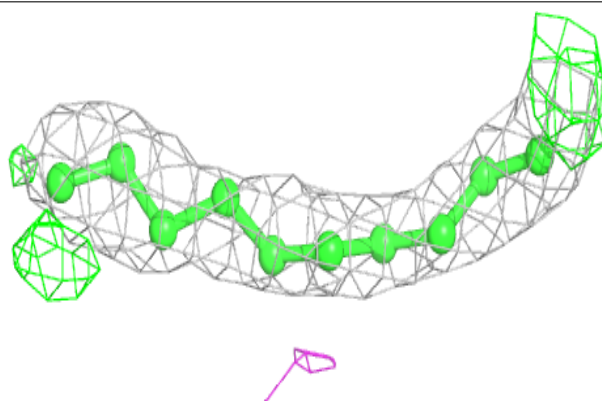


**Electron density around PLM D 203:**

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

**Electron density around PLM I 203:**

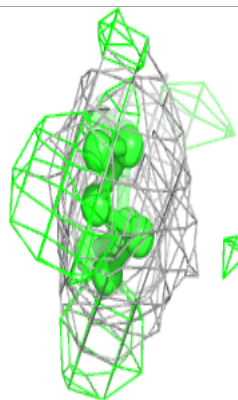
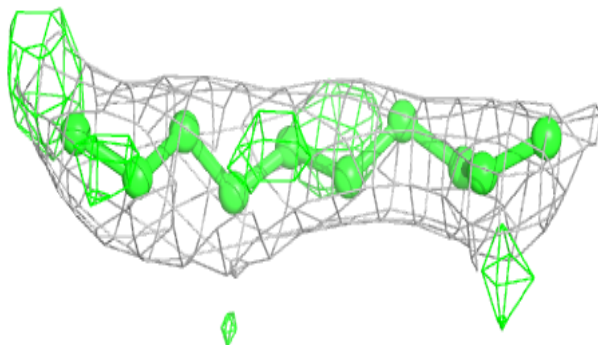
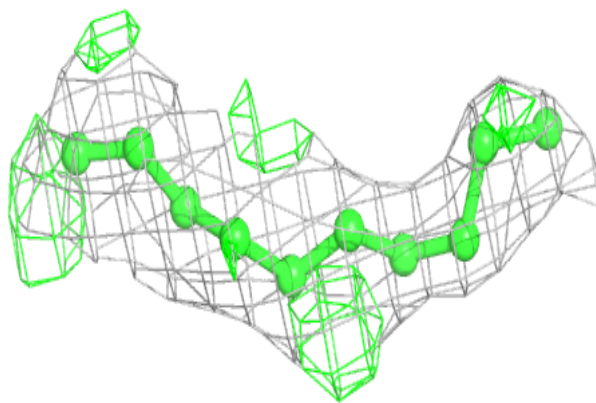
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



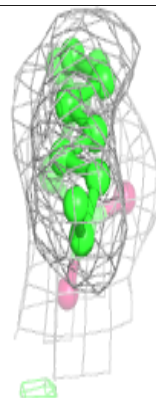
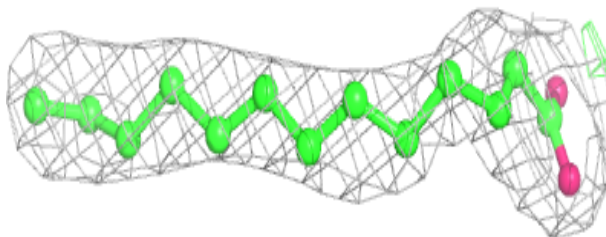
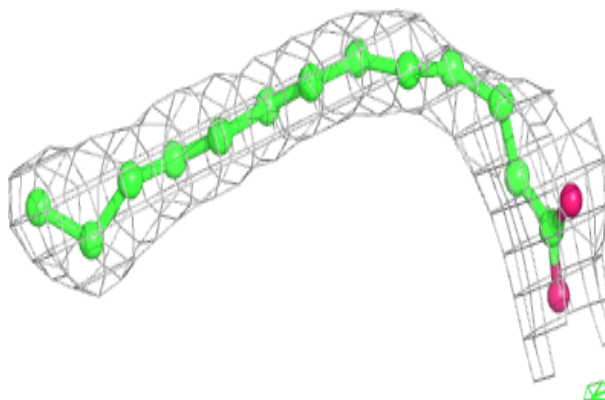


**Electron density around PLM G 204:**

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

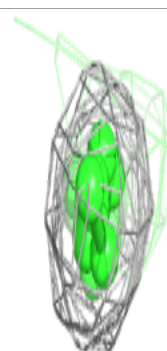
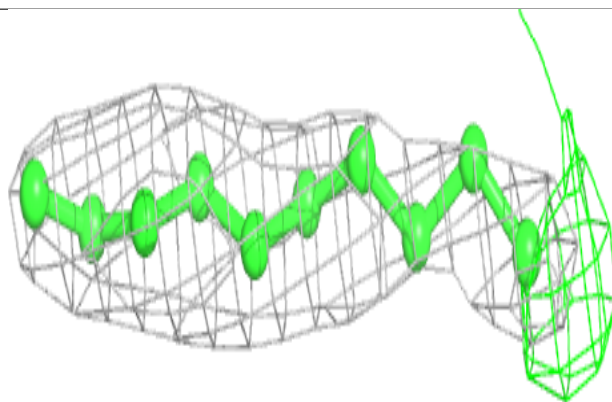
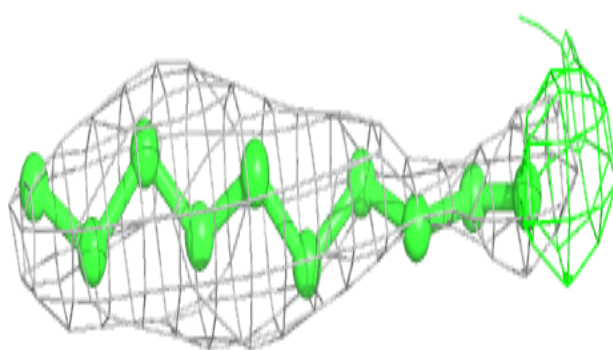
**Electron density around PLM D 206:**

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

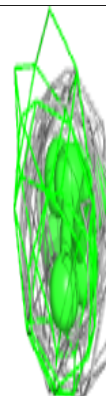
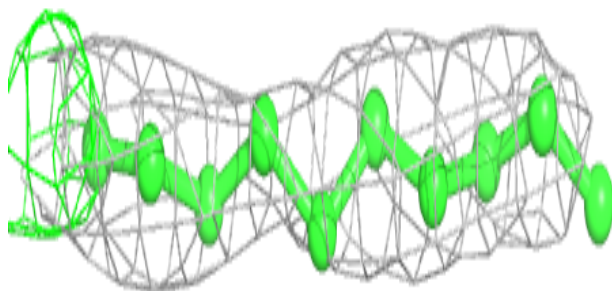
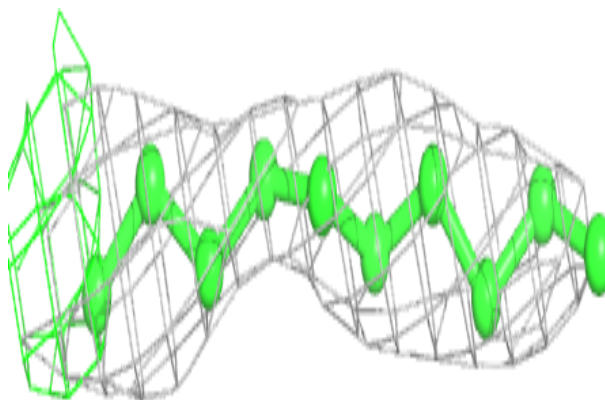


**Electron density around PLM A 205:**

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

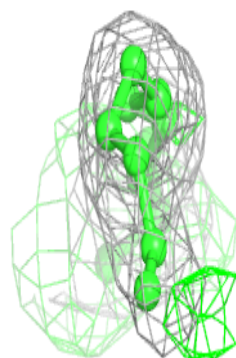
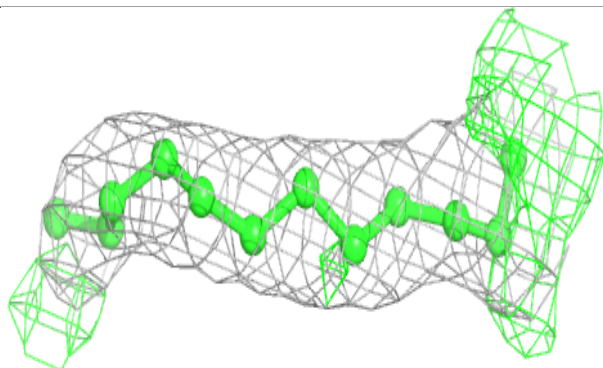
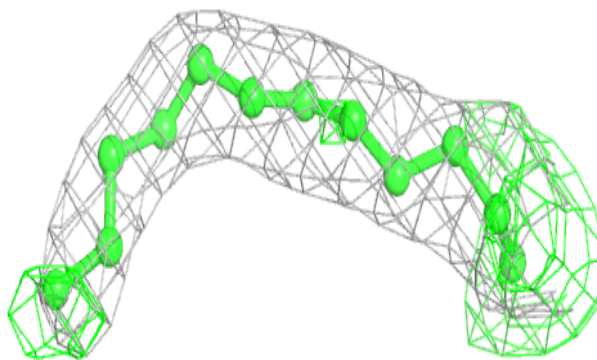
**Electron density around PLM F 205:**

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

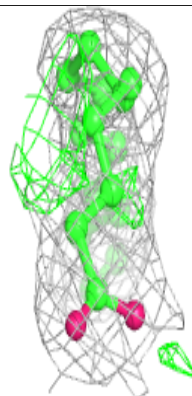
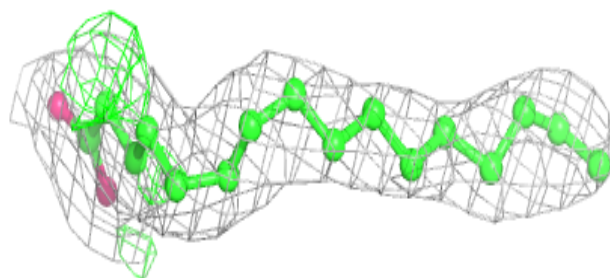
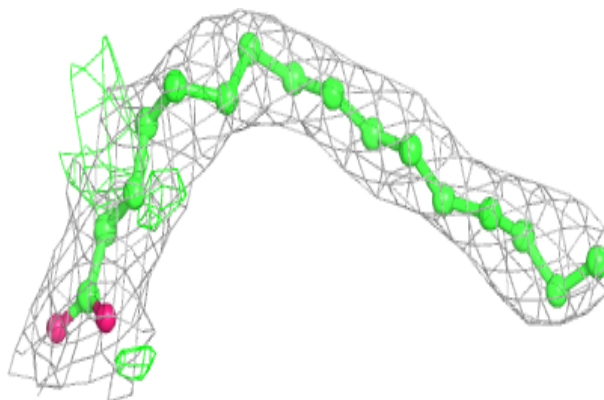


**Electron density around PLM B 203:**

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

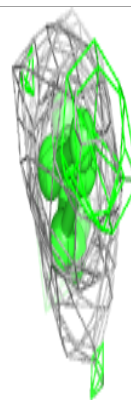
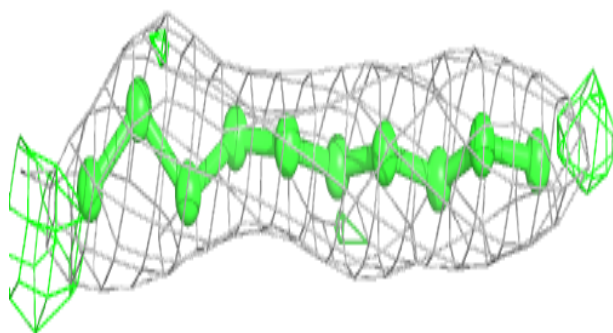
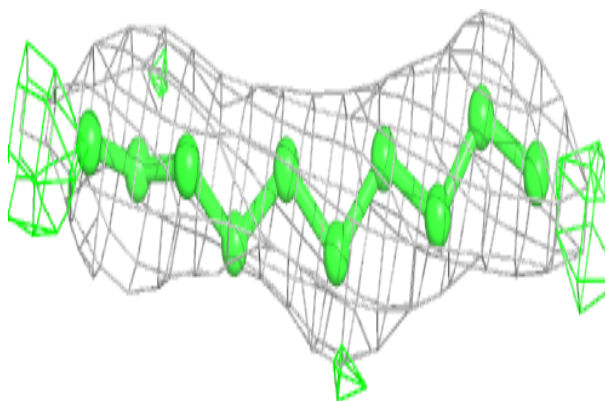
**Electron density around PLM I 204:**

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

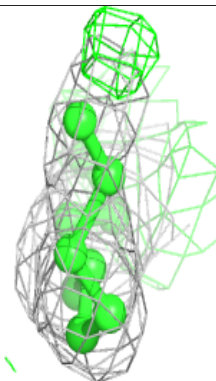
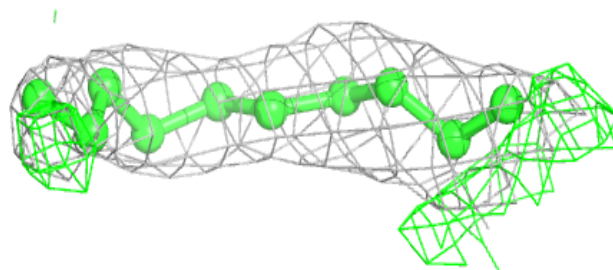
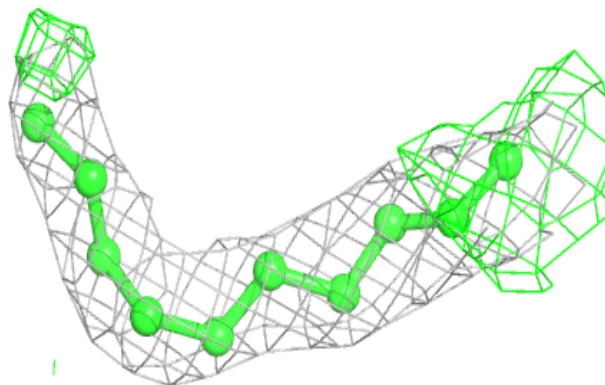


**Electron density around PLM L 206:**

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

**Electron density around PLM J 205:**

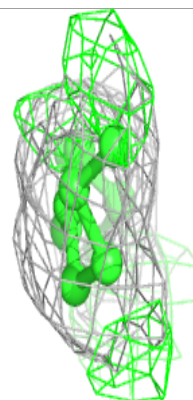
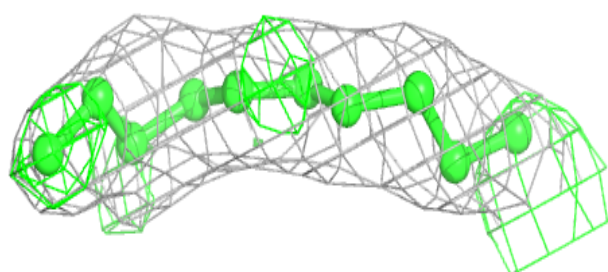
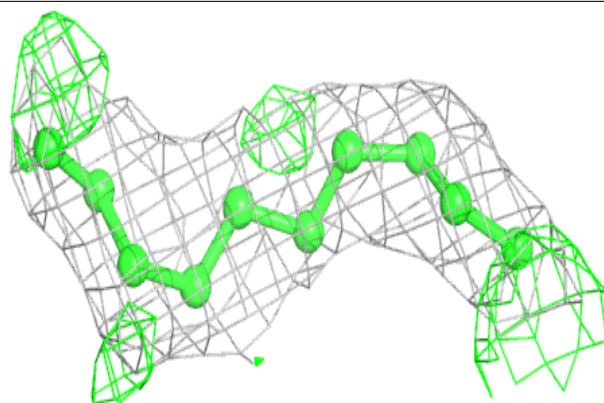
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



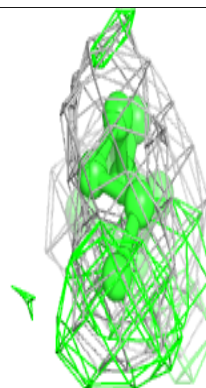
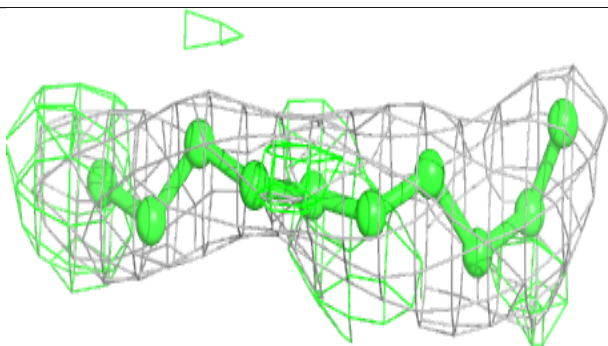
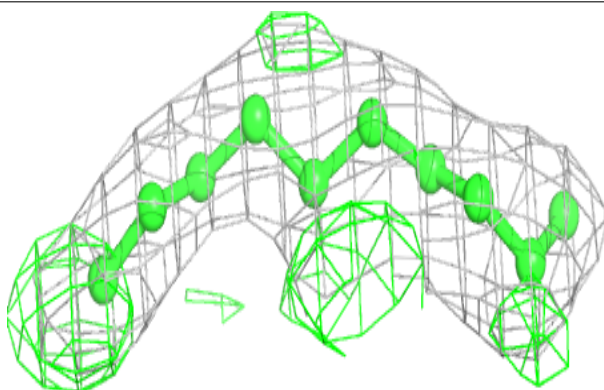


**Electron density around PLM B 207:**

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

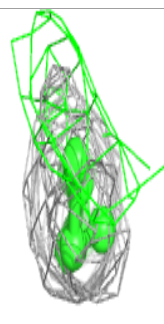
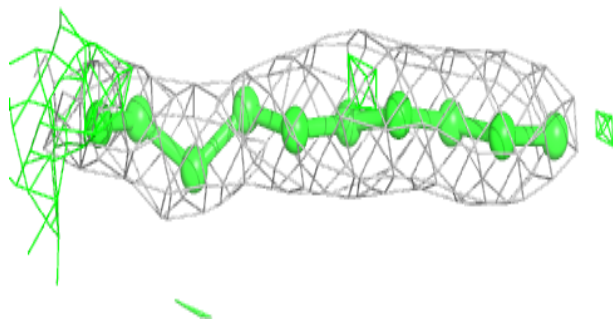
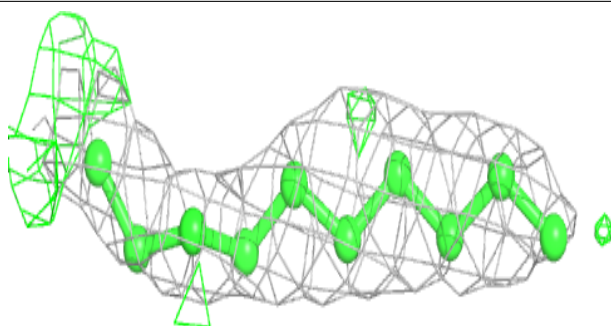
**Electron density around PLM F 203:**

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

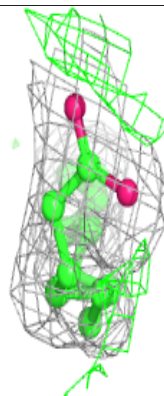
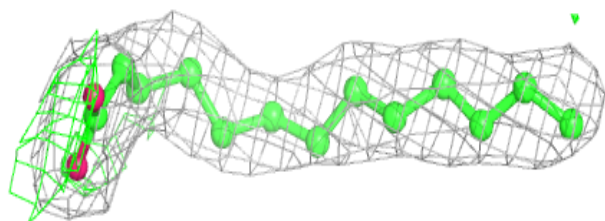
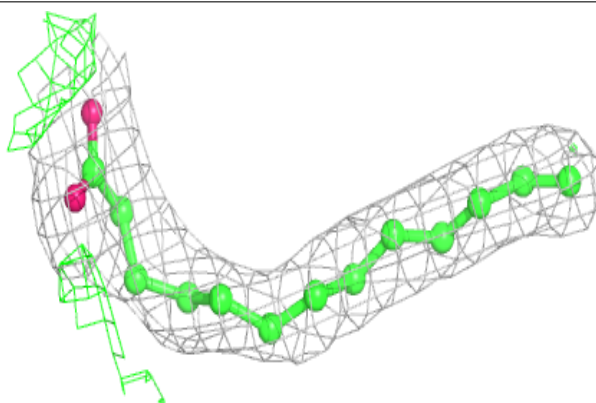


**Electron density around PLM E 202:**

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

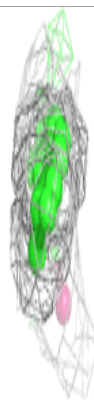
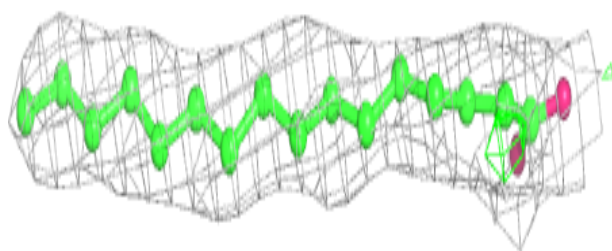
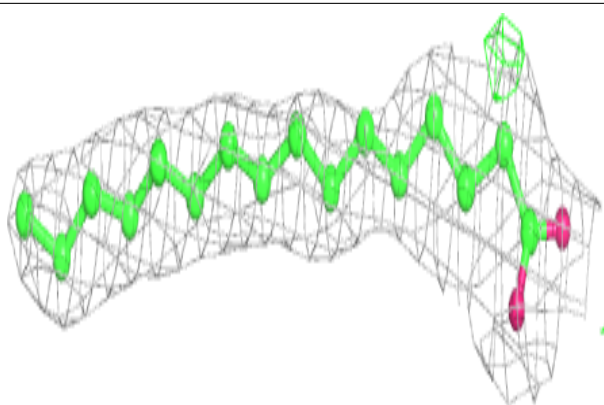
**Electron density around PLM J 207:**

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

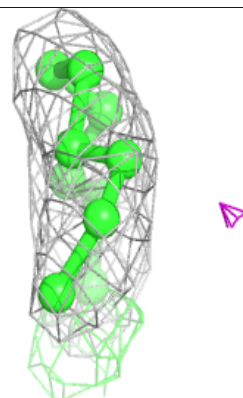
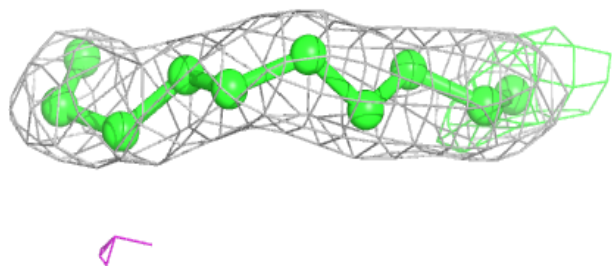
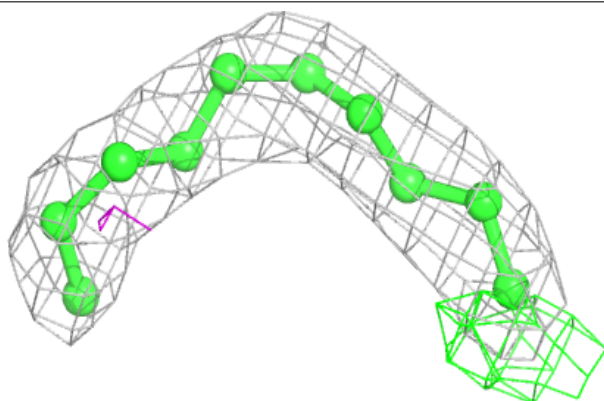


**Electron density around PLM A 204:**

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

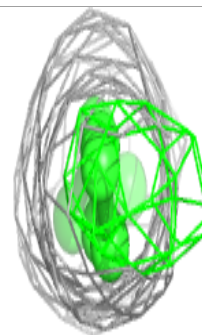
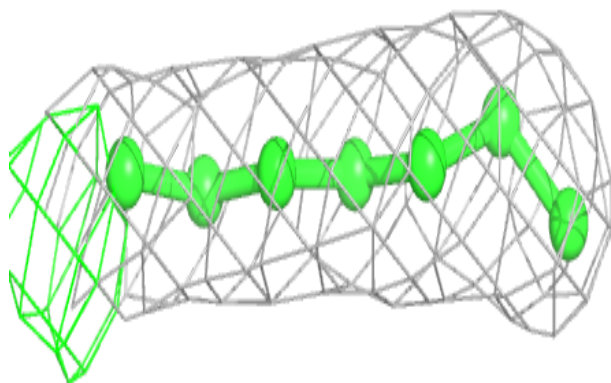
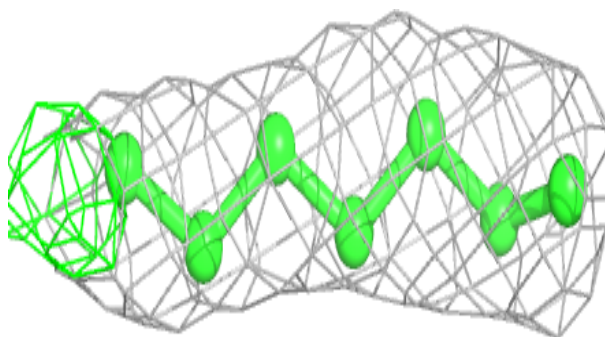
**Electron density around PLM A 203:**

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

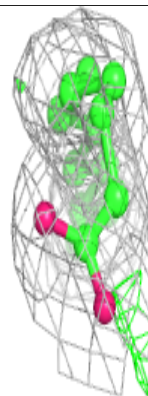
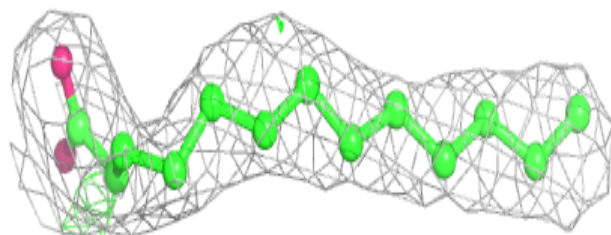
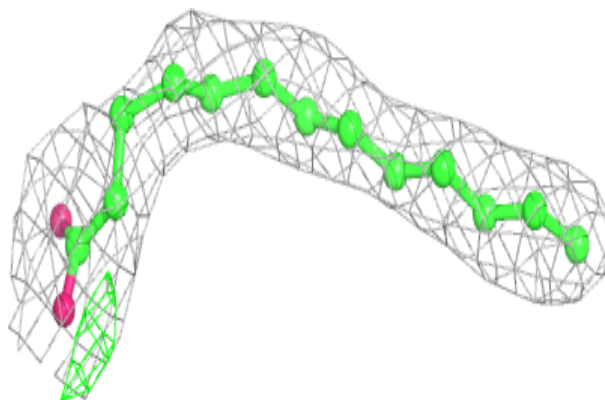


**Electron density around PLM E 203:**

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

**Electron density around PLM G 205:**

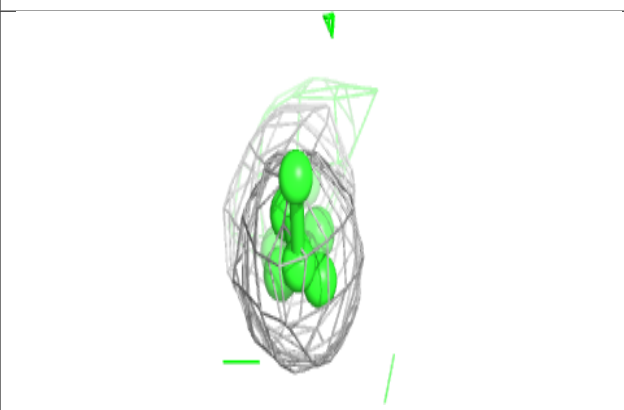
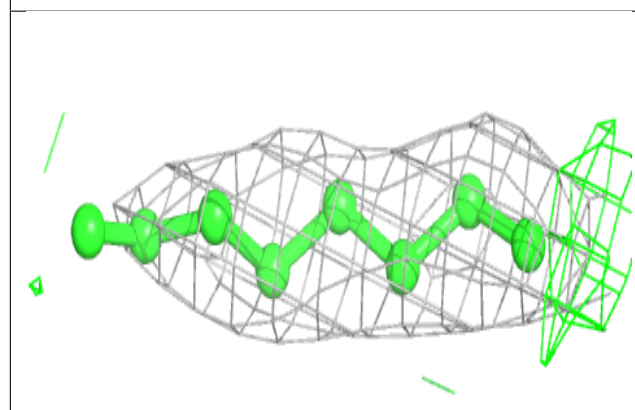
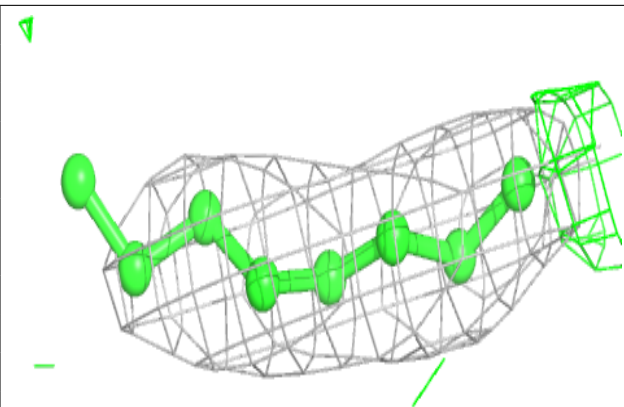
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



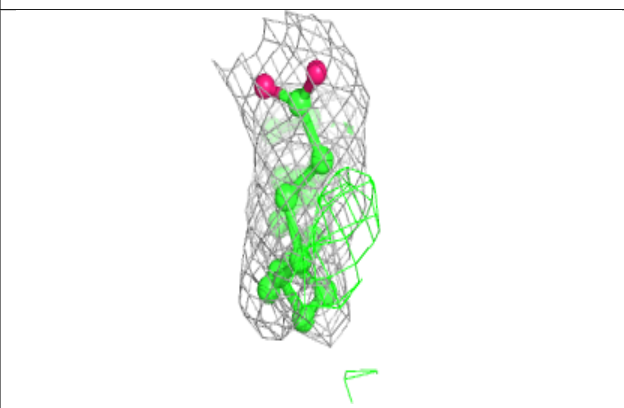
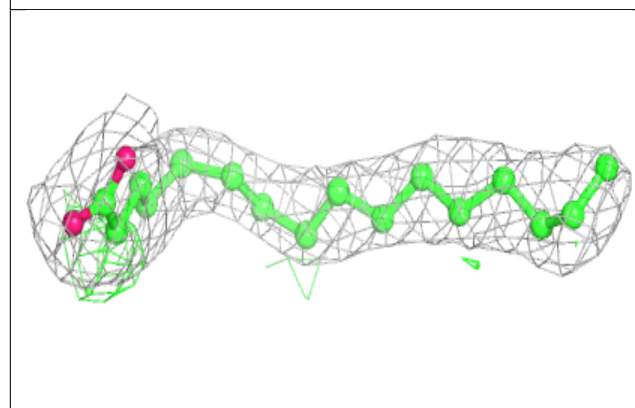
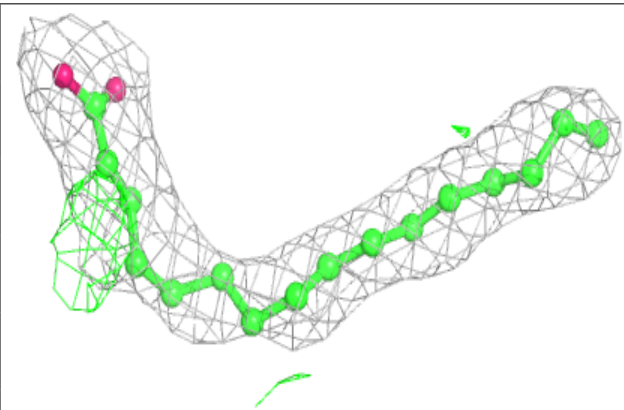


**Electron density around PLM F 202:**

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

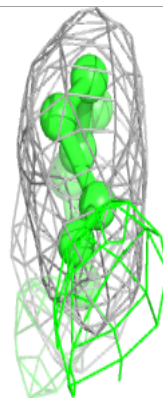
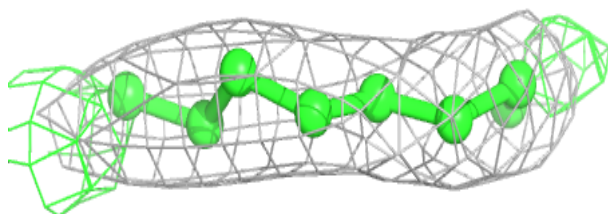
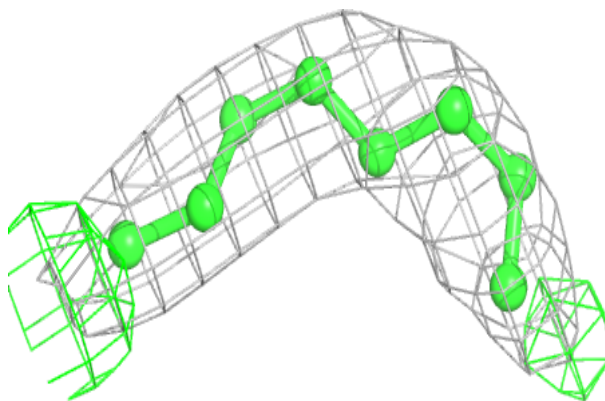
**Electron density around PLM D 205:**

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

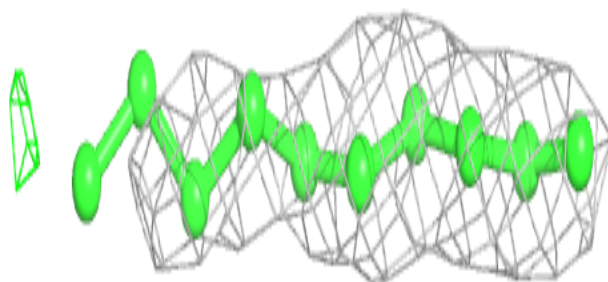
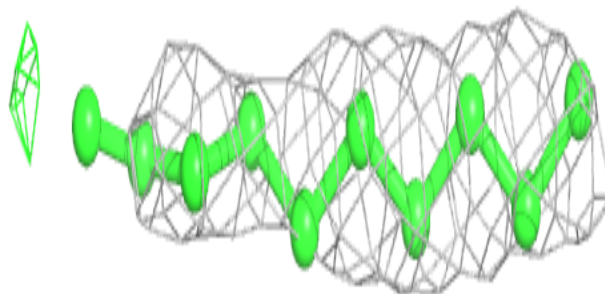


**Electron density around PLM L 204:**

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

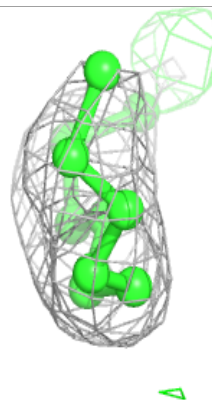
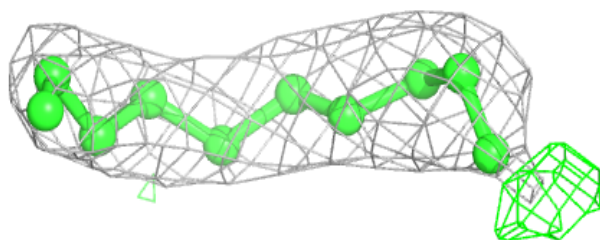
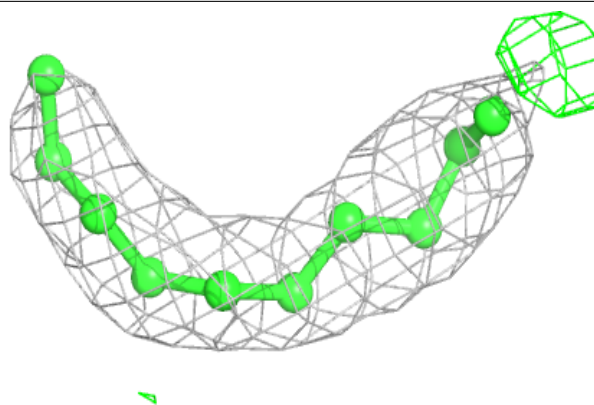
**Electron density around PLM B 204:**

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

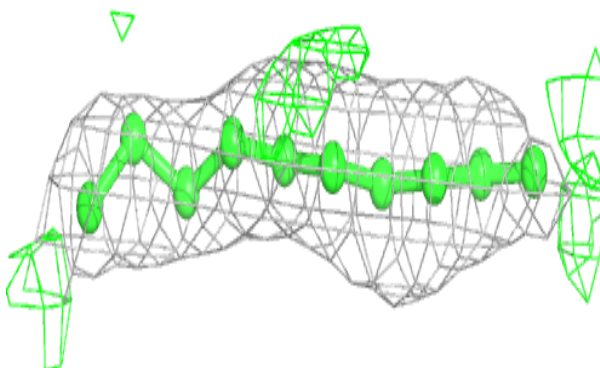
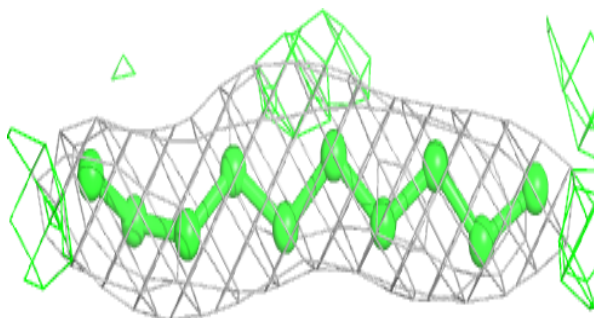


**Electron density around PLM C 206:**

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

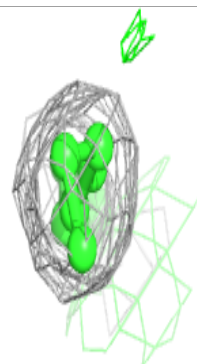
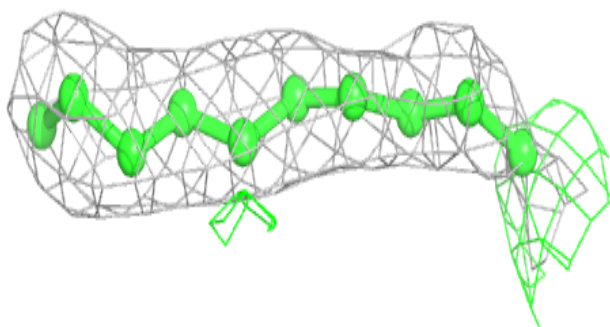
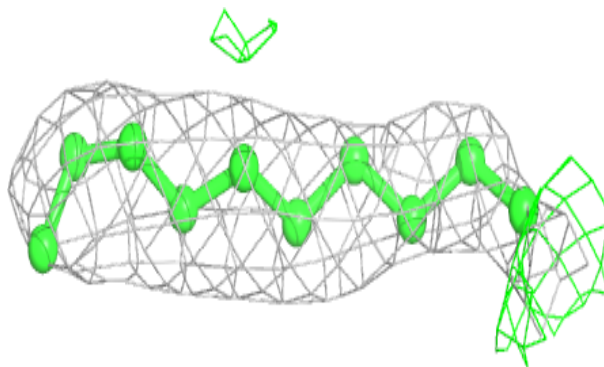
**Electron density around PLM B 208:**

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

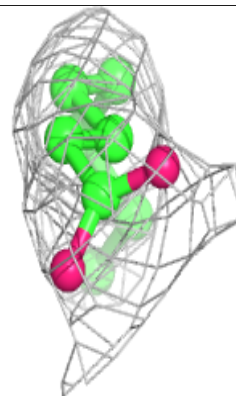
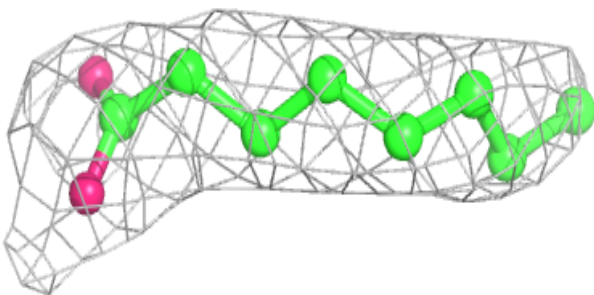
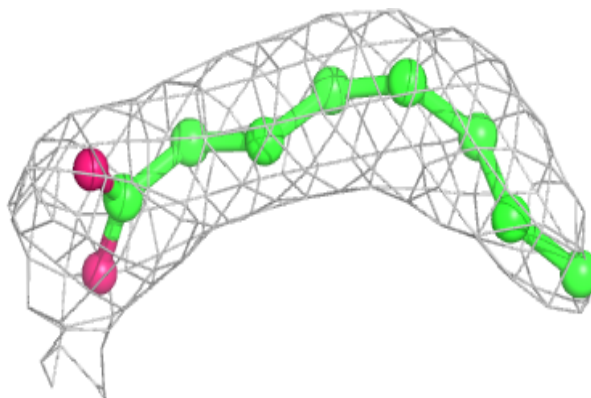


**Electron density around PLM E 204:**

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

**Electron density around PLM C 203:**

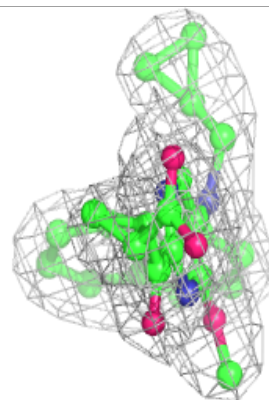
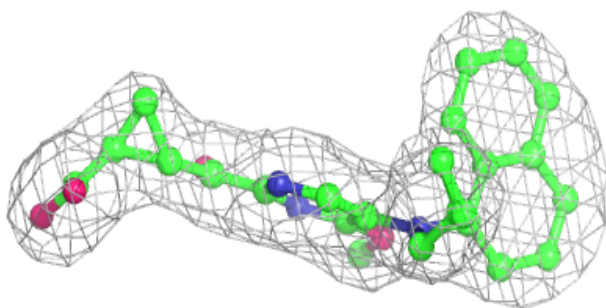
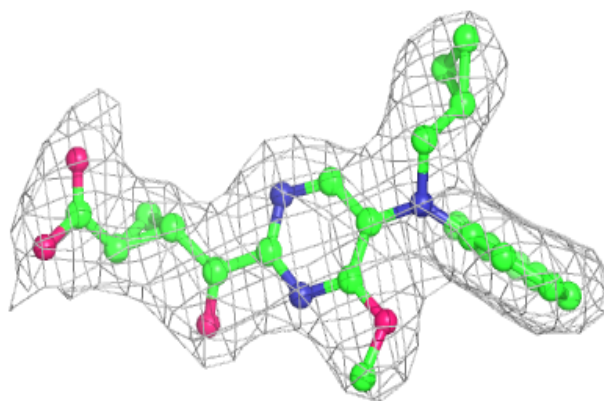
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



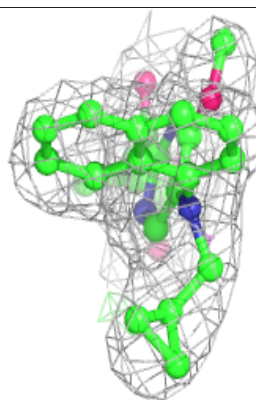
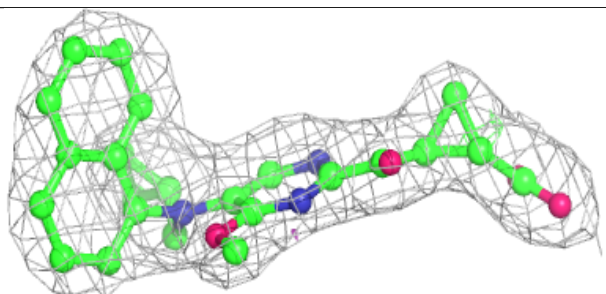
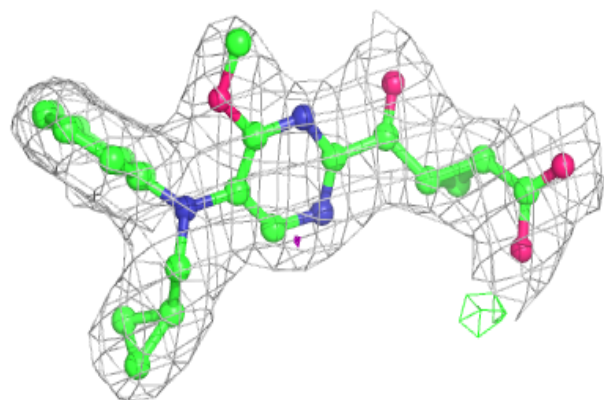


**Electron density around JUQ C 201:**

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

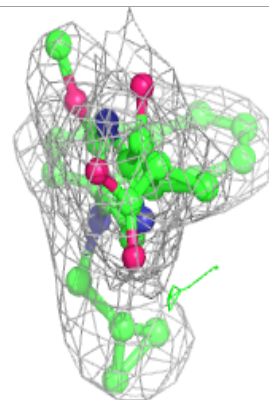
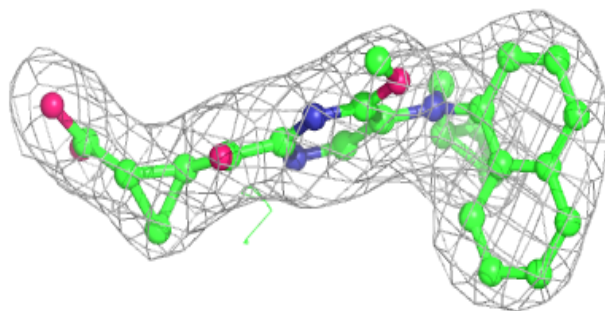
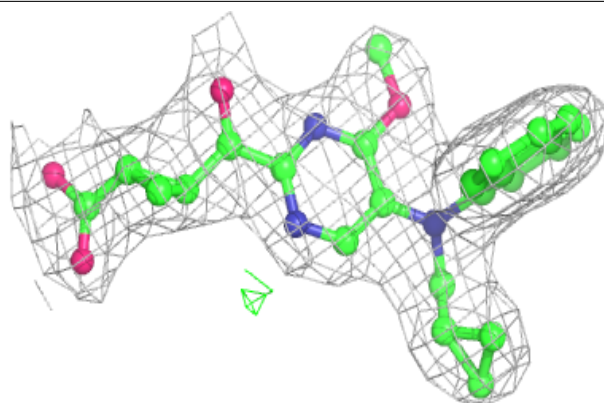
**Electron density around JUQ A 201:**

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

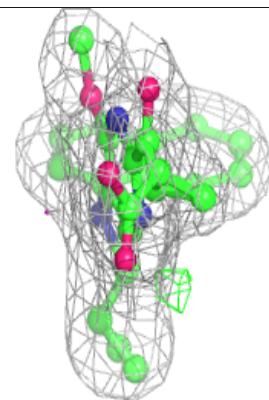
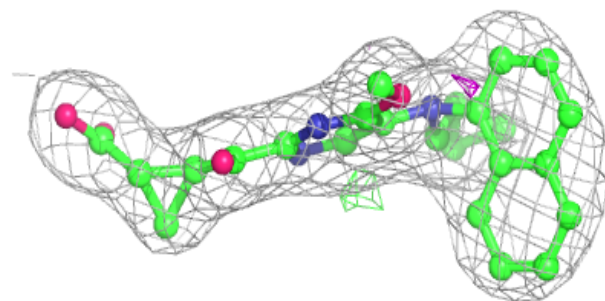
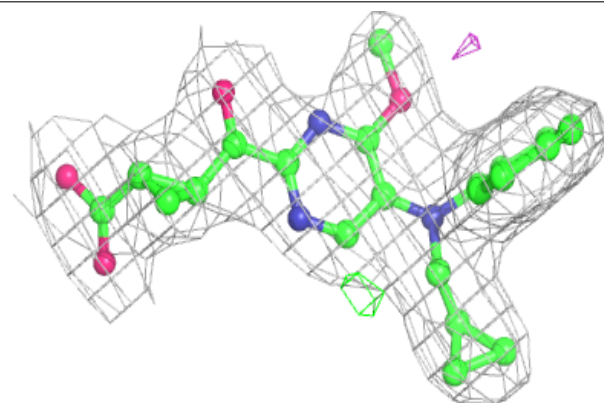


**Electron density around JUQ D 201:**

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

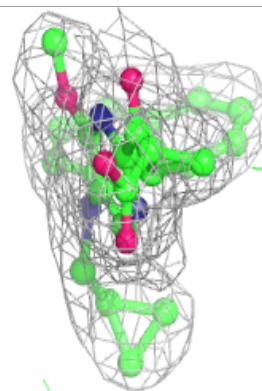
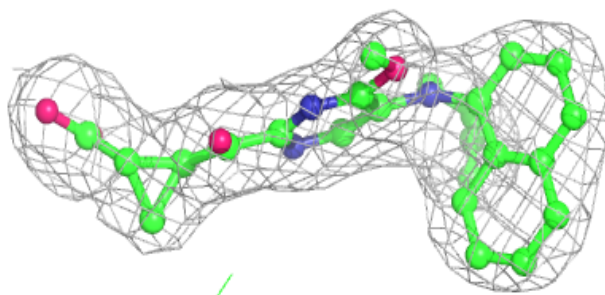
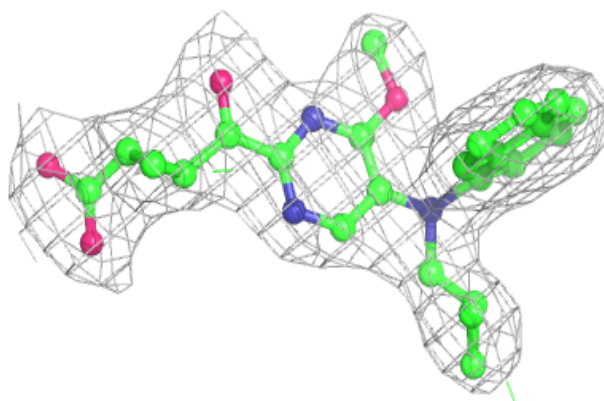
**Electron density around JUQ J 201:**

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

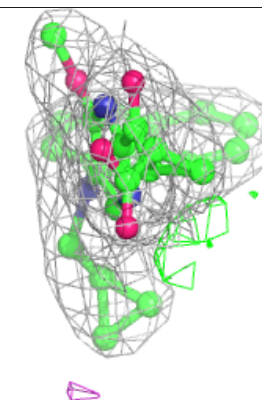
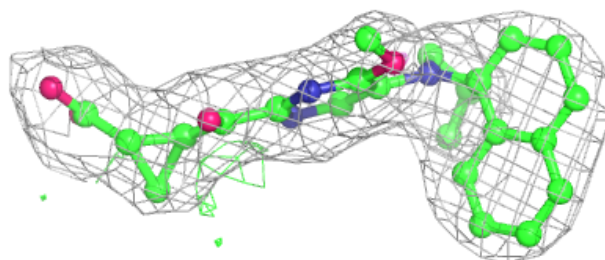
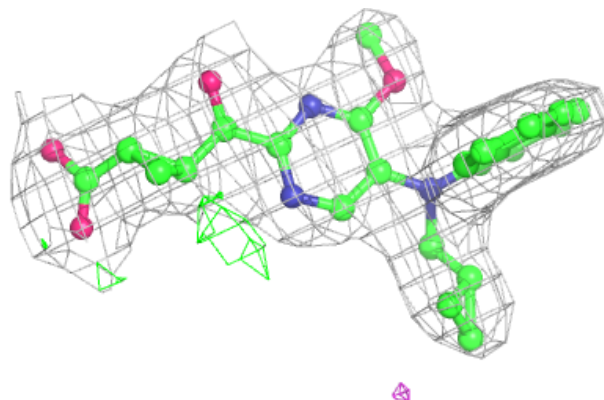


**Electron density around JUQ B 201:**

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

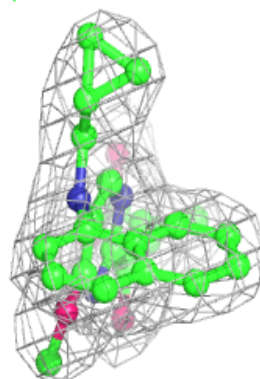
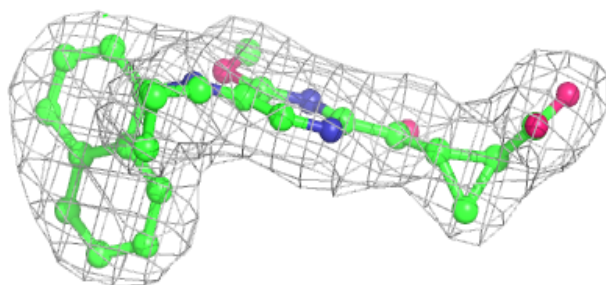
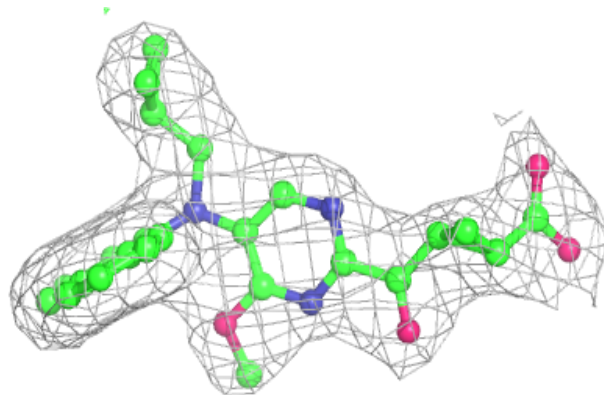
**Electron density around JUQ H 201:**

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

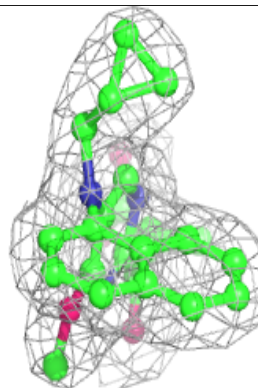
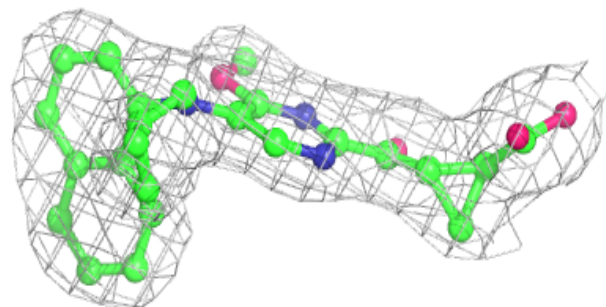
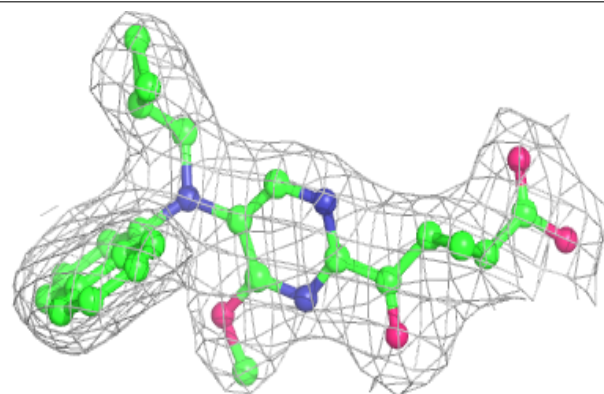


**Electron density around JUQ L 201:**

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

**Electron density around JUQ F 201:**

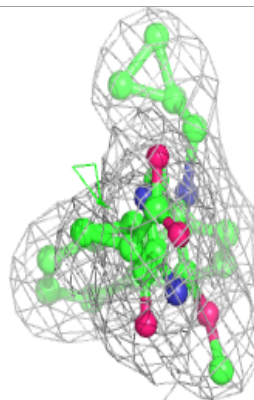
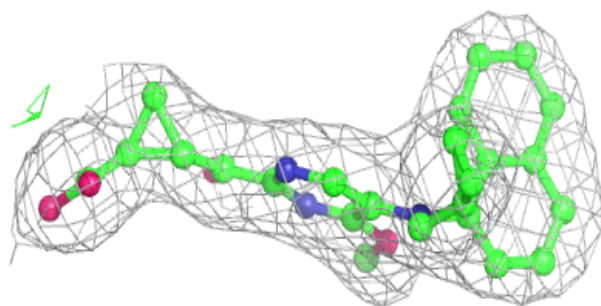
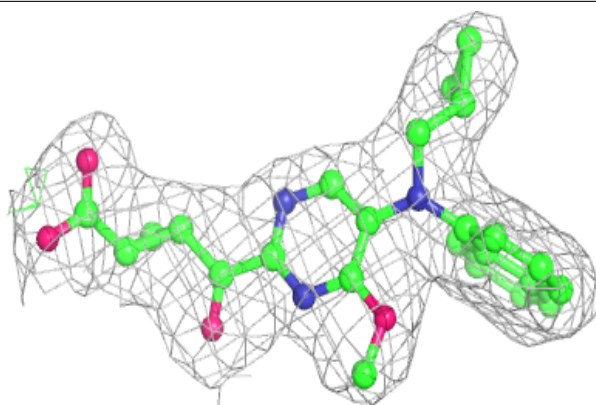
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



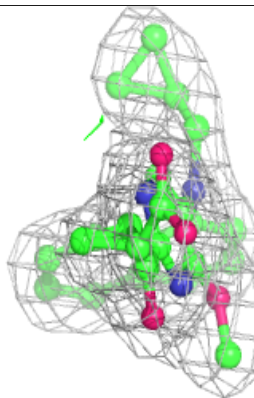
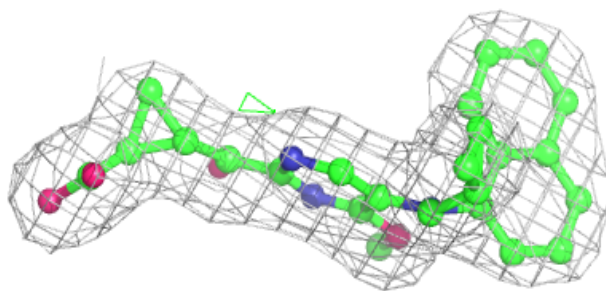
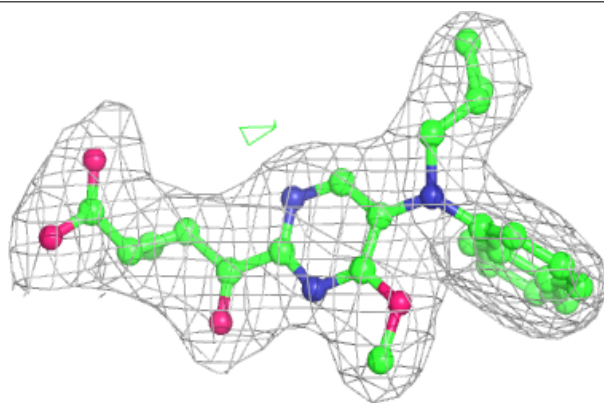


**Electron density around JUQ K 201:**

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

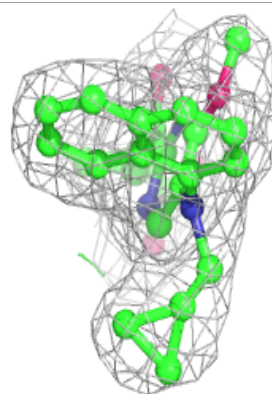
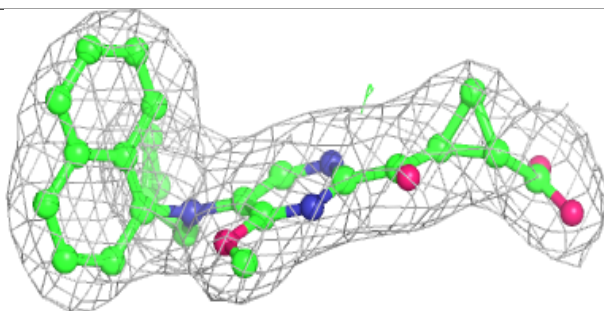
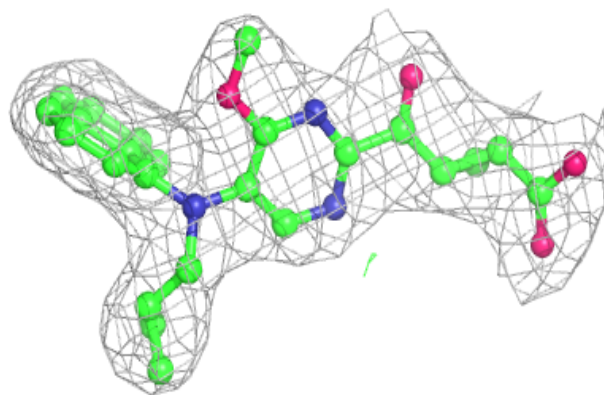
**Electron density around JUQ G 201:**

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

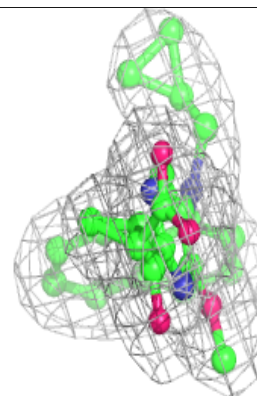
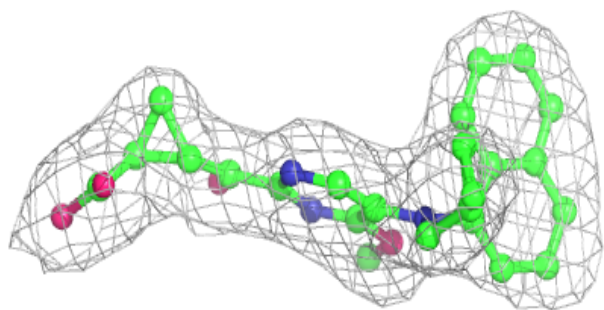
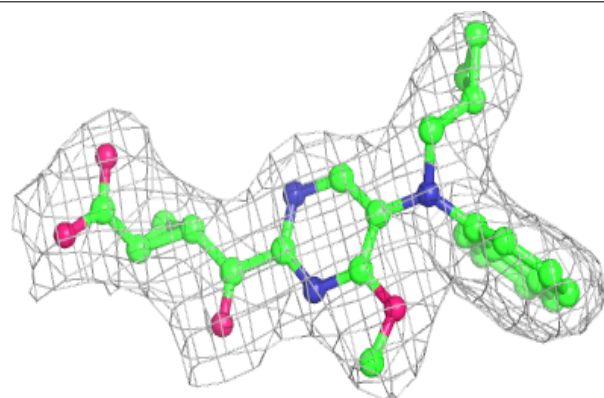


**Electron density around JUQ I 201:**

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

**Electron density around JUQ E 201:**

$2mF_o-DF_c$  (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.