



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

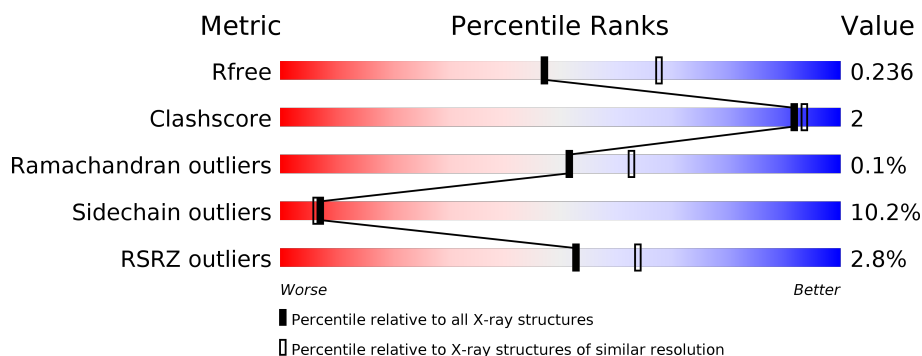
1 Overall quality at a glance

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 ≥ 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	 80% 13% •• 5%
1	H	157	 82% 12% • •
1	I	157	 81% 13% • 6%
1	J	157	 81% 12% •• 5%
1	K	157	 75% 17% • • •
1	L	157	 78% 15% • 6%

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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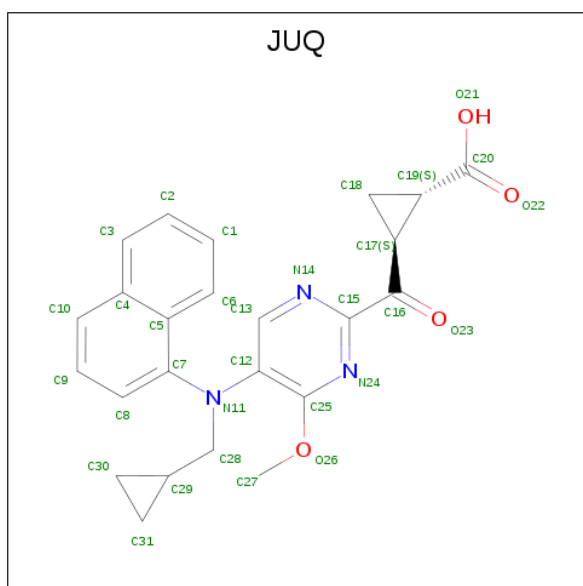
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	expression tag	UNP Q16873
G	-6	MET	-	initiating methionine	UNP Q16873
G	-5	ALA	-	expression tag	UNP Q16873
G	-4	HIS	-	expression tag	UNP Q16873
G	-3	HIS	-	expression tag	UNP Q16873
G	-2	HIS	-	expression tag	UNP Q16873
G	-1	HIS	-	expression tag	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: C₂₄H₂₃N₃O₄) (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: C₁₆H₃₂O₂).



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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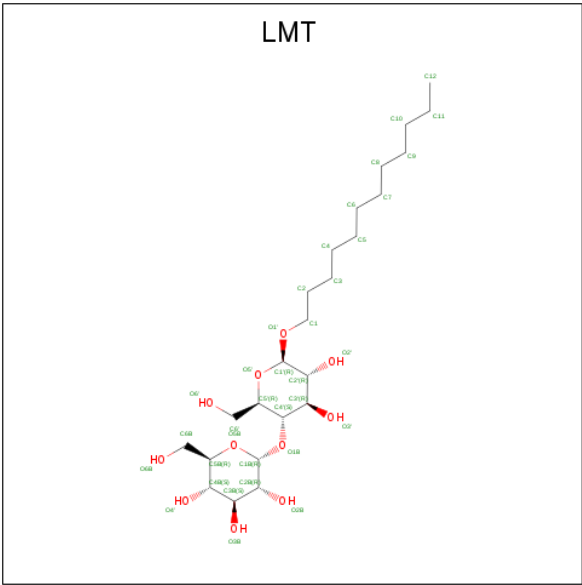
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0
4	D	1	Total C 10 10	0	0
4	D	1	Total C 10 10	0	0
4	D	1	Total C O 18 16 2	0	0
4	D	1	Total C O 15 13 2	0	0
4	E	1	Total C 10 10	0	0
4	E	1	Total C 7 7	0	0
4	E	1	Total C 10 10	0	0
4	F	1	Total C 8 8	0	0
4	F	1	Total C 10 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: C₂₄H₄₆O₁₁).



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

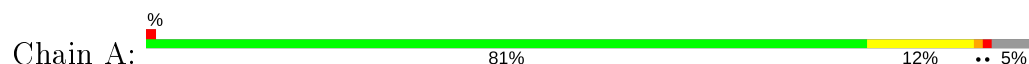
- Molecule 6 is water.

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

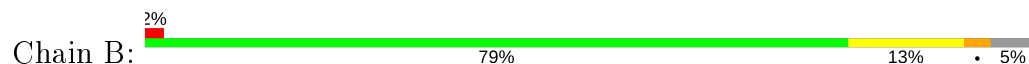
3 Residue-property plots [i](#)

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.

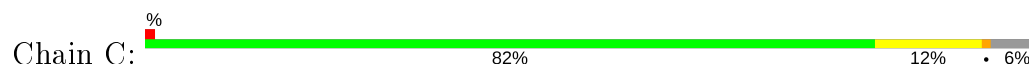
- Molecule 1: Leukotriene C4 synthase



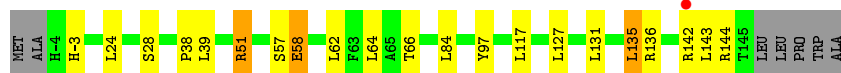
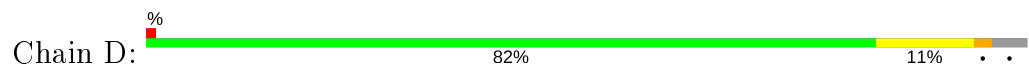
- Molecule 1: Leukotriene C4 synthase



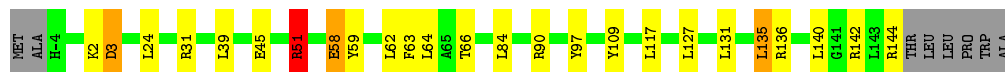
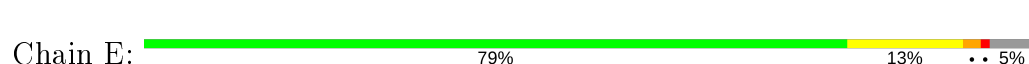
- Molecule 1: Leukotriene C4 synthase



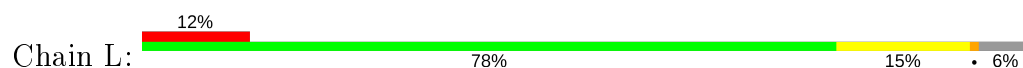
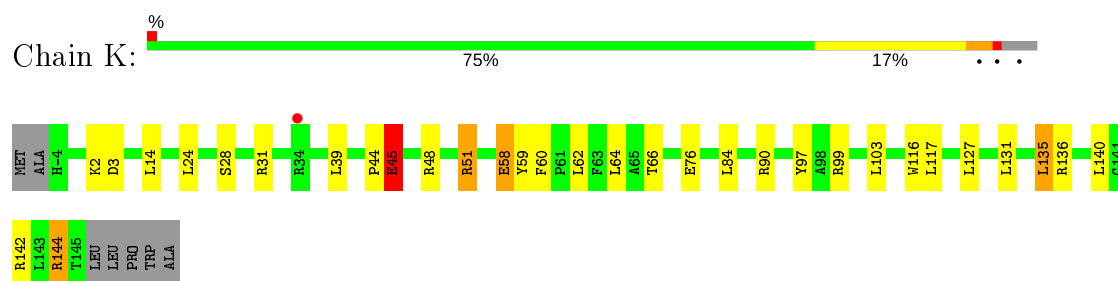
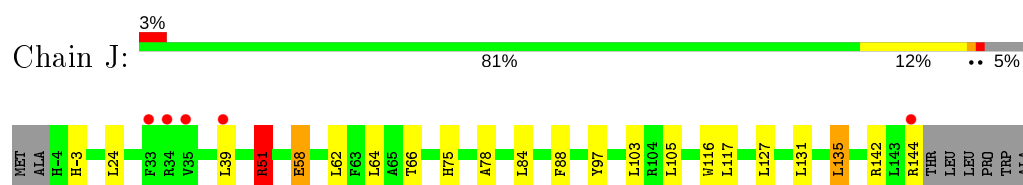
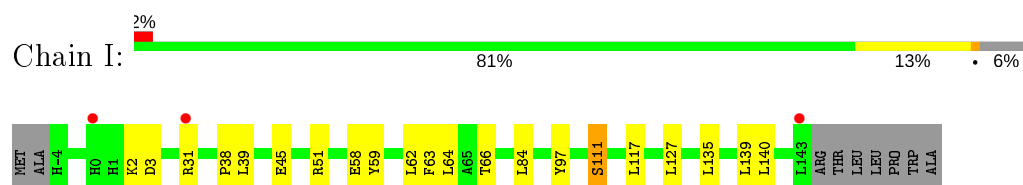
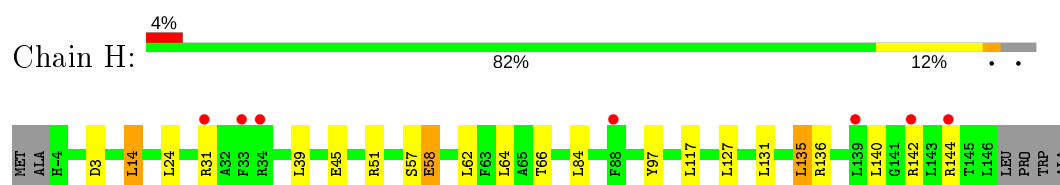
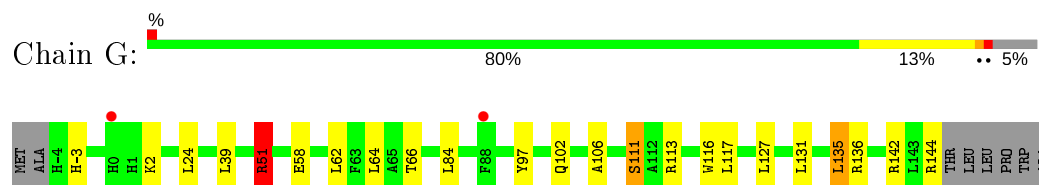
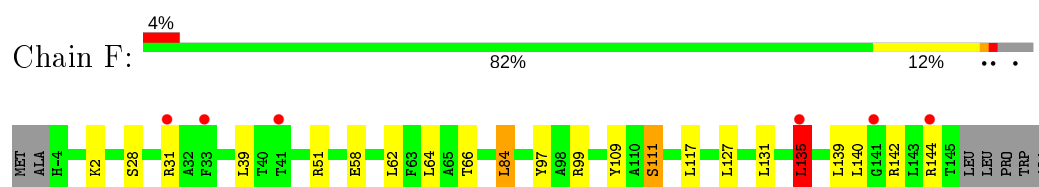
- Molecule 1: Leukotriene C4 synthase

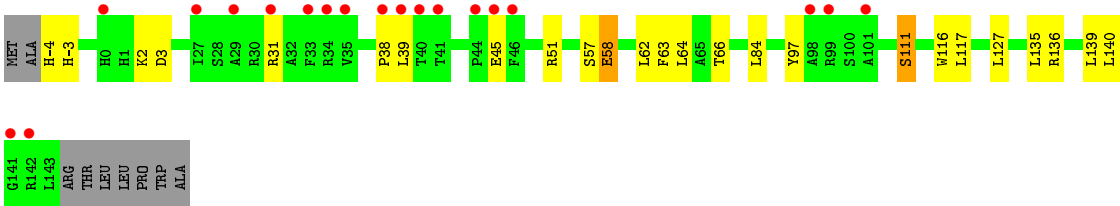


- Molecule 1: Leukotriene C4 synthase



- Molecule 1: Leukotriene C4 synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	51.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)

All (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
1	K	58	GLU	CD-OE1	8.12	1.34	1.25
1	J	58	GLU	CD-OE1	8.03	1.34	1.25
1	E	58	GLU	CD-OE1	7.72	1.34	1.25
1	G	111	SER	CB-OG	-7.62	1.32	1.42
1	I	58	GLU	CD-OE1	7.29	1.33	1.25
1	F	58	GLU	CD-OE1	7.19	1.33	1.25
1	I	63	PHE	CG-CD2	-7.06	1.28	1.38
1	C	111	SER	CB-OG	-6.99	1.33	1.42
1	H	58	GLU	CD-OE1	6.87	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	116	TRP	CG-CD1	6.77	1.46	1.36
1	C	58	GLU	CD-OE1	6.74	1.33	1.25
1	B	59	TYR	CE1-CZ	6.45	1.47	1.38
1	G	58	GLU	CD-OE1	6.40	1.32	1.25
1	F	109	TYR	CB-CG	6.35	1.61	1.51
1	H	57	SER	CB-OG	-6.35	1.34	1.42
1	B	51	ARG	CD-NE	-6.34	1.35	1.46
1	J	88	PHE	CG-CD2	6.30	1.48	1.38
1	L	-3	HIS	N-CA	6.07	1.58	1.46
1	K	90	ARG	CZ-NH1	-6.04	1.25	1.33
1	B	97	TYR	CE1-CZ	-6.03	1.30	1.38
1	L	58	GLU	CD-OE1	6.01	1.32	1.25
1	K	76	GLU	CD-OE2	5.97	1.32	1.25
1	K	116	TRP	CG-CD1	5.97	1.45	1.36
1	L	63	PHE	CG-CD2	-5.97	1.29	1.38
1	K	48	ARG	CZ-NH1	5.87	1.40	1.33
1	L	116	TRP	CG-CD1	5.84	1.45	1.36
1	L	57	SER	CB-OG	-5.72	1.34	1.42
1	E	90	ARG	CD-NE	-5.66	1.36	1.46
1	E	90	ARG	CZ-NH1	-5.66	1.25	1.33
1	B	28	SER	CB-OG	-5.62	1.34	1.42
1	C	63	PHE	CG-CD2	-5.60	1.30	1.38
1	L	-4	HIS	N-CA	5.57	1.57	1.46
1	L	111	SER	CB-OG	-5.53	1.35	1.42
1	E	63	PHE	CG-CD2	-5.53	1.30	1.38
1	K	90	ARG	CD-NE	-5.53	1.37	1.46
1	A	71	GLY	C-O	-5.29	1.15	1.23
1	K	99	ARG	CZ-NH1	-5.29	1.26	1.33
1	D	57	SER	CB-OG	-5.22	1.35	1.42
1	F	28	SER	CB-OG	-5.15	1.35	1.42
1	B	93	TYR	CE2-CZ	5.14	1.45	1.38
1	E	59	TYR	CE2-CZ	-5.09	1.31	1.38
1	D	28	SER	CB-OG	-5.08	1.35	1.42
1	B	59	TYR	CE2-CZ	-5.03	1.32	1.38
1	K	59	TYR	CZ-OH	5.02	1.46	1.37
1	B	90	ARG	CD-NE	-5.01	1.38	1.46
1	G	116	TRP	CE3-CZ3	5.01	1.47	1.38

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	E	51	ARG	NE-CZ-NH1	16.82	128.71	120.30
1	L	51	ARG	NE-CZ-NH1	-16.70	111.95	120.30
1	H	51	ARG	NE-CZ-NH1	-16.66	111.97	120.30
1	G	51	ARG	NE-CZ-NH1	16.61	128.60	120.30
1	A	51	ARG	NE-CZ-NH2	-16.58	112.01	120.30
1	B	51	ARG	NE-CZ-NH2	-15.90	112.35	120.30
1	E	51	ARG	NE-CZ-NH2	-15.74	112.43	120.30
1	J	51	ARG	NE-CZ-NH1	15.67	128.13	120.30
1	K	51	ARG	NE-CZ-NH1	15.56	128.08	120.30
1	K	51	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	F	51	ARG	NE-CZ-NH2	15.00	127.80	120.30
1	G	51	ARG	NE-CZ-NH2	-14.78	112.91	120.30
1	H	51	ARG	NE-CZ-NH2	14.75	127.67	120.30
1	D	51	ARG	NE-CZ-NH2	-14.65	112.97	120.30
1	L	51	ARG	NE-CZ-NH2	14.12	127.36	120.30
1	C	51	ARG	NE-CZ-NH2	13.92	127.26	120.30
1	J	51	ARG	NE-CZ-NH2	-13.75	113.42	120.30
1	I	51	ARG	NE-CZ-NH2	13.33	126.97	120.30
1	F	51	ARG	NE-CZ-NH1	-12.99	113.81	120.30
1	F	135	LEU	CA-CB-CG	10.56	139.59	115.30
1	L	-3	HIS	N-CA-C	10.10	138.27	111.00
1	F	99	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	F	135	LEU	CB-CG-CD2	8.61	125.64	111.00
1	F	31	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	L	31	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	135	LEU	CB-CG-CD1	8.02	124.64	111.00
1	L	135	LEU	CB-CG-CD1	8.00	124.61	111.00
1	L	31	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	I	135	LEU	CB-CG-CD1	7.92	124.47	111.00
1	C	31	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	E	31	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	31	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	D	142	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	142	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	E	31	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	K	31	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	F	31	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	B	31	ARG	NE-CZ-NH1	7.26	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	142	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	J	142	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	142	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	I	31	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	H	31	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	K	31	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	E	142	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	H	142	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	L	136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	K	142	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	H	31	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	31	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	58	GLU	OE1-CD-OE2	6.34	130.90	123.30
1	I	31	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	I	111	SER	CB-CA-C	6.25	121.97	110.10
1	K	45	GLU	CA-CB-CG	6.13	126.89	113.40
1	B	14	LEU	CB-CG-CD2	6.04	121.28	111.00
1	D	143	LEU	C-N-CA	-6.04	106.60	121.70
1	A	-4	HIS	N-CA-C	6.04	127.30	111.00
1	E	136	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	136	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	D	136	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	F	142	ARG	CG-CD-NE	-5.88	99.44	111.80
1	K	144	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	L	3	ASP	CB-CG-OD1	5.80	123.52	118.30
1	I	3	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	G	136	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	I	58	GLU	OE1-CD-OE2	5.65	130.08	123.30
1	G	2	LYS	CB-CA-C	-5.63	99.14	110.40
1	C	111	SER	CB-CA-C	5.62	120.77	110.10
1	F	31	ARG	CD-NE-CZ	5.59	131.43	123.60
1	K	58	GLU	OE1-CD-OE2	5.59	130.01	123.30
1	L	2	LYS	CB-CA-C	-5.57	99.26	110.40
1	B	136	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	58	GLU	CG-CD-OE2	-5.54	107.22	118.30
1	F	111	SER	CB-CA-C	5.54	120.62	110.10
1	I	31	ARG	CD-NE-CZ	5.54	131.35	123.60
1	H	14	LEU	CB-CG-CD2	5.51	120.37	111.00
1	B	2	LYS	CB-CA-C	-5.51	99.38	110.40
1	C	30	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	E	31	ARG	CD-NE-CZ	5.47	131.25	123.60
1	I	2	LYS	CB-CA-C	-5.45	99.50	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	136	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	L	111	SER	CB-CA-C	5.34	120.25	110.10
1	F	142	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	I	3	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	3	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	E	58	GLU	OE1-CD-OE2	5.31	129.67	123.30
1	D	142	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	K	14	LEU	CB-CG-CD2	5.30	120.01	111.00
1	C	31	ARG	CD-NE-CZ	5.28	131.00	123.60
1	G	58	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	E	2	LYS	CB-CA-C	-5.25	99.90	110.40
1	C	3	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	F	2	LYS	CB-CA-C	-5.20	99.99	110.40
1	K	31	ARG	CD-NE-CZ	5.20	130.88	123.60
1	L	31	ARG	CD-NE-CZ	5.19	130.87	123.60
1	F	111	SER	CA-CB-OG	-5.18	97.22	111.20
1	B	31	ARG	CD-NE-CZ	5.10	130.75	123.60
1	D	58	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	E	109	TYR	CB-CG-CD2	-5.09	117.94	121.00
1	E	58	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	H	31	ARG	CD-NE-CZ	5.07	130.70	123.60
1	A	-3	HIS	N-CA-C	5.07	124.68	111.00
1	J	58	GLU	OE1-CD-OE2	5.07	129.38	123.30
1	K	2	LYS	CB-CA-C	-5.05	100.29	110.40
1	E	3	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	K	136	ARG	NE-CZ-NH2	-5.02	117.79	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:G:102:GLN:OE1	1:J:105:LEU:HD12	1.81	0.76
1:J:75:HIS:HD2	1:J:78:ALA:H	1.33	0.75
1:A:44:PRO:HG2	1:K:103:LEU:HD11	1.68	0.74
1:I:59:TYR:OH	6:I:301:HOH:O	2.09	0.70
1:G:106:ALA:HB1	1:J:103:LEU:CD2	2.25	0.67
2:J:201:JUQ:C28	2:J:201:JUQ:C6	2.85	0.54
1:D:3:HIS:HE1	1:E:3:ASP:OD1	1.90	0.53
1:H:131:LEU:HG	1:H:135:LEU:HD22	1.91	0.53
1:J:3:HIS:HE1	1:K:3:ASP:OD1	1.93	0.52
1:E:131:LEU:HG	1:E:135:LEU:HD22	1.92	0.51
1:K:131:LEU:HG	1:K:135:LEU:HD22	1.92	0.51
1:A:131:LEU:HG	1:A:135:LEU:HD22	1.92	0.51
1:G:131:LEU:HG	1:G:135:LEU:HD22	1.93	0.50
1:J:131:LEU:HG	1:J:135:LEU:HD22	1.93	0.50
1:A:72:ILE:HD12	4:A:206:PLM:H61	1.94	0.50
1:B:131:LEU:HG	1:B:135:LEU:HD22	1.94	0.49
1:J:75:HIS:HD2	1:J:78:ALA:N	2.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PRO:HB2	1:E:51:ARG:HG3	1.94	0.49
1:D:131:LEU:HG	1:D:135:LEU:HD22	1.95	0.49
1:J:51:ARG:HG3	1:L:38:PRO:HB2	1.93	0.49
1:G:106:ALA:CB	1:J:103:LEU:HD23	2.37	0.48
1:L:62:LEU:O	1:L:66:THR:HG23	2.14	0.47
1:F:131:LEU:HG	1:F:135:LEU:HD12	1.97	0.46
1:A:103:LEU:HD11	1:K:44:PRO:HG2	1.97	0.46
1:B:62:LEU:O	1:B:66:THR:HG23	2.15	0.46
1:I:62:LEU:O	1:I:66:THR:HG23	2.16	0.45
1:D:62:LEU:O	1:D:66:THR:HG23	2.16	0.45
1:G:3:3:HIS:HE1	1:H:3:ASP:OD1	2.00	0.45
1:C:62:LEU:O	1:C:66:THR:HG23	2.18	0.44
1:K:62:LEU:O	1:K:66:THR:HG23	2.17	0.44
1:G:62:LEU:O	1:G:66:THR:HG23	2.18	0.43
1:J:75:HIS:CD2	1:J:78:ALA:H	2.23	0.43
1:A:62:LEU:O	1:A:66:THR:HG23	2.19	0.43
1:G:113:ARG:HH11	4:G:204:PLM:C7	2.31	0.43
1:G:51:ARG:HD3	6:G:305:HOH:O	2.19	0.43
1:F:62:LEU:O	1:F:66:THR:HG23	2.19	0.42
1:E:62:LEU:O	1:E:66:THR:HG23	2.19	0.42
1:F:84:LEU:HD21	4:F:202:PLM:HA2	2.02	0.42
1:J:62:LEU:O	1:J:66:THR:HG23	2.20	0.41
1:A:3:3:HIS:HE1	1:B:3:ASP:OD1	2.03	0.41
1:K:60:PHE:HD1	6:K:311:HOH:O	2.04	0.41
1:H:62:LEU:O	1:H:66:THR:HG23	2.19	0.41
1:G:51:ARG:HG3	1:I:38:PRO:HB2	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS
1	A	24	LEU
1	A	39	LEU
1	A	45	GLU
1	A	51	ARG
1	A	58	GLU
1	A	64	LEU
1	A	84	LEU
1	A	97	TYR
1	A	117	LEU
1	A	127	LEU
1	A	135	LEU
1	A	144	ARG
1	B	24	LEU
1	B	39	LEU
1	B	51	ARG
1	B	58	GLU
1	B	64	LEU
1	B	84	LEU
1	B	97	TYR
1	B	117	LEU
1	B	127	LEU
1	B	135	LEU
1	B	140	LEU
1	B	144	ARG
1	C	39	LEU
1	C	45	GLU
1	C	58	GLU
1	C	64	LEU
1	C	84	LEU

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Mol	Chain	Res	Type
1	C	97	TYR
1	C	117	LEU
1	C	127	LEU
1	C	139	LEU
1	C	140	LEU
1	D	24	LEU
1	D	39	LEU
1	D	51	ARG
1	D	58	GLU
1	D	64	LEU
1	D	84	LEU
1	D	97	TYR
1	D	117	LEU
1	D	127	LEU
1	D	135	LEU
1	E	24	LEU
1	E	39	LEU
1	E	45	GLU
1	E	51	ARG
1	E	58	GLU
1	E	64	LEU
1	E	84	LEU
1	E	97	TYR
1	E	117	LEU
1	E	127	LEU
1	E	135	LEU
1	E	140	LEU
1	E	144	ARG
1	F	39	LEU
1	F	64	LEU
1	F	84	LEU
1	F	97	TYR
1	F	111	SER
1	F	117	LEU
1	F	127	LEU
1	F	135	LEU
1	F	139	LEU
1	F	140	LEU
1	F	144	ARG
1	G	24	LEU
1	G	39	LEU
1	G	51	ARG

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Mol	Chain	Res	Type
1	G	64	LEU
1	G	84	LEU
1	G	97	TYR
1	G	111	SER
1	G	117	LEU
1	G	127	LEU
1	G	135	LEU
1	G	144	ARG
1	H	14	LEU
1	H	24	LEU
1	H	39	LEU
1	H	45	GLU
1	H	58	GLU
1	H	64	LEU
1	H	84	LEU
1	H	97	TYR
1	H	117	LEU
1	H	127	LEU
1	H	135	LEU
1	H	140	LEU
1	H	144	ARG
1	I	39	LEU
1	I	45	GLU
1	I	64	LEU
1	I	84	LEU
1	I	97	TYR
1	I	111	SER
1	I	117	LEU
1	I	127	LEU
1	I	139	LEU
1	I	140	LEU
1	J	24	LEU
1	J	39	LEU
1	J	51	ARG
1	J	58	GLU
1	J	64	LEU
1	J	84	LEU
1	J	97	TYR
1	J	117	LEU
1	J	127	LEU
1	J	135	LEU
1	J	144	ARG

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Mol	Chain	Res	Type
1	K	24	LEU
1	K	28	SER
1	K	39	LEU
1	K	45	GLU
1	K	51	ARG
1	K	58	GLU
1	K	64	LEU
1	K	84	LEU
1	K	97	TYR
1	K	117	LEU
1	K	127	LEU
1	K	135	LEU
1	K	140	LEU
1	K	144	ARG
1	L	39	LEU
1	L	45	GLU
1	L	58	GLU
1	L	64	LEU
1	L	84	LEU
1	L	97	TYR
1	L	111	SER
1	L	117	LEU
1	L	127	LEU
1	L	139	LEU
1	L	140	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS
1	A	55	ASN
1	B	55	ASN
1	D	-3	HIS
1	D	55	ASN
1	E	55	ASN
1	G	-3	HIS
1	G	55	ASN
1	H	55	ASN
1	J	-3	HIS
1	J	55	ASN
1	J	75	HIS
1	K	55	ASN

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

All (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
2	H	201	JUQ	C17-C16	-3.61	1.47	1.52
2	K	201	JUQ	C15-C16	-3.43	1.46	1.52
2	A	201	JUQ	C15-C16	-3.38	1.46	1.52
2	B	201	JUQ	O26-C25	3.17	1.40	1.35
2	K	201	JUQ	O26-C25	3.01	1.39	1.35
2	E	201	JUQ	C17-C16	-2.91	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	JUQ	C28-N11	2.90	1.50	1.46
2	F	201	JUQ	C25-N24	2.81	1.36	1.32
2	C	201	JUQ	C7-N11	2.53	1.47	1.43
2	E	201	JUQ	C7-N11	2.52	1.47	1.43
5	B	209	LMT	O1'-C1'	2.37	1.44	1.40
2	H	201	JUQ	C28-N11	2.34	1.49	1.46
2	E	201	JUQ	C15-C16	-2.30	1.48	1.52
2	H	201	JUQ	O26-C25	2.29	1.38	1.35
2	J	201	JUQ	O23-C16	2.27	1.25	1.22
2	H	201	JUQ	C6-C5	-2.25	1.37	1.42
2	J	201	JUQ	C25-N24	2.23	1.35	1.32
2	B	201	JUQ	C25-N24	2.22	1.35	1.32
2	I	201	JUQ	C15-C16	-2.22	1.48	1.52
2	B	201	JUQ	C15-C16	-2.15	1.48	1.52
2	L	201	JUQ	O23-C16	2.15	1.25	1.22
2	B	201	JUQ	C6-C5	-2.15	1.37	1.42
2	G	201	JUQ	O26-C25	2.15	1.38	1.35
2	L	201	JUQ	C7-C5	-2.08	1.38	1.42
2	D	201	JUQ	C7-C5	-2.06	1.38	1.42
2	C	201	JUQ	C15-C16	-2.06	1.49	1.52
2	E	201	JUQ	C28-N11	2.06	1.49	1.46
2	I	201	JUQ	C7-C5	-2.02	1.38	1.42
2	F	201	JUQ	C28-N11	2.01	1.49	1.46
2	C	201	JUQ	C25-N24	2.01	1.35	1.32

All (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
2	L	201	JUQ	C27-O26-C25	-5.78	111.48	117.21
2	L	201	JUQ	C25-C12-N11	5.41	125.54	119.99
2	L	201	JUQ	C28-N11-C12	-5.28	104.21	116.67
2	F	201	JUQ	C25-C12-N11	5.19	125.31	119.99
2	C	201	JUQ	C8-C7-N11	5.18	125.87	120.58
2	C	201	JUQ	C25-C12-N11	4.89	125.01	119.99
2	A	201	JUQ	C7-N11-C12	4.84	129.80	120.15
2	I	201	JUQ	C7-N11-C12	4.75	129.63	120.15
2	G	201	JUQ	C27-O26-C25	-4.69	112.57	117.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	JUQ	C7-N11-C12	4.63	129.39	120.15
2	B	201	JUQ	C27-O26-C25	-4.63	112.63	117.21
2	E	201	JUQ	C25-C12-N11	4.62	124.73	119.99
2	H	201	JUQ	C7-N11-C12	4.51	129.15	120.15
2	F	201	JUQ	C27-O26-C25	-4.49	112.76	117.21
2	D	201	JUQ	C7-N11-C12	4.30	128.72	120.15
2	E	201	JUQ	C7-N11-C12	4.29	128.72	120.15
2	D	201	JUQ	C25-C12-N11	4.09	124.19	119.99
2	L	201	JUQ	C8-C7-N11	4.04	124.70	120.58
2	G	201	JUQ	C7-N11-C12	3.93	128.00	120.15
2	J	201	JUQ	C28-N11-C12	-3.91	107.44	116.67
2	K	201	JUQ	C7-N11-C12	3.88	127.89	120.15
5	B	209	LMT	C1B-O5B-C5B	3.79	121.13	113.69
2	C	201	JUQ	C6-C5-C7	-3.65	116.44	122.74
2	H	201	JUQ	C27-O26-C25	-3.63	113.61	117.21
2	B	201	JUQ	C7-N11-C12	3.62	127.38	120.15
2	I	201	JUQ	C25-C12-N11	3.51	123.59	119.99
2	E	201	JUQ	C6-C5-C7	-3.47	116.76	122.74
2	J	201	JUQ	C7-N11-C12	3.41	126.95	120.15
2	C	201	JUQ	C6-C5-C4	3.38	122.26	117.89
2	B	201	JUQ	C8-C7-C5	-3.33	113.99	119.94
2	L	201	JUQ	C6-C5-C7	-3.32	117.01	122.74
2	G	201	JUQ	C25-C12-N11	3.32	123.39	119.99
2	B	201	JUQ	C28-N11-C12	-3.25	108.99	116.67
2	H	201	JUQ	C12-C13-N14	3.23	125.28	121.22
2	L	201	JUQ	C9-C10-C4	-3.22	115.41	120.44
2	G	201	JUQ	C28-N11-C12	-3.17	109.19	116.67
2	E	201	JUQ	C12-C13-N14	3.16	125.18	121.22
2	B	201	JUQ	C6-C5-C7	-3.13	117.34	122.74
2	L	201	JUQ	C12-C13-N14	3.11	125.12	121.22
2	J	201	JUQ	C28-N11-C7	-3.11	109.34	116.67
2	G	201	JUQ	C12-C13-N14	3.10	125.11	121.22
2	F	201	JUQ	C7-N11-C12	3.08	126.30	120.15
2	B	201	JUQ	C7-C5-C4	3.06	123.22	118.14
2	K	201	JUQ	C9-C10-C4	-3.05	115.67	120.44
2	E	201	JUQ	C8-C7-C5	-3.00	114.58	119.94
2	J	201	JUQ	C31-C29-C28	-2.99	106.58	120.30
2	C	201	JUQ	C12-C13-N14	2.97	124.95	121.22
2	L	201	JUQ	C28-N11-C7	2.96	123.66	116.67
2	B	201	JUQ	C15-C16-C17	2.93	122.12	118.07
2	I	201	JUQ	C12-C13-N14	2.92	124.89	121.22
2	B	201	JUQ	C25-C12-N11	2.92	122.99	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	201	JUQ	C10-C4-C5	2.85	122.88	119.12
2	E	201	JUQ	C9-C8-C7	2.81	124.58	120.66
2	L	201	JUQ	C7-N11-C12	2.80	125.74	120.15
2	D	201	JUQ	C6-C5-C4	2.78	121.48	117.89
2	C	201	JUQ	C10-C4-C5	2.76	122.75	119.12
2	E	201	JUQ	C10-C4-C5	2.75	122.73	119.12
2	K	201	JUQ	C12-C13-N14	2.74	124.66	121.22
2	I	201	JUQ	C6-C5-C4	2.73	121.42	117.89
2	K	201	JUQ	C6-C5-C7	-2.72	118.04	122.74
2	A	201	JUQ	C16-C15-N24	-2.72	114.11	117.35
2	H	201	JUQ	C6-C5-C7	-2.71	118.06	122.74
2	F	201	JUQ	C12-C25-N24	2.66	126.12	121.58
2	C	201	JUQ	C16-C15-N24	-2.65	114.18	117.35
2	E	201	JUQ	C12-C25-N24	2.65	126.10	121.58
2	F	201	JUQ	C12-C13-N14	2.65	124.54	121.22
2	A	201	JUQ	C18-C17-C19	2.65	60.93	58.89
2	G	201	JUQ	C8-C7-C5	-2.64	115.22	119.94
2	F	201	JUQ	C16-C15-N24	-2.60	114.25	117.35
2	L	201	JUQ	C18-C19-C20	2.57	125.03	120.02
2	A	201	JUQ	C25-C12-N11	2.55	122.61	119.99
2	E	201	JUQ	C6-C5-C4	2.55	121.19	117.89
2	C	201	JUQ	C9-C10-C4	-2.55	116.46	120.44
2	K	201	JUQ	C30-C29-C28	-2.55	108.61	120.30
2	B	201	JUQ	C16-C15-N24	-2.54	114.33	117.35
2	F	201	JUQ	C18-C19-C20	2.53	124.95	120.02
2	K	201	JUQ	C7-C5-C4	2.53	122.33	118.14
2	B	201	JUQ	C8-C7-N11	2.51	123.14	120.58
2	G	201	JUQ	C10-C4-C5	2.50	122.41	119.12
2	L	201	JUQ	C8-C7-C5	-2.50	115.48	119.94
2	F	201	JUQ	O23-C16-C17	2.49	123.45	120.28
2	E	201	JUQ	C17-C18-C19	-2.49	59.28	61.33
2	L	201	JUQ	C6-C5-C4	2.49	121.11	117.89
2	B	201	JUQ	C10-C4-C3	-2.48	117.38	123.19
2	C	201	JUQ	C15-C16-C17	2.45	121.47	118.07
2	K	201	JUQ	C8-C7-C5	-2.43	115.60	119.94
2	G	201	JUQ	C10-C4-C3	-2.37	117.64	123.19
2	A	201	JUQ	C17-C18-C19	-2.37	59.38	61.33
2	I	201	JUQ	C6-C5-C7	-2.37	118.66	122.74
2	K	201	JUQ	C18-C19-C20	2.36	124.62	120.02
2	E	201	JUQ	C7-C5-C4	2.35	122.05	118.14
2	L	201	JUQ	O23-C16-C17	2.35	123.27	120.28
2	D	201	JUQ	C18-C19-C20	2.33	124.56	120.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	JUQ	C15-C16-C17	2.33	121.29	118.07
2	G	201	JUQ	O26-C25-N24	2.32	122.20	119.01
2	G	201	JUQ	C9-C8-C7	2.30	123.87	120.66
2	B	201	JUQ	C9-C10-C4	-2.28	116.88	120.44
2	A	201	JUQ	N14-C15-N24	2.28	127.56	125.27
2	A	201	JUQ	O23-C16-C17	2.25	123.15	120.28
2	L	201	JUQ	C7-C5-C4	2.25	121.88	118.14
2	E	201	JUQ	C9-C10-C4	-2.24	116.95	120.44
2	D	201	JUQ	C16-C15-N24	-2.23	114.69	117.35
2	K	201	JUQ	C10-C4-C3	-2.21	118.02	123.19
2	H	201	JUQ	C9-C10-C4	-2.19	117.03	120.44
2	B	201	JUQ	C28-N11-C7	2.18	121.83	116.67
2	I	201	JUQ	C10-C4-C3	-2.18	118.10	123.19
2	C	201	JUQ	C8-C7-C5	-2.17	116.06	119.94
2	G	201	JUQ	C9-C10-C4	-2.13	117.11	120.44
2	G	201	JUQ	N14-C15-N24	2.12	127.40	125.27
2	H	201	JUQ	C7-C5-C4	2.12	121.66	118.14
2	A	201	JUQ	C12-C13-N14	2.11	123.87	121.22
2	C	201	JUQ	C27-O26-C25	-2.11	115.12	117.21
2	I	201	JUQ	C8-C7-N11	2.09	122.71	120.58
2	C	201	JUQ	C18-C17-C19	2.09	60.50	58.89
2	J	201	JUQ	C12-C13-N14	2.09	123.84	121.22
4	G	203	PLM	CD-CC-CB	2.08	124.97	114.42
2	I	201	JUQ	C17-C18-C19	-2.07	59.62	61.33
2	B	201	JUQ	C9-C8-C7	2.07	123.55	120.66
2	H	201	JUQ	C10-C4-C3	-2.06	118.37	123.19
2	I	201	JUQ	C10-C4-C5	2.05	121.82	119.12
2	B	201	JUQ	C12-C13-N14	2.02	123.75	121.22
2	I	201	JUQ	C16-C15-N24	-2.02	114.94	117.35
2	G	201	JUQ	C2-C1-C6	-2.01	117.62	120.44
2	E	201	JUQ	C10-C4-C3	-2.01	118.49	123.19

There are no chirality outliers.

All (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
2	F	201	JUQ	C29-C28-N11-C7

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Mol	Chain	Res	Type	Atoms
2	F	201	JUQ	C29-C28-N11-C12
4	J	207	PLM	C1-C2-C3-C4
2	J	201	JUQ	C13-C12-N11-C28
2	J	201	JUQ	C29-C28-N11-C12
4	A	207	PLM	C1-C2-C3-C4
4	G	205	PLM	C1-C2-C3-C4
2	E	201	JUQ	O23-C16-C17-C18
2	E	201	JUQ	C29-C28-N11-C12
4	L	205	PLM	C1-C2-C3-C4
4	B	206	PLM	C1-C2-C3-C4
2	L	201	JUQ	C13-C12-N11-C28
2	L	201	JUQ	C25-C12-N11-C28
2	L	201	JUQ	O23-C16-C17-C18
2	L	201	JUQ	C29-C28-N11-C7
2	L	201	JUQ	C29-C28-N11-C12
2	G	201	JUQ	C29-C28-N11-C7
2	G	201	JUQ	C29-C28-N11-C12
2	B	201	JUQ	C29-C28-N11-C7
2	B	201	JUQ	C29-C28-N11-C12
2	K	201	JUQ	C29-C28-N11-C7
2	K	201	JUQ	C29-C28-N11-C12
2	H	201	JUQ	O23-C16-C17-C18
2	H	201	JUQ	C12-C25-O26-C27
4	J	205	PLM	CC-CD-CE-CF
4	D	206	PLM	C2-C3-C4-C5
4	D	203	PLM	C8-C9-CA-CB
4	D	203	PLM	CB-CC-CD-CE
4	L	205	PLM	C2-C3-C4-C5
4	C	206	PLM	CA-CB-CC-CD
4	F	203	PLM	C9-CA-CB-CC
4	B	203	PLM	CC-CD-CE-CF
4	C	203	PLM	C3-C4-C5-C6
4	C	203	PLM	C4-C5-C6-C7
4	B	206	PLM	C8-C9-CA-CB
4	J	207	PLM	C2-C3-C4-C5
4	B	203	PLM	CB-CC-CD-CE
4	C	204	PLM	C9-CA-CB-CC
4	B	206	PLM	C5-C6-C7-C8
4	L	203	PLM	C9-CA-CB-CC
4	D	205	PLM	C4-C5-C6-C7
4	A	203	PLM	CB-CC-CD-CE
4	F	202	PLM	C9-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
4	F	203	PLM	CC-CD-CE-CF
4	J	207	PLM	C5-C6-C7-C8
4	G	204	PLM	CB-CC-CD-CE
4	F	205	PLM	CB-CC-CD-CE
4	A	205	PLM	CB-CC-CD-CE
4	J	205	PLM	C8-C9-CA-CB
4	L	205	PLM	C5-C6-C7-C8
4	G	203	PLM	C8-C9-CA-CB
4	C	207	PLM	C9-CA-CB-CC
2	G	201	JUQ	C13-C12-N11-C28
4	C	204	PLM	C8-C9-CA-CB
4	I	203	PLM	CA-CB-CC-CD
4	B	206	PLM	C2-C3-C4-C5
4	L	203	PLM	C8-C9-CA-CB
4	C	206	PLM	C9-CA-CB-CC
4	B	206	PLM	C6-C7-C8-C9
4	A	207	PLM	C5-C6-C7-C8
4	A	203	PLM	C7-C8-C9-CA
4	L	205	PLM	C4-C5-C6-C7
4	B	203	PLM	C7-C8-C9-CA
4	J	207	PLM	C4-C5-C6-C7
4	B	203	PLM	CA-CB-CC-CD
4	L	206	PLM	CC-CD-CE-CF
4	D	204	PLM	CB-CC-CD-CE
4	A	206	PLM	C3-C4-C5-C6
4	C	204	PLM	C4-C5-C6-C7
4	D	205	PLM	CC-CD-CE-CF
4	B	208	PLM	C7-C8-C9-CA
4	D	203	PLM	CD-CE-CF-CG
4	A	206	PLM	C4-C5-C6-C7
4	D	206	PLM	CA-CB-CC-CD
4	L	205	PLM	C8-C9-CA-CB
4	C	204	PLM	CD-CE-CF-CG
4	J	206	PLM	C4-C5-C6-C7
4	B	204	PLM	CB-CC-CD-CE
4	A	205	PLM	CA-CB-CC-CD
2	J	201	JUQ	N11-C28-C29-C30
2	L	201	JUQ	N11-C28-C29-C30
4	L	203	PLM	C5-C6-C7-C8
4	B	206	PLM	C3-C4-C5-C6
4	G	204	PLM	C7-C8-C9-CA
2	J	201	JUQ	O23-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	E	202	PLM	CD-CE-CF-CG
4	J	204	PLM	C9-CA-CB-CC
4	I	204	PLM	C3-C4-C5-C6
4	E	203	PLM	CA-CB-CC-CD
4	A	207	PLM	C2-C3-C4-C5
4	G	205	PLM	C2-C3-C4-C5
4	B	203	PLM	C6-C7-C8-C9
4	B	206	PLM	C7-C8-C9-CA
4	L	204	PLM	C7-C8-C9-CA
4	I	203	PLM	C8-C9-CA-CB
4	I	204	PLM	CC-CD-CE-CF
4	F	205	PLM	C8-C9-CA-CB
4	F	204	PLM	C7-C8-C9-CA
4	B	203	PLM	C8-C9-CA-CB
4	H	203	PLM	CD-CE-CF-CG
4	I	203	PLM	CC-CD-CE-CF
2	I	201	JUQ	C13-C12-N11-C28
2	C	201	JUQ	C13-C12-N11-C28
2	F	201	JUQ	C13-C12-N11-C28
2	E	201	JUQ	C13-C12-N11-C28
2	B	201	JUQ	C13-C12-N11-C28
2	K	201	JUQ	C13-C12-N11-C28
2	H	201	JUQ	C13-C12-N11-C28
4	E	202	PLM	CB-CC-CD-CE
4	F	205	PLM	C7-C8-C9-CA
4	C	206	PLM	C8-C9-CA-CB
4	I	203	PLM	CB-CC-CD-CE
4	B	204	PLM	CA-CB-CC-CD
4	H	203	PLM	CA-CB-CC-CD
4	E	202	PLM	CC-CD-CE-CF
4	C	205	PLM	CD-CE-CF-CG
4	A	207	PLM	CA-CB-CC-CD
4	E	204	PLM	C9-CA-CB-CC
4	B	204	PLM	CC-CD-CE-CF
4	A	206	PLM	C5-C6-C7-C8
4	L	203	PLM	CA-CB-CC-CD
2	I	201	JUQ	C25-C12-N11-C28
2	A	201	JUQ	C25-C12-N11-C28
2	D	201	JUQ	C25-C12-N11-C28
4	I	204	PLM	C4-C5-C6-C7
4	B	205	PLM	CB-CC-CD-CE
4	A	207	PLM	C9-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
4	C	204	PLM	C3-C4-C5-C6
2	C	201	JUQ	C29-C28-N11-C7
2	C	201	JUQ	C29-C28-N11-C12
2	E	201	JUQ	C29-C28-N11-C7
2	H	201	JUQ	C29-C28-N11-C7
2	H	201	JUQ	C29-C28-N11-C12
4	L	206	PLM	CB-CC-CD-CE
4	A	204	PLM	C3-C4-C5-C6
4	F	205	PLM	C9-CA-CB-CC
4	H	203	PLM	C8-C9-CA-CB
4	F	202	PLM	CA-CB-CC-CD
4	F	205	PLM	CA-CB-CC-CD
4	B	203	PLM	CD-CE-CF-CG
4	D	206	PLM	C9-CA-CB-CC
4	L	205	PLM	C7-C8-C9-CA
2	A	201	JUQ	C13-C12-N11-C28
2	D	201	JUQ	C13-C12-N11-C28
4	C	207	PLM	C7-C8-C9-CA
4	F	203	PLM	CA-CB-CC-CD
4	A	207	PLM	C4-C5-C6-C7
4	C	206	PLM	C7-C8-C9-CA
4	D	203	PLM	CC-CD-CE-CF
4	B	208	PLM	C9-CA-CB-CC
2	H	201	JUQ	N24-C25-O26-C27
4	F	205	PLM	CC-CD-CE-CF
4	L	203	PLM	C2-C3-C4-C5
2	A	201	JUQ	O23-C16-C17-C18
2	D	201	JUQ	O23-C16-C17-C18
4	G	205	PLM	C5-C6-C7-C8
4	B	208	PLM	C8-C9-CA-CB
4	A	205	PLM	C8-C9-CA-CB
4	D	204	PLM	CA-CB-CC-CD
4	D	206	PLM	C5-C6-C7-C8
4	B	206	PLM	C9-CA-CB-CC
4	A	203	PLM	CA-CB-CC-CD
5	B	209	LMT	O1'-C1-C2-C3
4	J	207	PLM	CA-CB-CC-CD
4	B	207	PLM	CB-CC-CD-CE
4	I	204	PLM	CB-CC-CD-CE
4	C	205	PLM	C9-CA-CB-CC
4	B	207	PLM	C7-C8-C9-CA
4	J	207	PLM	C7-C8-C9-CA

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Mol	Chain	Res	Type	Atoms
2	E	201	JUQ	C25-C12-N11-C28
4	C	205	PLM	CA-CB-CC-CD
4	J	206	PLM	CA-CB-CC-CD
4	A	205	PLM	CC-CD-CE-CF
4	I	204	PLM	CD-CE-CF-CG
4	G	205	PLM	C4-C5-C6-C7
4	F	205	PLM	CD-CE-CF-CG
2	B	201	JUQ	O23-C16-C17-C18
2	D	201	JUQ	C15-C16-C17-C18
2	J	201	JUQ	C15-C16-C17-C18
2	E	201	JUQ	C15-C16-C17-C18
2	L	201	JUQ	C15-C16-C17-C18
2	H	201	JUQ	C15-C16-C17-C18
4	H	203	PLM	C9-CA-CB-CC
2	I	201	JUQ	C5-C7-N11-C28
2	A	201	JUQ	C5-C7-N11-C28
2	D	201	JUQ	C5-C7-N11-C28
2	E	201	JUQ	C5-C7-N11-C28
4	L	203	PLM	CD-CE-CF-CG
4	A	203	PLM	CC-CD-CE-CF
4	I	204	PLM	C5-C6-C7-C8
4	A	206	PLM	CC-CD-CE-CF
4	A	205	PLM	C7-C8-C9-CA
4	G	203	PLM	CA-CB-CC-CD
4	G	204	PLM	CD-CE-CF-CG

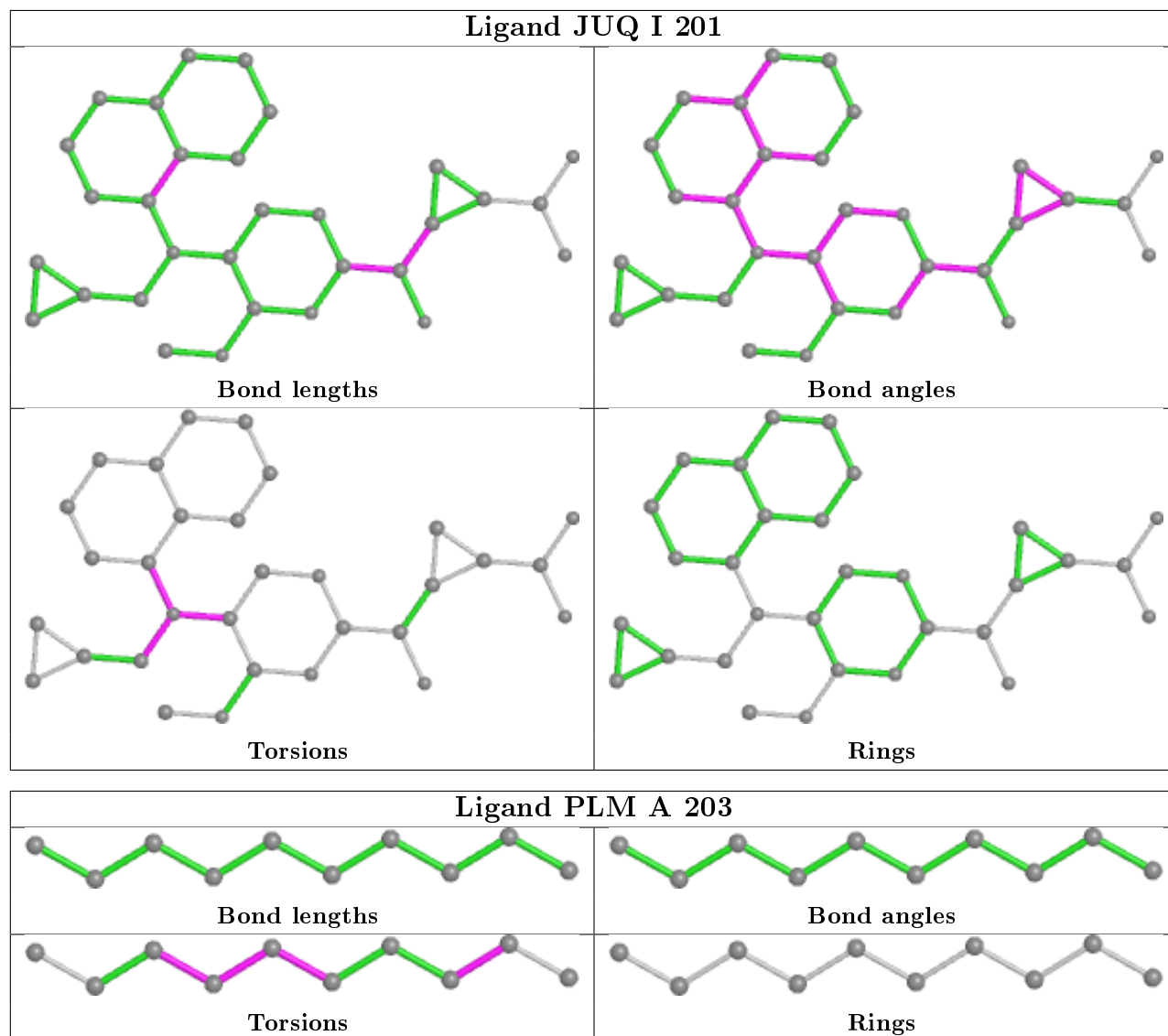
There are no ring outliers.

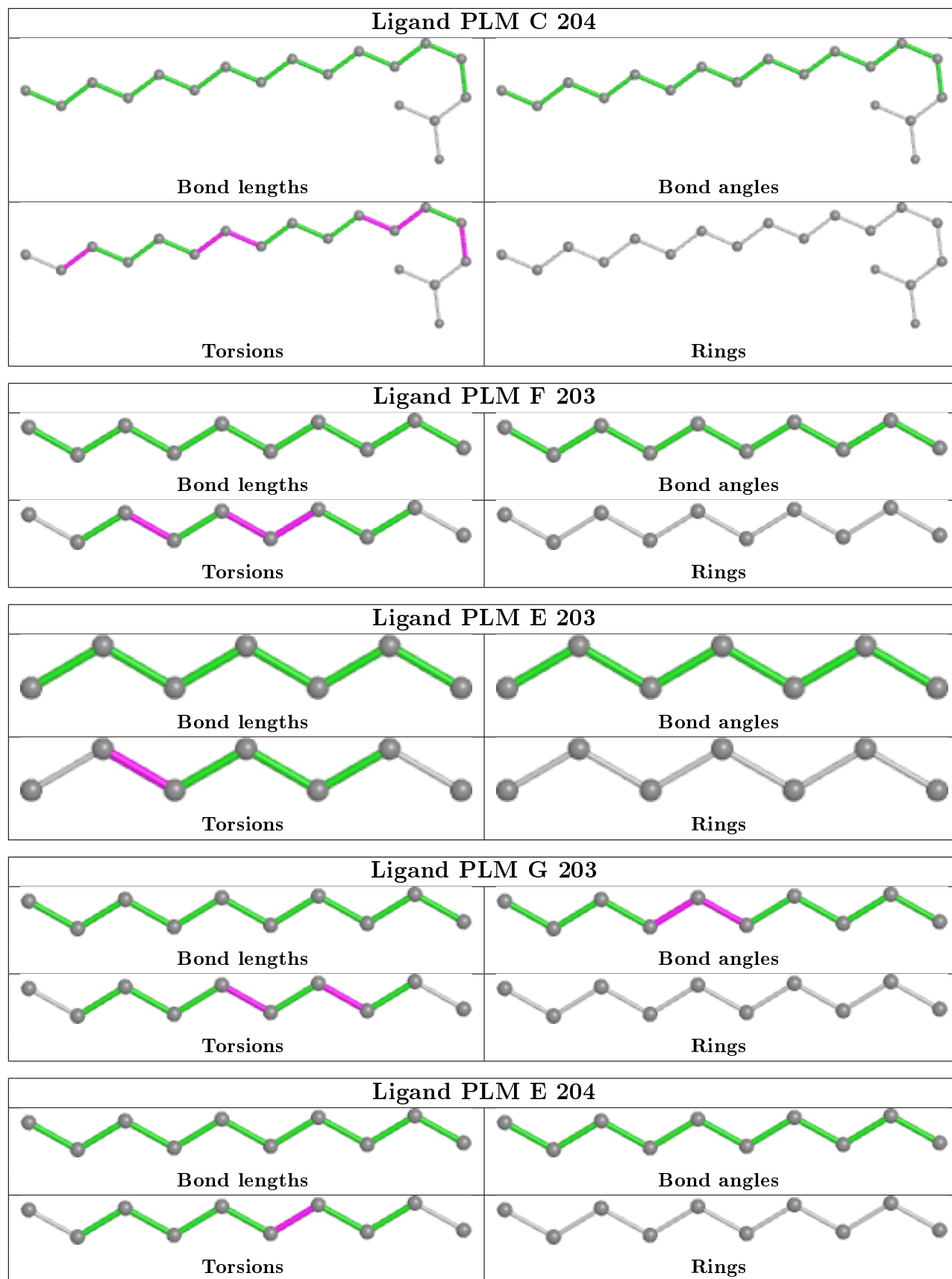
4 monomers are involved in 4 short contacts:

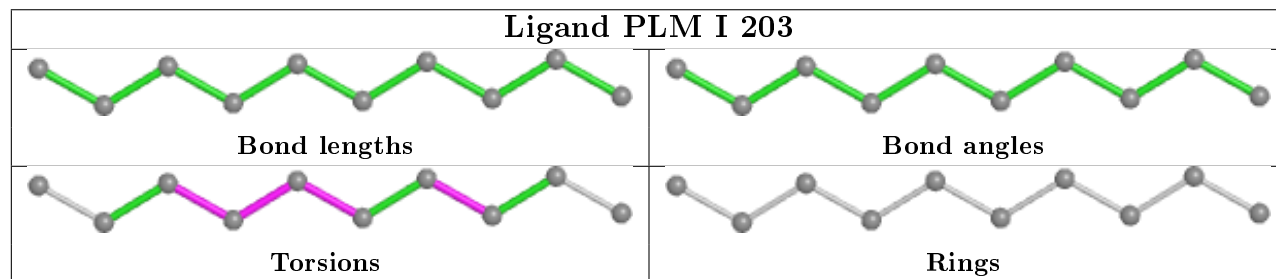
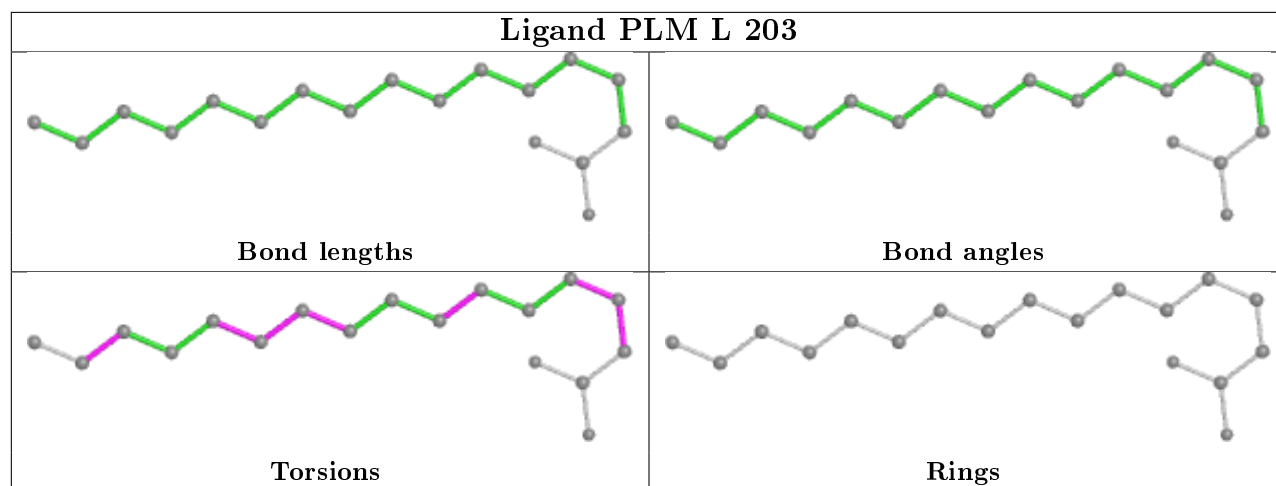
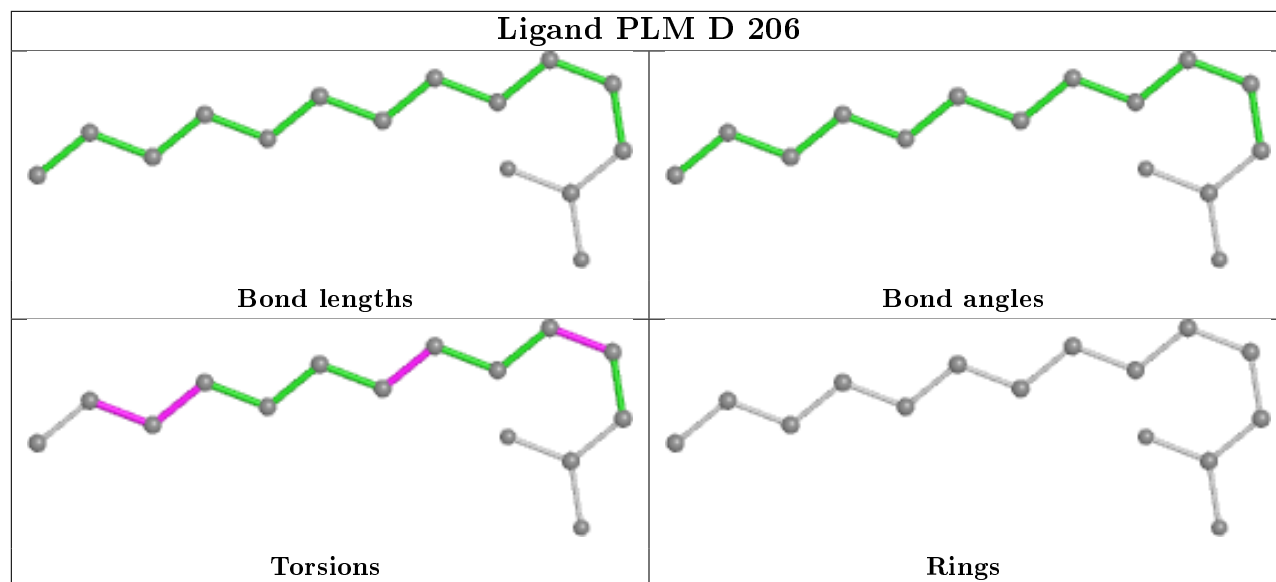
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	201	JUQ	1	0
4	G	204	PLM	1	0
4	F	202	PLM	1	0
4	A	206	PLM	1	0

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

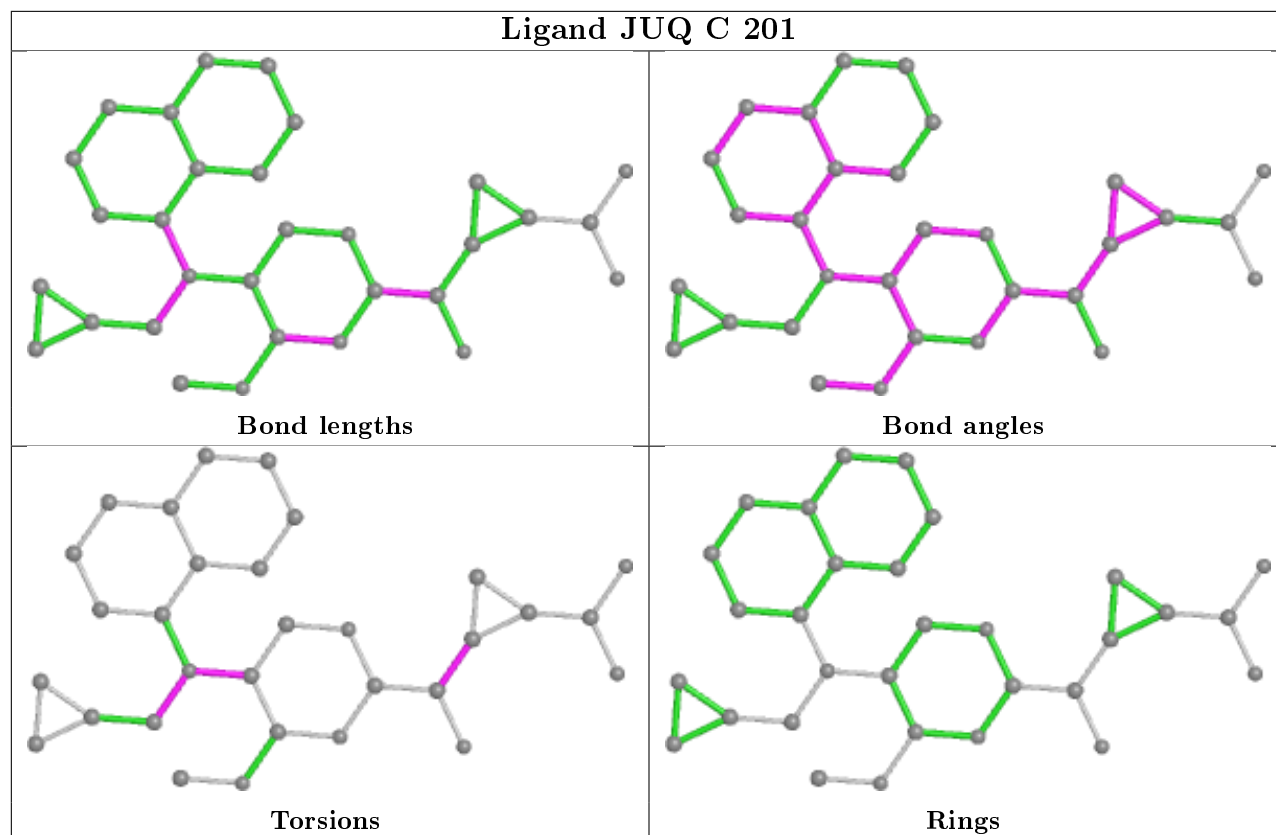
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



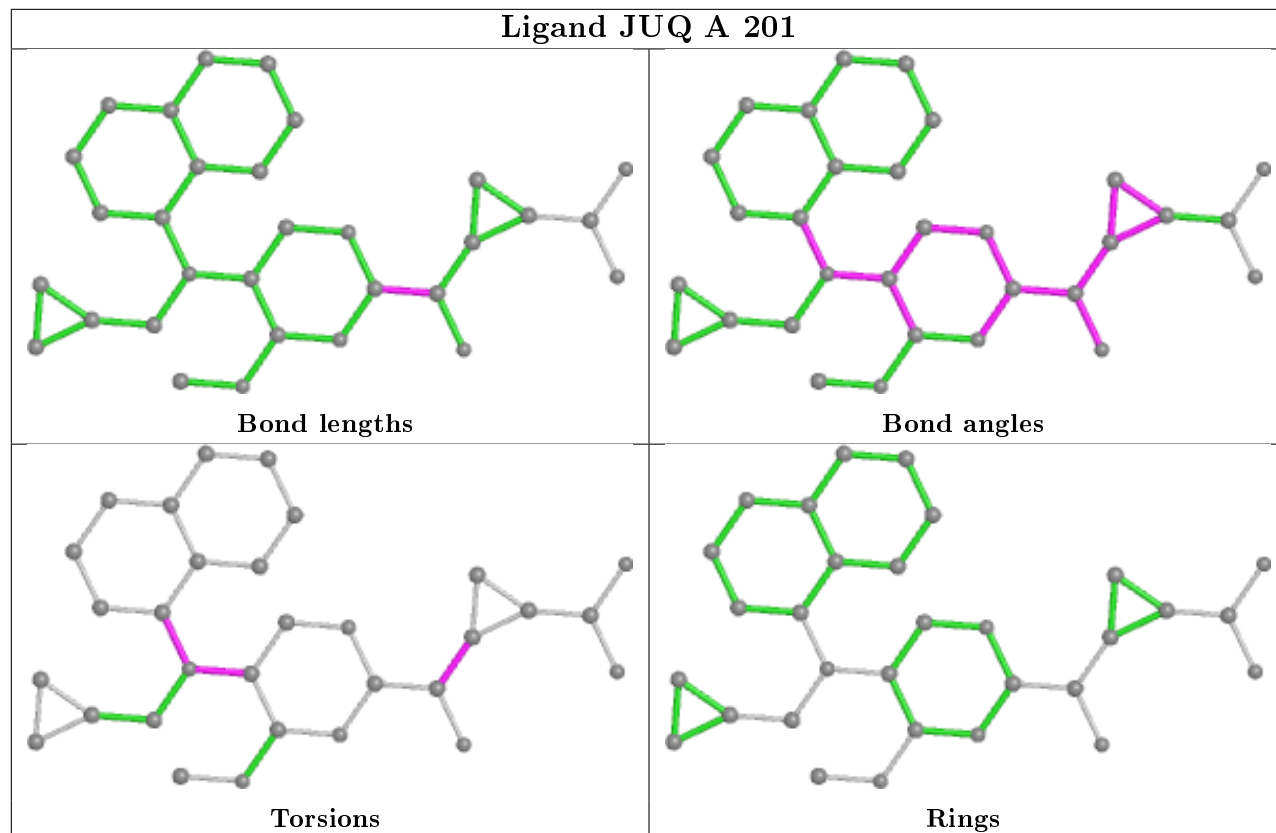


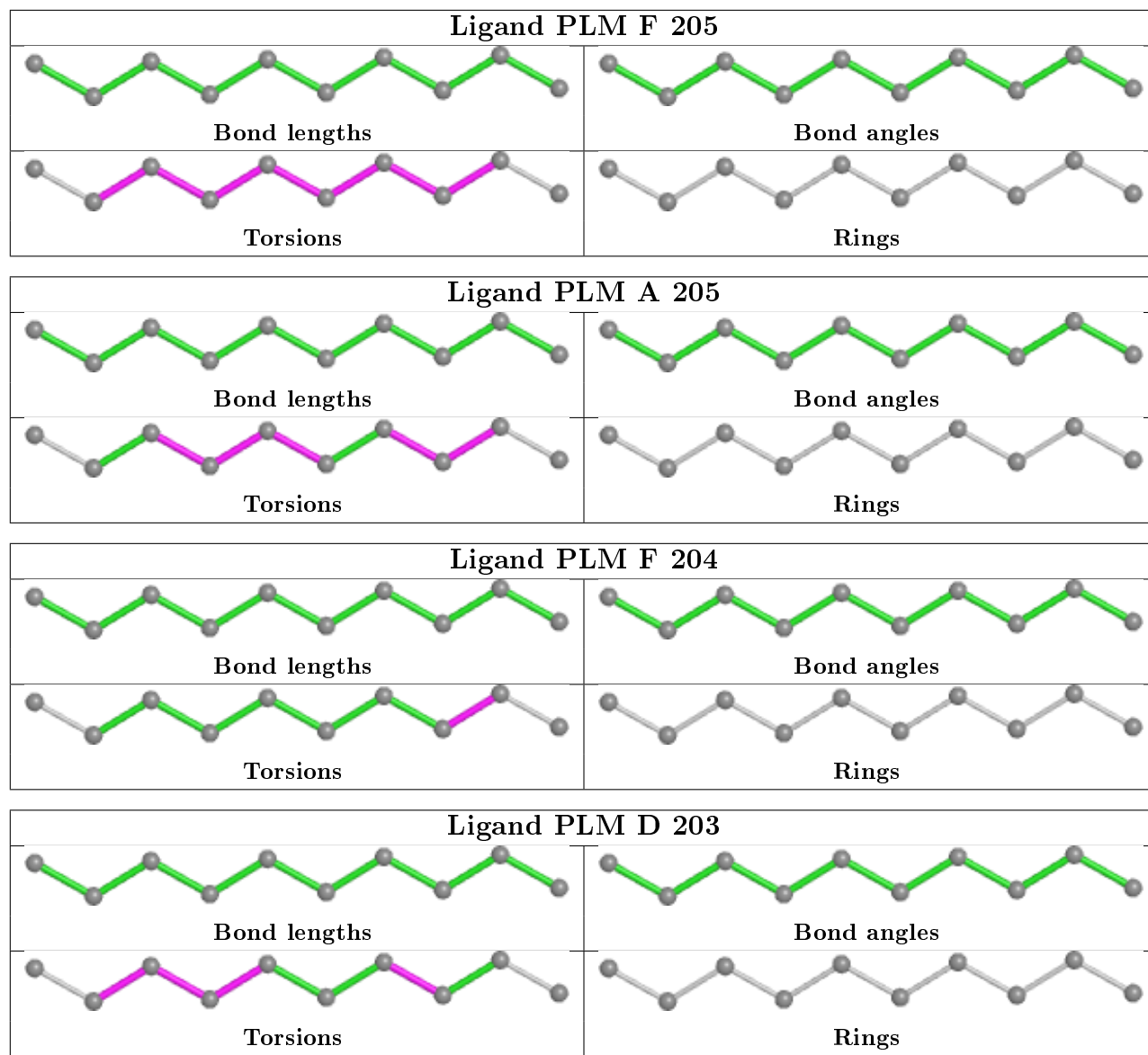


Ligand JUQ C 201

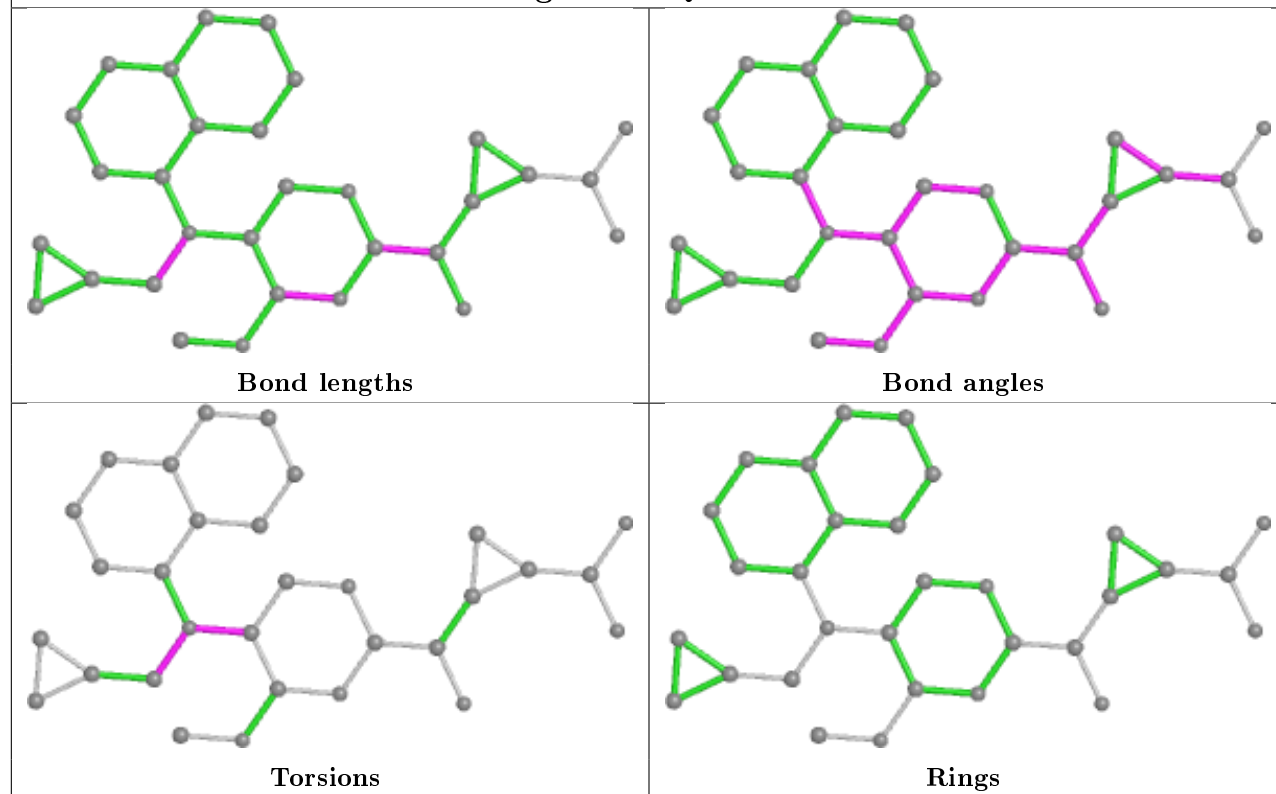


Ligand JUQ A 201

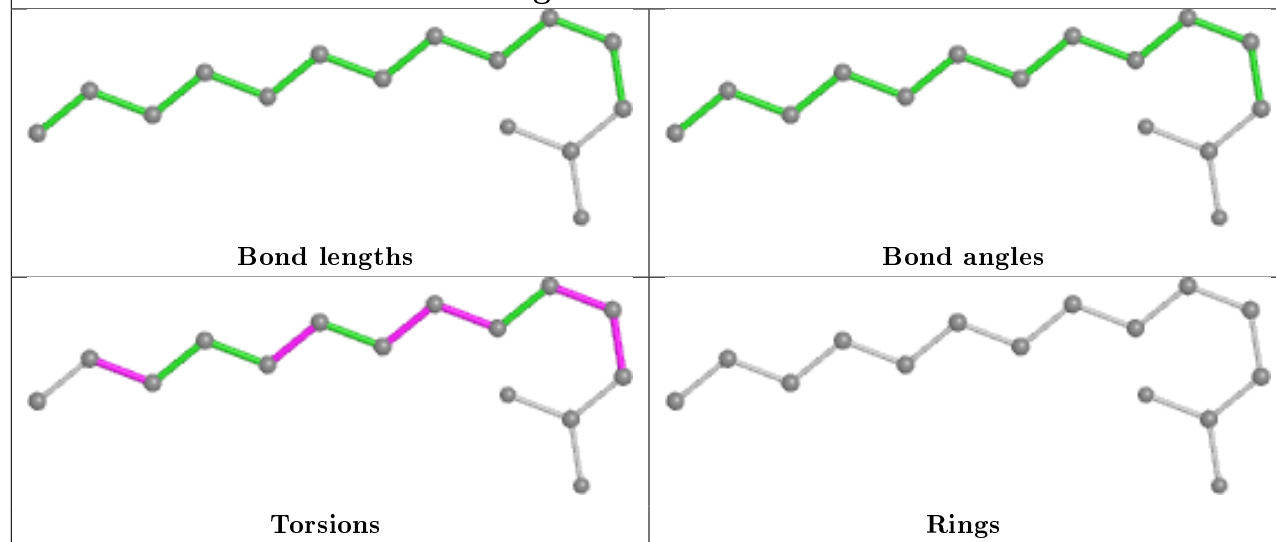




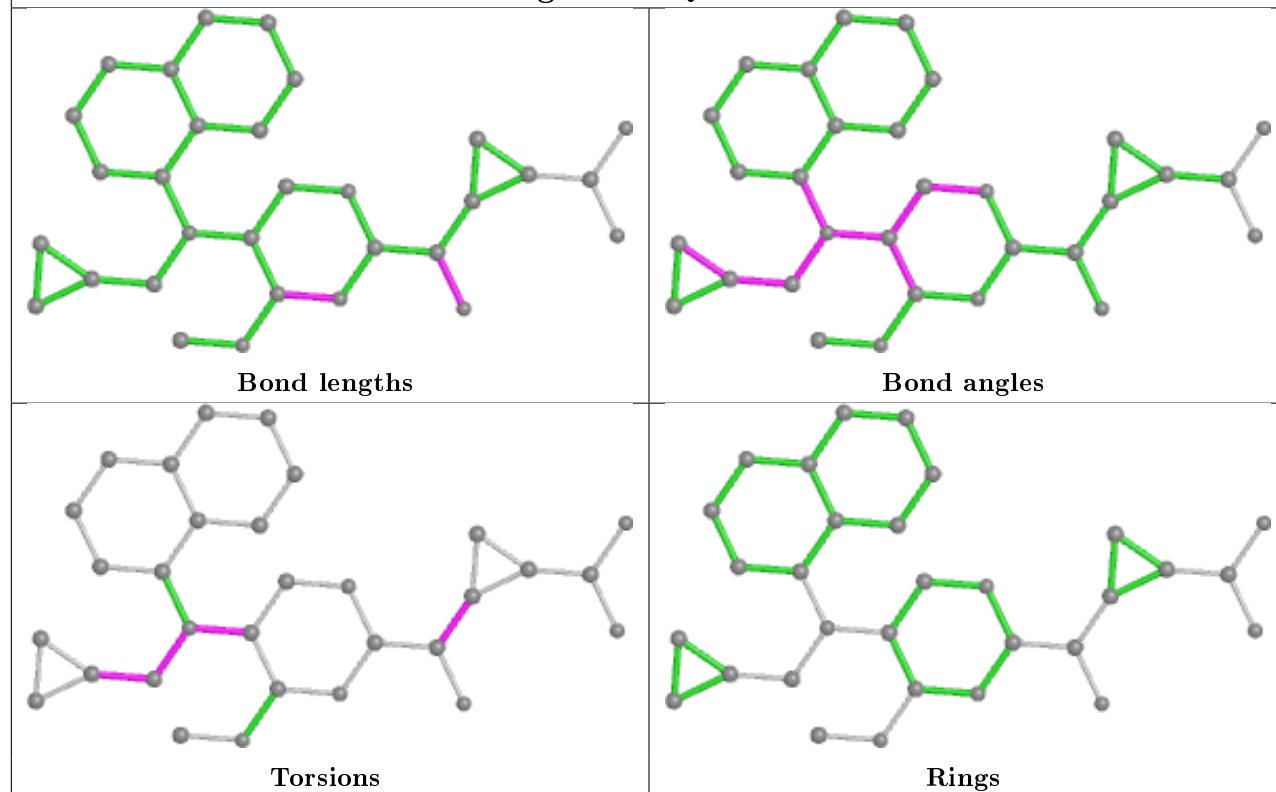
Ligand JUQ F 201



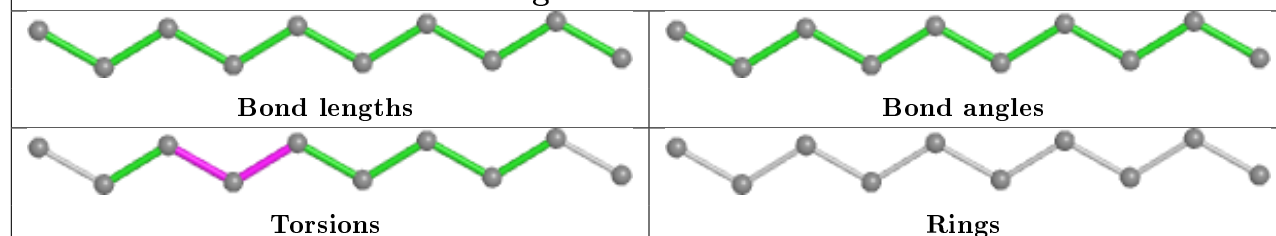
Ligand PLM J 207



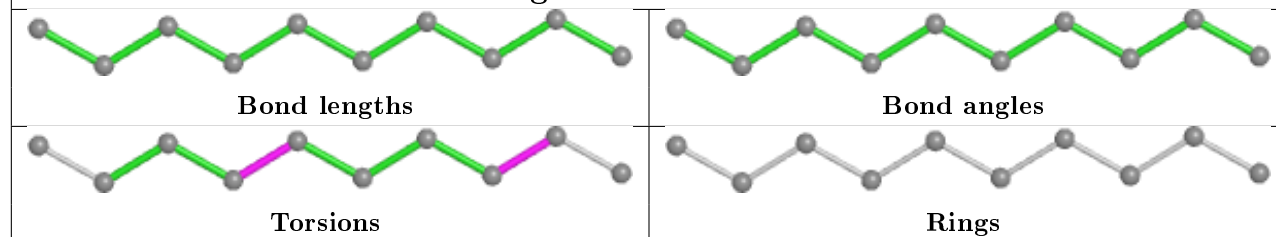
Ligand JUQ J 201

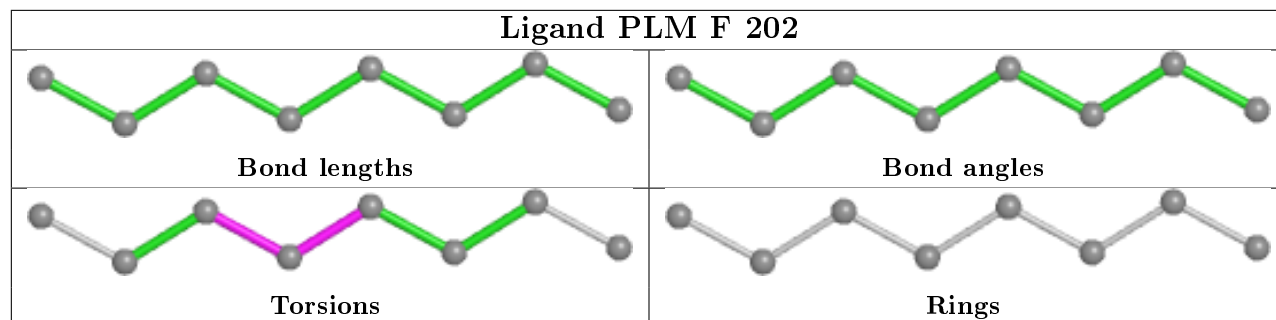
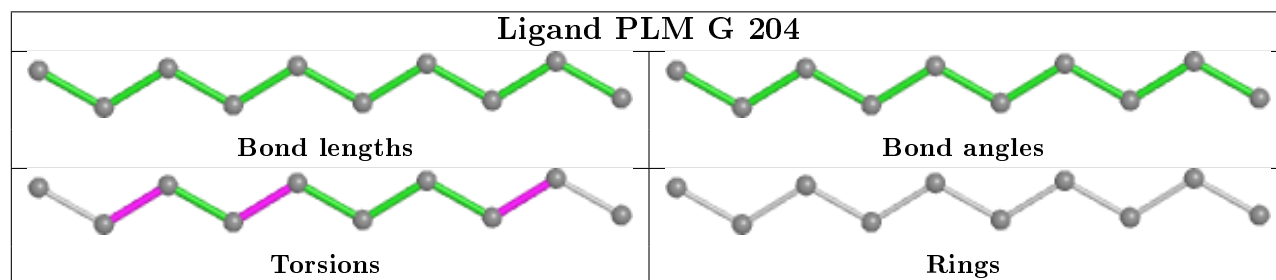
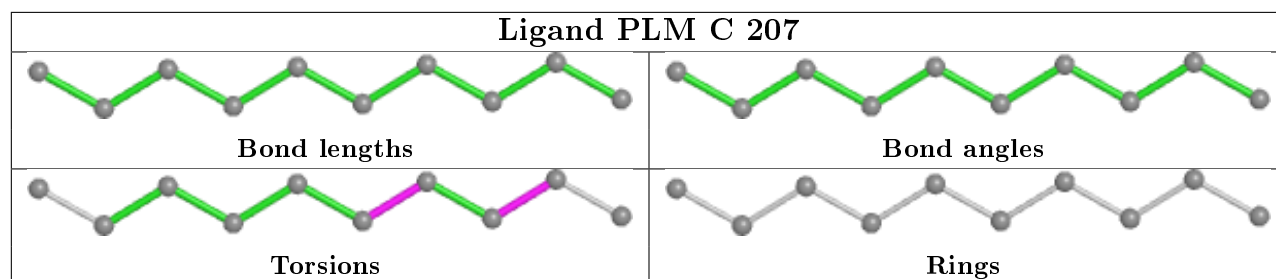
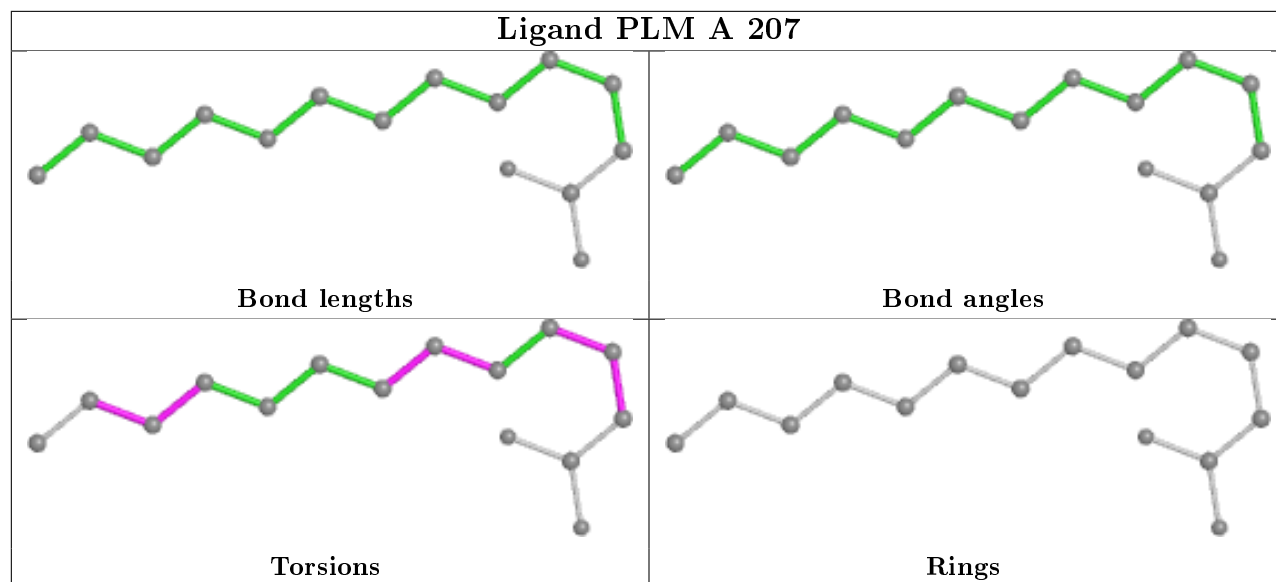


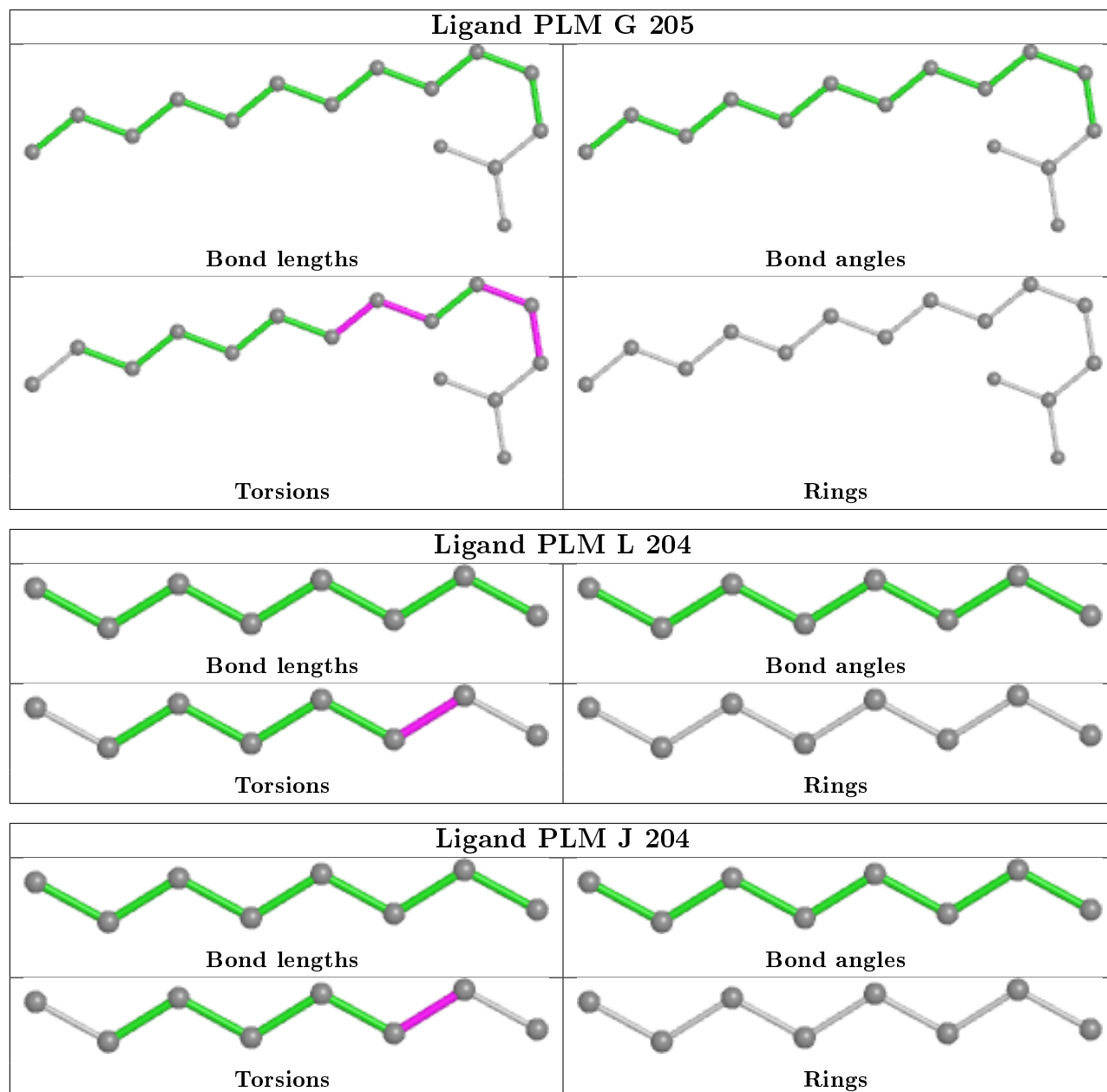
Ligand PLM L 206

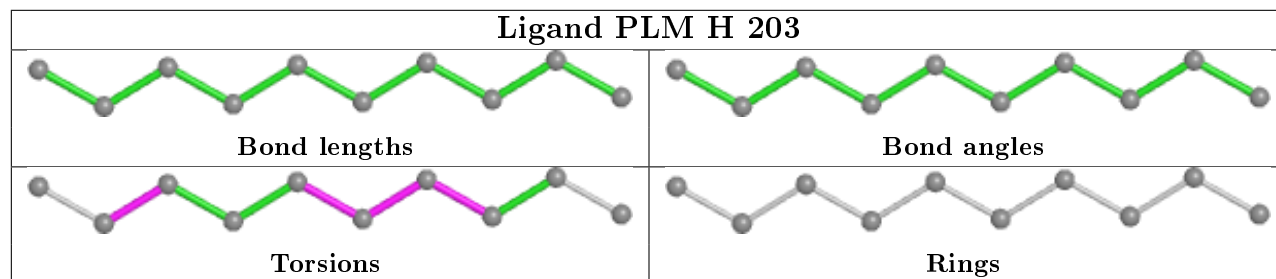
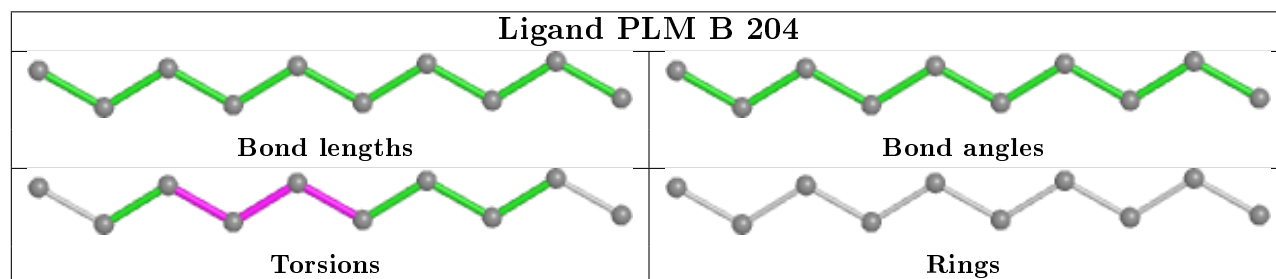
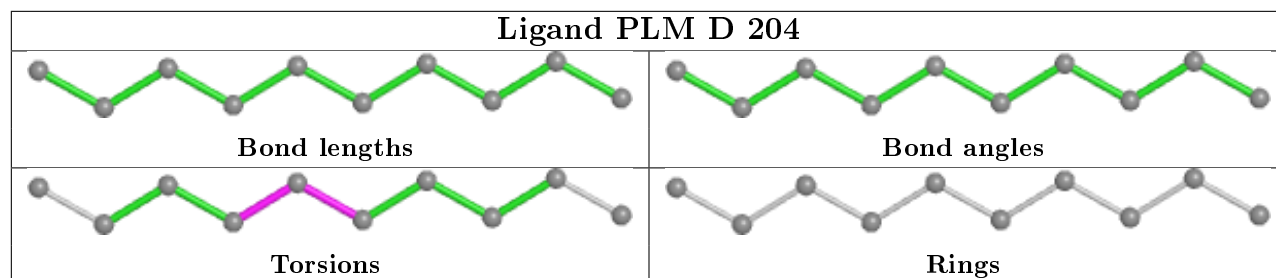
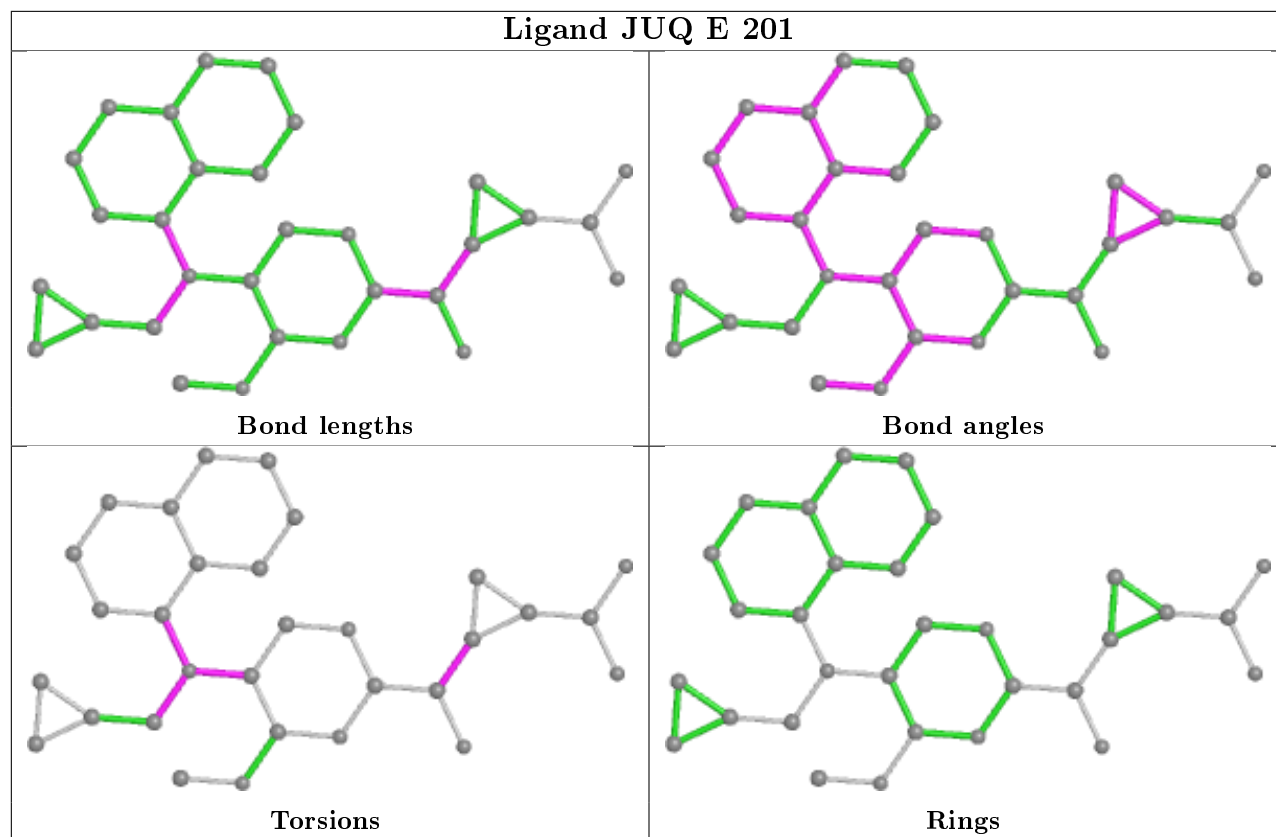


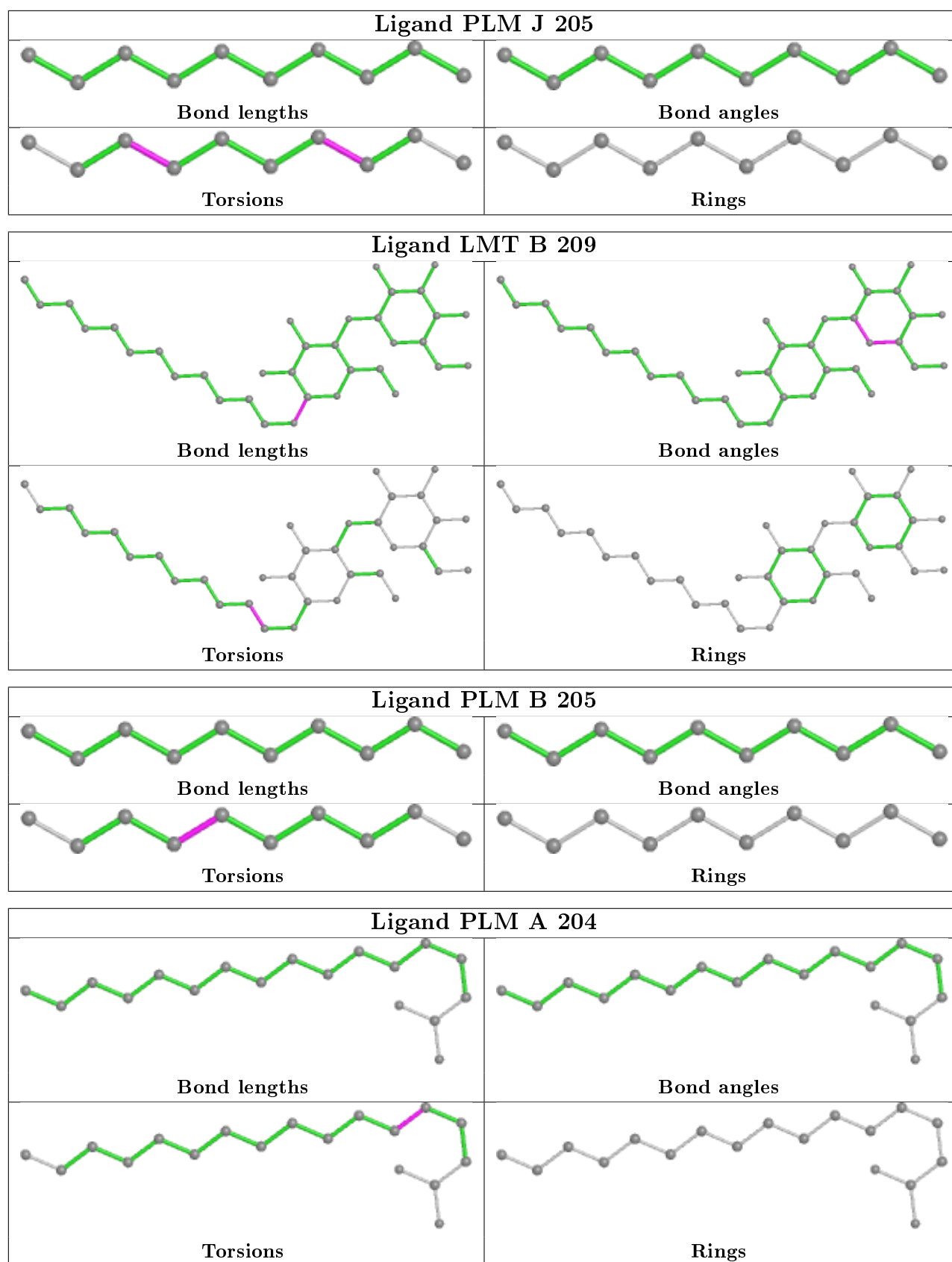
Ligand PLM B 207

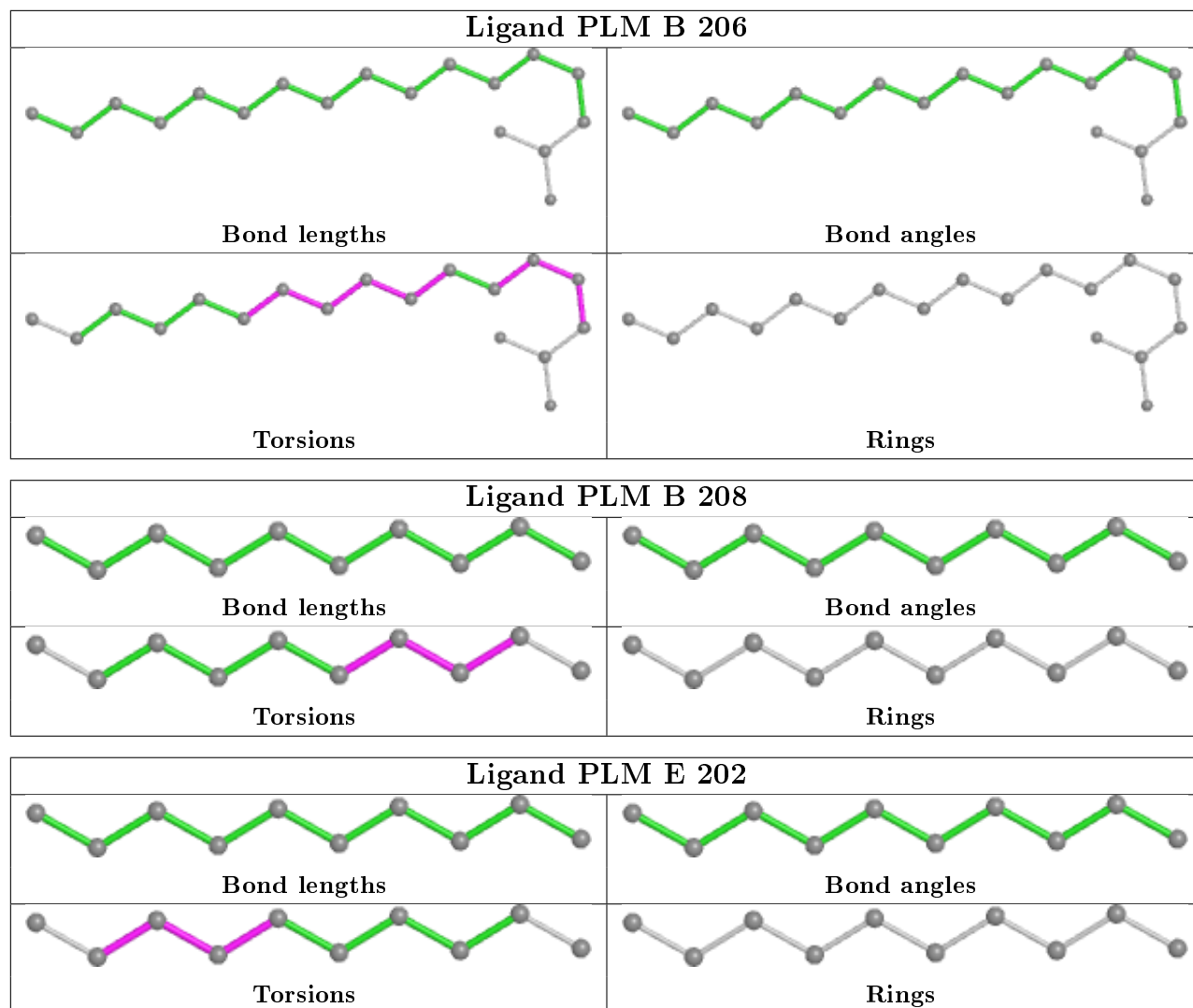




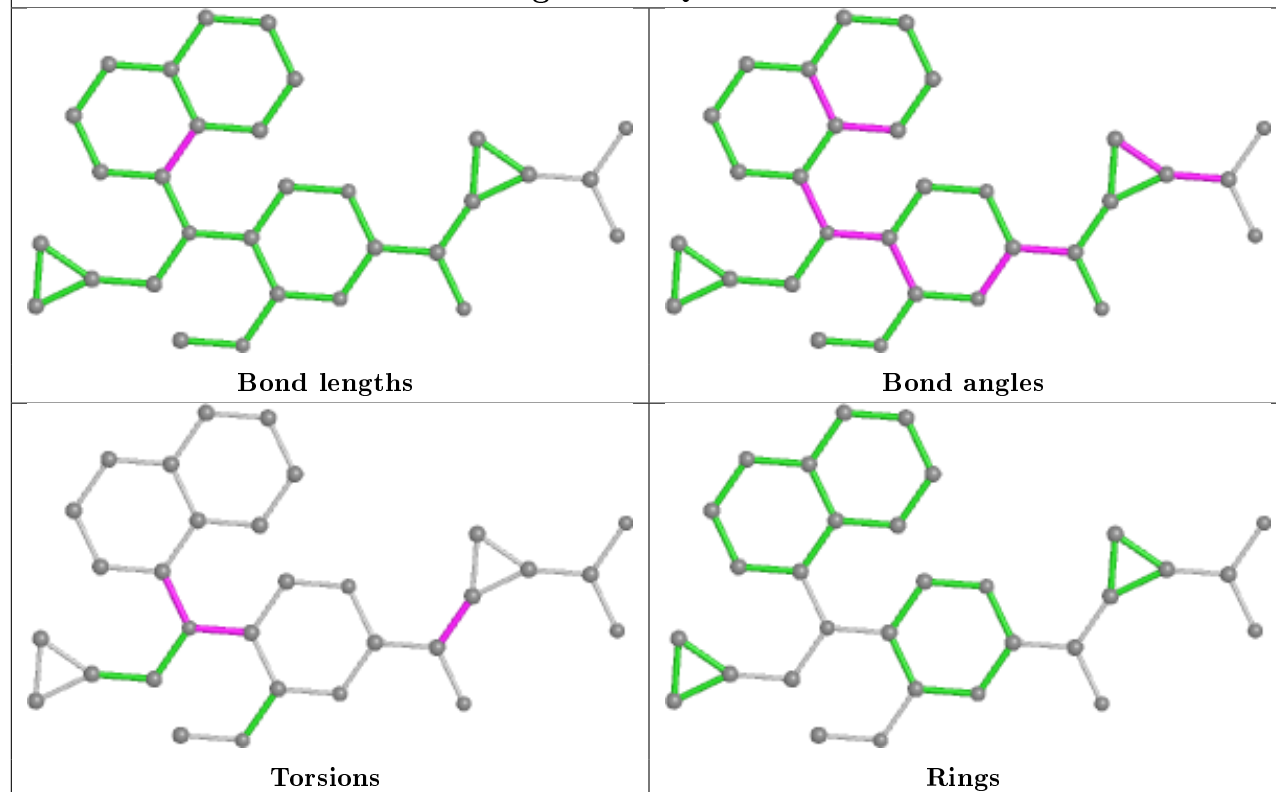




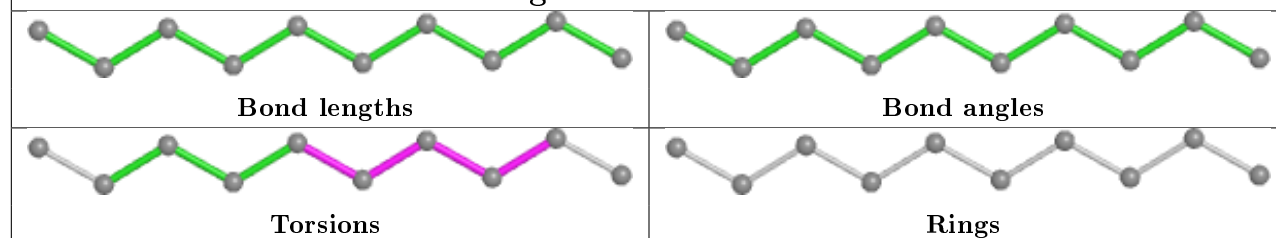




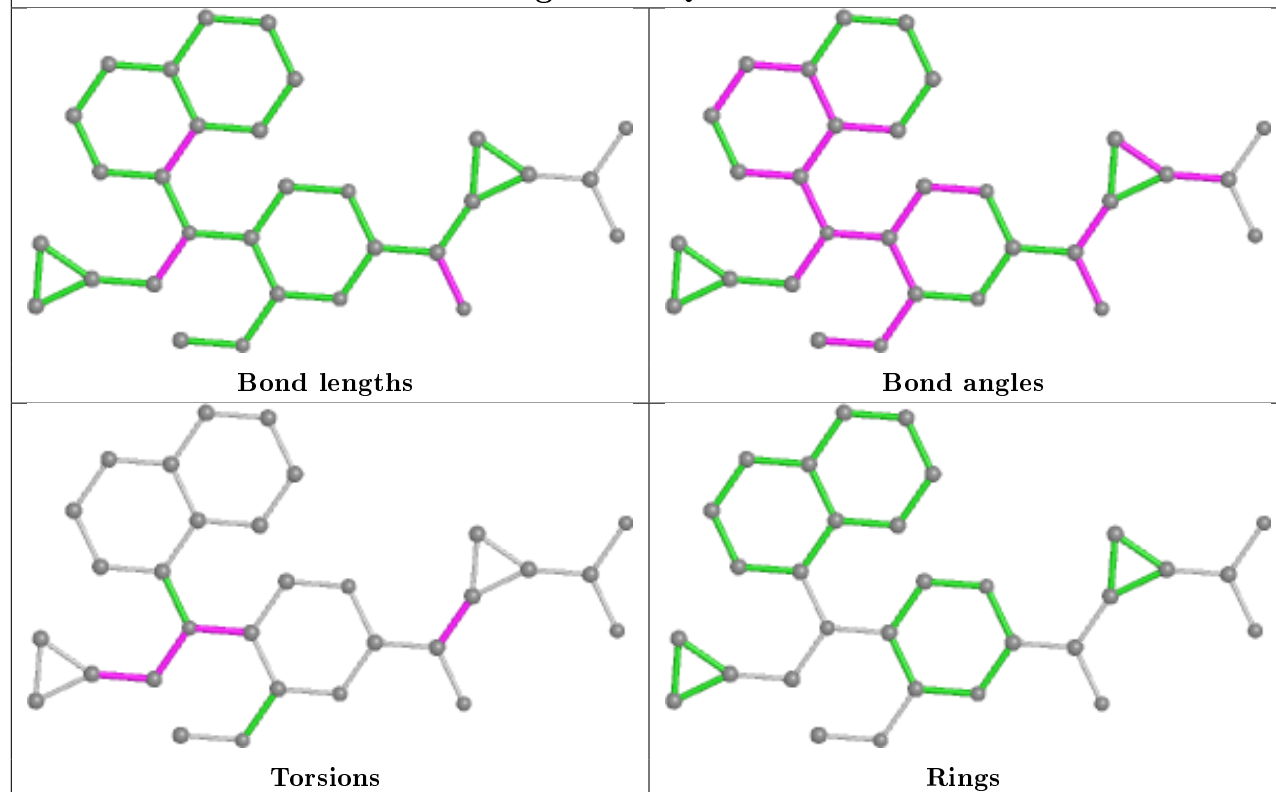
Ligand JUQ D 201



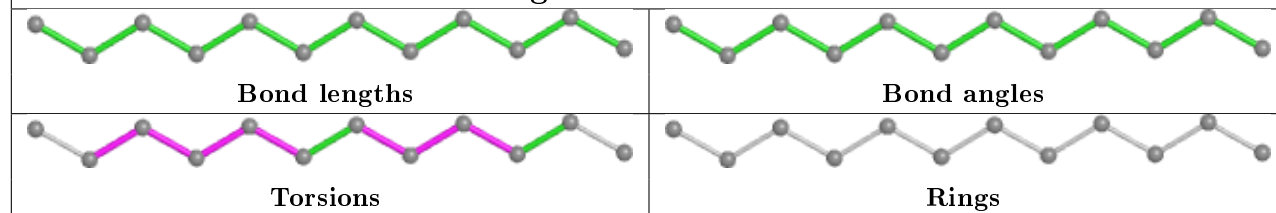
Ligand PLM C 206

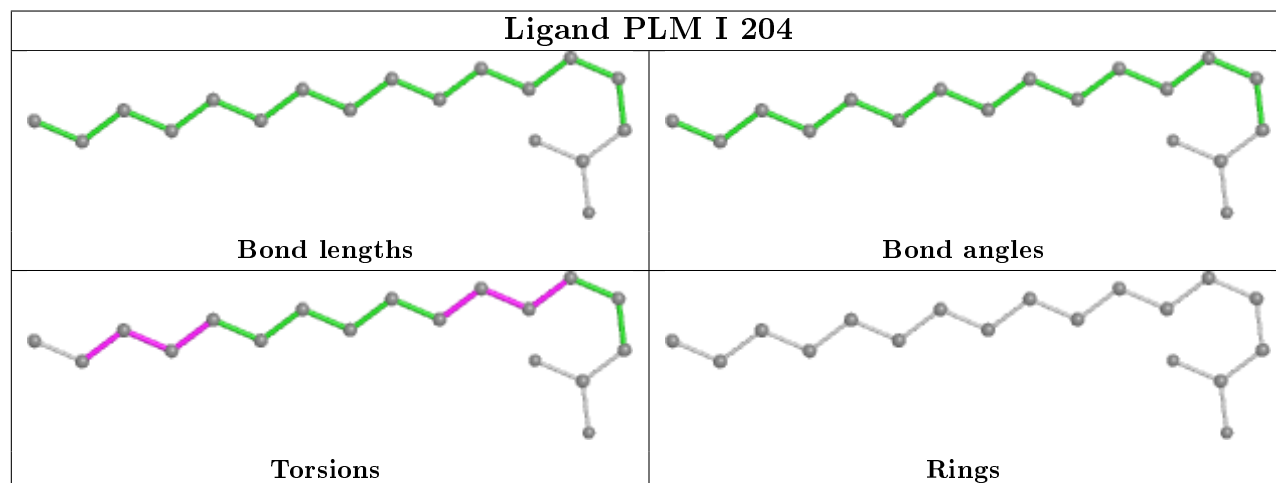
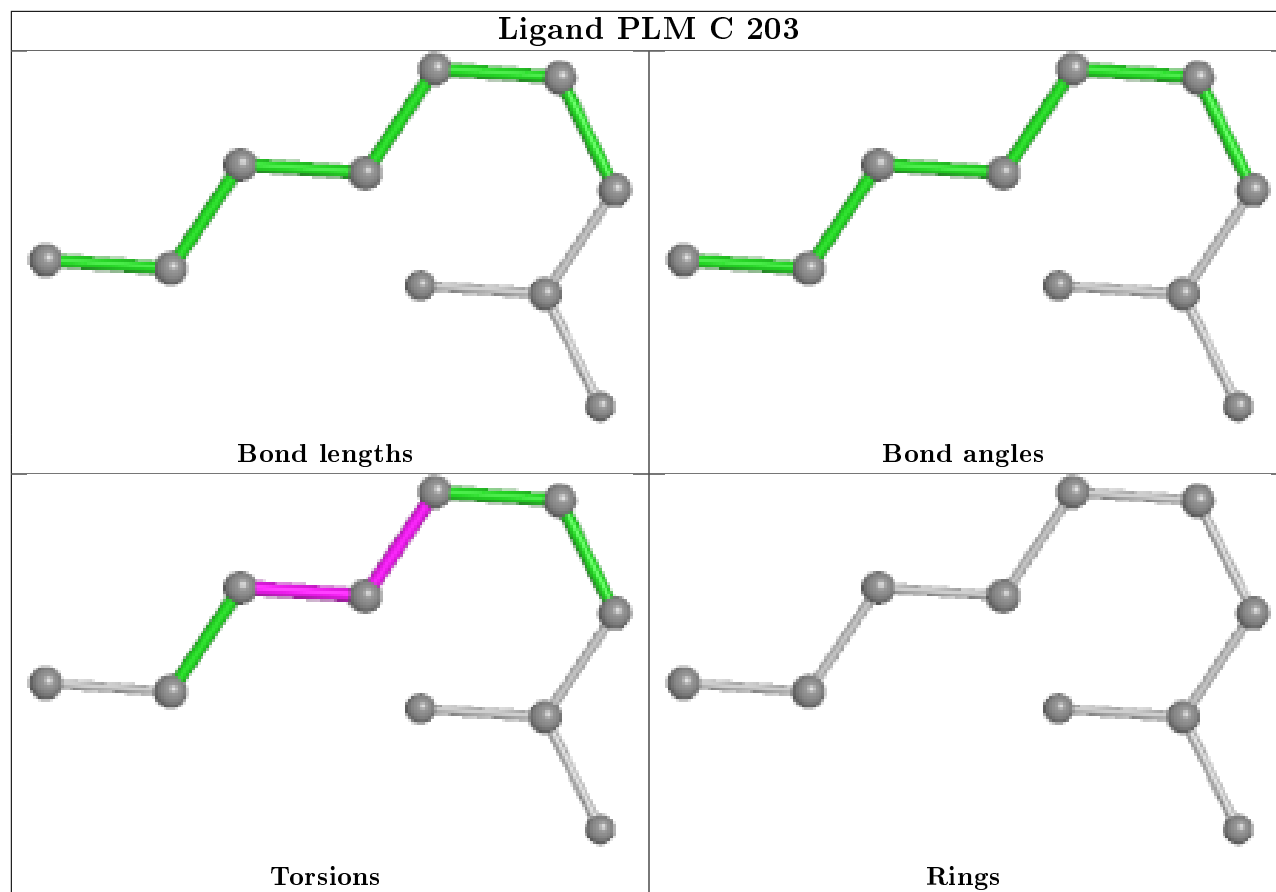


Ligand JUQ L 201

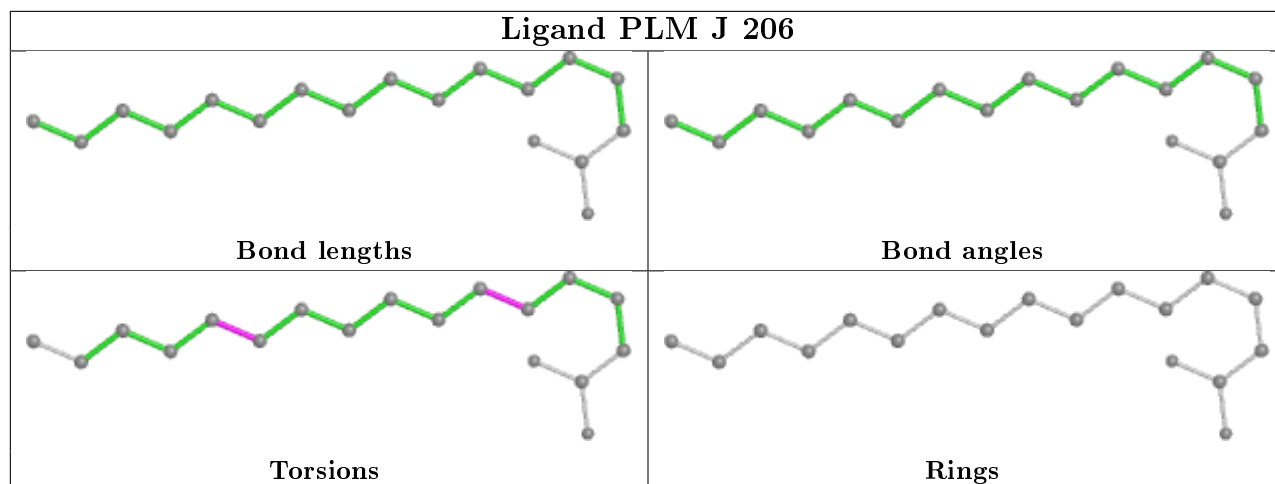


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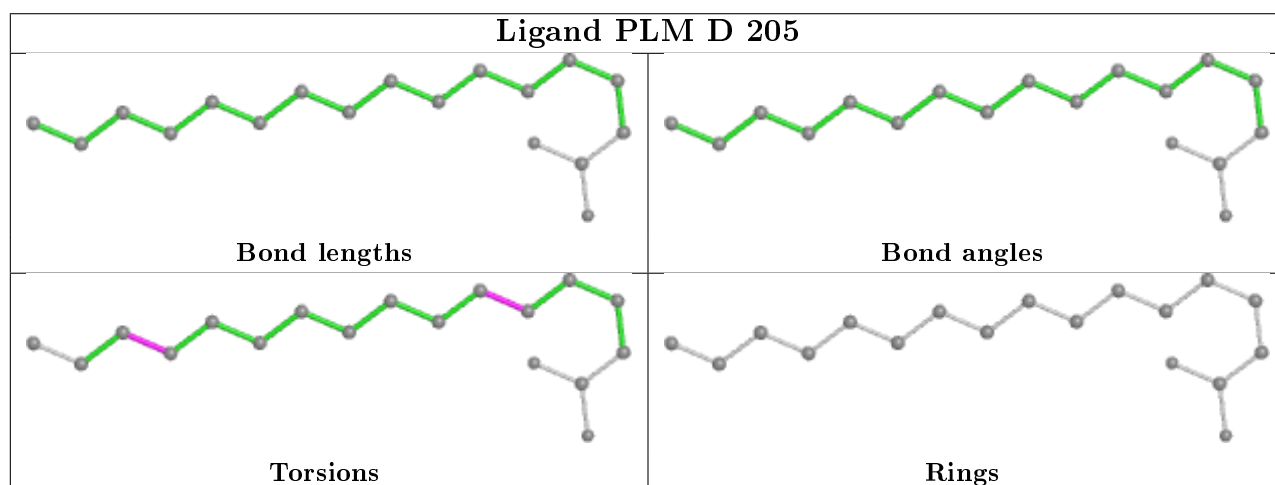




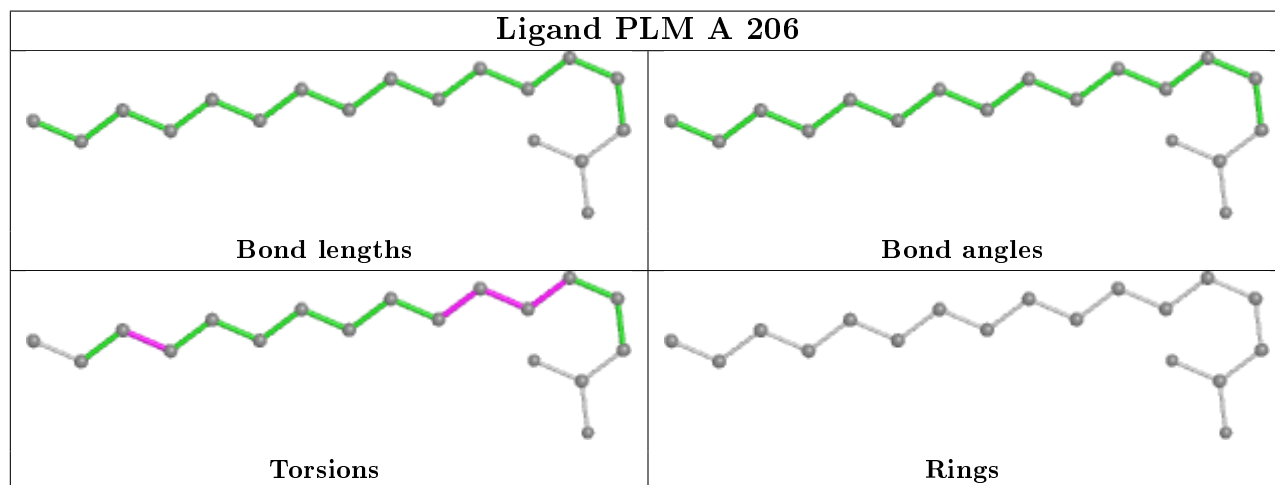
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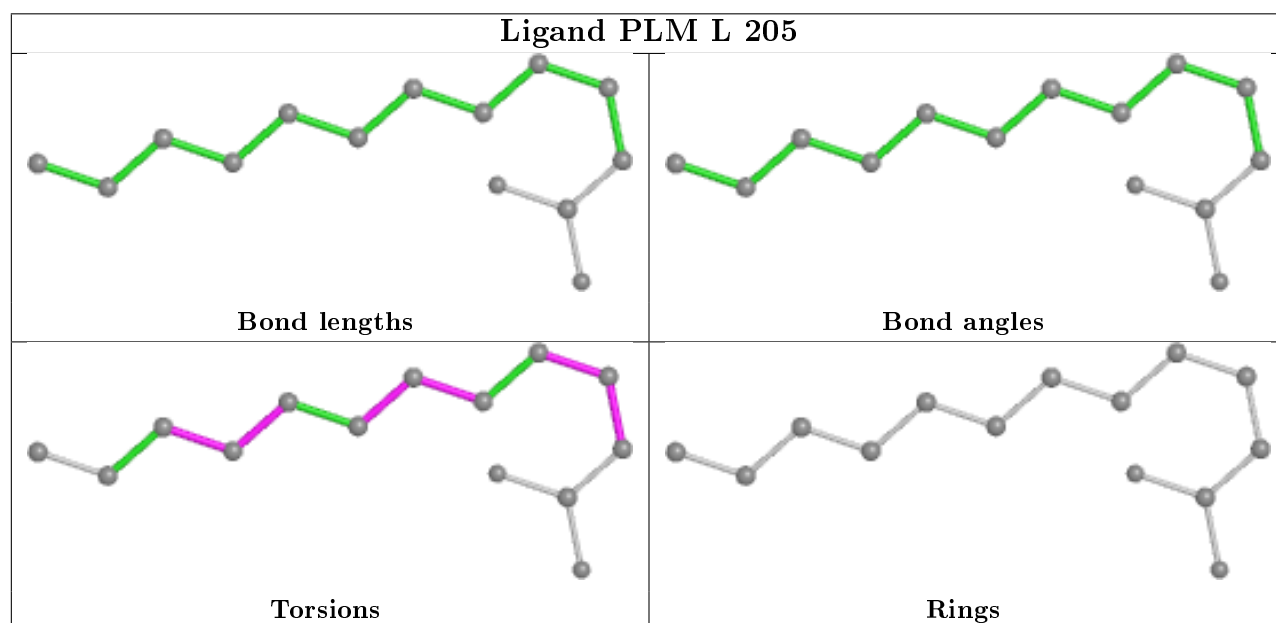
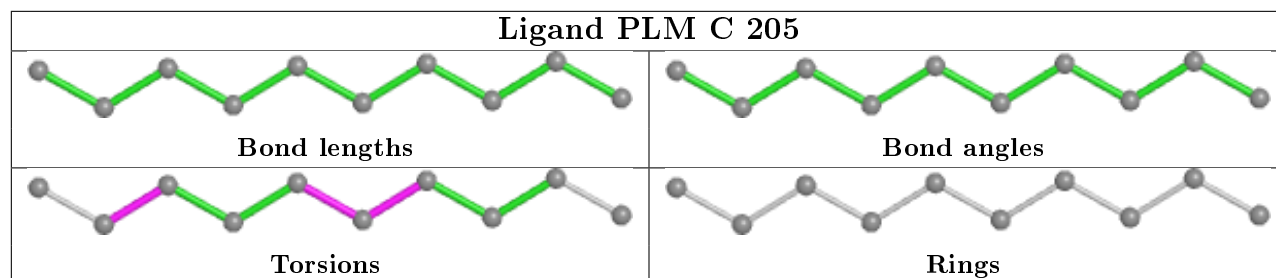
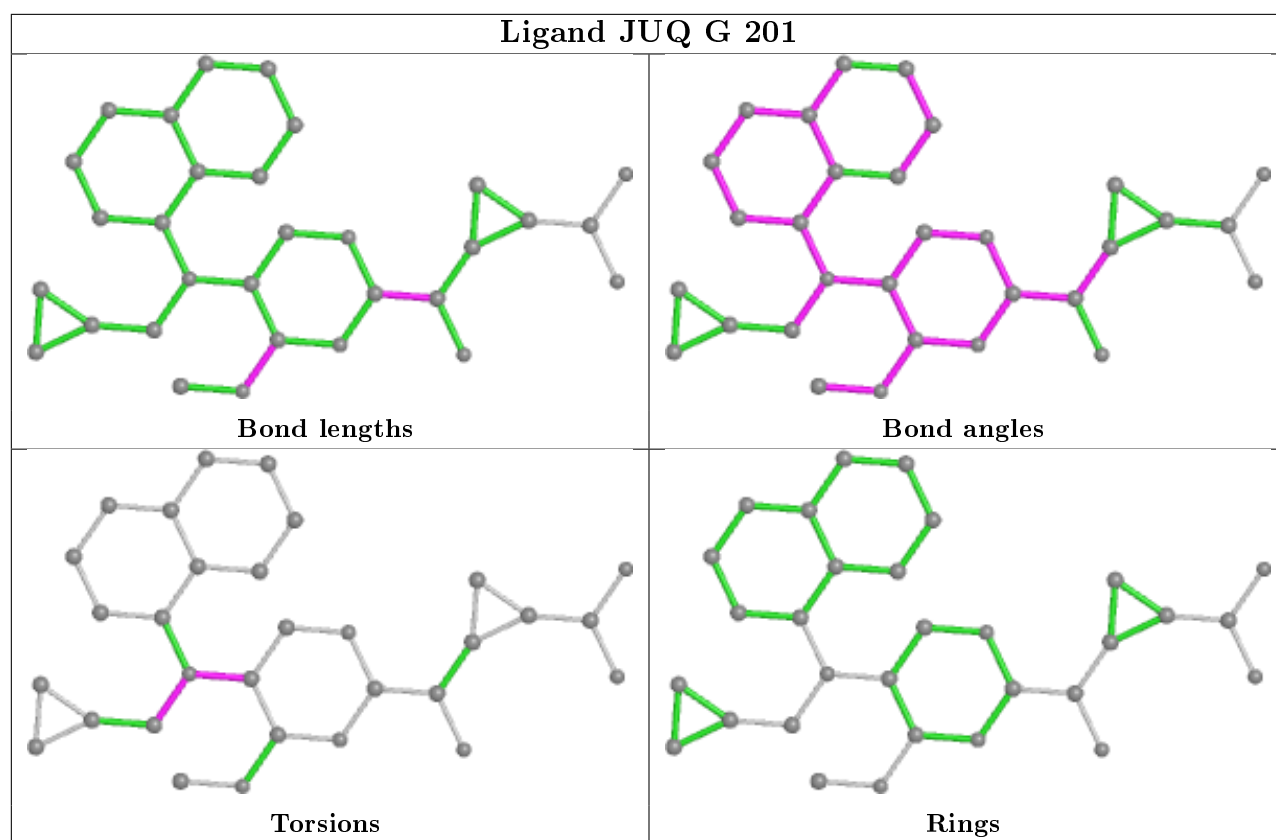


Ligand PLM D 205

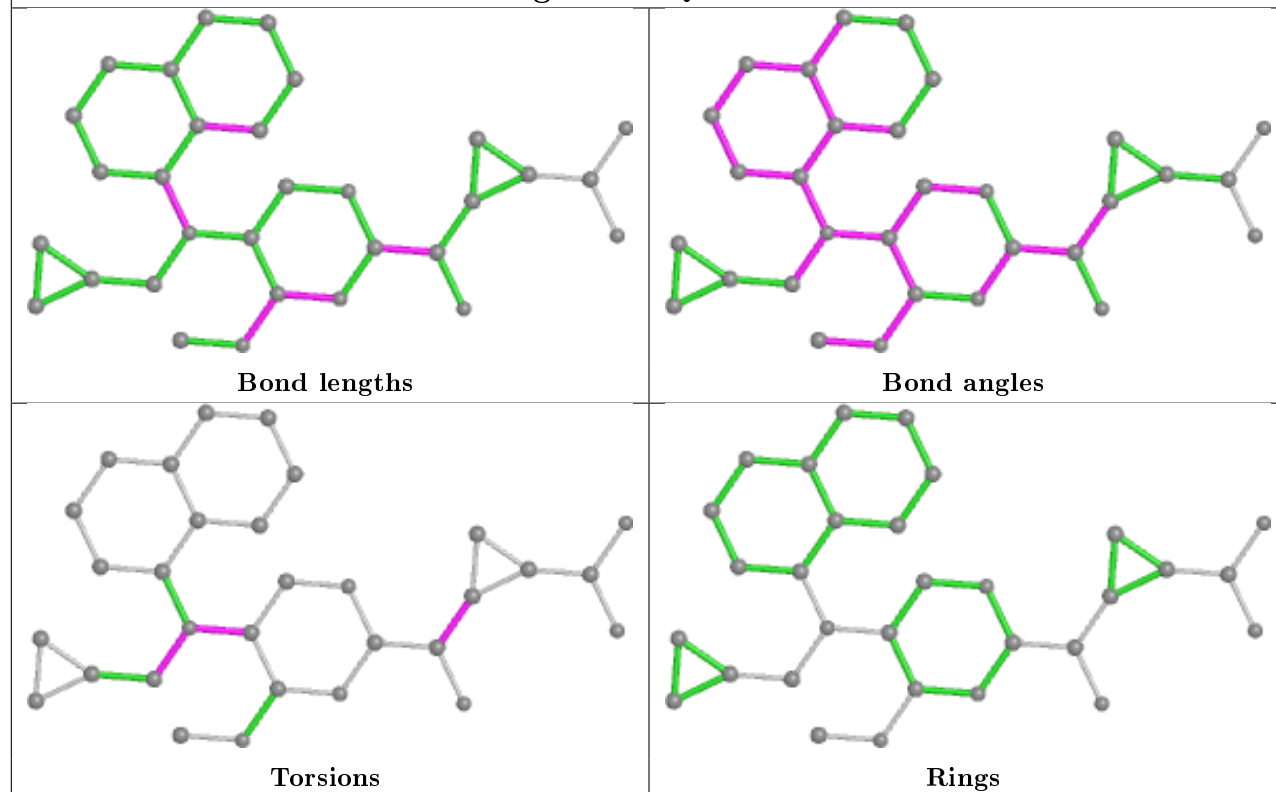


Ligand PLM A 206

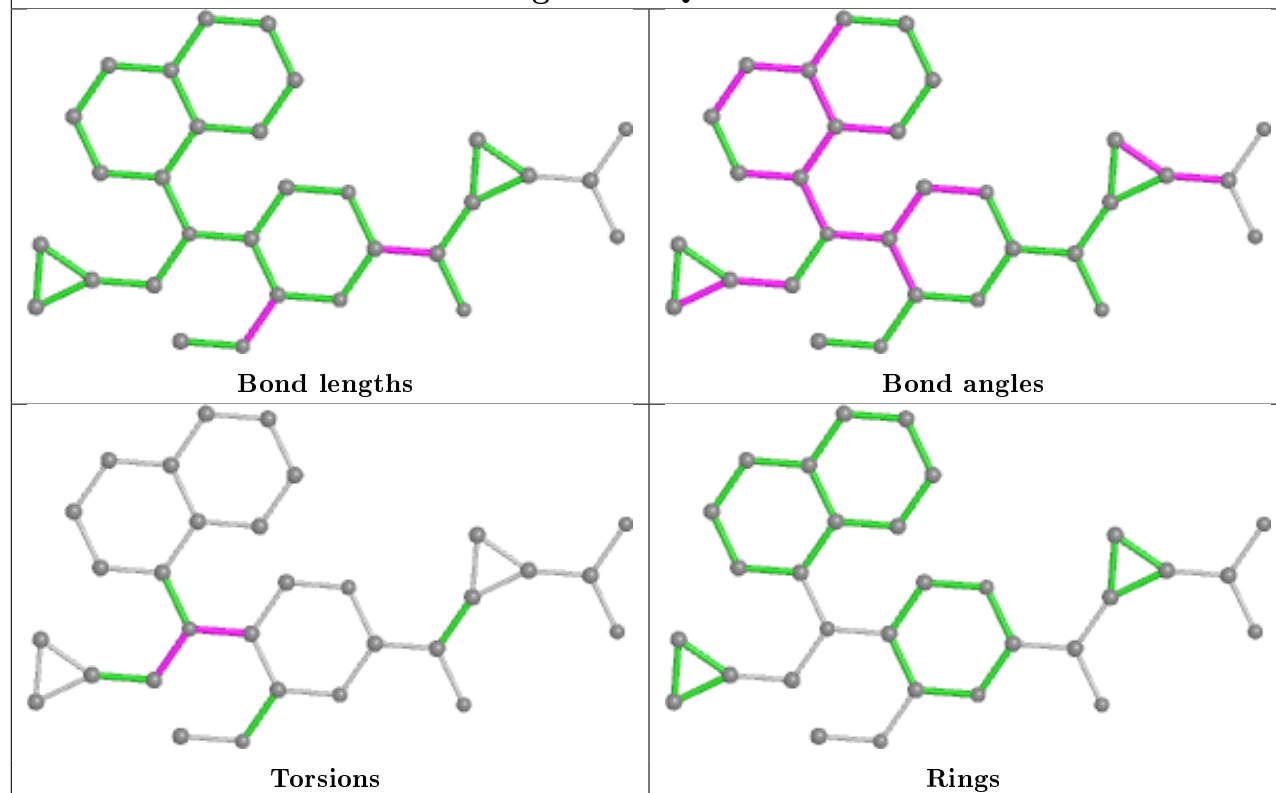


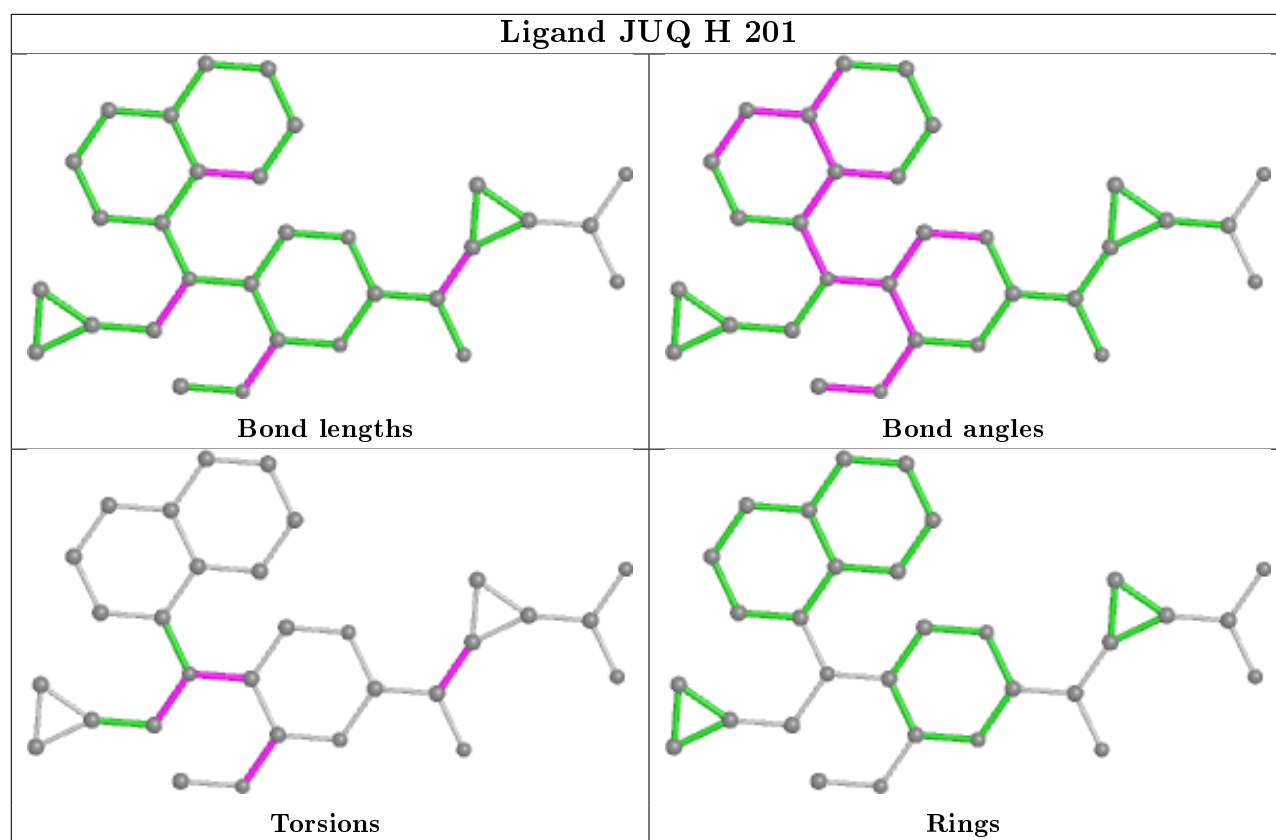


Ligand JUQ B 201



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	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

All (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
1	J	39	LEU	3.8
1	L	46	PHE	3.8
1	F	141	GLY	3.6
1	J	35	VAL	3.5
1	H	33	PHE	3.3
1	L	41	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	38	PRO	3.3
1	I	0	HIS	3.2
1	L	142	ARG	3.0
1	L	141	GLY	3.0
1	L	45	GLU	2.9
1	L	33	PHE	2.9
1	H	88	PHE	2.9
1	J	33	PHE	2.9
1	L	31	ARG	2.8
1	C	34	ARG	2.8
1	H	142	ARG	2.7
1	G	88	PHE	2.7
1	L	44	PRO	2.6
1	A	34	ARG	2.6
1	K	34	ARG	2.6
1	L	29	ALA	2.6
1	F	41	THR	2.4
1	D	142	ARG	2.4
1	H	34	ARG	2.4
1	B	88	PHE	2.4
1	B	143	LEU	2.4
1	L	27	ILE	2.3
1	F	31	ARG	2.3
1	I	31	ARG	2.2
1	F	33	PHE	2.2
1	H	144	ARG	2.2
1	L	99	ARG	2.2
1	L	101	ALA	2.2
1	I	143	LEU	2.2
1	L	0	HIS	2.1
1	F	135	LEU	2.1
1	C	141	GLY	2.1
1	F	144	ARG	2.1
1	G	0	HIS	2.1
1	L	40	THR	2.1
1	J	144	ARG	2.1
1	H	139	LEU	2.1
1	B	36	SER	2.1
1	H	31	ARG	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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

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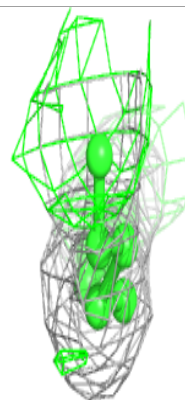
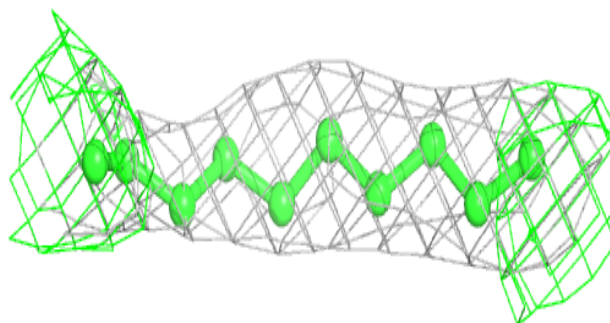
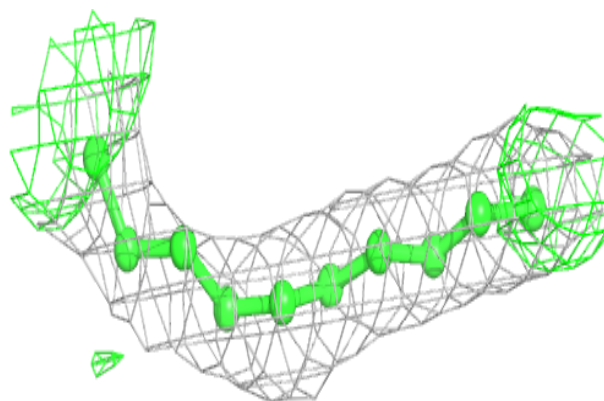
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PLM	B	207	10/18	0.84	0.22	69,88,96,100	0
4	PLM	F	203	10/18	0.85	0.15	72,86,98,100	0
4	PLM	E	202	10/18	0.85	0.19	71,76,85,89	0
4	PLM	J	207	15/18	0.86	0.21	60,74,85,88	0
4	PLM	J	203	10/18	0.86	0.24	67,69,75,77	0
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

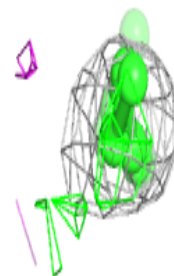
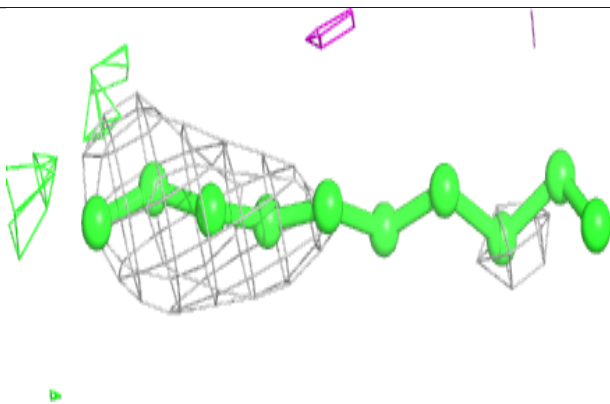
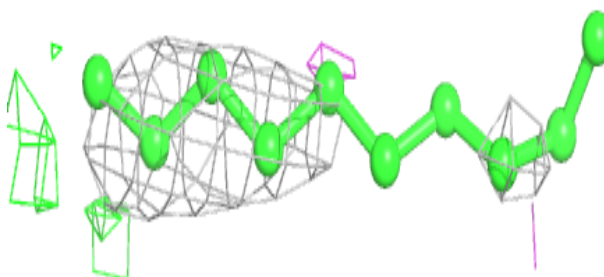
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

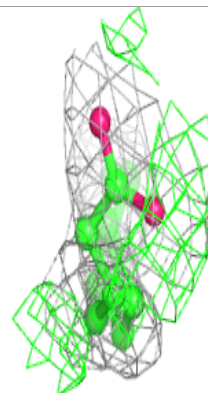
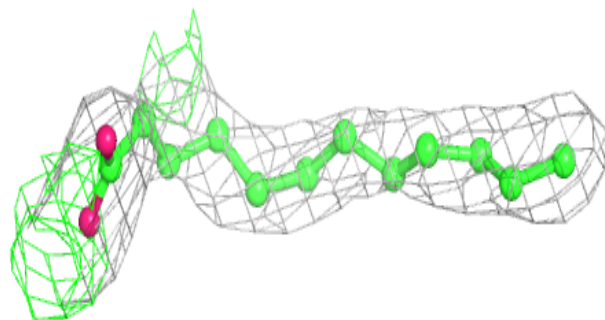
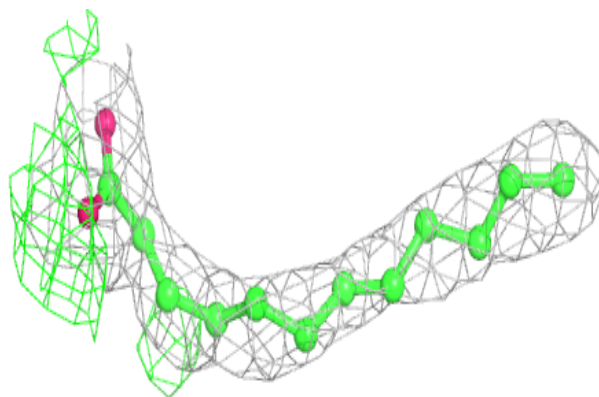
**Electron density around PLM F 204:**

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

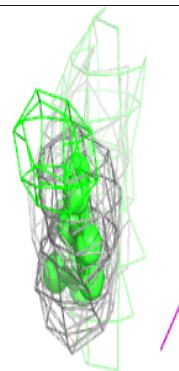
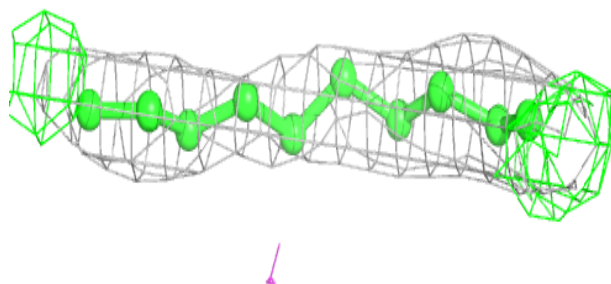
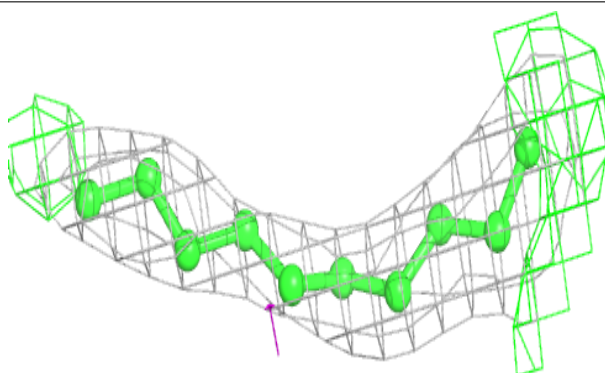


Electron density around PLM L 205:

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

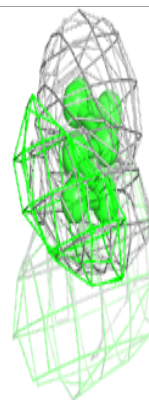
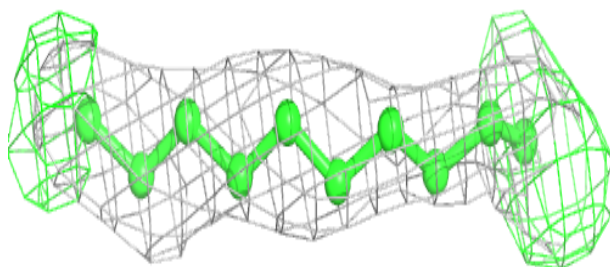
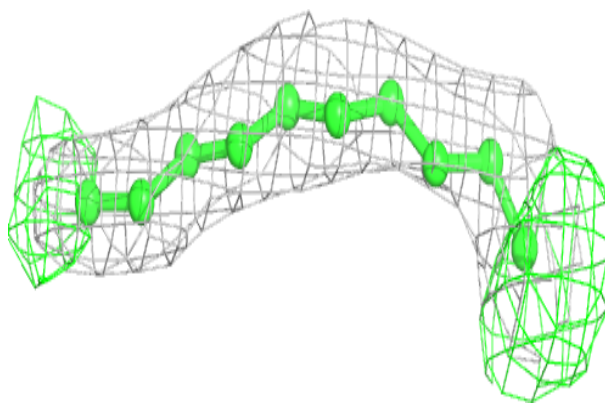
**Electron density around PLM D 204:**

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

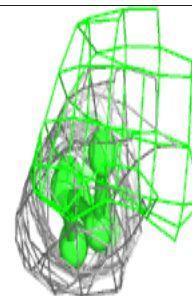
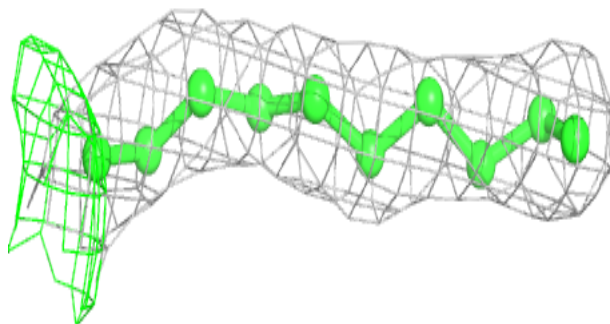
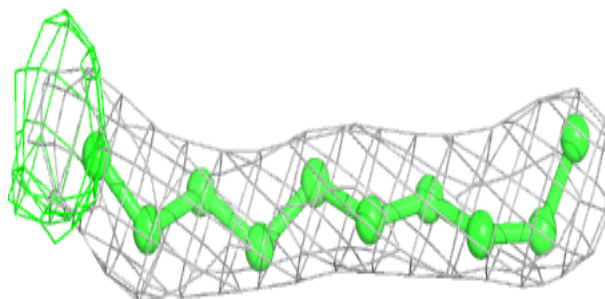


Electron density around PLM B 205:

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

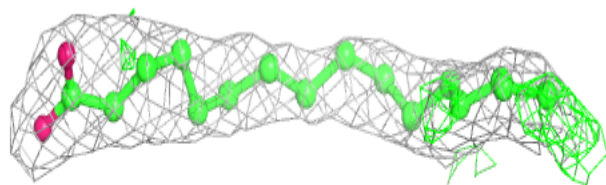
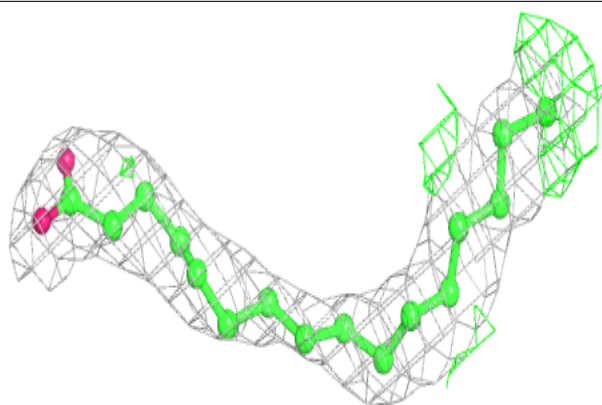
**Electron density around PLM H 203:**

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

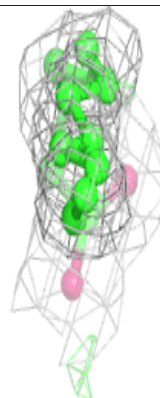
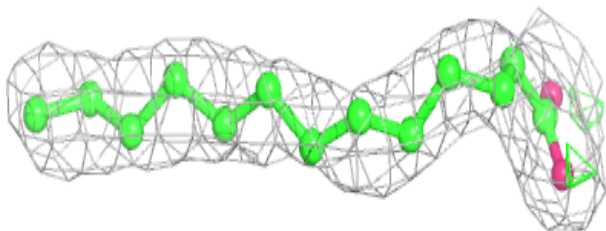
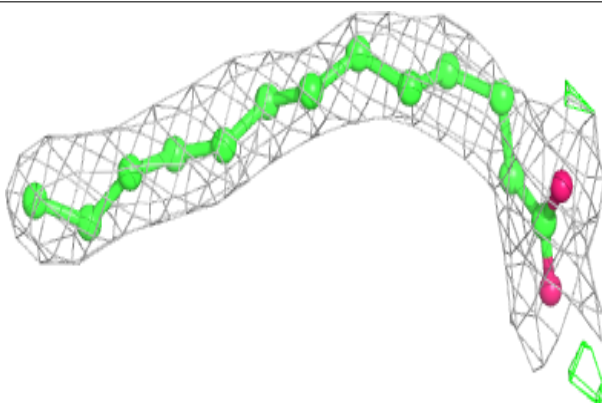


Electron density around PLM L 203:

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

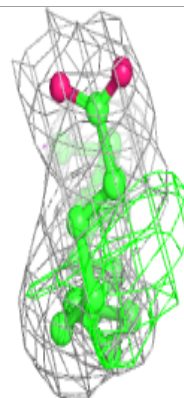
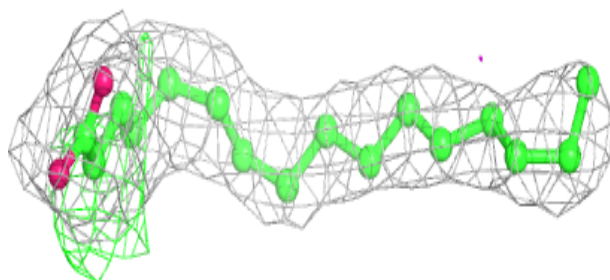
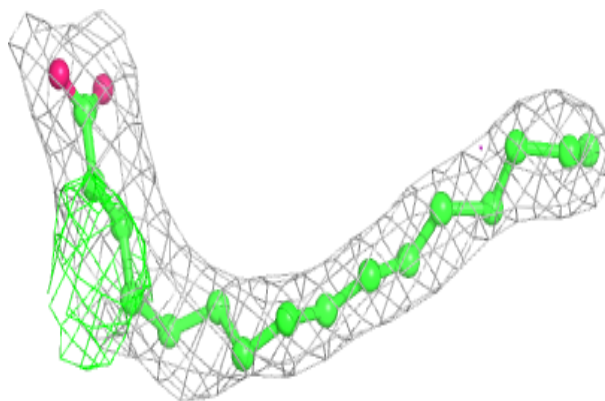
**Electron density around PLM A 207:**

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

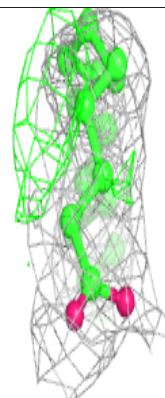
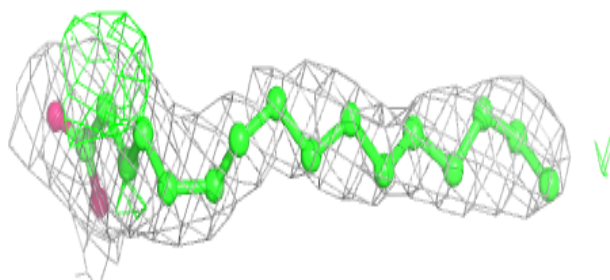
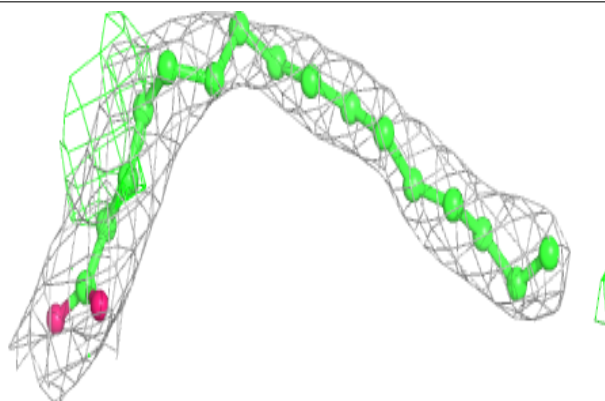


Electron density around PLM J 206:

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

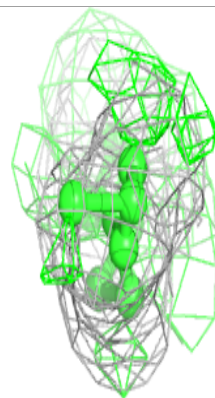
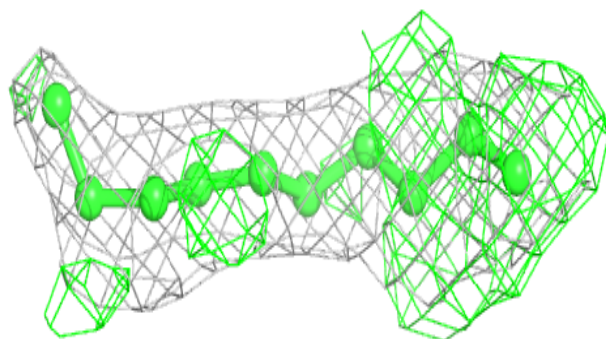
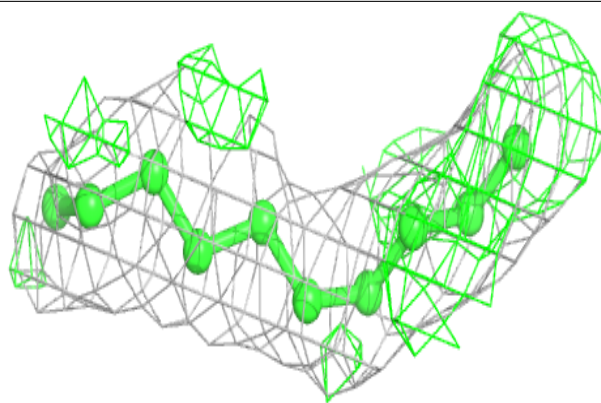
**Electron density around PLM A 206:**

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

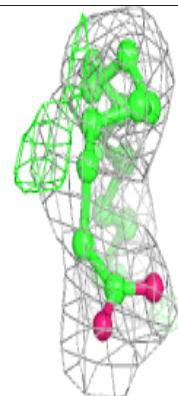
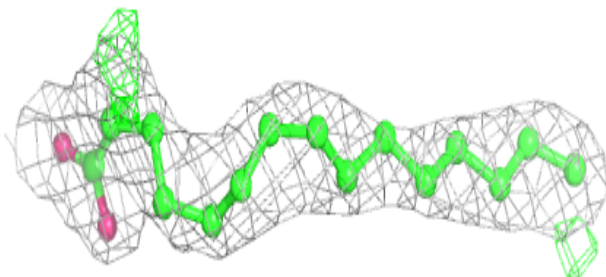
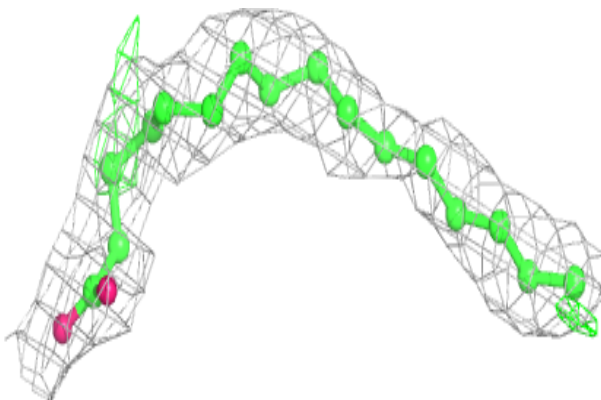


Electron density around PLM C 205:

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

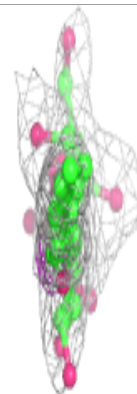
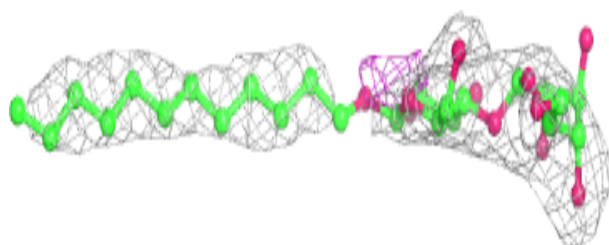
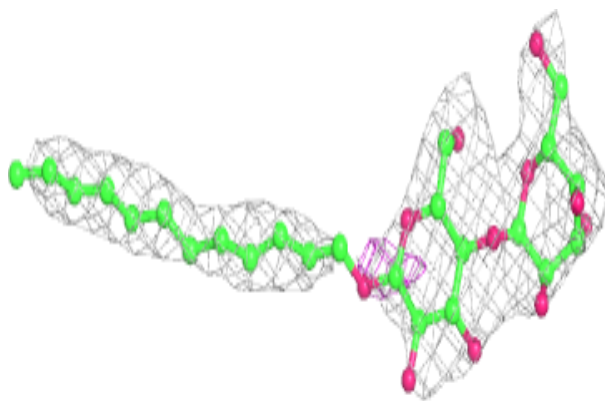
**Electron density around PLM B 206:**

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

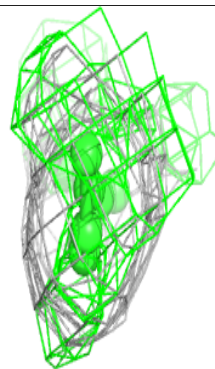
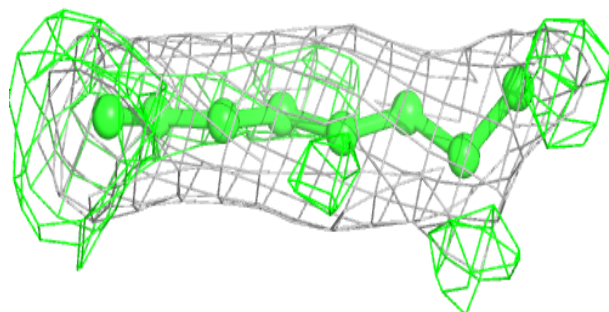
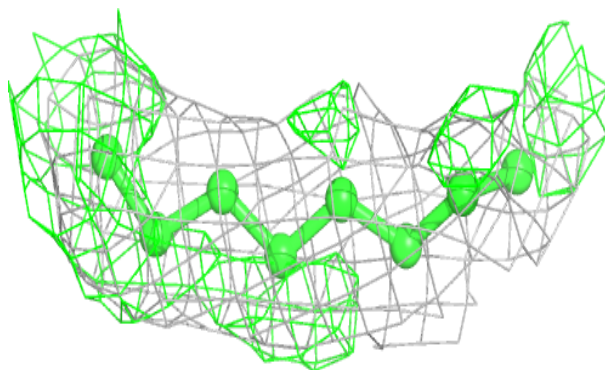


Electron density around LMT B 209:

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

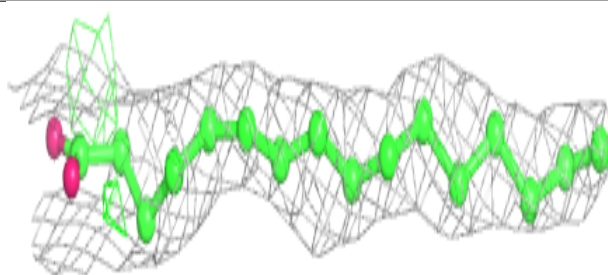
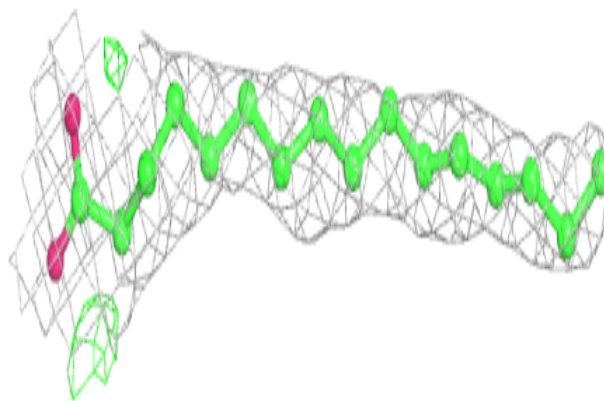
**Electron density around PLM J 204:**

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

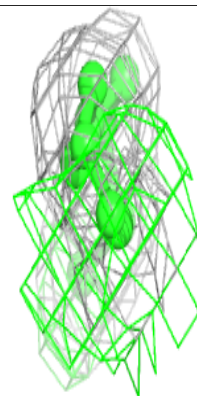
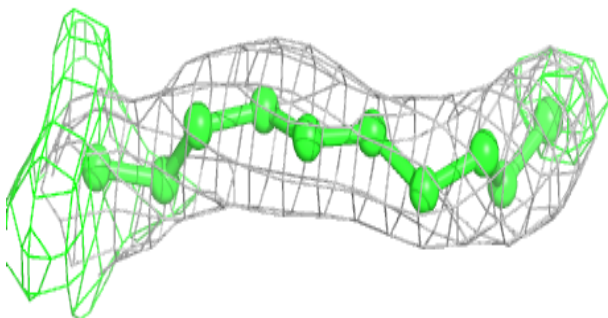
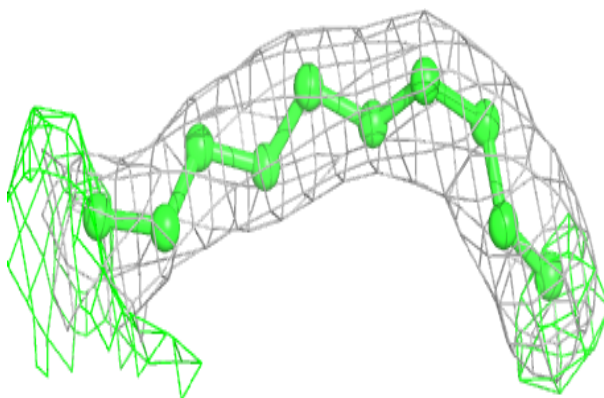


Electron density around PLM C 204:

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

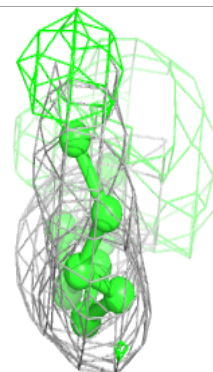
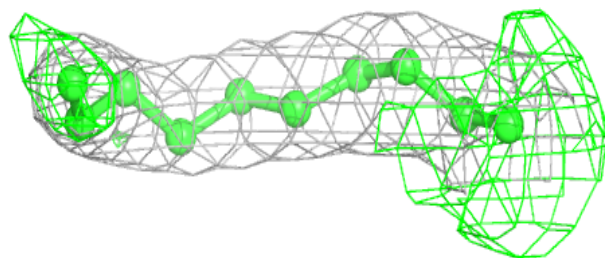
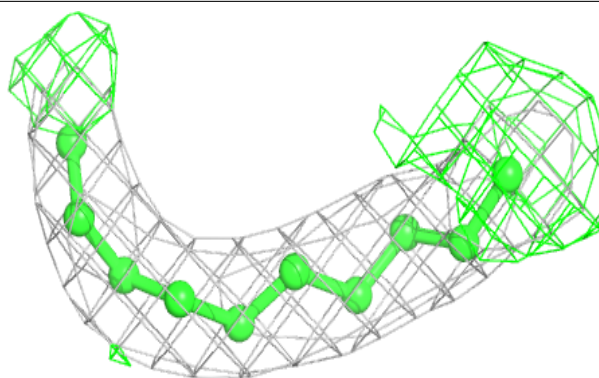
**Electron density around PLM G 203:**

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

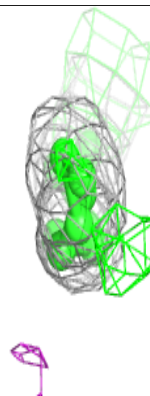
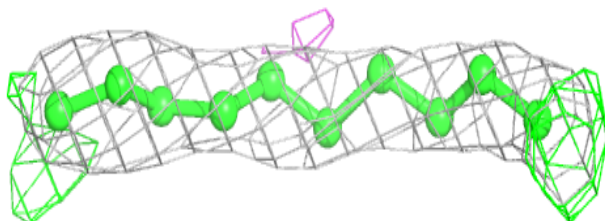
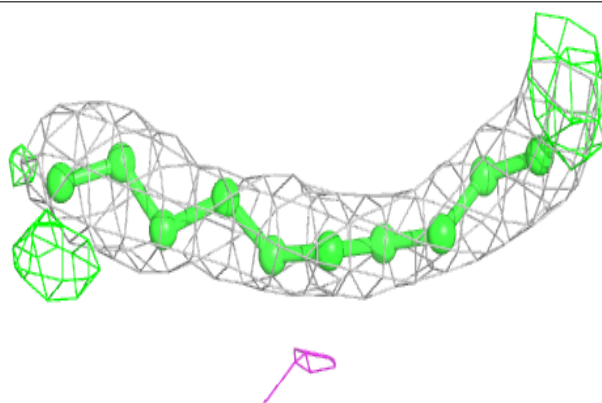


Electron density around PLM D 203:

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

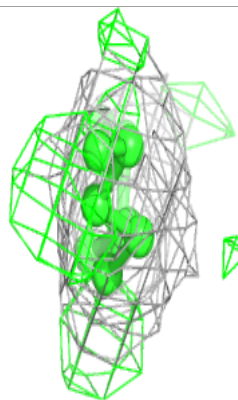
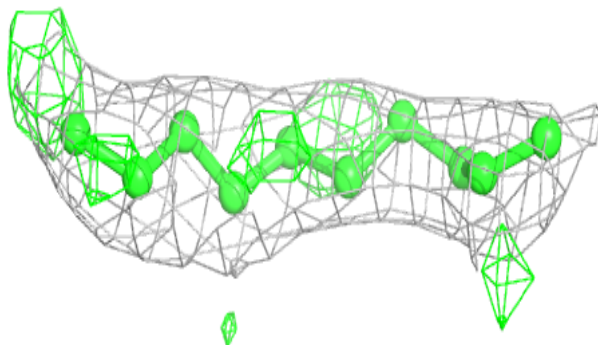
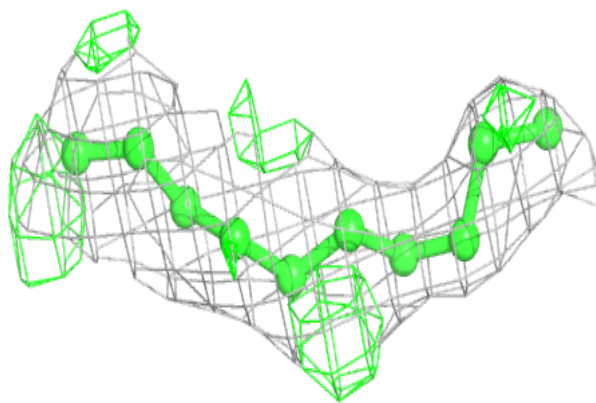
**Electron density around PLM I 203:**

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

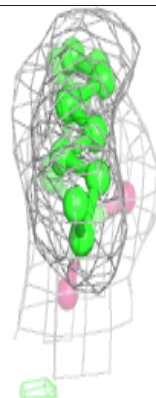
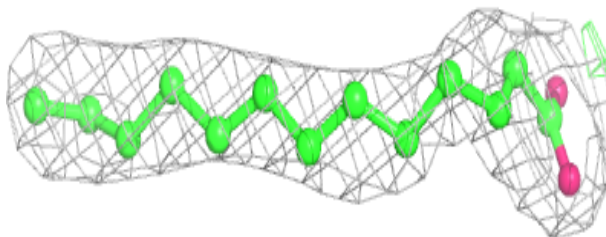
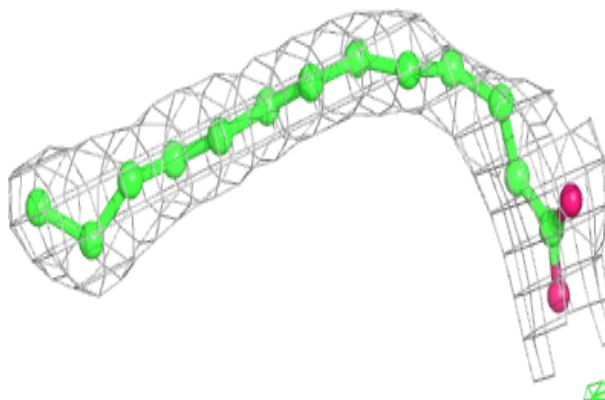


Electron density around PLM G 204:

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

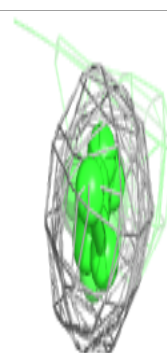
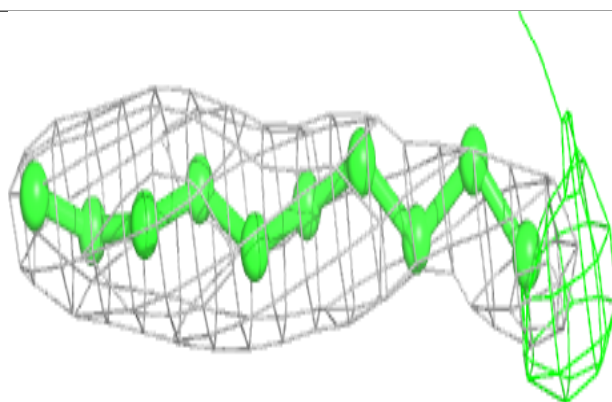
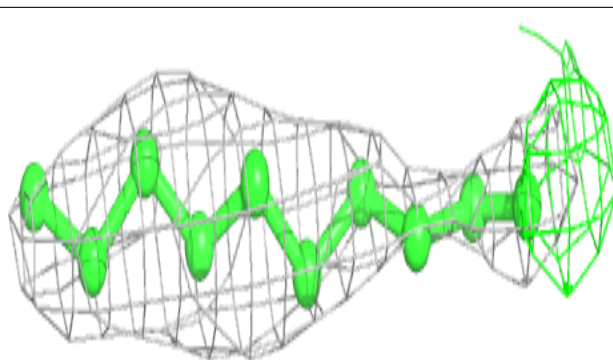
**Electron density around PLM D 206:**

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

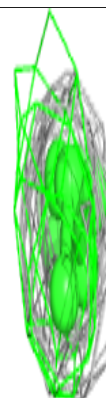
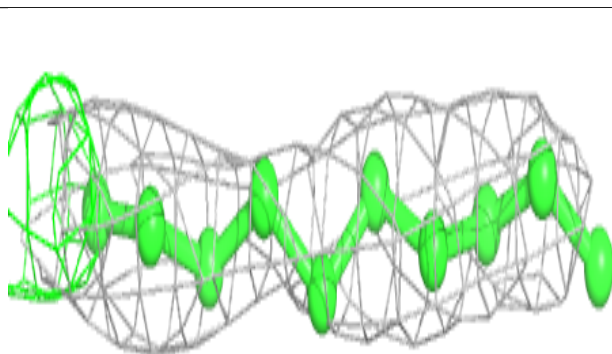
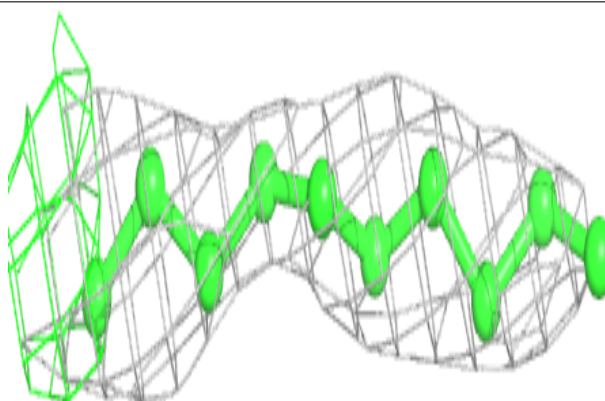


Electron density around PLM A 205:

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

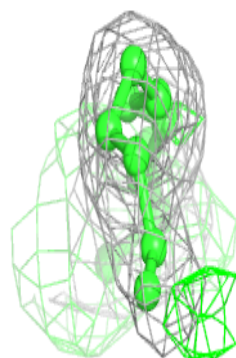
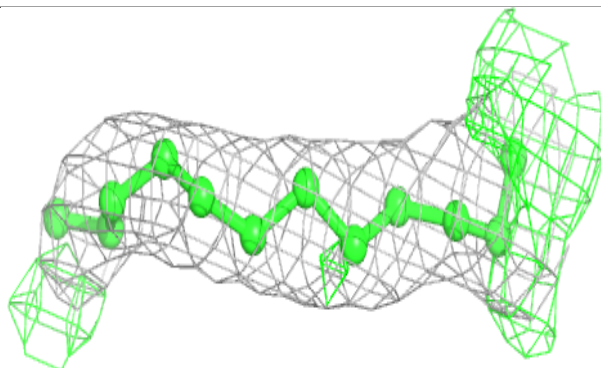
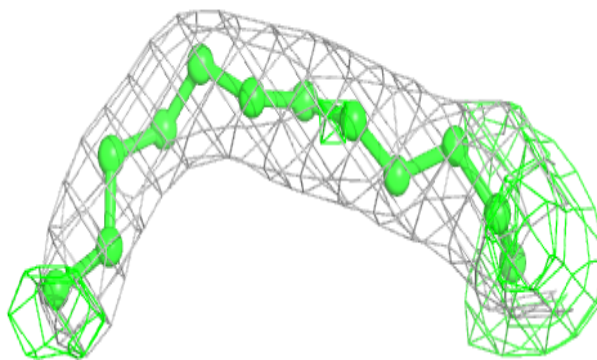
**Electron density around PLM F 205:**

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

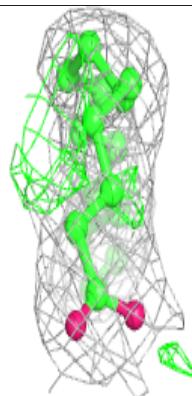
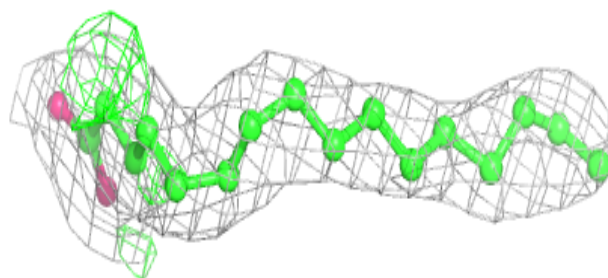
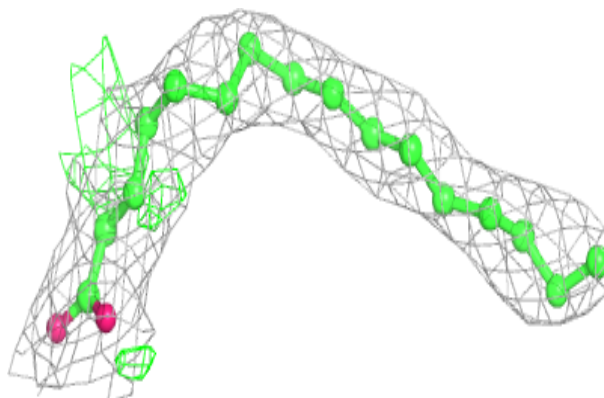


Electron density around PLM B 203:

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

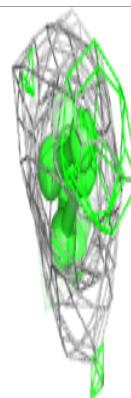
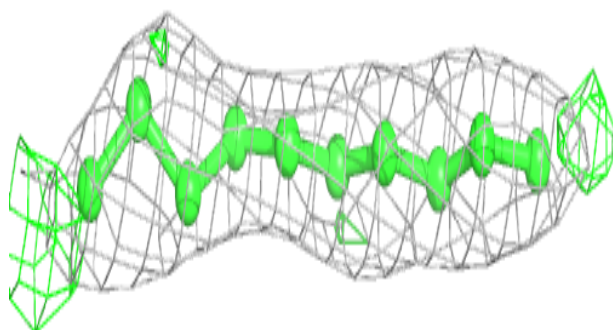
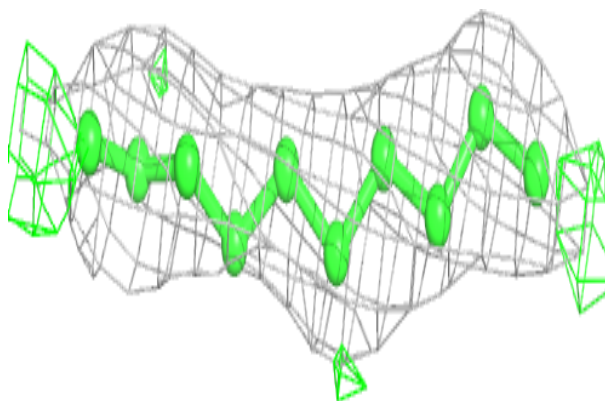
**Electron density around PLM I 204:**

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

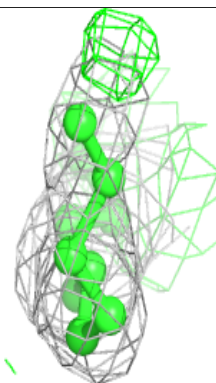
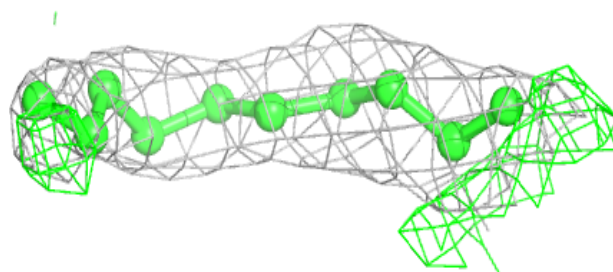
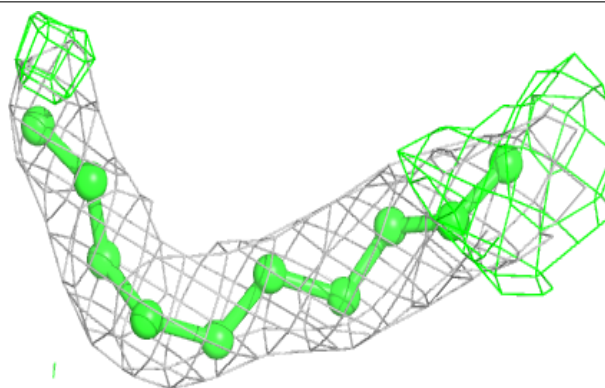


Electron density around PLM L 206:

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

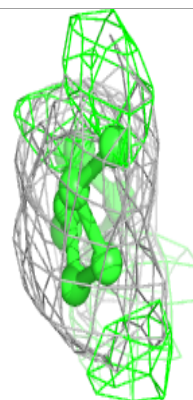
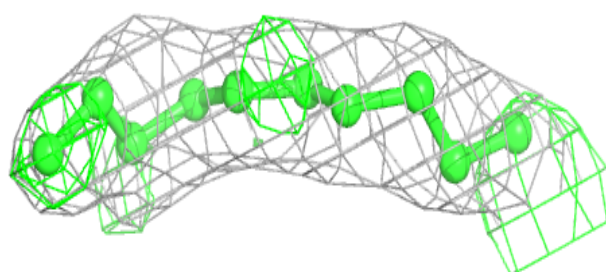
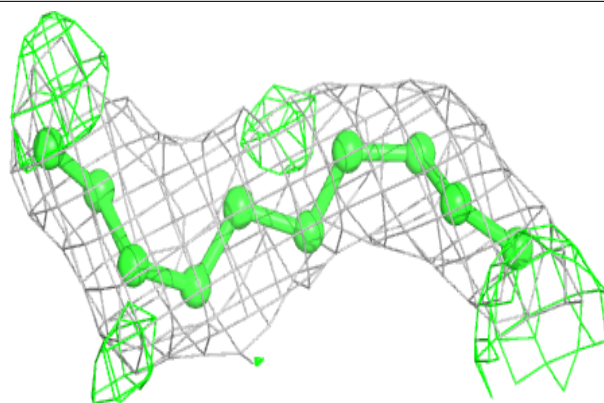
**Electron density around PLM J 205:**

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

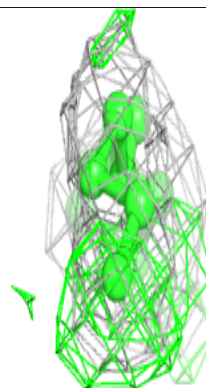
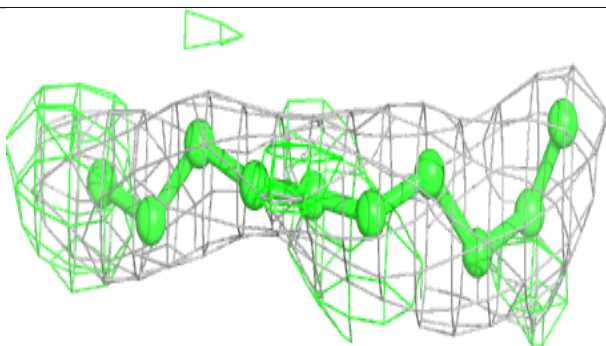
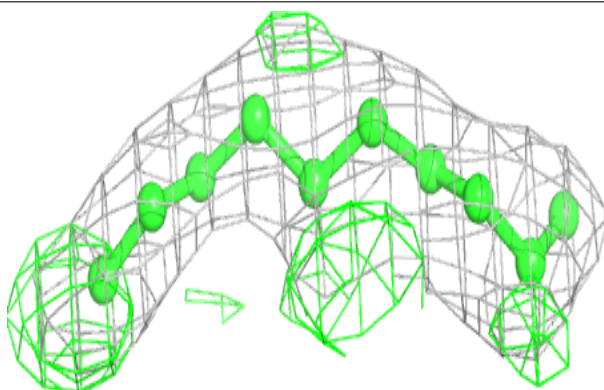


Electron density around PLM B 207:

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

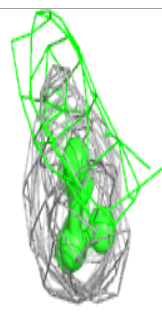
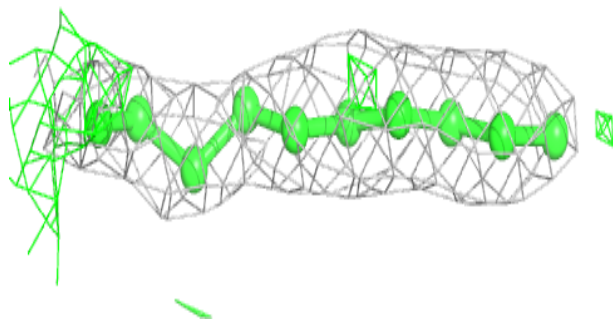
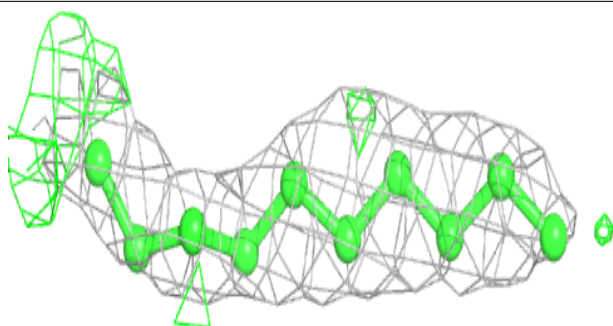
**Electron density around PLM F 203:**

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

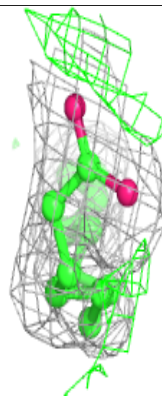
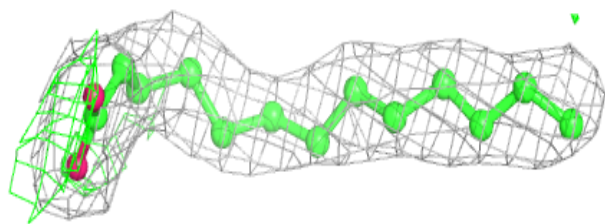
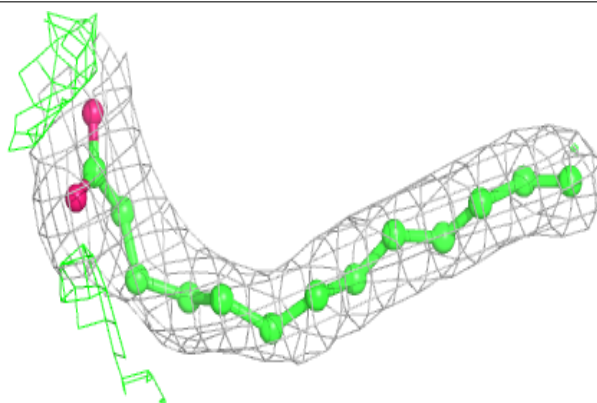


Electron density around PLM E 202:

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

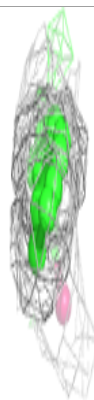
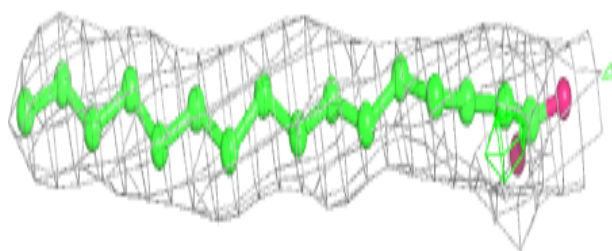
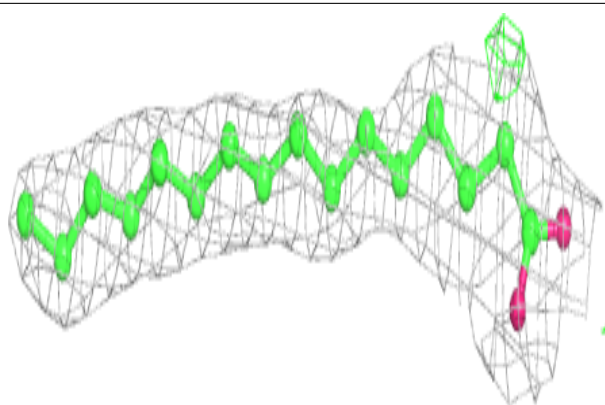
**Electron density around PLM J 207:**

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

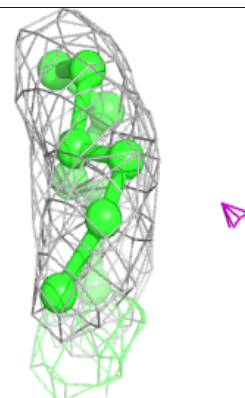
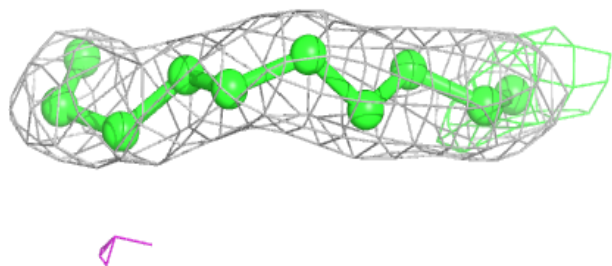
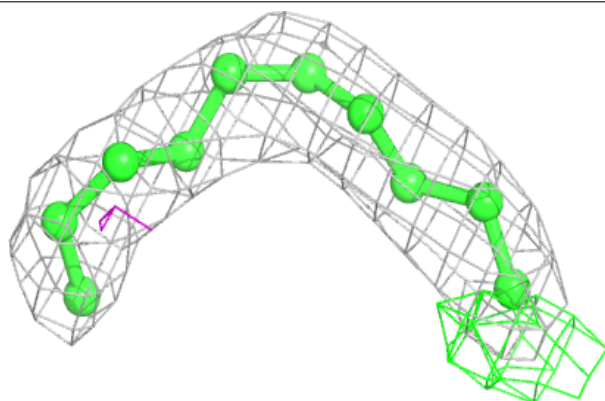


Electron density around PLM A 204:

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

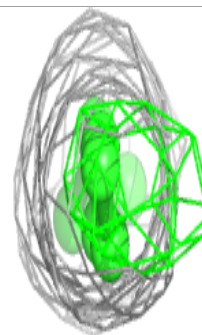
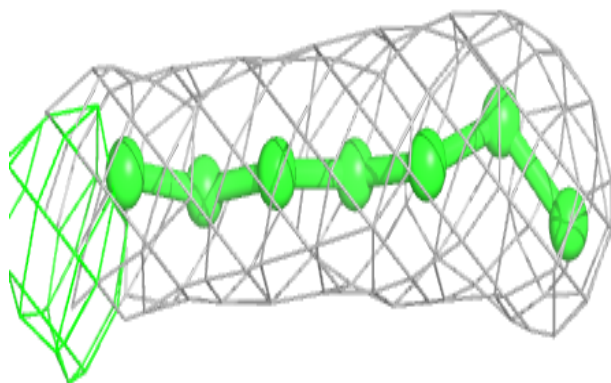
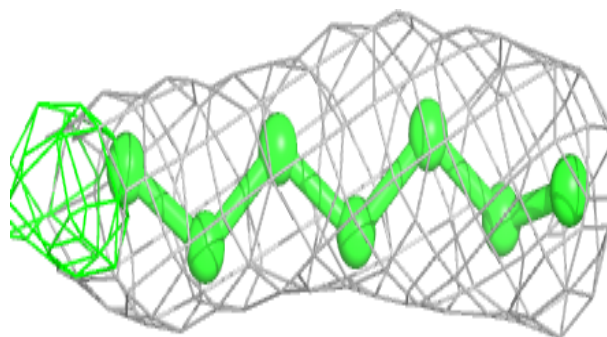
**Electron density around PLM A 203:**

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

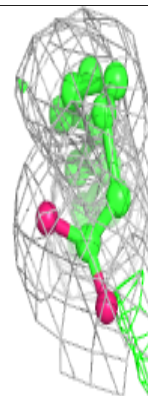
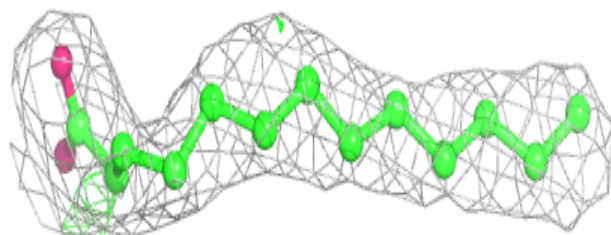
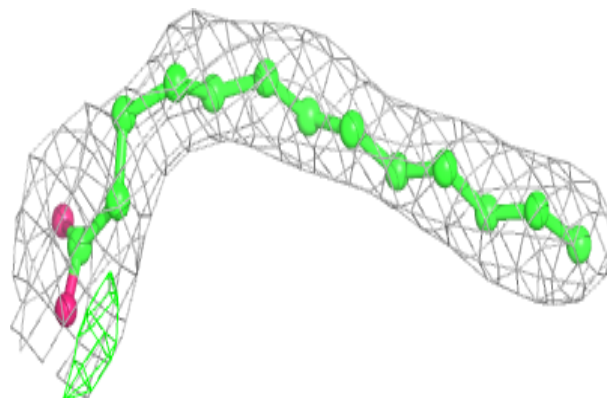


Electron density around PLM E 203:

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

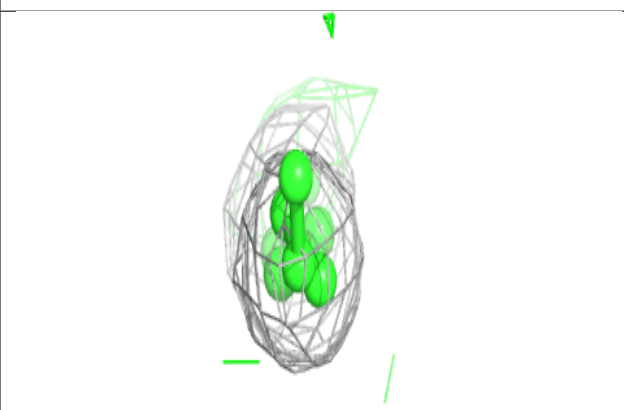
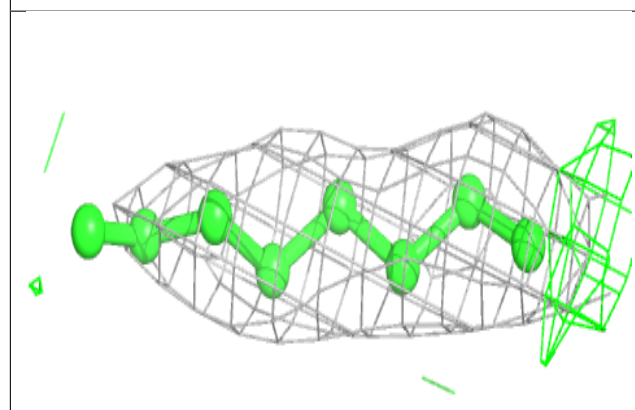
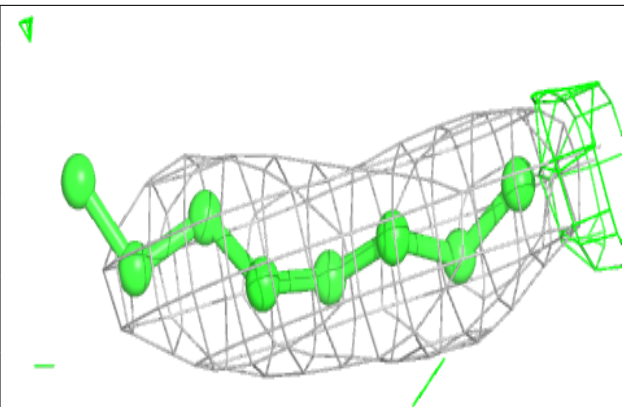
**Electron density around PLM G 205:**

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

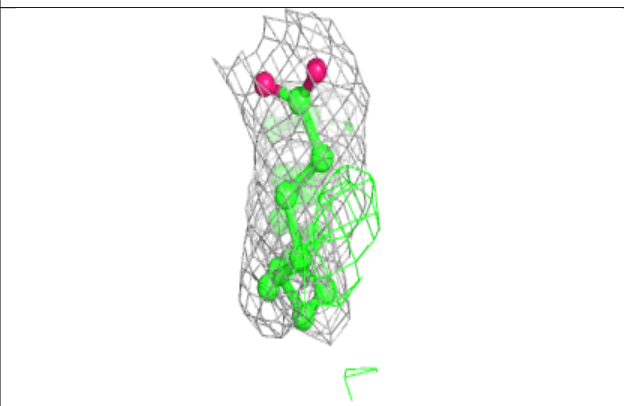
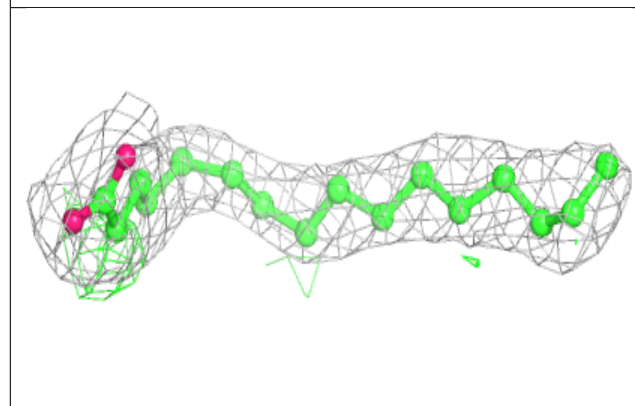
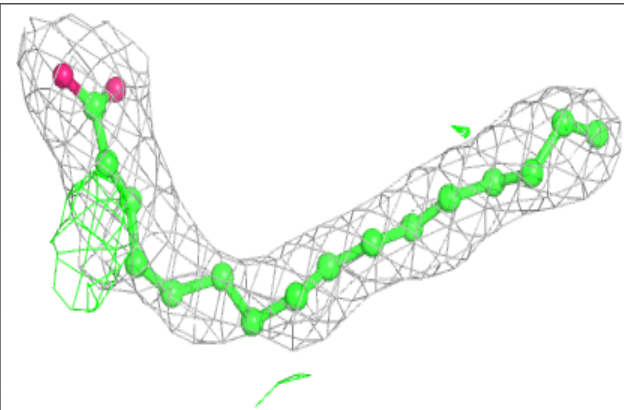


Electron density around PLM F 202:

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

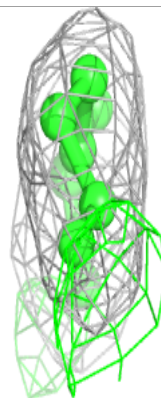
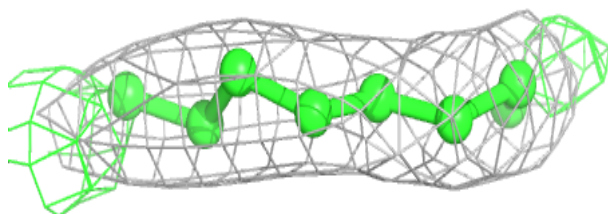
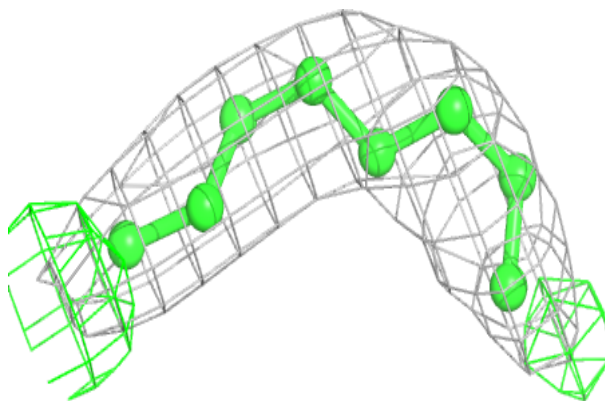
**Electron density around PLM D 205:**

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

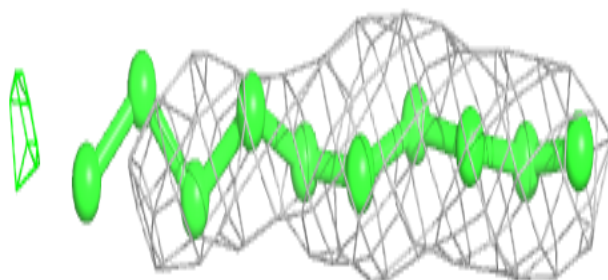
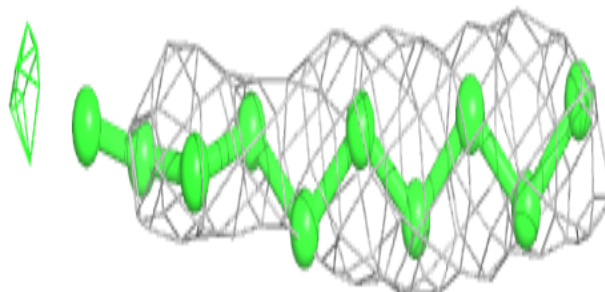


Electron density around PLM L 204:

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

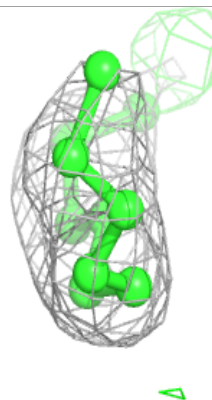
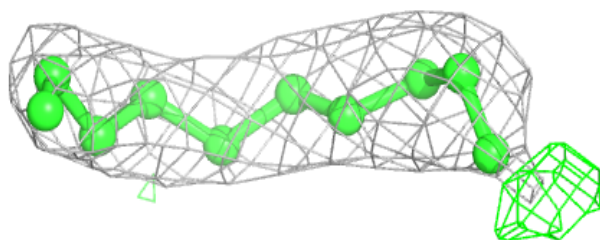
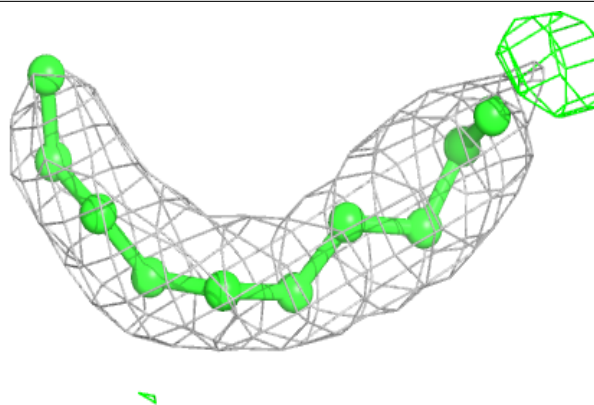
**Electron density around PLM B 204:**

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

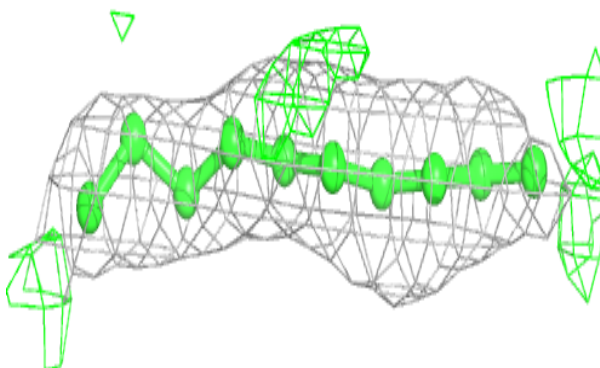
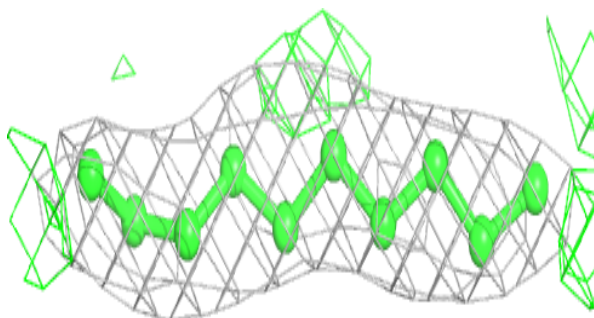


Electron density around PLM C 206:

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

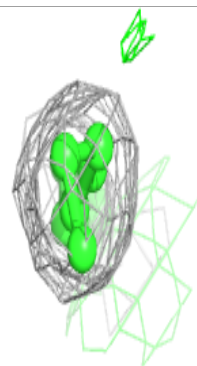
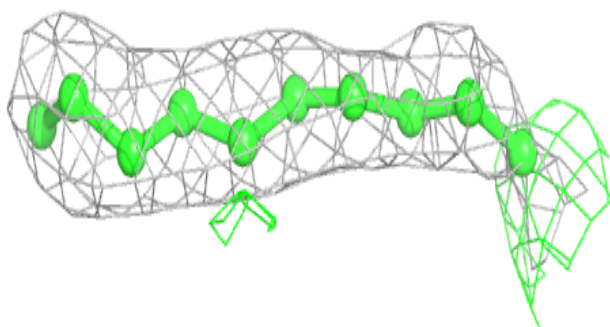
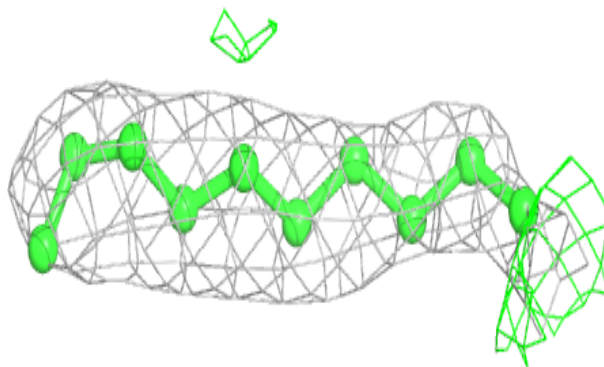
**Electron density around PLM B 208:**

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

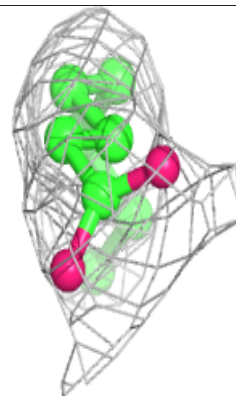
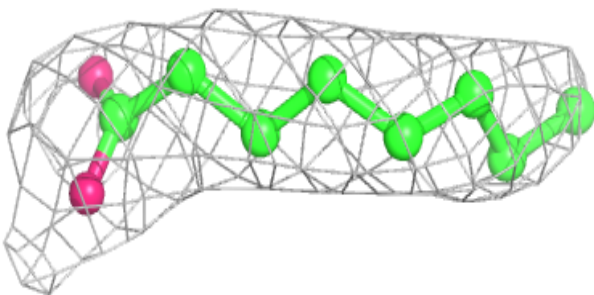
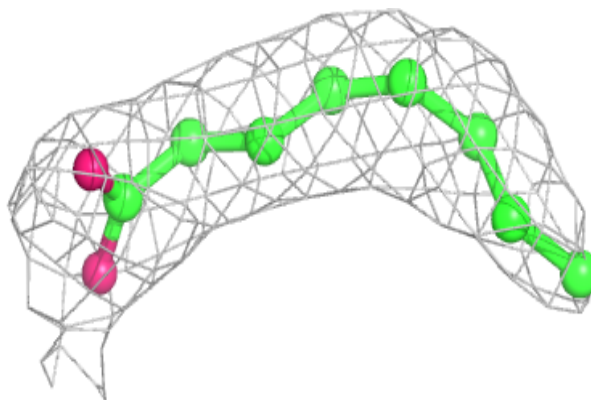


Electron density around PLM E 204:

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

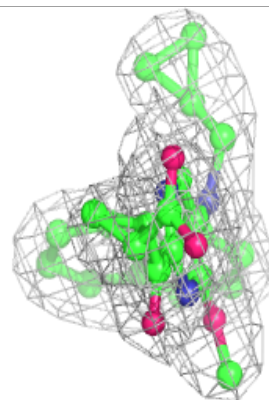
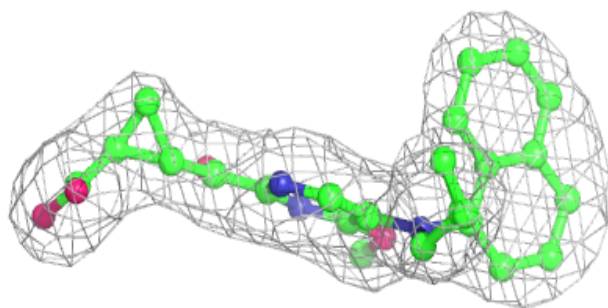
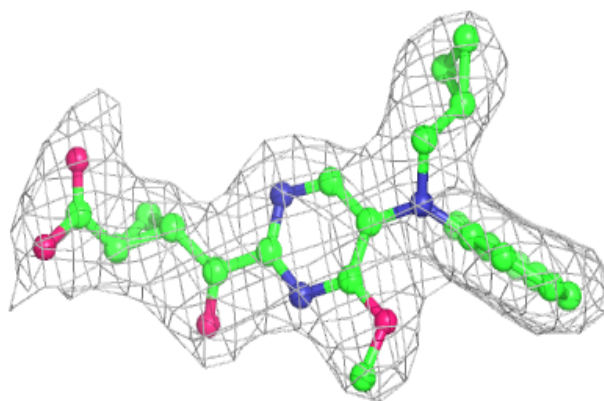
**Electron density around PLM C 203:**

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

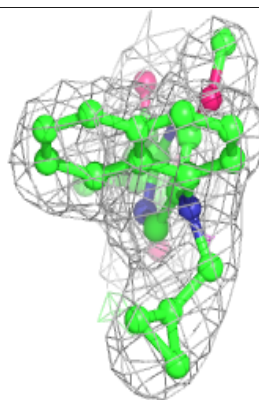
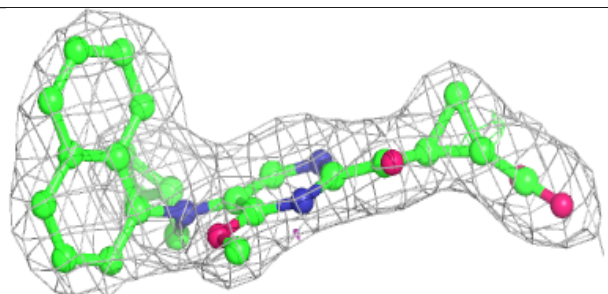
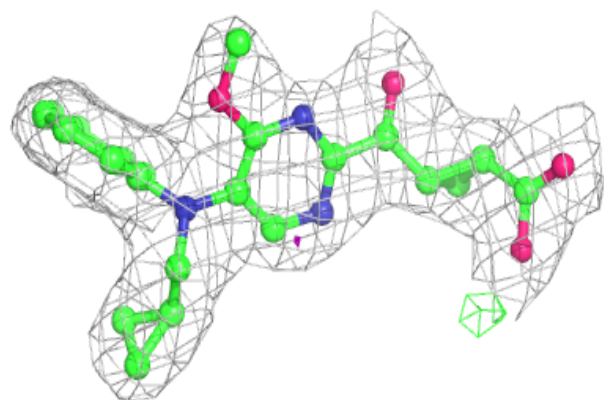


Electron density around JUQ C 201:

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

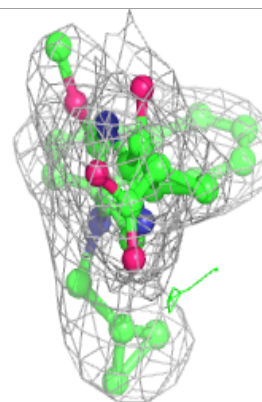
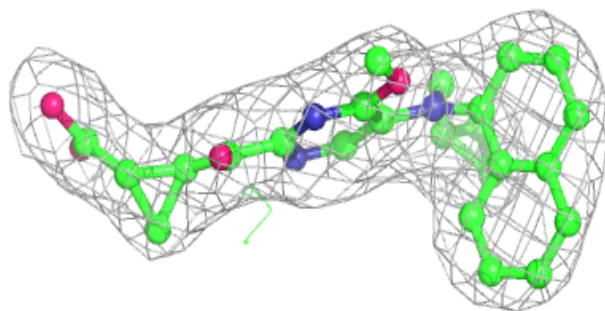
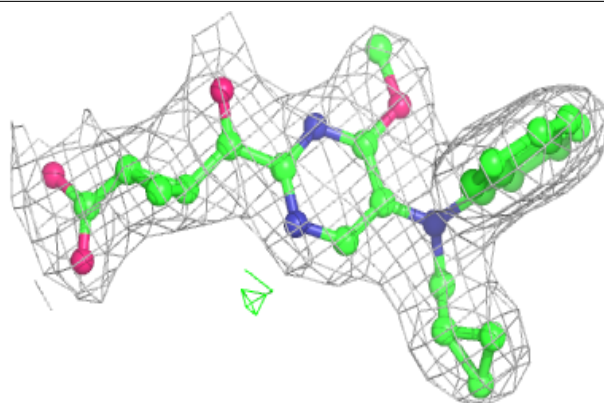
**Electron density around JUQ A 201:**

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

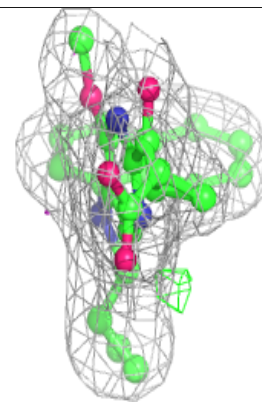
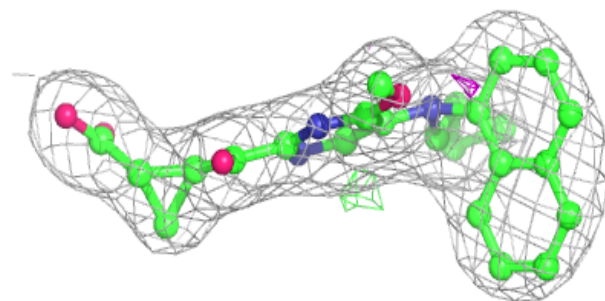
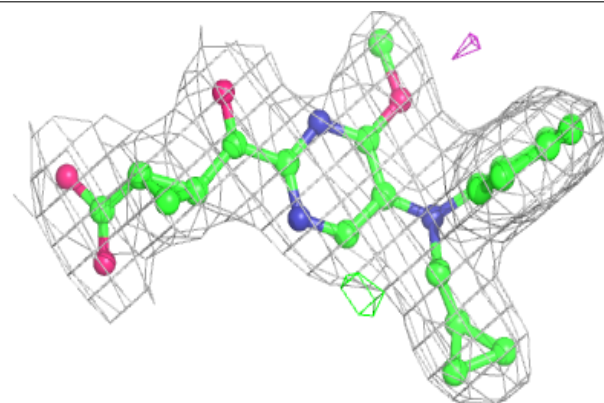


Electron density around JUQ D 201:

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

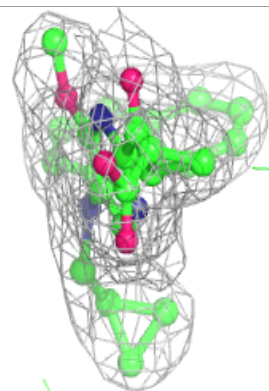
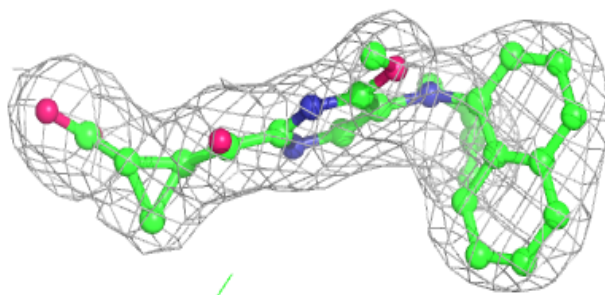
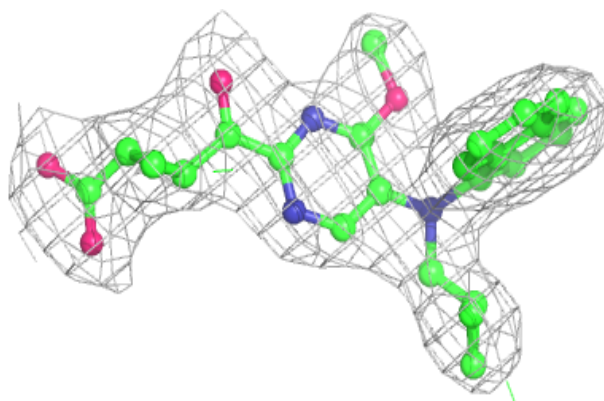
**Electron density around JUQ J 201:**

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

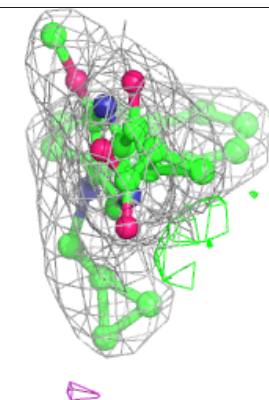
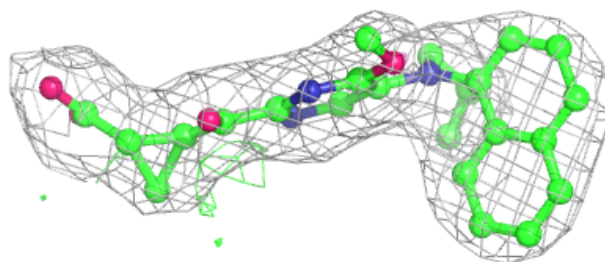
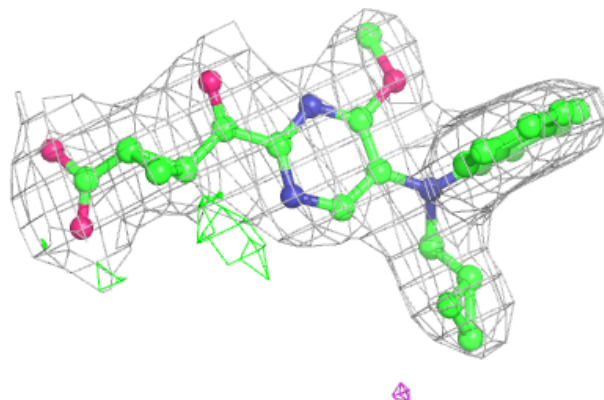


Electron density around JUQ B 201:

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

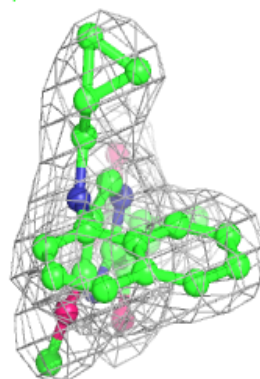
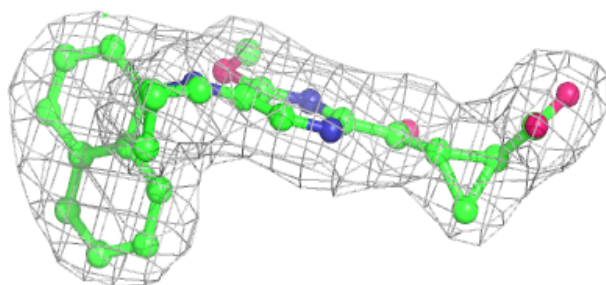
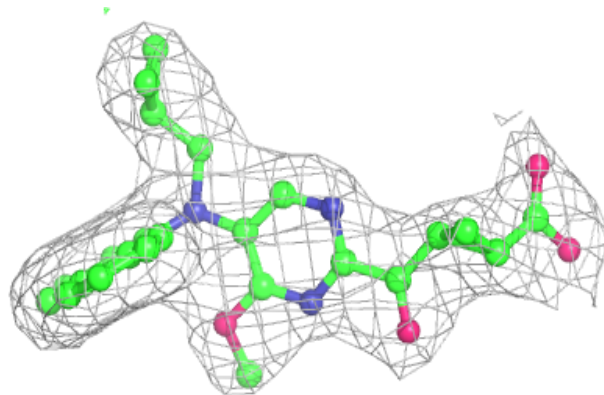
**Electron density around JUQ H 201:**

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

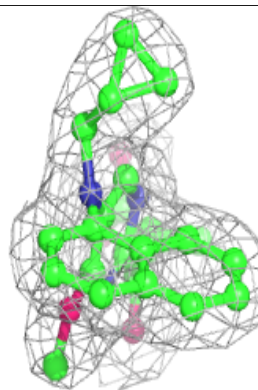
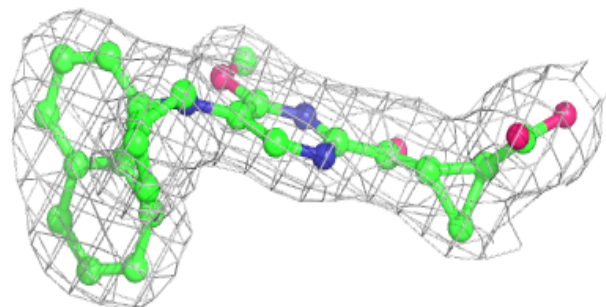
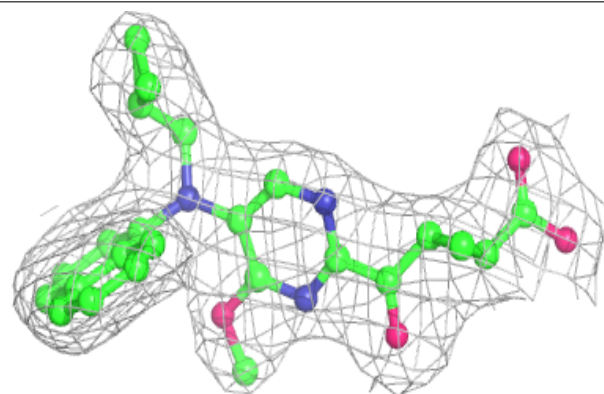


Electron density around JUQ L 201:

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

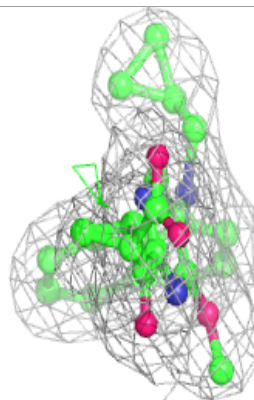
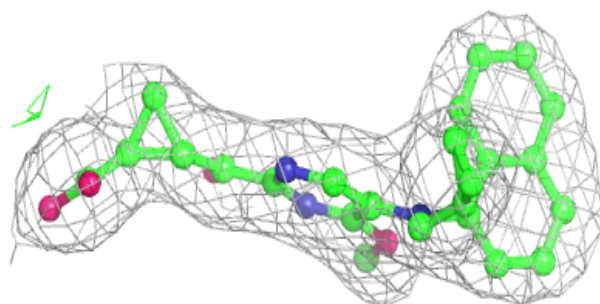
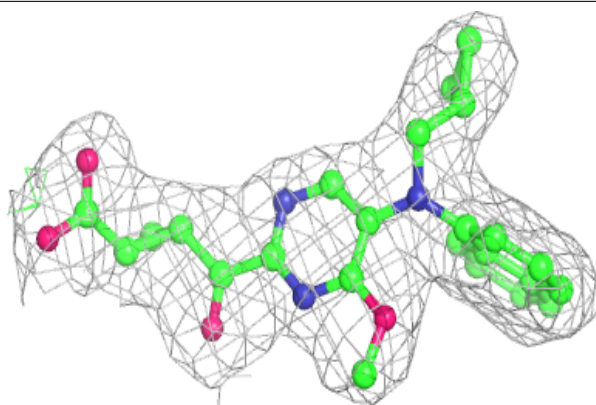
**Electron density around JUQ F 201:**

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

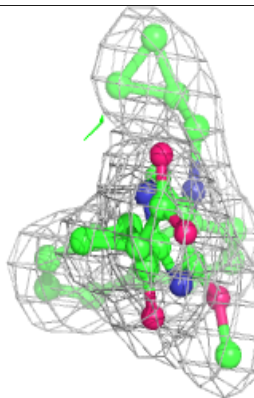
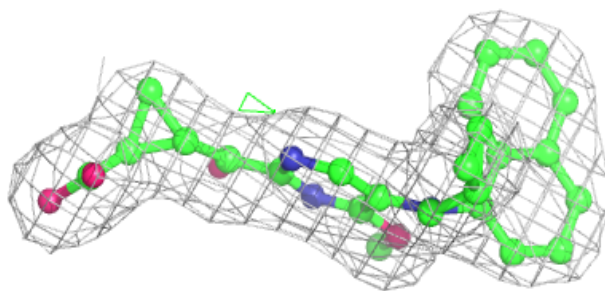
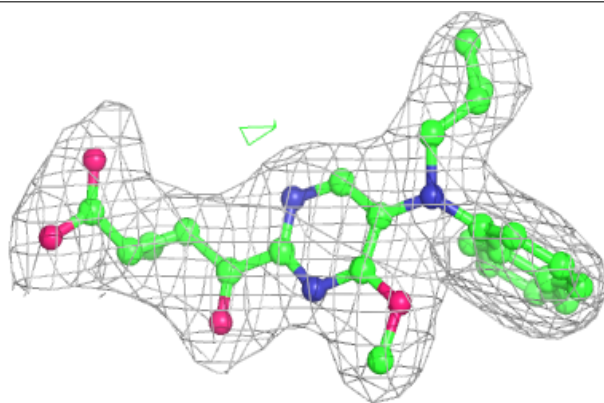


Electron density around JUQ K 201:

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

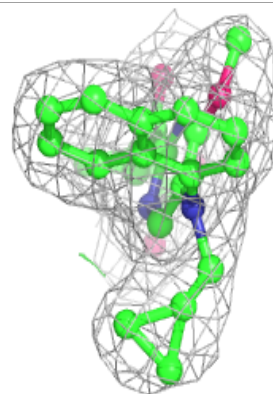
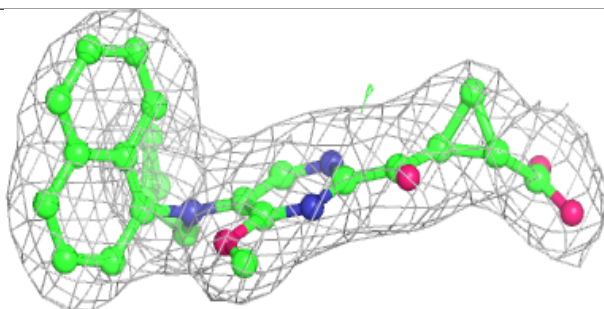
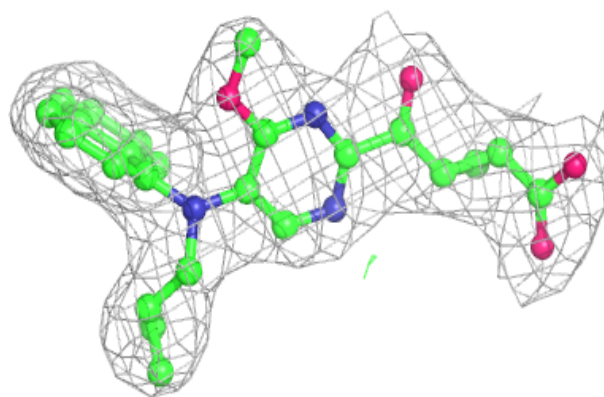
**Electron density around JUQ G 201:**

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

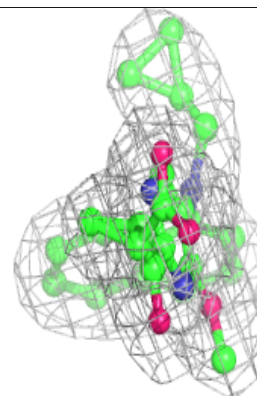
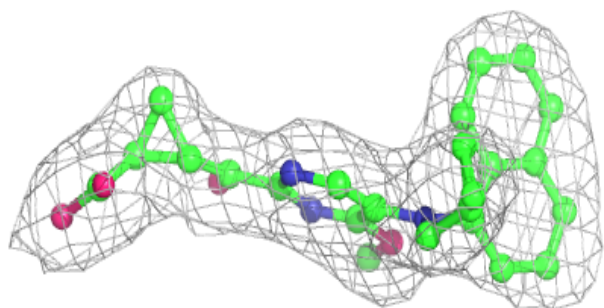
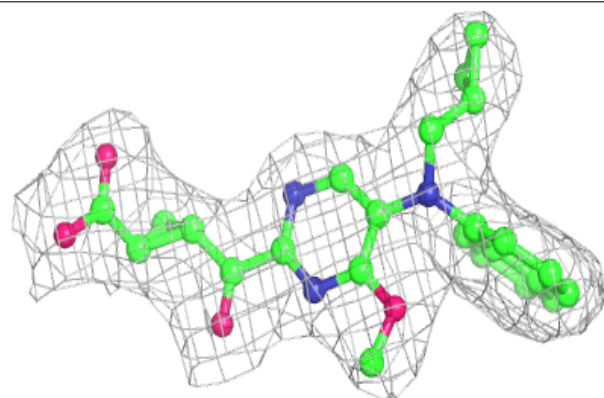


Electron density around JUQ I 201:

$2mF_o - DF_c$ (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

There are no such residues in this entry.