wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 01:15 AM EDT

PDB ID	:	5O9H
Title	:	Crystal structure of thermostabilised human C5a anaphylatoxin chemotactic receptor 1 (C5aR) in complex with NDT9513727
Authors	:	Robertson, N.; Rappas, M.; Dore, A.S.; Brown, J.; Bottegoni, G.; Koglin, M.; Cansfield, J.; Jazayeri, A.; Cooke, R.M.; Marshall, F.H.
Deposited on	:	2017-06-19
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

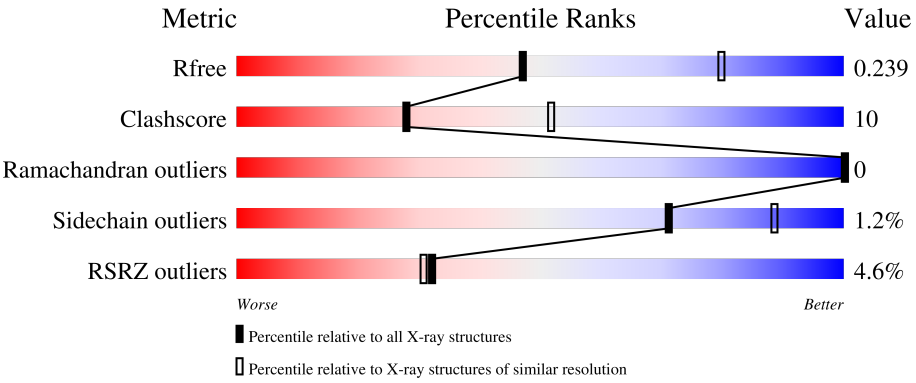
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	317	3% 74% 19% 7%
1	B	317	5% 79% 14% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TLA	A	402	X	X	-	-
3	TLA	A	403	X	X	-	-
3	TLA	B	402	X	X	-	-
4	OLA	A	408	-	-	-	X
4	OLA	B	419	-	-	X	-
5	CIT	B	420	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5349 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 C5a anaphylatoxin chemotactic receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2324	1555	380	377	12			
1	B	295	Total	C	N	O	S	0	0	0
			2338	1562	383	381	12			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP P21730
A	85	ALA	SER	engineered mutation	UNP P21730
A	91	ALA	ILE	engineered mutation	UNP P21730
A	142	ALA	ILE	engineered mutation	UNP P21730
A	146	ARG	ASN	engineered mutation	UNP P21730
A	156	LEU	ALA	engineered mutation	UNP P21730
A	172	ALA	PHE	engineered mutation	UNP P21730
A	232	ALA	ARG	engineered mutation	UNP P21730
A	234	GLU	ALA	engineered mutation	UNP P21730
A	311	GLU	LEU	engineered mutation	UNP P21730
A	317	GLU	SER	engineered mutation	UNP P21730
A	321	GLU	ASN	engineered mutation	UNP P21730
A	334	ALA	-	expression tag	UNP P21730
A	335	ALA	-	expression tag	UNP P21730
A	336	ALA	-	expression tag	UNP P21730
A	337	HIS	-	expression tag	UNP P21730
A	338	HIS	-	expression tag	UNP P21730
A	339	HIS	-	expression tag	UNP P21730
A	340	HIS	-	expression tag	UNP P21730
A	341	HIS	-	expression tag	UNP P21730
A	342	HIS	-	expression tag	UNP P21730
A	343	HIS	-	expression tag	UNP P21730
A	344	HIS	-	expression tag	UNP P21730
A	345	HIS	-	expression tag	UNP P21730
A	346	HIS	-	expression tag	UNP P21730

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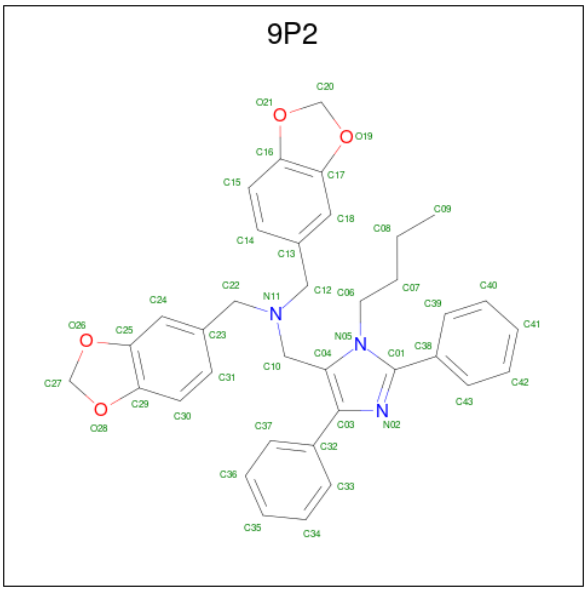
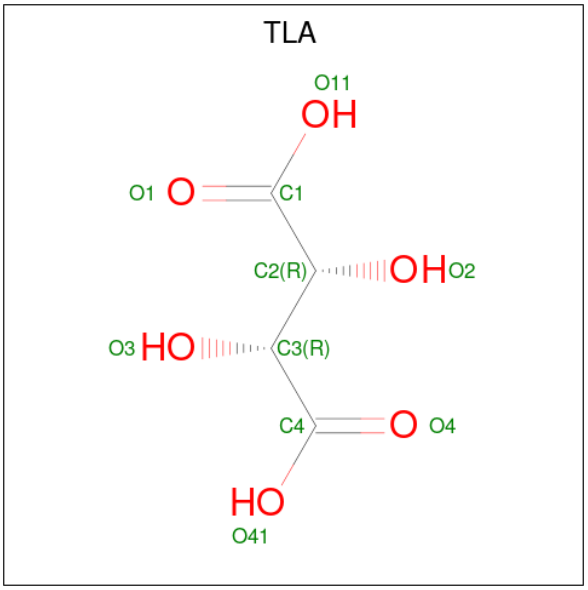
Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	initiating methionine	UNP P21730
B	85	ALA	SER	engineered mutation	UNP P21730
B	91	ALA	ILE	engineered mutation	UNP P21730
B	142	ALA	ILE	engineered mutation	UNP P21730
B	146	ARG	ASN	engineered mutation	UNP P21730
B	156	LEU	ALA	engineered mutation	UNP P21730
B	172	ALA	PHE	engineered mutation	UNP P21730
B	232	ALA	ARG	engineered mutation	UNP P21730
B	234	GLU	ALA	engineered mutation	UNP P21730
B	311	GLU	LEU	engineered mutation	UNP P21730
B	317	GLU	SER	engineered mutation	UNP P21730
B	321	GLU	ASN	engineered mutation	UNP P21730
B	334	ALA	-	expression tag	UNP P21730
B	335	ALA	-	expression tag	UNP P21730
B	336	ALA	-	expression tag	UNP P21730
B	337	HIS	-	expression tag	UNP P21730
B	338	HIS	-	expression tag	UNP P21730
B	339	HIS	-	expression tag	UNP P21730
B	340	HIS	-	expression tag	UNP P21730
B	341	HIS	-	expression tag	UNP P21730
B	342	HIS	-	expression tag	UNP P21730
B	343	HIS	-	expression tag	UNP P21730
B	344	HIS	-	expression tag	UNP P21730
B	345	HIS	-	expression tag	UNP P21730
B	346	HIS	-	expression tag	UNP P21730

- Molecule 2 is 1-(1,3-benzodioxol-5-yl)- {N}-(1,3-benzodioxol-5-ylmethyl)- {N}-[(3-butyl-2,5-diphenyl-imidazol-4-yl)methyl]methanamine (three-letter code: 9P2) (formula: $C_{36}H_{35}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	36	3	4		
2	B	1	Total	C	N	O	0	0
			43	36	3	4		

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			10	4	6			
3	A	1	Total	C	O		0	0
			10	4	6			

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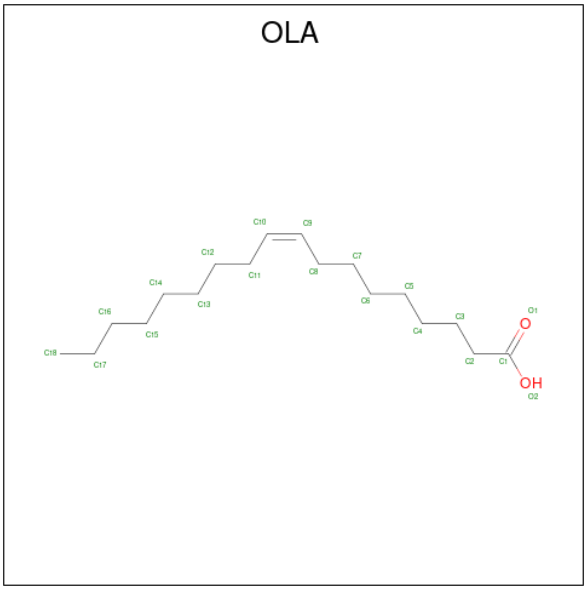
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 10 4 6	0	0

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 17 15 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C 15 15	0	0
4	A	1	Total C O 14 12 2	0	0
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C 12 12	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 20 18 2	0	0
4	A	1	Total C 13 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C 15 15	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 11 9 2	0	0
4	B	1	Total C O 13 11 2	0	0
4	B	1	Total C O 10 8 2	0	0
4	B	1	Total C O 15 13 2	0	0
4	B	1	Total C O 14 12 2	0	0
4	B	1	Total C O 13 11 2	0	0
4	B	1	Total C O 7 5 2	0	0
4	B	1	Total C O 16 14 2	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 14 12 2	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 14 12 2	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 16 14 2	0	0
4	B	1	Total C O 15 13 2	0	0

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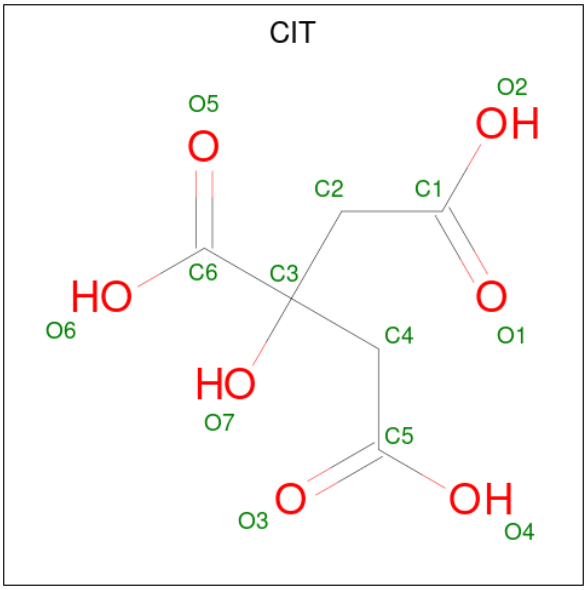
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 14 14	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 13 6 7	0	0

- Molecule 6 is water.

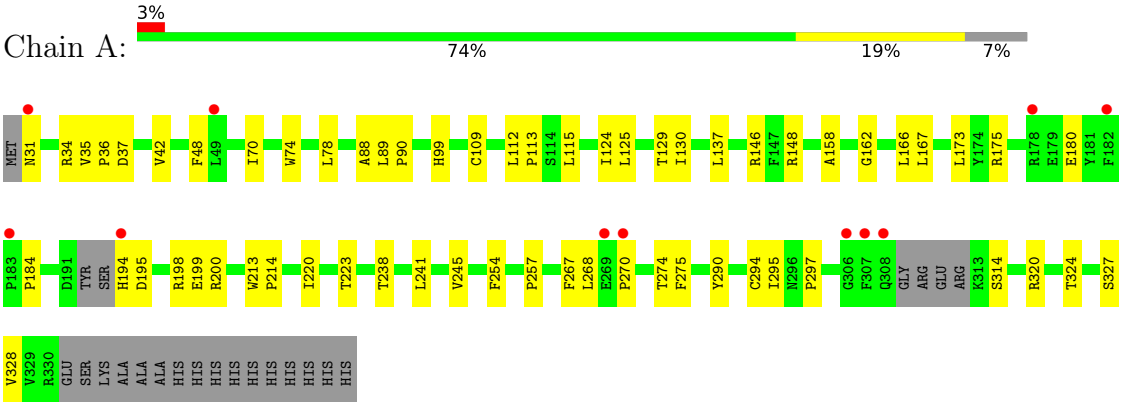
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	39	Total O 39 39	0	0
6	B	32	Total O 32 32	0	0

3 Residue-property plots (i)

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

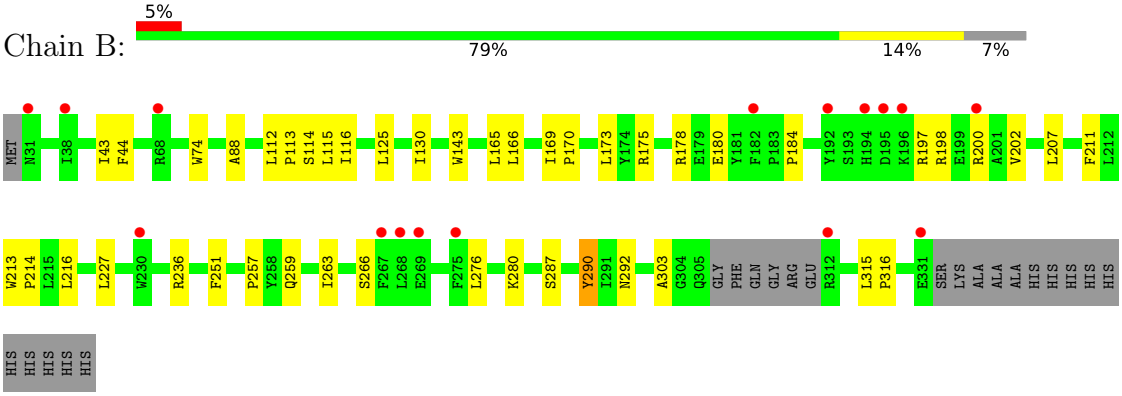
• Molecule 1: C5a anaphylatoxin chemotactic receptor 1

Chain A:



• Molecule 1: C5a anaphylatoxin chemotactic receptor 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.09Å 51.10Å 118.94Å 90.00° 106.73° 90.00°	Depositor
Resolution (Å)	19.89 – 2.70 34.59 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.89-2.70) 99.2 (34.59-2.70)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.238 0.211 , 0.239	Depositor DCC
R_{free} test set	1357 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 74.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5349	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TLA, CIT, OLA, 9P2

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	0.27	0/2384	0.44	0/3257
1	B	0.26	0/2399	0.44	0/3279
All	All	0.27	0/4783	0.44	0/6536

There are no bond length outliers.

There are no bond angle outliers.

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	2324	0	2442	46	0
1	B	2338	0	2456	33	1
2	A	43	0	0	0	0
2	B	43	0	0	1	0
3	A	20	0	4	2	1
3	B	10	0	2	0	0
4	A	237	0	361	28	0
4	B	250	0	362	32	0
5	B	13	0	5	0	0
6	A	39	0	0	1	0
6	B	32	0	0	1	0
All	All	5349	0	5632	108	1

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 10.

The worst 5 of 108 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:A:166:LEU:HG	4:B:419:OLA:H10	1.55	0.87
4:A:405:OLA:H71	4:A:406:OLA:H52	1.59	0.85
4:B:410:OLA:H10	4:B:417:OLA:H41	1.61	0.83
1:B:251:PHE:HA	1:B:292:ASN:HD21	1.45	0.81
1:A:162:GLY:HA3	4:A:416:OLA:H152	1.66	0.79

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:NH1	3:A:403:TLA:O11[2_856]	2.19	0.01

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	288/317 (91%)	284 (99%)	4 (1%)	0	100	100
1	B	291/317 (92%)	287 (99%)	4 (1%)	0	100	100
All	All	579/634 (91%)	571 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	252/271 (93%)	248 (98%)	4 (2%)	62 85
1	B	254/271 (94%)	252 (99%)	2 (1%)	81 93
All	All	506/542 (93%)	500 (99%)	6 (1%)	71 88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	SER
1	B	44	PHE
1	B	290	TYR
1	A	78	LEU
1	A	37	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	B	292	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

38 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	OLA	B	403	-	12,12,19	0.60	0	12,12,19	1.14	0
4	OLA	A	410	-	9,9,19	0.27	0	8,8,19	0.64	0
4	OLA	B	416	-	19,19,19	0.52	0	19,19,19	0.94	0
4	OLA	A	406	-	14,14,19	0.28	0	13,13,19	0.72	0
4	OLA	B	411	-	13,13,19	0.59	0	12,13,19	1.09	0
4	OLA	B	415	-	19,19,19	0.51	0	19,19,19	1.03	0
4	OLA	A	415	-	14,14,19	0.30	0	13,13,19	0.73	0
4	OLA	B	418	-	14,14,19	0.56	0	14,14,19	1.04	0
4	OLA	A	418	-	10,10,19	0.65	0	10,10,19	1.19	1 (10%)
4	OLA	A	404	-	16,16,19	0.52	0	16,16,19	1.03	0
4	OLA	A	405	-	19,19,19	0.51	0	19,19,19	0.99	0
4	OLA	B	408	-	6,6,19	0.78	0	6,6,19	1.34	1 (16%)
2	9P2	A	401	-	45,49,49	2.76	12 (26%)	59,68,68	1.20	5 (8%)
4	OLA	B	419	-	13,13,19	0.28	0	12,12,19	0.76	0
4	OLA	B	404	-	9,9,19	0.68	0	9,9,19	1.20	0
4	OLA	A	416	-	19,19,19	0.51	0	19,19,19	0.97	0
4	OLA	A	414	-	15,15,19	0.55	0	15,15,19	1.07	0
2	9P2	B	401	-	45,49,49	2.71	12 (26%)	59,68,68	1.20	7 (11%)
4	OLA	B	406	-	13,13,19	0.59	0	12,13,19	1.16	1 (8%)
4	OLA	B	414	-	8,8,19	0.31	0	7,7,19	0.74	0
4	OLA	B	417	-	15,15,19	0.54	0	15,15,19	1.04	0
4	OLA	A	417	-	19,19,19	0.50	0	19,19,19	1.02	0
5	CIT	B	420	-	12,12,12	1.32	1 (8%)	17,17,17	1.47	2 (11%)
4	OLA	A	411	-	17,17,19	0.52	0	17,17,19	1.06	1 (5%)
4	OLA	B	413	-	13,13,19	0.59	0	12,13,19	1.13	0
4	OLA	A	412	-	19,19,19	0.50	0	19,19,19	1.07	1 (5%)
4	OLA	A	413	-	12,12,19	0.29	0	11,11,19	0.70	0
3	TLA	A	403	-	9,9,9	1.14	0	12,12,12	3.55	8 (66%)
4	OLA	B	405	-	14,14,19	0.56	0	14,14,19	1.10	1 (7%)
4	OLA	A	409	-	11,11,19	0.31	0	10,10,19	0.69	0
3	TLA	B	402	-	9,9,9	1.11	0	12,12,12	3.60	8 (66%)
4	OLA	B	410	-	19,19,19	0.51	0	19,19,19	1.00	0
3	TLA	A	402	-	9,9,9	1.08	0	12,12,12	3.68	8 (66%)
4	OLA	B	412	-	19,19,19	0.52	0	19,19,19	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OLA	B	407	-	12,12,19	0.59	0	12,12,19	1.21	1 (8%)
4	OLA	A	408	-	15,15,19	0.54	0	15,15,19	1.06	0
4	OLA	B	409	-	15,15,19	0.54	0	15,15,19	1.01	1 (6%)
4	OLA	A	407	-	13,13,19	0.60	0	12,13,19	1.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	B	403	-	-	7/10/10/17	-
4	OLA	A	410	-	-	0/7/7/17	-
4	OLA	B	416	-	-	5/17/17/17	-
4	OLA	A	406	-	-	7/12/12/17	-
4	OLA	B	411	-	-	6/11/11/17	-
4	OLA	B	415	-	-	5/17/17/17	-
4	OLA	A	415	-	-	5/12/12/17	-
4	OLA	B	418	-	-	7/12/12/17	-
4	OLA	A	418	-	-	1/8/8/17	-
4	OLA	A	404	-	-	9/14/14/17	-
4	OLA	A	405	-	-	8/17/17/17	-
4	OLA	B	408	-	-	0/4/4/17	-
2	9P2	A	401	-	-	7/23/36/36	0/7/7/7
4	OLA	B	419	-	-	5/11/11/17	-
4	OLA	B	404	-	-	1/7/7/17	-
4	OLA	A	416	-	-	10/17/17/17	-
4	OLA	A	414	-	-	3/13/13/17	-
2	9P2	B	401	-	-	7/23/36/36	0/7/7/7
4	OLA	B	406	-	-	4/11/11/17	-
4	OLA	B	414	-	-	2/6/6/17	-
4	OLA	B	417	-	-	6/13/13/17	-
4	OLA	A	417	-	-	10/17/17/17	-
5	CIT	B	420	-	-	11/16/16/16	-
4	OLA	A	411	-	-	7/15/15/17	-
4	OLA	B	413	-	-	6/11/11/17	-
4	OLA	A	412	-	-	4/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	413	-	-	4/10/10/17	-
3	TLA	A	403	-	2/2/4/4	6/12/12/12	-
4	OLA	B	405	-	-	3/12/12/17	-
4	OLA	A	409	-	-	2/9/9/17	-
3	TLA	B	402	-	2/2/4/4	8/12/12/12	-
4	OLA	B	410	-	-	9/17/17/17	-
3	TLA	A	402	-	2/2/4/4	8/12/12/12	-
4	OLA	B	412	-	-	9/17/17/17	-
4	OLA	B	407	-	-	4/10/10/17	-
4	OLA	A	408	-	-	7/13/13/17	-
4	OLA	B	409	-	-	5/13/13/17	-
4	OLA	A	407	-	-	1/11/11/17	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	9P2	C32-C03	-10.61	1.37	1.49
2	B	401	9P2	C32-C03	-10.19	1.37	1.49
2	A	401	9P2	C24-C25	6.48	1.50	1.38
2	B	401	9P2	C24-C25	6.38	1.50	1.38
2	B	401	9P2	C18-C17	5.96	1.49	1.38

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	TLA	O3-C3-C2	6.15	122.45	110.23
3	A	402	TLA	O2-C2-C3	6.06	122.26	110.23
3	A	403	TLA	O2-C2-C3	5.57	121.29	110.23
3	B	402	TLA	C3-C2-C1	5.55	122.26	109.87
3	A	402	TLA	O3-C3-C2	5.51	121.17	110.23

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	402	TLA	C3
3	A	402	TLA	C2
3	A	403	TLA	C3
3	A	403	TLA	C2
3	B	402	TLA	C3

5 of 209 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	9P2	N02-C03-C32-C37
3	A	402	TLA	C1-C2-C3-C4
3	A	402	TLA	O2-C2-C3-O3
3	A	403	TLA	O11-C1-C2-O2
3	A	403	TLA	C1-C2-C3-C4

There are no ring outliers.

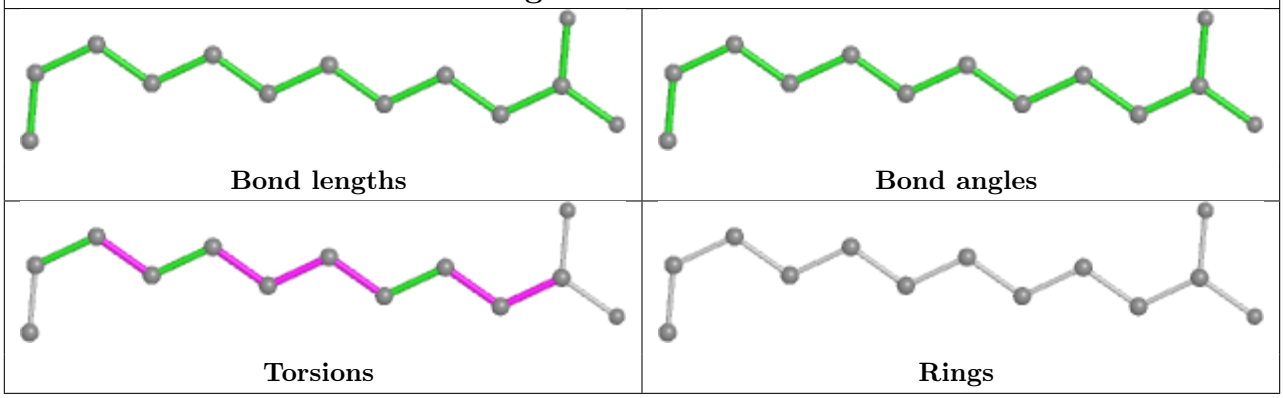
27 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	OLA	1	0
4	A	410	OLA	2	0
4	B	416	OLA	4	0
4	A	406	OLA	7	0
4	B	411	OLA	1	0
4	B	415	OLA	2	0
4	B	418	OLA	1	0
4	A	404	OLA	1	0
4	A	405	OLA	7	0
4	B	419	OLA	10	0
4	A	416	OLA	5	0
2	B	401	9P2	1	0
4	B	406	OLA	4	0
4	B	417	OLA	3	0
4	A	417	OLA	3	0
4	A	411	OLA	1	0
4	B	413	OLA	1	0
4	A	412	OLA	2	0
4	A	413	OLA	3	0
3	A	403	TLA	0	1
4	B	405	OLA	2	0
4	A	409	OLA	2	0
4	B	410	OLA	4	0
3	A	402	TLA	2	0
4	B	412	OLA	1	0
4	A	408	OLA	2	0
4	B	409	OLA	3	0

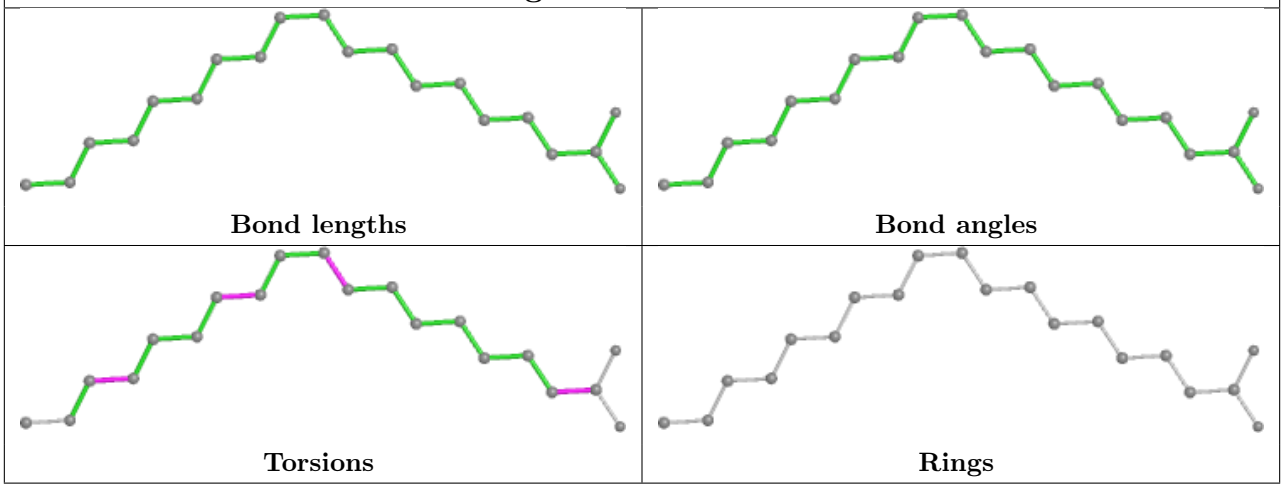
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

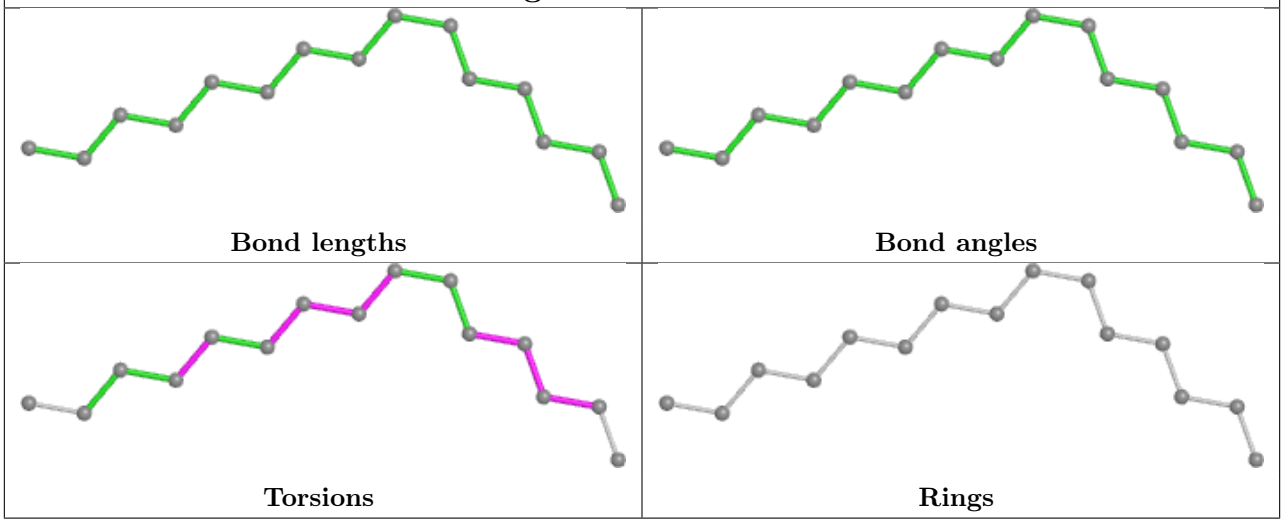
Ligand OLA B 403



Ligand OLA B 416



Ligand OLA A 406



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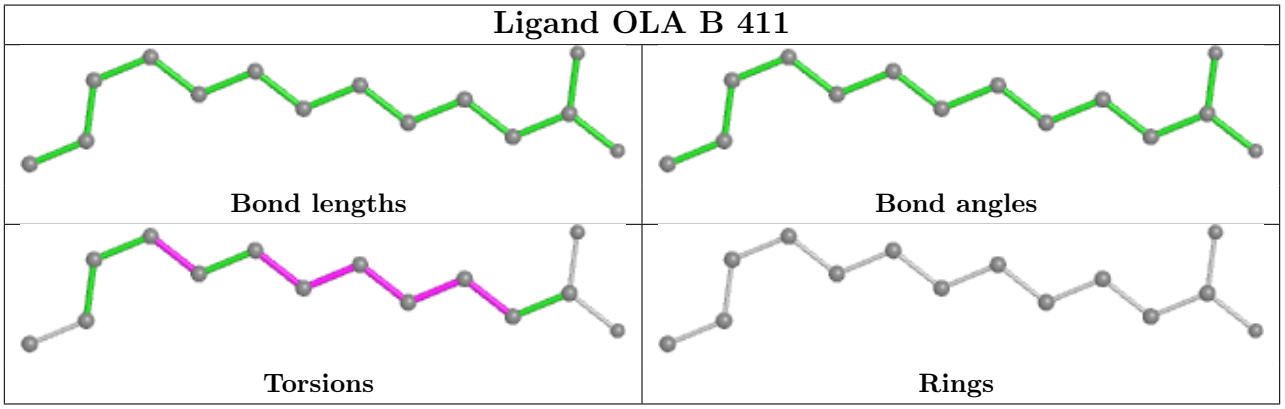

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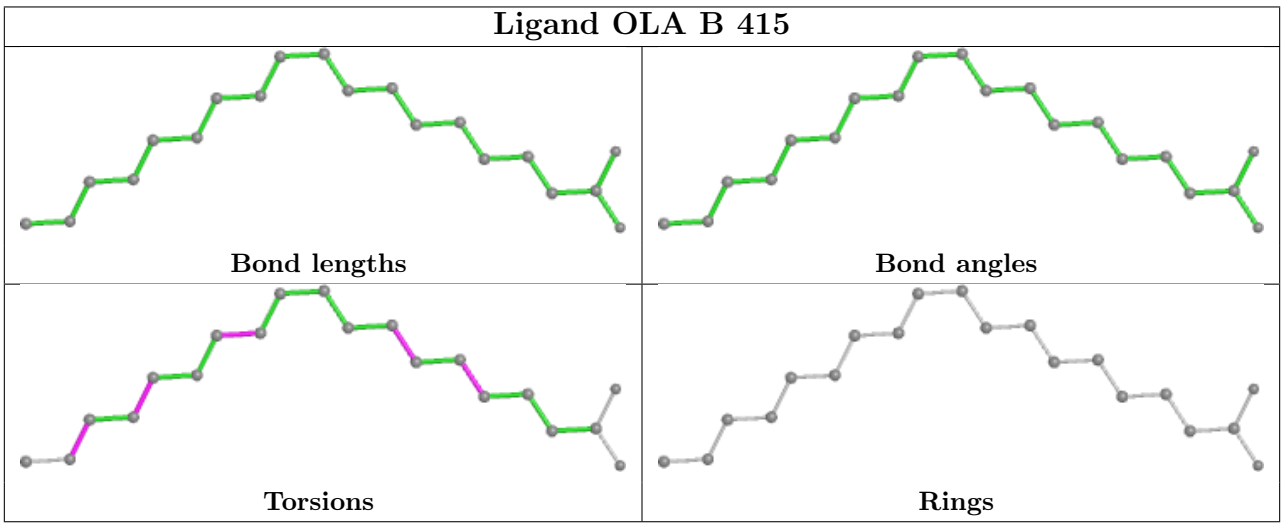

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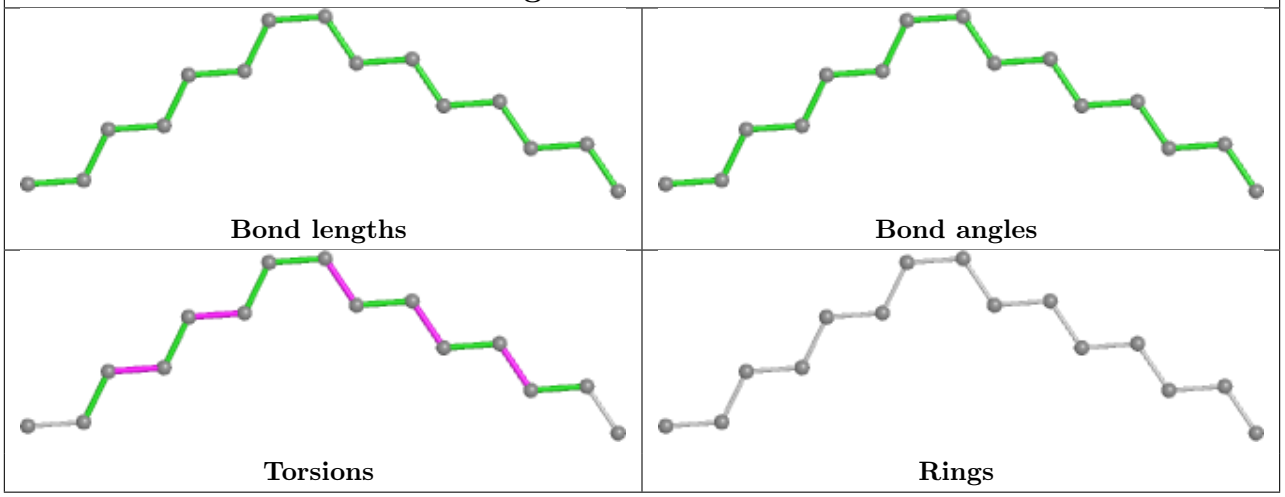

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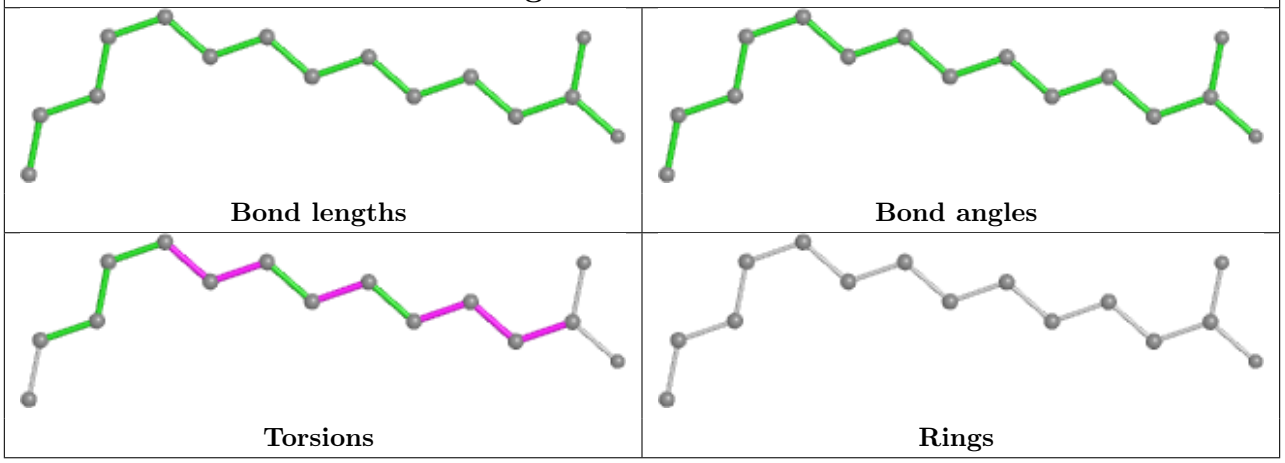

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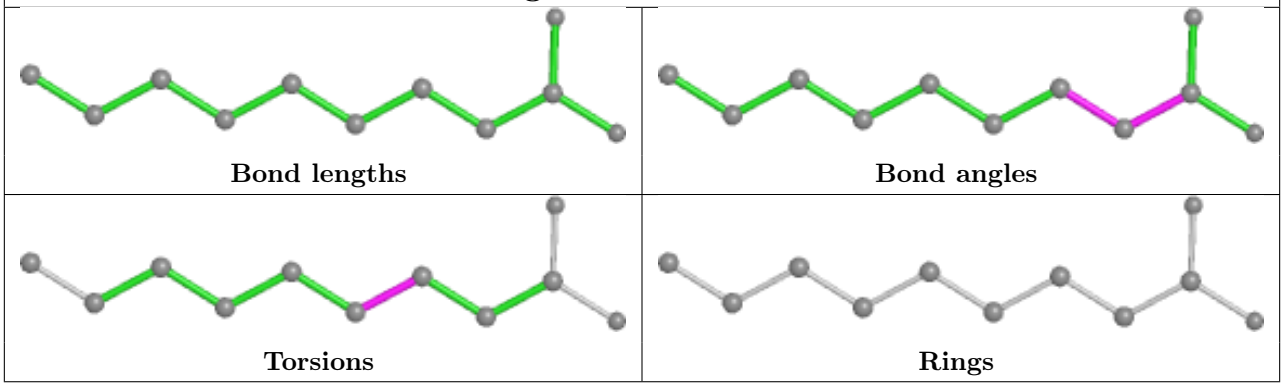

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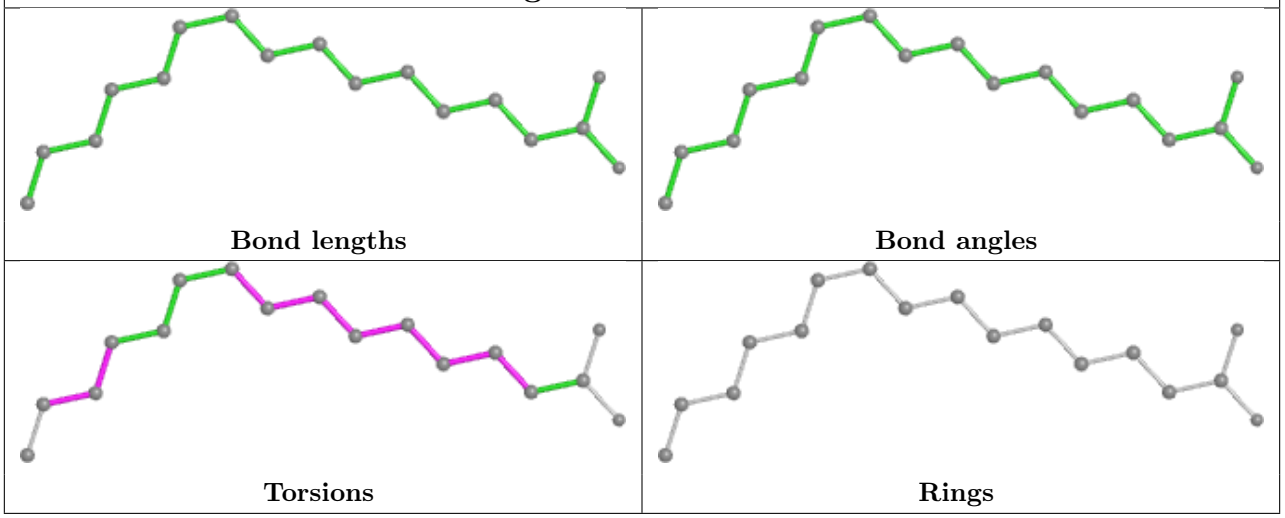

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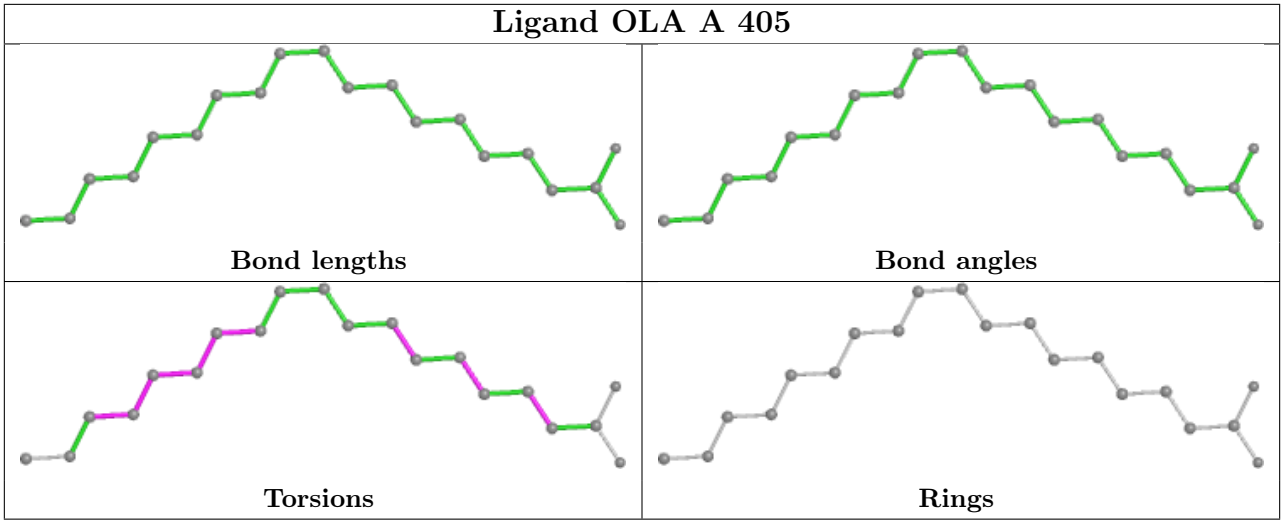

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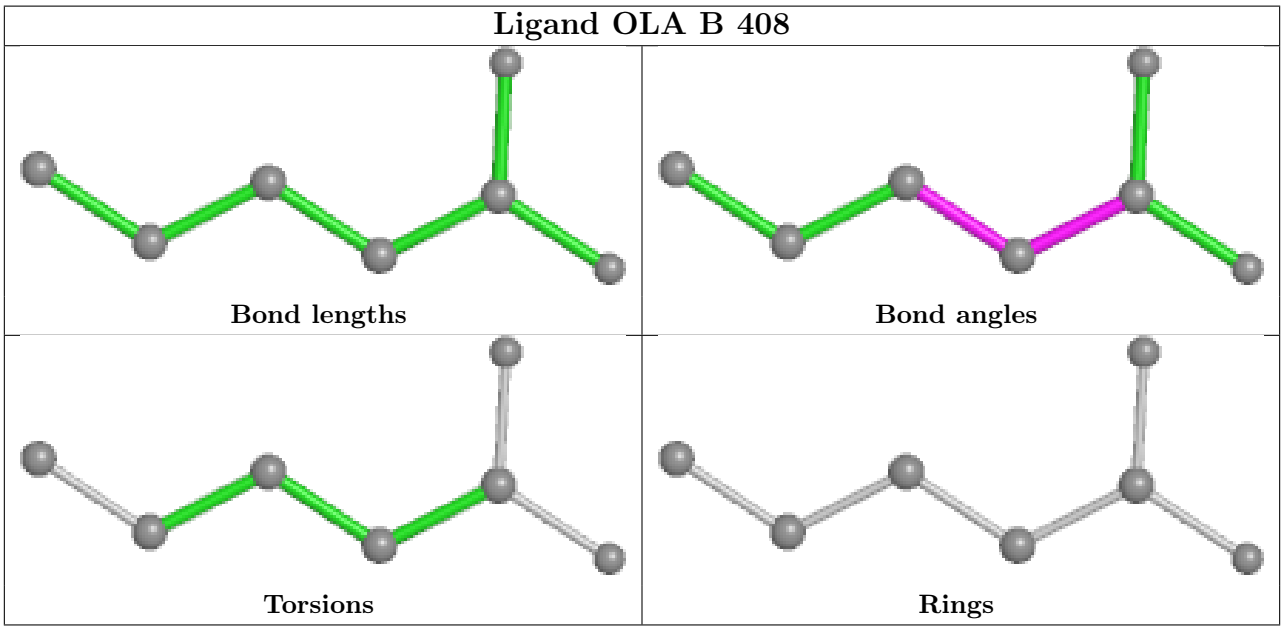
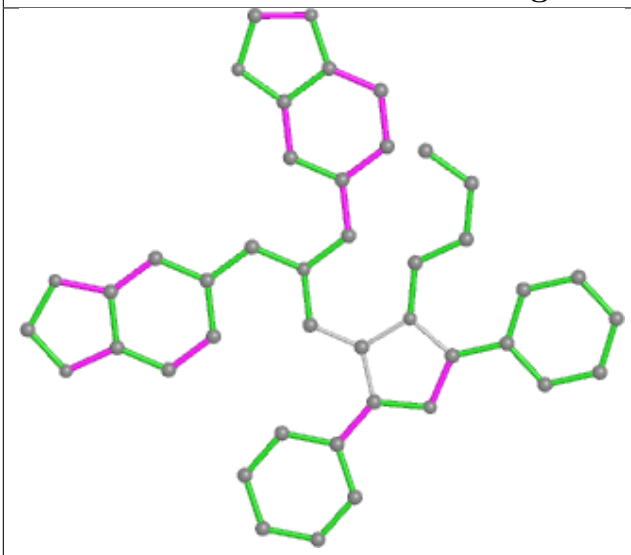
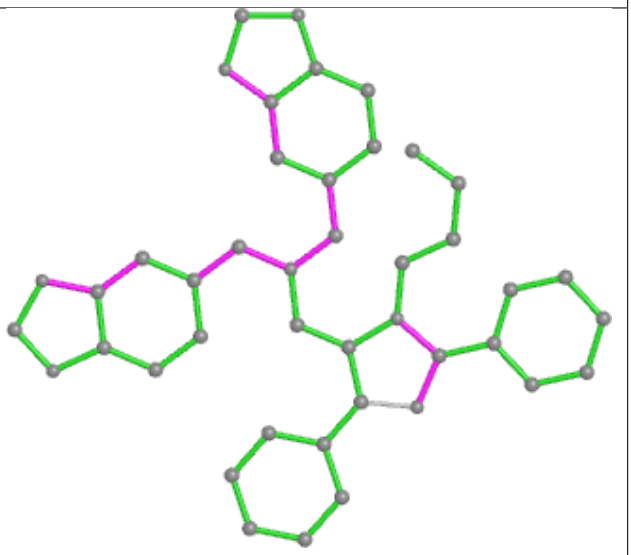


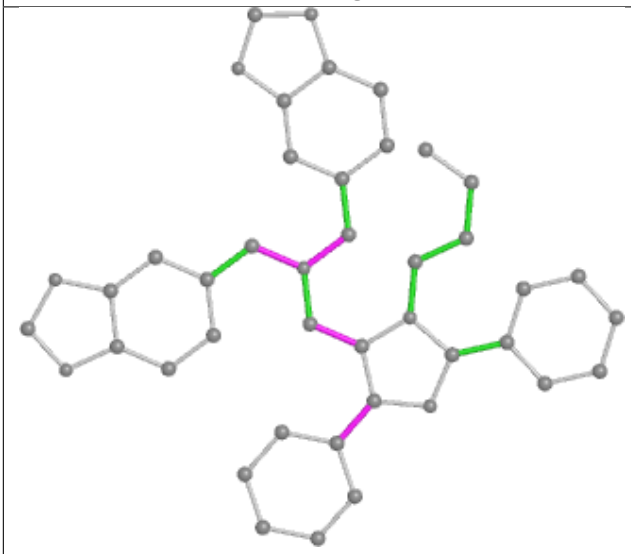
Ligand 9P2 A 401



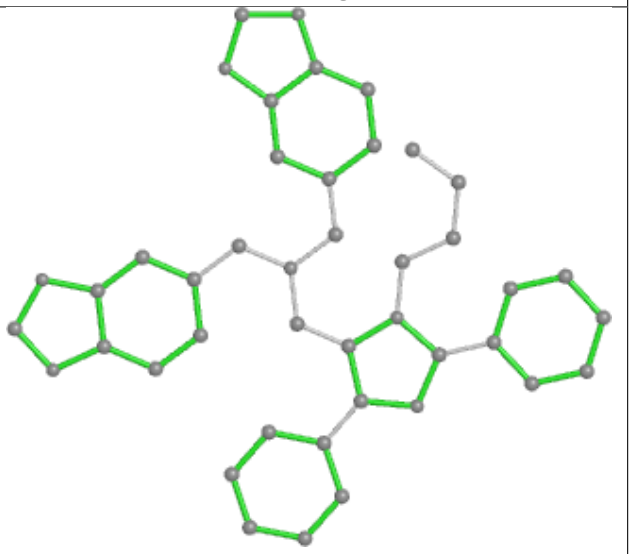
Bond lengths



Bond angles

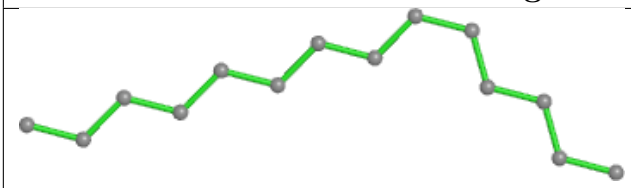


Torsions

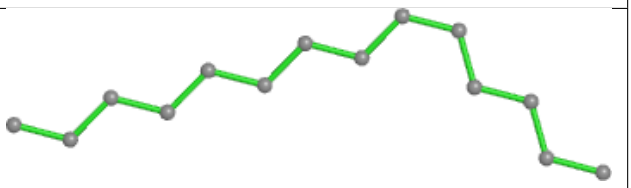


Rings

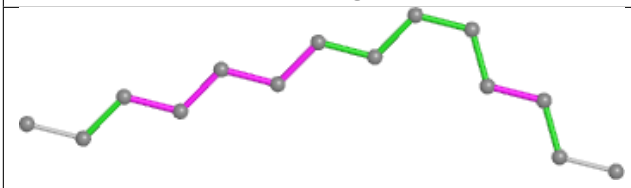
Ligand OLA B 419



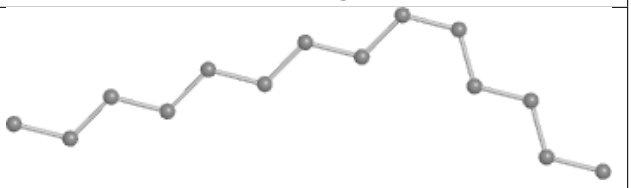
Bond lengths



Bond angles

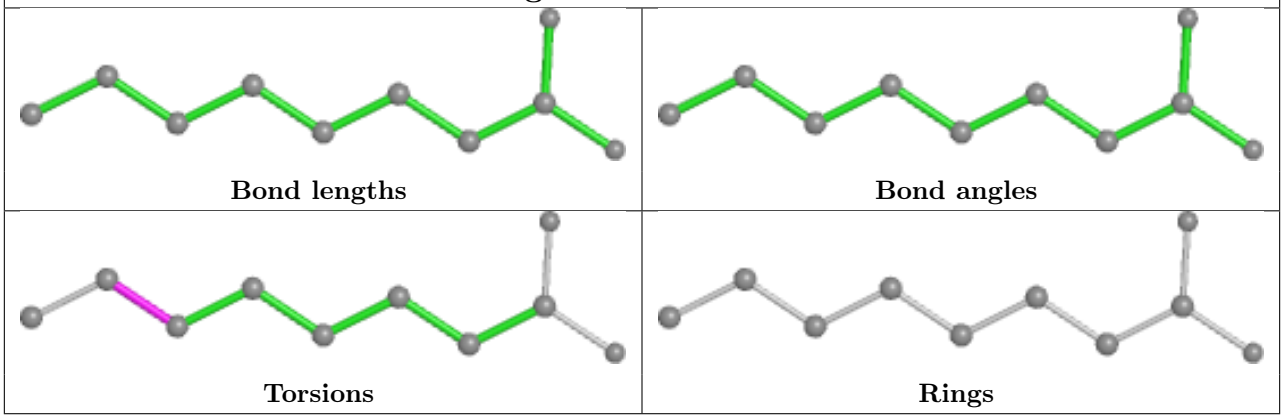


Torsions



Rings

Ligand OLA B 404



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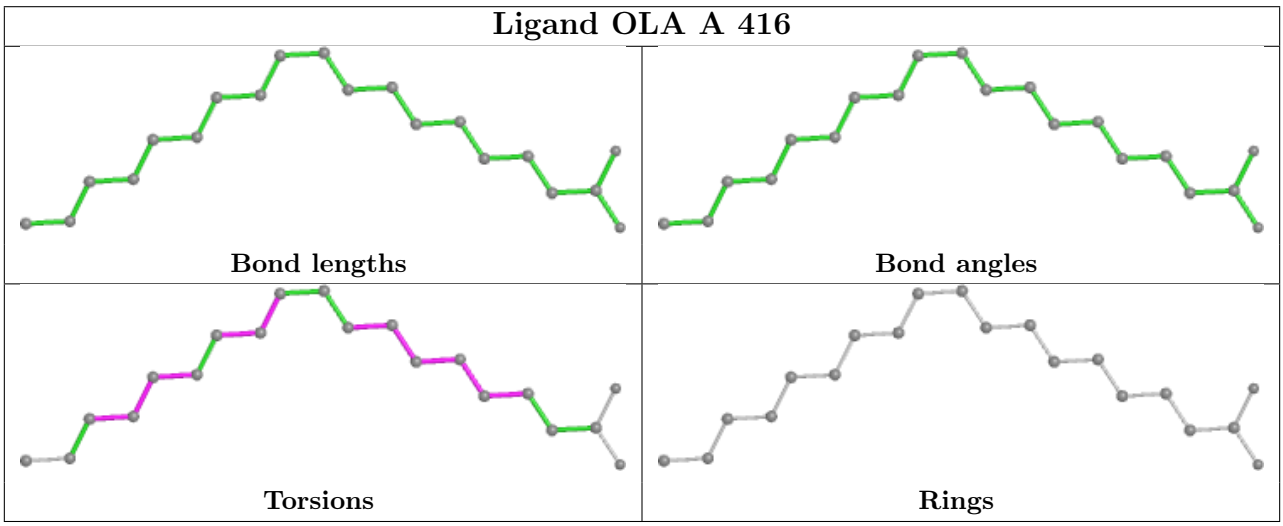
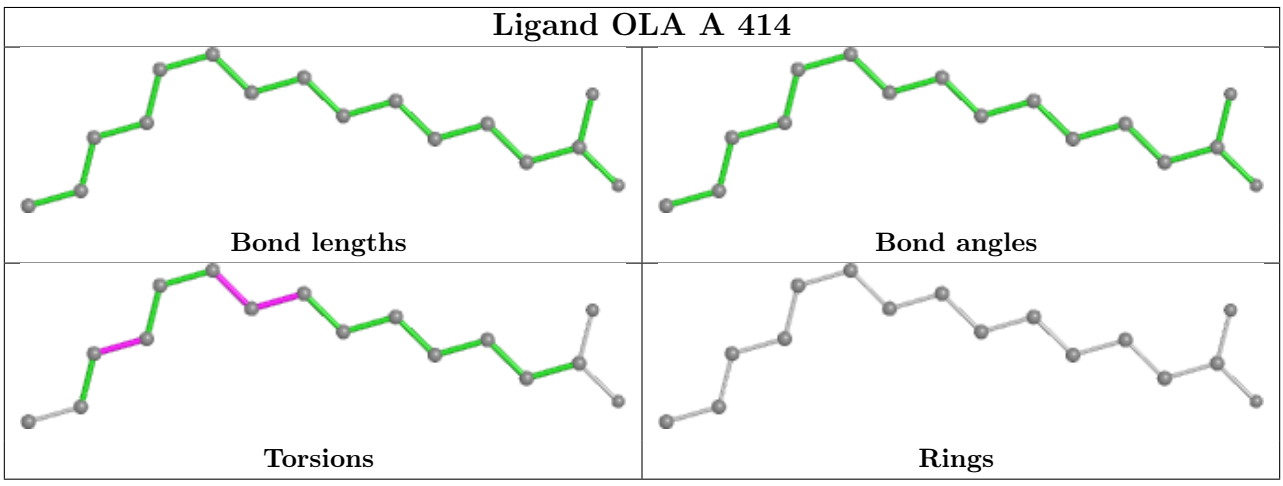
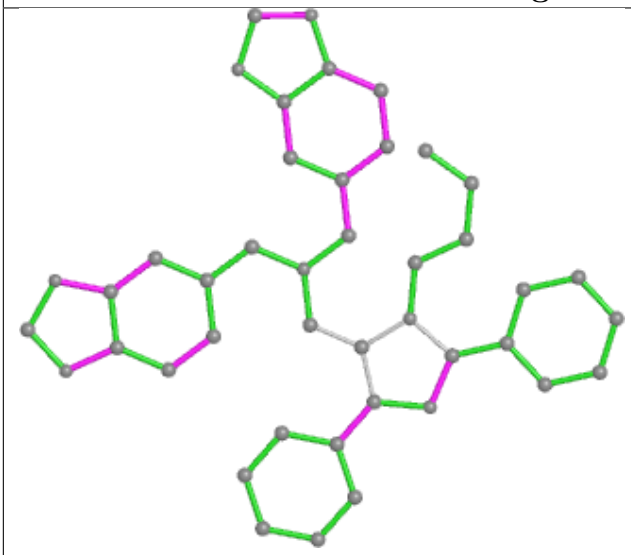


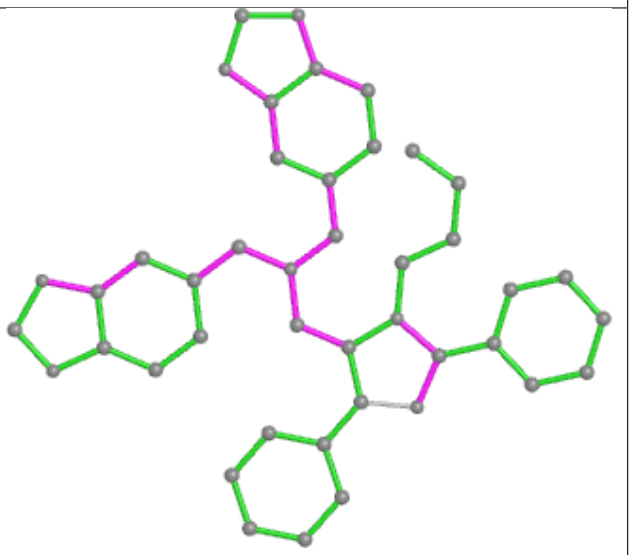
Ligand OLA A 414



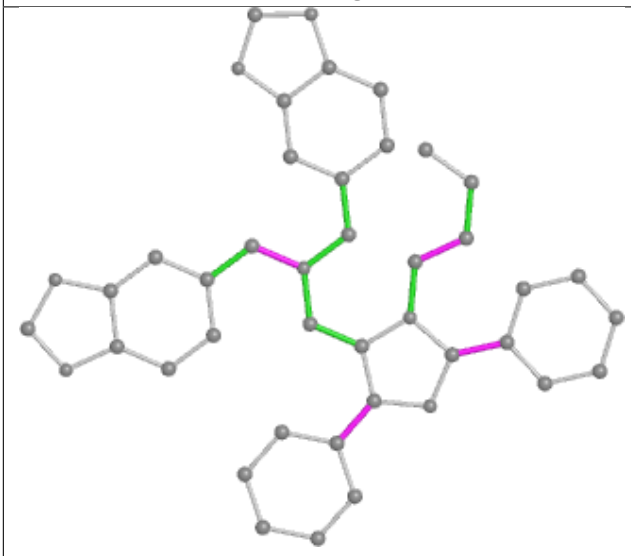
Ligand 9P2 B 401



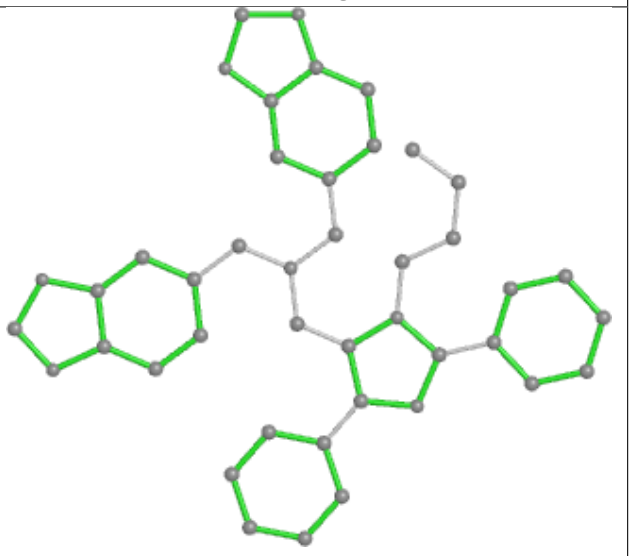
Bond lengths



Bond angles



Torsions



Rings

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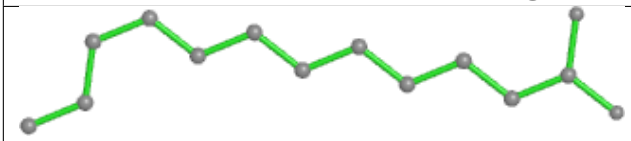
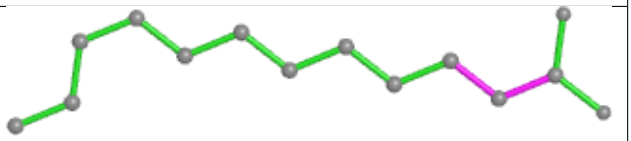
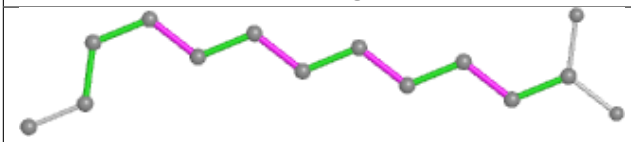


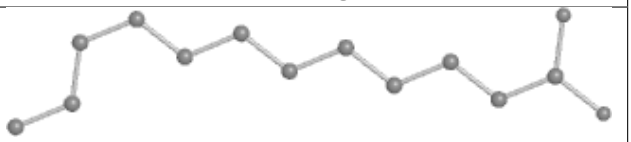
Bond lengths



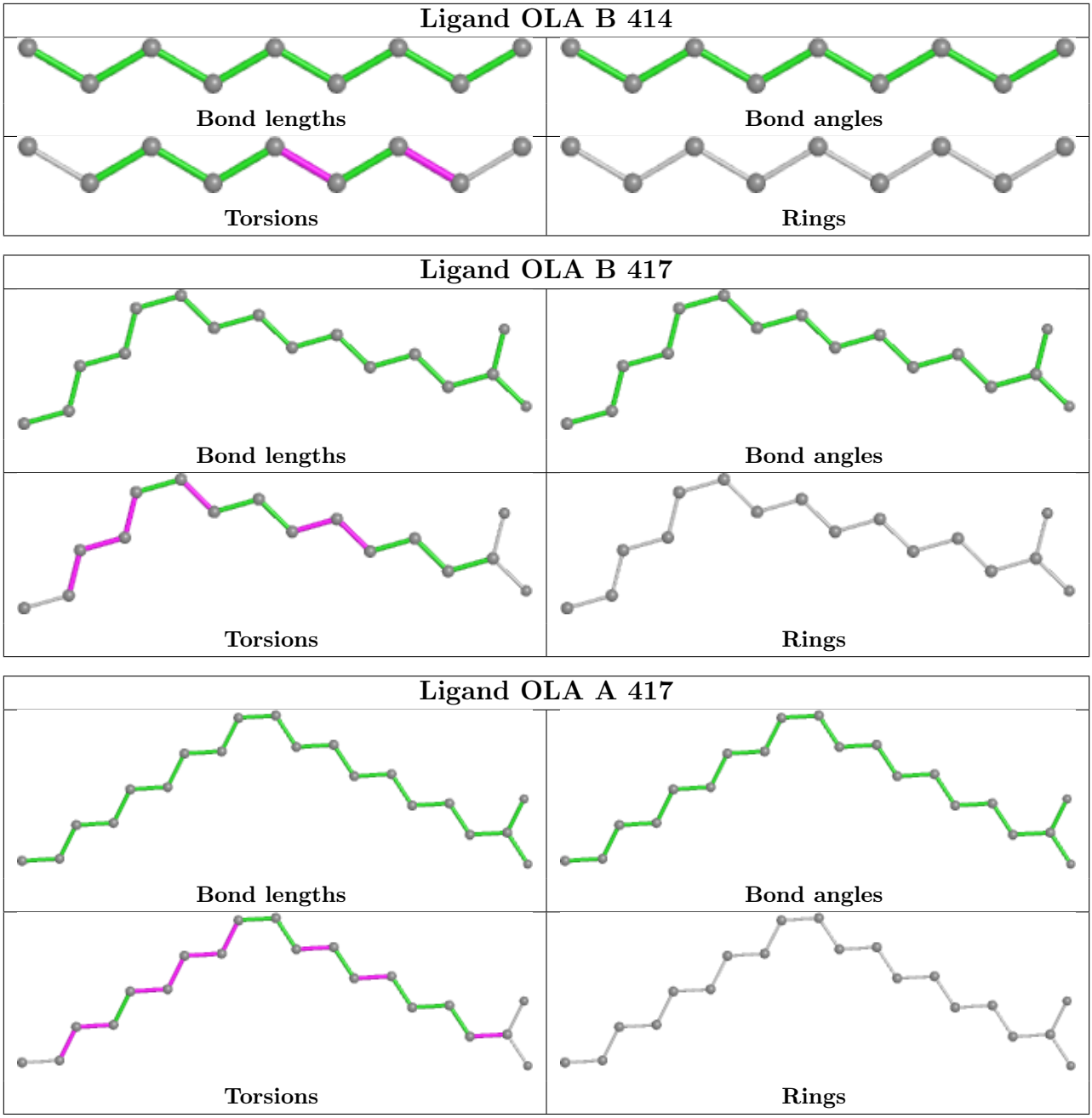
Bond angles



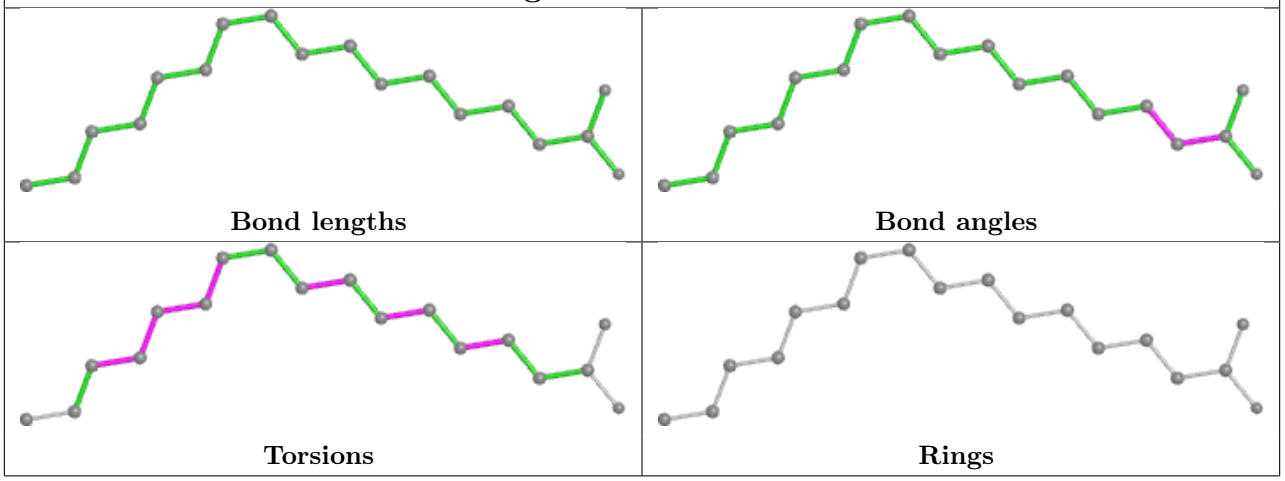
Torsions



Rings


Ligand OLA B 414
Bond lengths
Bond angles
Torsions
Rings
Ligand OLA B 417
Bond lengths
Bond angles
Torsions
Rings
Ligand OLA A 417
Bond lengths
Bond angles
Torsions
Rings

Ligand OLA A 411



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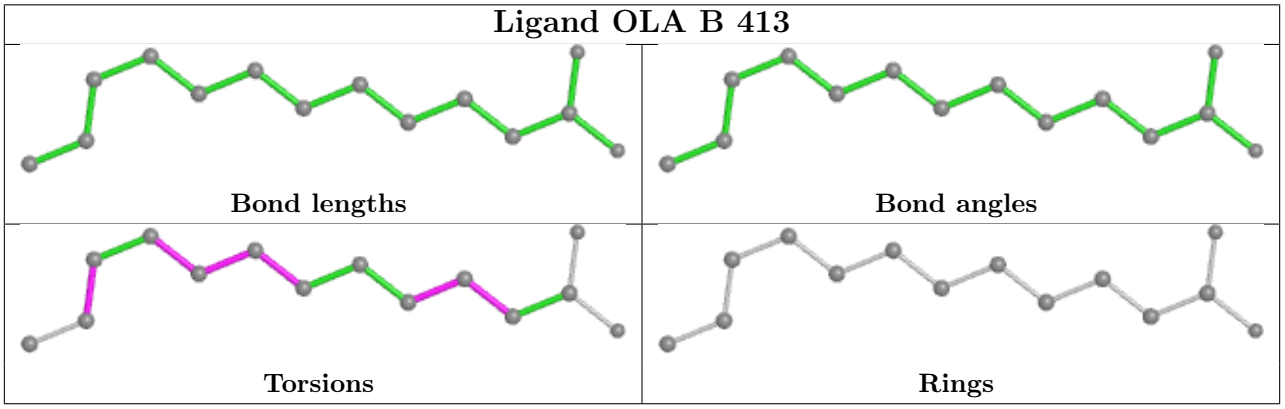

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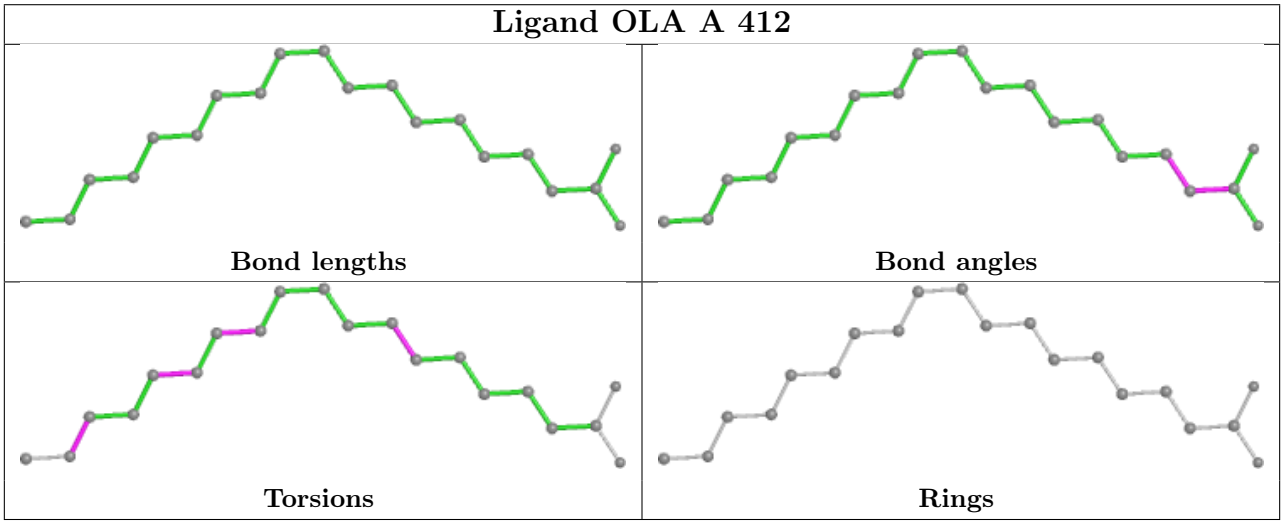

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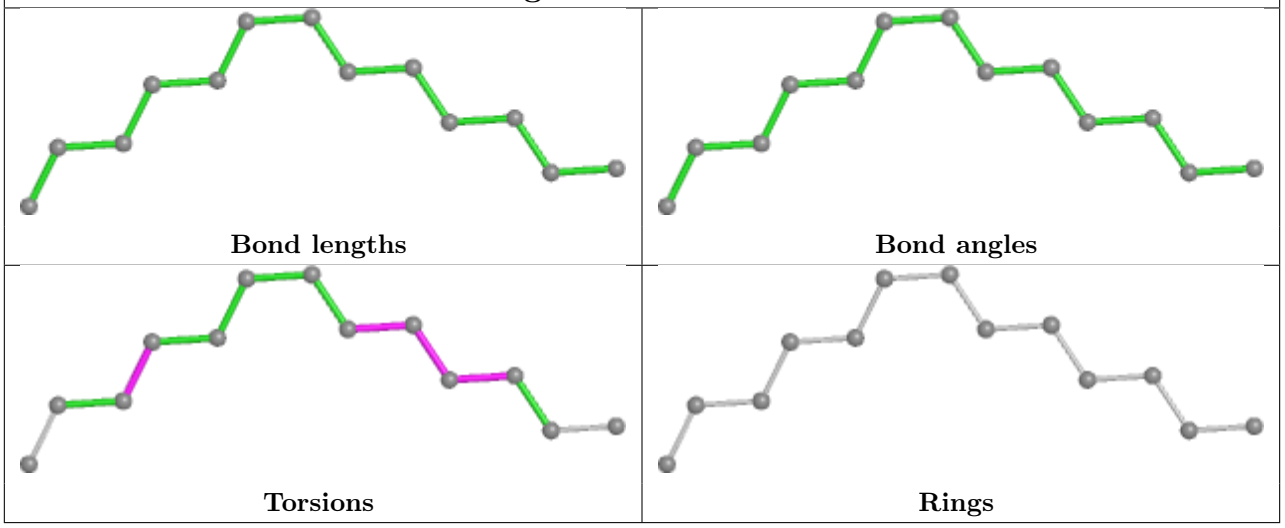

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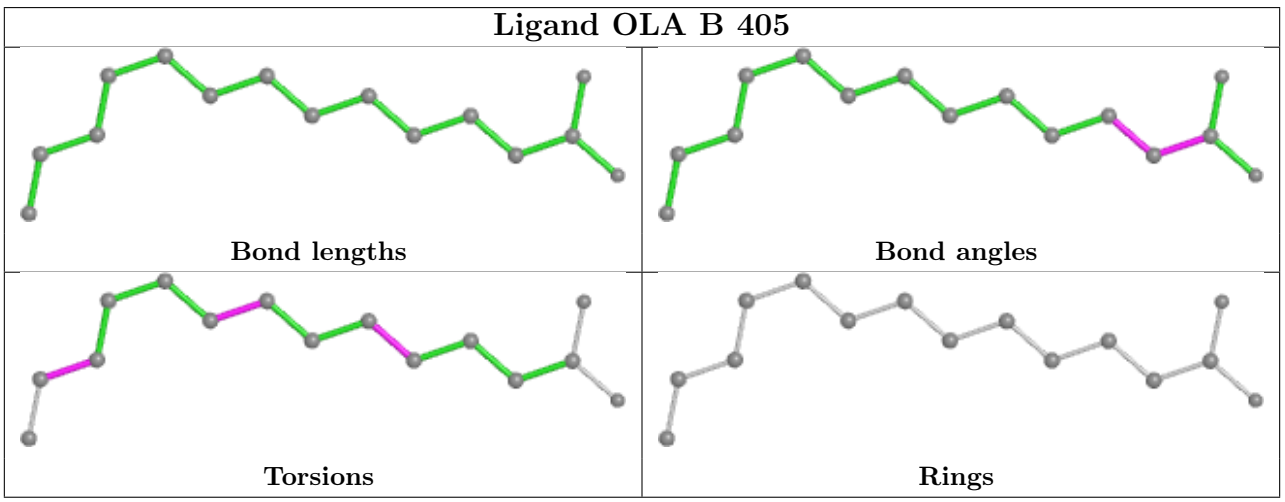

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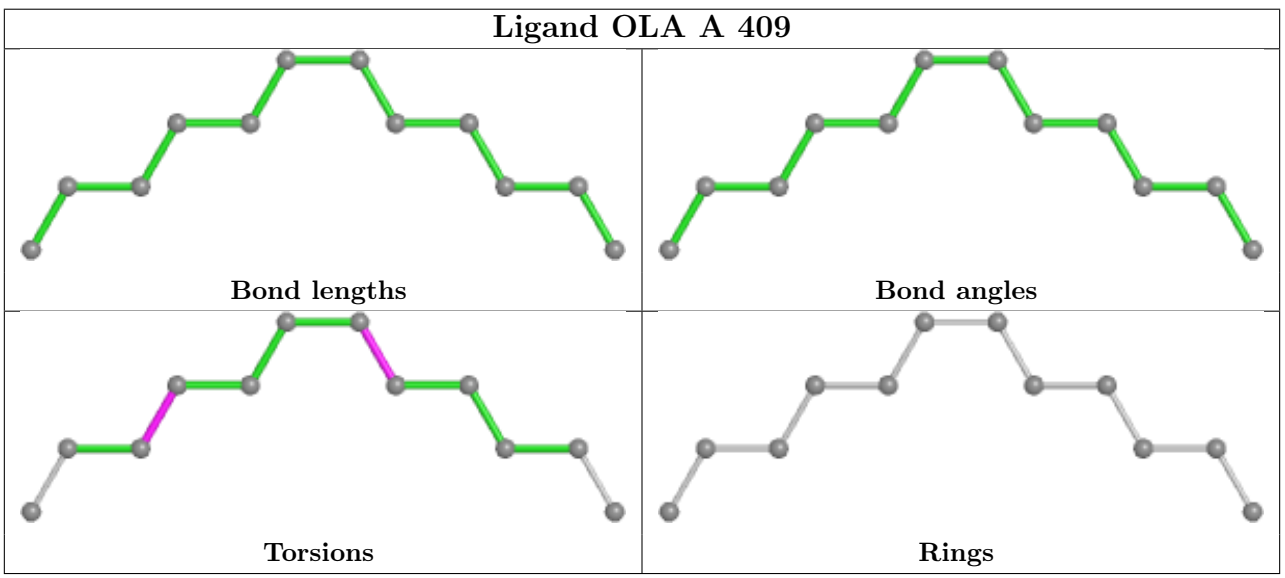

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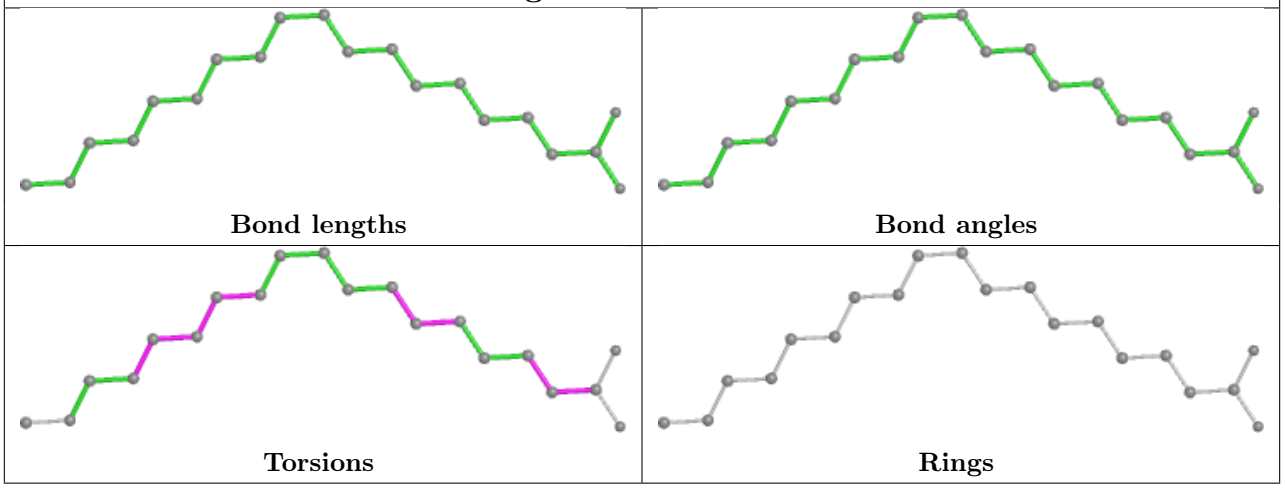
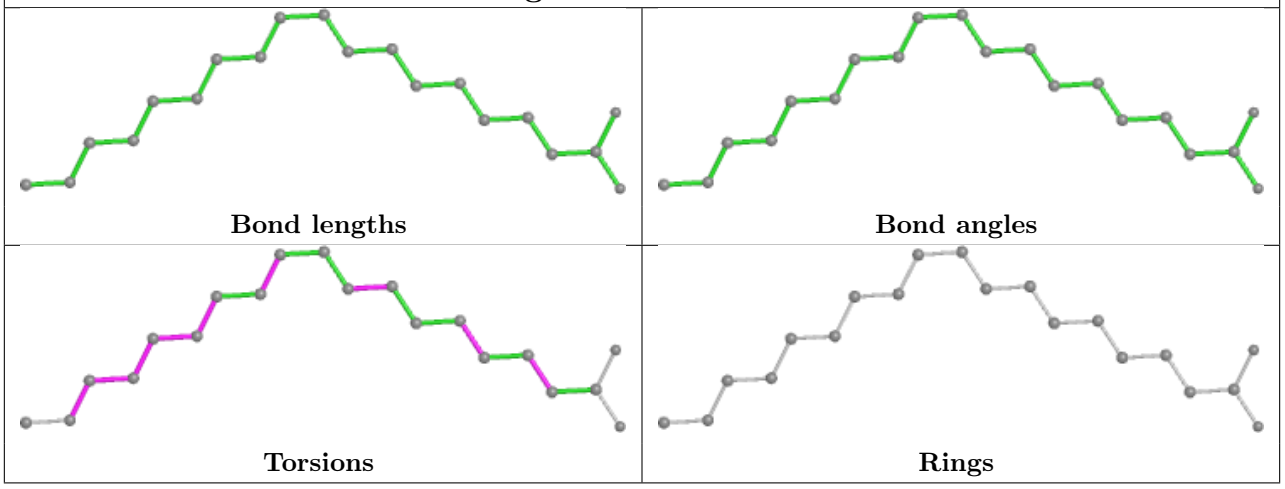
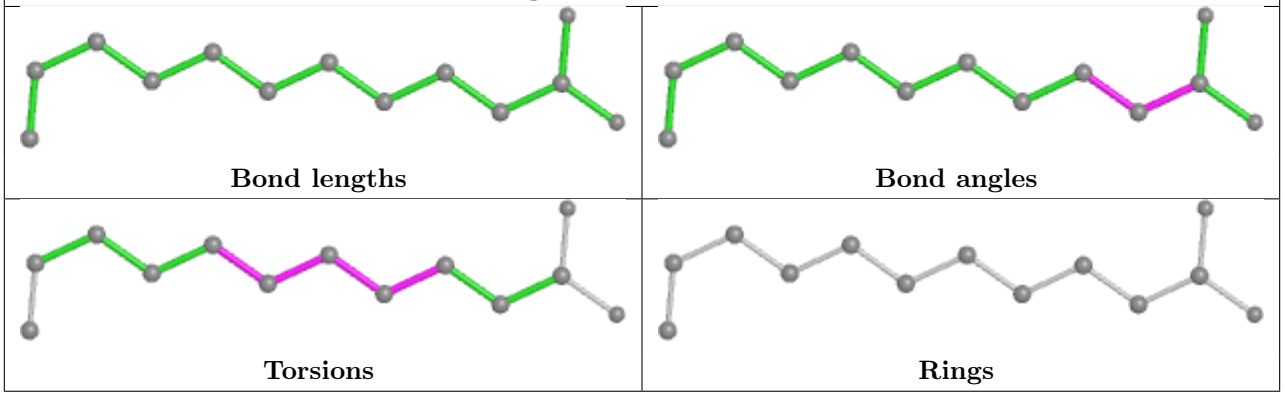
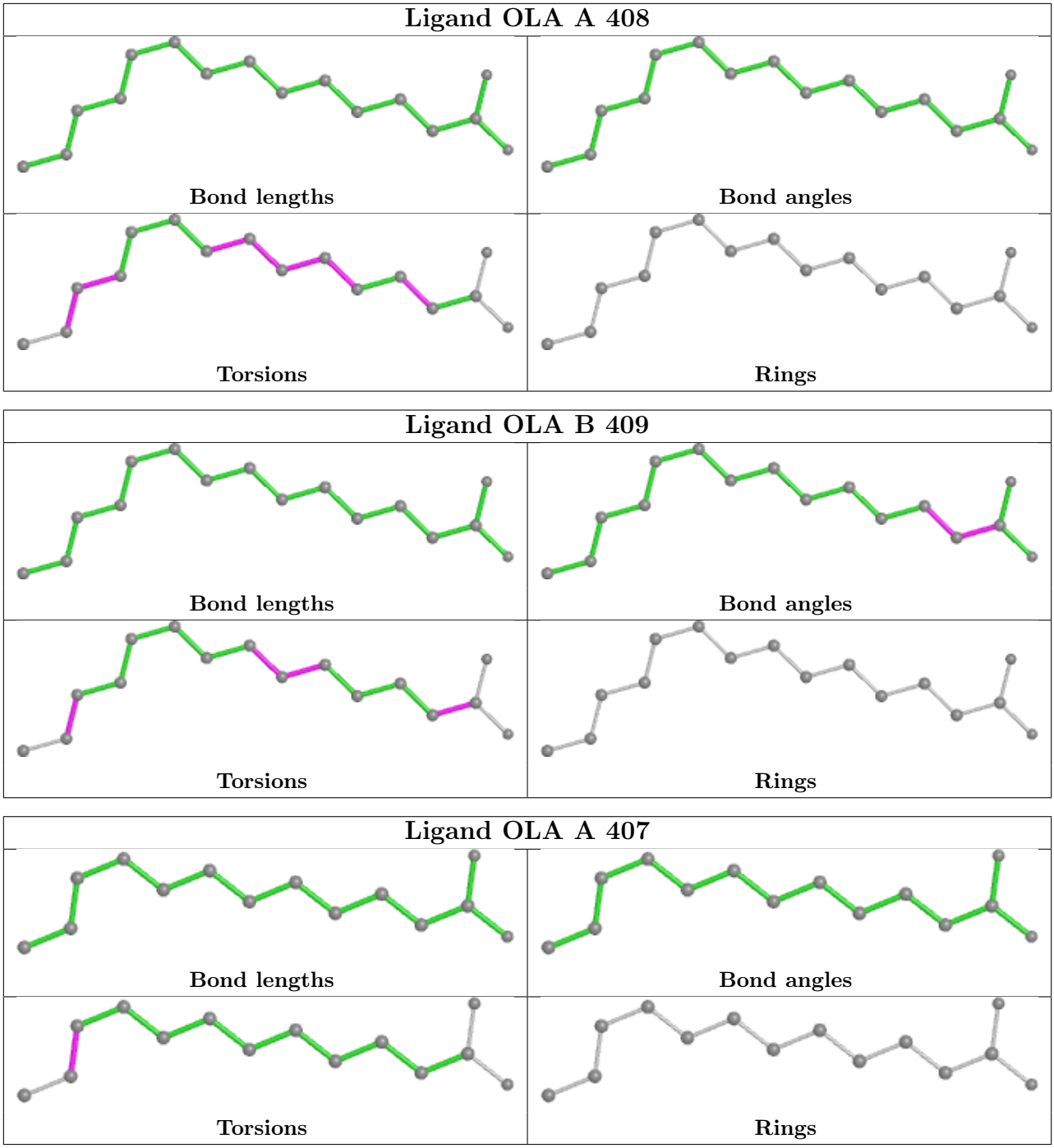


Ligand OLA B 412



Ligand OLA B 407





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	294/317 (92%)	0.02	11 (3%)	41	41	19, 41, 83, 108	0
1	B	295/317 (93%)	-0.03	16 (5%)	25	24	15, 39, 82, 125	0
All	All	589/634 (92%)	-0.01	27 (4%)	32	31	15, 40, 83, 125	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	ASN	6.3
1	A	182	PHE	6.0
1	B	195	ASP	5.2
1	B	196	LYS	4.8
1	B	194	HIS	4.4

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 monosaccharides in this entry.

6.4 Ligands

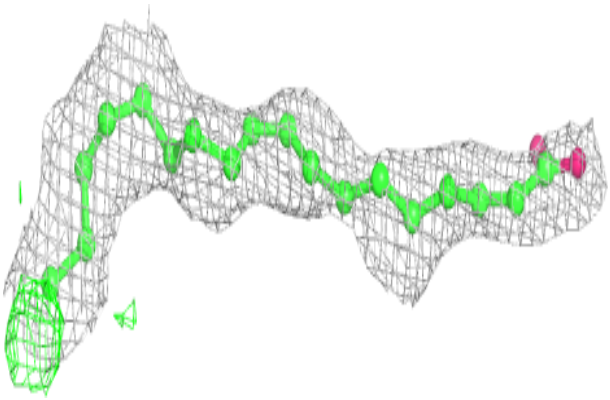
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

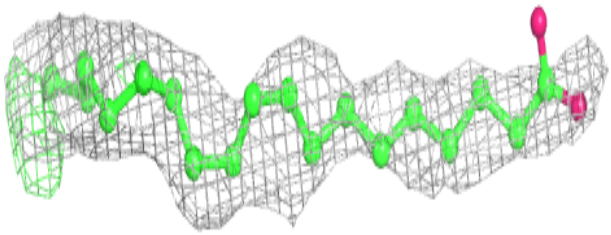
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CIT	B	420	13/13	0.69	0.47	82,92,102,118	0
4	OLA	B	412	20/20	0.76	0.36	38,63,93,98	0
4	OLA	B	411	14/20	0.77	0.34	63,73,89,91	0
4	OLA	A	405	20/20	0.77	0.28	40,55,77,81	0
4	OLA	B	418	15/20	0.77	0.37	40,58,87,94	0
4	OLA	B	403	13/20	0.77	0.27	41,55,65,70	0
4	OLA	A	408	16/20	0.78	0.45	58,71,77,82	0
3	TLA	A	403	10/10	0.78	0.32	43,71,85,101	0
4	OLA	A	409	12/20	0.80	0.36	55,63,77,80	0
4	OLA	B	406	14/20	0.80	0.41	42,58,82,84	0
4	OLA	A	411	18/20	0.80	0.51	51,59,67,71	0
4	OLA	B	404	10/20	0.81	0.27	33,41,68,79	0
4	OLA	B	413	14/20	0.81	0.47	39,51,64,82	0
4	OLA	A	410	10/20	0.82	0.22	46,62,68,73	0
4	OLA	A	412	20/20	0.82	0.46	38,57,78,81	0
4	OLA	B	416	20/20	0.82	0.28	40,60,79,82	0
4	OLA	A	416	20/20	0.82	0.30	19,45,71,86	0
4	OLA	A	418	11/20	0.82	0.41	52,65,92,99	0
4	OLA	B	415	20/20	0.83	0.30	33,57,73,74	0
4	OLA	A	407	14/20	0.83	0.26	44,61,73,76	0
4	OLA	B	409	16/20	0.83	0.31	38,59,97,103	0
4	OLA	B	410	20/20	0.83	0.24	37,62,77,80	0
3	TLA	A	402	10/10	0.84	0.25	38,59,71,87	0
4	OLA	A	417	20/20	0.84	0.26	37,56,95,95	0
4	OLA	A	415	15/20	0.84	0.31	36,52,69,71	0
4	OLA	B	405	15/20	0.85	0.24	40,57,78,85	0
4	OLA	A	406	15/20	0.86	0.28	33,57,72,76	0
4	OLA	B	414	9/20	0.86	0.27	46,52,58,64	0
4	OLA	B	417	16/20	0.87	0.25	45,60,74,80	0
4	OLA	B	407	13/20	0.88	0.25	32,37,62,64	0
4	OLA	B	419	14/20	0.89	0.21	32,46,61,65	0
4	OLA	A	414	16/20	0.89	0.28	37,56,67,74	0
4	OLA	B	408	7/20	0.90	0.16	27,32,47,52	0
4	OLA	A	413	13/20	0.91	0.19	38,47,55,62	0
3	TLA	B	402	10/10	0.91	0.24	40,59,68,81	0
4	OLA	A	404	17/20	0.91	0.22	25,44,64,69	0
2	9P2	A	401	43/43	0.95	0.18	18,26,43,51	0
2	9P2	B	401	43/43	0.96	0.17	17,27,37,41	0

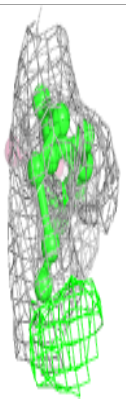
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA B 412:

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

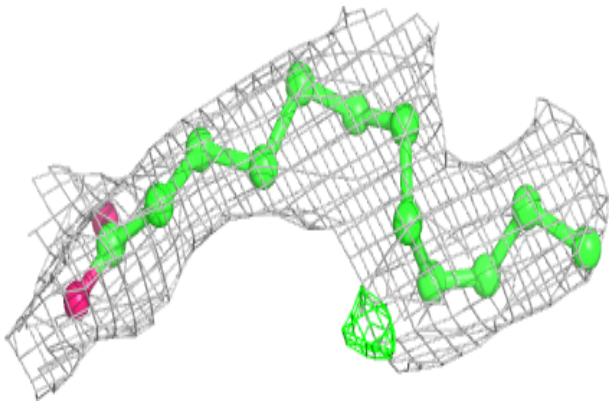


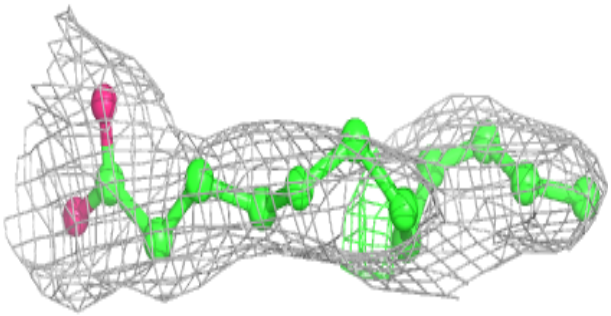


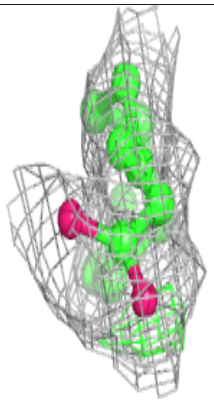


Electron density around OLA B 411:

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

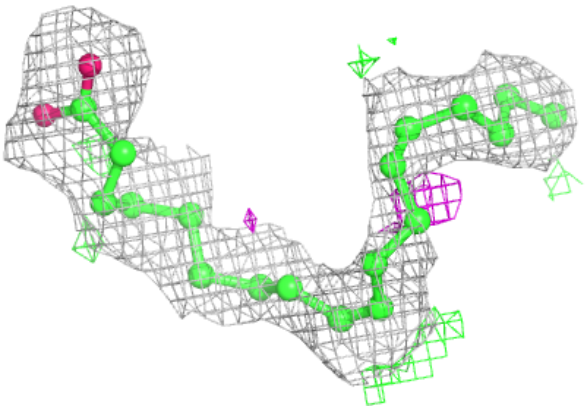


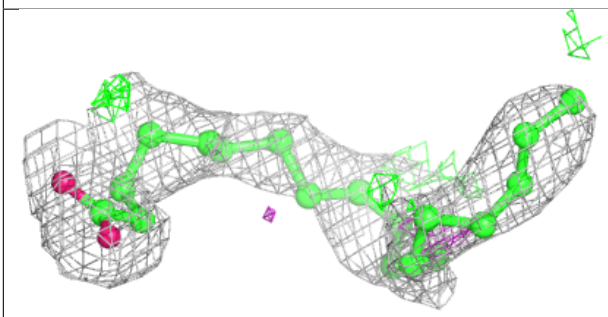


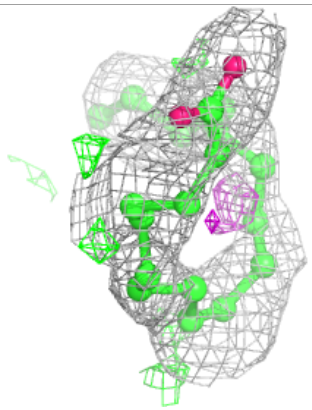


Electron density around OLA A 405:

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

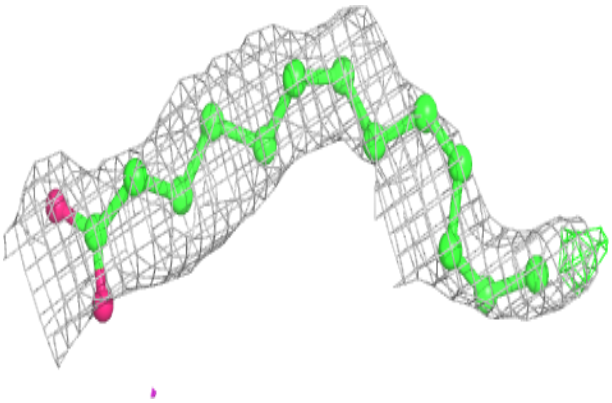


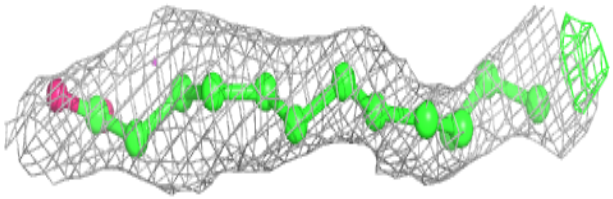


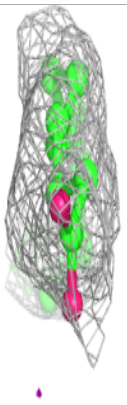


Electron density around OLA B 418:

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

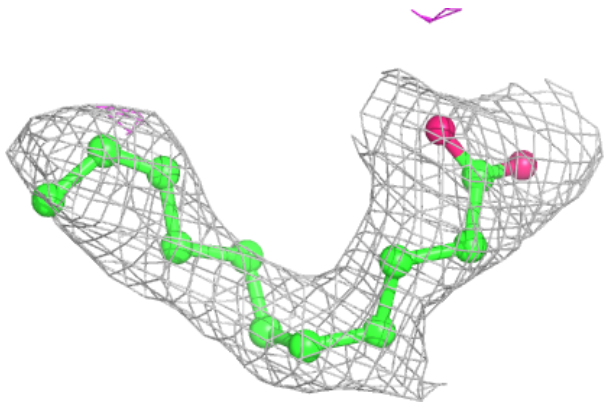


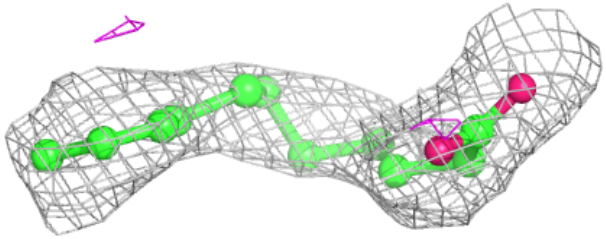


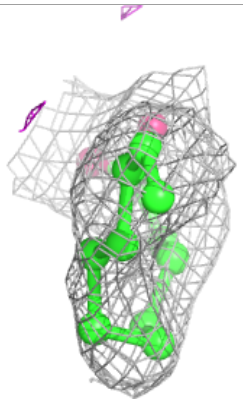


Electron density around OLA B 403:

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

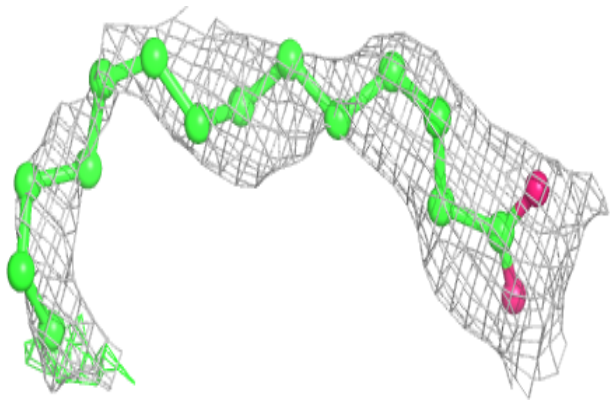


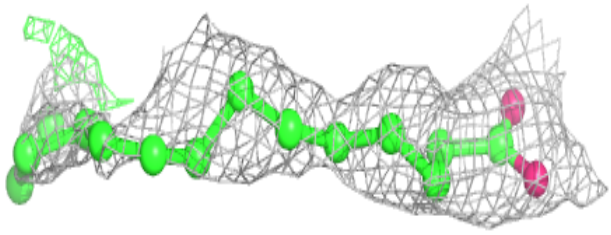


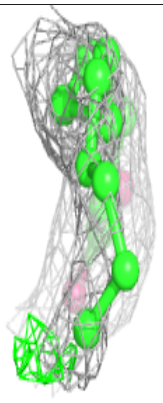


Electron density around OLA A 408:

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

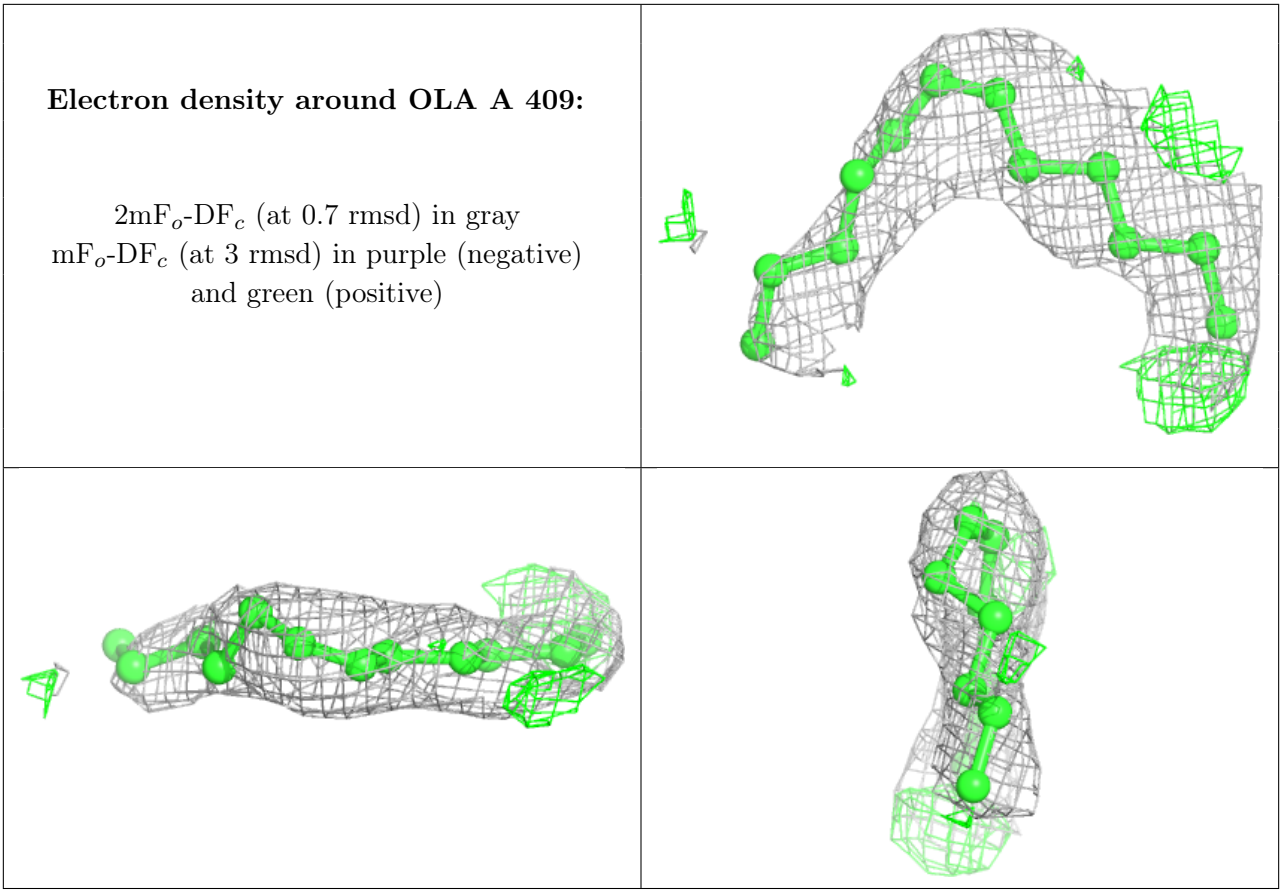






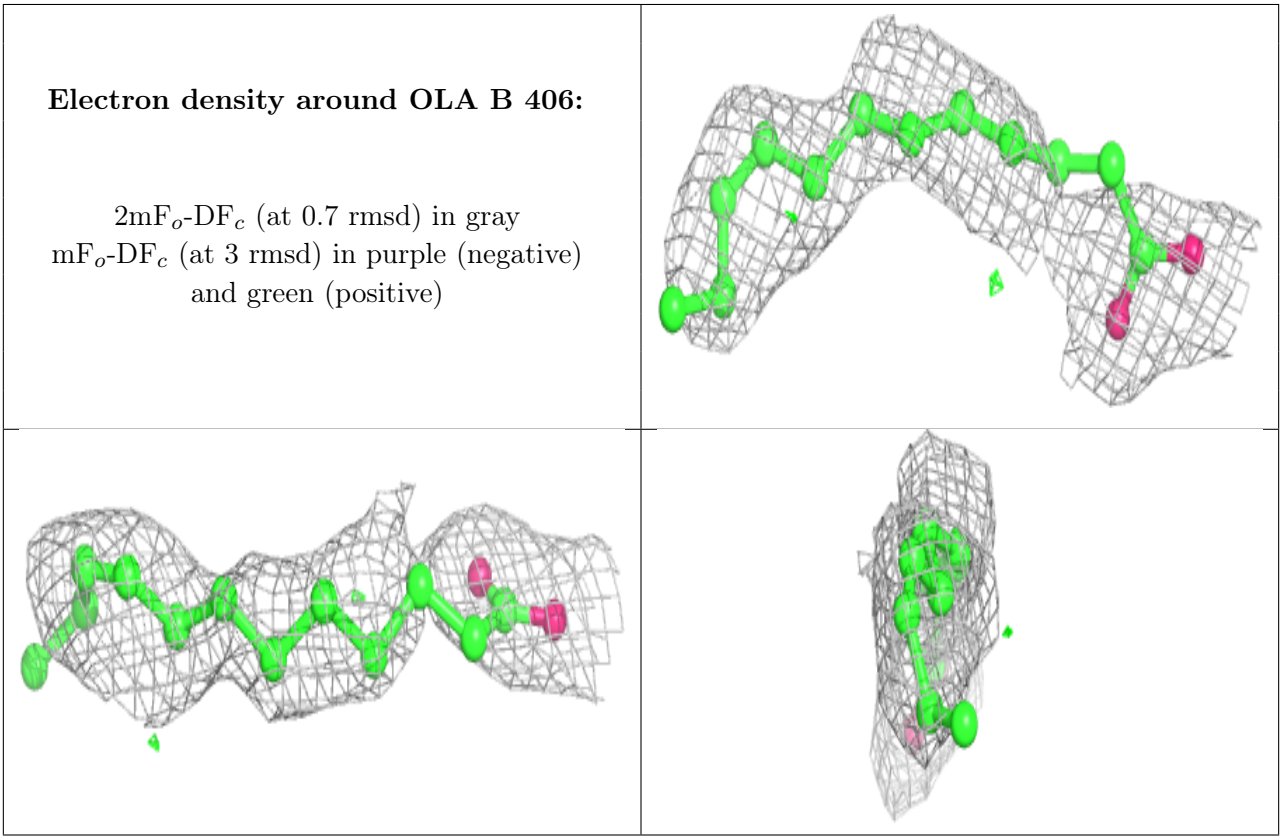
Electron density around OLA A 409:

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



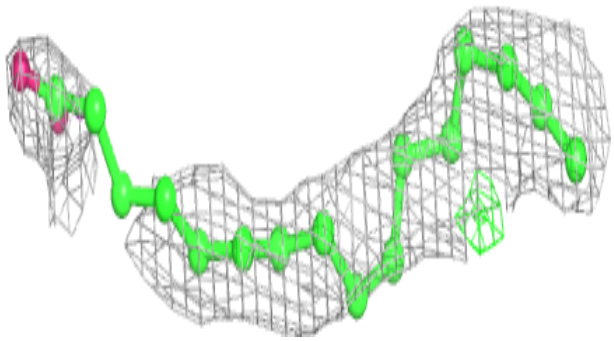
Electron density around OLA B 406:

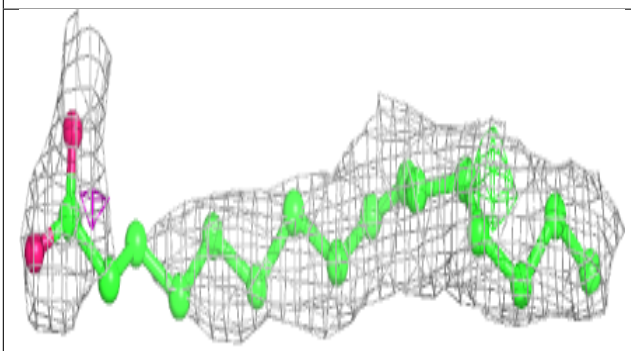
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

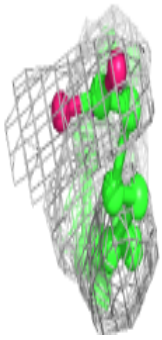


Electron density around OLA A 411:

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

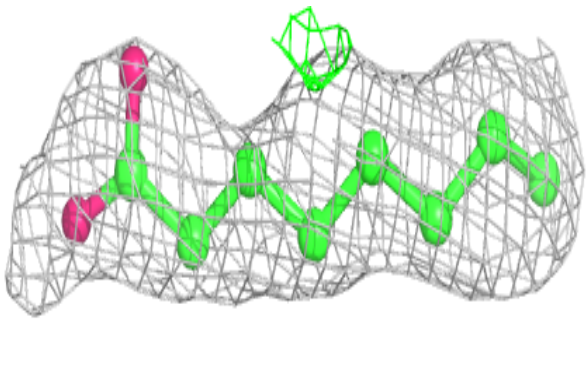


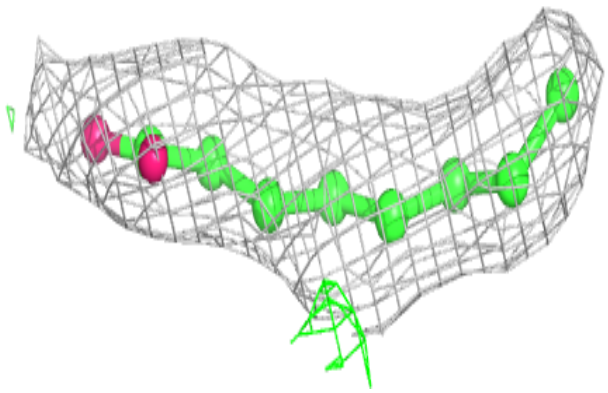


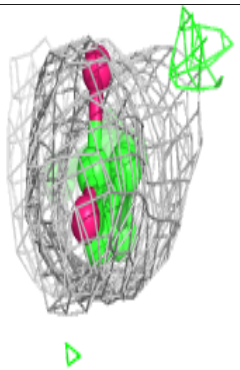


Electron density around OLA B 404:

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

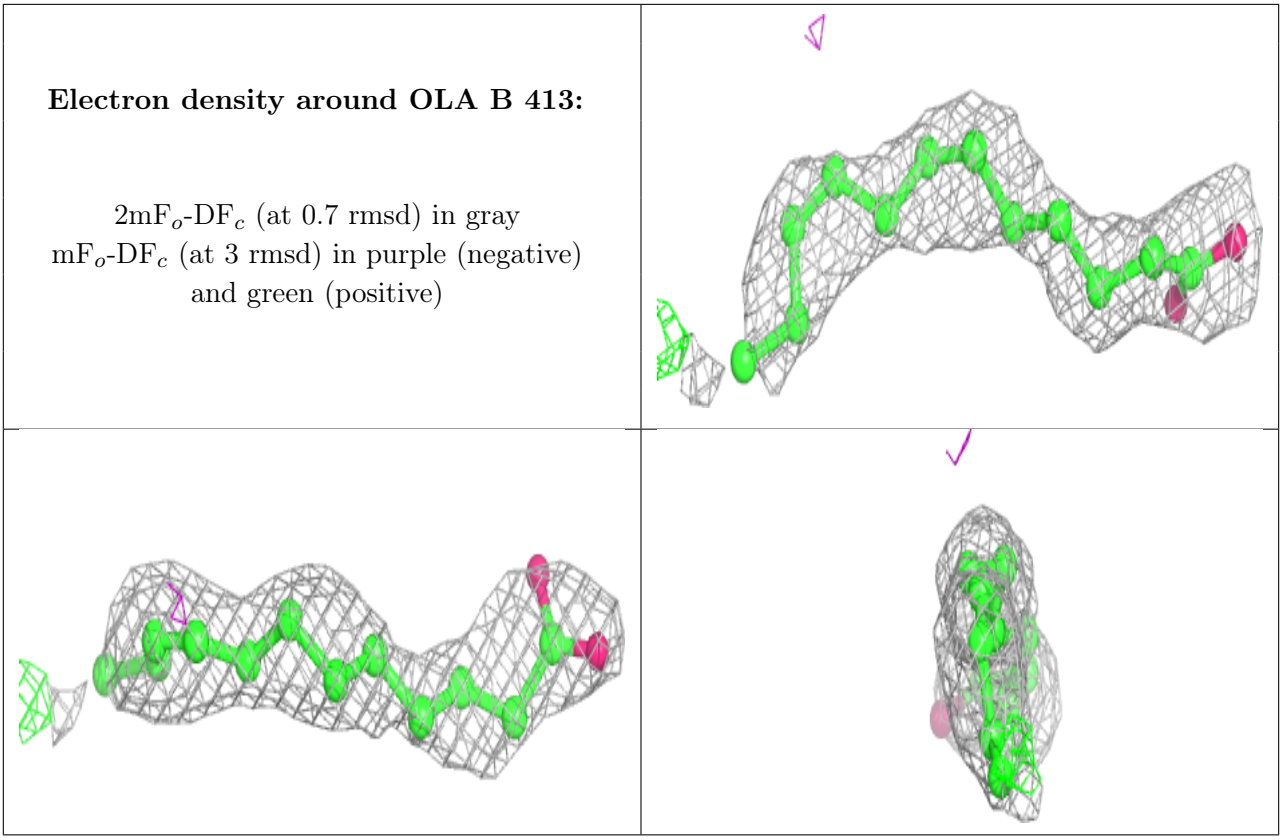






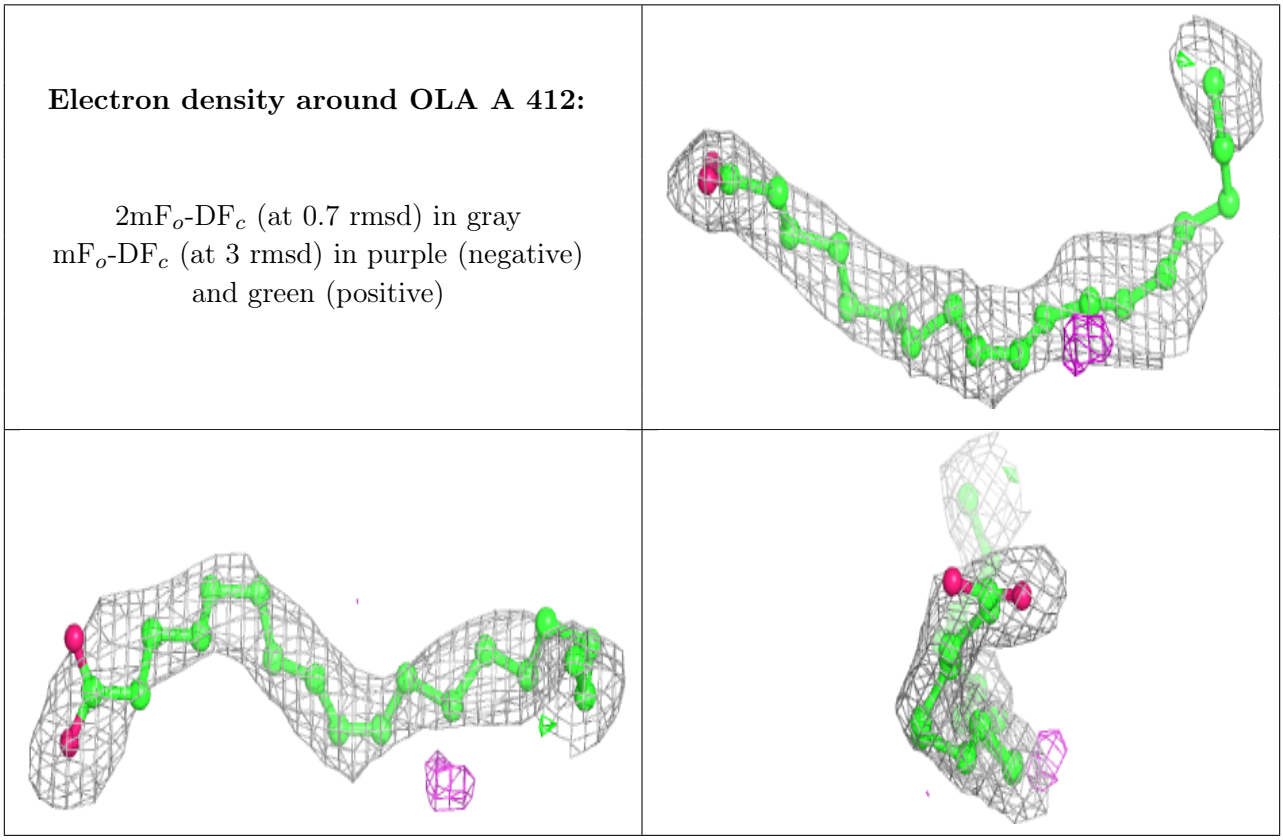
Electron density around OLA B 413:

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



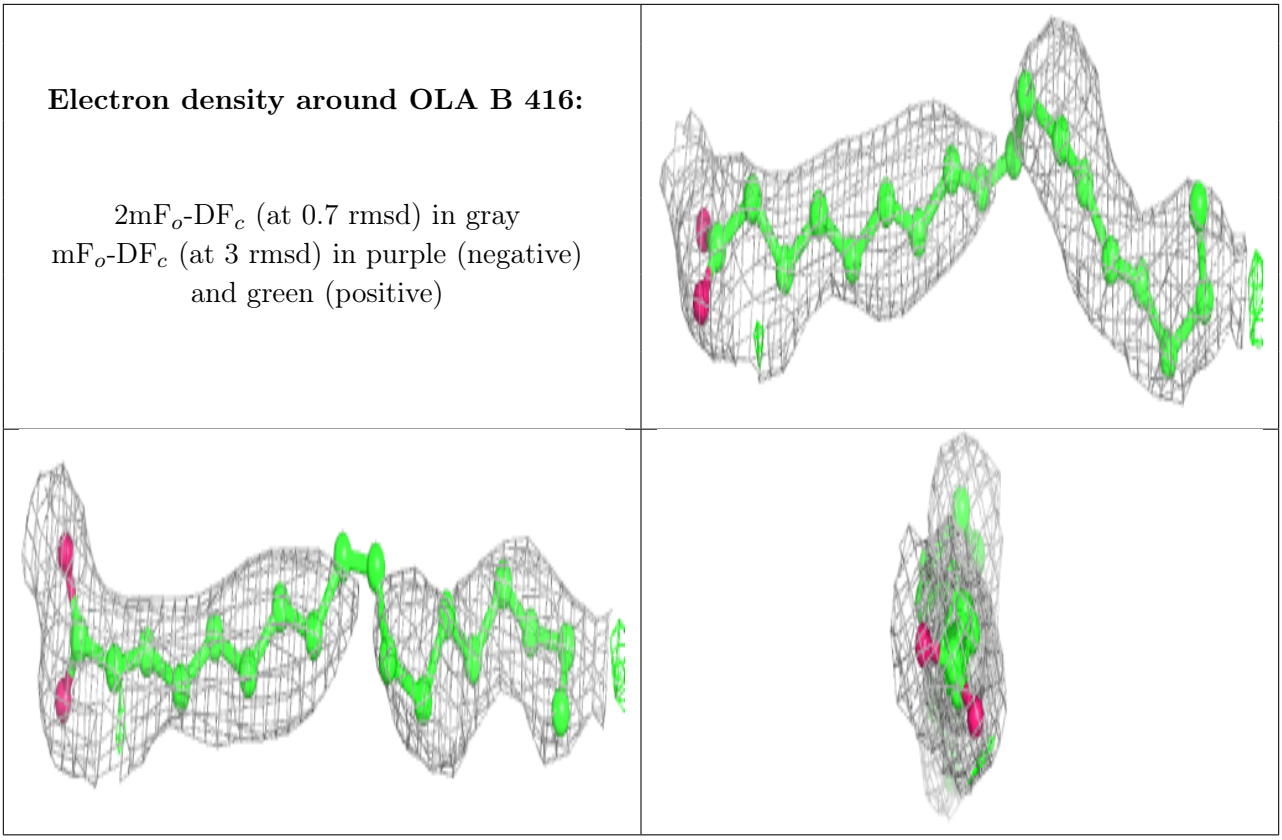
Electron density around OLA A 412:

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



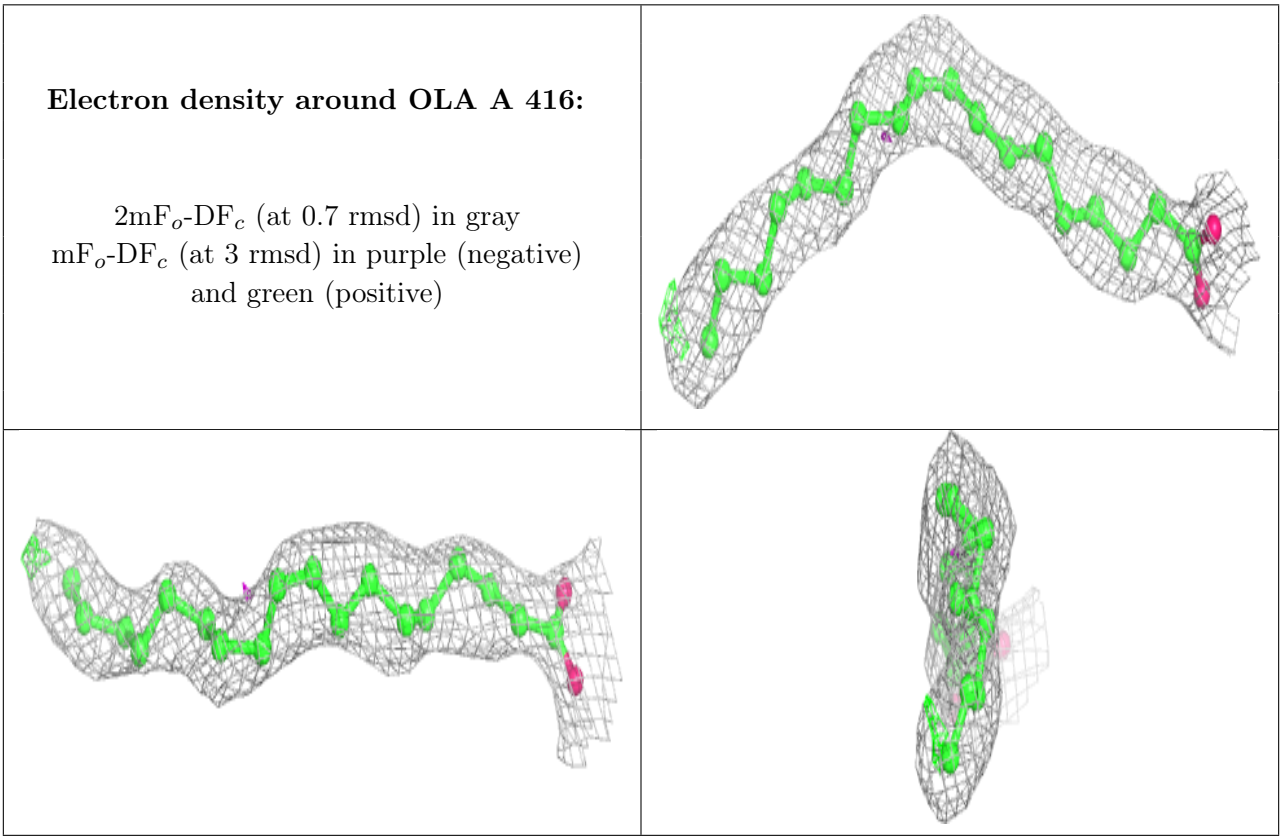
Electron density around OLA B 416:

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



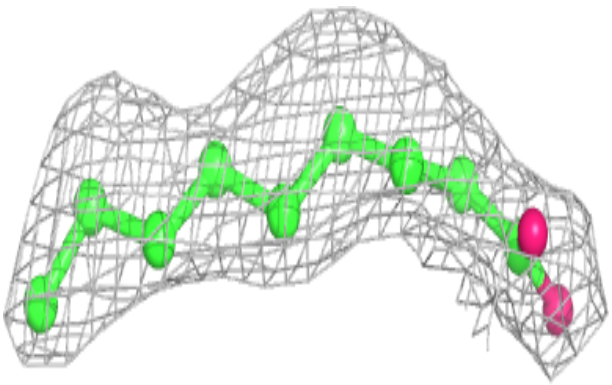
Electron density around OLA A 416:

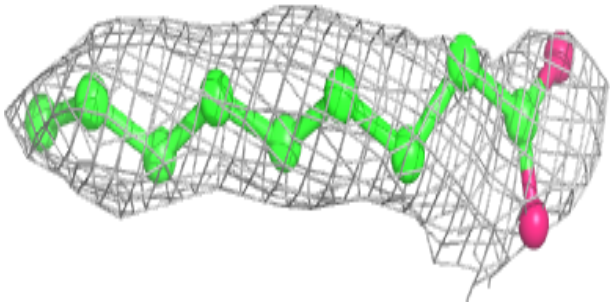
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

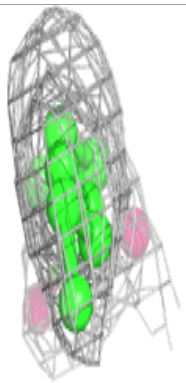


Electron density around OLA A 418:

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

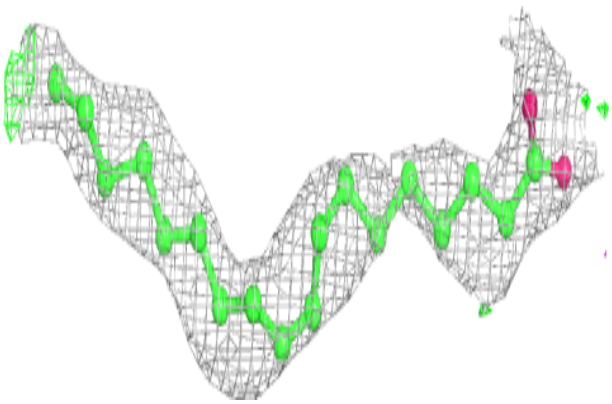


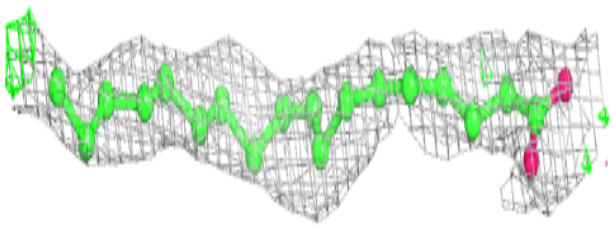


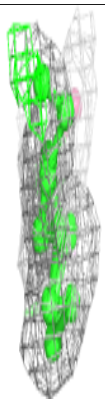


Electron density around OLA B 415:

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

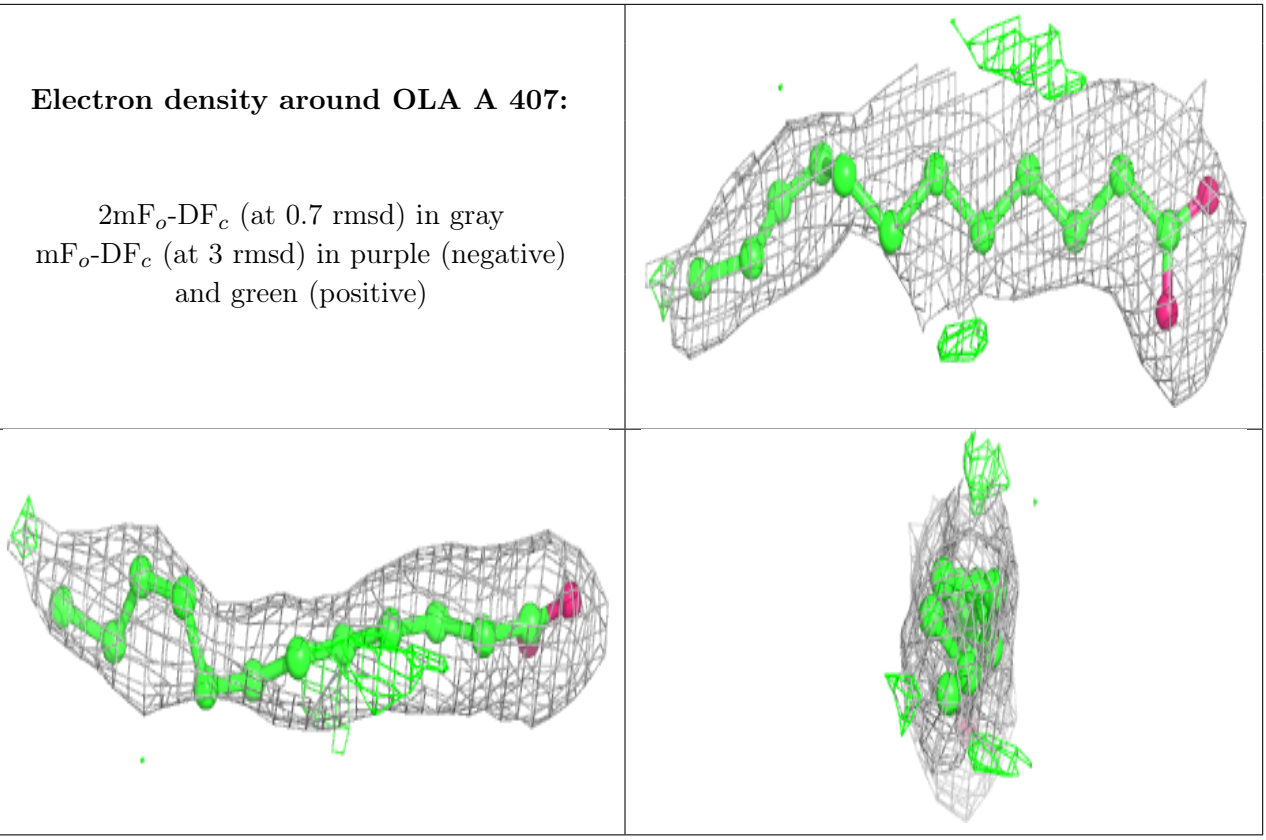






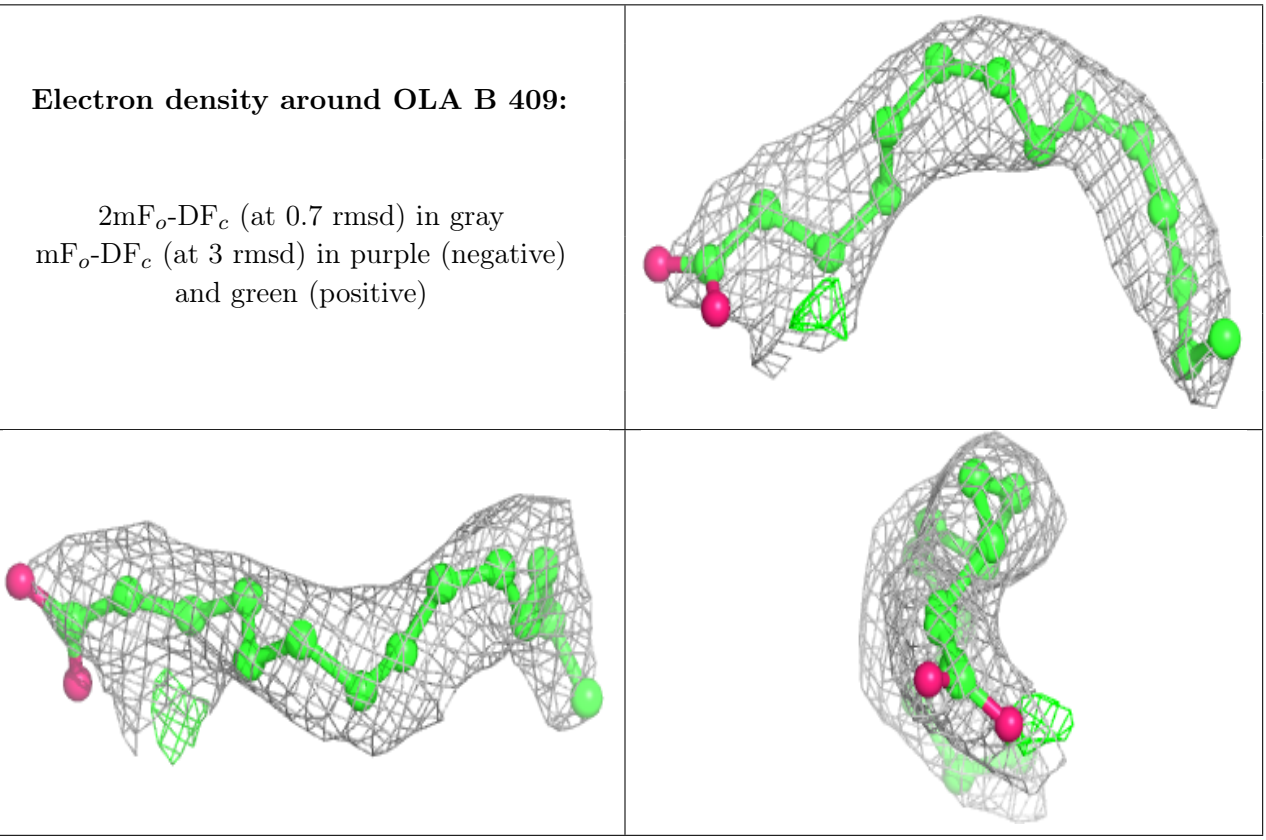
Electron density around OLA A 407:

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



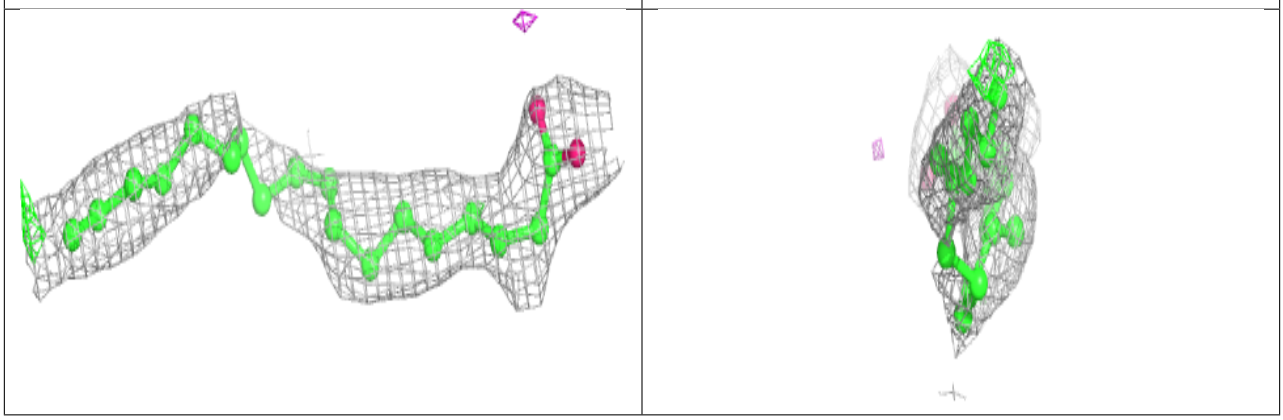
Electron density around OLA B 409:

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



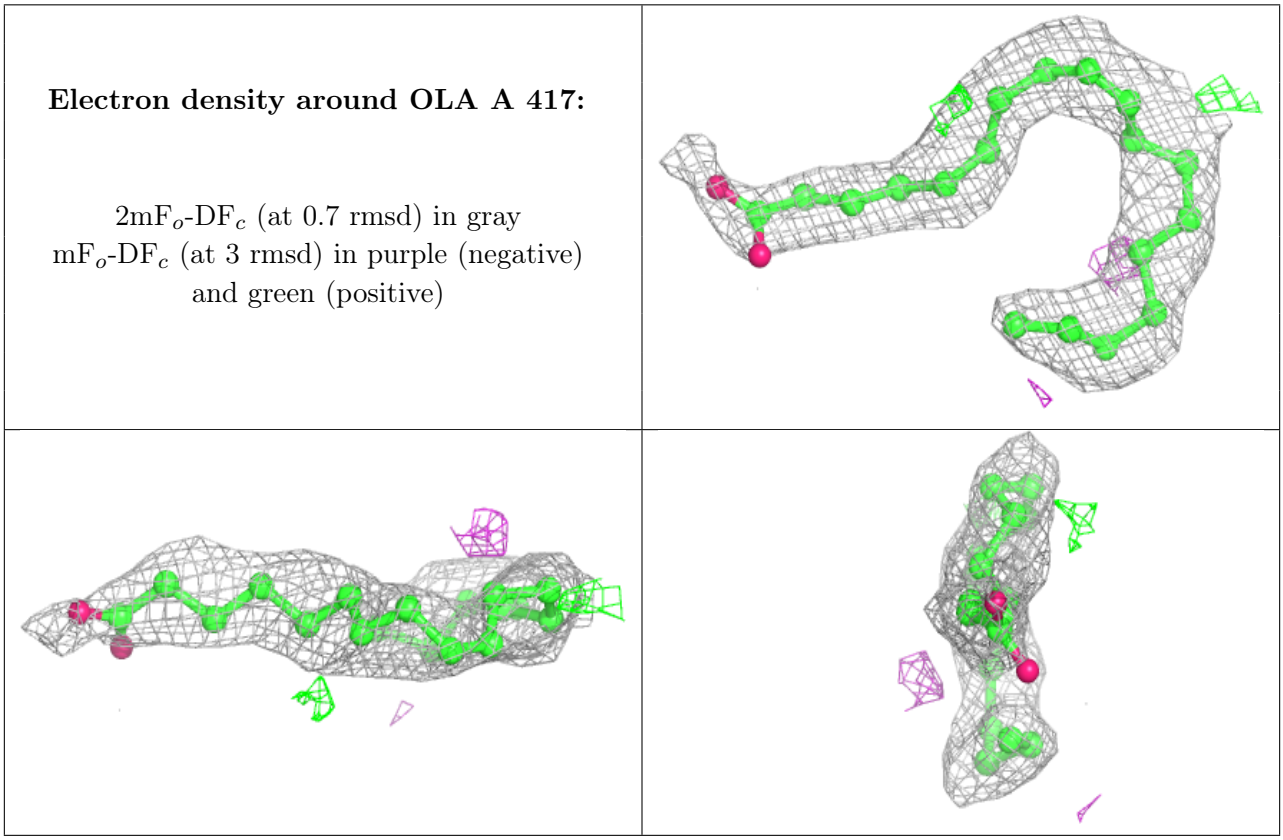
Electron density around OLA B 410:

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



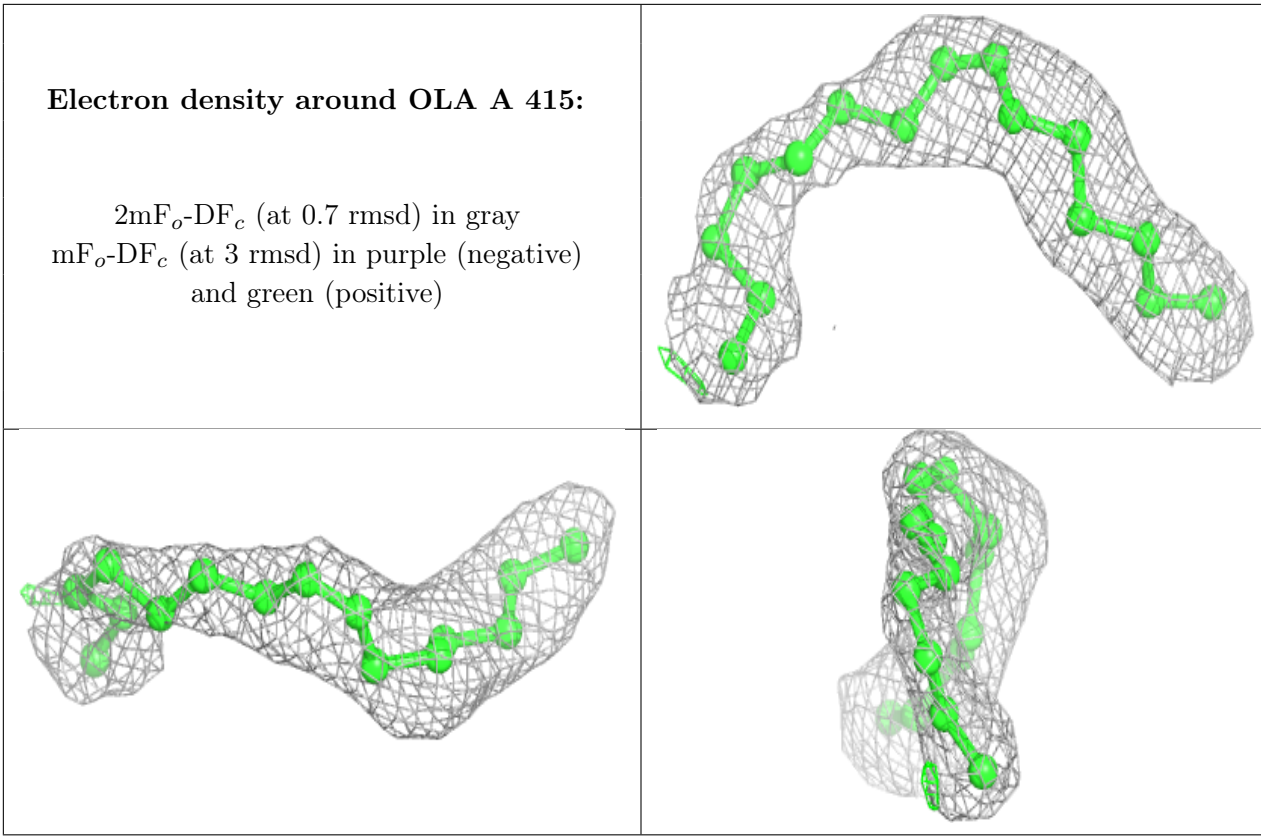
Electron density around OLA A 417:

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



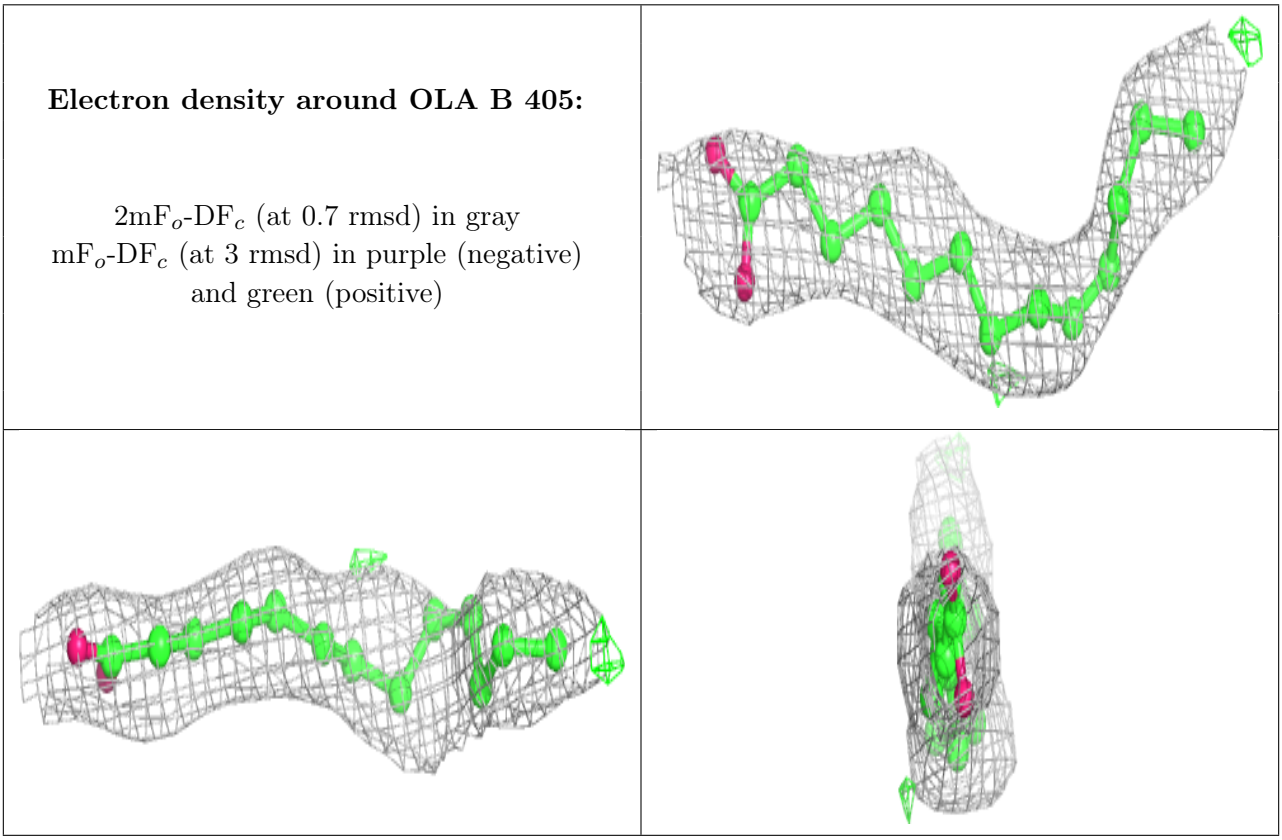
Electron density around OLA A 415:

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



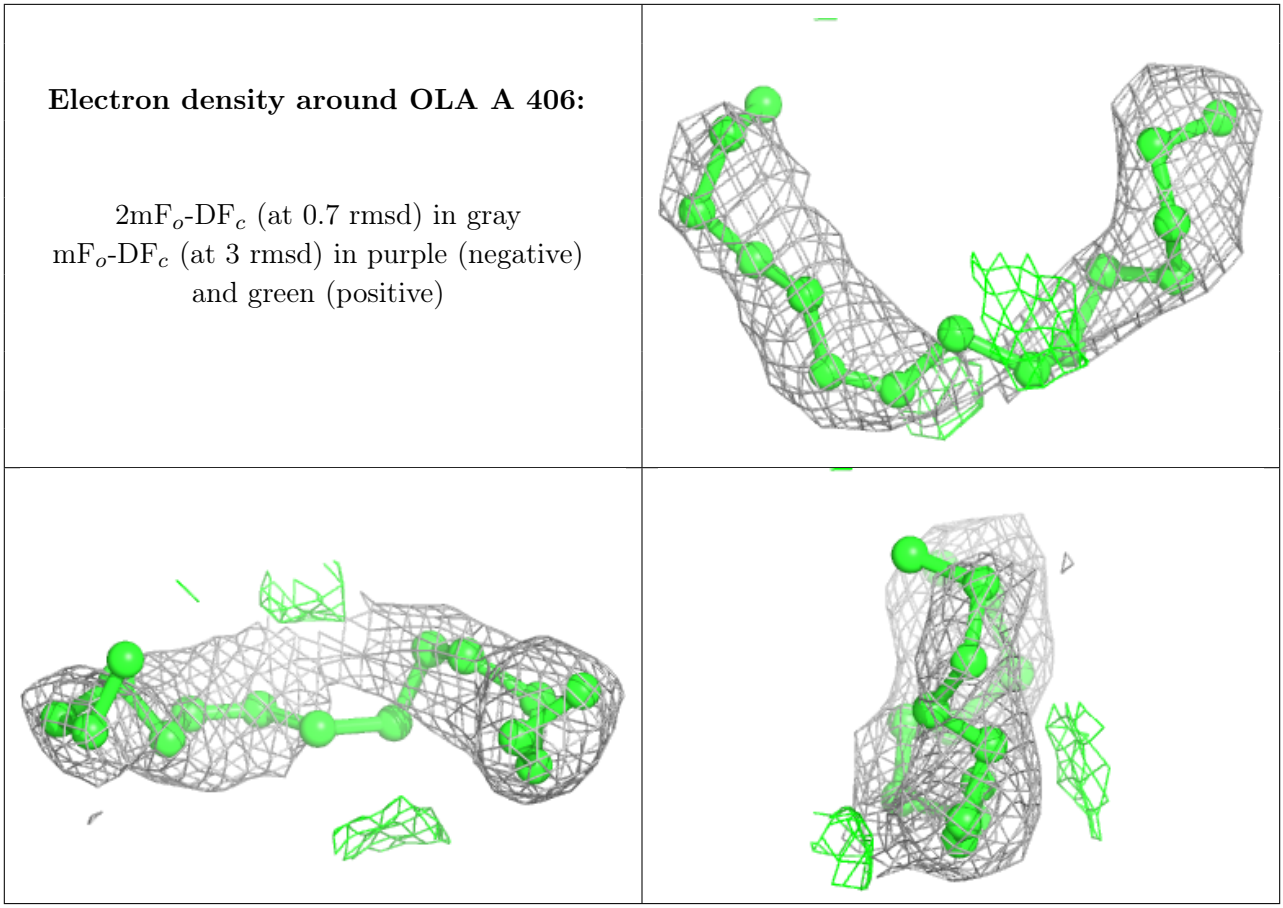
Electron density around OLA B 405:

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



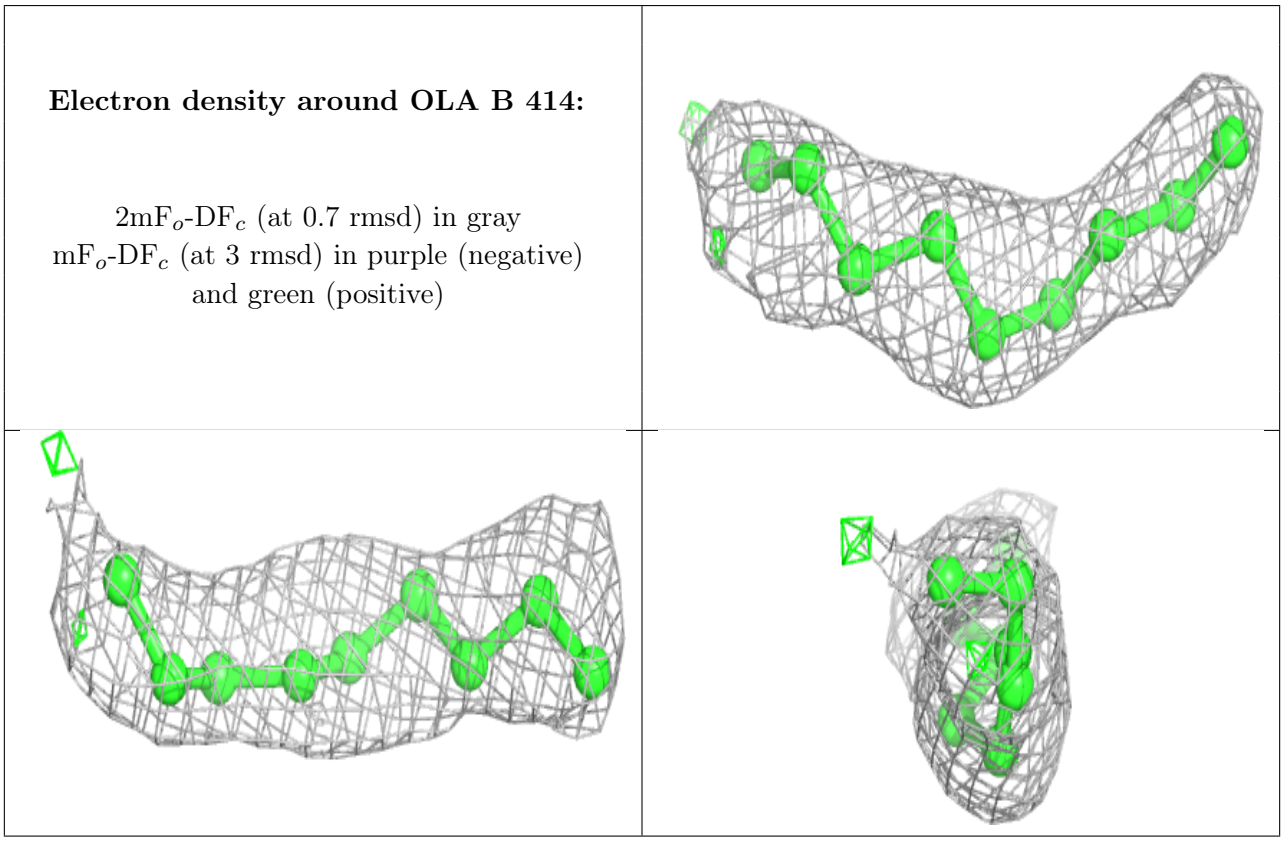
Electron density around OLA A 406:

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



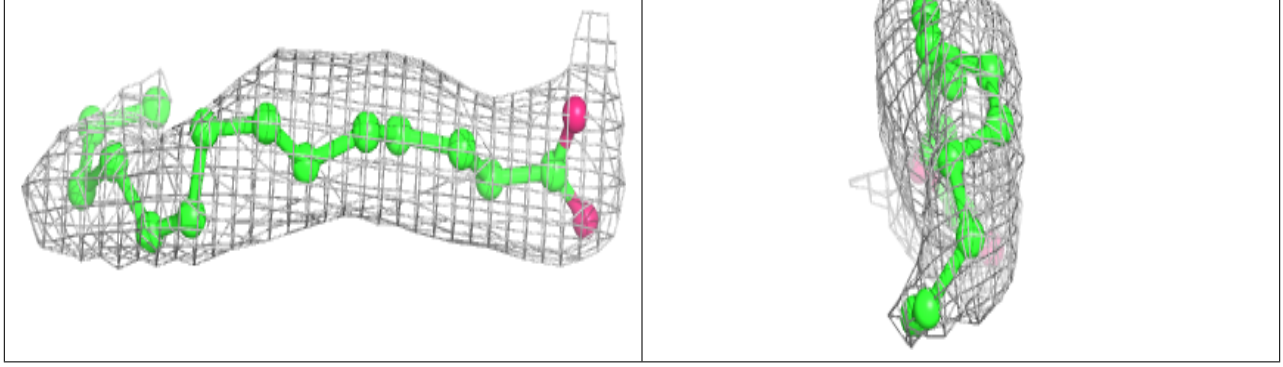
Electron density around OLA B 414:

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



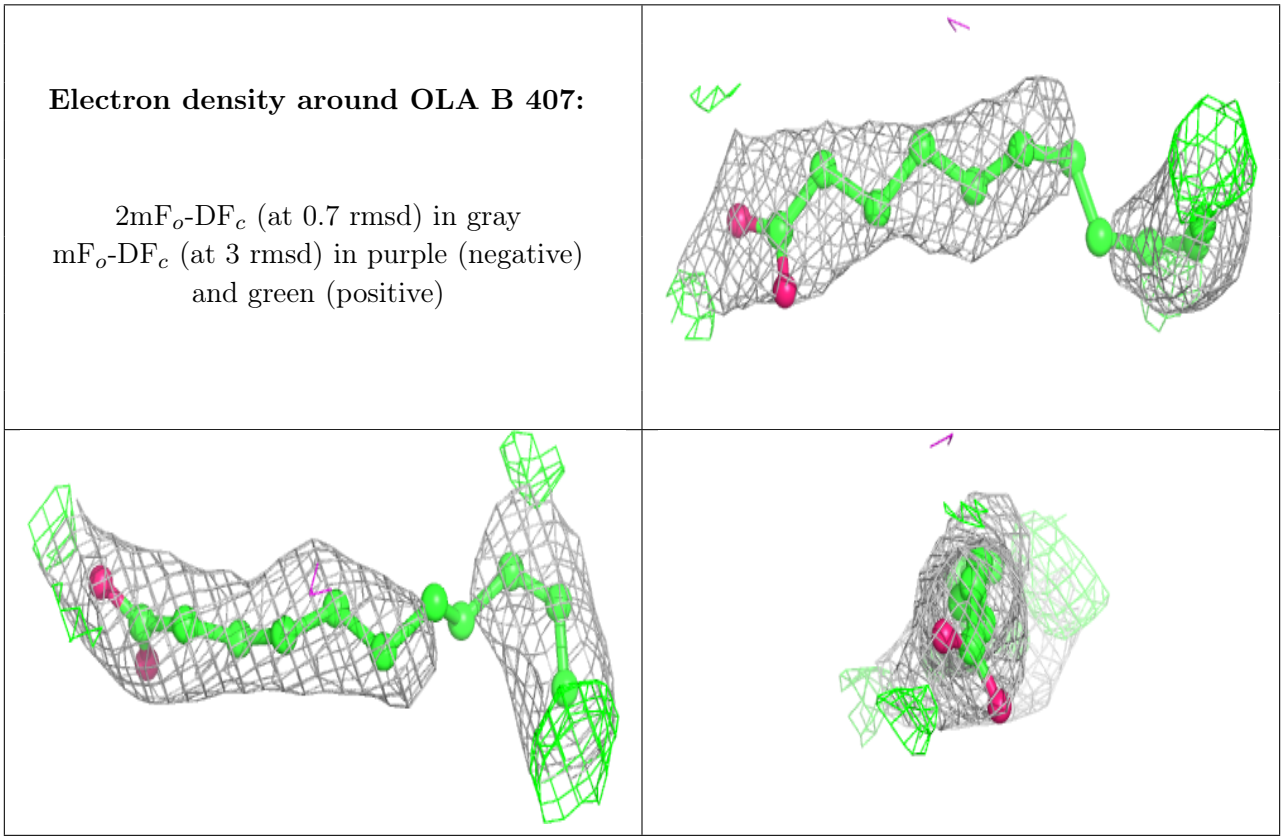
Electron density around OLA B 417:

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



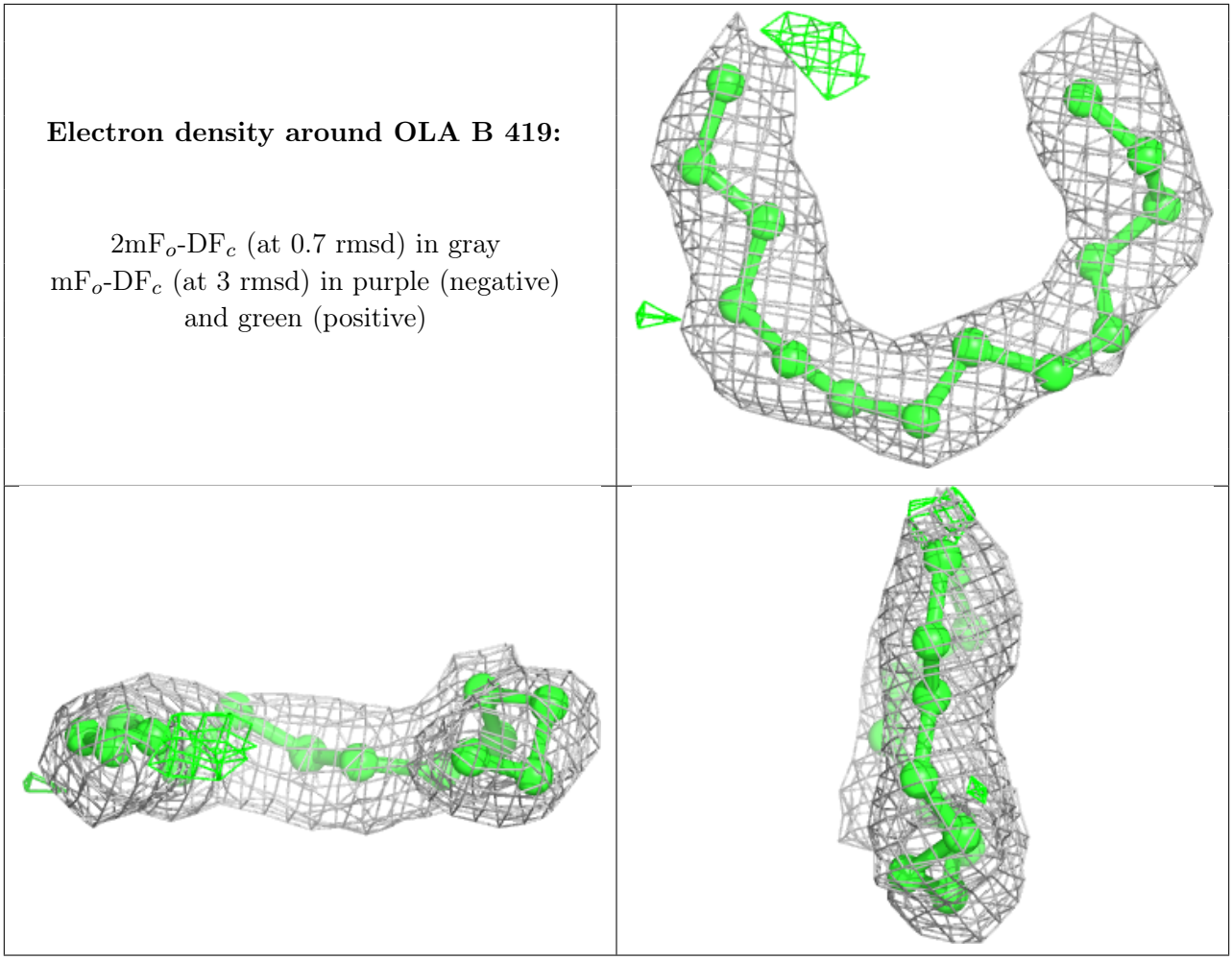
Electron density around OLA B 407:

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



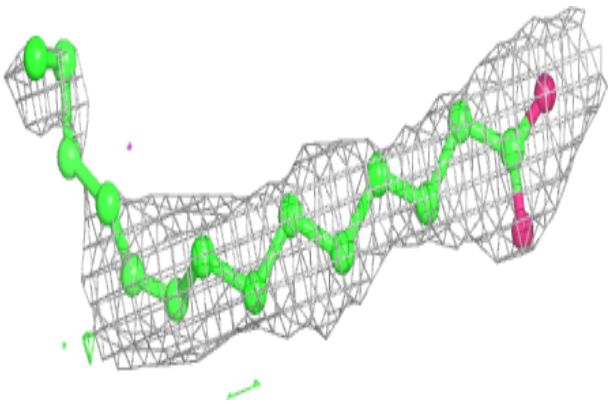
Electron density around OLA B 419:

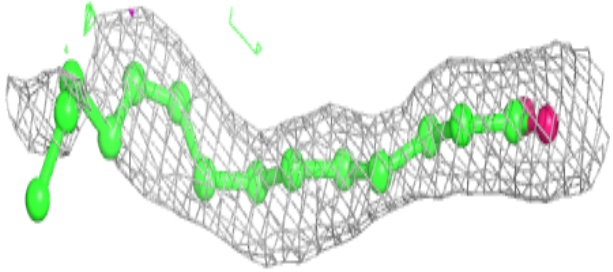
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

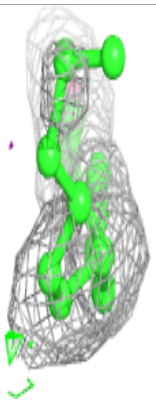


Electron density around OLA A 414:

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

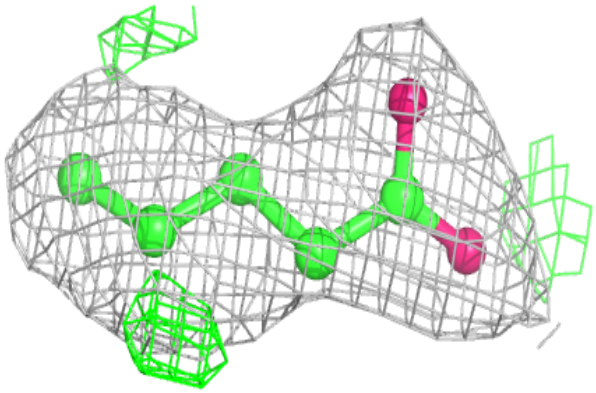


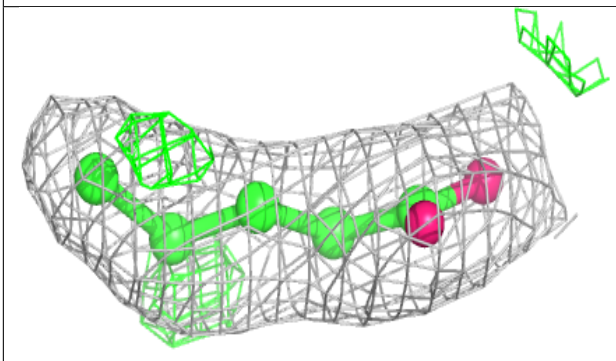


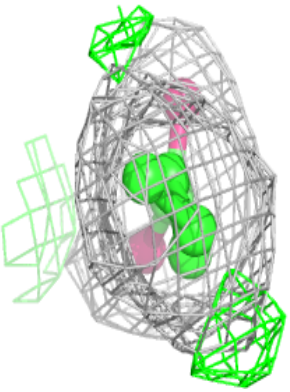


Electron density around OLA B 408:

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

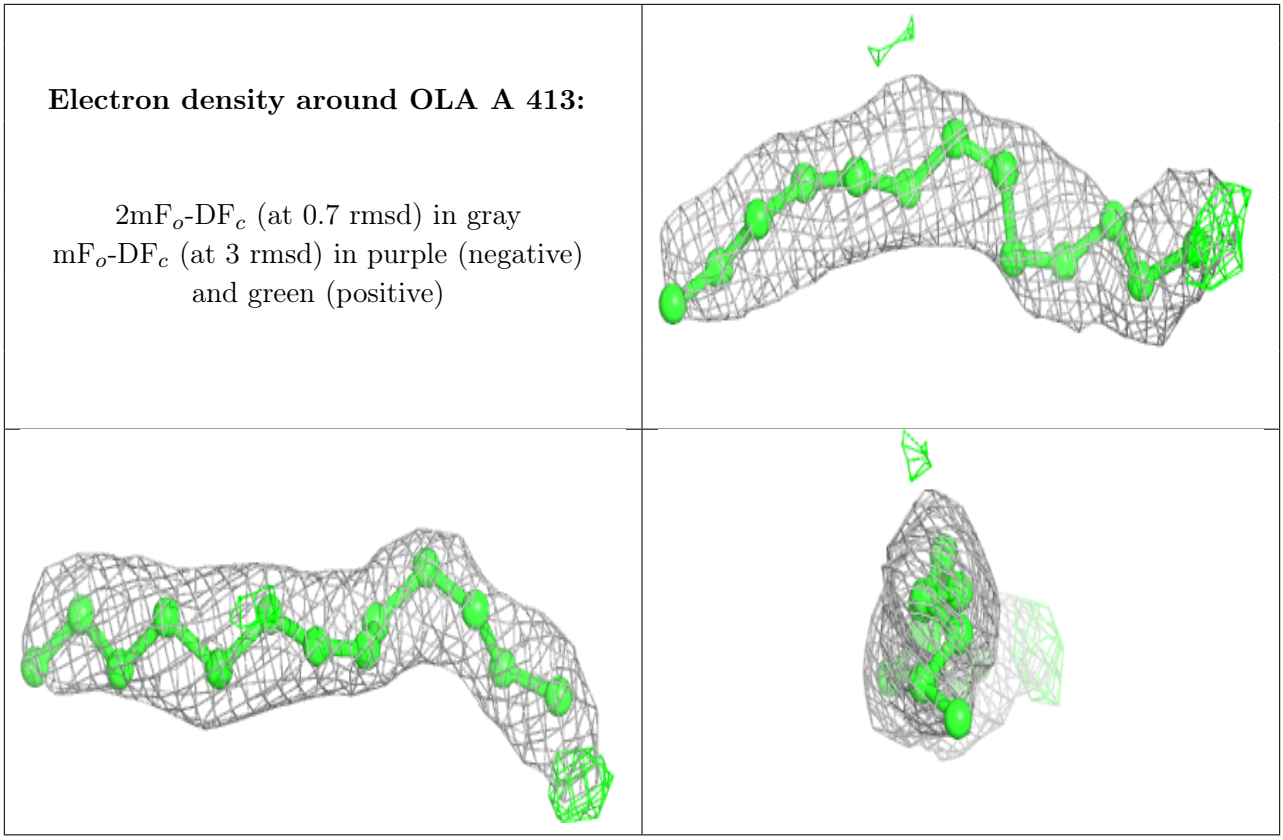






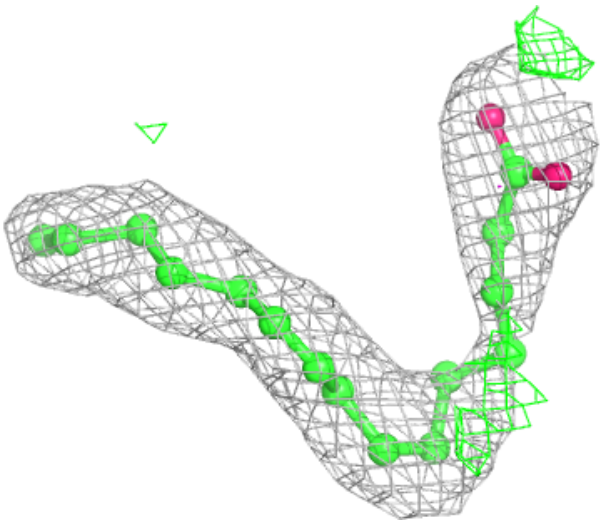
Electron density around OLA A 413:

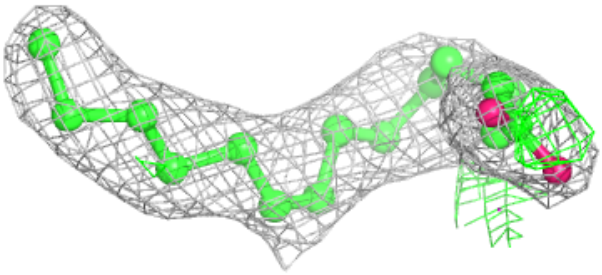
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA A 404:

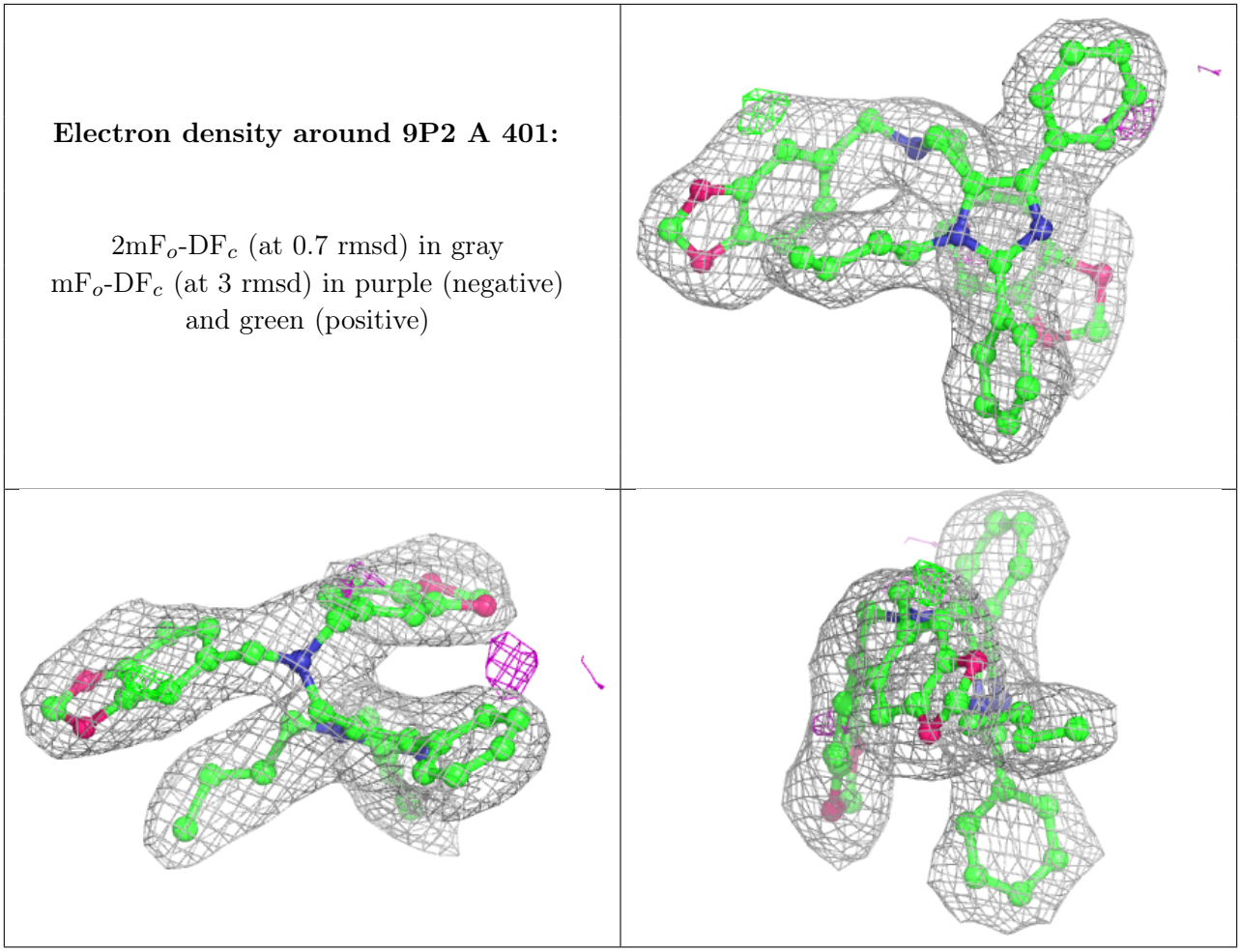
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





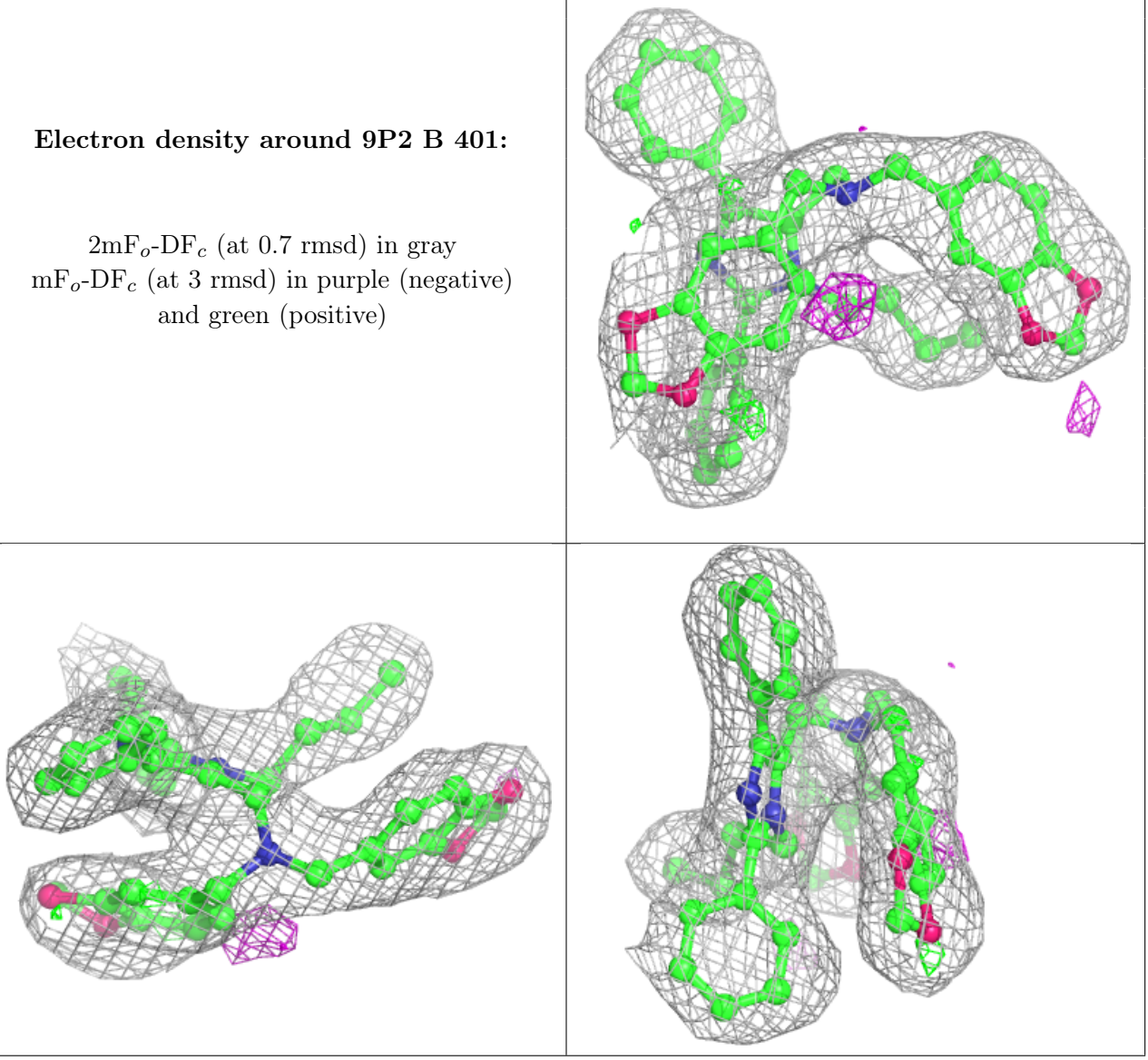
Electron density around 9P2 A 401:

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



Electron density around 9P2 B 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.