wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 10:06 pm BST

PDB ID	:	5IU4
Title	:	Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with ZM241385 at 1.7A resolution
Authors	:	Segala, E.; Guo, D.; Cheng, R.K.Y.; Bortolato, A.; Deflorian, F.; Dore, A.S.; Errey, J.C.; Heitman, L.H.; Ijzerman, A.P.; Marshall, F.H.; Cooke, R.M.
Deposited on	:	2016-03-17
Resolution	:	1.72 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 following versions of software and data (see references (1)) were used in the production of this report:

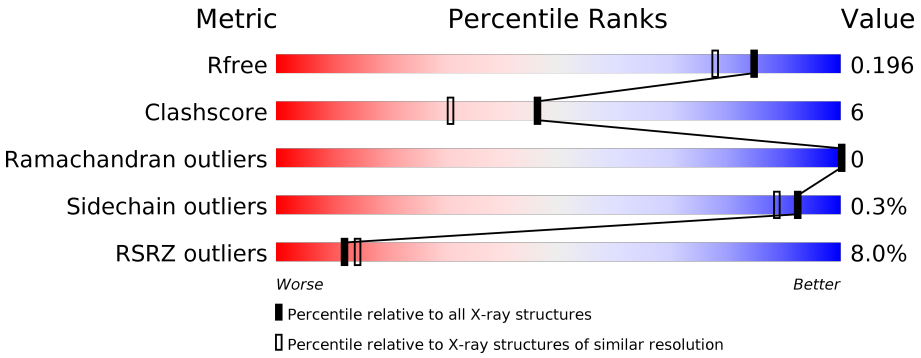
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 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 <=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	433	7% 78% 11% 10%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3835 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 Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3171	2070	531	546	24	0	24	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	54	LEU	ALA	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	318	ALA	GLY	engineered mutation	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274

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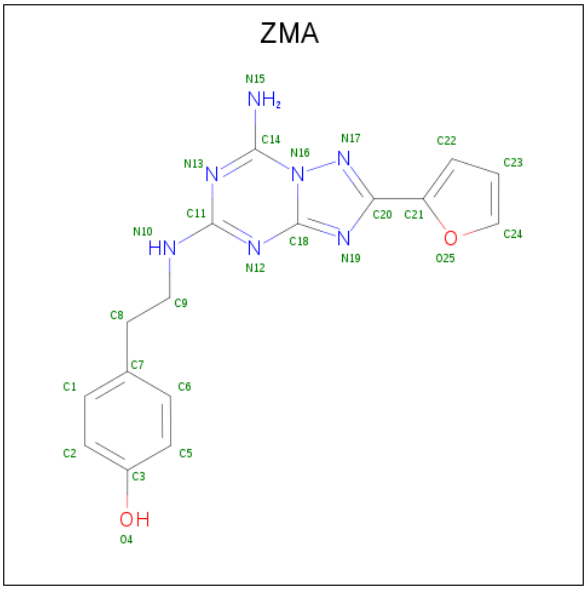
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

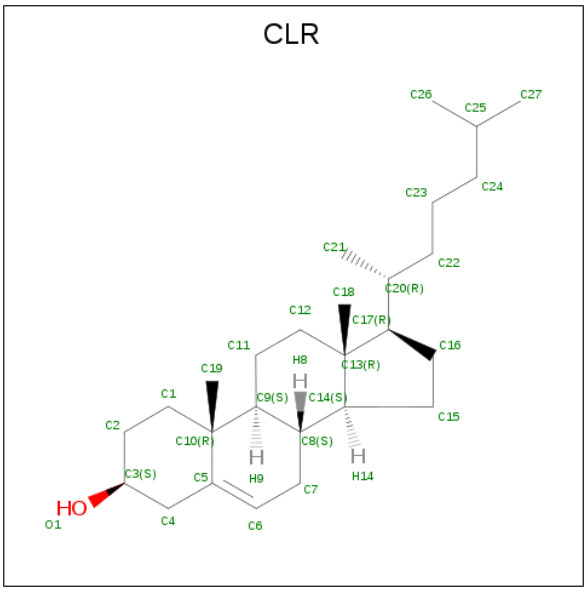
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is 4-{2-[(7-amino-2-furan-2-yl[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl} phenol (three-letter code: ZMA) (formula: $C_{16}H_{15}N_7O_2$).



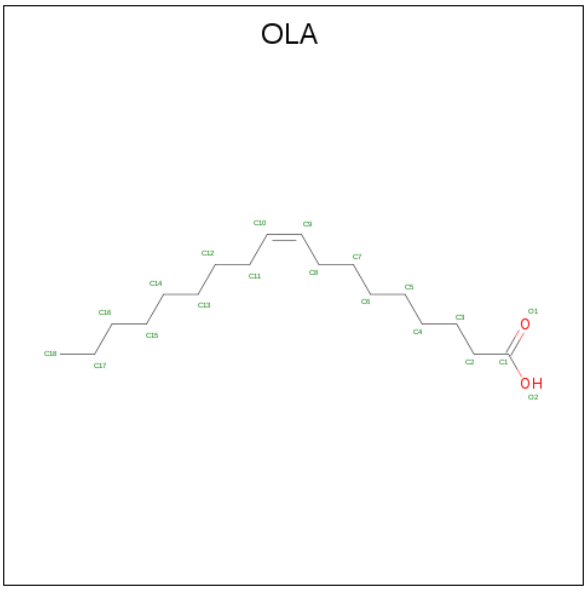
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 25 16 7 2	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



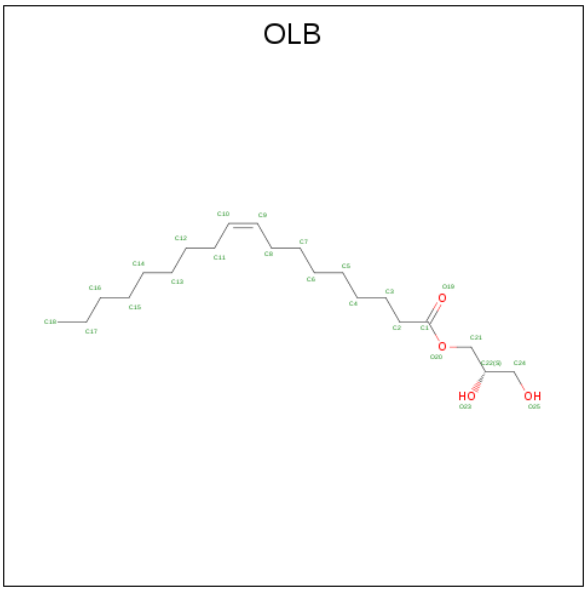
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



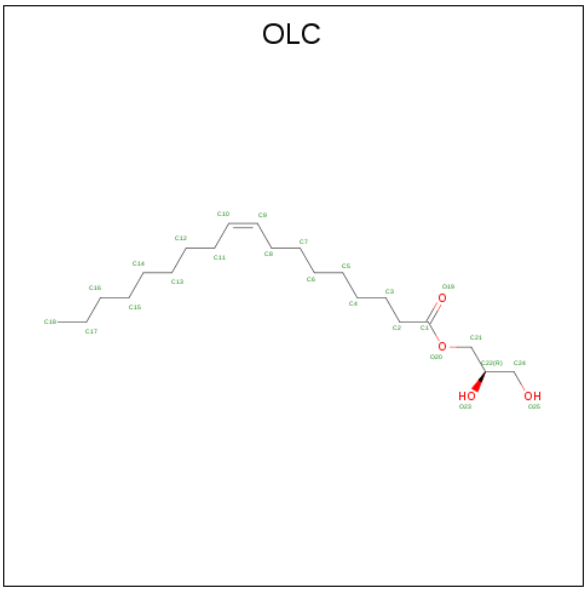
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C 7 7	0	0
5	A	1	Total C O 9 7 2	0	0
5	A	1	Total C O 18 16 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C O 12 10 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 14 12 2	0	0
5	A	1	Total C 7 7	0	0
5	A	1	Total C O 19 17 2	0	0
5	A	1	Total C 10 10	0	0
5	A	1	Total C 7 7	0	0
5	A	1	Total C O 17 15 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C 13 13	0	0
5	A	1	Total C O 17 15 2	0	0
5	A	1	Total C O 12 10 2	0	0
5	A	1	Total C 10 10	0	0

- Molecule 6 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 17 13 4	0	0
6	A	1	Total C O 19 15 4	0	0
6	A	1	Total C O 20 16 4	0	0

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 25 21 4	0	0
7	A	1	Total C O 19 15 4	0	0

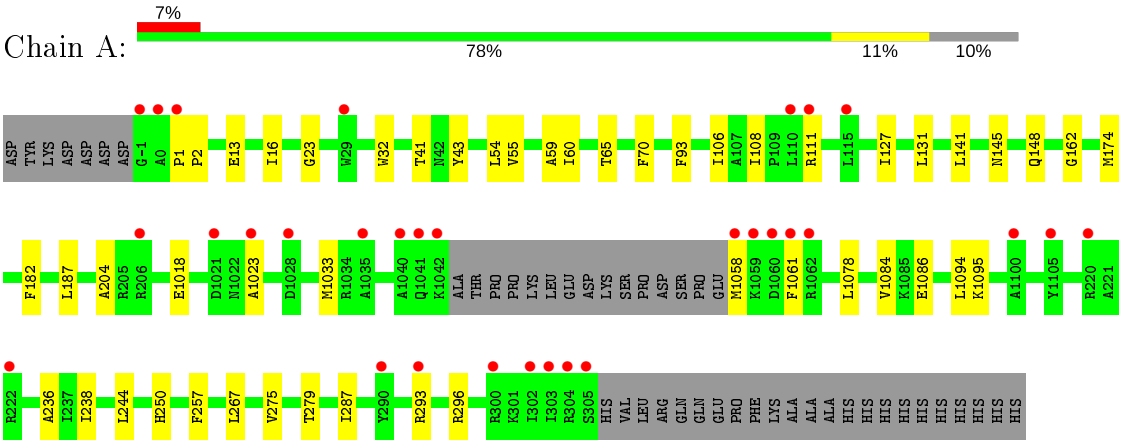
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	164	Total O 165 165	0	1

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: Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.43Å 179.60Å 139.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.73 – 1.72 33.73 – 1.72	Depositor EDS
% Data completeness (in resolution range)	93.0 (33.73-1.72) 92.2 (33.73-1.72)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 1.72Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.167 , 0.200 0.164 , 0.196	Depositor DCC
R_{free} test set	2440 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3835	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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: OLA, OLB, OLC, NA, ZMA, CLR

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	0.37	0/3244	0.50	0/4411

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	3171	0	3264	40	0
2	A	1	0	0	0	0
3	A	25	0	15	1	0
4	A	112	0	184	3	0
5	A	261	0	374	17	0
6	A	56	0	74	1	0
7	A	44	0	65	3	0
8	A	165	0	0	8	0
All	All	3835	0	3976	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 6.

The worst 5 of 48 close contacts within the same asymmetric unit are listed below, sorted by their

clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2411:OLA:H122	5:A:2420:OLA:C15	2.08	0.83
4:A:2403:CLR:H272	7:A:2429:OLC:H14A	1.63	0.80
1:A:162:GLY:O	8:A:2501:HOH:O	2.05	0.73
4:A:2405:CLR:H262	5:A:2418:OLA:H183	1.71	0.72
1:A:267[A]:LEU:HD21	5:A:2410:OLA:H21	1.74	0.70

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	408/433 (94%)	406 (100%)	2 (0%)	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	336/353 (95%)	335 (100%)	1 (0%)	92 89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\#\|Z\| > 2$
5	OLA	A	2422	-	12,12,19	0.39	0	11,11,19	0.44	0
5	OLA	A	2416	-	6,6,19	0.27	0	5,5,19	0.19	0
4	CLR	A	2405	-	31,31,31	0.71	0	48,48,48	0.86	0
5	OLA	A	2424	-	8,11,19	0.49	0	7,11,19	0.41	0
5	OLA	A	2411	-	16,19,19	0.46	0	15,19,19	0.30	0
6	OLB	A	2428	-	19,19,24	0.88	2 (10%)	20,20,25	0.95	1 (5%)
7	OLC	A	2429	-	24,24,24	0.80	2 (8%)	25,25,25	0.78	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	OLA	A	2410	-	14,17,19	0.43	0	13,17,19	0.28	0
5	OLA	A	2413	-	8,11,19	0.44	0	7,11,19	0.44	0
6	OLB	A	2426	-	16,16,24	0.99	2 (12%)	17,17,25	1.06	1 (5%)
3	ZMA	A	2401	-	21,28,28	0.83	0	22,39,39	2.80	5 (22%)
5	OLA	A	2412	-	11,14,19	0.36	0	10,14,19	0.30	0
7	OLC	A	2430	-	18,18,24	0.92	2 (11%)	18,19,25	0.99	1 (5%)
5	OLA	A	2408	-	6,6,19	0.27	0	5,5,19	0.17	0
5	OLA	A	2414	-	4,7,19	0.28	0	3,7,19	0.17	0
6	OLB	A	2427	-	18,18,24	0.88	1 (5%)	18,19,25	1.17	1 (5%)
5	OLA	A	2421	-	7,10,19	0.23	0	6,10,19	0.36	0
5	OLA	A	2425	-	9,9,19	0.61	0	8,8,19	0.21	0
5	OLA	A	2406	-	16,19,19	0.42	0	15,19,19	0.27	0
4	CLR	A	2402	-	31,31,31	0.70	0	48,48,48	1.05	3 (6%)
5	OLA	A	2415	-	10,13,19	0.44	0	8,13,19	0.27	0
5	OLA	A	2423	-	13,16,19	0.33	0	12,16,19	0.47	0
5	OLA	A	2420	-	13,16,19	0.36	0	12,16,19	0.37	0
5	OLA	A	2407	-	11,14,19	0.35	0	10,14,19	0.35	0
4	CLR	A	2403	-	31,31,31	0.85	1 (3%)	48,48,48	1.05	2 (4%)
5	OLA	A	2418	-	9,9,19	0.52	0	8,8,19	0.40	0
4	CLR	A	2404	-	31,31,31	0.73	0	48,48,48	0.86	0
5	OLA	A	2417	-	15,18,19	0.43	0	14,18,19	0.27	0
5	OLA	A	2419	-	6,6,19	0.25	0	5,5,19	0.36	0
5	OLA	A	2409	-	5,8,19	0.20	0	4,8,19	0.25	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
5	OLA	A	2422	-	-	3/10/10/17	-
5	OLA	A	2416	-	-	3/4/4/17	-
4	CLR	A	2405	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2424	-	-	4/7/9/17	-
5	OLA	A	2411	-	-	6/15/17/17	-
6	OLB	A	2428	-	-	10/19/19/24	-
7	OLC	A	2429	-	-	12/24/24/24	-
5	OLA	A	2410	-	-	8/13/15/17	-
5	OLA	A	2413	-	-	4/7/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLB	A	2426	-	-	7/16/16/24	-
3	ZMA	A	2401	-	-	0/6/10/10	0/4/4/4
5	OLA	A	2412	-	-	3/10/12/17	-
7	OLC	A	2430	-	-	7/18/18/24	-
5	OLA	A	2408	-	-	2/4/4/17	-
5	OLA	A	2414	-	-	2/3/5/17	-
6	OLB	A	2427	-	-	7/18/18/24	-
5	OLA	A	2421	-	-	5/6/8/17	-
5	OLA	A	2425	-	-	4/7/7/17	-
5	OLA	A	2406	-	-	7/15/17/17	-
4	CLR	A	2402	-	-	8/10/68/68	0/4/4/4
5	OLA	A	2415	-	-	5/9/11/17	-
5	OLA	A	2423	-	-	7/12/14/17	-
5	OLA	A	2420	-	-	4/12/14/17	-
5	OLA	A	2407	-	-	5/10/12/17	-
4	CLR	A	2403	-	-	2/10/68/68	0/4/4/4
5	OLA	A	2418	-	-	4/7/7/17	-
4	CLR	A	2404	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2417	-	-	4/14/16/17	-
5	OLA	A	2419	-	-	1/4/4/17	-
5	OLA	A	2409	-	-	2/4/6/17	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2430	OLC	O20-C1	2.54	1.40	1.33
6	A	2426	OLB	O20-C1	2.39	1.40	1.33
6	A	2428	OLB	O20-C1	2.37	1.40	1.33
7	A	2429	OLC	O20-C1	2.35	1.40	1.33
7	A	2429	OLC	O20-C21	-2.31	1.39	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2401	ZMA	N15-C14-N16	9.32	124.25	117.97
3	A	2401	ZMA	N17-C20-N19	5.40	118.13	114.56
3	A	2401	ZMA	C9-C8-C7	-4.89	101.54	112.87
6	A	2427	OLB	O20-C1-C2	3.47	122.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2426	OLB	O20-C1-C2	3.11	121.65	111.91

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2424	OLA	C1-C2-C3-C4
5	A	2413	OLA	C1-C2-C3-C4
7	A	2430	OLC	O20-C21-C22-O23
6	A	2427	OLB	O20-C21-C22-C24
5	A	2406	OLA	C1-C2-C3-C4

There are no ring outliers.

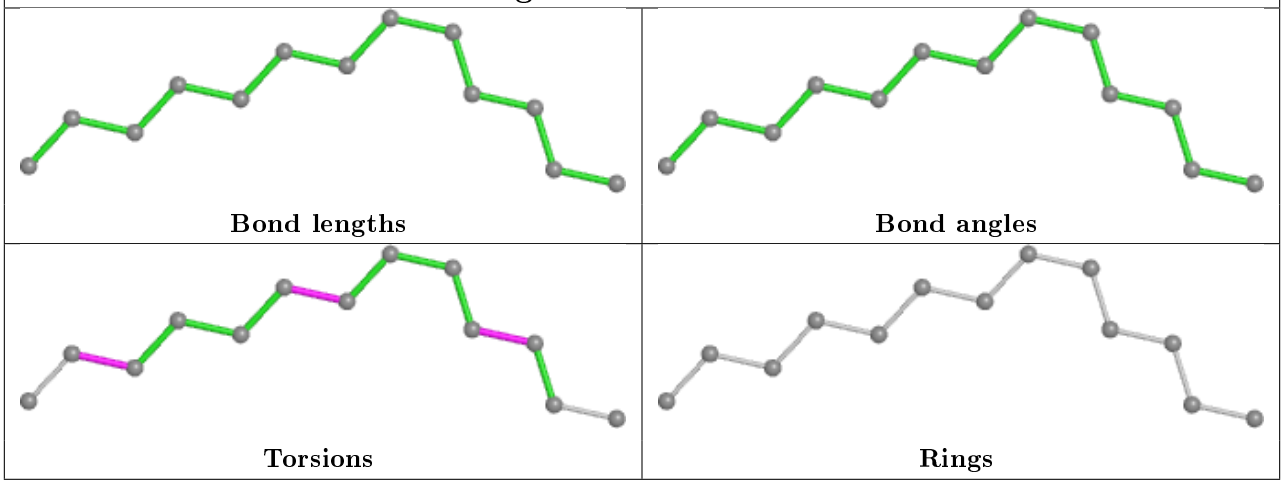
16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2405	CLR	1	0
5	A	2411	OLA	3	0
6	A	2428	OLB	1	0
7	A	2429	OLC	1	0
5	A	2410	OLA	2	0
3	A	2401	ZMA	1	0
7	A	2430	OLC	2	0
5	A	2408	OLA	2	0
5	A	2421	OLA	1	0
5	A	2425	OLA	1	0
4	A	2402	CLR	1	0
5	A	2423	OLA	1	0
5	A	2420	OLA	5	0
4	A	2403	CLR	2	0
5	A	2418	OLA	2	0
5	A	2417	OLA	3	0

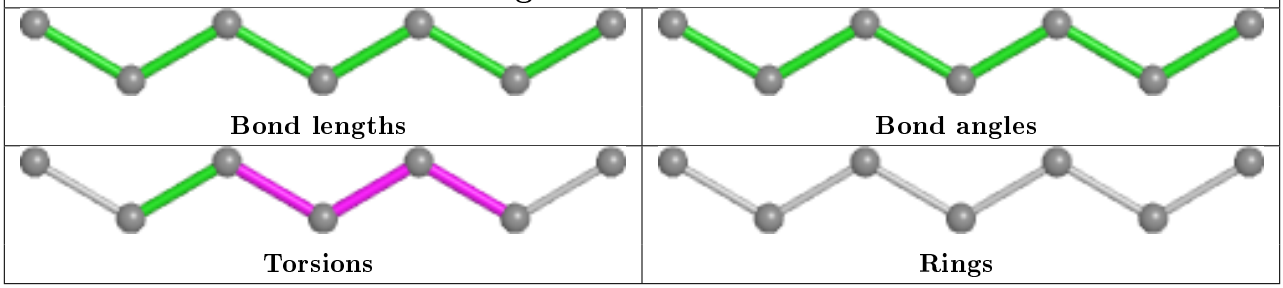
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

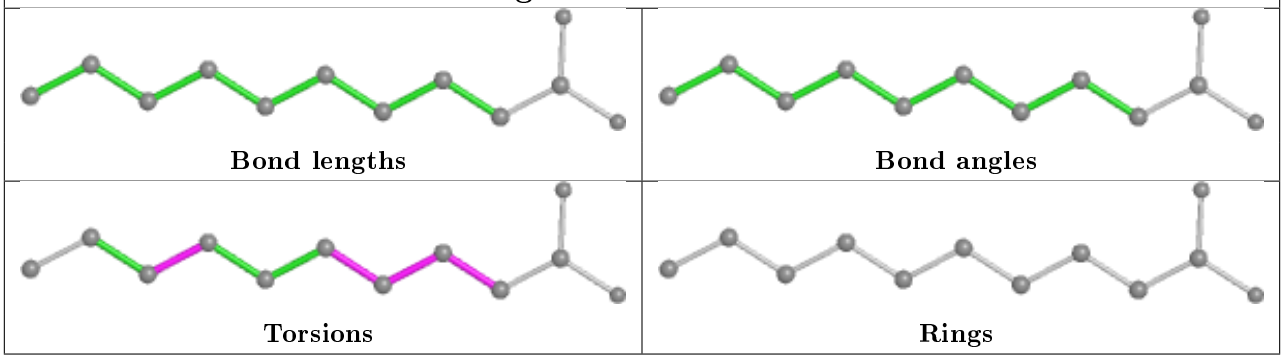
Ligand OLA A 2422



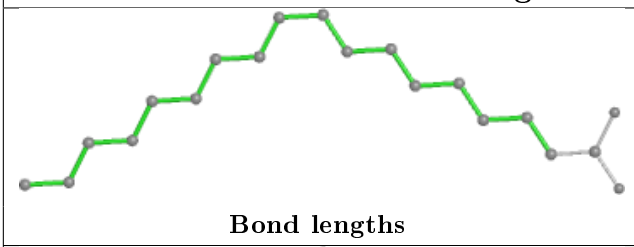
Ligand OLA A 2416



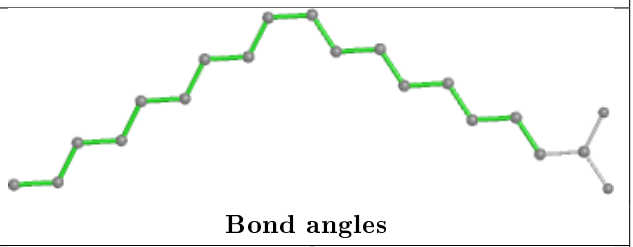
Ligand OLA A 2424



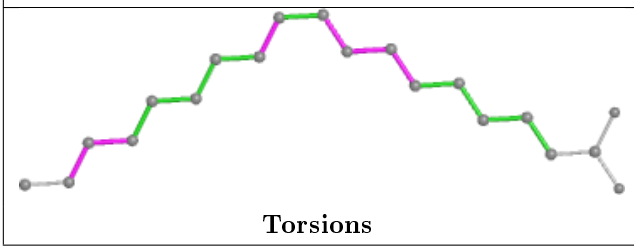
Ligand OLA A 2411



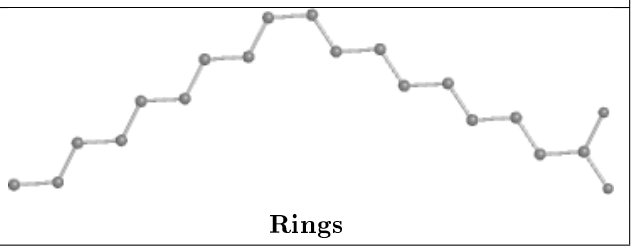
Bond lengths



Bond angles

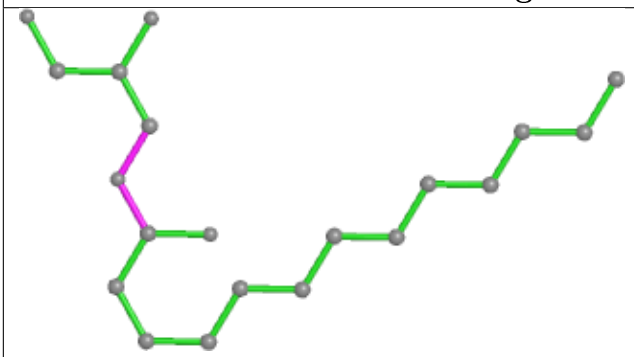


Torsions

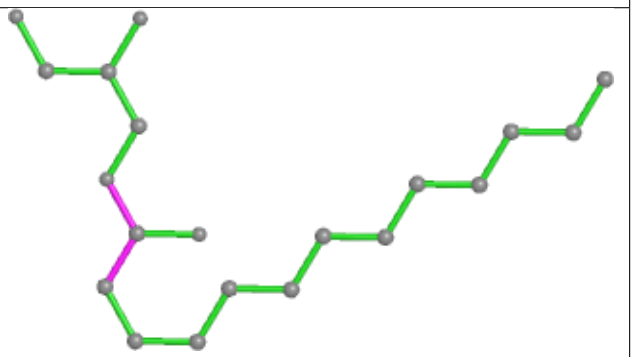


Rings

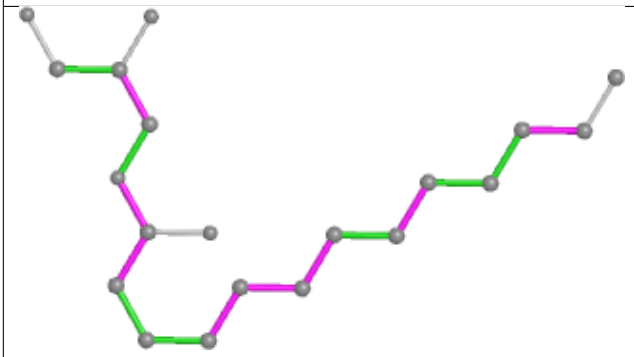
Ligand OLB A 2428



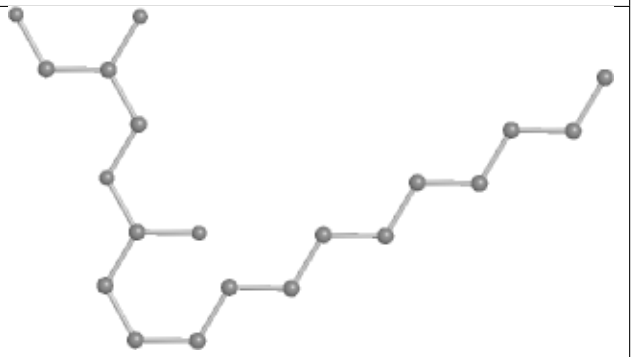
Bond lengths



Bond angles

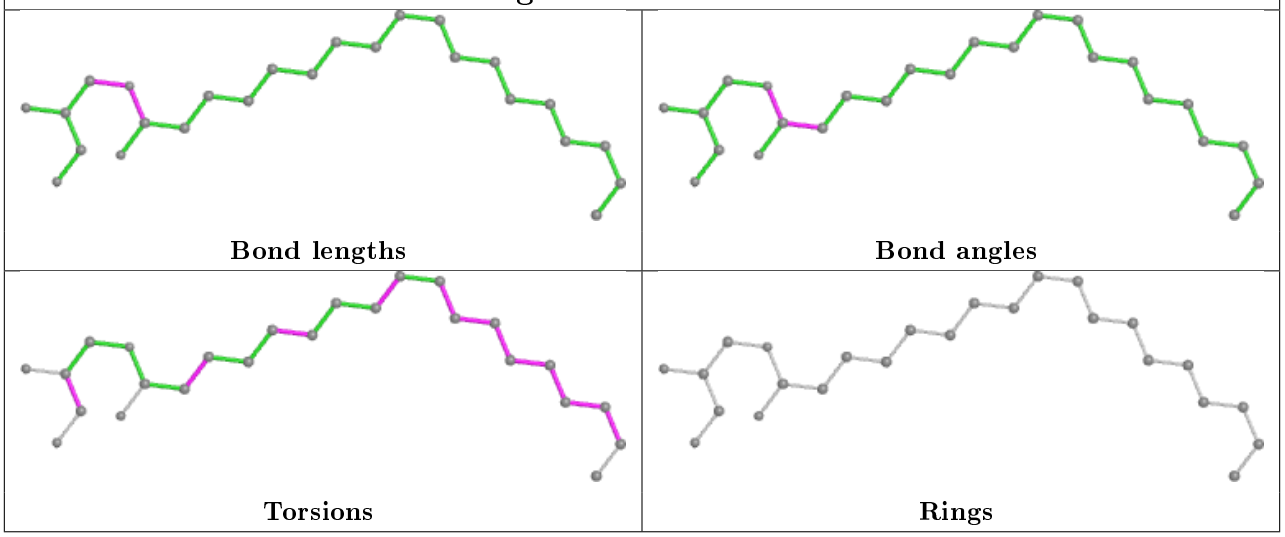


Torsions

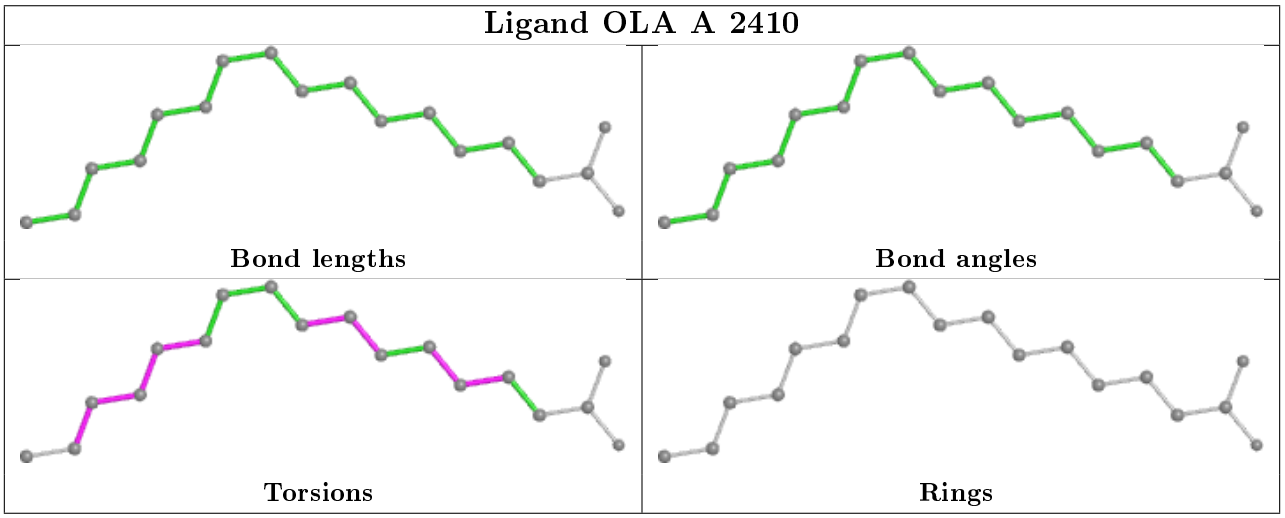


Rings

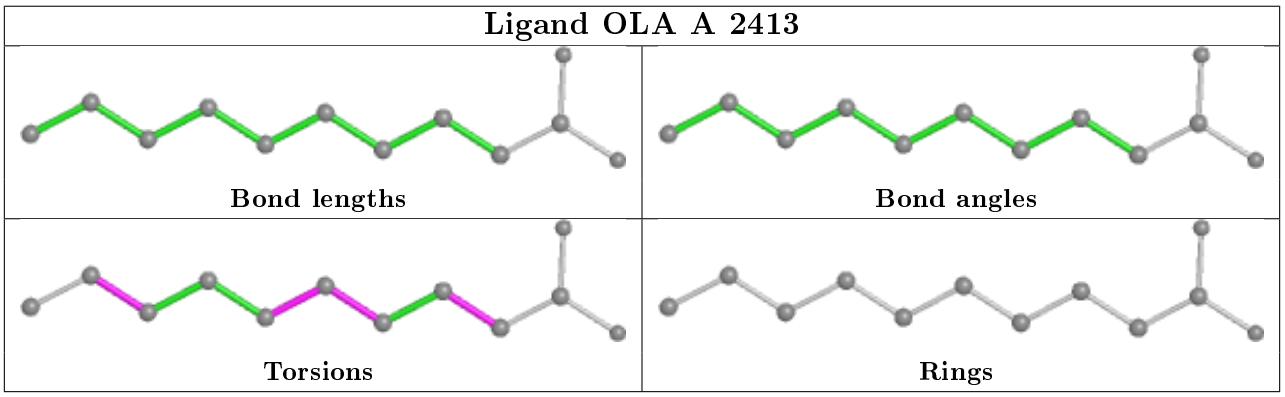
Ligand OLC A 2429



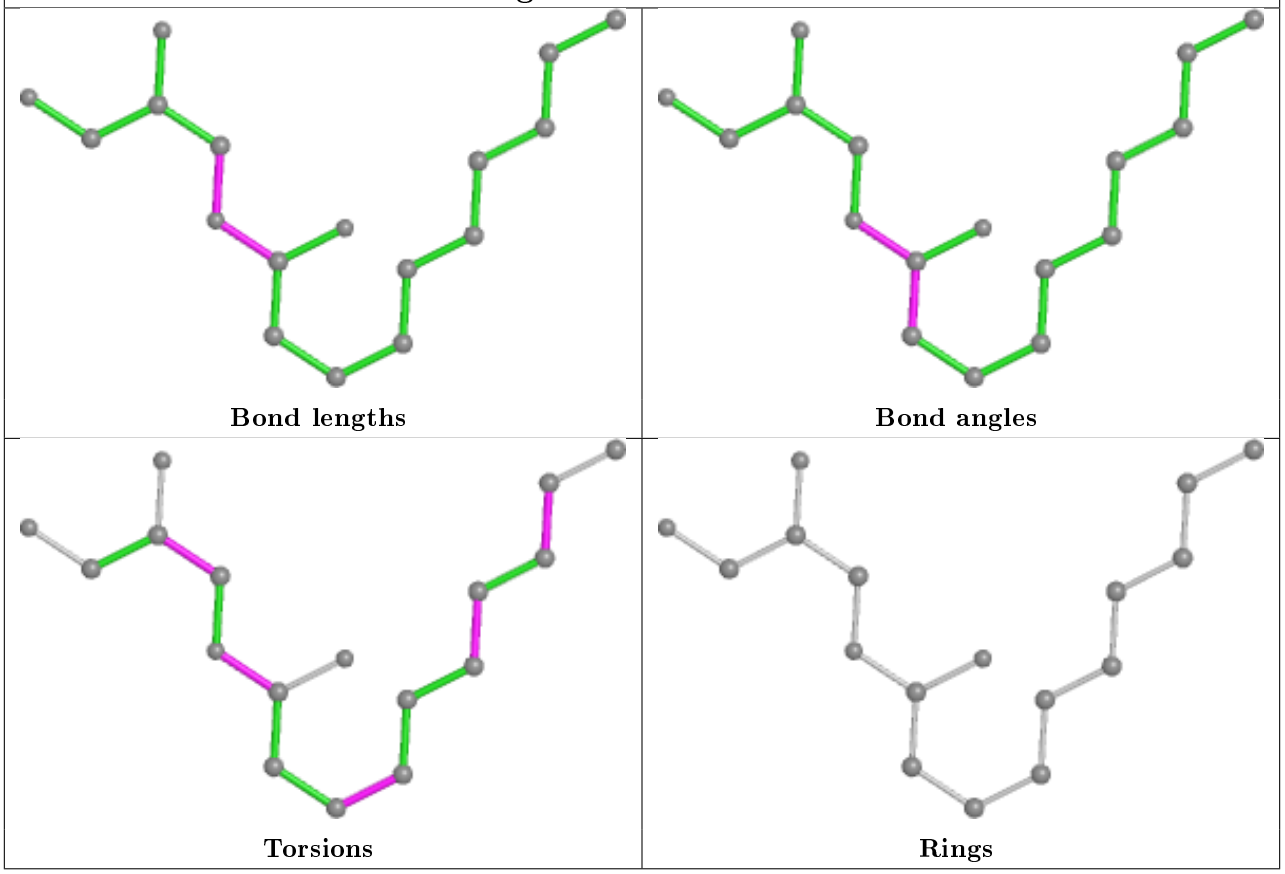
Ligand OLA A 2410



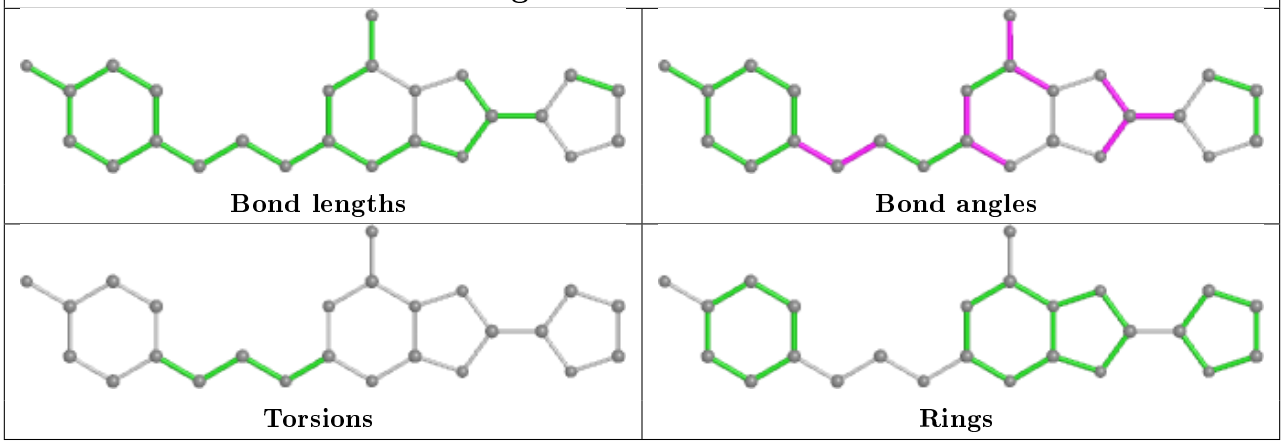
Ligand OLA A 2413



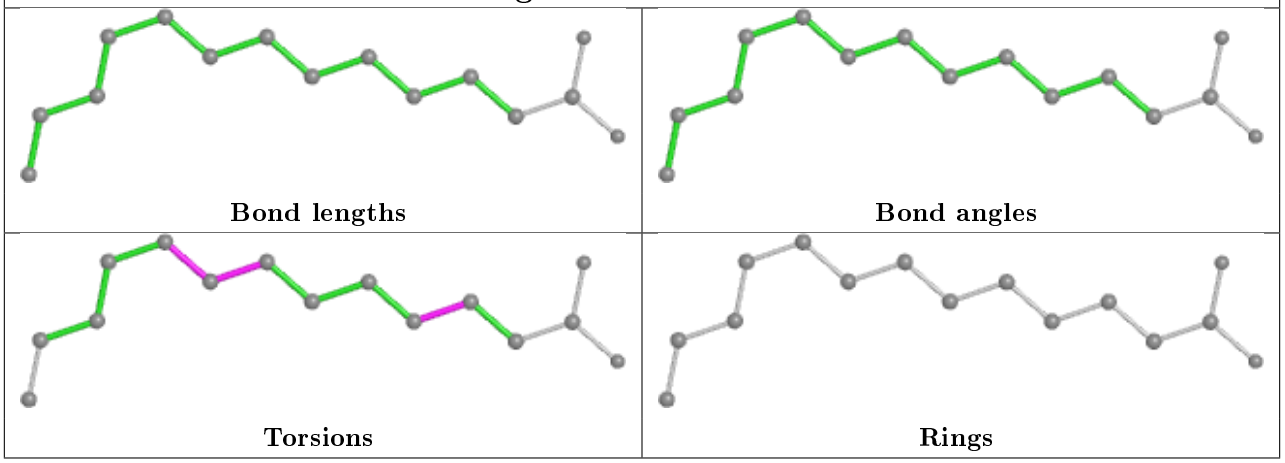
Ligand OLB A 2426



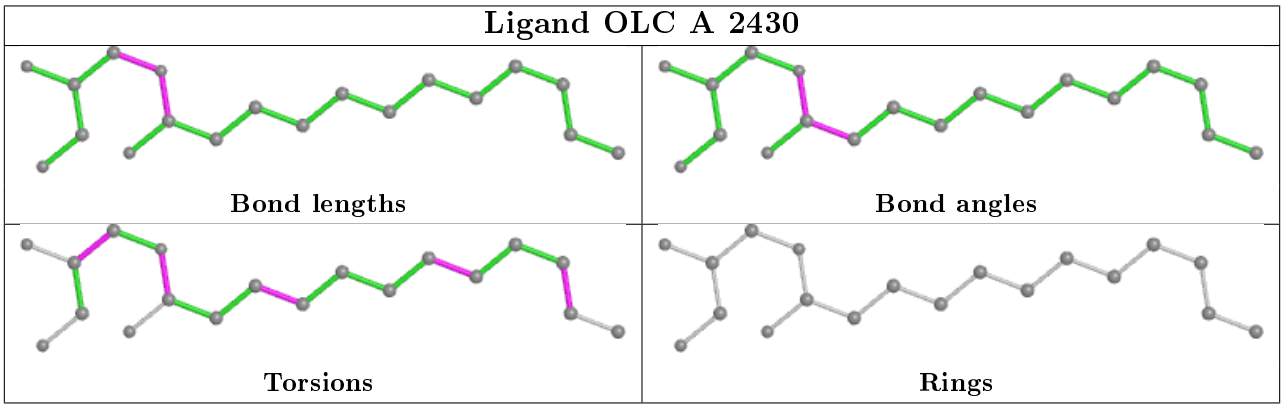
Ligand ZMA A 2401



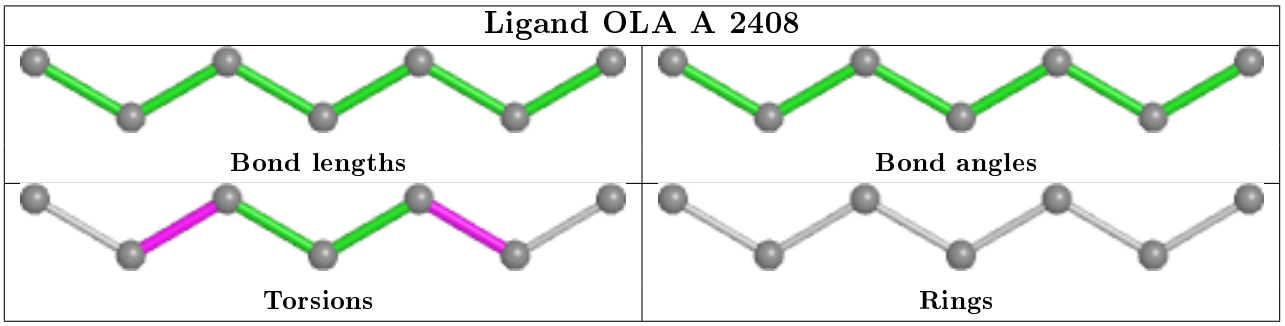
Ligand OLA A 2412



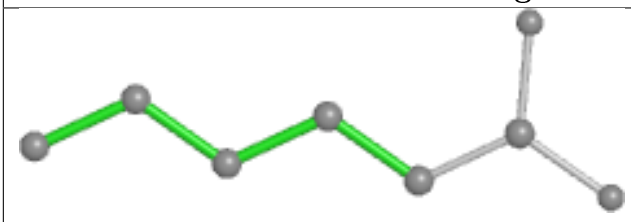
Ligand OLC A 2430



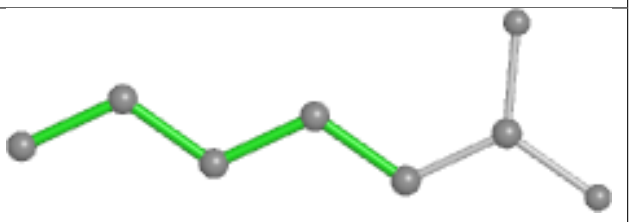
Ligand OLA A 2408



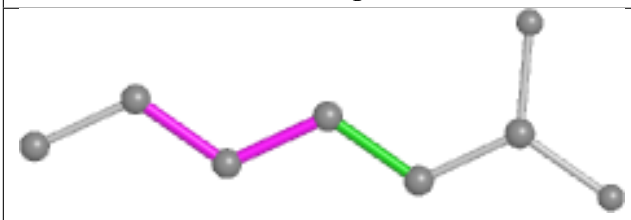
Ligand OLA A 2414



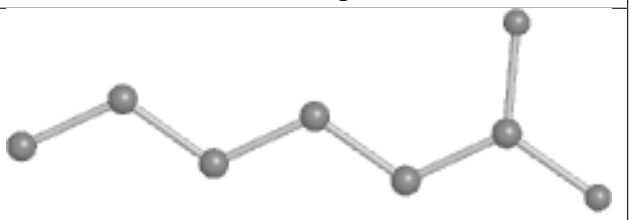
Bond lengths



Bond angles

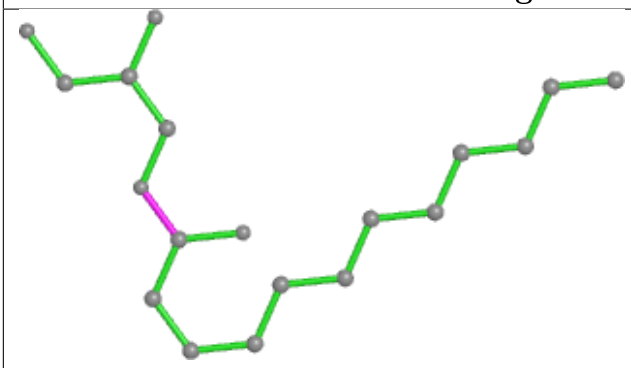


Torsions

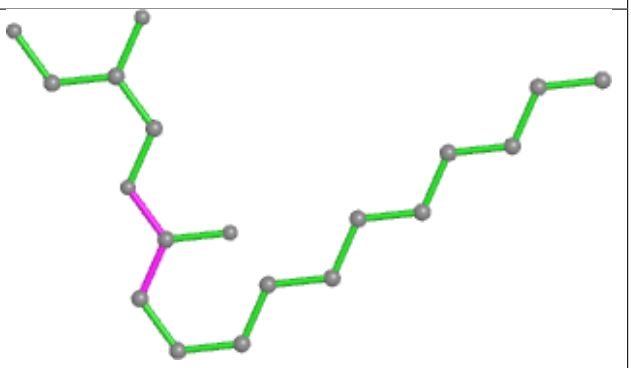


Rings

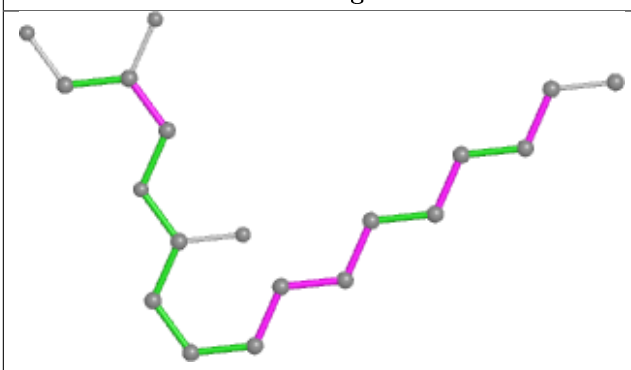
Ligand OLB A 2427



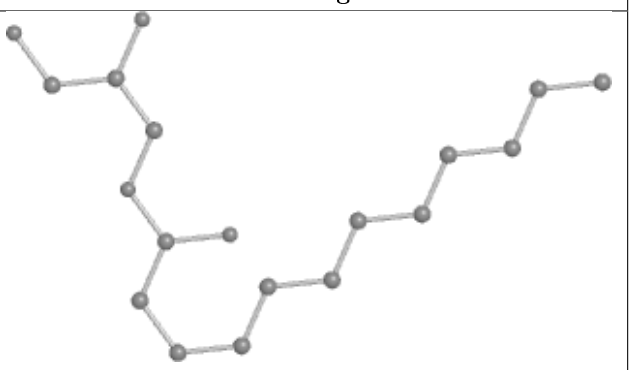
Bond lengths



Bond angles

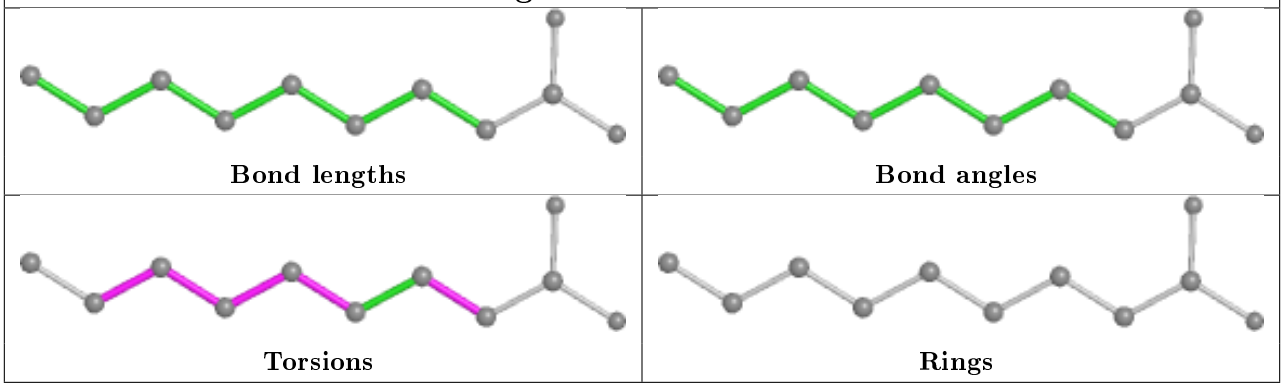


Torsions

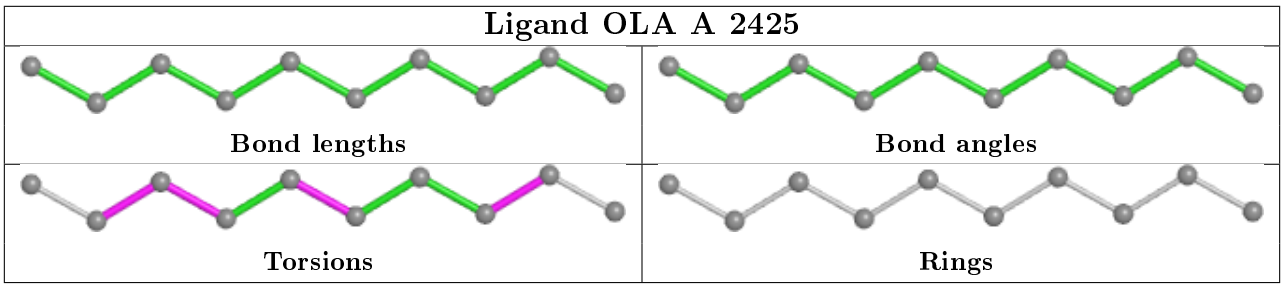


Rings

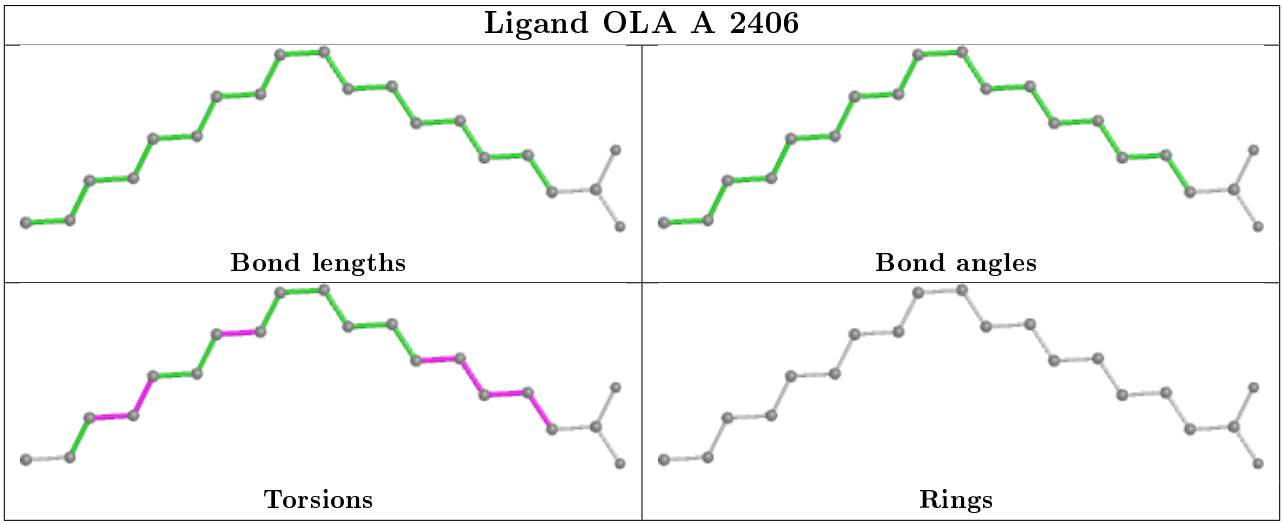
Ligand OLA A 2421



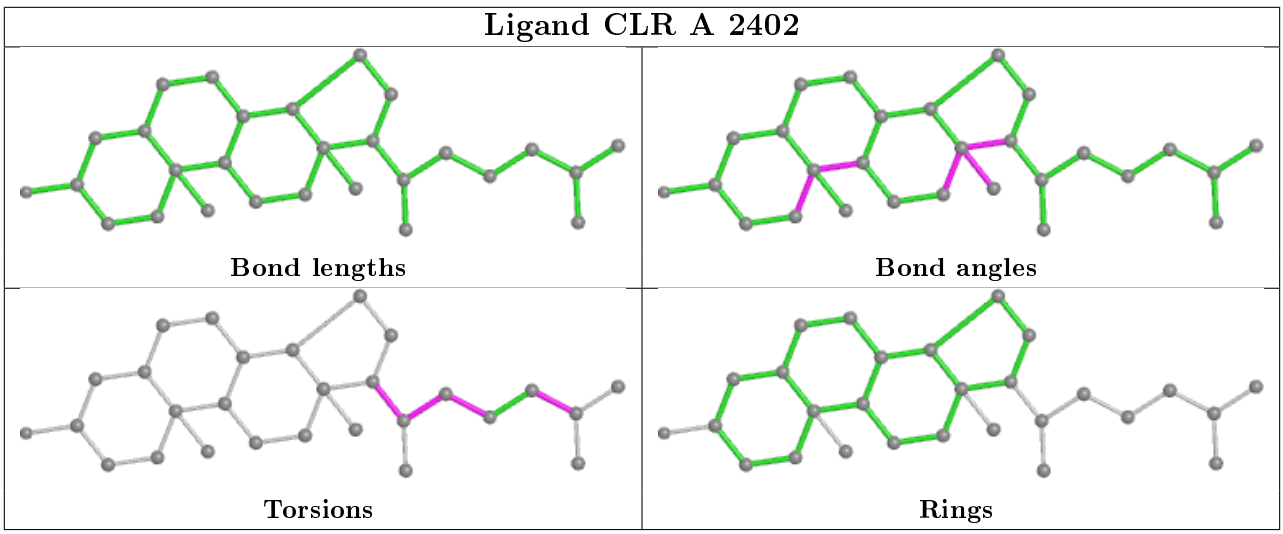
Ligand OLA A 2425



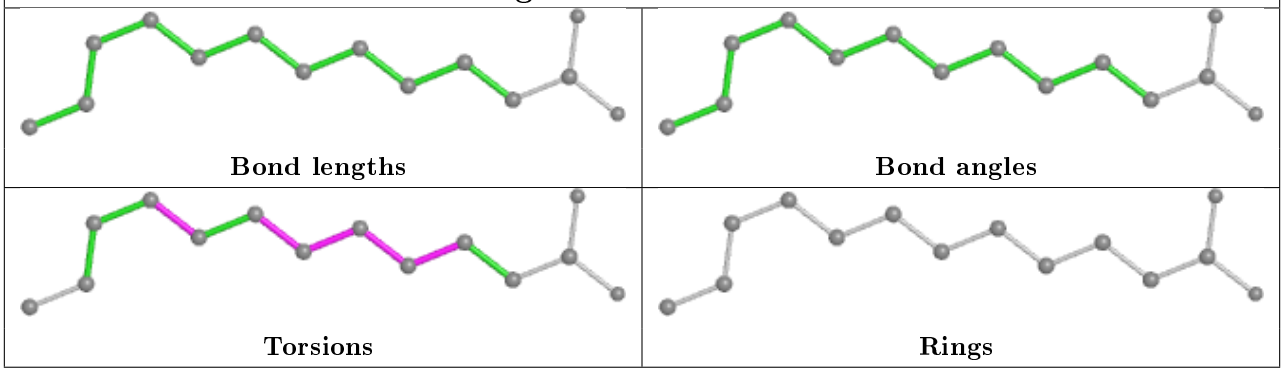
Ligand OLA A 2406



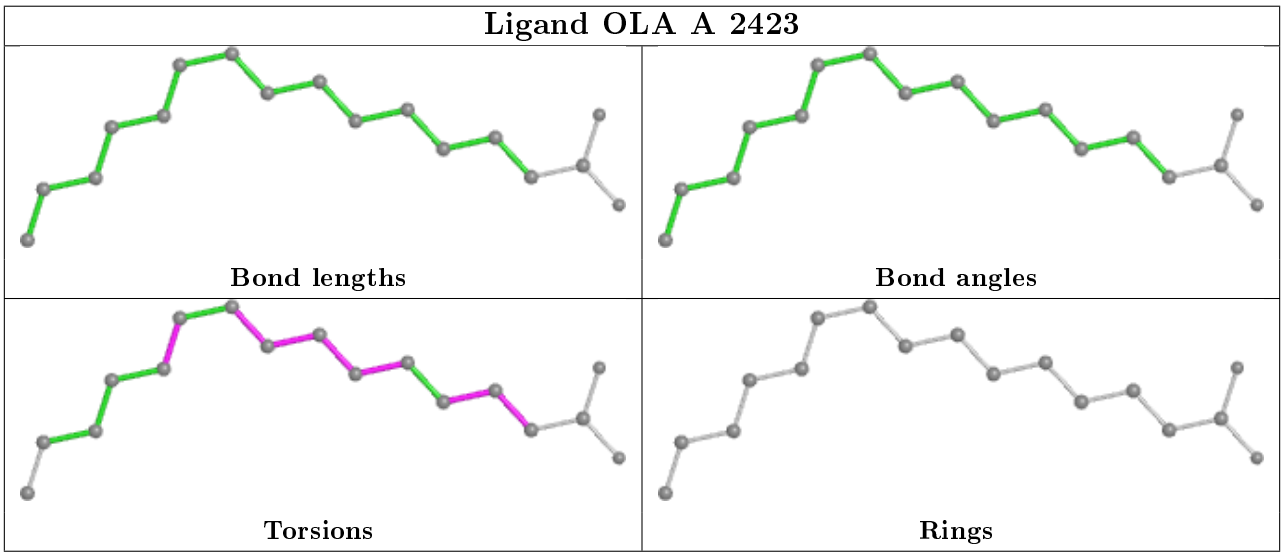
Ligand CLR A 2402



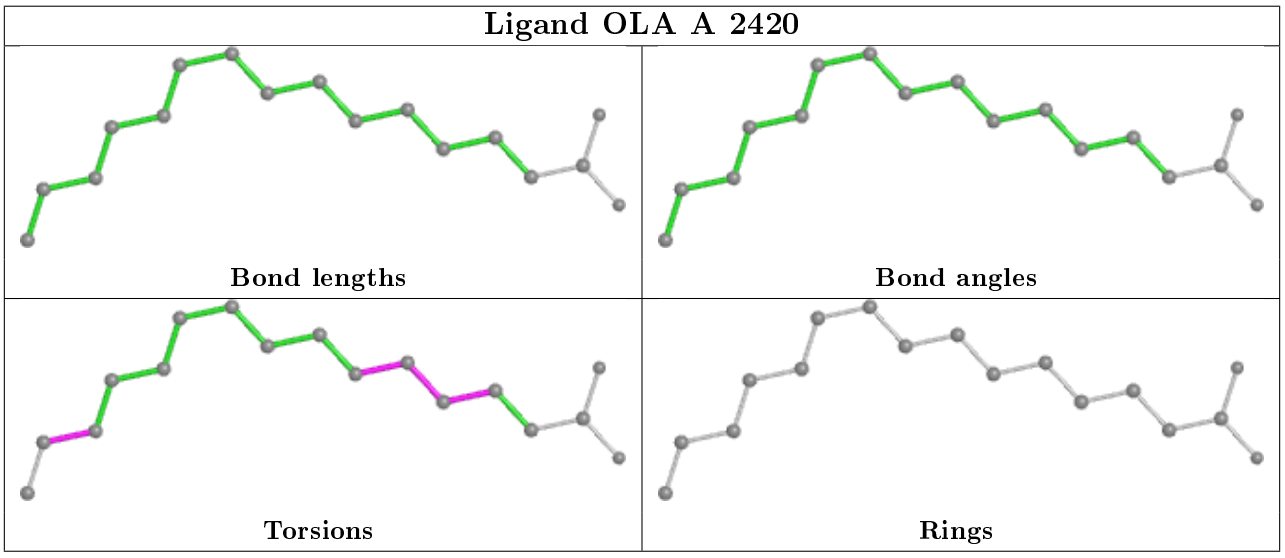
Ligand OLA A 2415



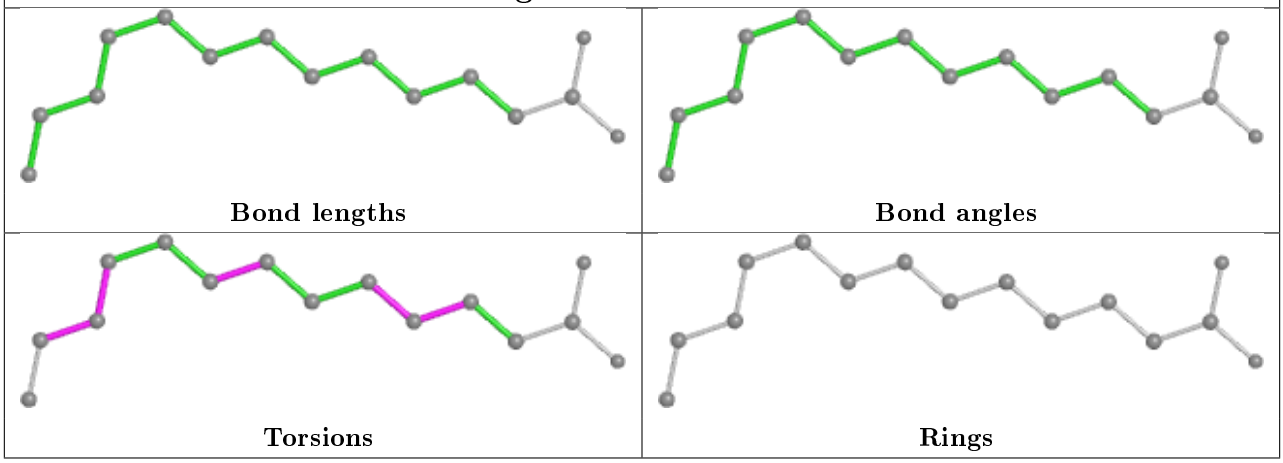
Ligand OLA A 2423



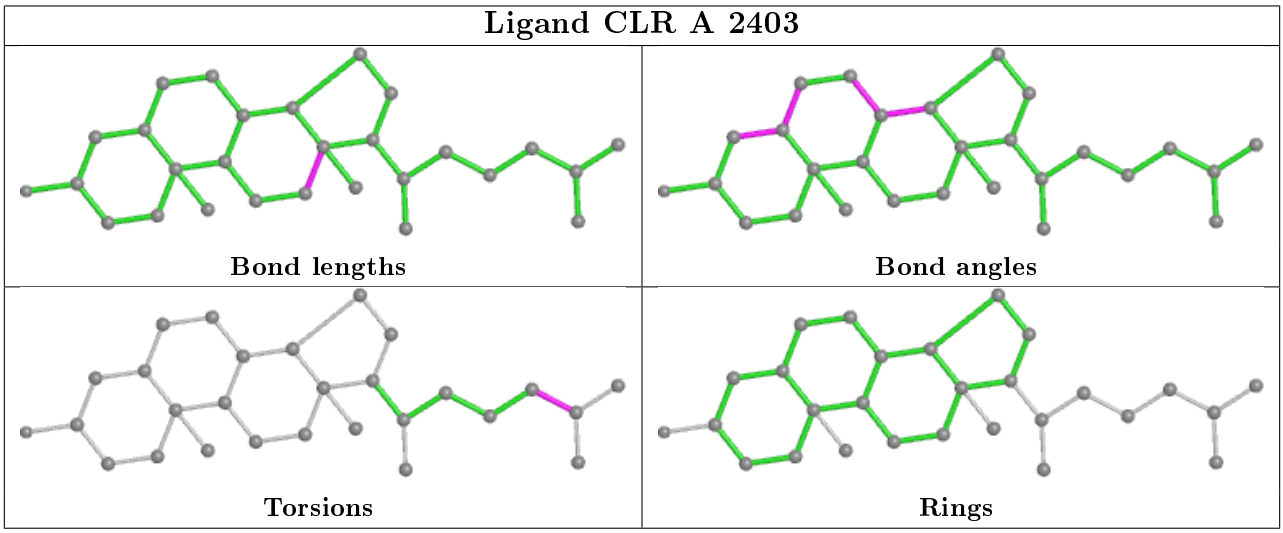
Ligand OLA A 2420



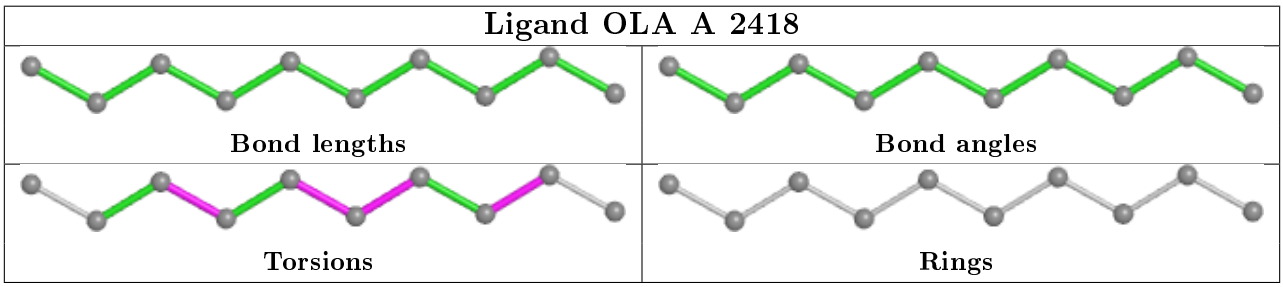
Ligand OLA A 2407

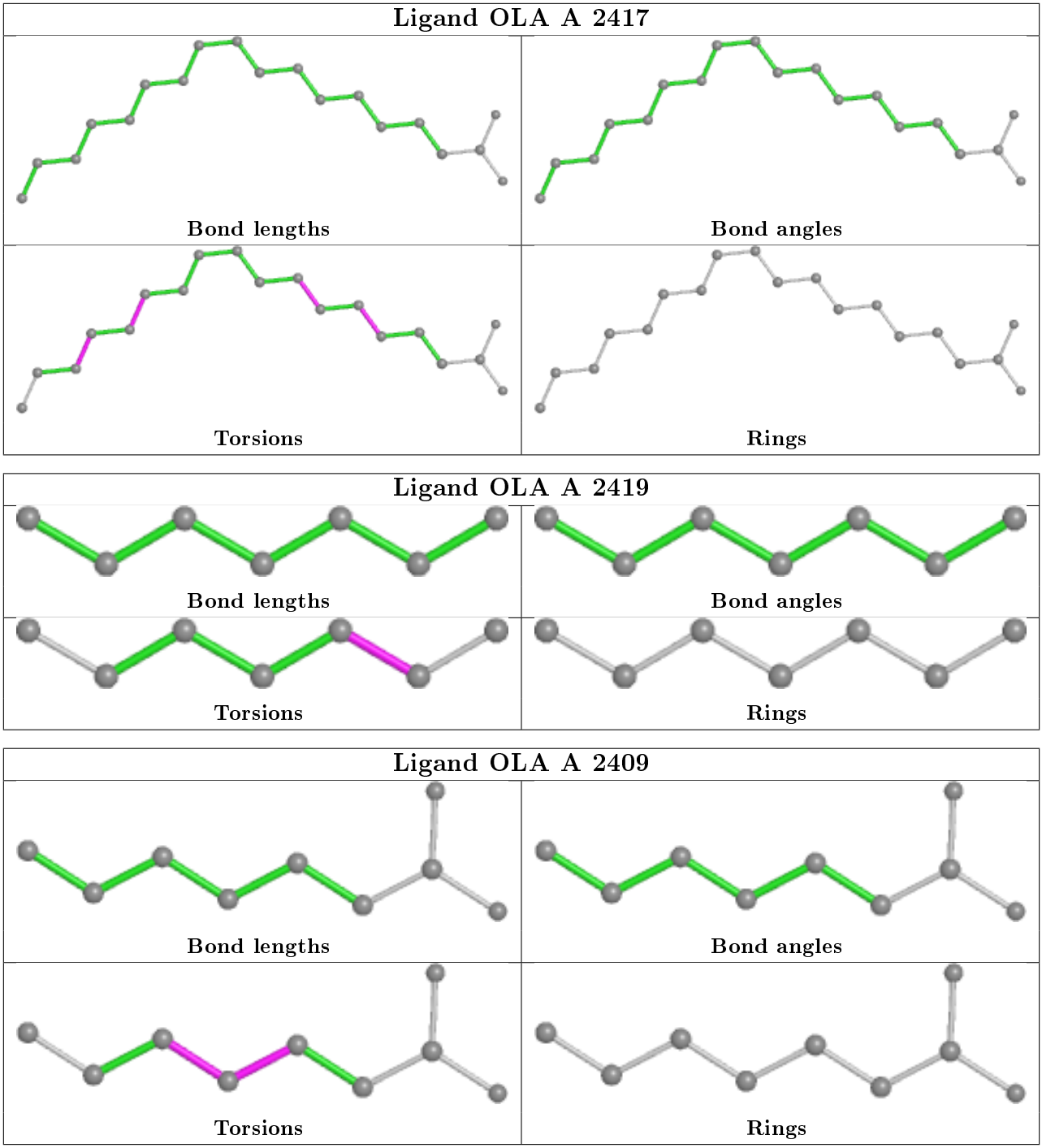


Ligand CLR A 2403



Ligand OLA A 2418





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	388/433 (89%)	0.26	31 (7%)	12	14	10, 27, 77, 106	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1058	MET	8.9
1	A	1061	PHE	7.4
1	A	1059	LYS	6.5
1	A	110	LEU	5.4
1	A	304	ARG	4.6

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	OLA	A	2421	11/20	0.65	0.19	53,59,65,66	0
5	OLA	A	2411	20/20	0.66	0.21	44,62,71,73	0

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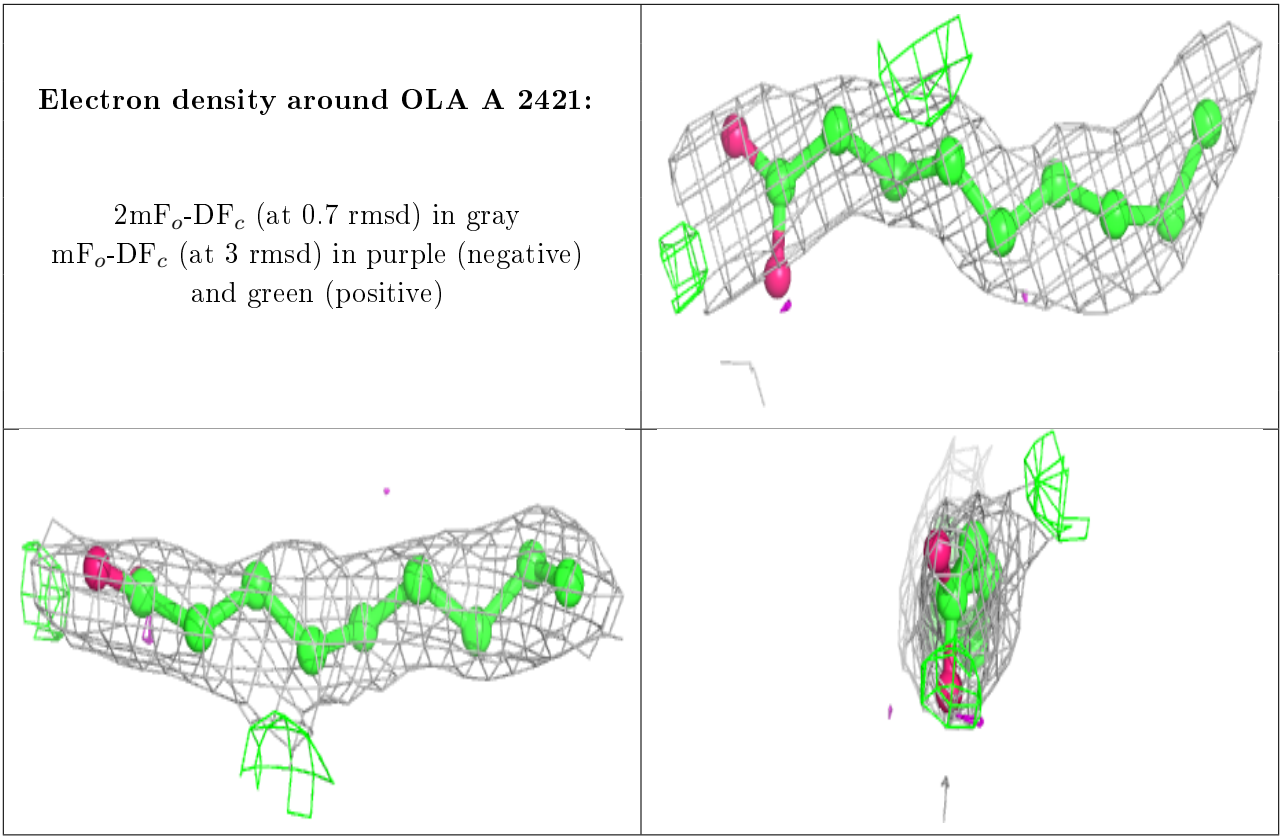
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CLR	A	2402	28/28	0.67	0.31	113,119,121,122	0
5	OLA	A	2413	12/20	0.73	0.28	45,54,68,69	0
5	OLA	A	2424	12/20	0.75	0.14	53,61,75,77	0
5	OLA	A	2415	14/20	0.76	0.17	50,61,65,66	0
7	OLC	A	2430	19/25	0.77	0.20	44,51,67,67	0
6	OLB	A	2428	20/25	0.78	0.24	52,63,82,82	0
5	OLA	A	2412	15/20	0.79	0.18	58,61,77,80	0
5	OLA	A	2416	7/20	0.79	0.12	58,60,62,63	0
5	OLA	A	2414	8/20	0.79	0.15	53,57,62,63	0
5	OLA	A	2417	19/20	0.79	0.16	55,60,64,64	0
6	OLB	A	2426	17/25	0.80	0.17	57,63,73,73	0
5	OLA	A	2407	15/20	0.81	0.17	49,59,65,68	0
5	OLA	A	2408	7/20	0.82	0.14	51,54,57,59	0
5	OLA	A	2425	10/20	0.84	0.12	41,47,50,50	0
6	OLB	A	2427	19/25	0.87	0.19	45,57,74,78	0
5	OLA	A	2422	13/20	0.87	0.11	44,47,52,52	0
5	OLA	A	2418	10/20	0.89	0.18	41,46,48,50	0
5	OLA	A	2406	20/20	0.90	0.10	37,48,56,57	0
5	OLA	A	2420	17/20	0.90	0.13	39,45,54,54	0
5	OLA	A	2410	18/20	0.90	0.11	47,53,63,65	0
5	OLA	A	2419	7/20	0.90	0.09	59,60,71,71	0
5	OLA	A	2409	9/20	0.90	0.12	33,39,54,56	0
5	OLA	A	2423	17/20	0.91	0.12	41,43,60,67	0
2	NA	A	2400	1/1	0.92	0.10	33,33,33,33	0
7	OLC	A	2429	25/25	0.93	0.14	40,49,67,72	0
4	CLR	A	2404	28/28	0.97	0.06	15,19,30,37	0
4	CLR	A	2403	28/28	0.97	0.07	14,20,41,49	0
4	CLR	A	2405	28/28	0.98	0.06	14,17,41,44	0
3	ZMA	A	2401	25/25	0.98	0.12	9,12,35,43	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.

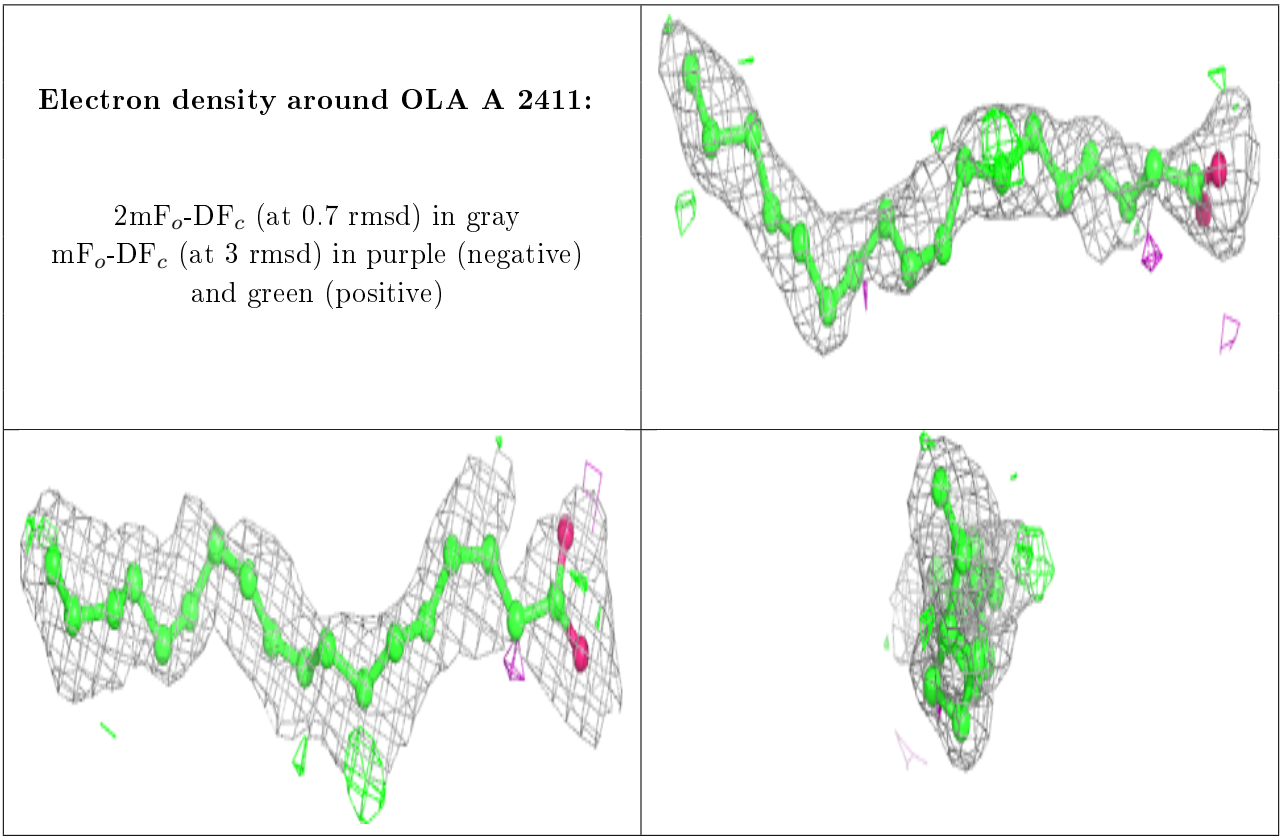
Electron density around OLA A 2421:

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



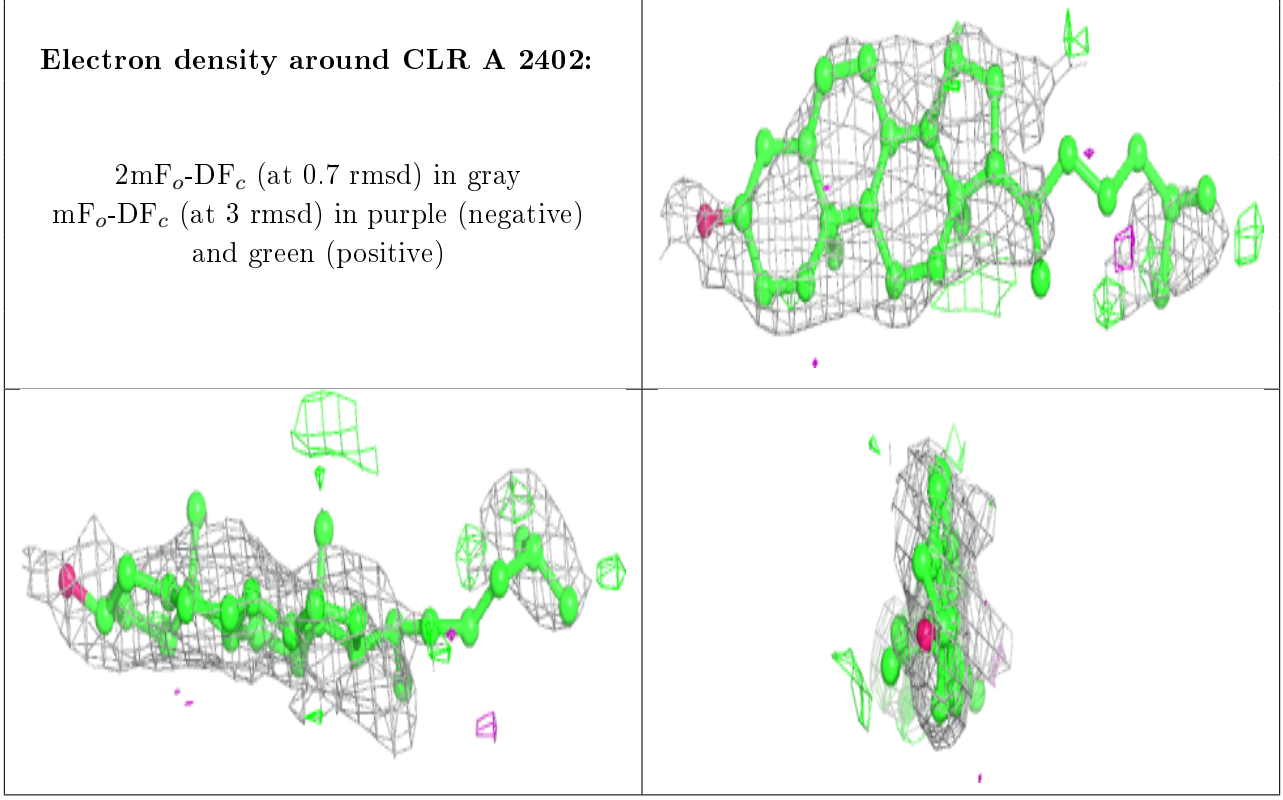
Electron density around OLA A 2411:

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



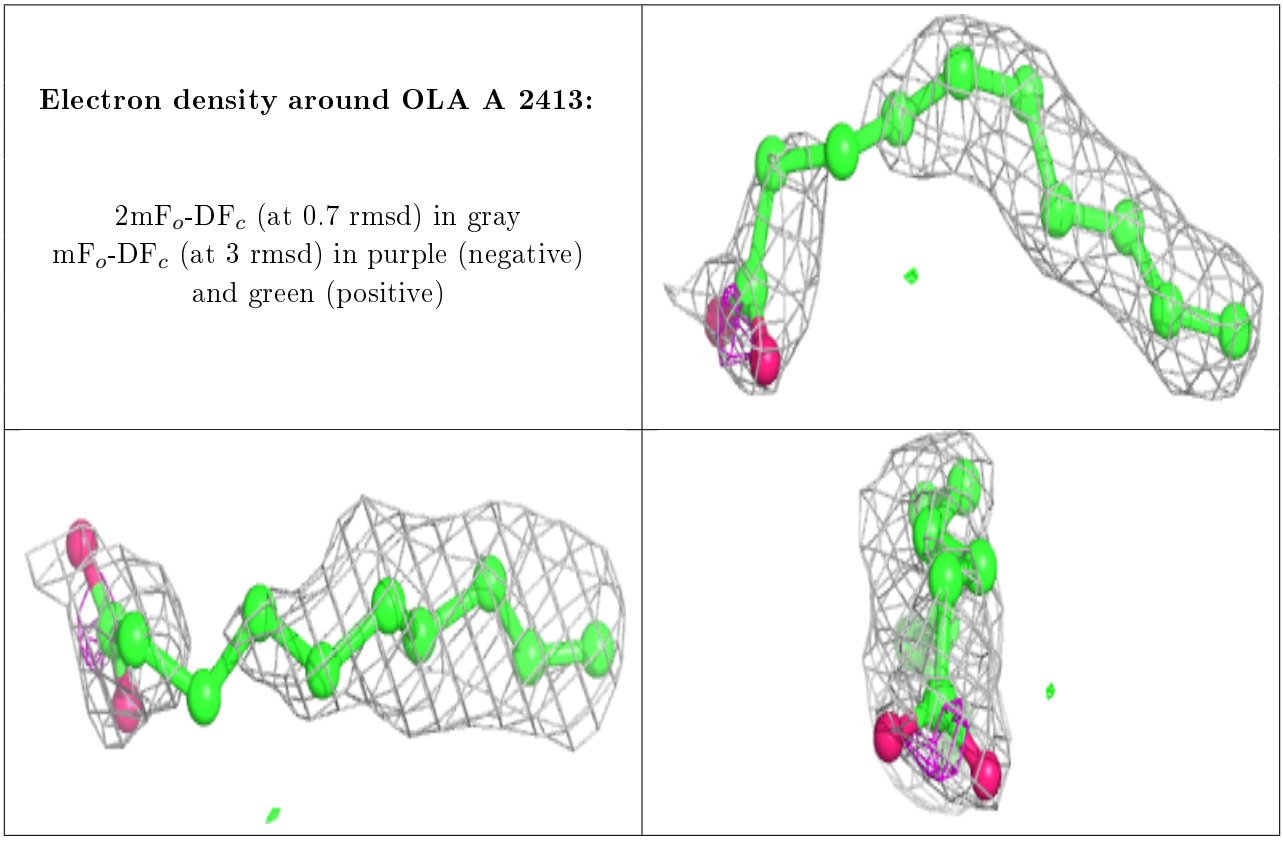
Electron density around CLR A 2402:

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



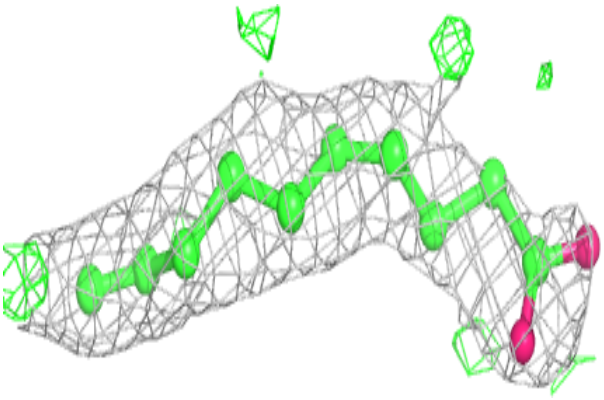
Electron density around OLA A 2413:

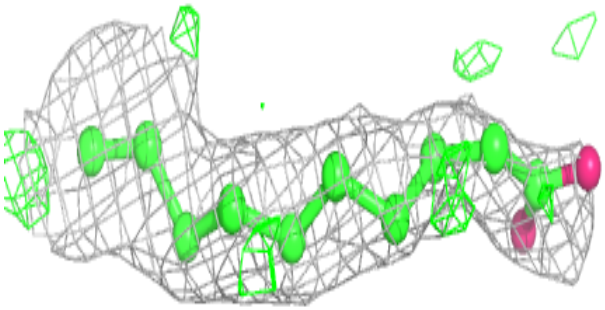
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

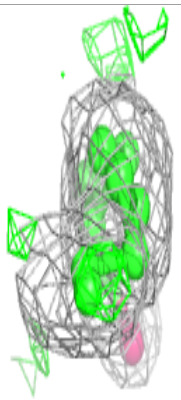


Electron density around OLA A 2424:

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

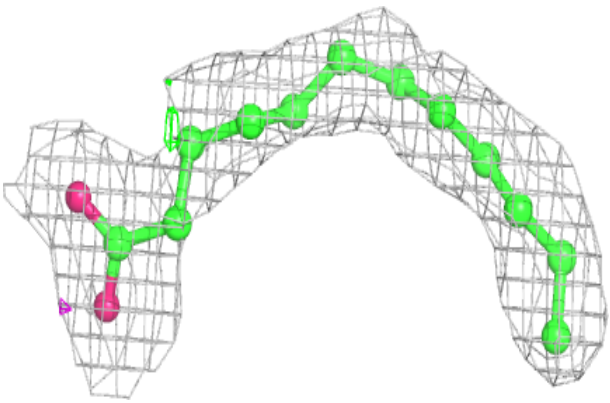


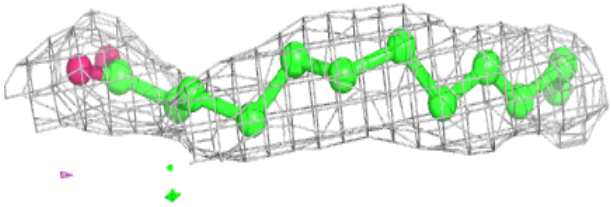


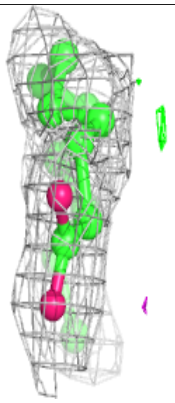


Electron density around OLA A 2415:

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

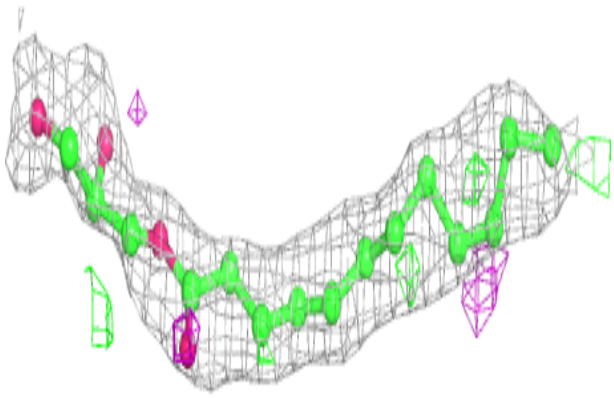


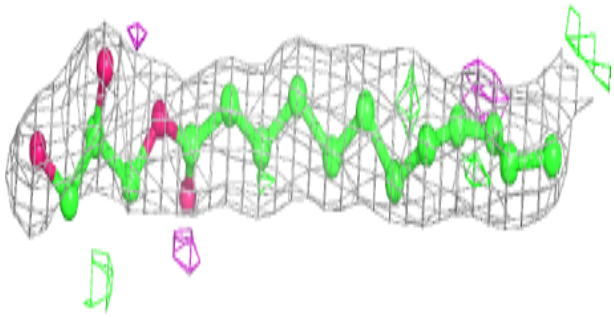


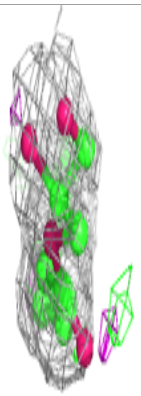


Electron density around OLC A 2430:

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

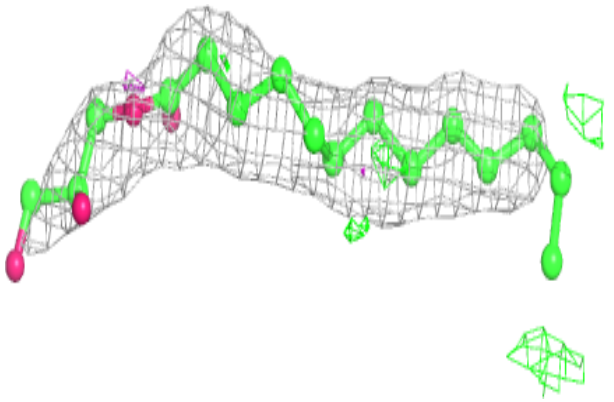


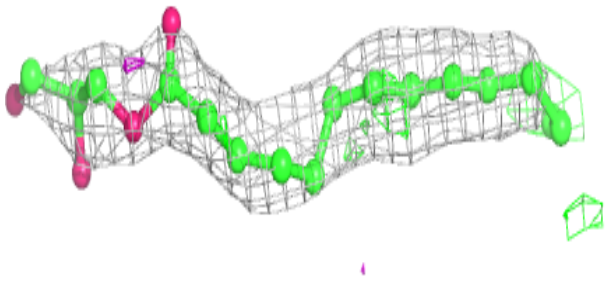


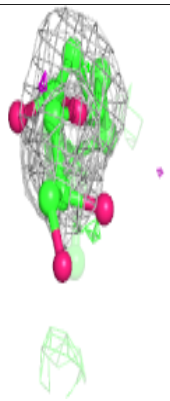


Electron density around OLB A 2428:

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

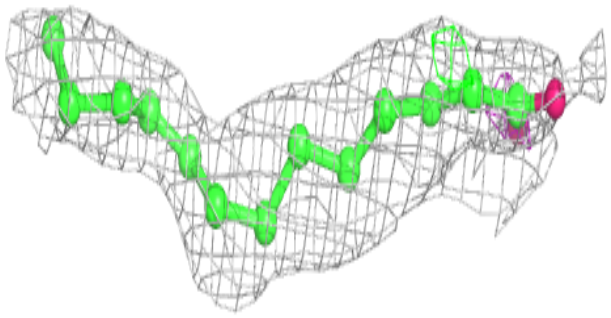


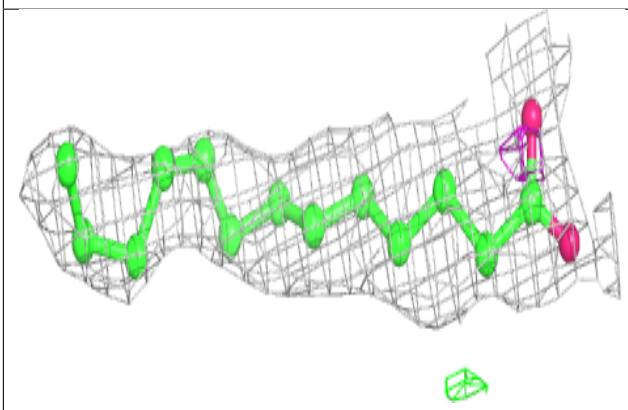


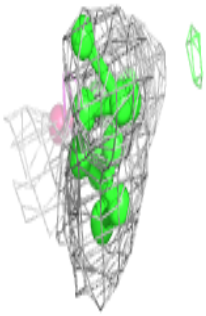


Electron density around OLA A 2412:

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

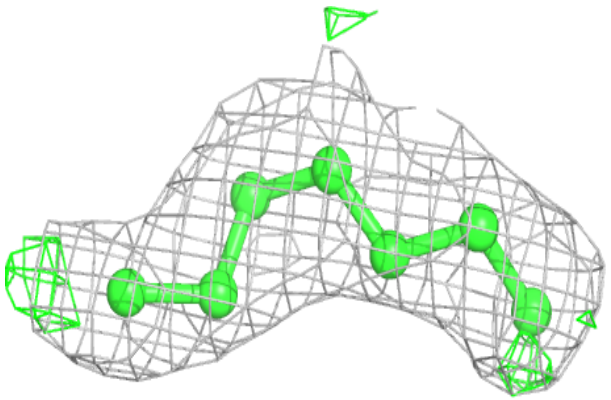


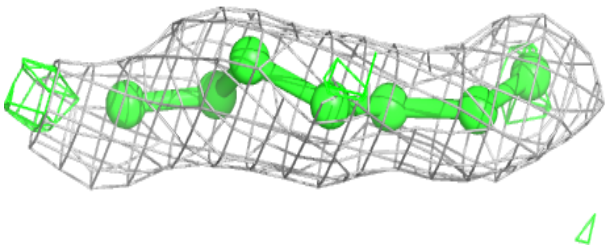


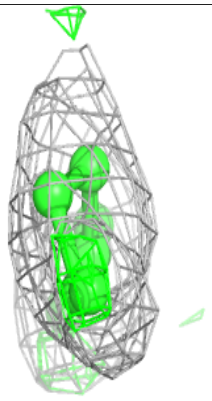


Electron density around OLA A 2416:

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

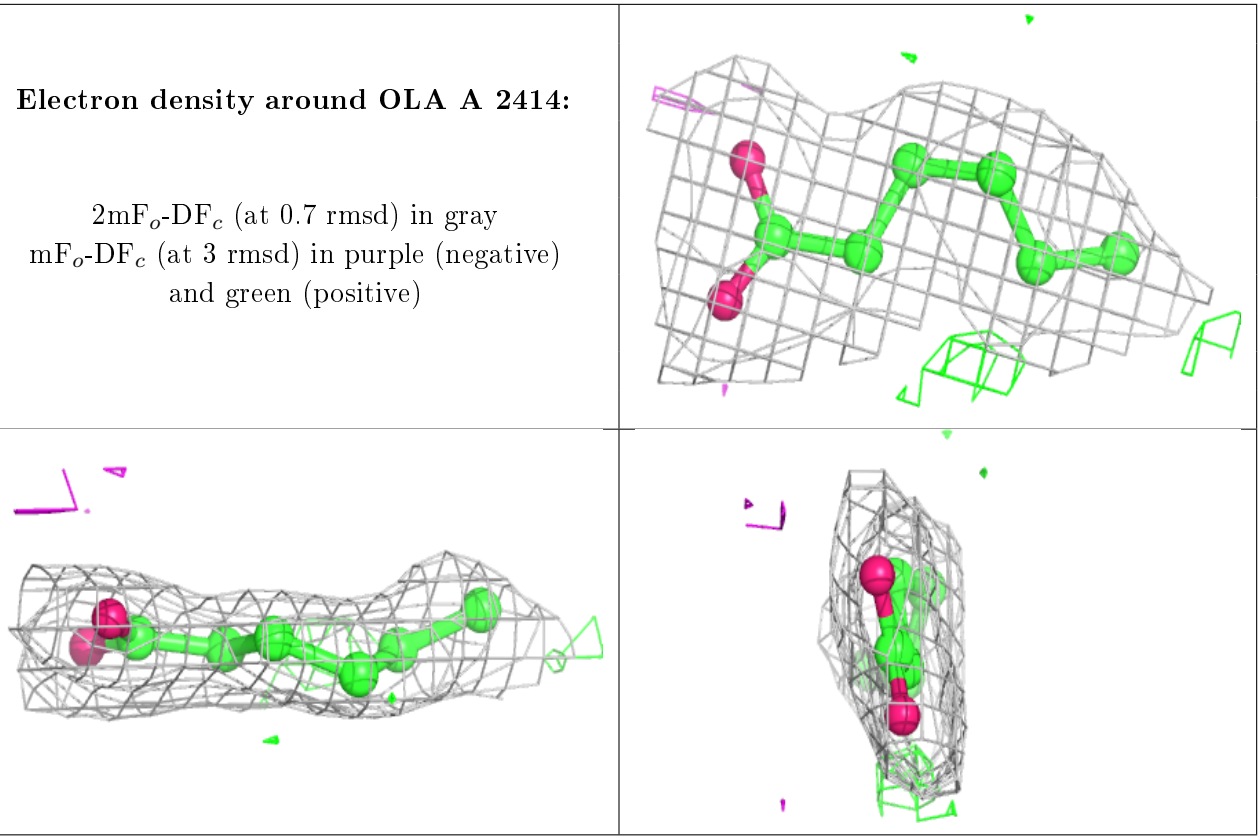






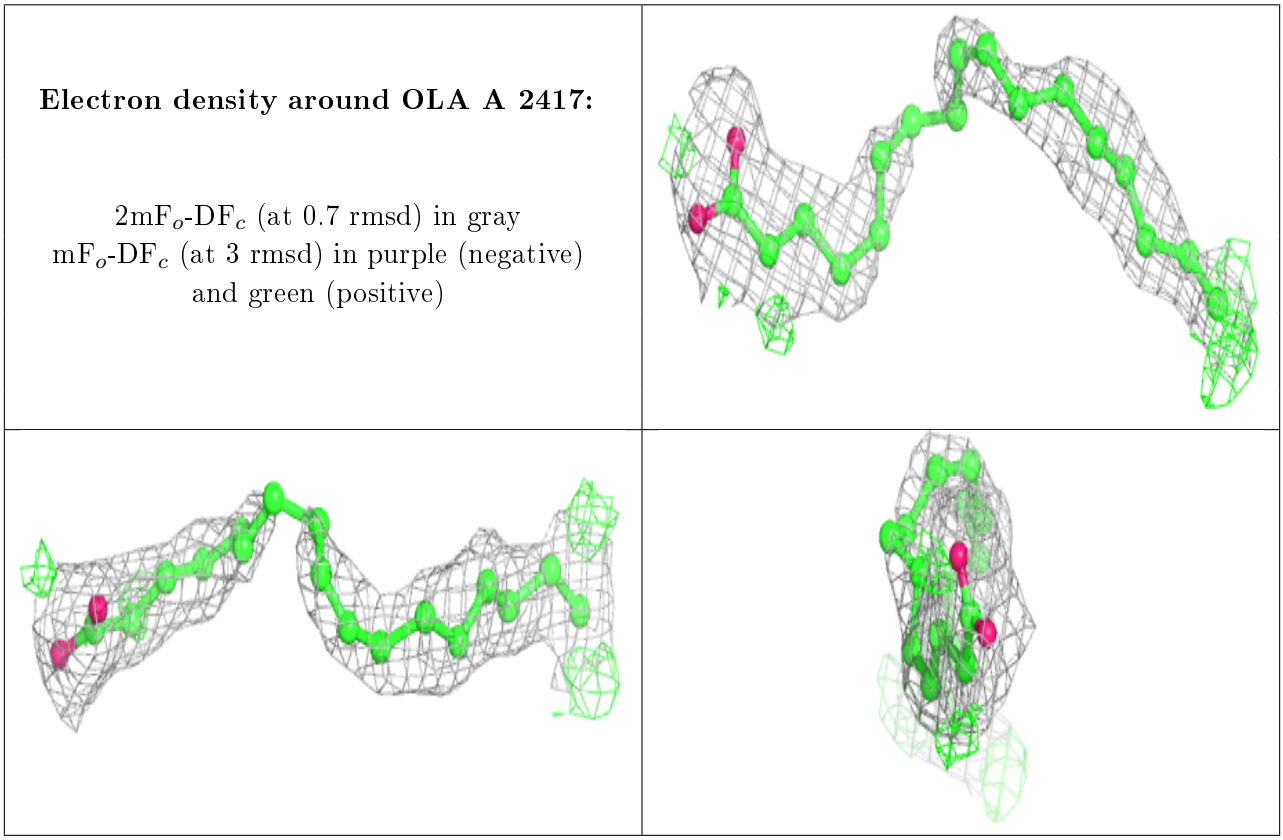
Electron density around OLA A 2414:

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



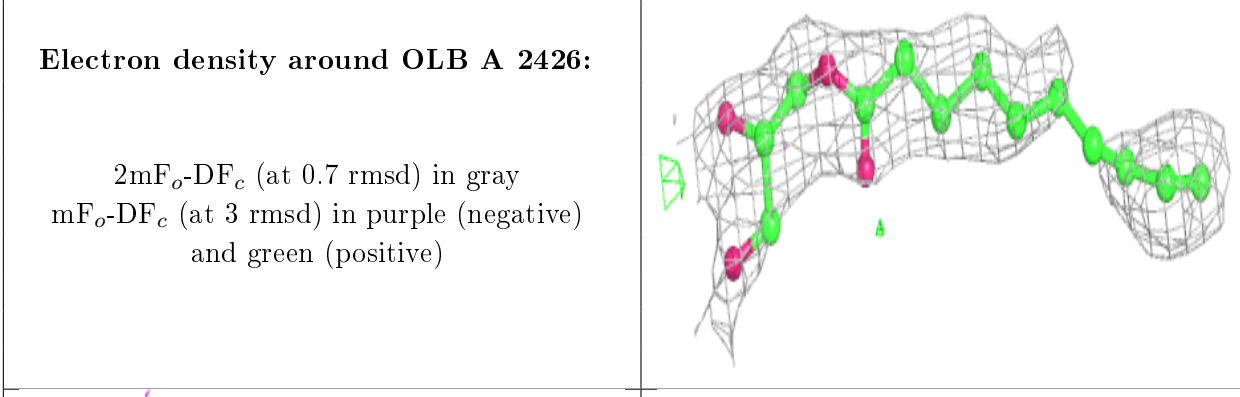
Electron density around OLA A 2417:

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



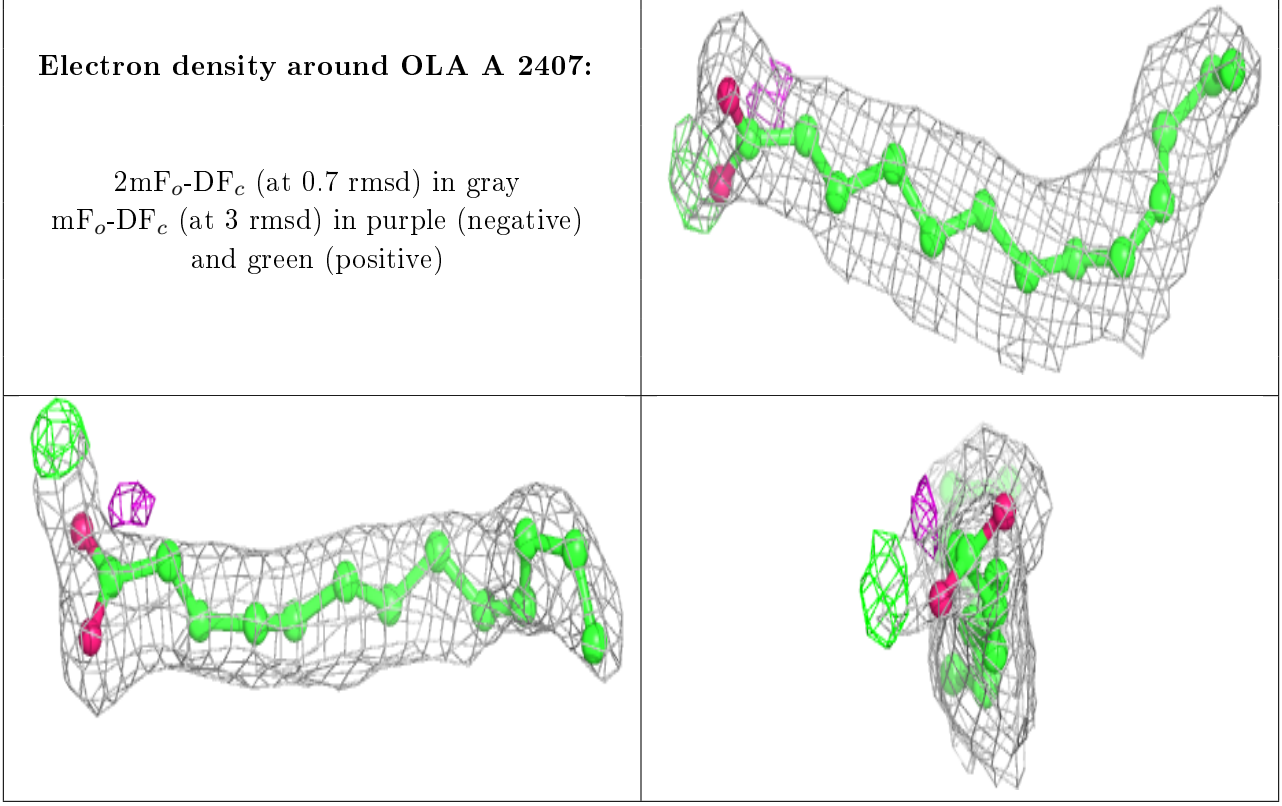
Electron density around OLB A 2426:

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



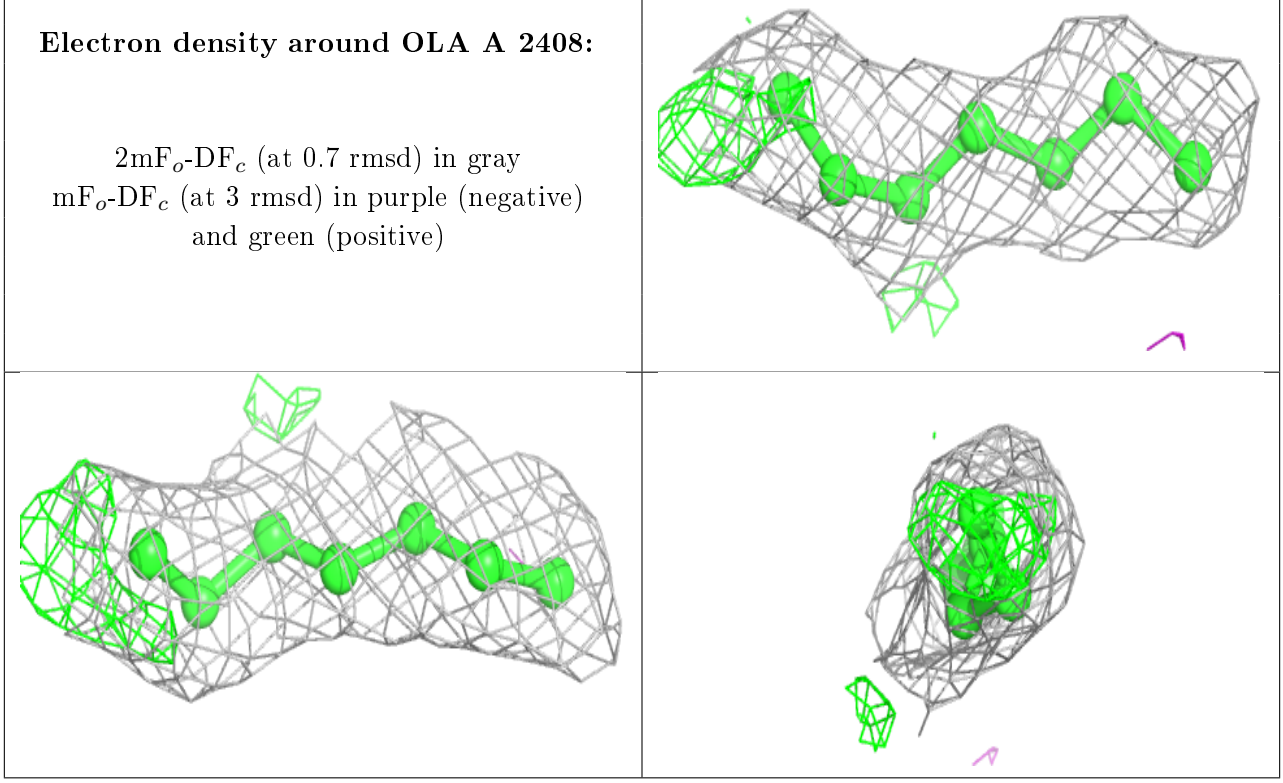
Electron density around OLA A 2407:

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



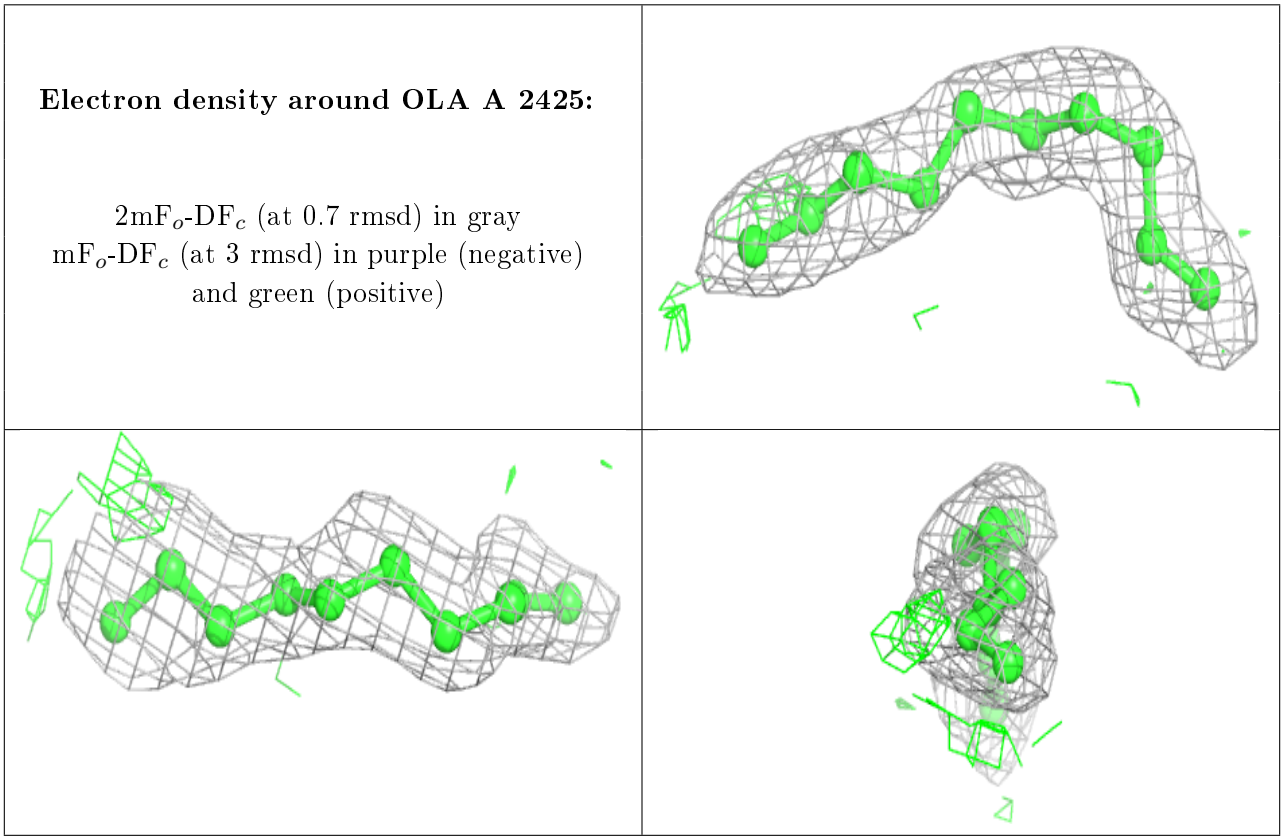
Electron density around OLA A 2408:

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



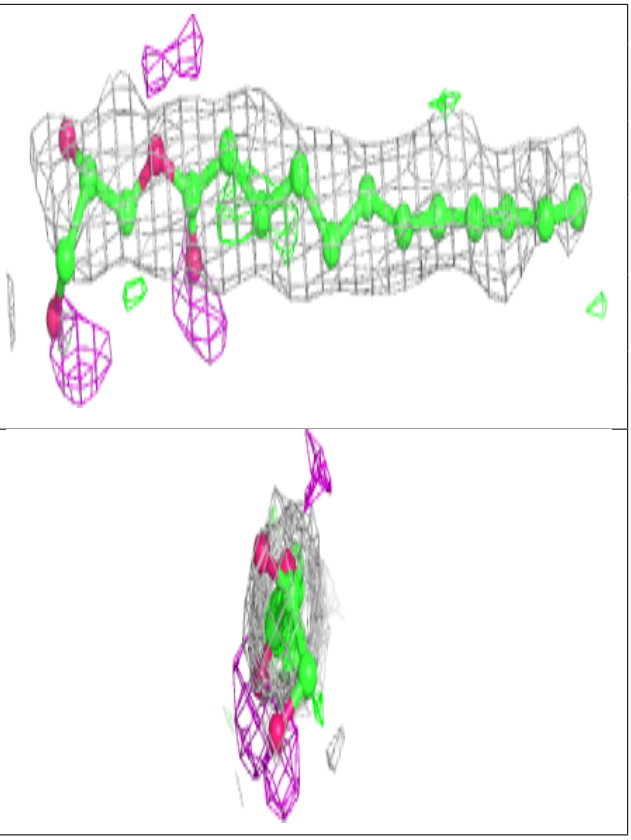
Electron density around OLA A 2425:

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



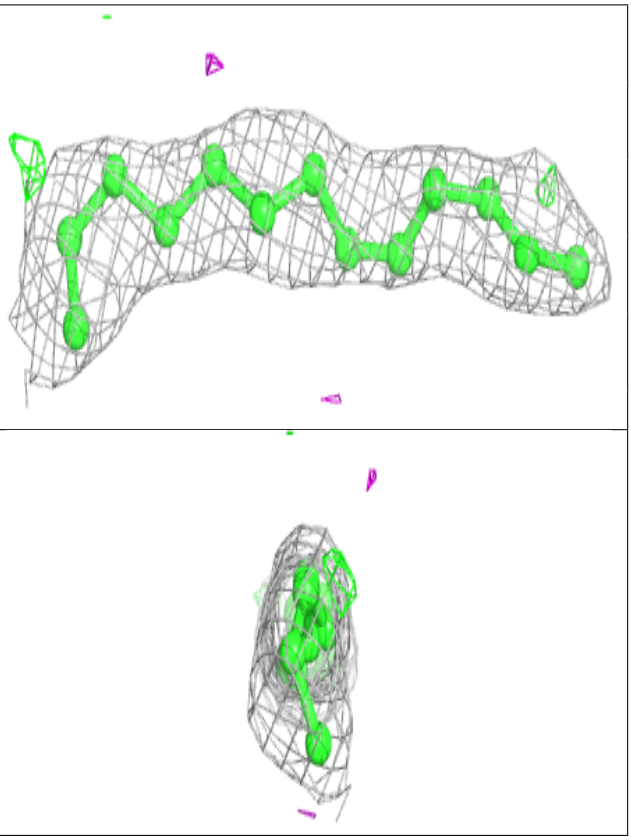
Electron density around OLB A 2427:

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



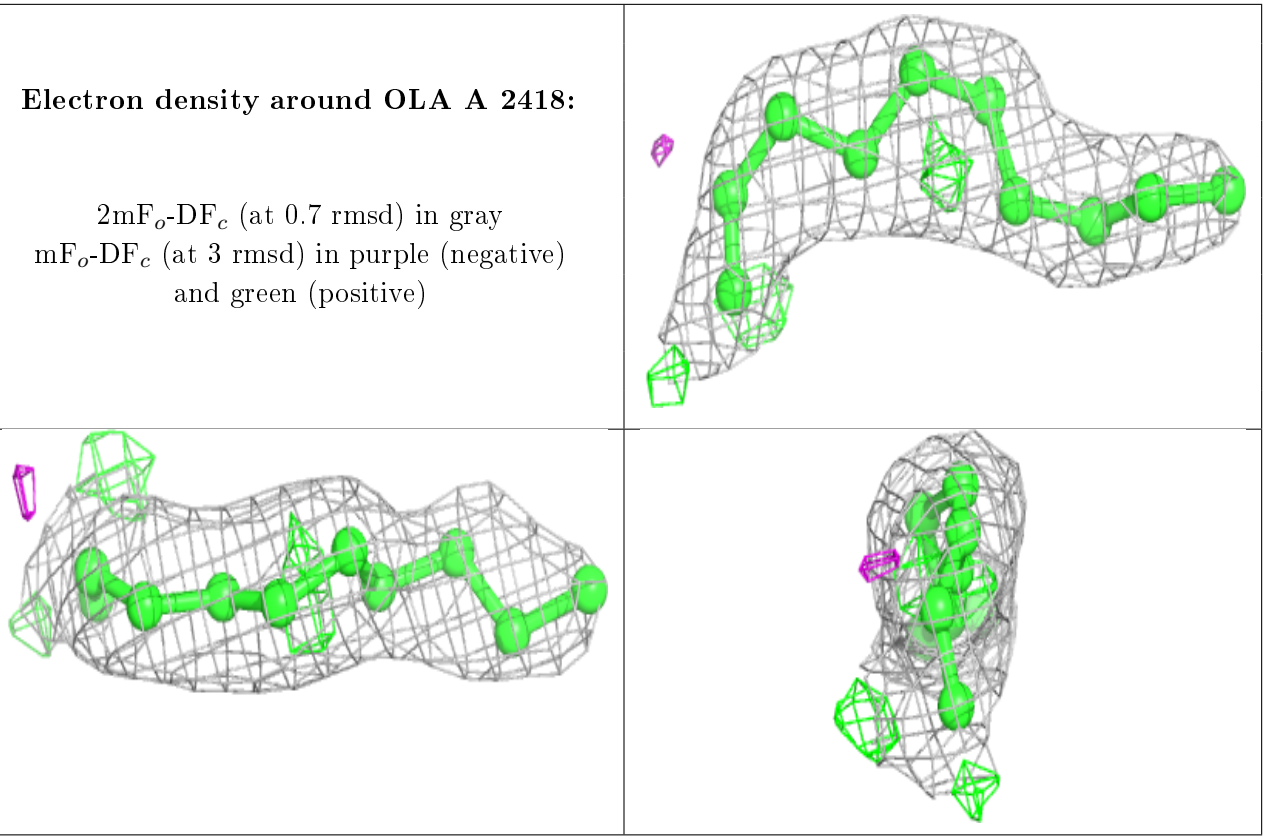
Electron density around OLA A 2422:

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



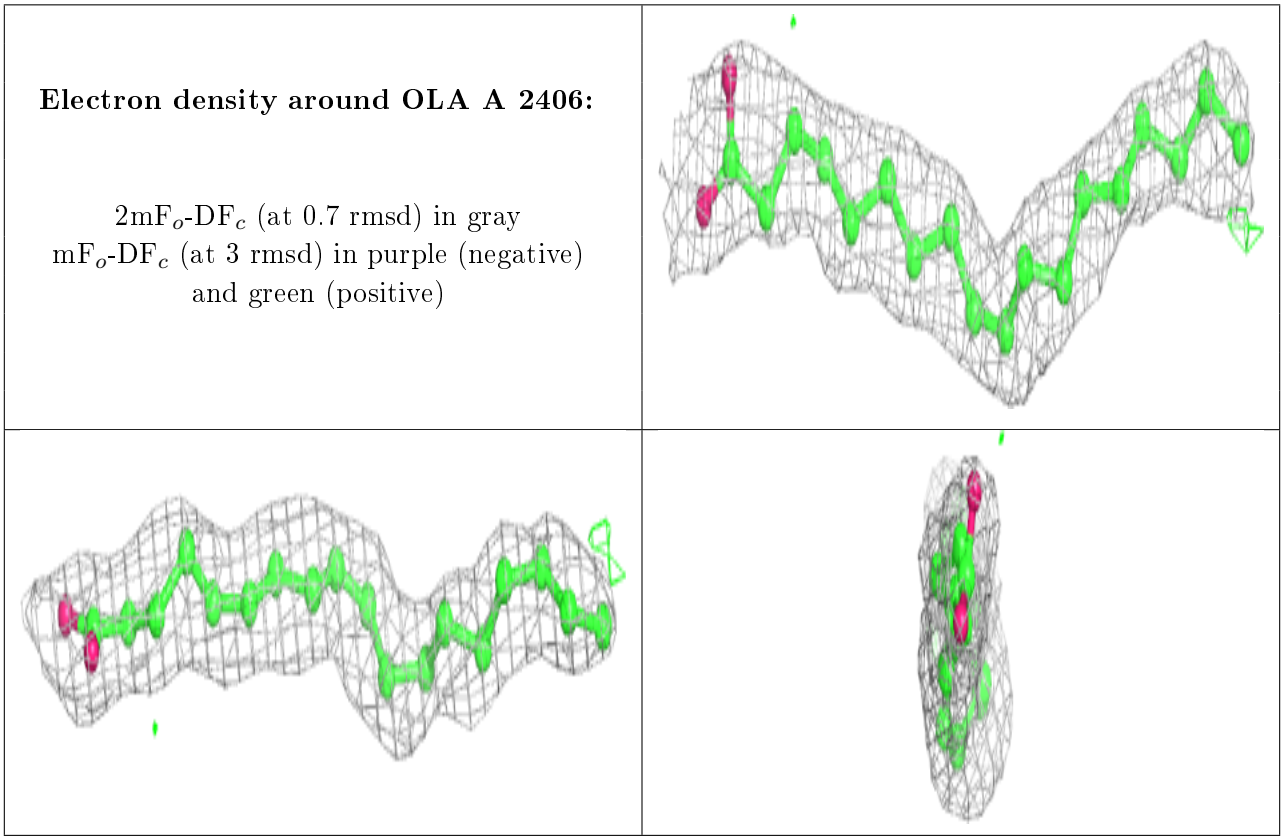
Electron density around OLA A 2418:

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



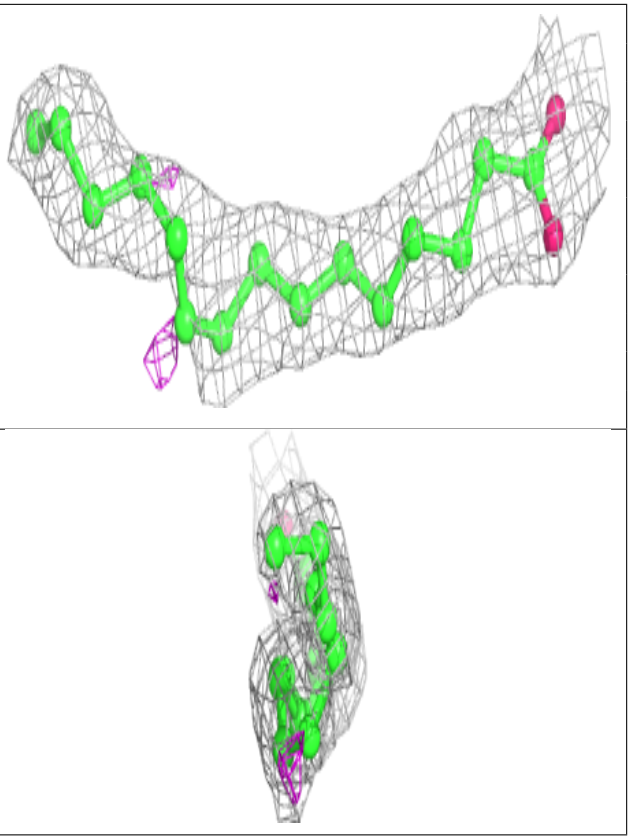
Electron density around OLA A 2406:

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



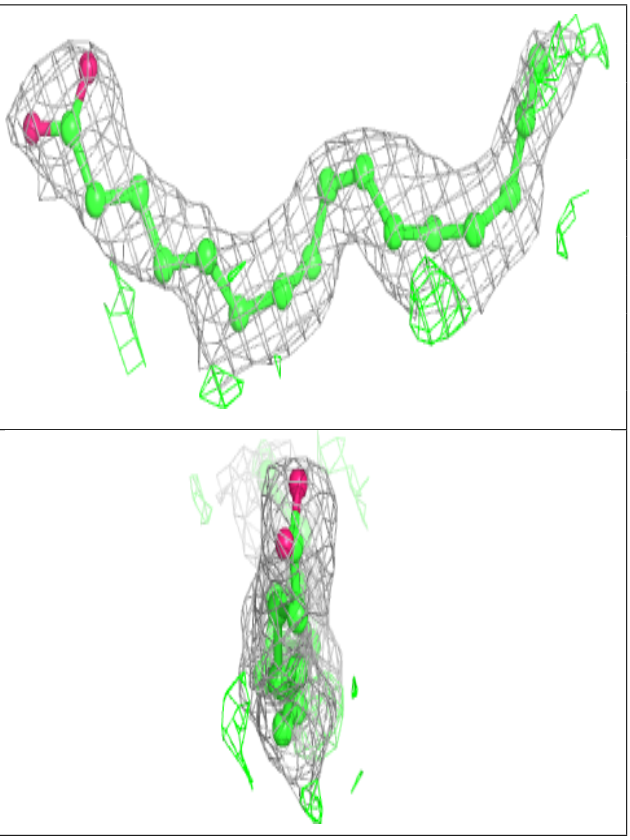
Electron density around OLA A 2420:

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



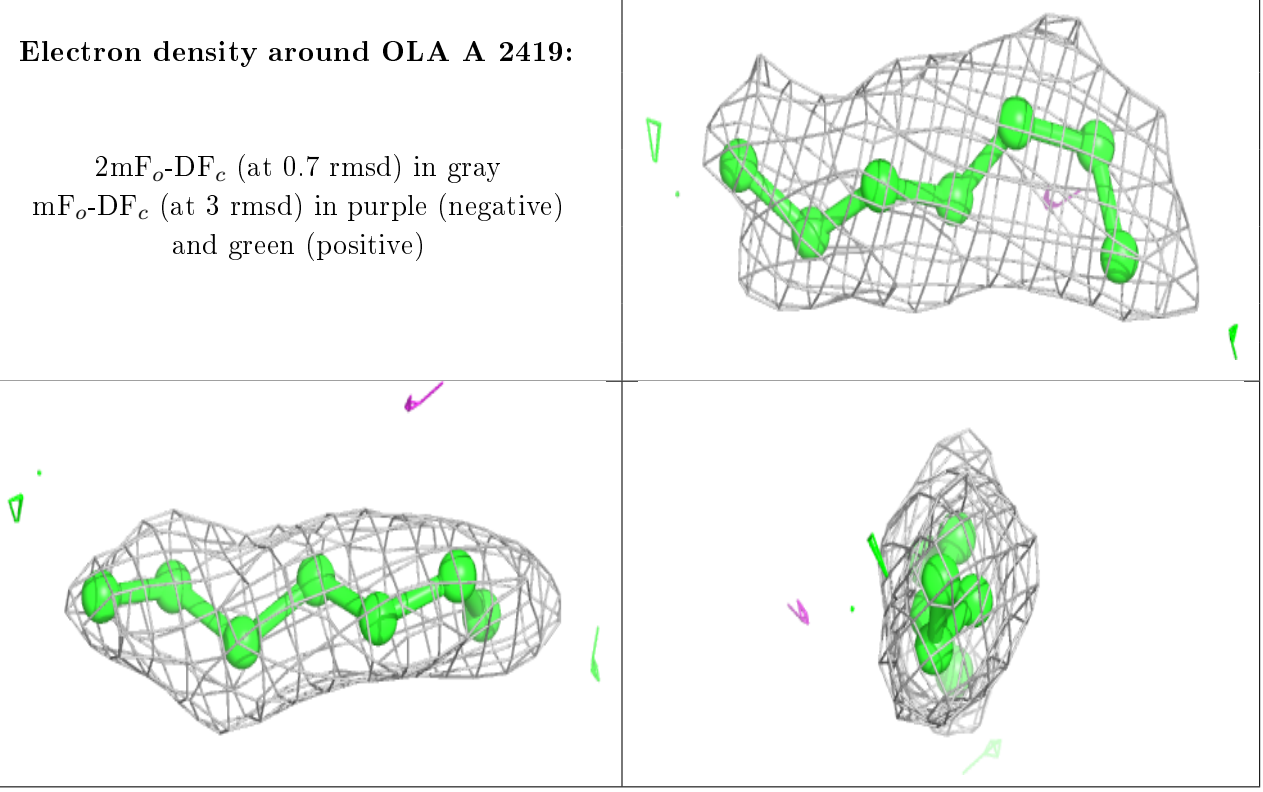
Electron density around OLA A 2410:

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



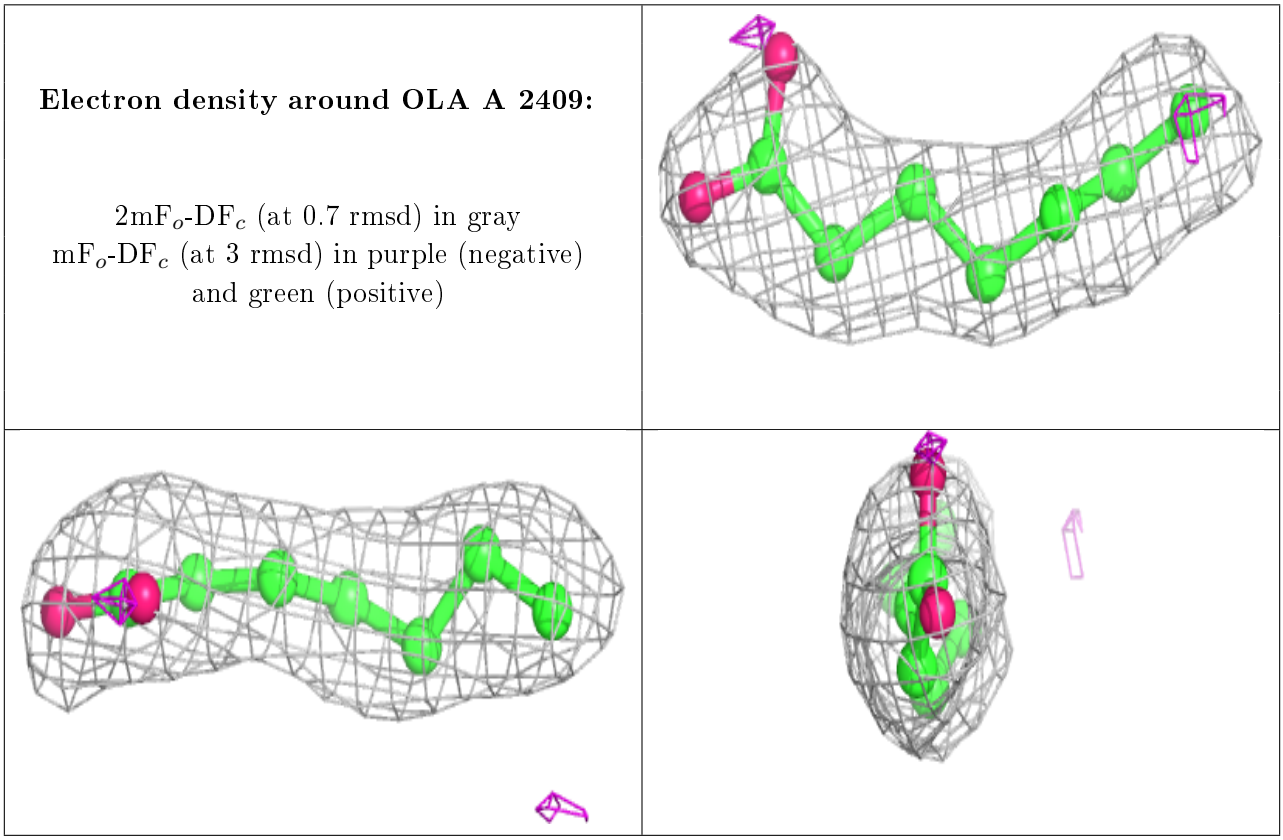
Electron density around OLA A 2419:

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



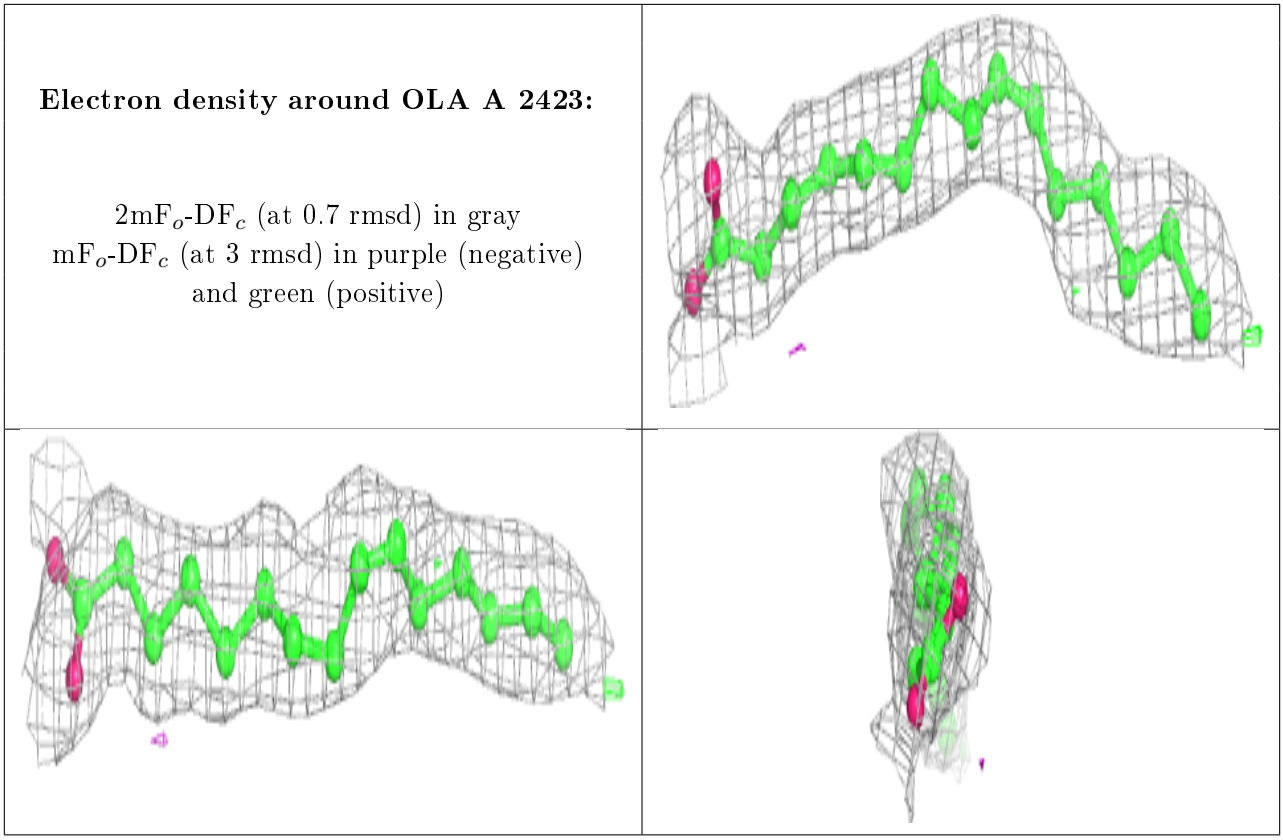
Electron density around OLA A 2409:

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



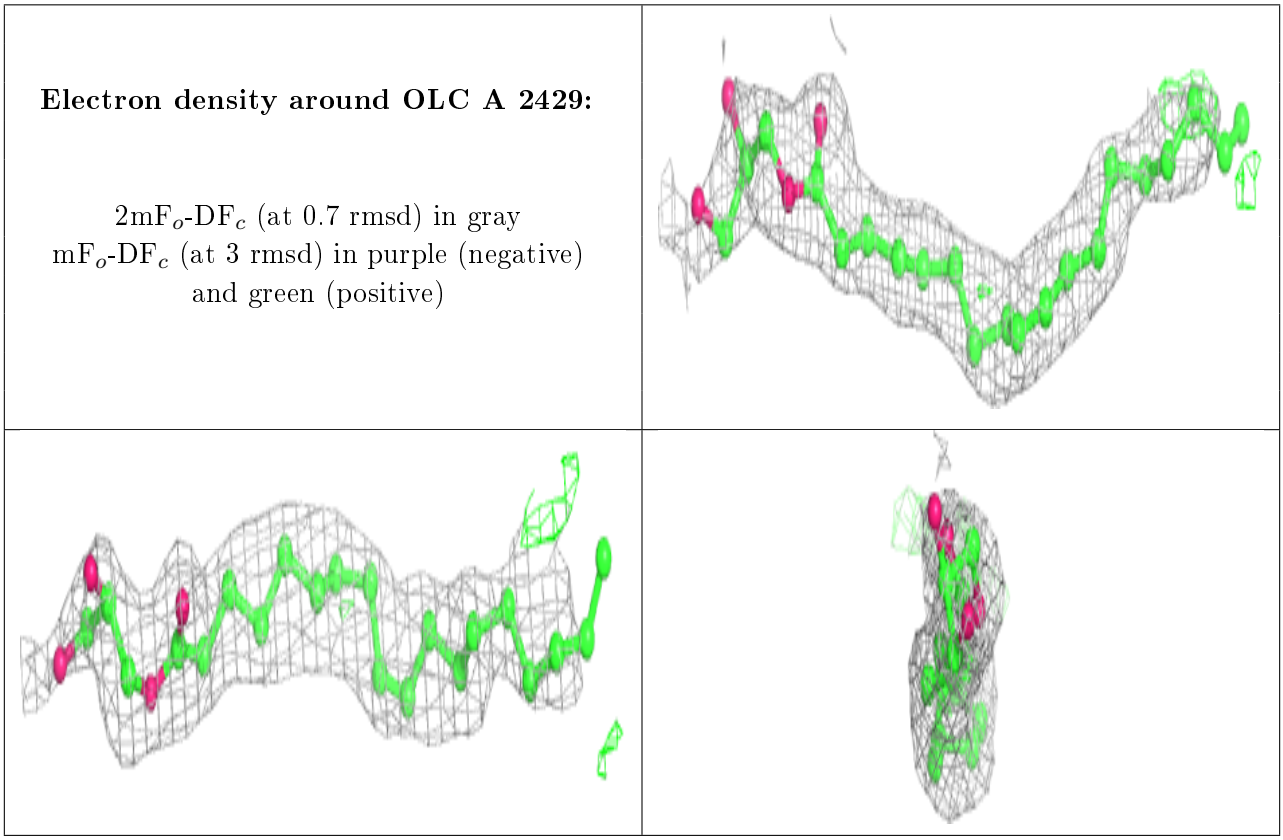
Electron density around OLA A 2423:

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



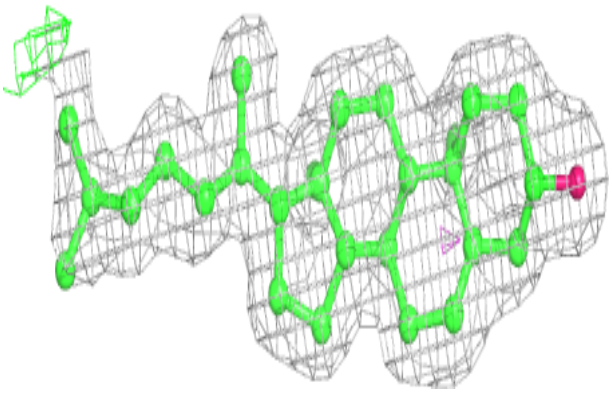
Electron density around OLC A 2429:

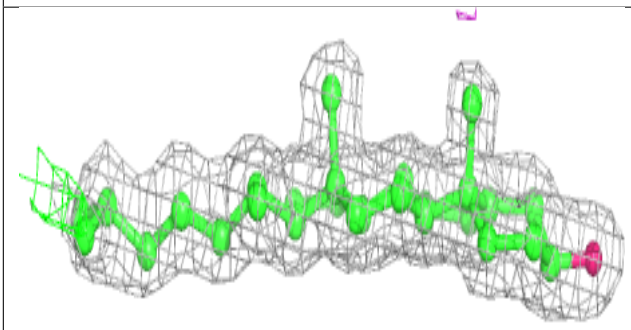
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

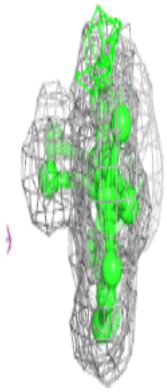


Electron density around CLR A 2403:

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

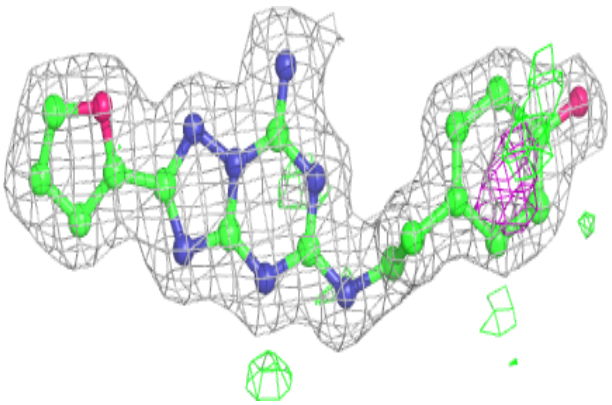


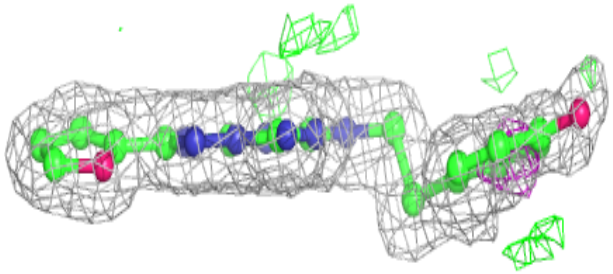


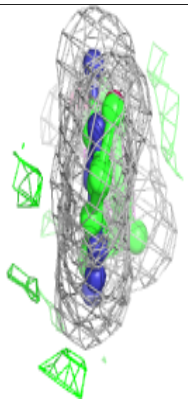


Electron density around ZMA A 2401:

$2mF_o$-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.