Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 03:01 PM BST

PDB ID	:	5IUA
Title	:	Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with compound 12b at 2.2A resolution
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Deposited on	:	2016-03-17
Resolution	:	2.20 Å(reported)

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

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

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

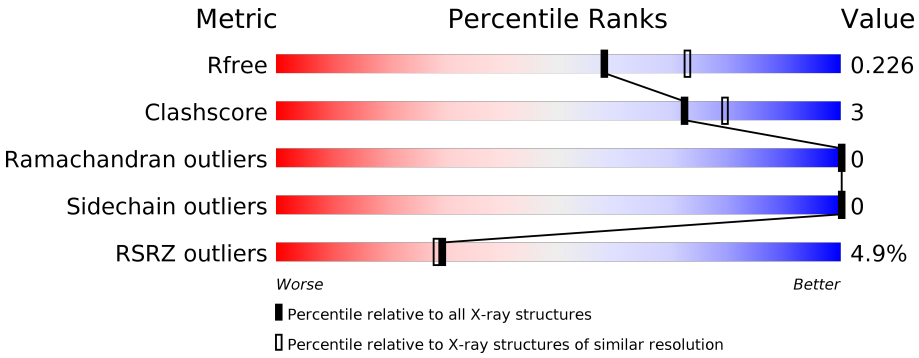
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	4% 85% 5% 10%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3810 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	3144	2053	527	541	23	0	21	0

There are 35 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	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	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	316	ALA	-	expression tag	UNP P29274
A	317	ALA	-	expression tag	UNP P29274
A	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274

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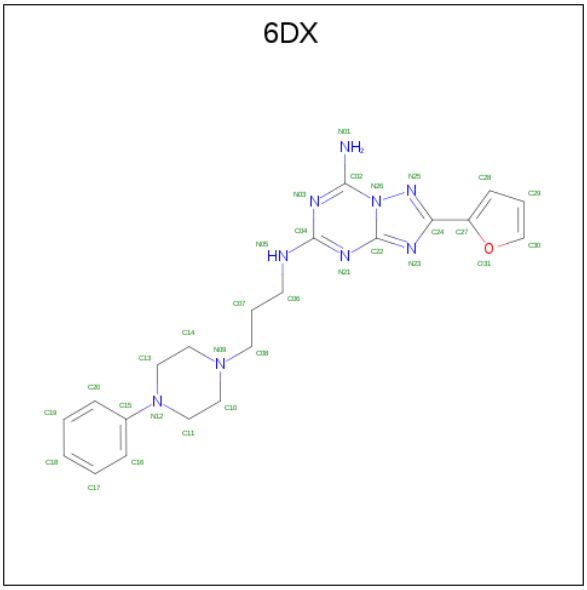
Chain	Residue	Modelled	Actual	Comment	Reference
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	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).

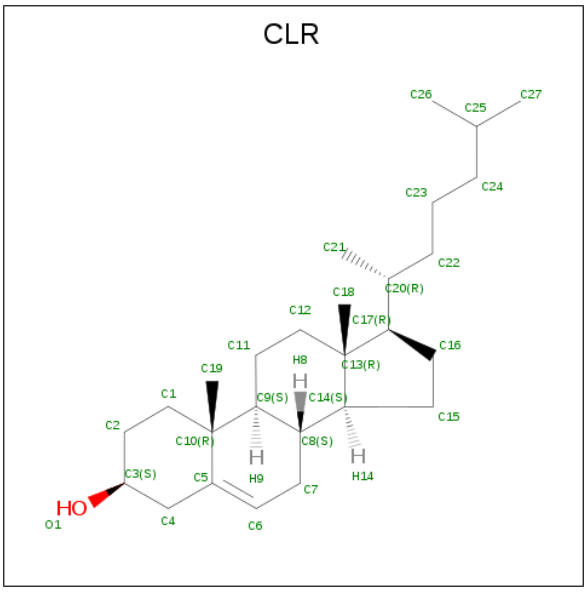
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is 2-(furan-2-yl)-N 5 -[3-(4-phenylpiperazin-1-yl)propyl][1,2,4]triazolo[1,5-a][1,3,5]triazine-5,7-diamine (three-letter code: 6DX) (formula: $C_{21}H_{25}N_9O$).



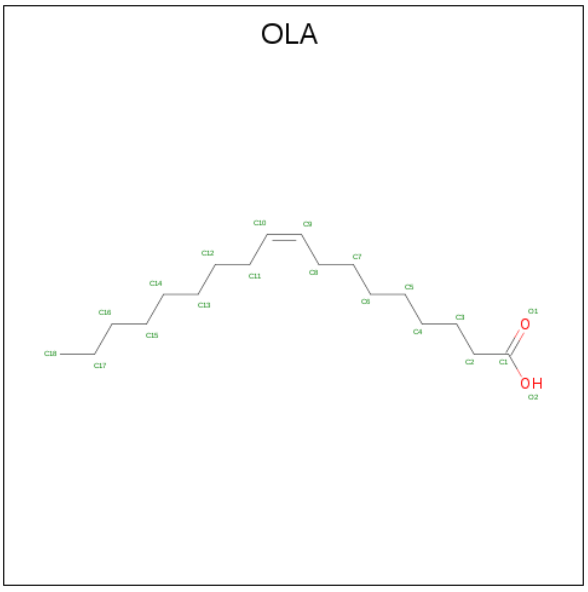
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 31 21 9 1	0	0

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



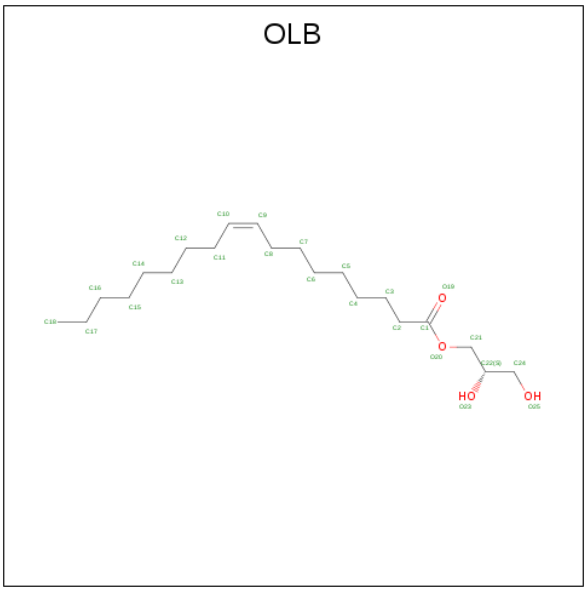
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0

- 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 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 O 19 17 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C 15 15	0	0
5	A	1	Total C O 14 12 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 8 8	0	0
5	A	1	Total C 12 12	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 16 12 4	0	0
6	A	1	Total C O 22 18 4	0	0
6	A	1	Total C O 19 15 4	0	0
6	A	1	Total C O 25 21 4	0	0
6	A	1	Total C O 20 16 4	0	0
6	A	1	Total C O 21 17 4	0	0

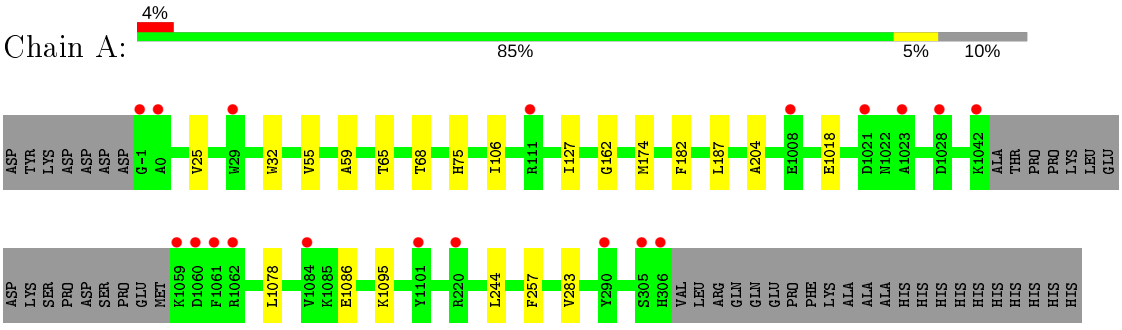
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	131	Total O 131 131	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: 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	39.56Å 179.98Å 139.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.82 – 2.20 33.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (33.82-2.20) 94.4 (33.82-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.200 , 0.233 0.193 , 0.226	Depositor DCC
R_{free} test set	1205 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3810	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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, NA, CLR, 6DX

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	0.24	0/3221	0.36	0/4379

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	3144	0	3238	17	0
2	A	1	0	0	0	0
3	A	31	0	0	0	0
4	A	112	0	184	3	0
5	A	232	0	330	12	0
6	A	159	0	220	6	0
7	A	131	0	0	3	0
All	All	3810	0	3972	26	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 3.

All (26) 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:2417:OLA:H72	6:A:2428:OLB:H19	1.80	0.62
1:A:25:VAL:HG22	5:A:2415:OLA:H132	1.85	0.57
1:A:32:TRP:CE3	5:A:2415:OLA:H71	2.40	0.56
1:A:162:GLY:O	7:A:2501:HOH:O	2.18	0.56
1:A:65:THR:HG21	6:A:2427:OLB:H4A	1.88	0.56
4:A:2402:CLR:H12	4:A:2403:CLR:H72	1.89	0.55
1:A:68:THR:HA	6:A:2425:OLB:H24A	1.89	0.55
5:A:2410:OLA:H81	5:A:2414:OLA:C12	2.38	0.54
1:A:68:THR:HG22	6:A:2425:OLB:H21	1.89	0.53
1:A:75:HIS:ND1	7:A:2504:HOH:O	2.33	0.53
1:A:174[B]:MET:SD	7:A:2576:HOH:O	2.60	0.51
5:A:2410:OLA:H111	5:A:2414:OLA:C12	2.41	0.50
1:A:244[B]:LEU:HG	5:A:2421:OLA:H61	1.96	0.47
1:A:1078:LEU:HD13	1:A:1086:GLU:HG2	1.97	0.46
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.99	0.45
1:A:127:ILE:HD13	5:A:2410:OLA:H62	1.99	0.44
1:A:1018:GLU:OE2	1:A:1095:LYS:NZ	2.45	0.44
4:A:2405:CLR:H232	4:A:2405:CLR:H211	1.86	0.43
1:A:182:PHE:CE1	1:A:187[B]:LEU:HG	2.54	0.43
4:A:2402:CLR:H271	5:A:2417:OLA:H142	2.00	0.42
5:A:2410:OLA:H152	5:A:2410:OLA:H122	1.53	0.42
1:A:106:ILE:HD11	1:A:204:ALA:HB2	2.02	0.42
1:A:174[A]:MET:HG3	1:A:257:PHE:HB2	2.03	0.41
5:A:2417:OLA:C8	6:A:2428:OLB:H221	2.51	0.40
5:A:2410:OLA:H152	6:A:2430:OLB:C14	2.51	0.40
1:A:283:VAL:HG12	5:A:2419:OLA:H71	2.04	0.40

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	405/433 (94%)	403 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	333/353 (94%)	333 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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	155	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	2410	-	16,19,19	0.44	0	15,19,19	0.23	0
4	CLR	A	2403	-	31,31,31	0.65	0	48,48,48	1.06	2 (4%)
5	OLA	A	2422	-	11,11,19	0.41	0	10,10,19	0.29	0
6	OLB	A	2425	-	15,15,24	0.99	2 (13%)	16,16,25	0.91	1 (6%)
5	OLA	A	2421	-	7,7,19	0.24	0	6,6,19	0.22	0
5	OLA	A	2411	-	11,14,19	0.37	0	10,14,19	0.29	0
5	OLA	A	2412	-	8,11,19	0.46	0	7,11,19	0.48	0
4	CLR	A	2405	-	31,31,31	0.71	0	48,48,48	0.94	0
4	CLR	A	2402	-	31,31,31	0.70	0	48,48,48	1.04	2 (4%)
5	OLA	A	2413	-	4,7,19	0.27	0	3,7,19	0.14	0
4	CLR	A	2404	-	31,31,31	0.68	0	48,48,48	1.00	1 (2%)
5	OLA	A	2409	-	14,17,19	0.40	0	13,17,19	0.23	0
5	OLA	A	2415	-	15,18,19	0.42	0	14,18,19	0.24	0
6	OLB	A	2423	-	16,16,24	0.98	2 (12%)	17,17,25	1.00	1 (5%)
5	OLA	A	2407	-	11,14,19	0.36	0	10,14,19	0.30	0
5	OLA	A	2419	-	11,14,19	0.38	0	10,14,19	0.34	0
5	OLA	A	2414	-	10,13,19	0.42	0	8,13,19	0.30	0
5	OLA	A	2406	-	16,19,19	0.42	0	15,19,19	0.27	0
6	OLB	A	2427	-	18,18,24	0.93	2 (11%)	18,19,25	0.90	1 (5%)
5	OLA	A	2416	-	7,10,19	0.24	0	6,10,19	0.34	0
5	OLA	A	2418	-	10,13,19	0.42	0	8,13,19	0.34	0
5	OLA	A	2408	-	5,8,19	0.25	0	4,8,19	0.18	0
6	OLB	A	2424	-	18,18,24	0.91	2 (11%)	18,19,25	0.92	1 (5%)
6	OLB	A	2428	-	24,24,24	0.80	2 (8%)	25,25,25	0.83	1 (4%)
6	OLB	A	2429	-	19,19,24	0.89	2 (10%)	20,20,25	0.87	1 (5%)
5	OLA	A	2417	-	14,14,19	0.42	0	13,13,19	0.28	0
3	6DX	A	2401	-	28,35,35	2.85	9 (32%)	31,48,48	2.17	6 (19%)
6	OLB	A	2430	-	20,20,24	0.88	2 (10%)	21,21,25	0.83	1 (4%)
6	OLB	A	2426	-	21,21,24	0.84	2 (9%)	22,22,25	0.93	1 (4%)
5	OLA	A	2420	-	6,6,19	0.26	0	5,5,19	0.15	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	2410	-	-	8/15/17/17	-
4	CLR	A	2403	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2422	-	-	6/9/9/17	-
6	OLB	A	2425	-	-	8/15/15/24	-
5	OLA	A	2421	-	-	2/5/5/17	-
5	OLA	A	2411	-	-	7/10/12/17	-
5	OLA	A	2412	-	-	4/7/9/17	-
4	CLR	A	2405	-	-	1/10/68/68	0/4/4/4
4	CLR	A	2402	-	-	8/10/68/68	0/4/4/4
5	OLA	A	2413	-	-	1/3/5/17	-
4	CLR	A	2404	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2409	-	-	8/13/15/17	-
5	OLA	A	2415	-	-	5/14/16/17	-
6	OLB	A	2423	-	-	8/16/16/24	-
5	OLA	A	2407	-	-	5/10/12/17	-
5	OLA	A	2419	-	-	4/10/12/17	-
5	OLA	A	2414	-	-	4/9/11/17	-
5	OLA	A	2406	-	-	9/15/17/17	-
6	OLB	A	2427	-	-	6/18/18/24	-
5	OLA	A	2416	-	-	4/6/8/17	-
5	OLA	A	2418	-	-	5/9/11/17	-
5	OLA	A	2408	-	-	2/4/6/17	-
6	OLB	A	2424	-	-	4/18/18/24	-
6	OLB	A	2428	-	-	11/24/24/24	-
6	OLB	A	2429	-	-	8/19/19/24	-
5	OLA	A	2417	-	-	5/12/12/17	-
3	6DX	A	2401	-	-	2/11/25/25	0/5/5/5
6	OLB	A	2430	-	-	10/20/20/24	-
6	OLB	A	2426	-	-	13/21/21/24	-
5	OLA	A	2420	-	-	3/4/4/17	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2401	6DX	C08-N09	-8.57	1.27	1.47
3	A	2401	6DX	C11-N12	-5.68	1.37	1.46
3	A	2401	6DX	C13-N12	-5.66	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2401	6DX	C04-N05	5.43	1.42	1.34
3	A	2401	6DX	C02-N01	4.50	1.43	1.34
3	A	2401	6DX	C15-N12	3.17	1.47	1.38
3	A	2401	6DX	C14-N09	-2.72	1.39	1.46
3	A	2401	6DX	C10-N09	-2.63	1.39	1.46
6	A	2427	OLB	O20-C1	2.45	1.40	1.33
6	A	2430	OLB	O20-C1	2.42	1.40	1.33
6	A	2428	OLB	O20-C1	2.42	1.40	1.33
6	A	2429	OLB	O20-C1	2.42	1.40	1.33
6	A	2425	OLB	O20-C1	2.40	1.40	1.33
6	A	2426	OLB	O20-C1	2.40	1.40	1.33
6	A	2423	OLB	O20-C1	2.38	1.40	1.33
6	A	2424	OLB	O20-C1	2.32	1.40	1.33
3	A	2401	6DX	C22-N23	2.19	1.38	1.35
6	A	2428	OLB	O20-C21	-2.15	1.40	1.45
6	A	2423	OLB	O20-C21	-2.13	1.40	1.45
6	A	2429	OLB	O20-C21	-2.12	1.40	1.45
6	A	2425	OLB	O20-C21	-2.09	1.40	1.45
6	A	2424	OLB	O20-C21	-2.09	1.40	1.45
6	A	2426	OLB	O20-C21	-2.07	1.40	1.45
6	A	2427	OLB	O20-C21	-2.07	1.40	1.45
6	A	2430	OLB	O20-C21	-2.05	1.40	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2401	6DX	N25-C24-N23	-9.21	108.46	114.56
3	A	2401	6DX	N21-C04-N03	-3.79	120.23	126.23
6	A	2423	OLB	O20-C1-C2	2.89	120.97	111.91
6	A	2426	OLB	O20-C1-C2	2.87	120.90	111.91
6	A	2427	OLB	O20-C1-C2	2.78	120.65	111.91
3	A	2401	6DX	N01-C02-N03	2.73	120.62	117.03
6	A	2424	OLB	O20-C1-C2	2.72	120.44	111.91
6	A	2425	OLB	O20-C1-C2	2.71	120.40	111.91
6	A	2429	OLB	O20-C1-C2	2.66	120.26	111.91
6	A	2430	OLB	O20-C1-C2	2.65	120.24	111.91
4	A	2403	CLR	C18-C13-C17	-2.65	106.78	111.71
6	A	2428	OLB	O20-C1-C2	2.64	120.19	111.91
3	A	2401	6DX	N01-C02-N26	2.61	119.73	117.97
3	A	2401	6DX	C06-N05-C04	-2.37	119.65	123.75
3	A	2401	6DX	C14-N09-C10	2.37	114.17	108.83
4	A	2403	CLR	C12-C13-C17	2.36	120.11	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2402	CLR	C1-C10-C9	2.30	111.95	108.73
4	A	2402	CLR	C12-C13-C17	2.22	119.90	116.57
4	A	2404	CLR	C12-C13-C17	2.03	119.61	116.57

There are no chirality outliers.

All (161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2429	OLB	C10-C11-C12-C13
6	A	2425	OLB	C21-C22-C24-O25
5	A	2412	OLA	C1-C2-C3-C4
5	A	2407	OLA	C1-C2-C3-C4
5	A	2419	OLA	C10-C11-C12-C13
5	A	2406	OLA	C1-C2-C3-C4
5	A	2418	OLA	C1-C2-C3-C4
5	A	2418	OLA	C9-C10-C11-C12
6	A	2428	OLB	O20-C21-C22-O23
6	A	2428	OLB	O20-C21-C22-C24
6	A	2426	OLB	C21-C22-C24-O25
6	A	2425	OLB	O19-C1-O20-C21
6	A	2428	OLB	O19-C1-O20-C21
6	A	2425	OLB	C2-C1-O20-C21
6	A	2428	OLB	C2-C1-O20-C21
5	A	2413	OLA	C2-C3-C4-C5
5	A	2419	OLA	C5-C6-C7-C8
5	A	2410	OLA	C12-C13-C14-C15
6	A	2429	OLB	C2-C1-O20-C21
6	A	2430	OLB	C2-C1-O20-C21
6	A	2430	OLB	O20-C21-C22-C24
5	A	2415	OLA	C3-C4-C5-C6
6	A	2430	OLB	O20-C21-C22-O23
6	A	2425	OLB	C1-C2-C3-C4
6	A	2430	OLB	C1-C2-C3-C4
6	A	2430	OLB	O19-C1-O20-C21
4	A	2405	CLR	C22-C23-C24-C25
6	A	2425	OLB	O23-C22-C24-O25
6	A	2427	OLB	C1-C2-C3-C4
6	A	2424	OLB	C1-C2-C3-C4
6	A	2426	OLB	C1-C2-C3-C4
6	A	2429	OLB	O19-C1-O20-C21
4	A	2402	CLR	C13-C17-C20-C22
6	A	2423	OLB	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
5	A	2417	OLA	C11-C12-C13-C14
6	A	2423	OLB	O20-C21-C22-C24
5	A	2412	OLA	C4-C5-C6-C7
6	A	2424	OLB	C3-C4-C5-C6
5	A	2410	OLA	C2-C3-C4-C5
5	A	2410	OLA	C11-C12-C13-C14
4	A	2402	CLR	C13-C17-C20-C21
5	A	2409	OLA	C2-C3-C4-C5
5	A	2409	OLA	C12-C13-C14-C15
6	A	2426	OLB	O20-C21-C22-O23
5	A	2406	OLA	C3-C4-C5-C6
5	A	2406	OLA	C4-C5-C6-C7
5	A	2410	OLA	C6-C7-C8-C9
5	A	2411	OLA	C6-C7-C8-C9
6	A	2428	OLB	C1-C2-C3-C4
6	A	2429	OLB	C4-C5-C6-C7
5	A	2406	OLA	C14-C15-C16-C17
5	A	2410	OLA	C14-C15-C16-C17
6	A	2425	OLB	C5-C6-C7-C8
6	A	2429	OLB	C2-C3-C4-C5
5	A	2416	OLA	C2-C3-C4-C5
6	A	2427	OLB	C2-C3-C4-C5
5	A	2407	OLA	C2-C3-C4-C5
5	A	2414	OLA	C2-C3-C4-C5
5	A	2412	OLA	C3-C4-C5-C6
6	A	2426	OLB	O23-C22-C24-O25
5	A	2415	OLA	C11-C12-C13-C14
5	A	2422	OLA	C10-C11-C12-C13
5	A	2409	OLA	C6-C7-C8-C9
5	A	2406	OLA	C10-C11-C12-C13
6	A	2426	OLB	C6-C7-C8-C9
3	A	2401	6DX	C16-C15-N12-C11
6	A	2428	OLB	C14-C15-C16-C17
5	A	2421	OLA	C2-C3-C4-C5
5	A	2417	OLA	C13-C14-C15-C16
6	A	2424	OLB	C9-C10-C11-C12
5	A	2414	OLA	C5-C6-C7-C8
5	A	2409	OLA	C10-C11-C12-C13
5	A	2418	OLA	C6-C7-C8-C9
6	A	2430	OLB	C10-C11-C12-C13
6	A	2423	OLB	C2-C1-O20-C21
6	A	2426	OLB	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
4	A	2402	CLR	C16-C17-C20-C21
6	A	2425	OLB	C3-C4-C5-C6
5	A	2408	OLA	C3-C4-C5-C6
5	A	2421	OLA	C4-C5-C6-C7
5	A	2407	OLA	C6-C7-C8-C9
3	A	2401	6DX	C20-C15-N12-C11
5	A	2409	OLA	C3-C4-C5-C6
6	A	2427	OLB	C6-C7-C8-C9
4	A	2402	CLR	C21-C20-C22-C23
6	A	2428	OLB	C4-C5-C6-C7
6	A	2423	OLB	O19-C1-O20-C21
6	A	2426	OLB	O19-C1-O20-C21
4	A	2402	CLR	C16-C17-C20-C22
5	A	2414	OLA	C4-C5-C6-C7
5	A	2422	OLA	C4-C5-C6-C7
6	A	2430	OLB	C2-C3-C4-C5
5	A	2417	OLA	C5-C6-C7-C8
5	A	2409	OLA	C5-C6-C7-C8
5	A	2420	OLA	C2-C3-C4-C5
5	A	2422	OLA	C5-C6-C7-C8
5	A	2417	OLA	C4-C5-C6-C7
6	A	2426	OLB	C3-C4-C5-C6
5	A	2416	OLA	C6-C7-C8-C9
5	A	2407	OLA	C5-C6-C7-C8
5	A	2417	OLA	C15-C16-C17-C18
5	A	2415	OLA	C5-C6-C7-C8
6	A	2428	OLB	O23-C22-C24-O25
5	A	2422	OLA	C12-C13-C14-C15
6	A	2426	OLB	C11-C12-C13-C14
5	A	2406	OLA	C13-C14-C15-C16
4	A	2402	CLR	C23-C24-C25-C27
5	A	2406	OLA	C12-C13-C14-C15
4	A	2402	CLR	C20-C22-C23-C24
4	A	2402	CLR	C23-C24-C25-C26
5	A	2411	OLA	C3-C4-C5-C6
6	A	2426	OLB	C12-C13-C14-C15
6	A	2427	OLB	C3-C4-C5-C6
6	A	2429	OLB	O23-C22-C24-O25
5	A	2416	OLA	C1-C2-C3-C4
6	A	2423	OLB	C7-C8-C9-C10
5	A	2409	OLA	C11-C12-C13-C14
6	A	2428	OLB	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	A	2419	OLA	C6-C7-C8-C9
6	A	2426	OLB	C7-C8-C9-C10
6	A	2430	OLB	C5-C6-C7-C8
5	A	2408	OLA	C4-C5-C6-C7
5	A	2411	OLA	C2-C3-C4-C5
6	A	2423	OLB	C5-C6-C7-C8
5	A	2422	OLA	C9-C10-C11-C12
5	A	2411	OLA	C10-C11-C12-C13
6	A	2430	OLB	C3-C4-C5-C6
6	A	2426	OLB	C9-C10-C11-C12
5	A	2412	OLA	C7-C8-C9-C10
5	A	2410	OLA	C13-C14-C15-C16
5	A	2422	OLA	C11-C12-C13-C14
6	A	2425	OLB	O20-C21-C22-O23
6	A	2427	OLB	O23-C22-C24-O25
6	A	2427	OLB	C4-C5-C6-C7
6	A	2426	OLB	C2-C3-C4-C5
5	A	2420	OLA	C1-C2-C3-C4
5	A	2409	OLA	C13-C14-C15-C16
6	A	2428	OLB	C21-C22-C24-O25
5	A	2406	OLA	C7-C8-C9-C10
5	A	2416	OLA	C4-C5-C6-C7
6	A	2429	OLB	C9-C10-C11-C12
6	A	2430	OLB	C9-C10-C11-C12
5	A	2414	OLA	C6-C7-C8-C9
5	A	2410	OLA	C7-C8-C9-C10
5	A	2410	OLA	C9-C10-C11-C12
5	A	2418	OLA	C7-C8-C9-C10
6	A	2428	OLB	C7-C8-C9-C10
5	A	2411	OLA	C4-C5-C6-C7
6	A	2423	OLB	C3-C4-C5-C6
5	A	2411	OLA	C9-C10-C11-C12
5	A	2411	OLA	C7-C8-C9-C10
6	A	2423	OLB	C2-C3-C4-C5
5	A	2419	OLA	C3-C4-C5-C6
5	A	2418	OLA	C5-C6-C7-C8
5	A	2420	OLA	C3-C4-C5-C6
5	A	2406	OLA	C2-C3-C4-C5
6	A	2429	OLB	C21-C22-C24-O25
6	A	2424	OLB	C21-C22-C24-O25
5	A	2407	OLA	C9-C10-C11-C12
5	A	2415	OLA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
5	A	2415	OLA	C14-C15-C16-C17

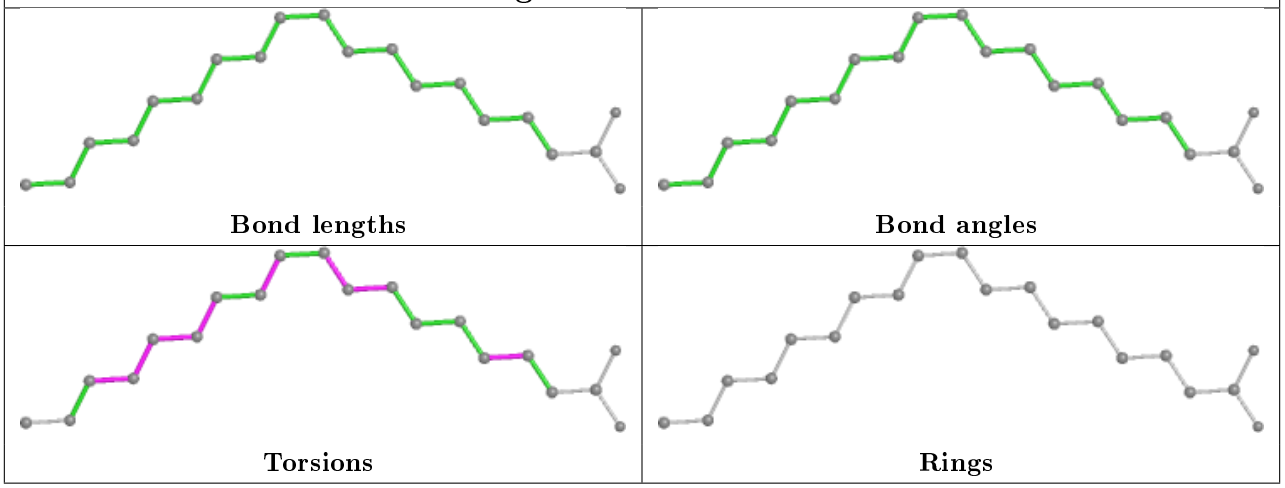
There are no ring outliers.

13 monomers are involved in 17 short contacts:

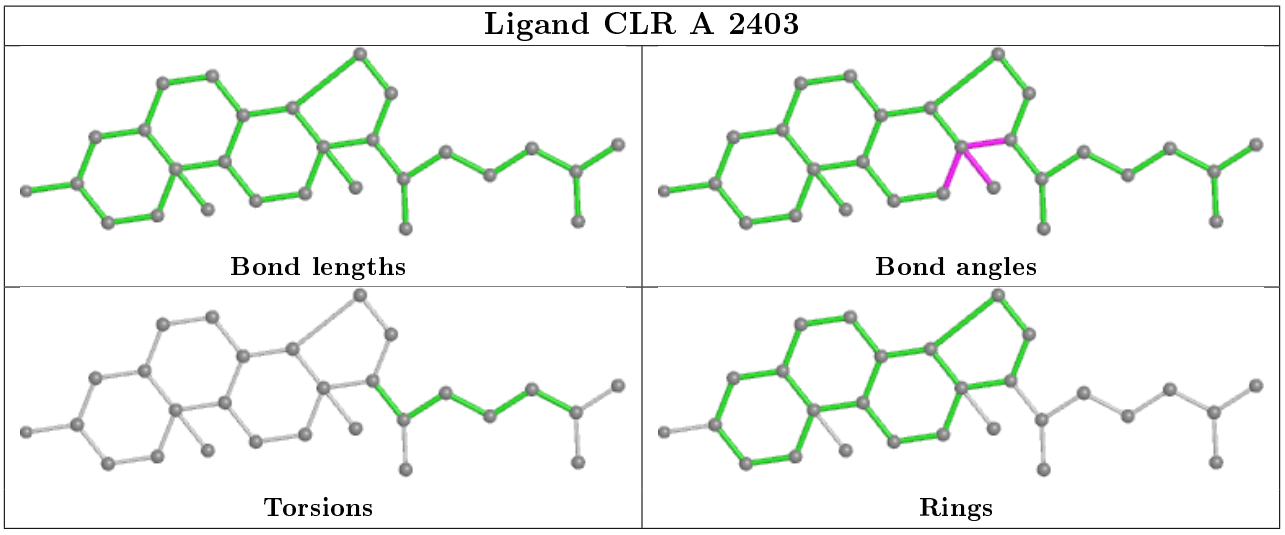
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2410	OLA	5	0
4	A	2403	CLR	1	0
6	A	2425	OLB	2	0
5	A	2421	OLA	1	0
4	A	2405	CLR	1	0
4	A	2402	CLR	2	0
5	A	2415	OLA	2	0
5	A	2419	OLA	1	0
5	A	2414	OLA	2	0
6	A	2427	OLB	1	0
6	A	2428	OLB	2	0
5	A	2417	OLA	3	0
6	A	2430	OLB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 2410



Ligand CLR A 2403



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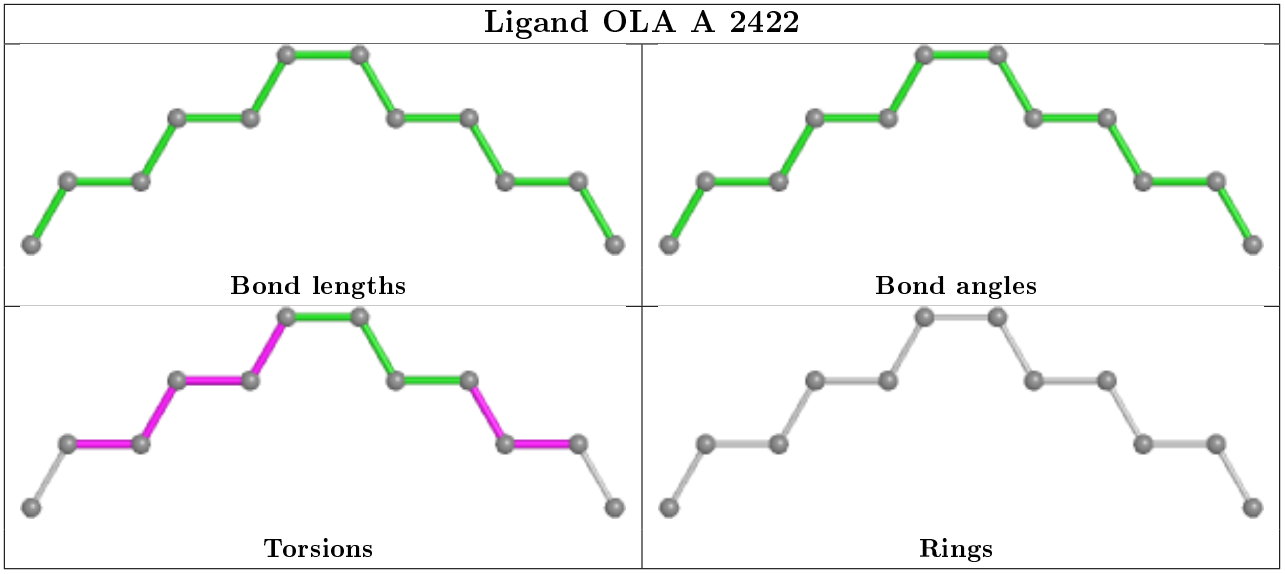
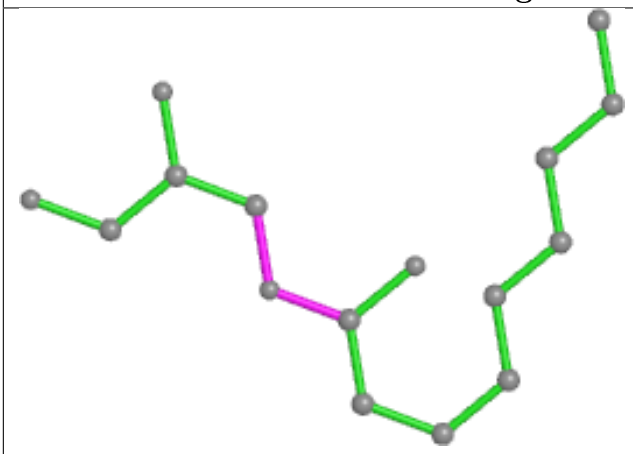
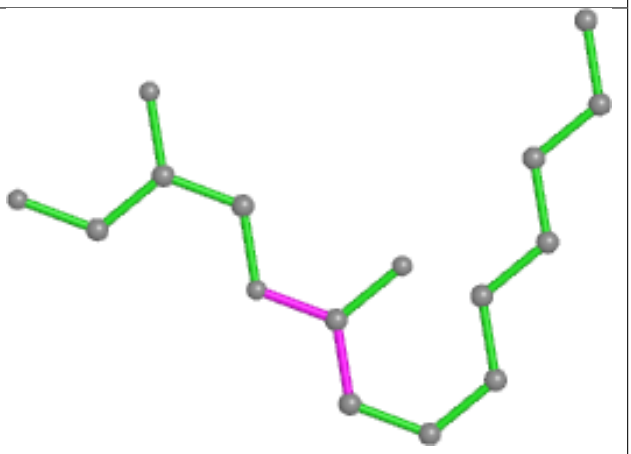


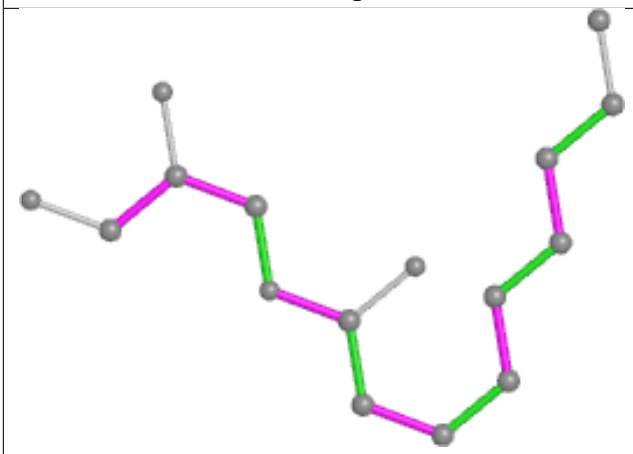
Ligand OLB A 2425



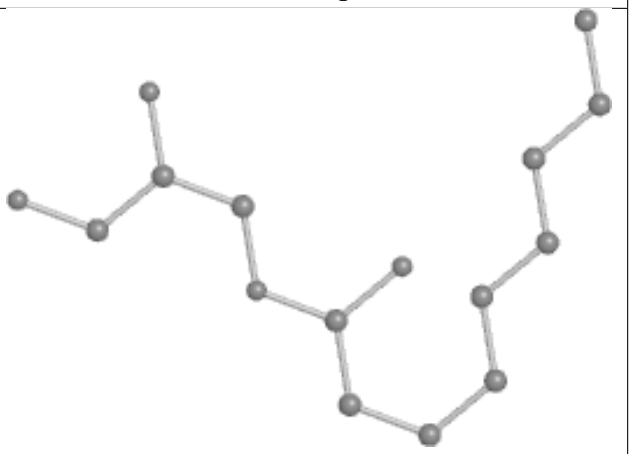
Bond lengths



Bond angles

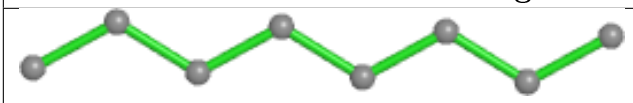


Torsions



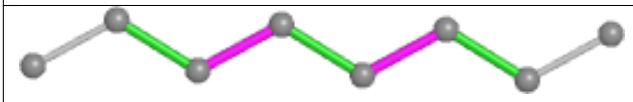
Rings

Ligand OLA A 2421

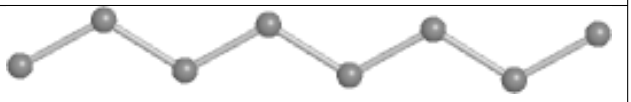


Bond lengths

Bond angles

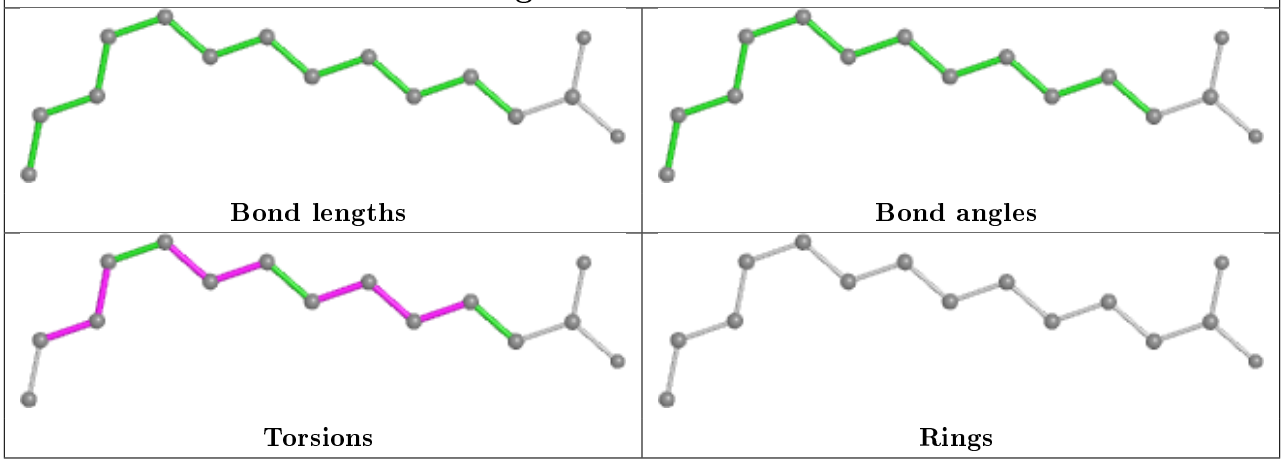


Torsions

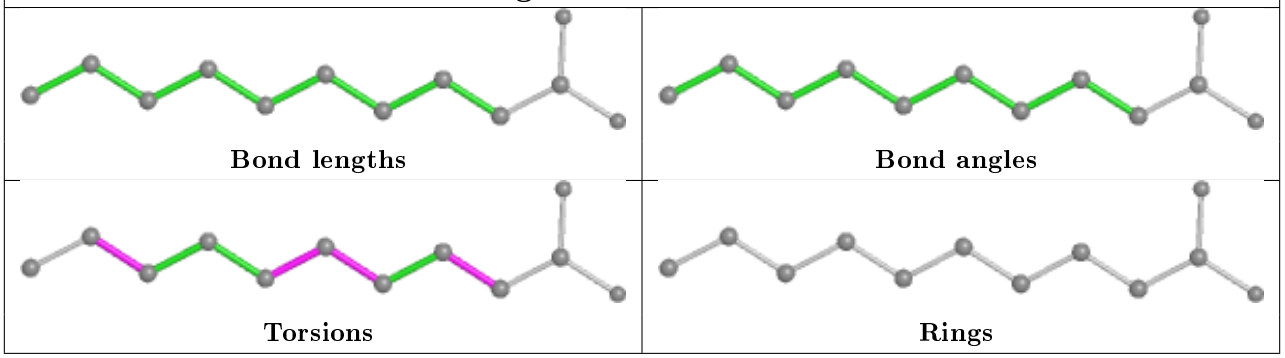


Rings

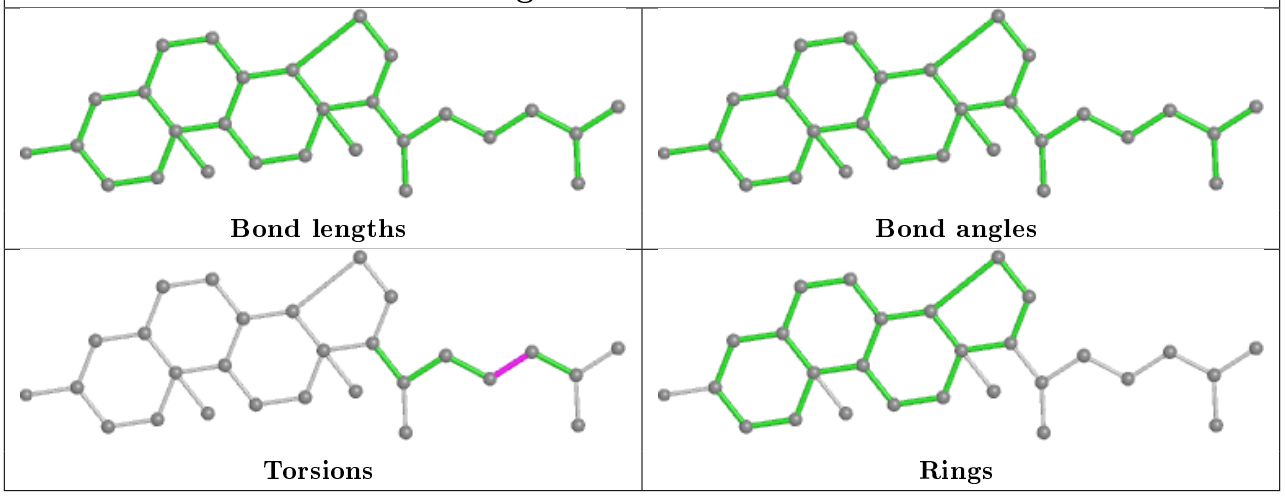
Ligand OLA A 2411



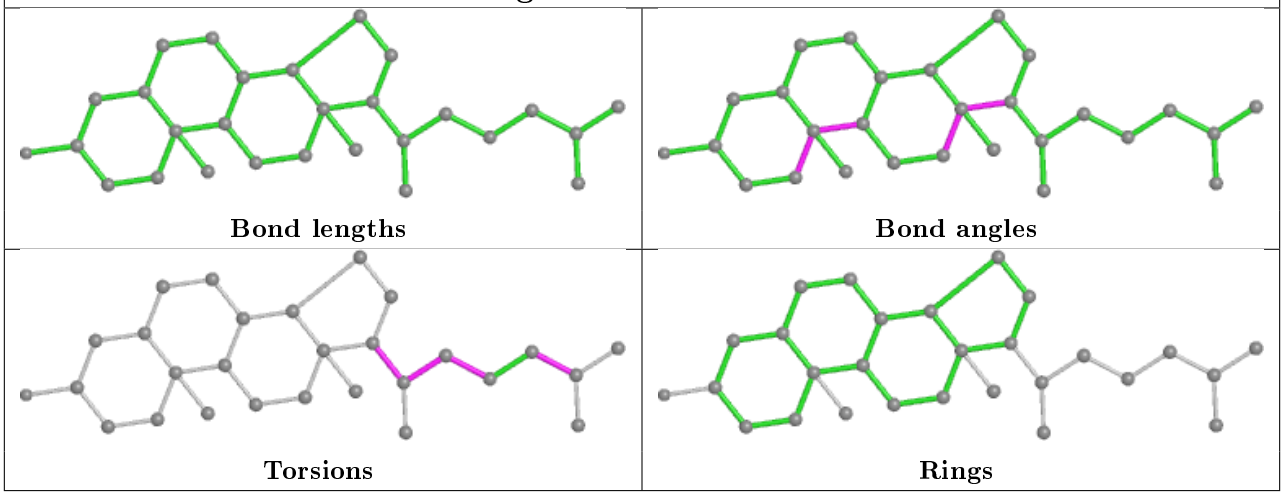
Ligand OLA A 2412



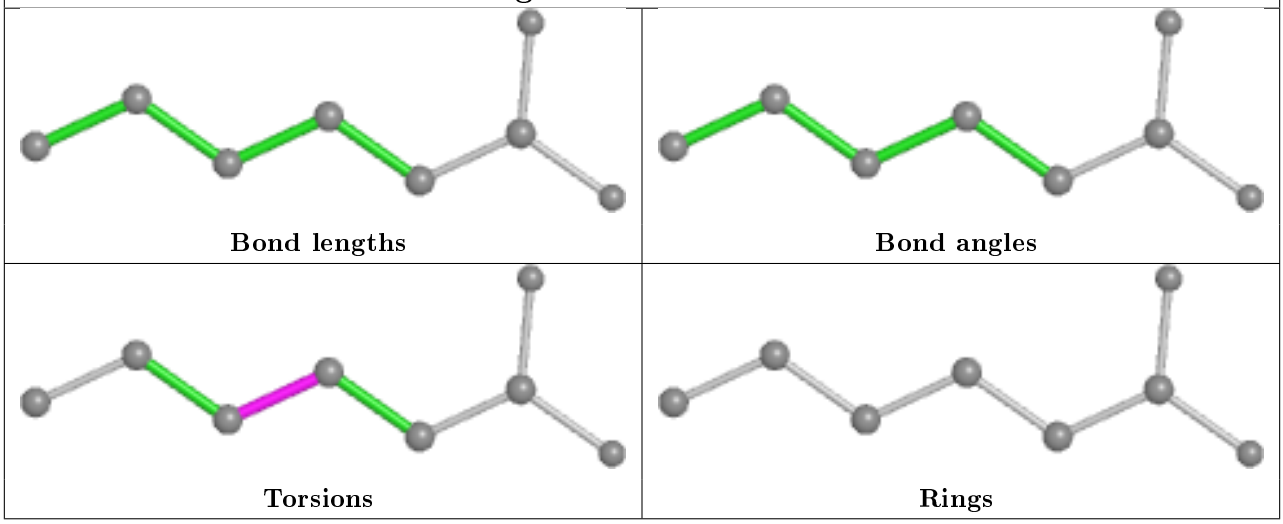
Ligand CLR A 2405



Ligand CLR A 2402



Ligand OLA A 2413



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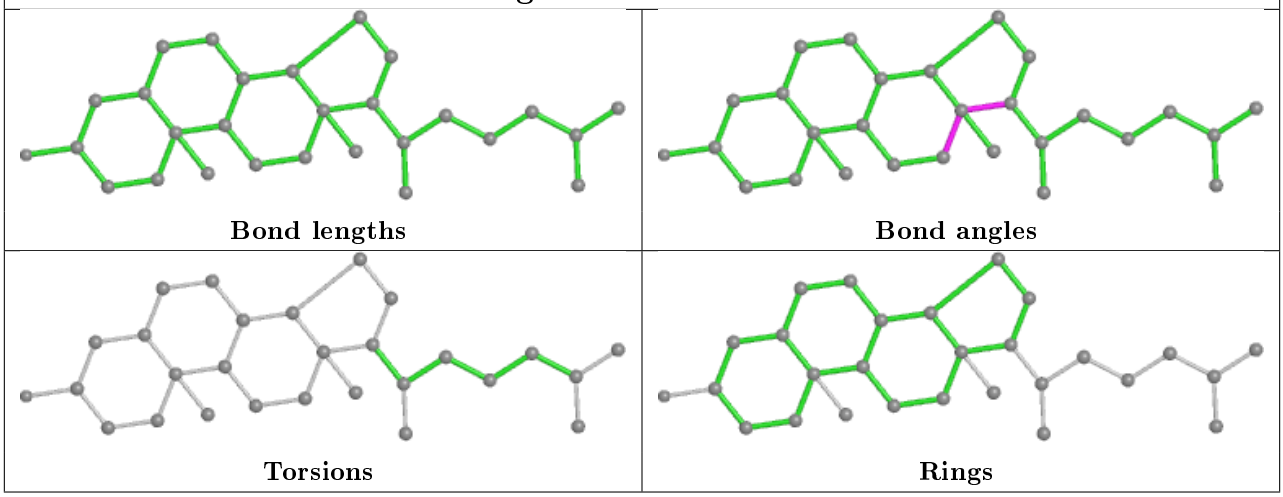
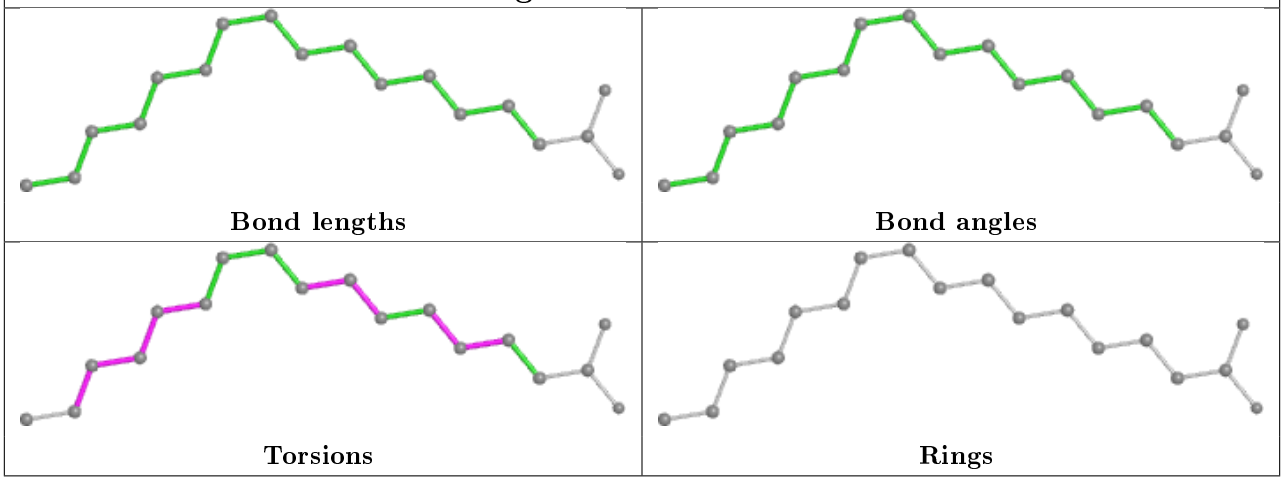


Ligand OLA A 2409



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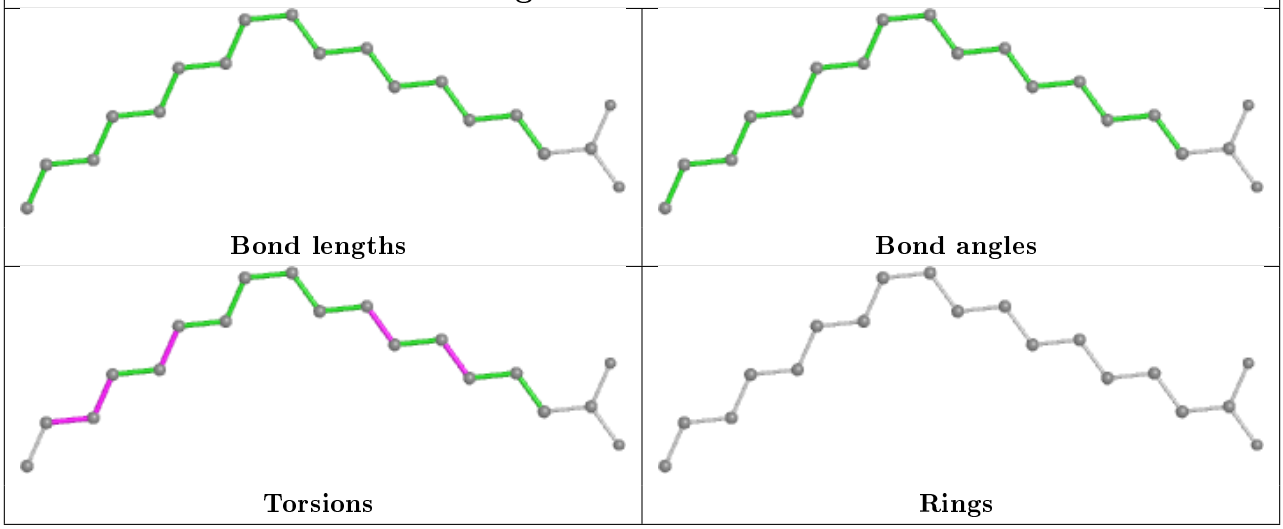

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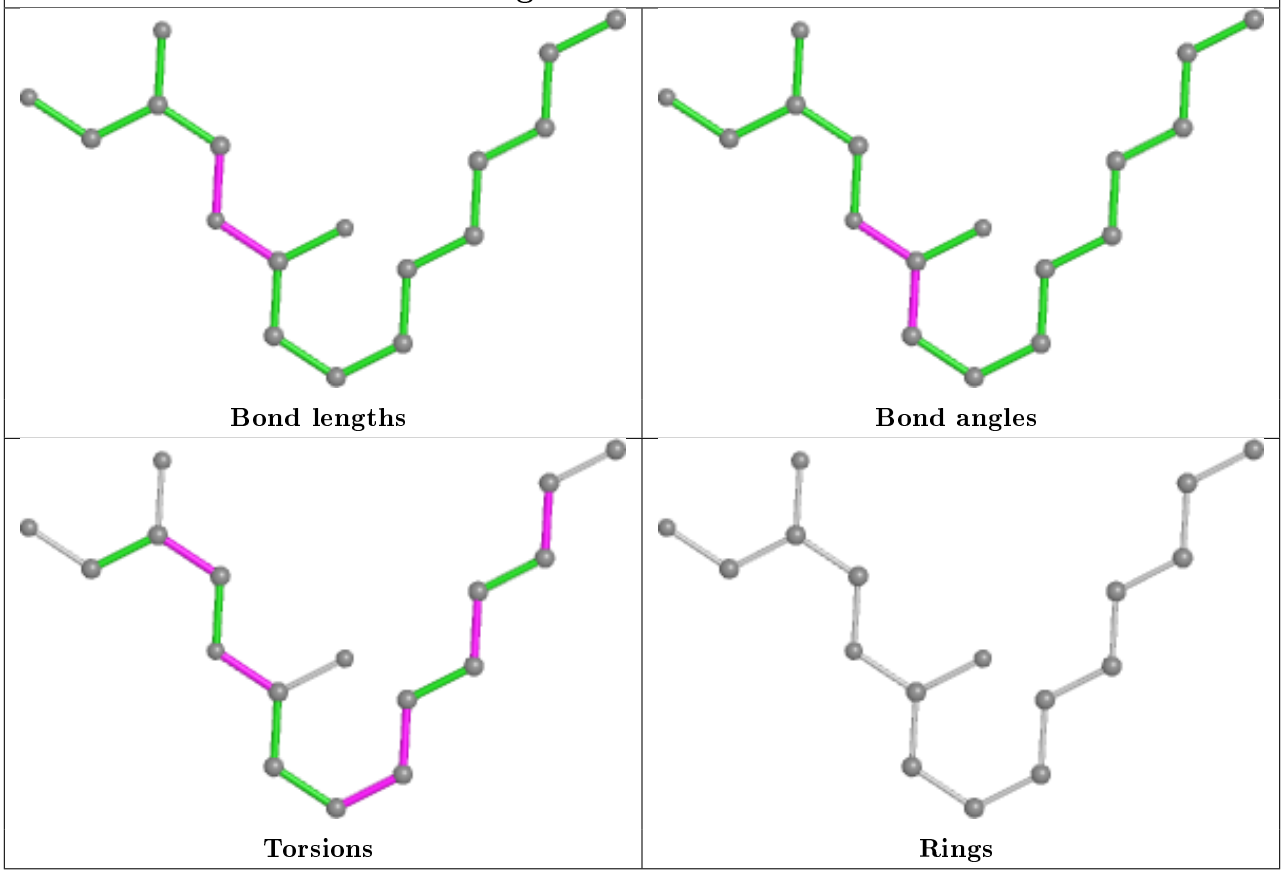

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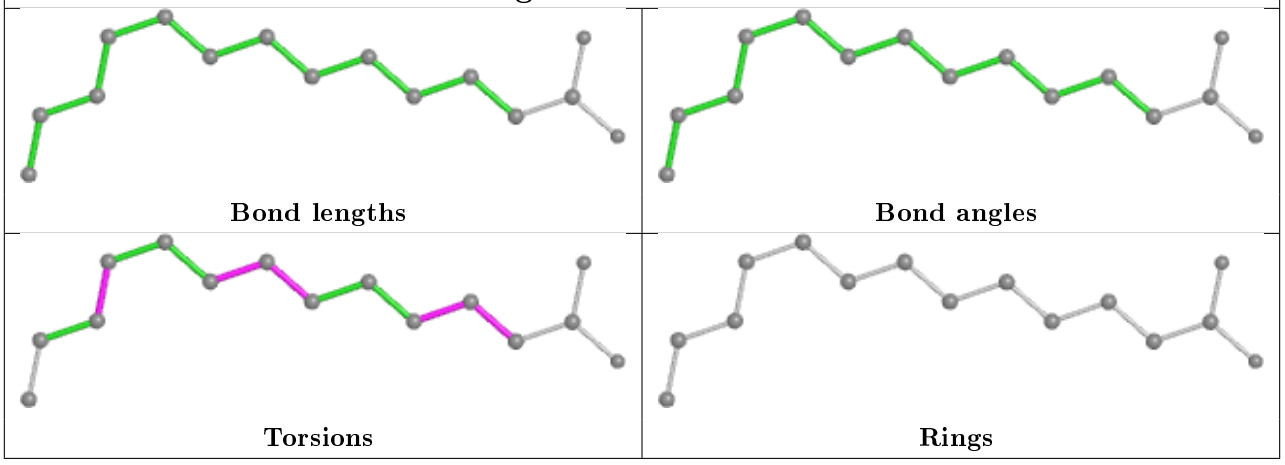
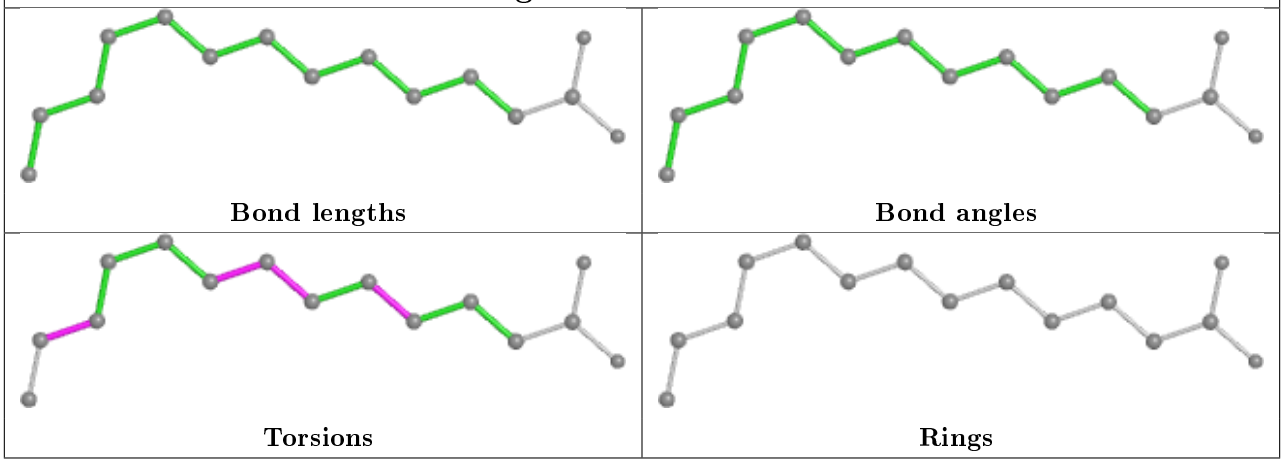
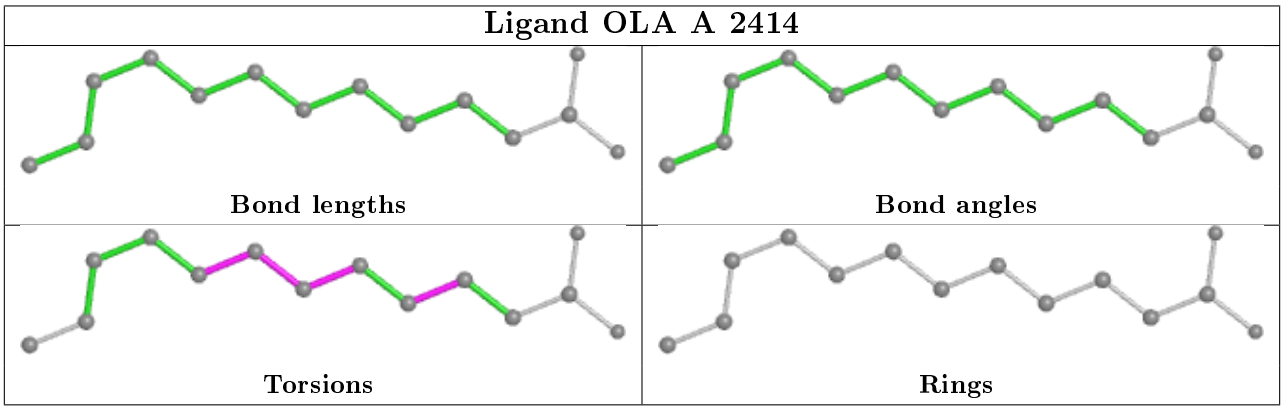


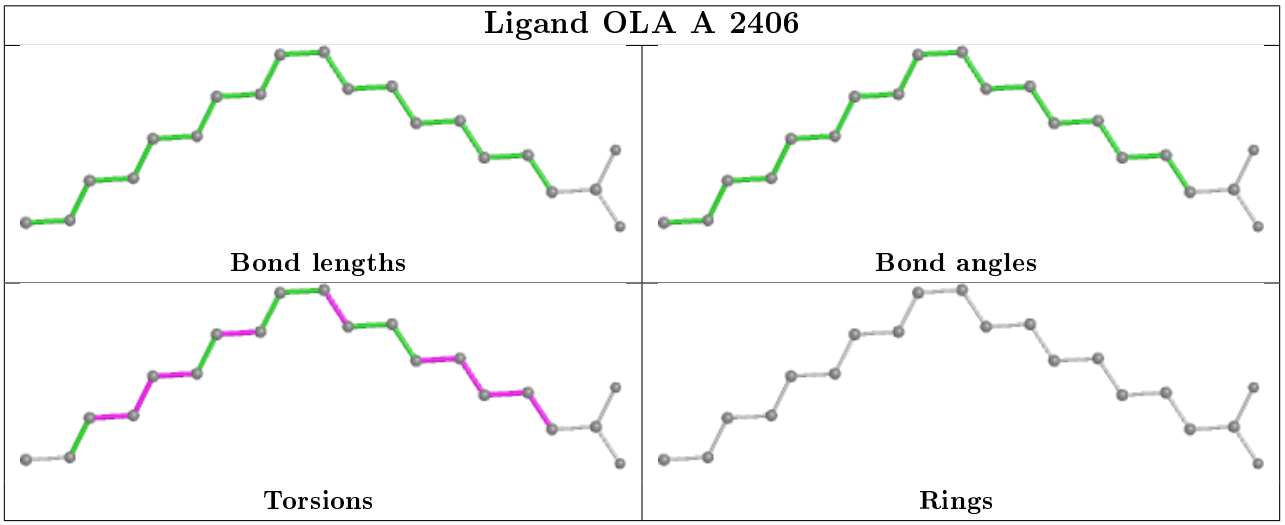
Ligand OLA A 2419



Ligand OLA A 2414



Ligand OLA A 2406



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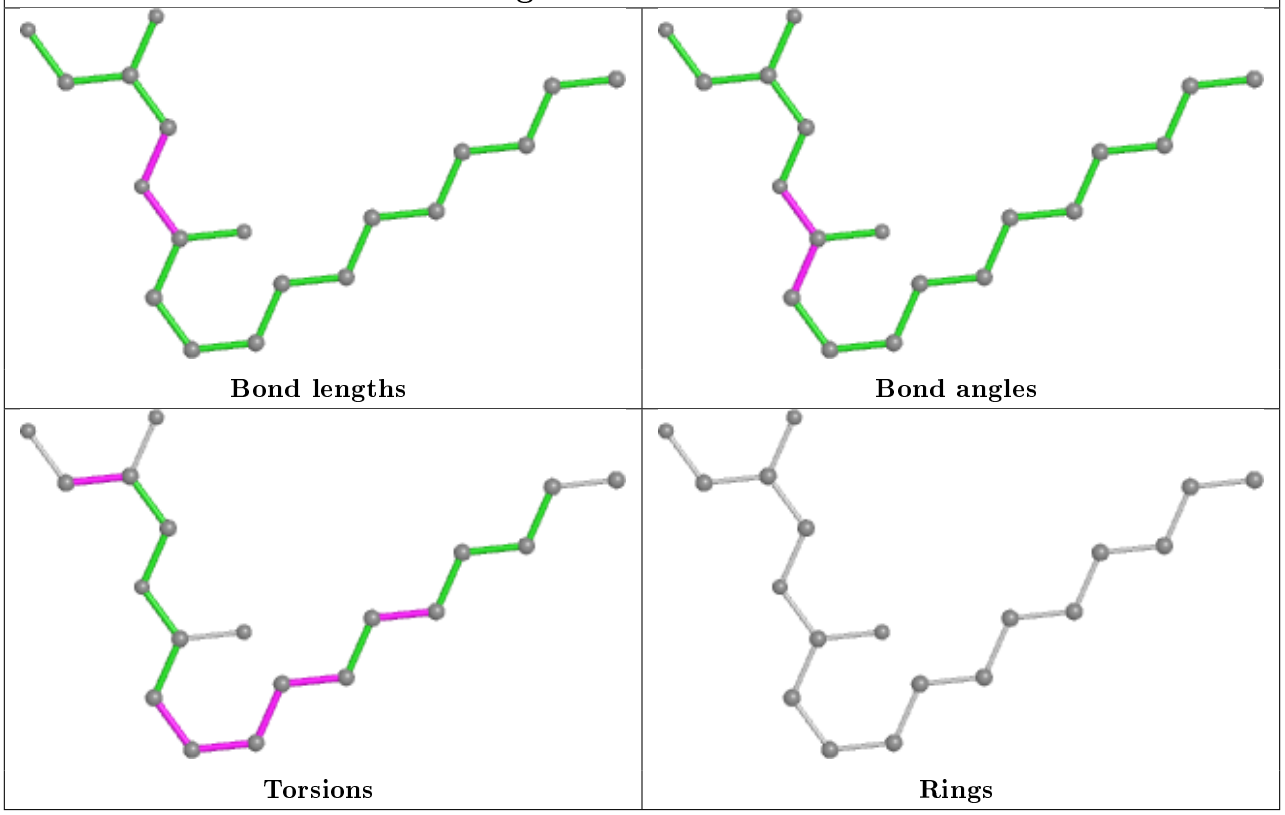
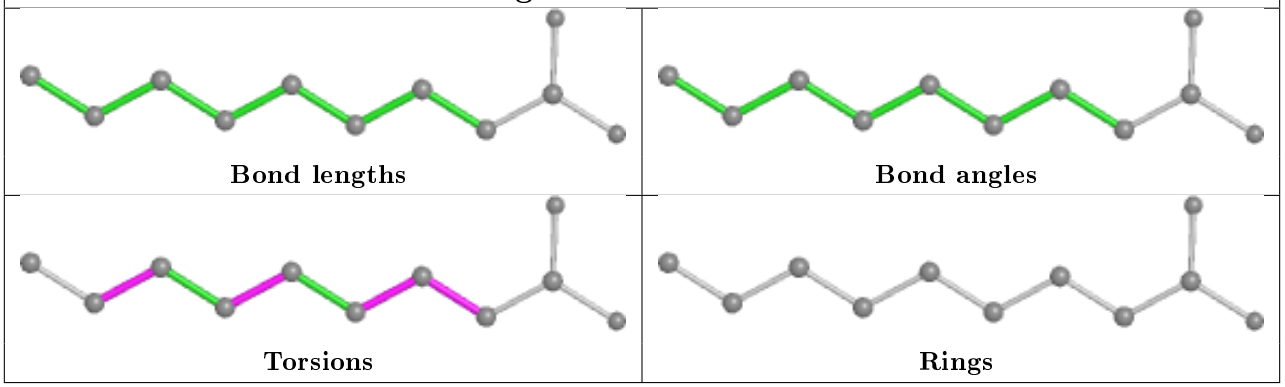
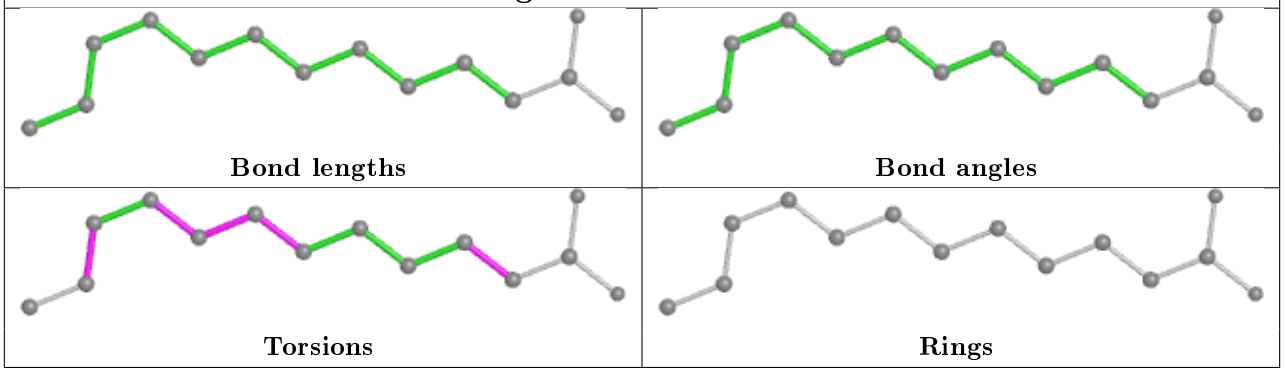


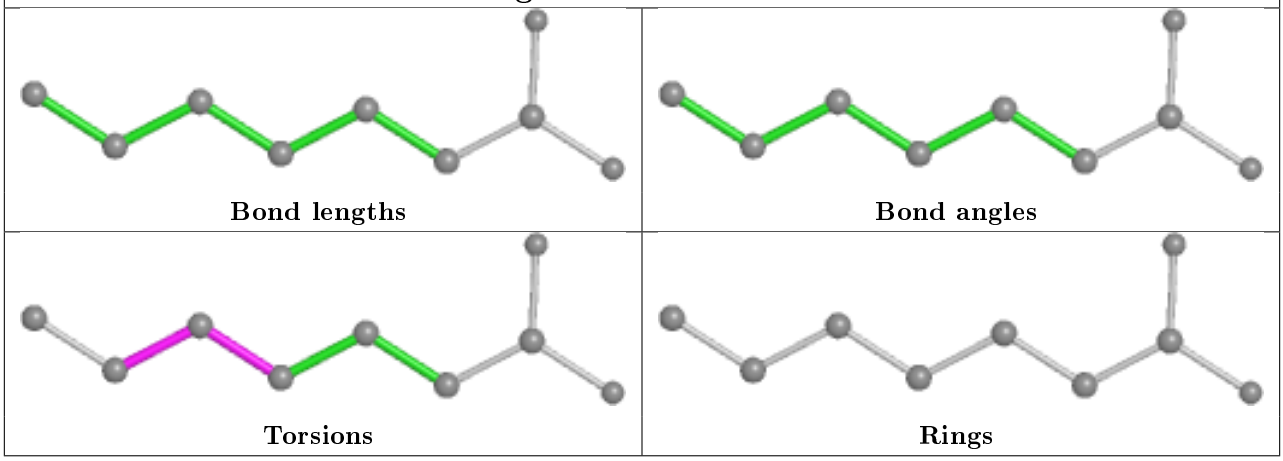
Ligand OLA A 2416



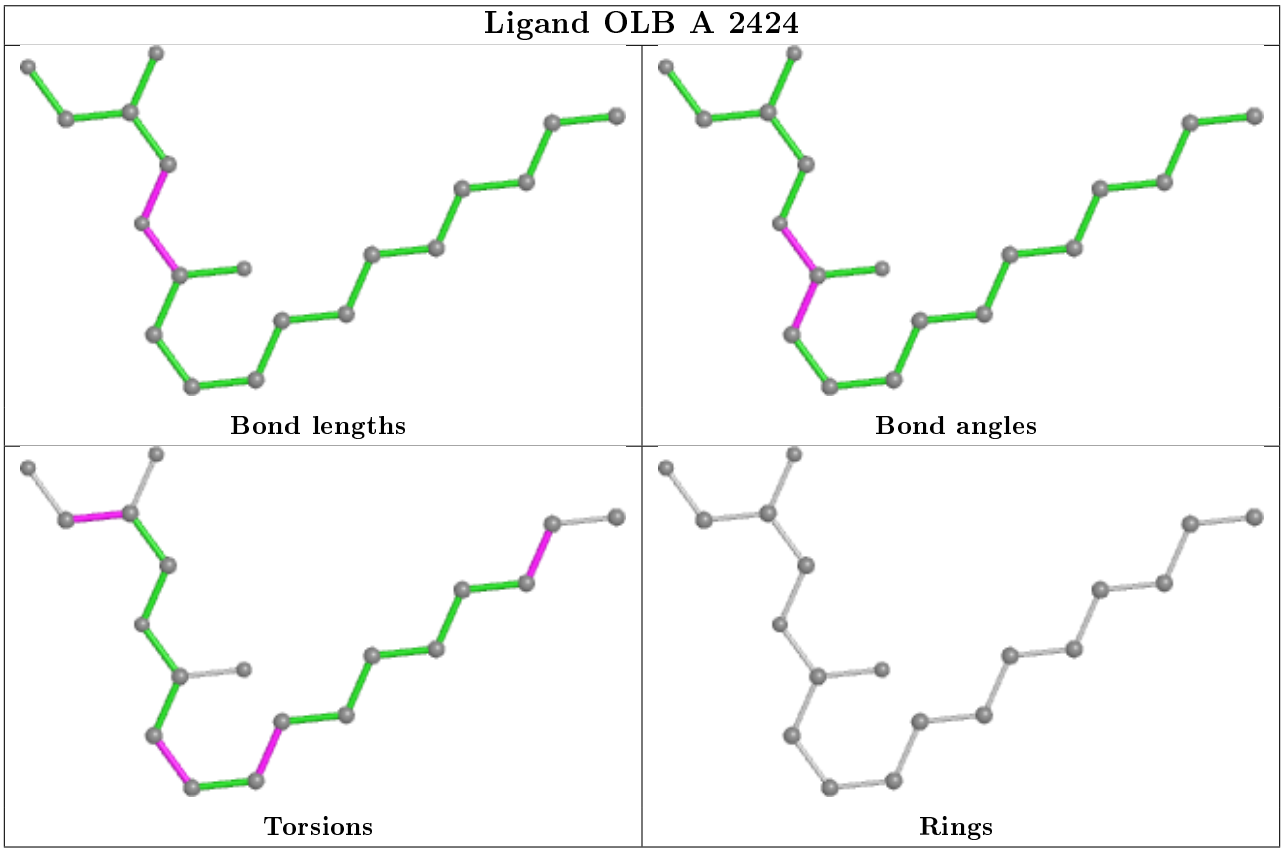
Ligand OLA A 2418



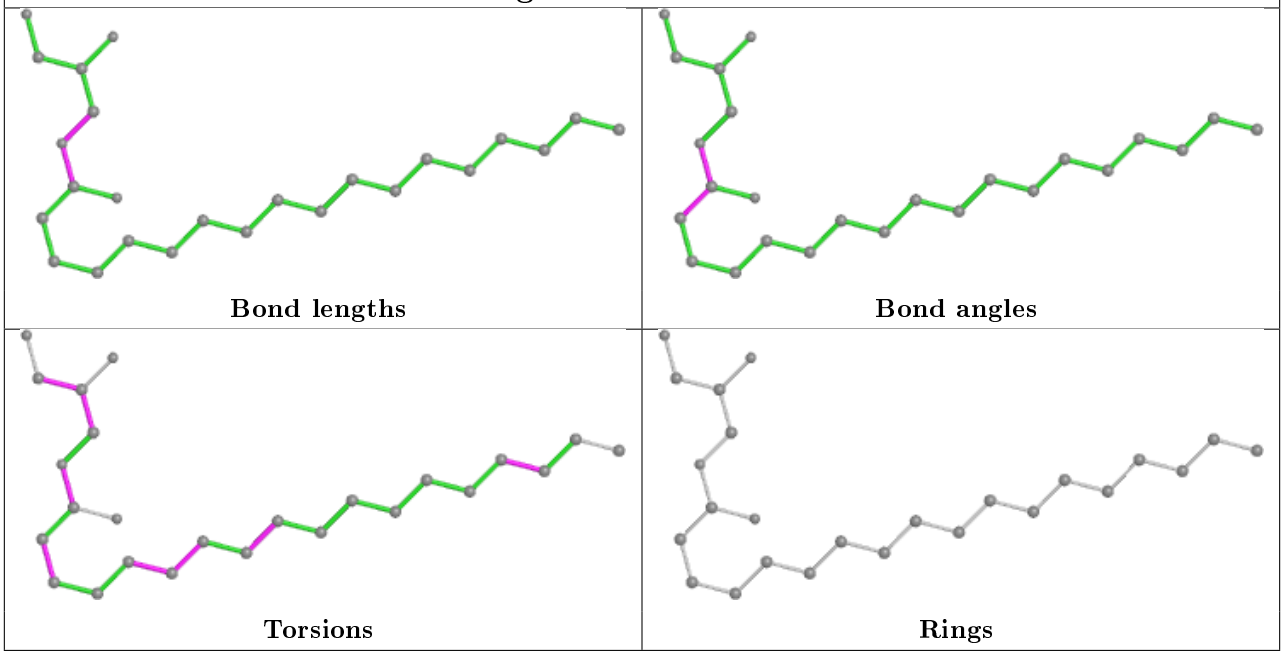
Ligand OLA A 2408



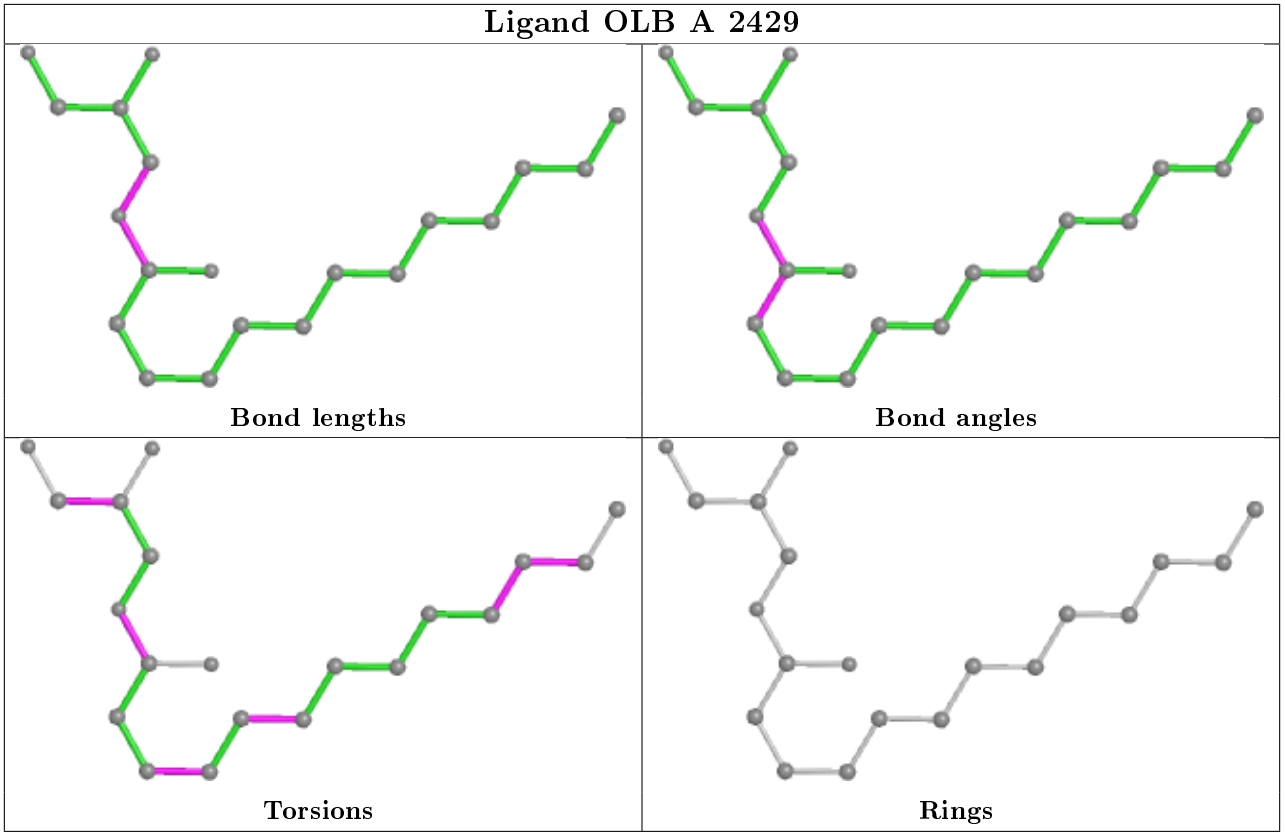
Ligand OLB A 2424



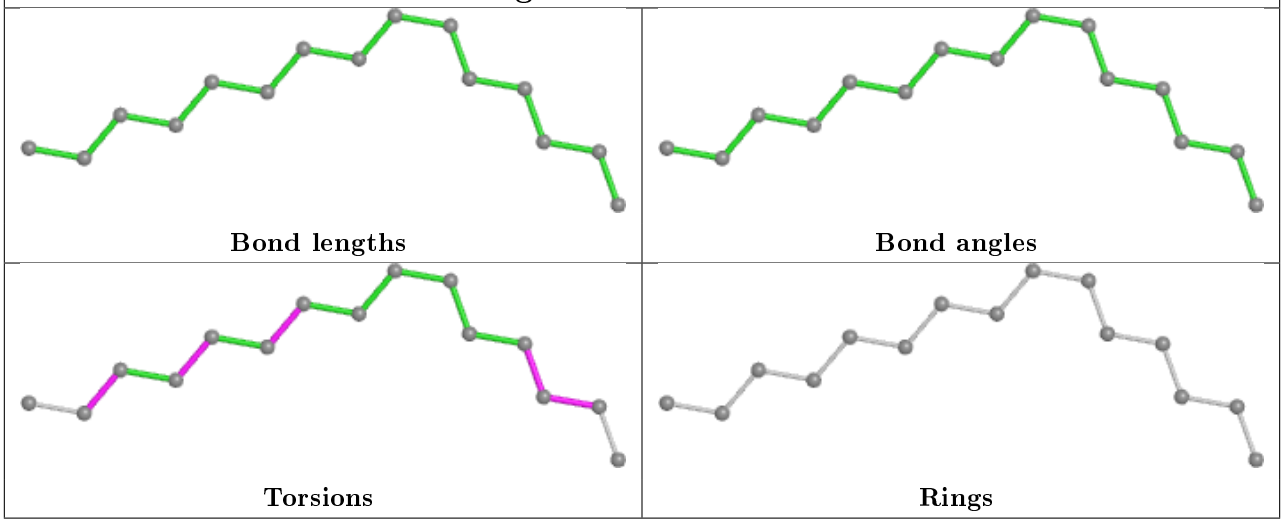
Ligand OLB A 2428



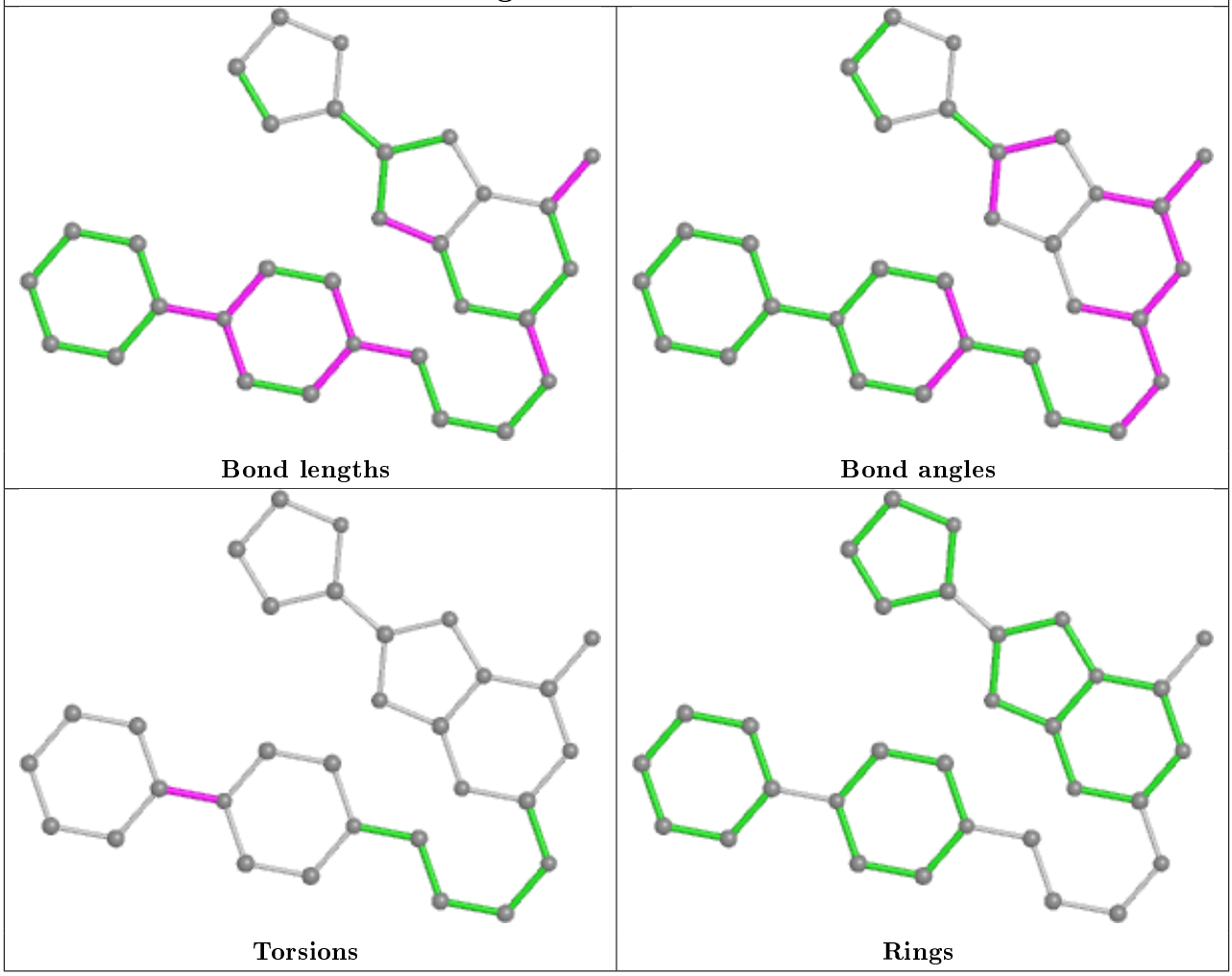
Ligand OLB A 2429



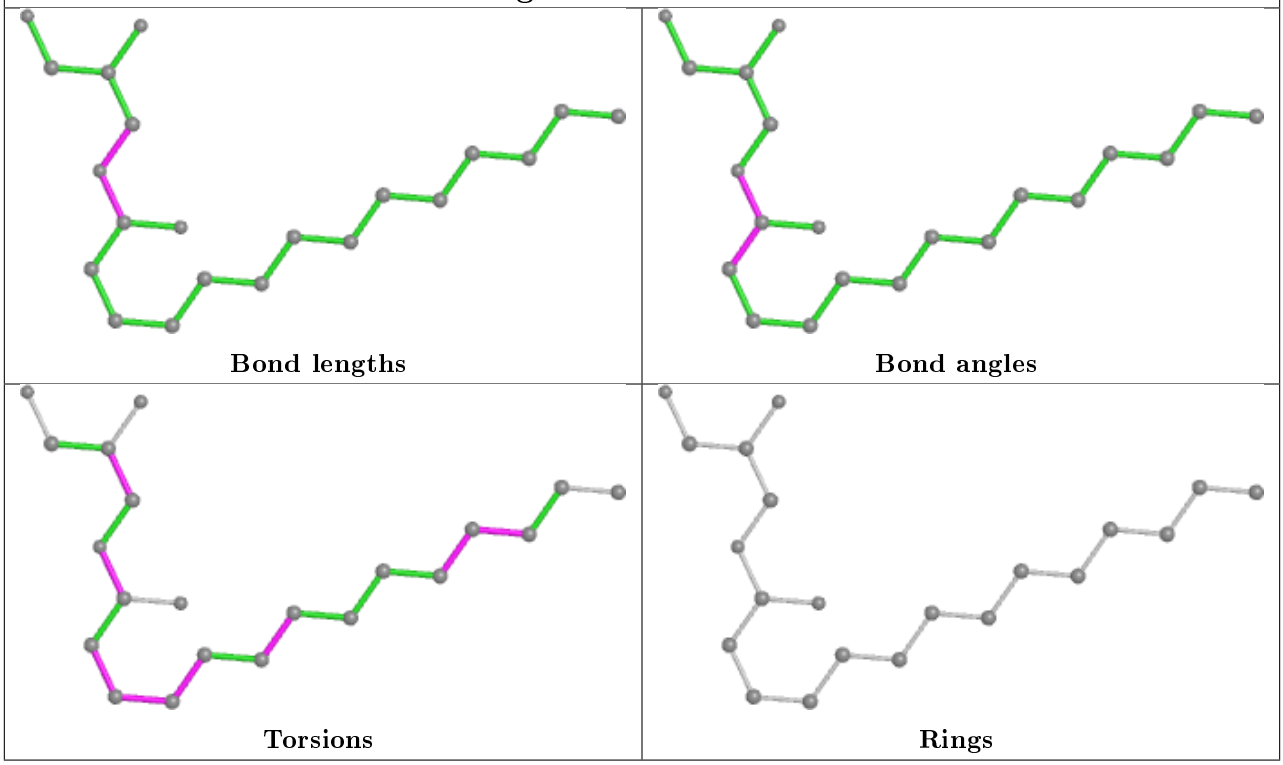
Ligand OLA A 2417



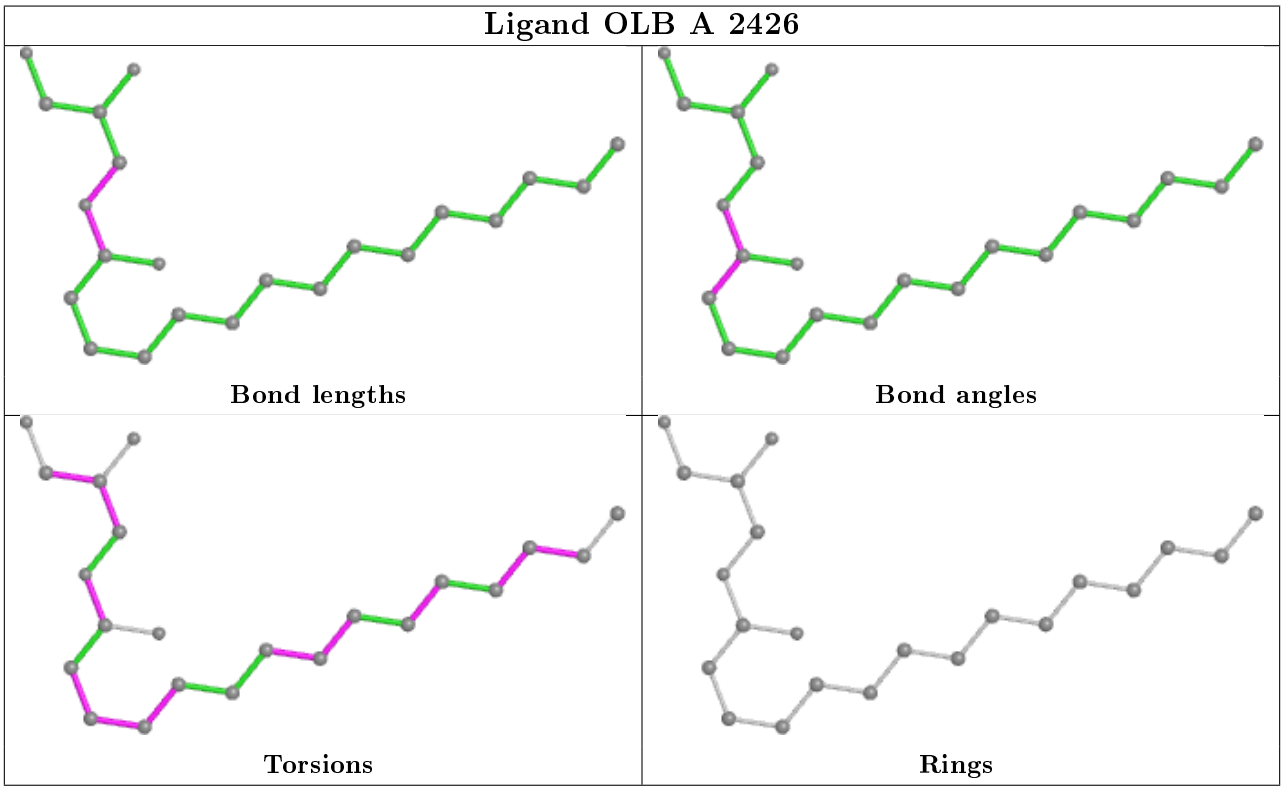
Ligand 6DX A 2401

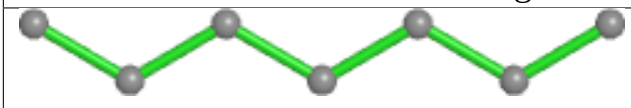
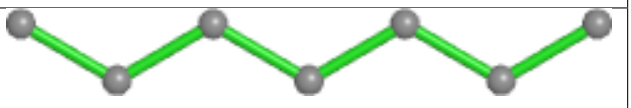
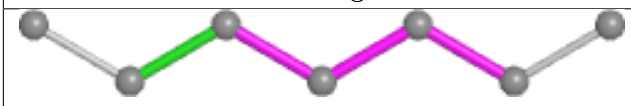
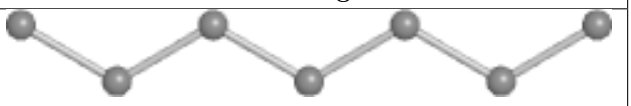


Ligand OLB A 2430



Ligand OLB A 2426



Ligand OLA A 2420	
 Bond lengths	 Bond angles
 Torsions	 Rings

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%)	-0.12	19 (4%) 29 28	11, 26, 66, 103	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	ASP	4.2
1	A	-1	GLY	4.2
1	A	1061	PHE	4.1
1	A	1062	ARG	3.7
1	A	306	HIS	3.7
1	A	1059	LYS	3.5
1	A	1008	GLU	2.6
1	A	220	ARG	2.5
1	A	1101	TYR	2.4
1	A	1060	ASP	2.4
1	A	111	ARG	2.4
1	A	0	ALA	2.3
1	A	305	SER	2.3
1	A	29	TRP	2.3
1	A	1023	ALA	2.2
1	A	1028	ASP	2.1
1	A	1042	LYS	2.1
1	A	290	TYR	2.1
1	A	1084	VAL	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

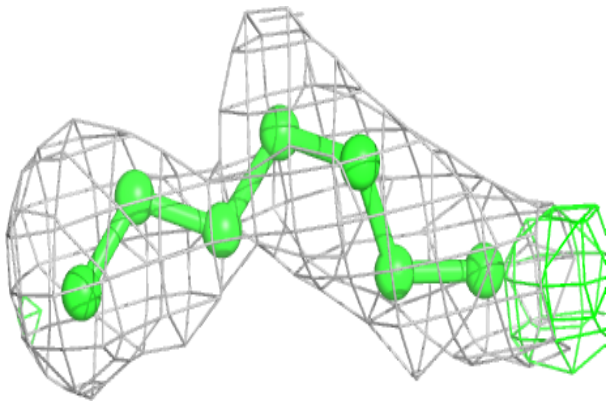
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

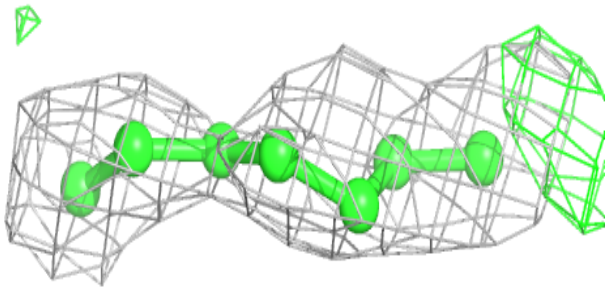
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	OLA	A	2420	7/20	0.54	0.20	52,54,55,55	0
4	CLR	A	2402	28/28	0.58	0.35	92,96,100,101	0
5	OLA	A	2413	8/20	0.62	0.18	52,56,61,63	0
5	OLA	A	2410	20/20	0.62	0.25	43,53,63,65	0
5	OLA	A	2414	14/20	0.64	0.23	44,57,60,60	0
6	OLB	A	2428	25/25	0.69	0.25	38,49,72,74	0
6	OLB	A	2429	20/25	0.71	0.28	39,52,89,91	0
5	OLA	A	2415	19/20	0.73	0.22	46,52,68,69	0
6	OLB	A	2425	16/25	0.76	0.20	44,70,82,82	0
5	OLA	A	2421	8/20	0.76	0.14	45,46,48,48	0
5	OLA	A	2411	15/20	0.76	0.22	62,63,73,74	0
5	OLA	A	2418	14/20	0.78	0.19	41,52,65,67	0
5	OLA	A	2419	15/20	0.78	0.19	37,41,64,67	0
5	OLA	A	2412	12/20	0.78	0.28	35,48,61,62	0
6	OLB	A	2430	21/25	0.79	0.24	40,50,58,60	0
5	OLA	A	2416	11/20	0.79	0.20	44,56,81,81	0
6	OLB	A	2423	17/25	0.80	0.19	55,60,64,66	0
5	OLA	A	2407	15/20	0.81	0.23	45,51,66,67	0
5	OLA	A	2409	18/20	0.82	0.17	40,51,62,66	0
5	OLA	A	2422	12/20	0.83	0.24	40,44,48,50	0
5	OLA	A	2417	15/20	0.85	0.17	45,49,56,56	0
6	OLB	A	2427	19/25	0.86	0.17	33,37,65,67	0
6	OLB	A	2426	22/25	0.86	0.18	37,43,66,69	0
5	OLA	A	2408	9/20	0.86	0.23	29,38,53,60	0
6	OLB	A	2424	19/25	0.87	0.17	40,49,63,64	0
5	OLA	A	2406	20/20	0.90	0.15	26,44,60,61	0
4	CLR	A	2405	28/28	0.93	0.11	19,26,43,45	0
4	CLR	A	2404	28/28	0.94	0.11	21,26,39,46	0
4	CLR	A	2403	28/28	0.94	0.10	19,25,41,42	0
3	6DX	A	2401	31/31	0.95	0.18	12,21,60,62	0
2	NA	A	2400	1/1	0.96	0.13	31,31,31,31	0

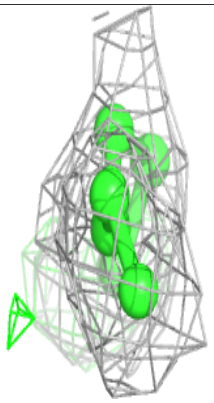
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 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 CLR A 2402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
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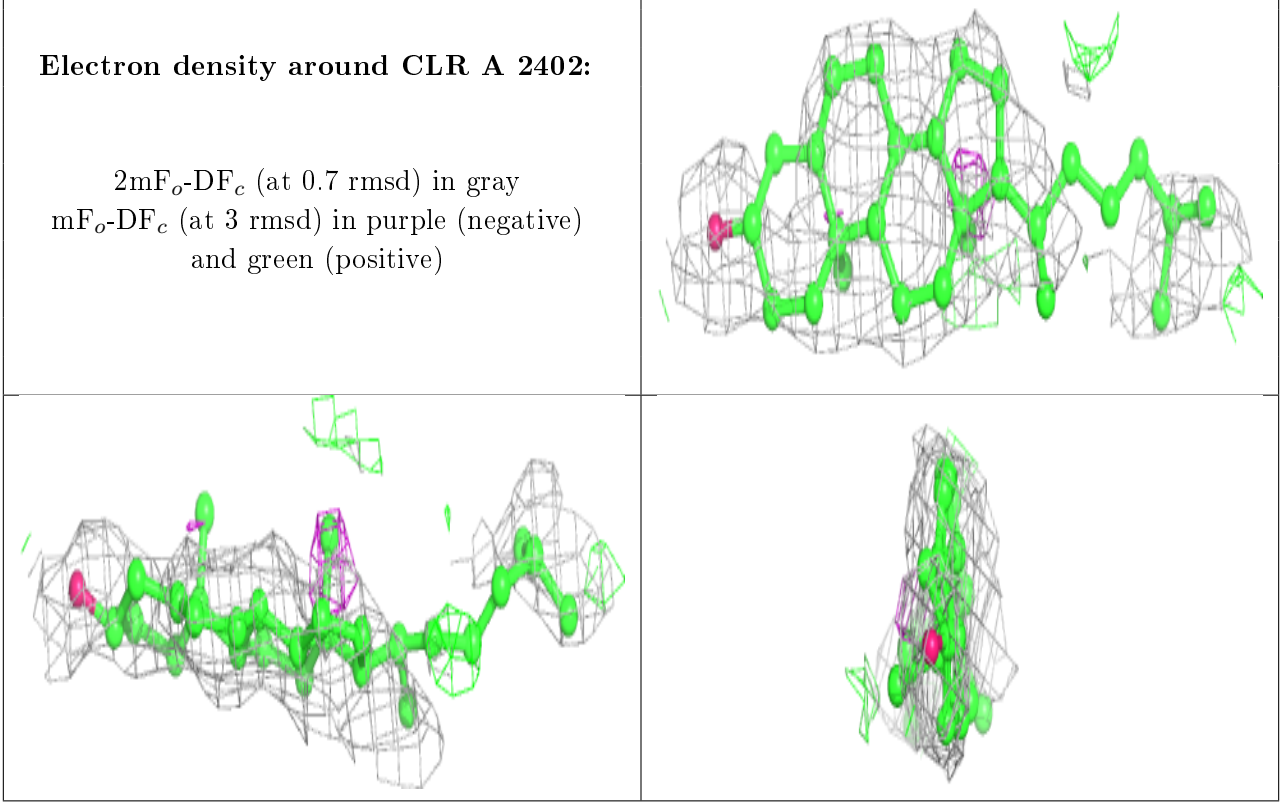
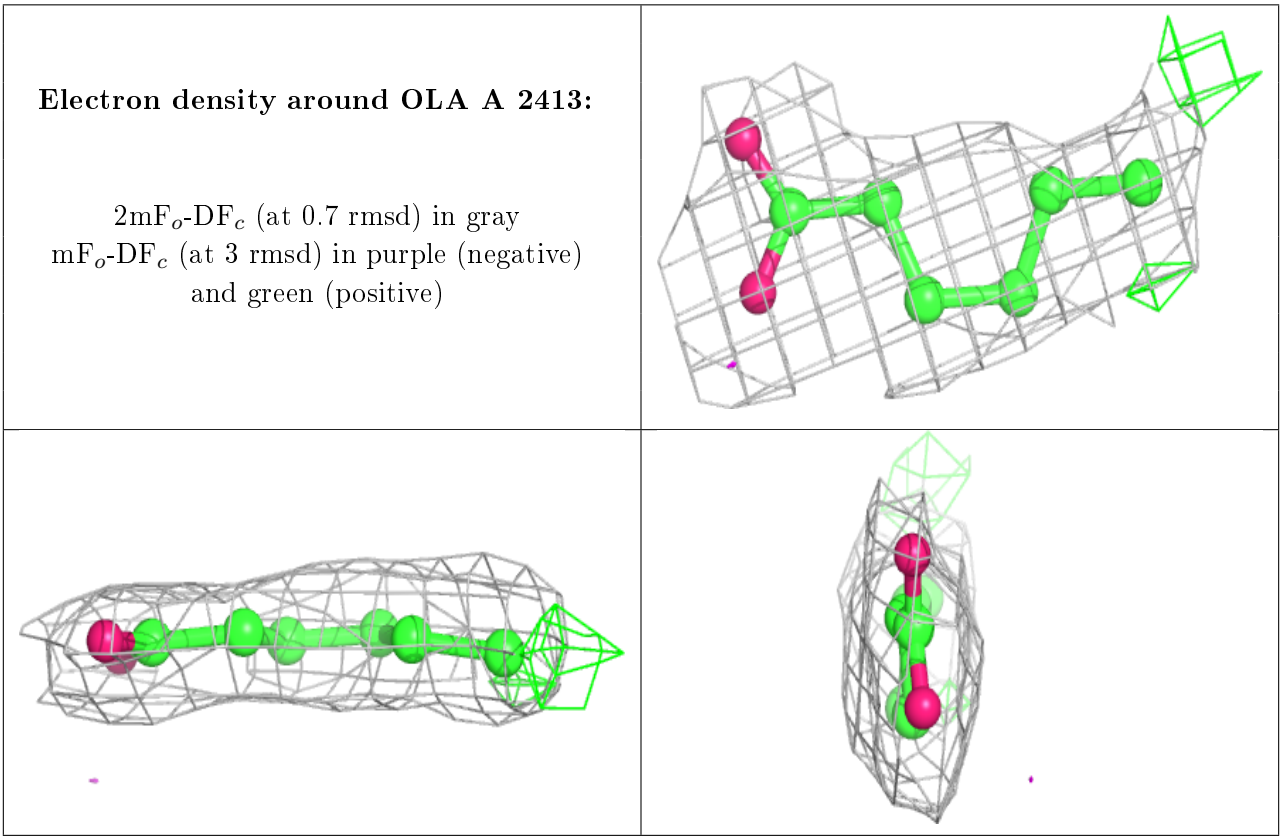


Electron density around OLA A 2413:

$2mF_o$-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 2410:

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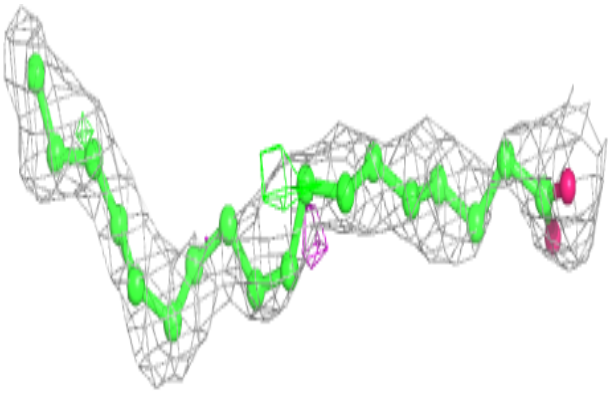
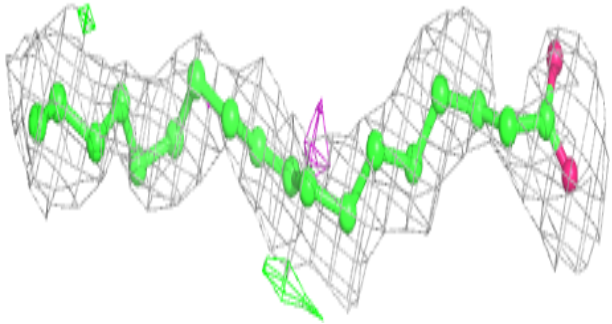
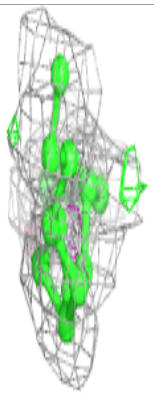
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

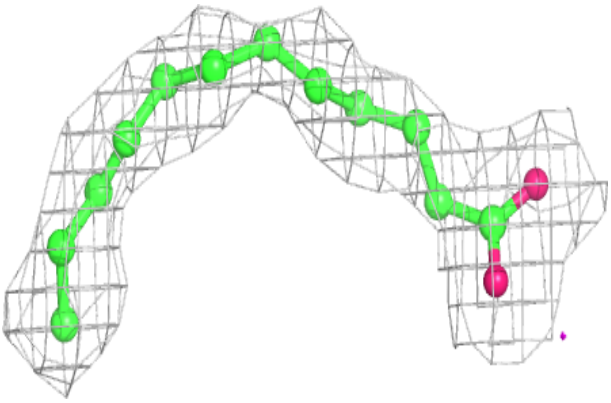


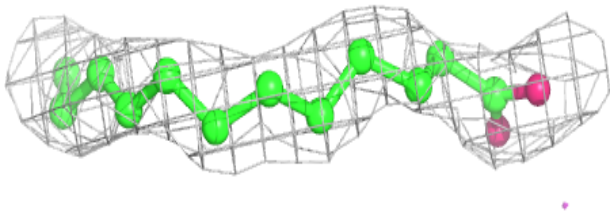


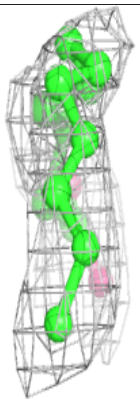


Electron density around OLA A 2414:

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







Electron density around OLB A 2428:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
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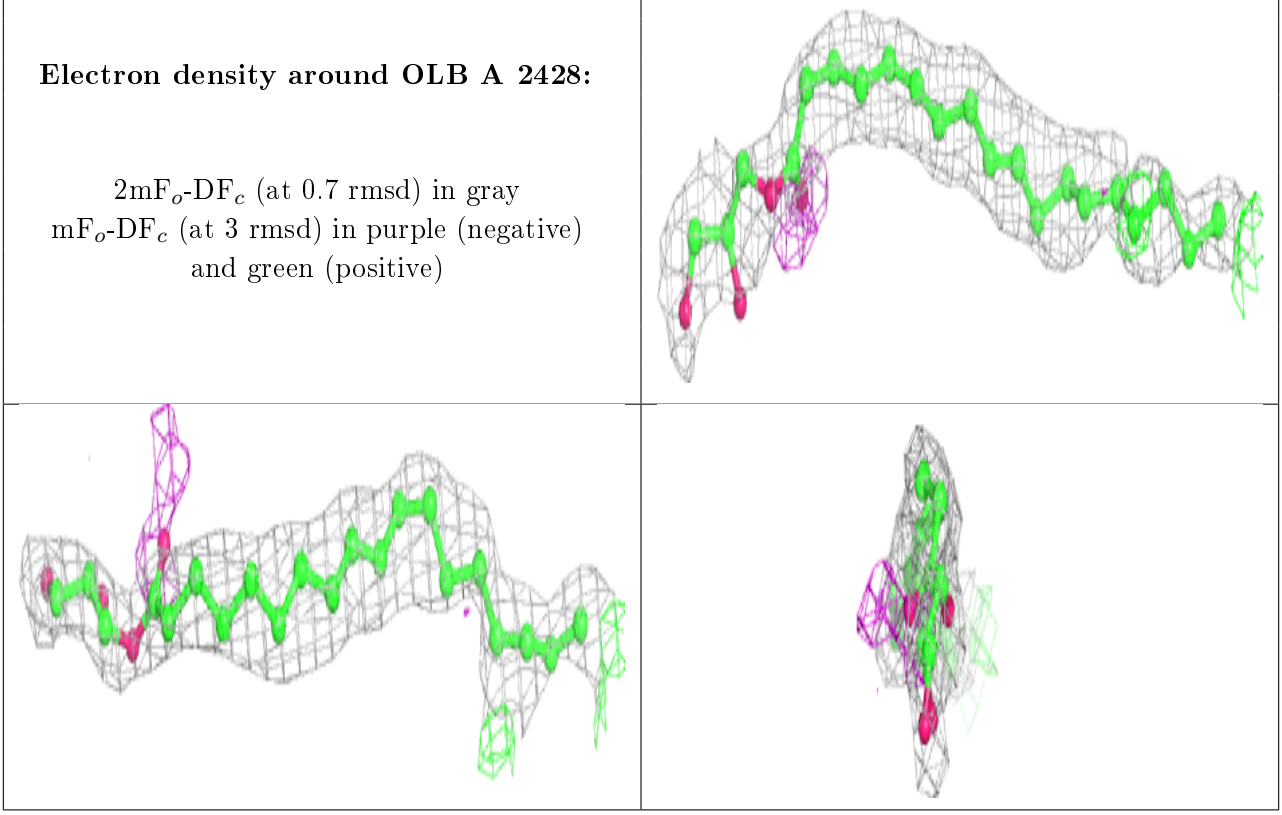
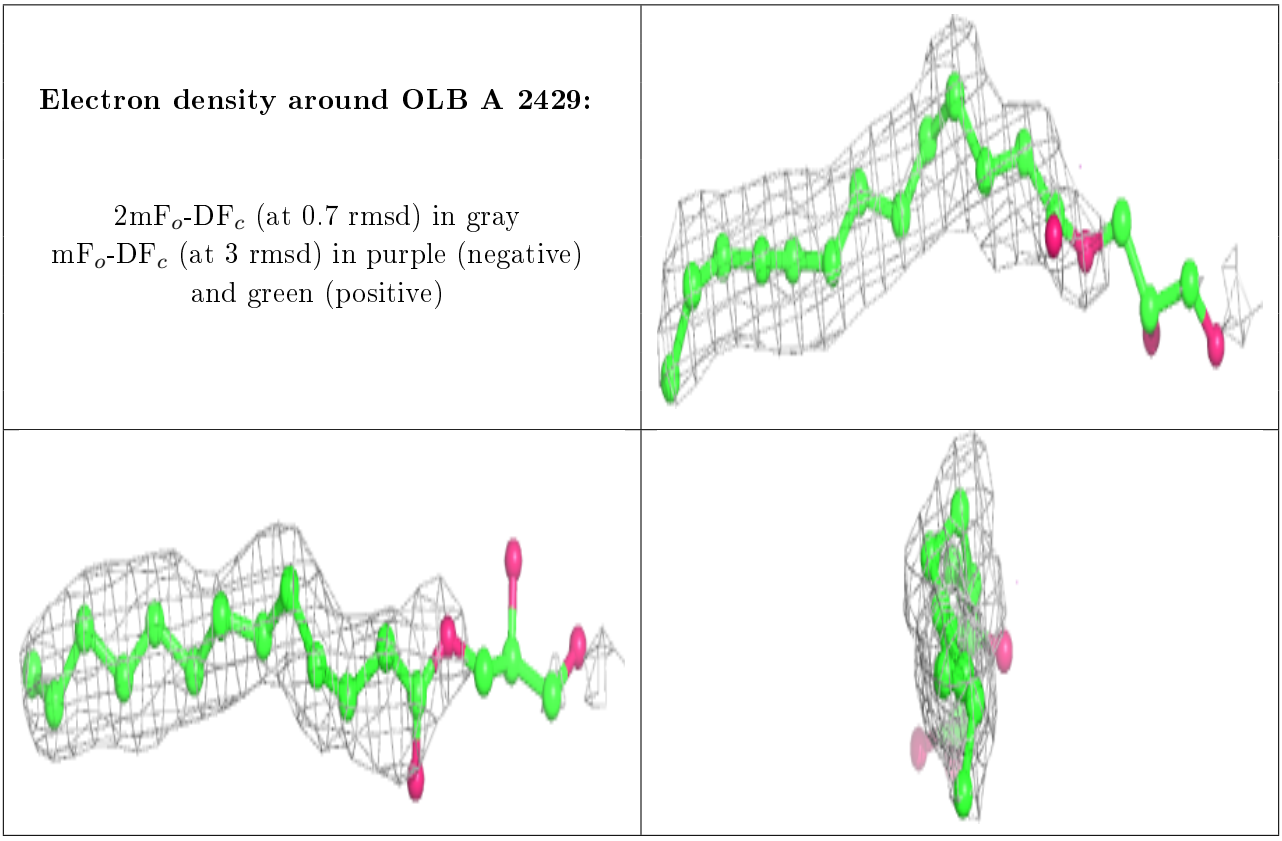


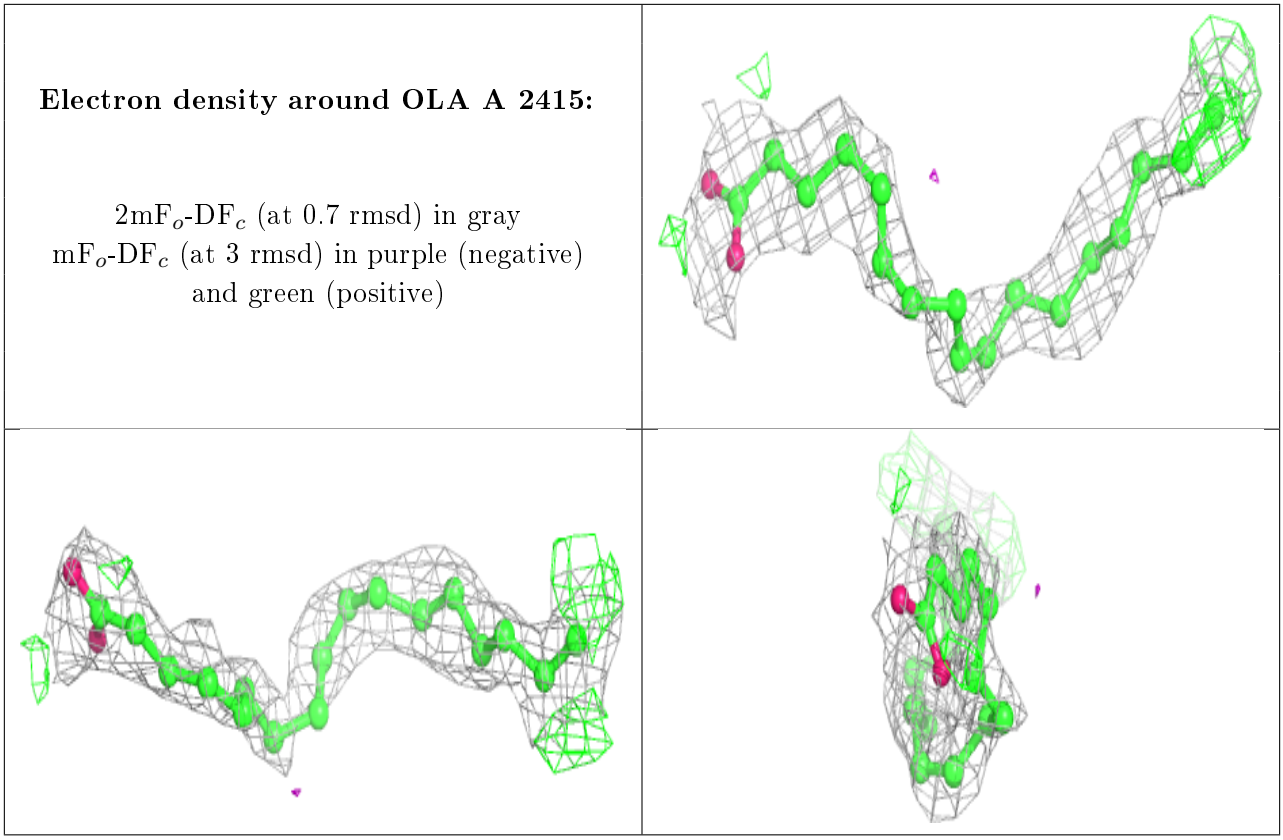
Electron density around OLB A 2429:

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



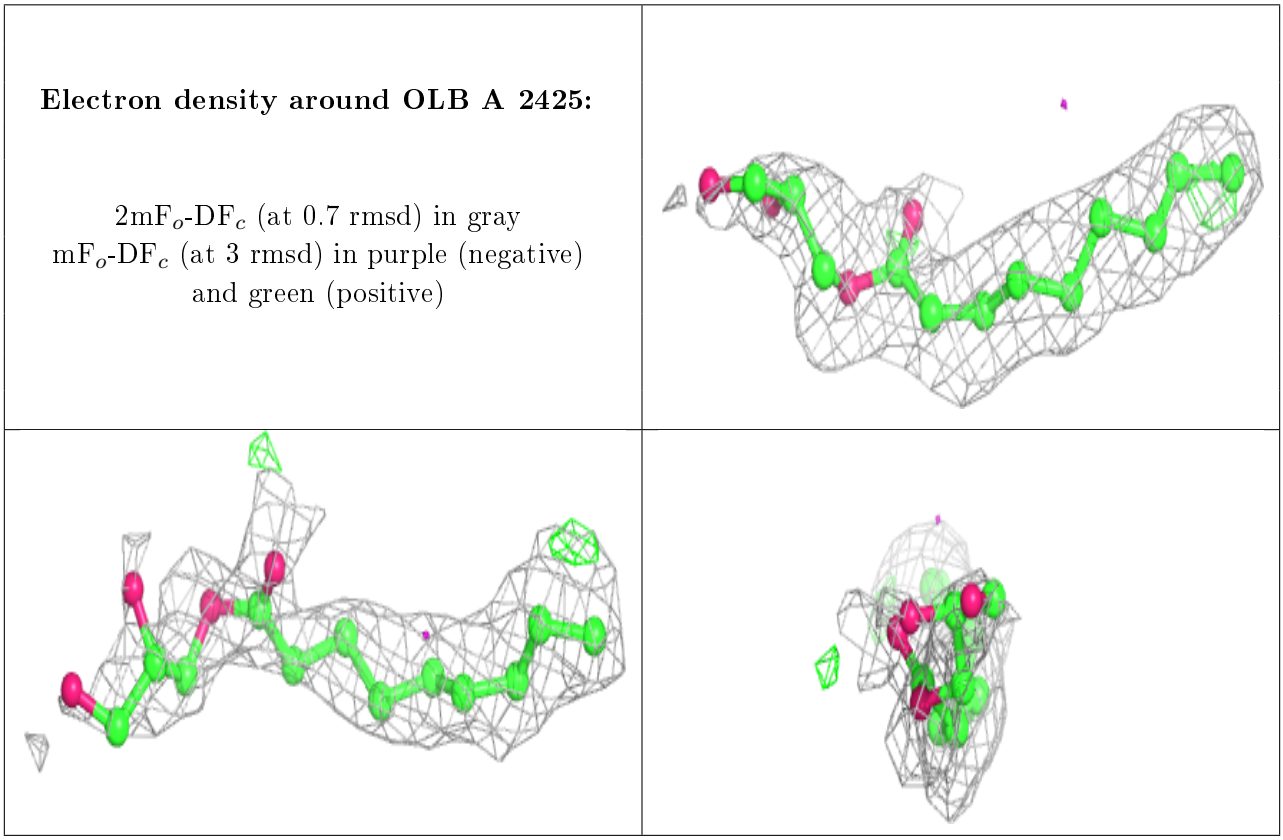
Electron density around OLA A 2415:

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



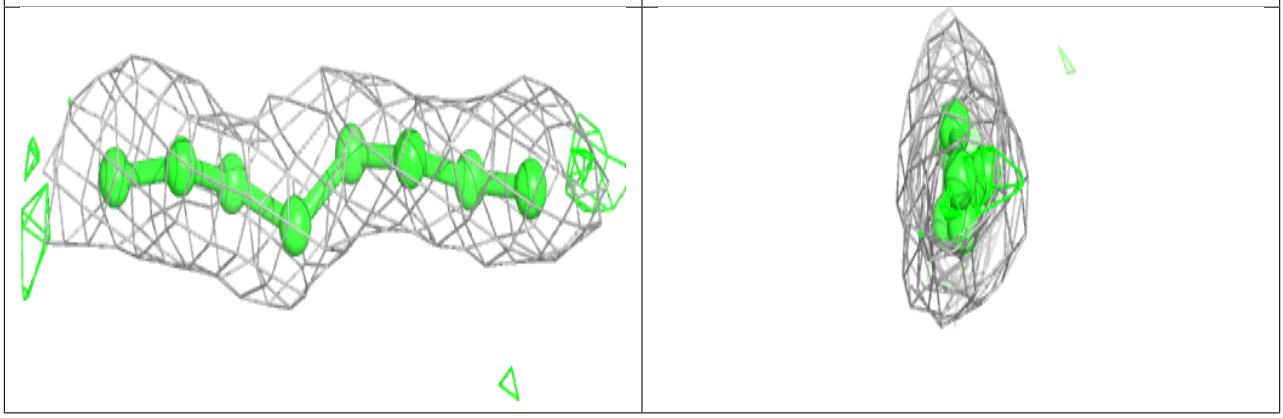
Electron density around OLB A 2425:

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



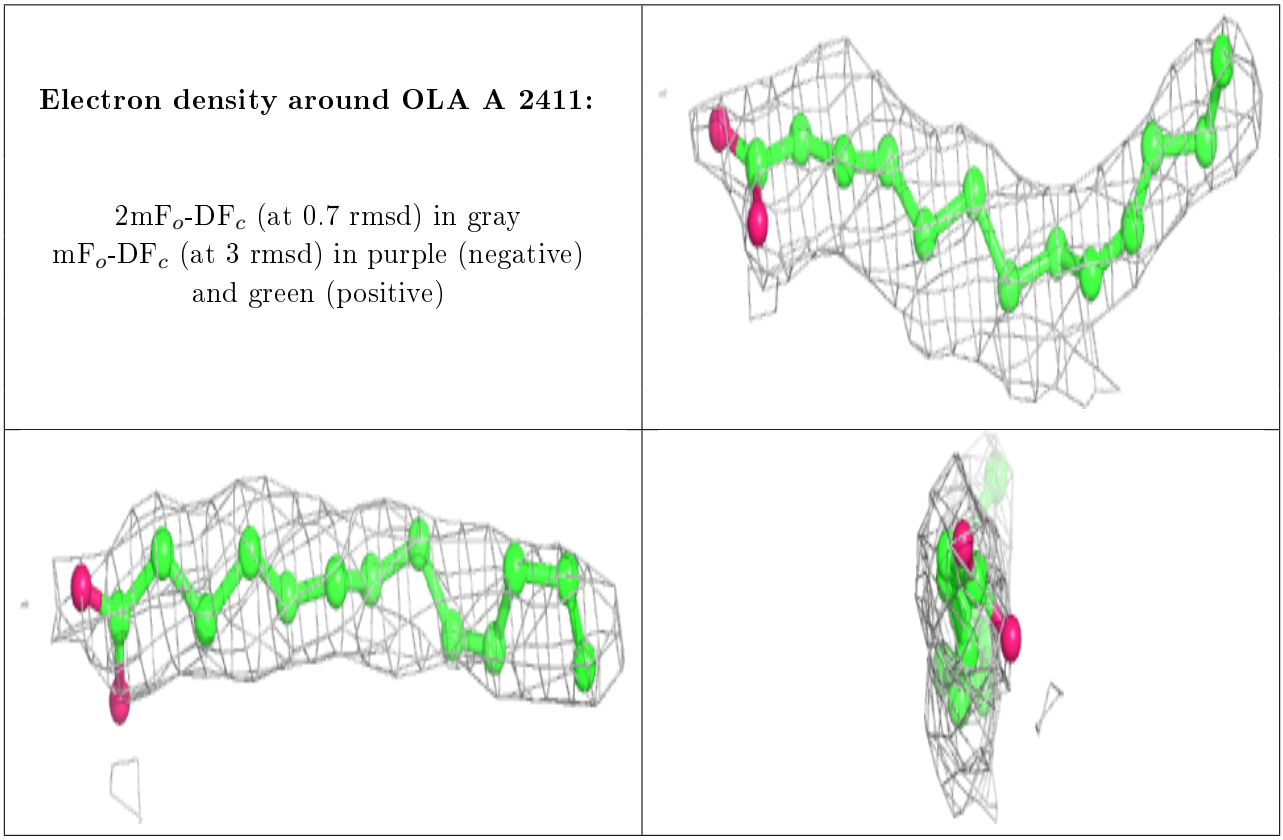
Electron density around OLA A 2421:

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



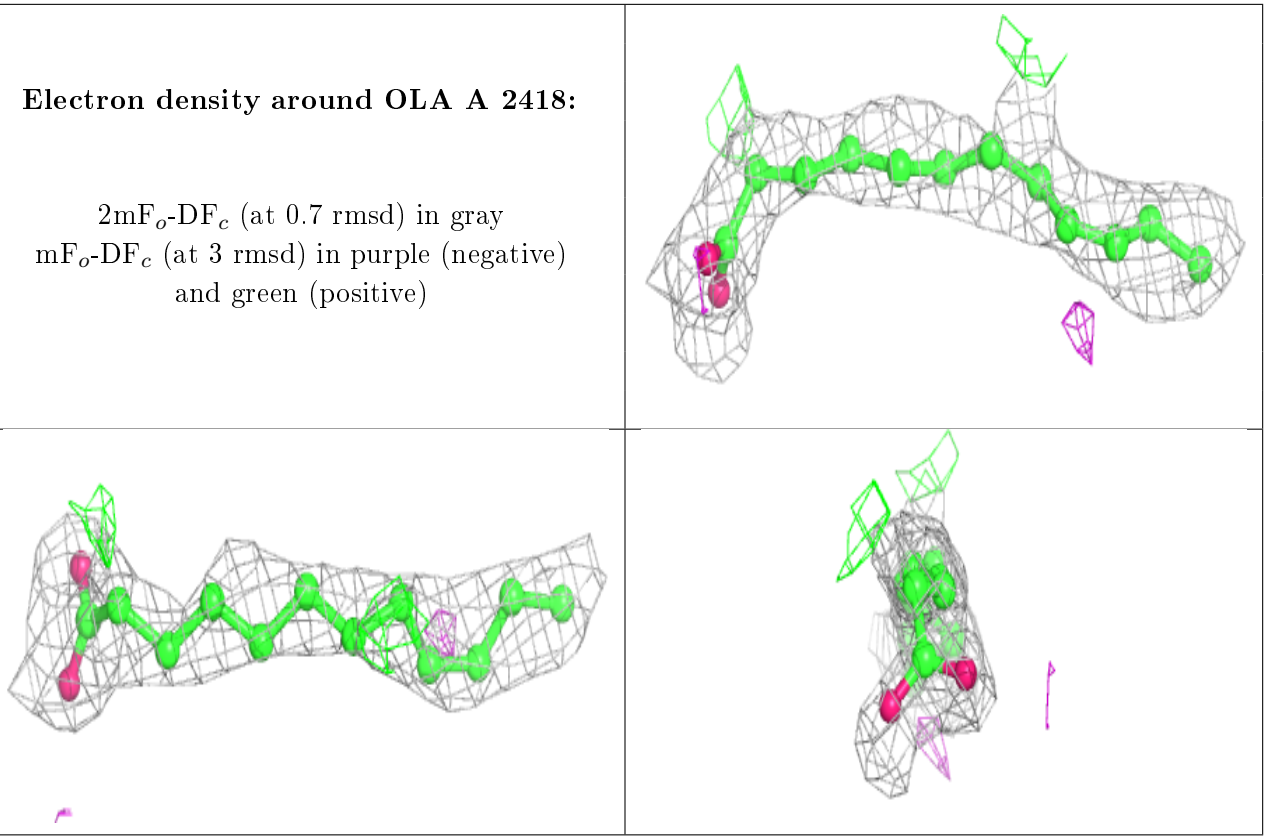
Electron density around OLA A 2411:

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



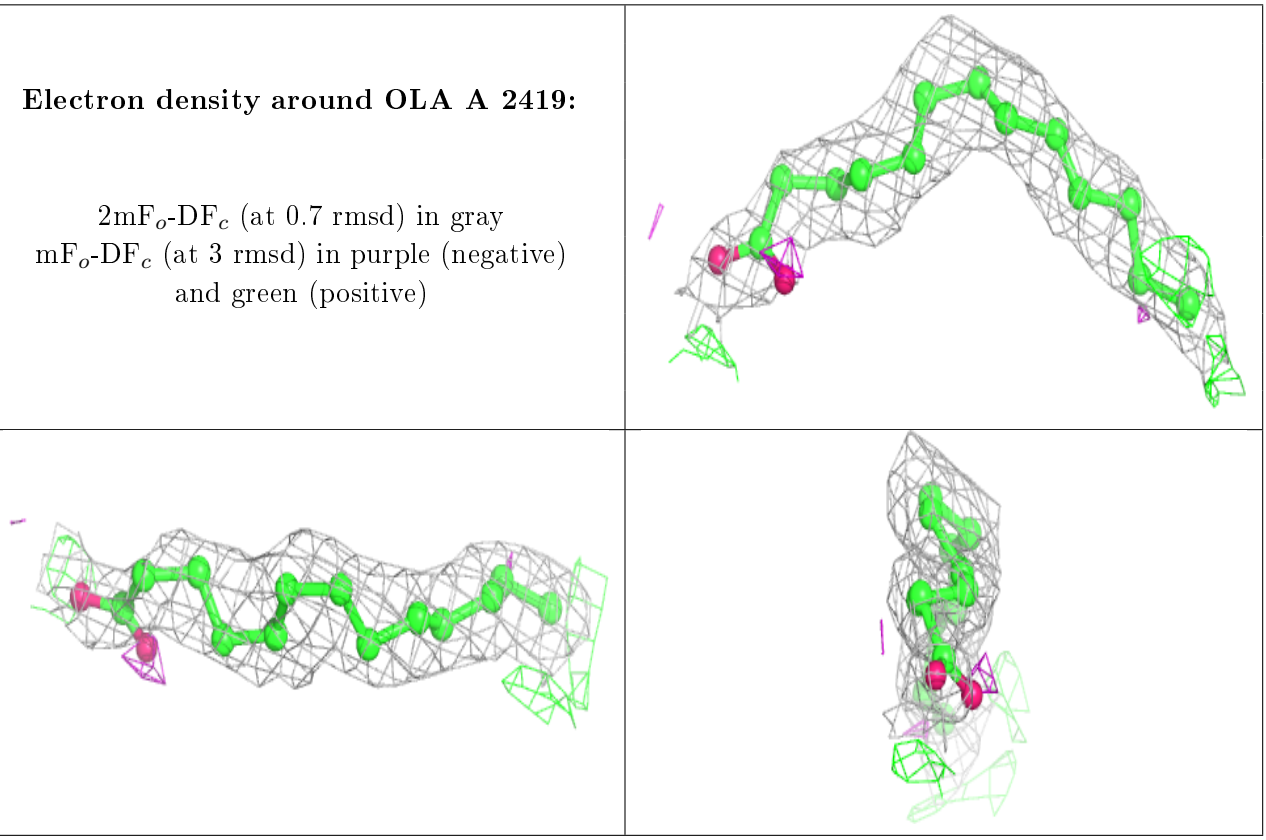
Electron density around OLA A 2418:

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



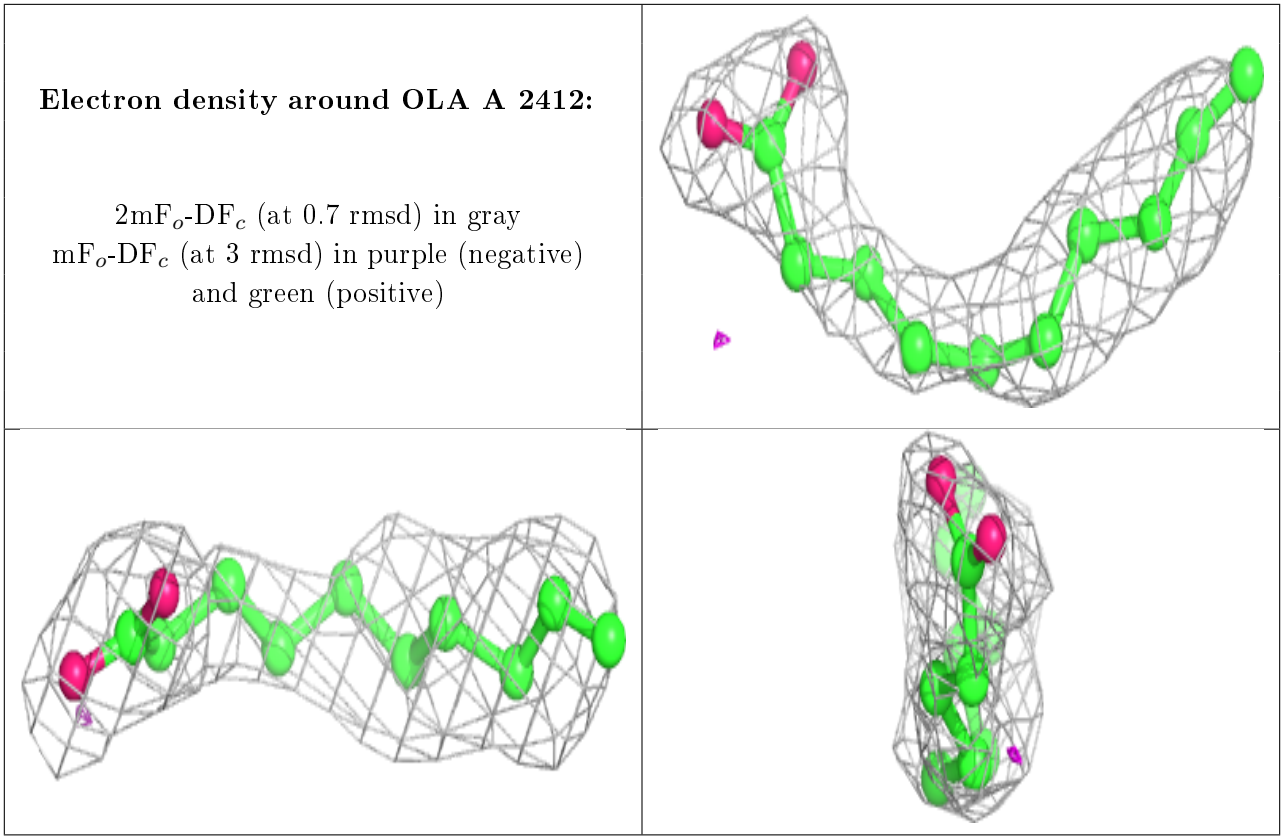
Electron density around OLA A 2419:

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



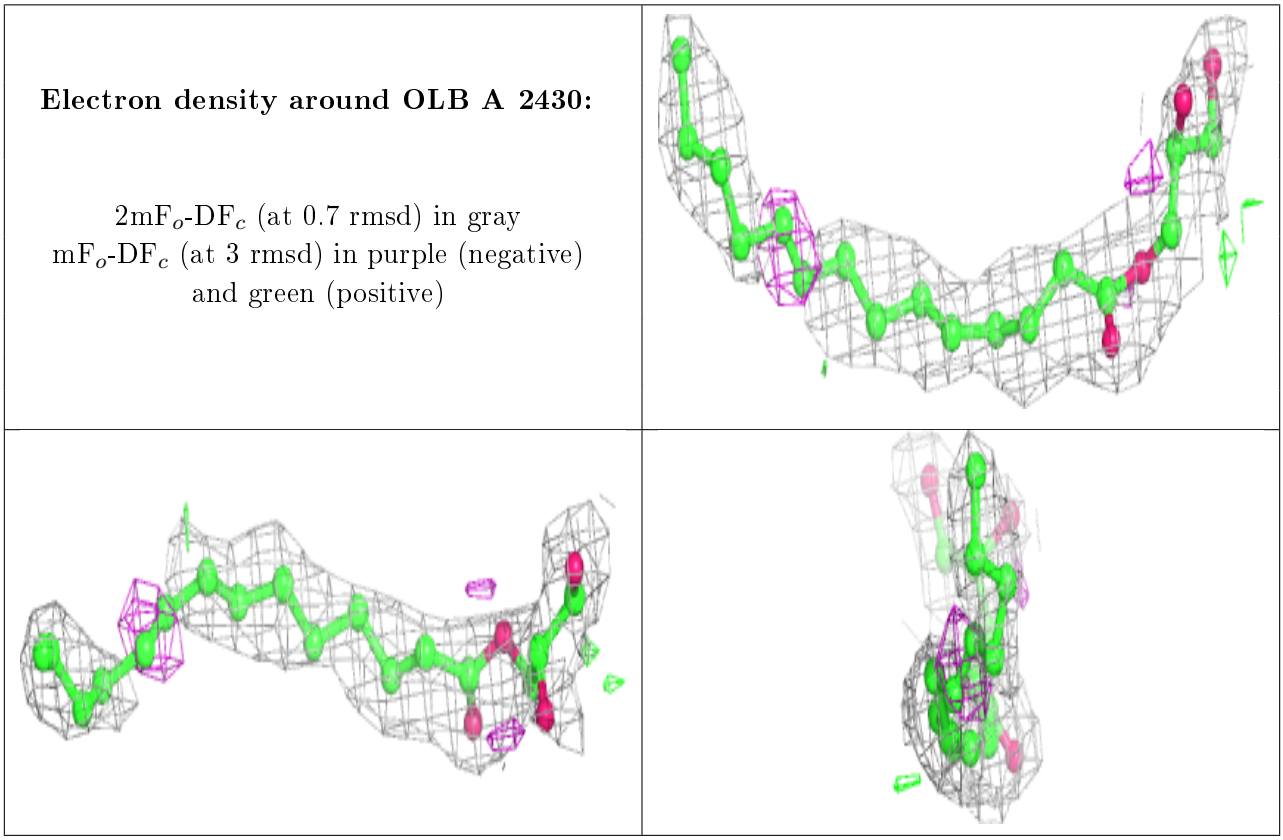
Electron density around OLA A 2412:

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



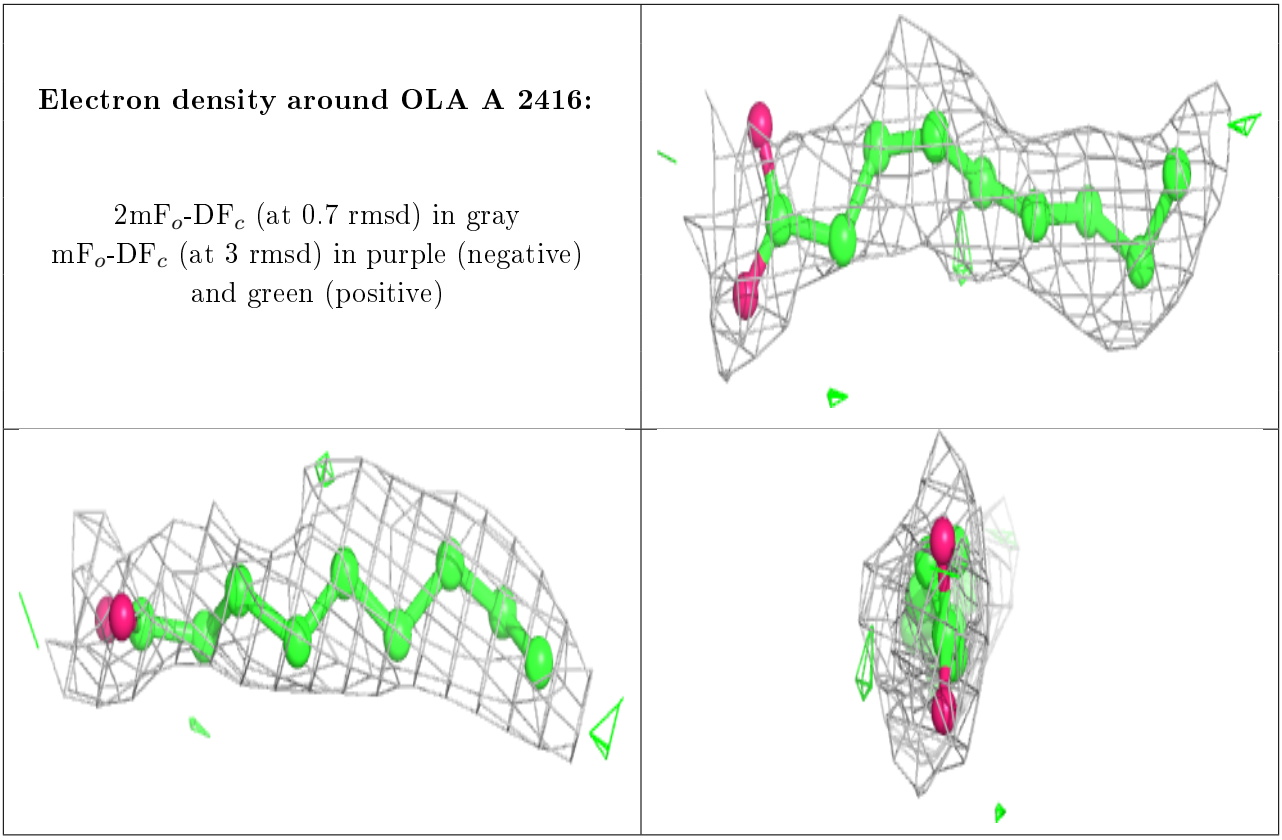
Electron density around OLB A 2430:

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



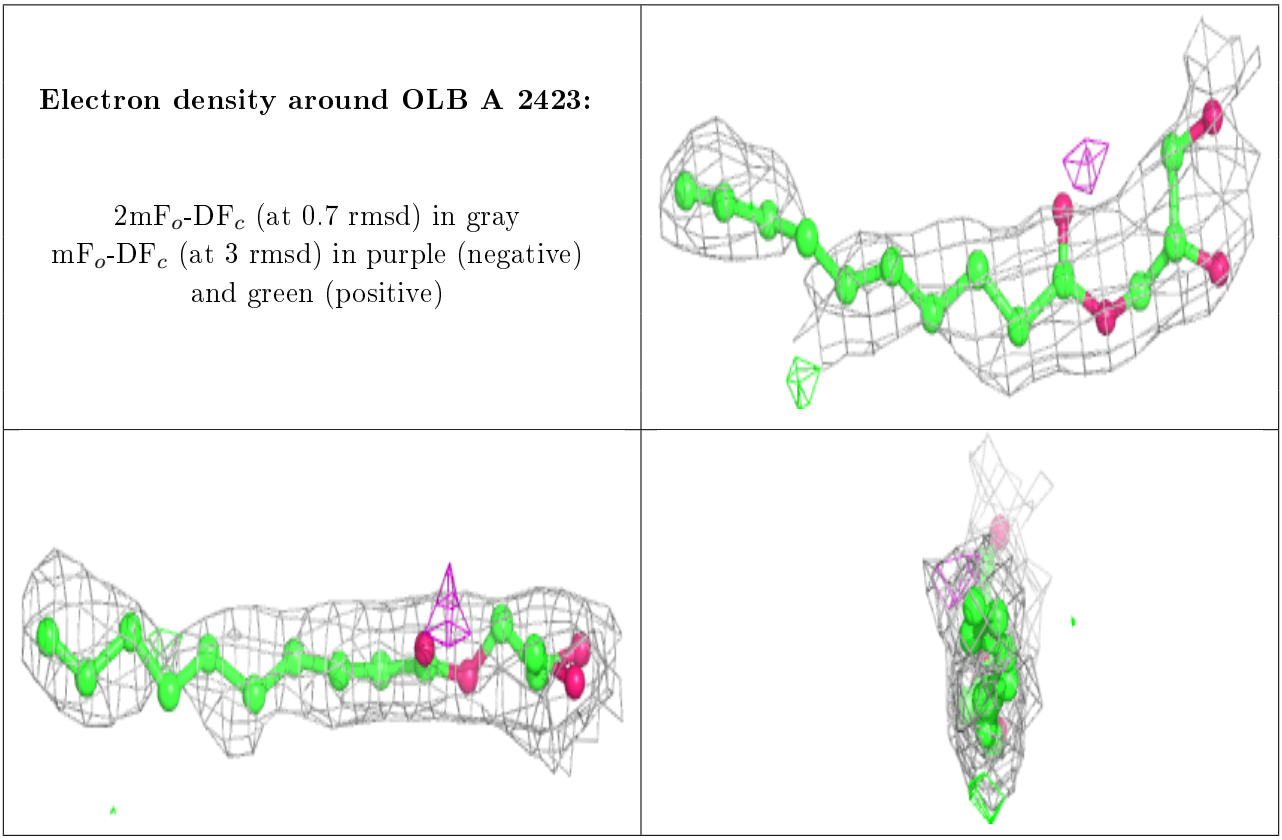
Electron density around OLA A 2416:

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



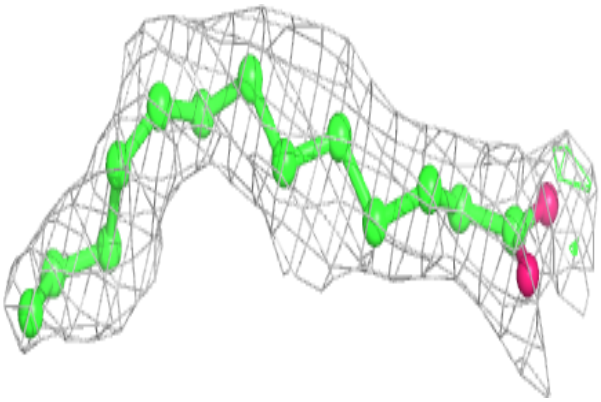
Electron density around OLB A 2423:

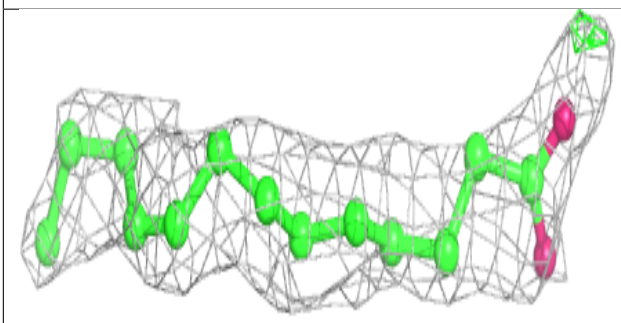
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

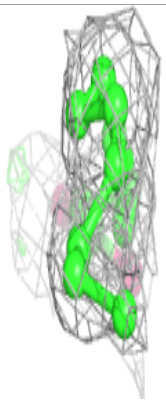


Electron density around OLA A 2407:

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

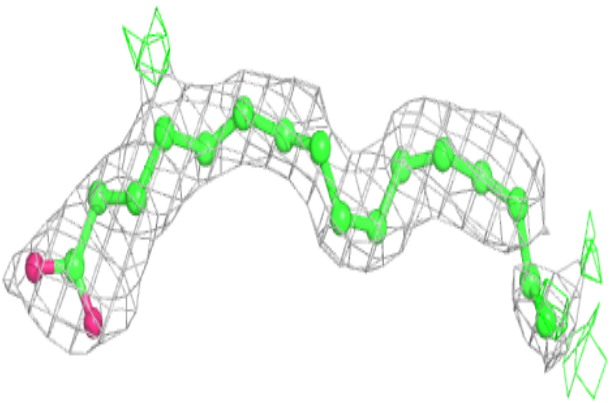


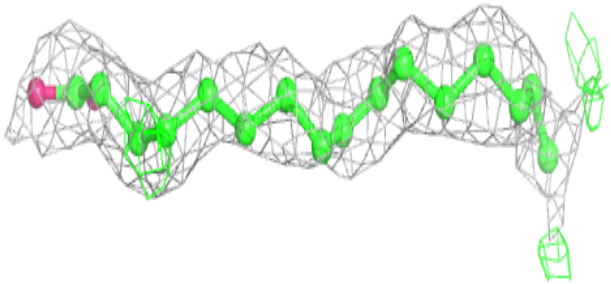


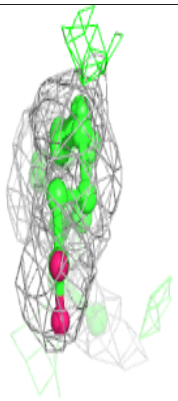


Electron density around OLA A 2409:

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

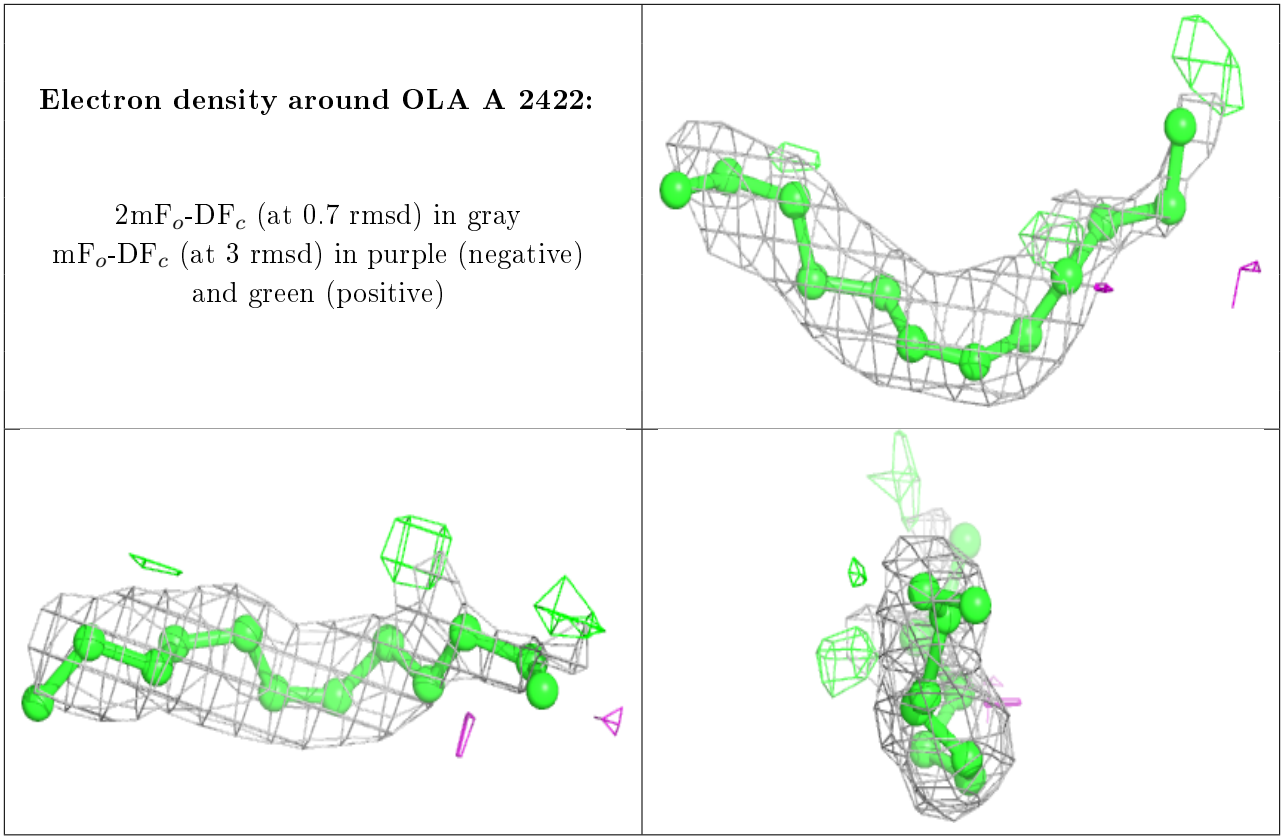






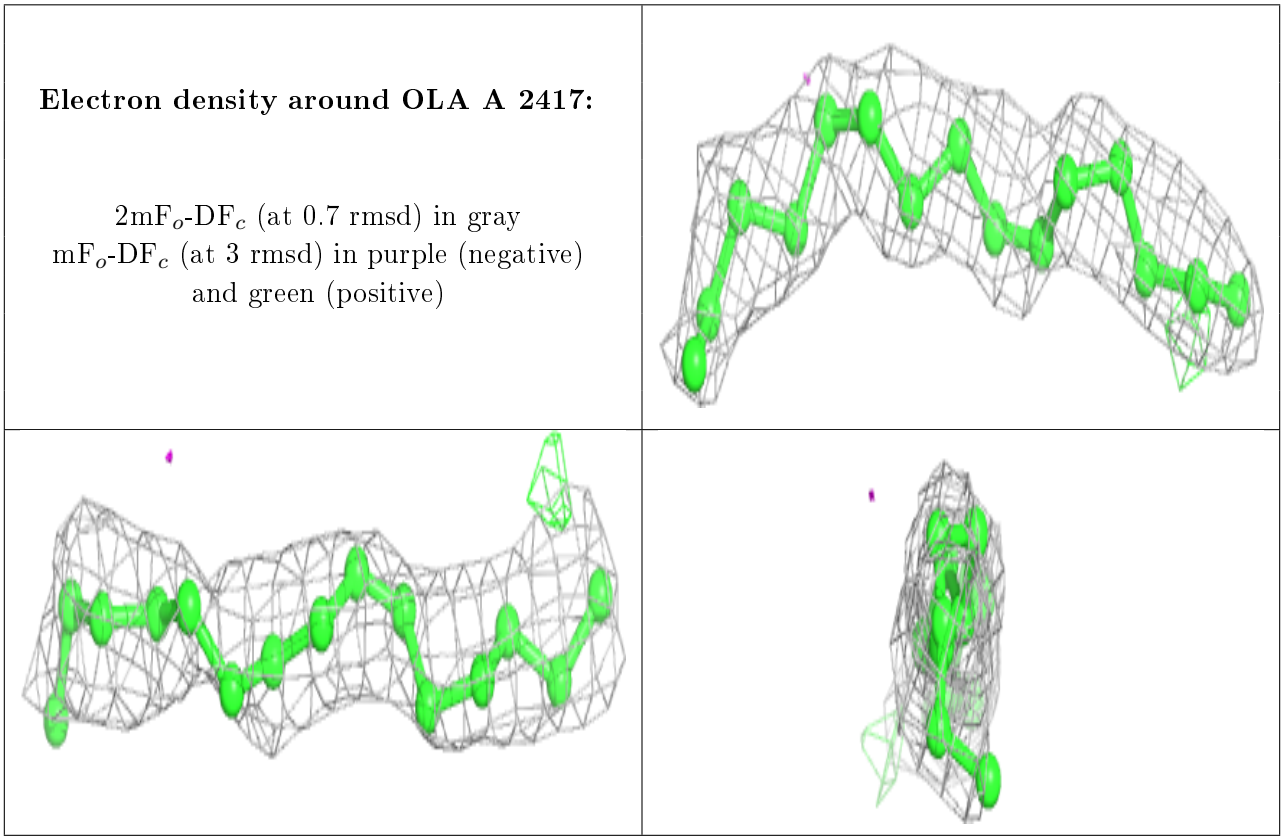
Electron density around OLA A 2422:

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



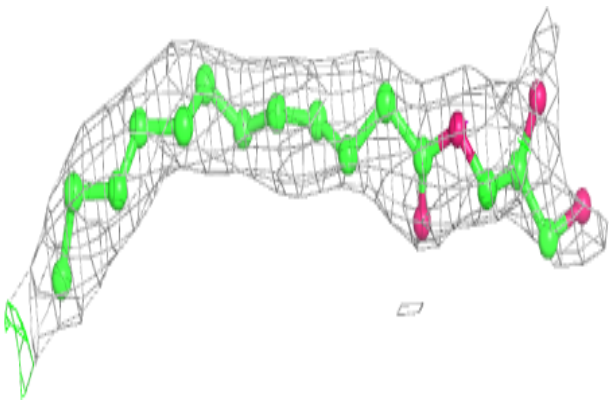
Electron density around OLA A 2417:

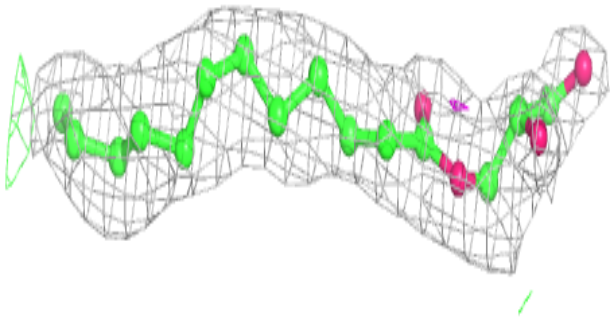
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

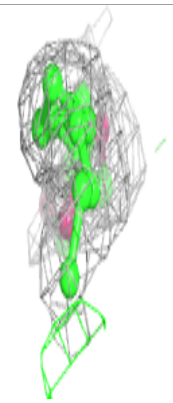


Electron density around OLB A 2427:

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

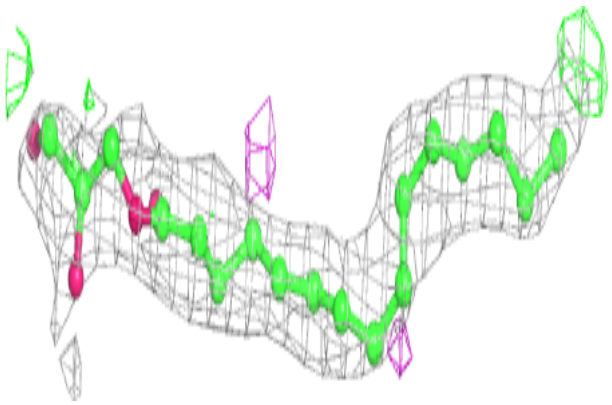


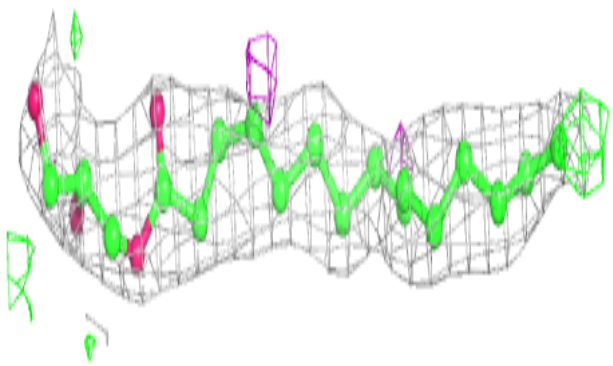


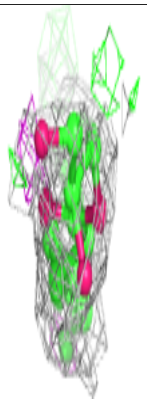


Electron density around OLB A 2426:

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

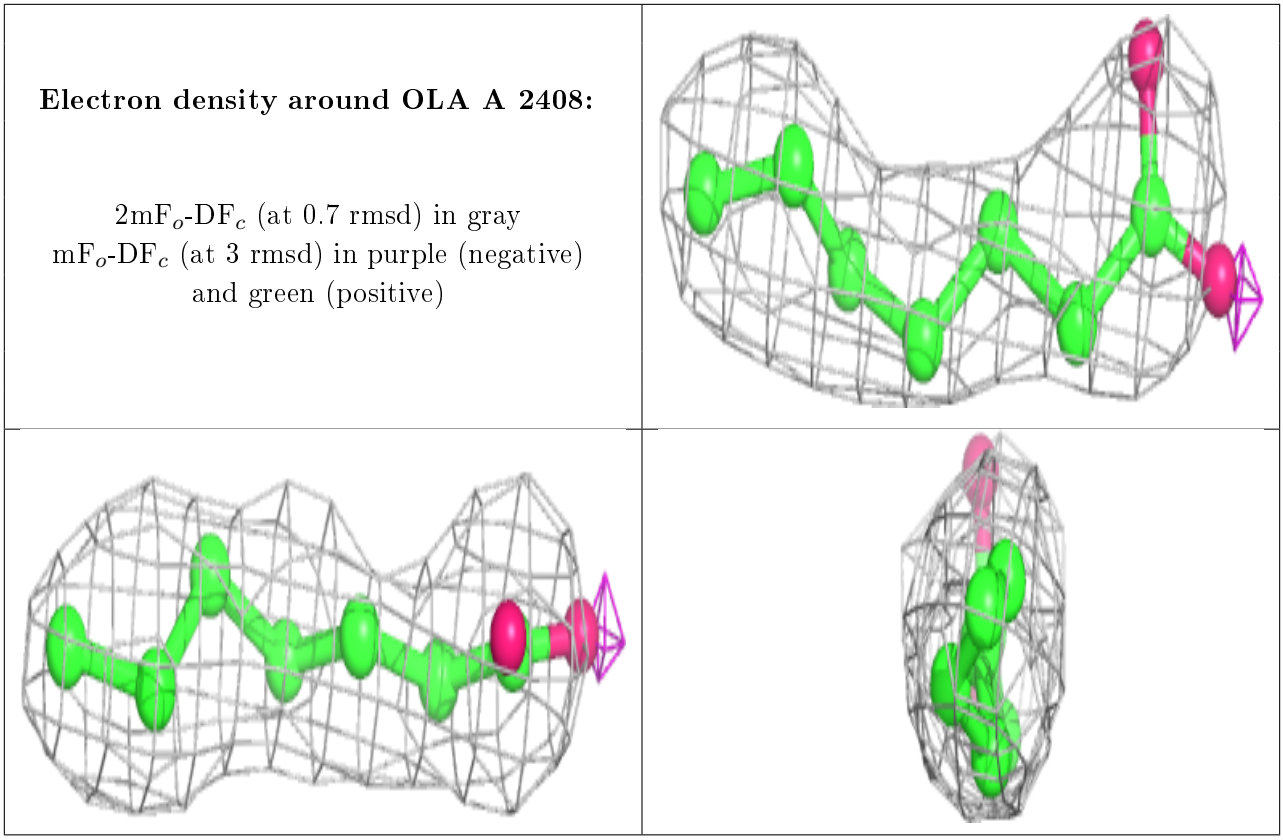






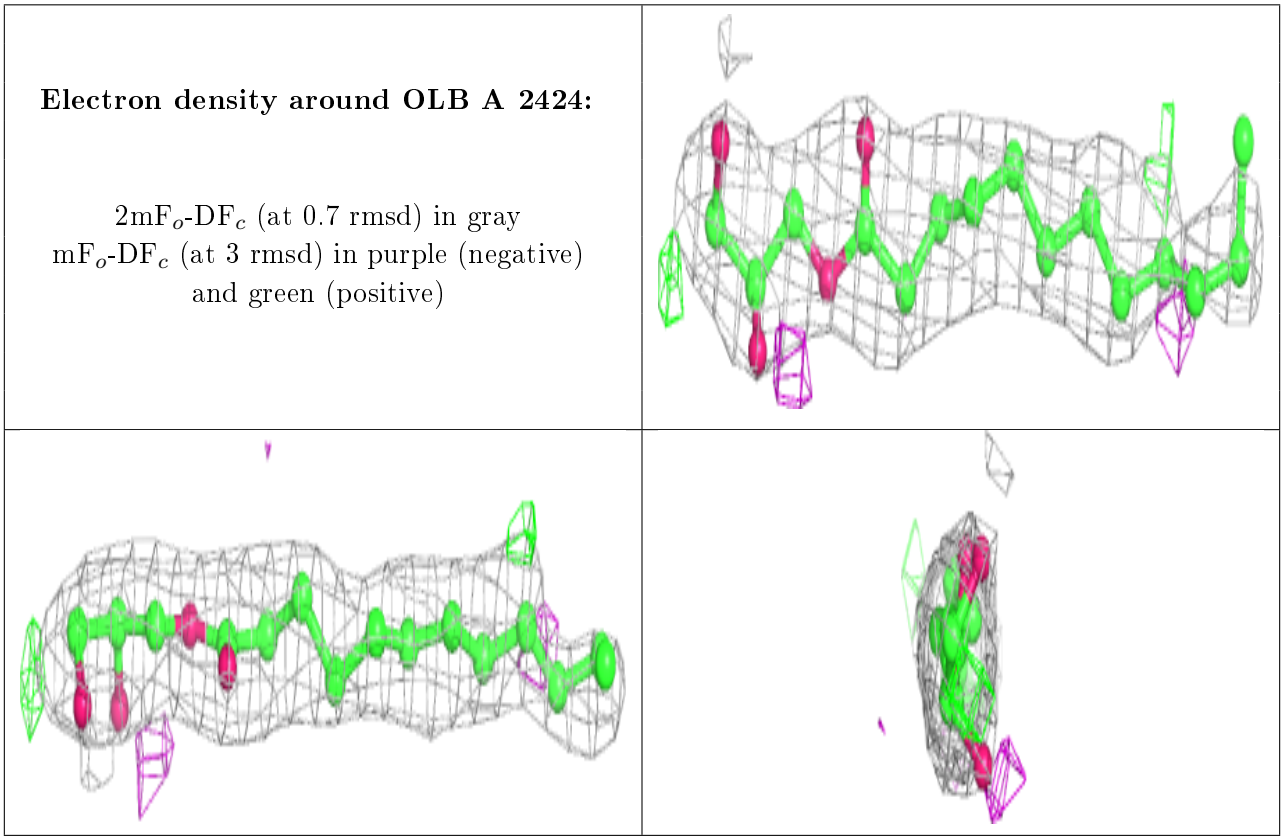
Electron density around OLA A 2408:

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



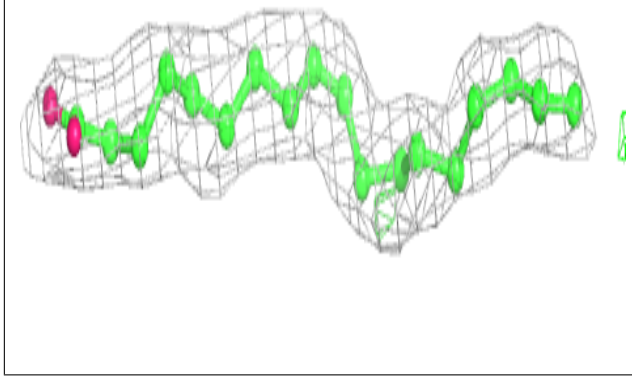
Electron density around OLB A 2424:

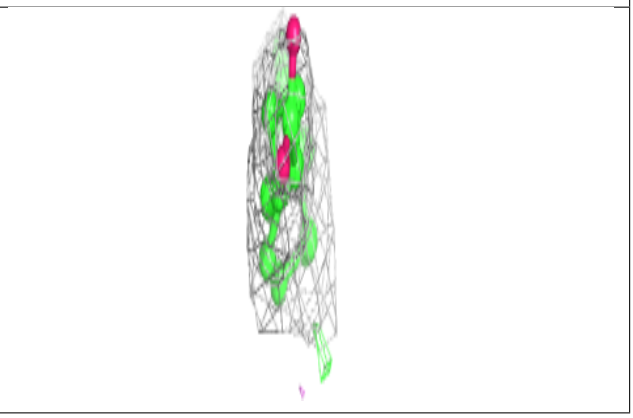
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA A 2406:

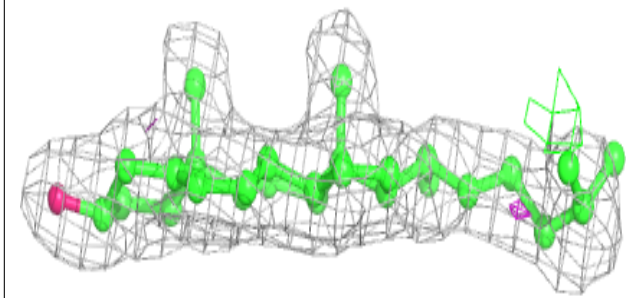
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

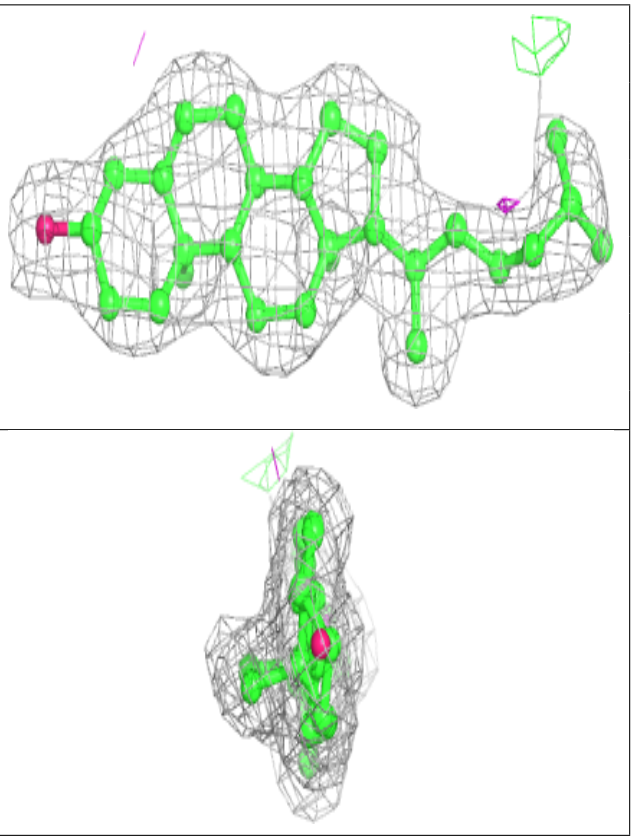




Electron density around CLR A 2405:

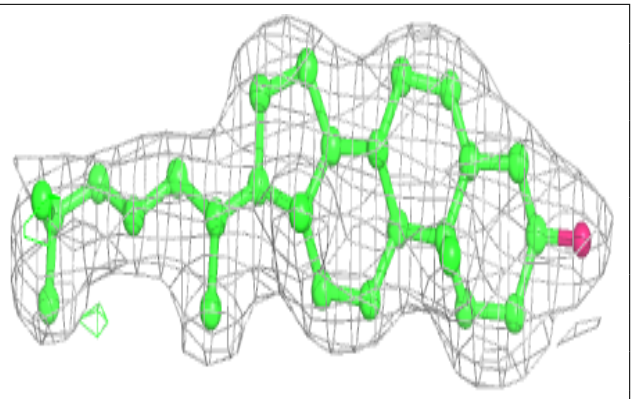
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

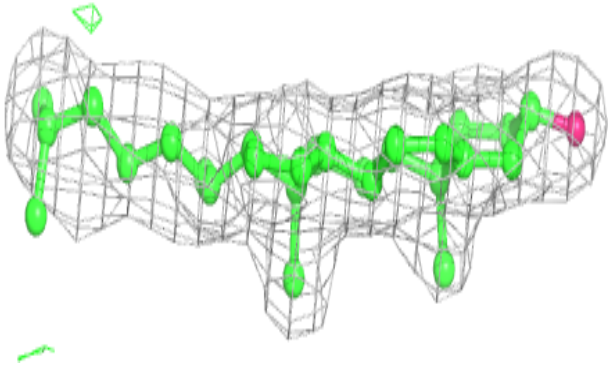


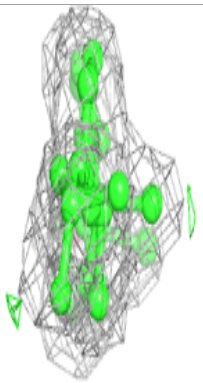


Electron density around CLR A 2404:

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

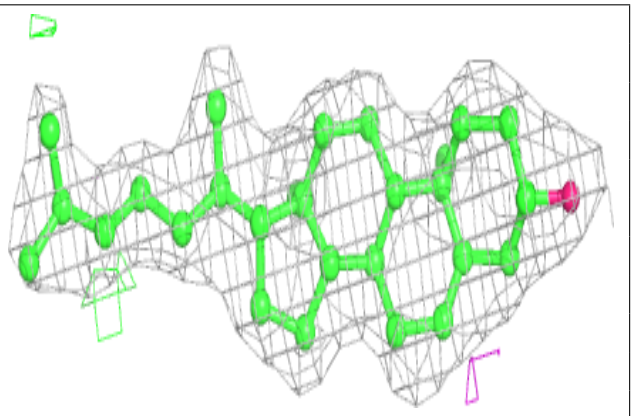


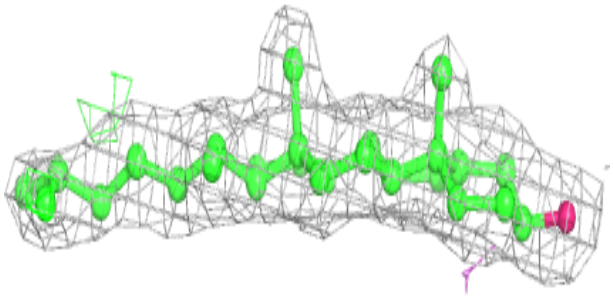


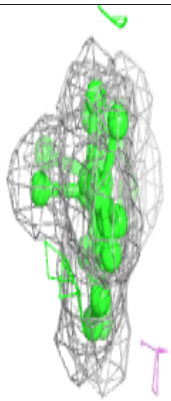


Electron density around CLR A 2403:

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

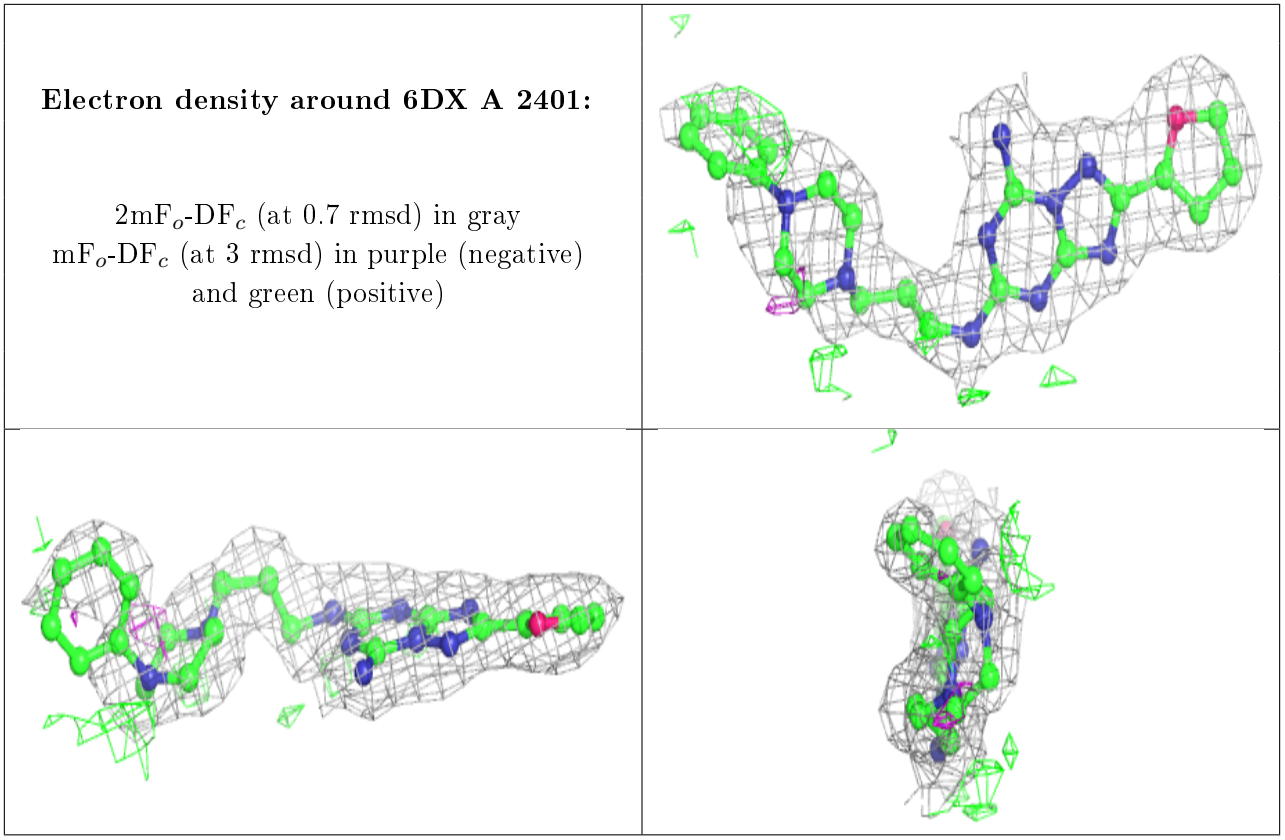






Electron density around 6DX A 2401:

$2mF_o$-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

There are no such residues in this entry.