Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:33 am BST

PDB ID	:	4EIY
Title	:	Crystal structure of the chimeric protein of A2aAR-BRIL in complex with ZM241385 at 1.8A resolution
Authors	:	Liu, W.; Chun, E.; Thompson, A.A.; Chubukov, P.; Xu, F.; Katritch, V.; Han, G.W.; Heitman, L.H.; Ijzerman, A.P.; Cherezov, V.; Stevens, R.C.; GPCR Network (GPCR)
Deposited on	:	2012-04-06
Resolution	:	1.80 Å(reported)

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

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

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

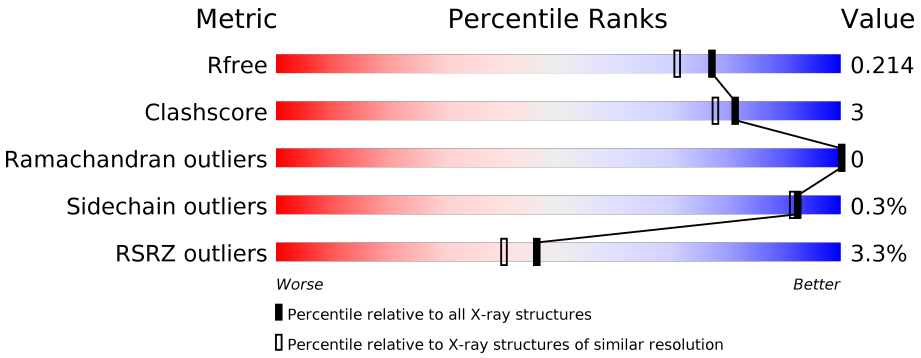
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	447	3% 81% 6% 13%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3771 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 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3105	2024	522	537	22	0	12	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	EXPRESSION TAG	UNP P29274
A	-23	LYS	-	EXPRESSION TAG	UNP P29274
A	-22	THR	-	EXPRESSION TAG	UNP P29274
A	-21	ILE	-	EXPRESSION TAG	UNP P29274
A	-20	ILE	-	EXPRESSION TAG	UNP P29274
A	-19	ALA	-	EXPRESSION TAG	UNP P29274
A	-18	LEU	-	EXPRESSION TAG	UNP P29274
A	-17	SER	-	EXPRESSION TAG	UNP P29274
A	-16	TYR	-	EXPRESSION TAG	UNP P29274
A	-15	ILE	-	EXPRESSION TAG	UNP P29274
A	-14	PHE	-	EXPRESSION TAG	UNP P29274
A	-13	CYS	-	EXPRESSION TAG	UNP P29274
A	-12	LEU	-	EXPRESSION TAG	UNP P29274
A	-11	VAL	-	EXPRESSION TAG	UNP P29274
A	-10	PHE	-	EXPRESSION TAG	UNP P29274
A	-9	ALA	-	EXPRESSION TAG	UNP P29274
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	1007	TRP	MET	ENGINEERED MUTATION	UNP P0ABE7

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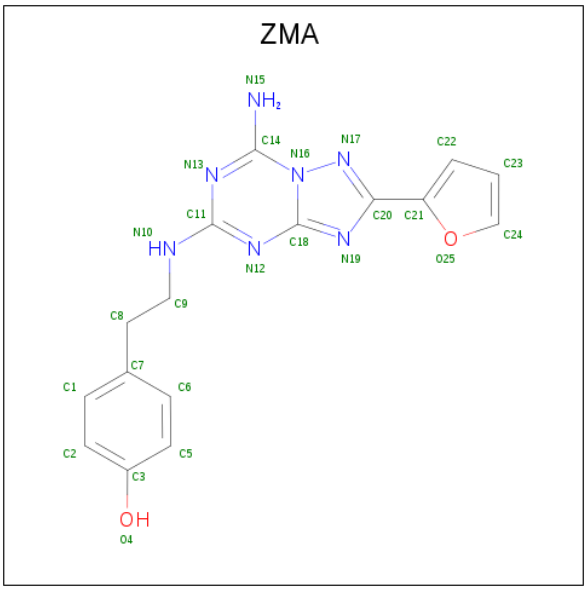
Chain	Residue	Modelled	Actual	Comment	Reference
A	1102	ILE	HIS	ENGINEERED MUTATION	UNP P0ABE7
A	1106	LEU	ARG	ENGINEERED MUTATION	UNP P0ABE7
A	317	HIS	-	EXPRESSION TAG	UNP P29274
A	318	HIS	-	EXPRESSION TAG	UNP P29274
A	319	HIS	-	EXPRESSION TAG	UNP P29274
A	320	HIS	-	EXPRESSION TAG	UNP P29274
A	321	HIS	-	EXPRESSION TAG	UNP P29274
A	322	HIS	-	EXPRESSION TAG	UNP P29274
A	323	HIS	-	EXPRESSION TAG	UNP P29274
A	324	HIS	-	EXPRESSION TAG	UNP P29274
A	325	HIS	-	EXPRESSION TAG	UNP P29274
A	326	HIS	-	EXPRESSION TAG	UNP P29274

- Molecule 2 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: $C_{16}H_{15}N_7O_2$).

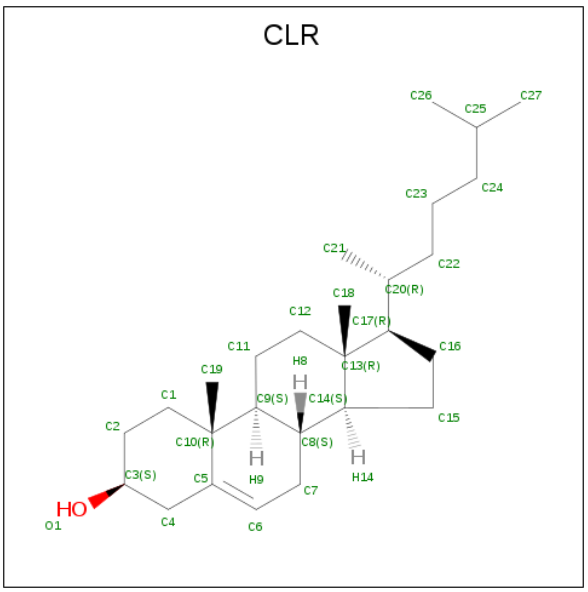


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 25 16 7 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

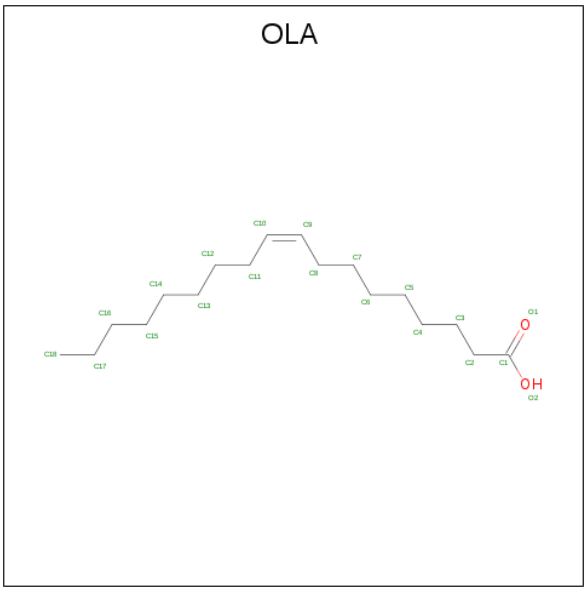
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

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



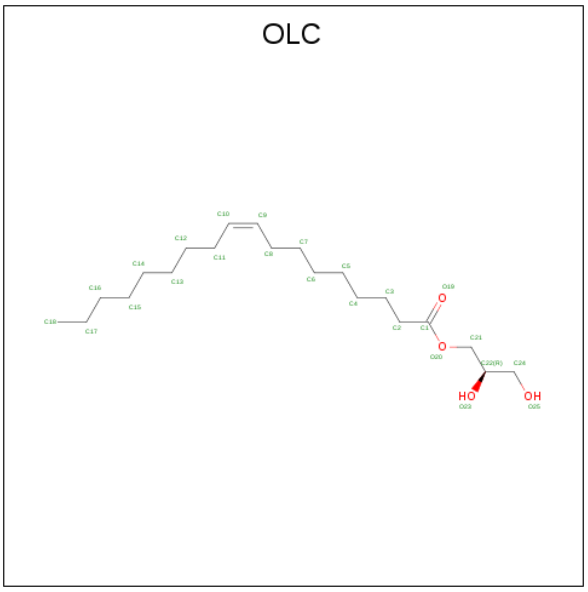
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0
4	A	1	Total C O 28 27 1	0	0

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



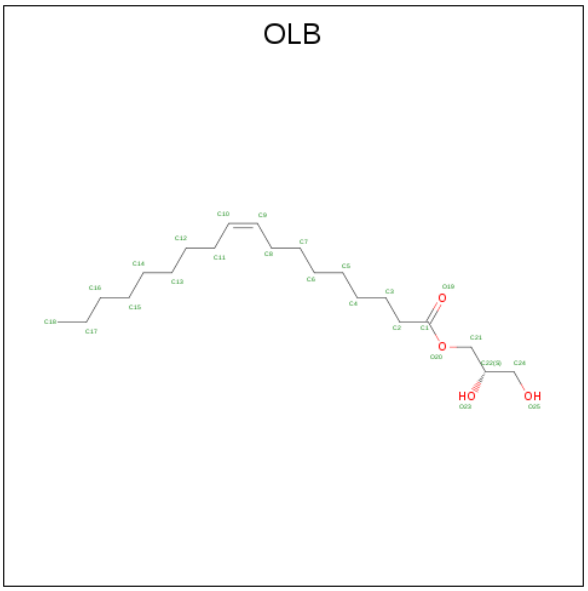
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C O 19 17 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C O 9 7 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 10 8 2	0	0
5	A	1	Total C O 9 7 2	0	0
5	A	1	Total C O 12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

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



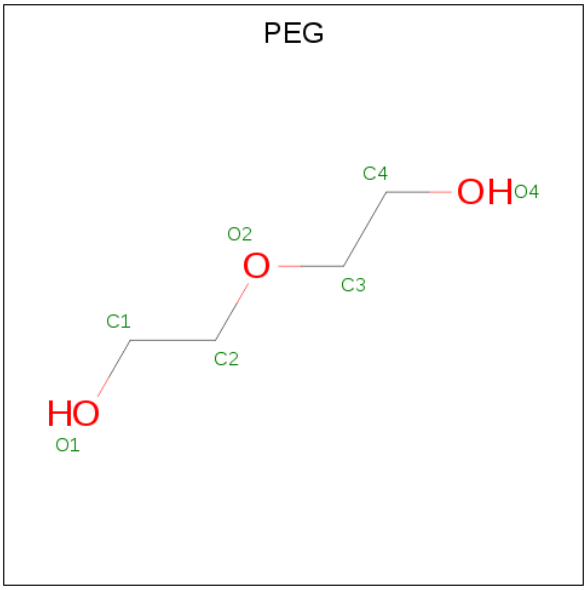
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 17 13 4	0	0
6	A	1	Total C O 15 11 4	0	0
6	A	1	Total C O 22 18 4	0	0
6	A	1	Total C O 17 13 4	0	0
6	A	1	Total C O 16 12 4	0	0
6	A	1	Total C O 21 17 4	0	0

- Molecule 7 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
7	A	1	Total C O 18 14 4	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0

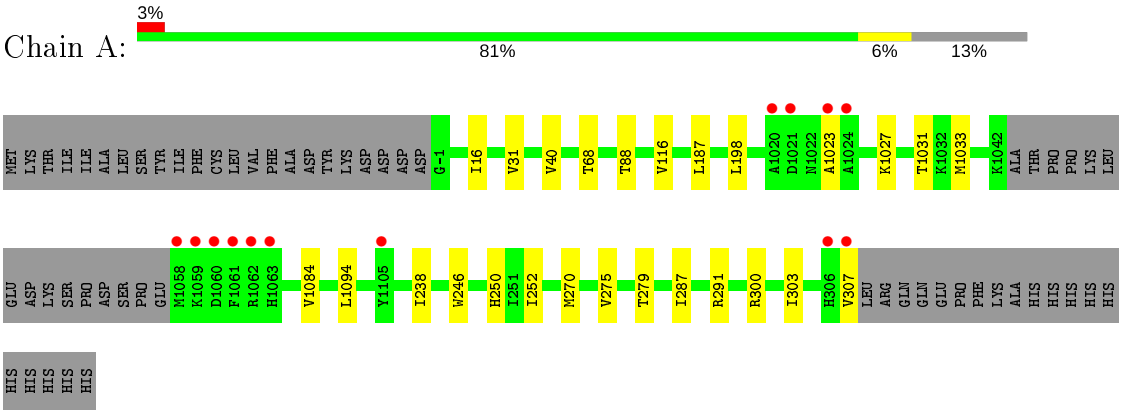
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	177	Total O 185 185	0	8

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 chimera



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.44Å 179.52Å 140.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 1.80 27.52 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.73-1.80) 94.5 (27.52-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.174 , 0.213 0.180 , 0.214	Depositor DCC
R_{free} test set	2221 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3771	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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, PEG, 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	0.66	0/3170	0.61	0/4313

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	3105	0	3158	19	0
2	A	25	0	15	1	0
3	A	1	0	0	0	0
4	A	84	0	138	2	0
5	A	231	0	324	3	0
6	A	108	0	144	0	0
7	A	18	0	23	1	0
8	A	14	0	20	0	0
9	A	185	0	0	0	0
All	All	3771	0	3822	19	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 (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:O	1:A:279[B]:THR:HG23	1.93	0.68
1:A:300[B]:ARG:HG2	1:A:300[B]:ARG:HH21	1.67	0.59
1:A:250:HIS:CE1	2:A:2401:ZMA:H24	2.39	0.57
1:A:31:VAL:HG12	7:A:2426:OLB:H24A	1.87	0.56
1:A:300[B]:ARG:NH2	1:A:300[B]:ARG:HG2	2.22	0.54
1:A:1027:LYS:O	1:A:1031:THR:HG23	2.15	0.47
1:A:1023:ALA:CA	1:A:1084:VAL:HG22	2.45	0.46
1:A:198[B]:LEU:HD23	5:A:2413:OLA:C2	2.46	0.45
1:A:303:ILE:HG23	1:A:307:VAL:CG2	2.47	0.45
1:A:1033:MET:CE	1:A:1094:LEU:HD13	2.47	0.45
1:A:252:ILE:HG21	1:A:270:MET:SD	2.58	0.44
1:A:238[B]:ILE:HD11	1:A:287:ILE:HB	1.99	0.43
1:A:16:ILE:HD11	1:A:275:VAL:HG13	2.01	0.42
1:A:198[B]:LEU:HD23	5:A:2413:OLA:C3	2.50	0.41
1:A:187:LEU:CD1	4:A:2405:CLR:H263	2.50	0.41
1:A:88[B]:THR:HG22	1:A:246:TRP:CZ2	2.55	0.41
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.51	0.40
1:A:187:LEU:HD11	4:A:2405:CLR:H263	2.02	0.40
1:A:68:THR:HG21	5:A:2406:OLA:H21	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	398/447 (89%)	394 (99%)	4 (1%)	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	326/374 (87%)	325 (100%)	1 (0%)	92 91

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

Mol	Chain	Res	Type
1	A	291	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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	$\#\|Z\|>2$
6	OLC	A	2428	-	20,20,24	1.13	1 (5%)	21,21,25	1.14	2 (9%)
5	OLA	A	2406	-	16,19,19	0.41	0	15,19,19	0.26	0
8	PEG	A	2430	-	6,6,6	0.52	0	5,5,5	0.17	0
5	OLA	A	2408	-	7,10,19	0.35	0	6,10,19	0.69	0
7	OLB	A	2426	-	17,17,24	1.19	1 (5%)	18,18,25	0.96	1 (5%)
5	OLA	A	2416	-	14,17,19	0.37	0	13,17,19	0.42	0
5	OLA	A	2420	-	11,14,19	0.28	0	10,14,19	0.68	0
5	OLA	A	2409	-	15,18,19	0.23	0	14,18,19	0.59	0
6	OLC	A	2423	-	14,14,24	1.26	1 (7%)	15,15,25	0.87	1 (6%)
5	OLA	A	2421	-	15,18,19	0.26	0	14,18,19	0.57	0
5	OLA	A	2414	-	5,8,19	0.30	0	4,8,19	0.51	0
5	OLA	A	2419	-	11,14,19	0.36	0	10,14,19	0.37	0
5	OLA	A	2417	-	16,19,19	0.40	0	15,19,19	0.44	0
5	OLA	A	2407	-	11,14,19	0.30	0	10,14,19	0.49	0
6	OLC	A	2425	-	16,16,24	1.20	1 (6%)	17,17,25	1.36	2 (11%)
5	OLA	A	2418	-	16,19,19	0.37	0	15,19,19	0.41	0
8	PEG	A	2429	-	6,6,6	0.51	0	5,5,5	0.27	0
5	OLA	A	2415	-	8,11,19	0.24	0	7,11,19	0.73	0
5	OLA	A	2411	-	5,8,19	0.14	0	4,8,19	0.91	0
6	OLC	A	2424	-	21,21,24	0.93	1 (4%)	22,22,25	0.76	0
2	ZMA	A	2401	-	21,28,28	0.63	0	22,39,39	2.43	4 (18%)
5	OLA	A	2413	-	6,9,19	0.36	0	5,9,19	0.36	0
4	CLR	A	2405	-	31,31,31	0.85	0	48,48,48	1.11	3 (6%)
6	OLC	A	2422	-	16,16,24	1.16	1 (6%)	17,17,25	1.17	2 (11%)
5	OLA	A	2412	-	4,7,19	0.36	0	3,7,19	0.54	0
6	OLC	A	2427	-	15,15,24	1.03	1 (6%)	16,16,25	1.24	2 (12%)
4	CLR	A	2404	-	31,31,31	0.75	0	48,48,48	1.58	7 (14%)
4	CLR	A	2403	-	31,31,31	0.69	0	48,48,48	0.97	1 (2%)
5	OLA	A	2410	-	7,10,19	0.25	0	6,10,19	0.80	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
6	OLC	A	2428	-	-	9/20/20/24	-
5	OLA	A	2406	-	-	10/15/17/17	-
8	PEG	A	2430	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	2408	-	-	1/6/8/17	-
7	OLB	A	2426	-	-	9/17/17/24	-
5	OLA	A	2416	-	-	5/13/15/17	-
5	OLA	A	2420	-	-	2/10/12/17	-
5	OLA	A	2409	-	-	3/14/16/17	-
6	OLC	A	2423	-	-	3/14/14/24	-
5	OLA	A	2421	-	-	5/14/16/17	-
5	OLA	A	2414	-	-	2/4/6/17	-
5	OLA	A	2419	-	-	4/10/12/17	-
5	OLA	A	2417	-	-	4/15/17/17	-
5	OLA	A	2407	-	-	5/10/12/17	-
6	OLC	A	2425	-	-	9/16/16/24	-
5	OLA	A	2418	-	-	8/15/17/17	-
8	PEG	A	2429	-	-	0/4/4/4	-
5	OLA	A	2415	-	-	3/7/9/17	-
5	OLA	A	2411	-	-	0/4/6/17	-
6	OLC	A	2424	-	-	7/21/21/24	-
2	ZMA	A	2401	-	-	0/6/10/10	0/4/4/4
5	OLA	A	2413	-	-	5/5/7/17	-
4	CLR	A	2405	-	-	2/10/68/68	0/4/4/4
6	OLC	A	2422	-	-	7/16/16/24	-
5	OLA	A	2412	-	-	0/3/5/17	-
6	OLC	A	2427	-	-	2/15/15/24	-
4	CLR	A	2404	-	-	2/10/68/68	0/4/4/4
4	CLR	A	2403	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2410	-	-	3/6/8/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2428	OLC	O20-C1	4.69	1.47	1.33
7	A	2426	OLB	O20-C1	4.65	1.46	1.33
6	A	2425	OLC	O20-C1	4.52	1.46	1.33
6	A	2423	OLC	O20-C1	4.48	1.46	1.33
6	A	2422	OLC	O20-C1	4.29	1.45	1.33
6	A	2424	OLC	O20-C1	3.88	1.44	1.33
6	A	2427	OLC	O20-C1	3.50	1.43	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2401	ZMA	N15-C14-N16	8.00	123.36	117.97
4	A	2404	CLR	C2-C3-C4	7.14	120.10	110.31
2	A	2401	ZMA	C9-C8-C7	-4.90	101.51	112.87
6	A	2425	OLC	O20-C1-C2	3.73	123.62	111.91
6	A	2428	OLC	O20-C1-C2	3.67	123.43	111.91
2	A	2401	ZMA	N17-C20-N19	3.51	116.88	114.56
6	A	2422	OLC	O20-C1-C2	3.35	122.43	111.91
2	A	2401	ZMA	N12-C11-N13	-3.28	121.05	126.23
4	A	2404	CLR	O1-C3-C4	3.07	116.26	109.68
4	A	2404	CLR	O1-C3-C2	2.94	117.64	110.16
6	A	2427	OLC	O20-C1-C2	2.87	120.90	111.91
6	A	2428	OLC	O20-C1-O19	-2.69	116.81	123.59
4	A	2404	CLR	C4-C5-C10	2.61	119.89	116.42
6	A	2425	OLC	O20-C1-O19	-2.54	117.18	123.59
6	A	2427	OLC	O20-C1-O19	-2.41	117.52	123.59
4	A	2405	CLR	C1-C2-C3	2.38	113.52	110.47
4	A	2404	CLR	C4-C5-C6	-2.35	117.22	120.61
6	A	2422	OLC	O20-C1-O19	-2.26	117.89	123.59
4	A	2405	CLR	C4-C5-C10	2.25	119.40	116.42
4	A	2404	CLR	C1-C2-C3	2.24	113.34	110.47
6	A	2423	OLC	O20-C1-C2	2.19	118.79	111.91
4	A	2404	CLR	C2-C1-C10	2.19	117.48	112.74
4	A	2405	CLR	C2-C3-C4	-2.18	107.32	110.31
7	A	2426	OLB	O20-C1-C2	2.15	118.67	111.91
4	A	2403	CLR	C7-C8-C14	-2.03	107.97	110.91

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2428	OLC	C21-C22-C24-O25
5	A	2406	OLA	C1-C2-C3-C4
5	A	2420	OLA	C10-C11-C12-C13
5	A	2414	OLA	C1-C2-C3-C4
5	A	2407	OLA	C10-C11-C12-C13
5	A	2413	OLA	C1-C2-C3-C4
5	A	2410	OLA	C1-C2-C3-C4
8	A	2430	PEG	O2-C3-C4-O4
6	A	2428	OLC	C2-C1-O20-C21
6	A	2428	OLC	O19-C1-O20-C21
6	A	2428	OLC	O23-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
4	A	2405	CLR	C22-C23-C24-C25
7	A	2426	OLB	C2-C1-O20-C21
6	A	2424	OLC	O20-C21-C22-O23
6	A	2422	OLC	C2-C1-O20-C21
5	A	2417	OLA	C10-C11-C12-C13
5	A	2409	OLA	C5-C6-C7-C8
5	A	2406	OLA	C3-C4-C5-C6
5	A	2417	OLA	C13-C14-C15-C16
6	A	2425	OLC	C2-C3-C4-C5
6	A	2424	OLC	O20-C21-C22-C24
5	A	2418	OLA	C12-C13-C14-C15
5	A	2407	OLA	C5-C6-C7-C8
7	A	2426	OLB	O19-C1-O20-C21
6	A	2425	OLC	C3-C4-C5-C6
7	A	2426	OLB	C22-C21-O20-C1
5	A	2406	OLA	C13-C14-C15-C16
6	A	2425	OLC	C5-C6-C7-C8
6	A	2422	OLC	C21-C22-C24-O25
5	A	2406	OLA	C14-C15-C16-C17
5	A	2406	OLA	C4-C5-C6-C7
5	A	2416	OLA	C2-C3-C4-C5
5	A	2421	OLA	C3-C4-C5-C6
6	A	2422	OLC	C5-C6-C7-C8
5	A	2418	OLA	C11-C12-C13-C14
6	A	2422	OLC	O19-C1-O20-C21
6	A	2427	OLC	C5-C6-C7-C8
5	A	2418	OLA	C5-C6-C7-C8
6	A	2423	OLC	C4-C5-C6-C7
5	A	2406	OLA	C10-C11-C12-C13
5	A	2421	OLA	C6-C7-C8-C9
5	A	2421	OLA	C10-C11-C12-C13
5	A	2419	OLA	C6-C7-C8-C9
5	A	2419	OLA	C3-C4-C5-C6
5	A	2418	OLA	C14-C15-C16-C17
7	A	2426	OLB	C4-C5-C6-C7
6	A	2424	OLC	C6-C7-C8-C9
6	A	2424	OLC	C5-C6-C7-C8
6	A	2428	OLC	C11-C12-C13-C14
5	A	2416	OLA	C4-C5-C6-C7
5	A	2410	OLA	C2-C3-C4-C5
6	A	2423	OLC	C3-C4-C5-C6
6	A	2424	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	A	2422	OLC	C2-C3-C4-C5
5	A	2406	OLA	C2-C3-C4-C5
5	A	2406	OLA	C11-C12-C13-C14
5	A	2413	OLA	C3-C4-C5-C6
6	A	2422	OLC	O23-C22-C24-O25
7	A	2426	OLB	C5-C6-C7-C8
5	A	2413	OLA	C4-C5-C6-C7
5	A	2418	OLA	C3-C4-C5-C6
5	A	2421	OLA	C14-C15-C16-C17
5	A	2417	OLA	C14-C15-C16-C17
5	A	2415	OLA	C4-C5-C6-C7
5	A	2419	OLA	C5-C6-C7-C8
8	A	2430	PEG	C4-C3-O2-C2
5	A	2407	OLA	C2-C3-C4-C5
6	A	2425	OLC	O23-C22-C24-O25
5	A	2416	OLA	C12-C13-C14-C15
6	A	2424	OLC	C11-C12-C13-C14
4	A	2404	CLR	C23-C24-C25-C27
5	A	2415	OLA	C6-C7-C8-C9
5	A	2419	OLA	C7-C8-C9-C10
6	A	2425	OLC	C4-C5-C6-C7
7	A	2426	OLB	O20-C21-C22-O23
5	A	2413	OLA	C2-C3-C4-C5
4	A	2404	CLR	C23-C24-C25-C26
6	A	2425	OLC	C2-C1-O20-C21
5	A	2408	OLA	C4-C5-C6-C7
5	A	2407	OLA	C6-C7-C8-C9
6	A	2428	OLC	C2-C3-C4-C5
6	A	2423	OLC	O20-C21-C22-O23
5	A	2418	OLA	C7-C8-C9-C10
5	A	2409	OLA	C4-C5-C6-C7
6	A	2427	OLC	C6-C7-C8-C9
5	A	2416	OLA	C5-C6-C7-C8
6	A	2424	OLC	C10-C11-C12-C13
5	A	2415	OLA	C5-C6-C7-C8
5	A	2413	OLA	C5-C6-C7-C8
5	A	2418	OLA	C4-C5-C6-C7
6	A	2422	OLC	C3-C4-C5-C6
7	A	2426	OLB	C2-C3-C4-C5
5	A	2410	OLA	C6-C7-C8-C9
6	A	2428	OLC	C6-C7-C8-C9
5	A	2406	OLA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	A	2425	OLC	C21-C22-C24-O25
5	A	2418	OLA	C9-C10-C11-C12
6	A	2425	OLC	O19-C1-O20-C21
6	A	2425	OLC	C7-C8-C9-C10
6	A	2428	OLC	C7-C8-C9-C10
7	A	2426	OLB	C6-C7-C8-C9
5	A	2420	OLA	C7-C8-C9-C10
5	A	2407	OLA	C9-C10-C11-C12
5	A	2421	OLA	C5-C6-C7-C8
7	A	2426	OLB	C7-C8-C9-C10
5	A	2409	OLA	C7-C8-C9-C10
5	A	2406	OLA	C7-C8-C9-C10
5	A	2416	OLA	C9-C10-C11-C12
5	A	2417	OLA	C15-C16-C17-C18
5	A	2414	OLA	C3-C4-C5-C6
4	A	2405	CLR	C20-C22-C23-C24
6	A	2428	OLC	C10-C11-C12-C13

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2406	OLA	1	0
7	A	2426	OLB	1	0
2	A	2401	ZMA	1	0
5	A	2413	OLA	2	0
4	A	2405	CLR	2	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.

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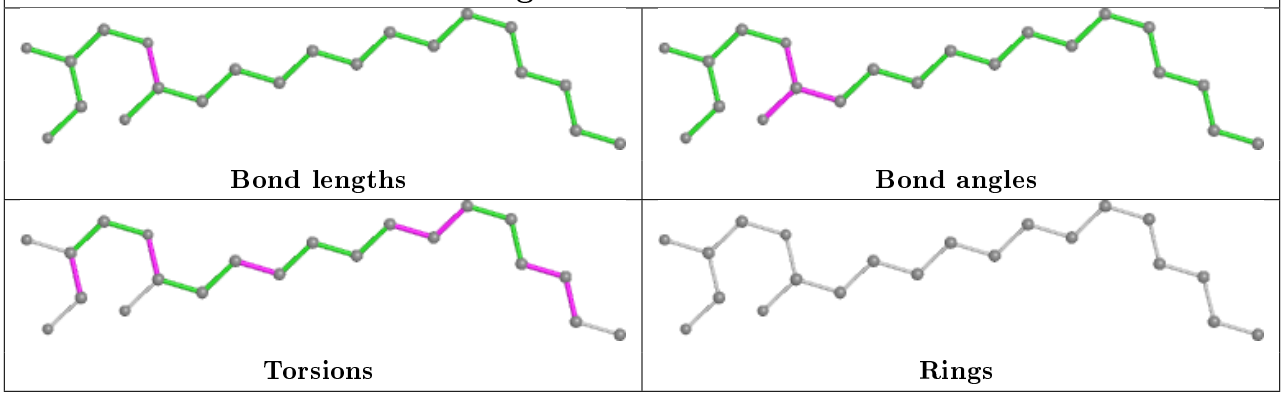

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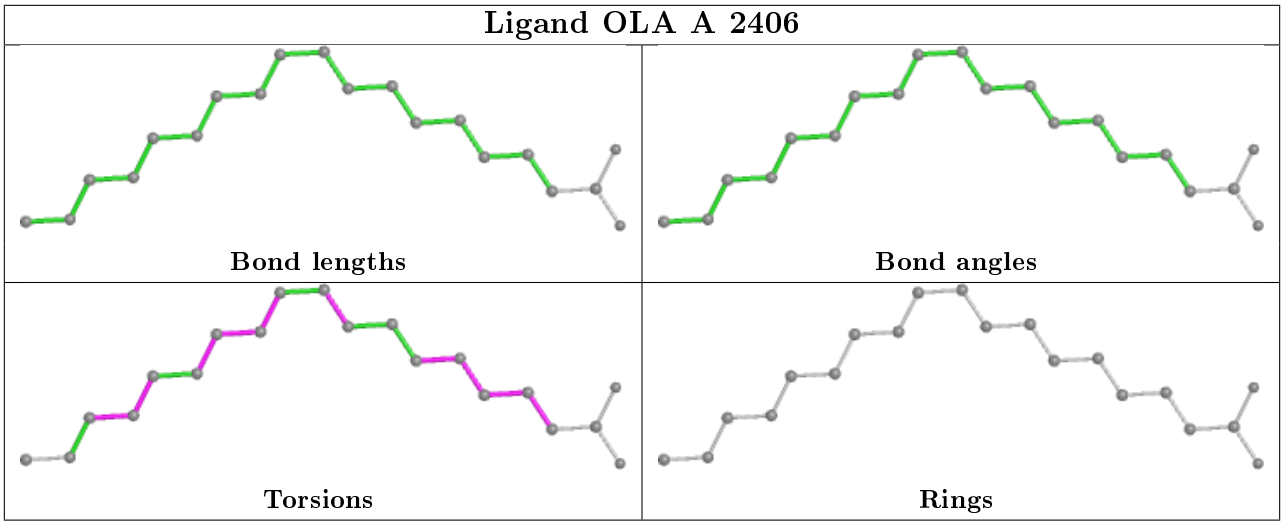

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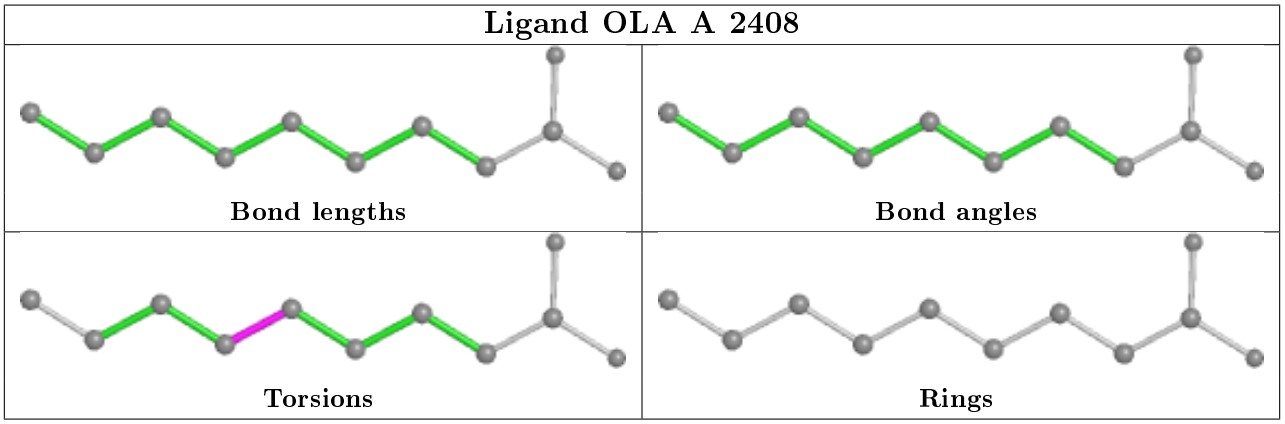

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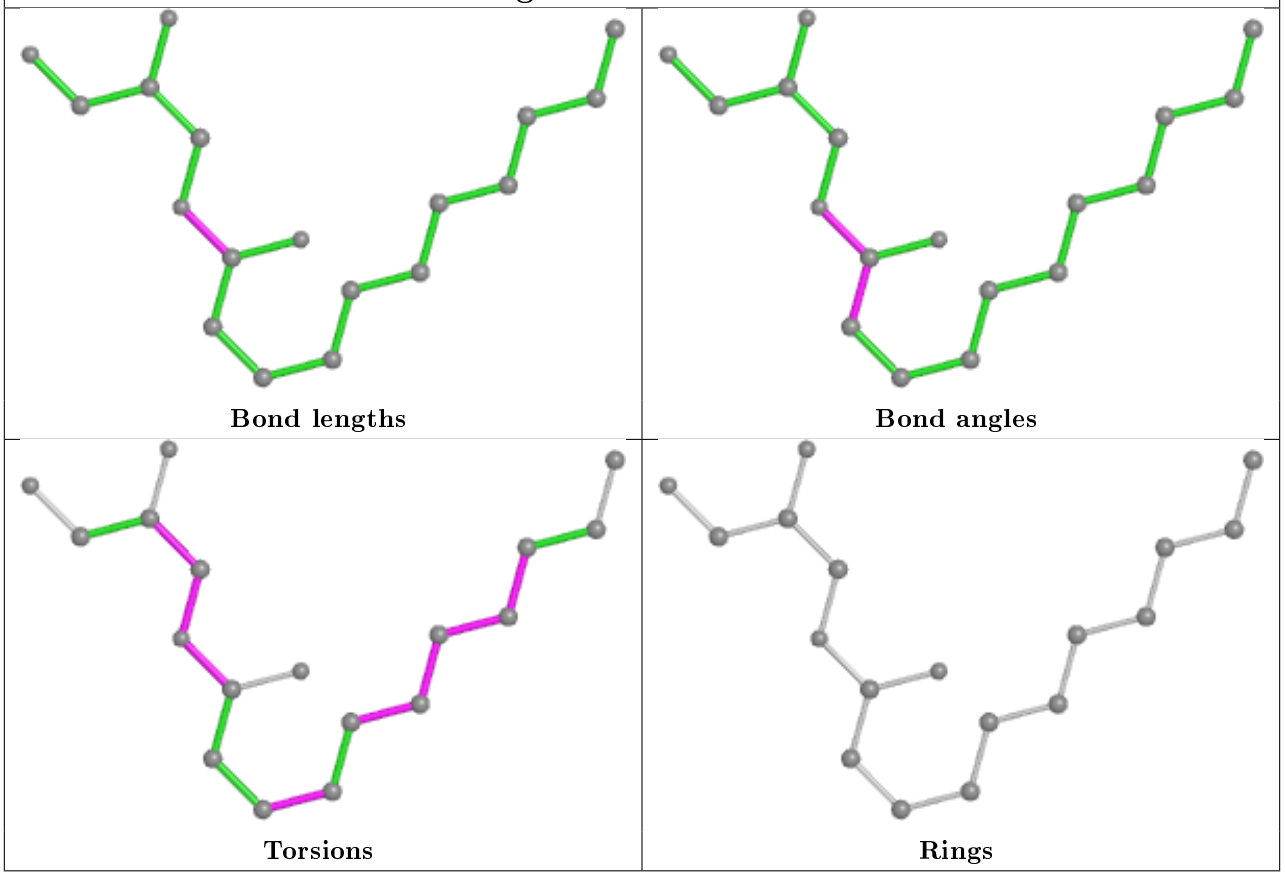

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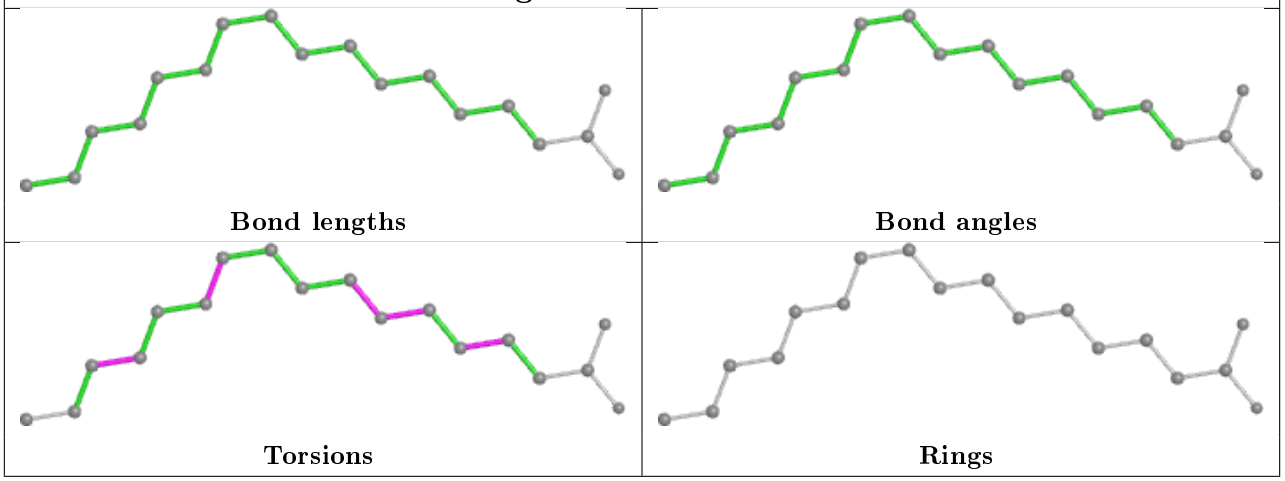

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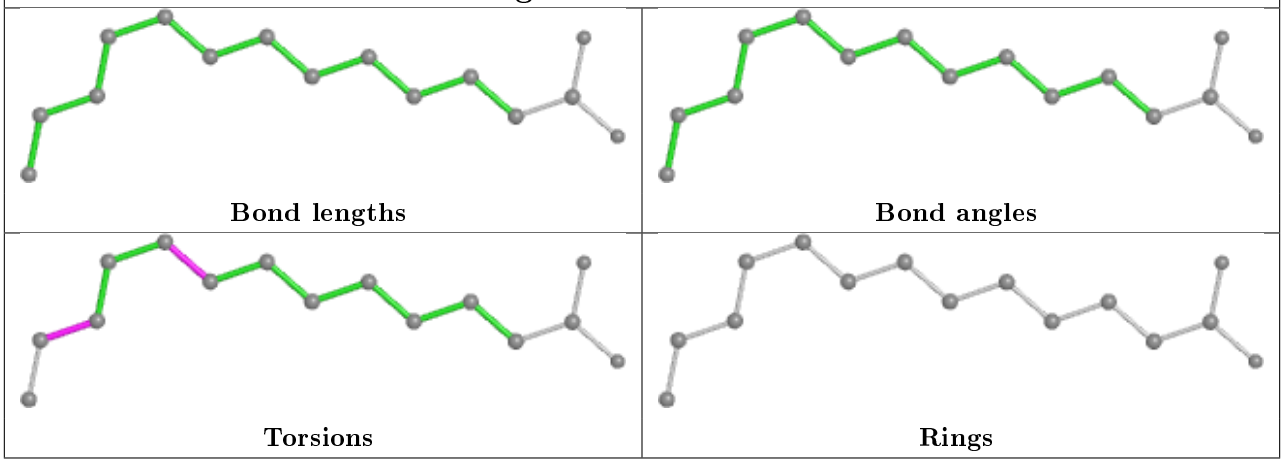

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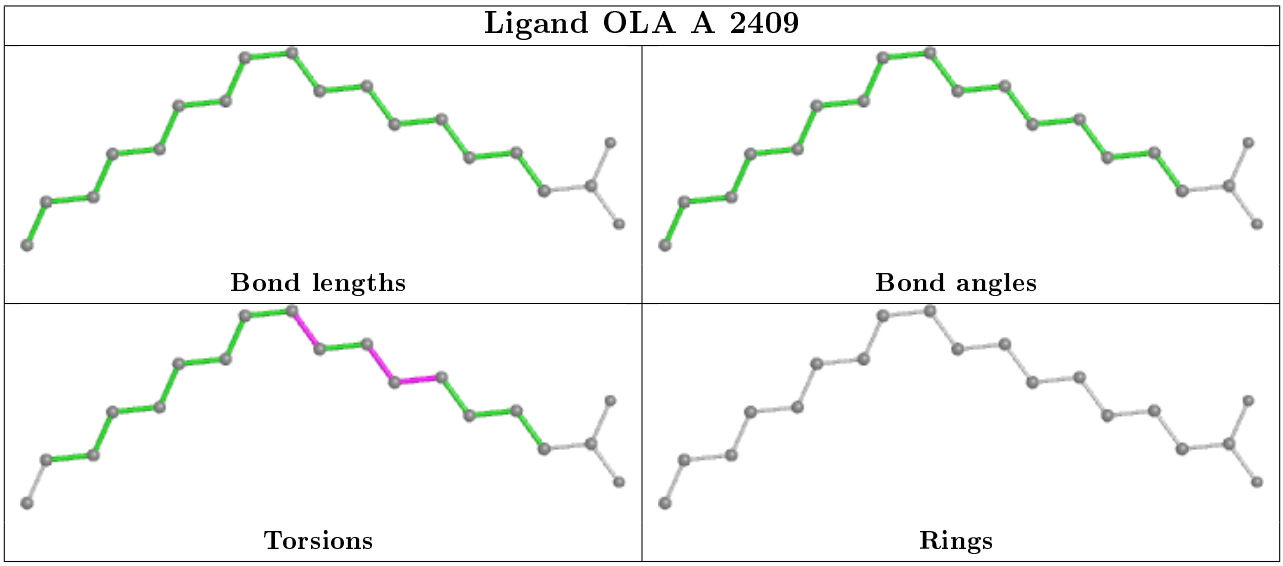

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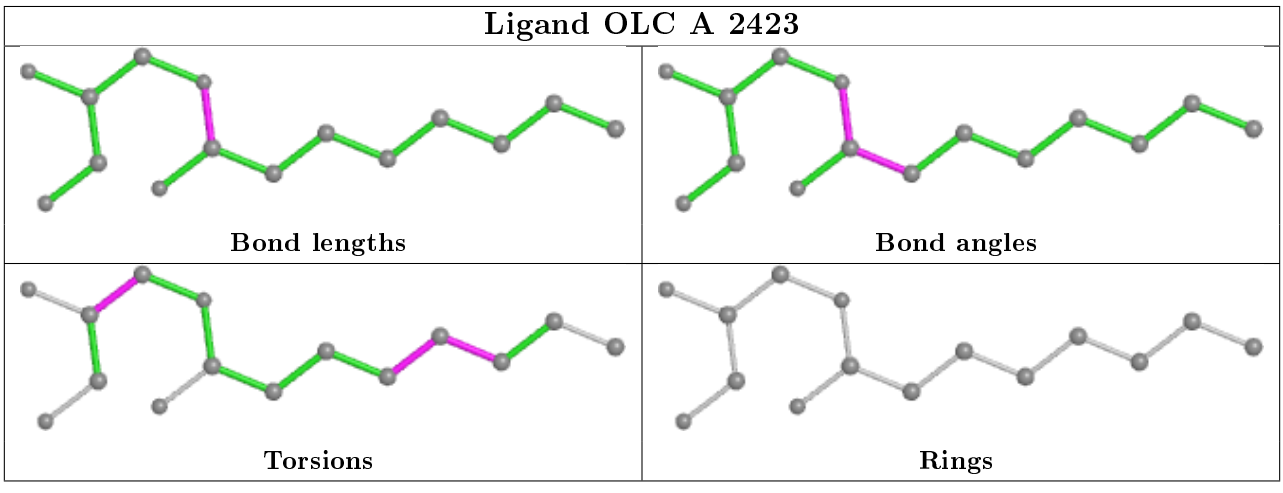

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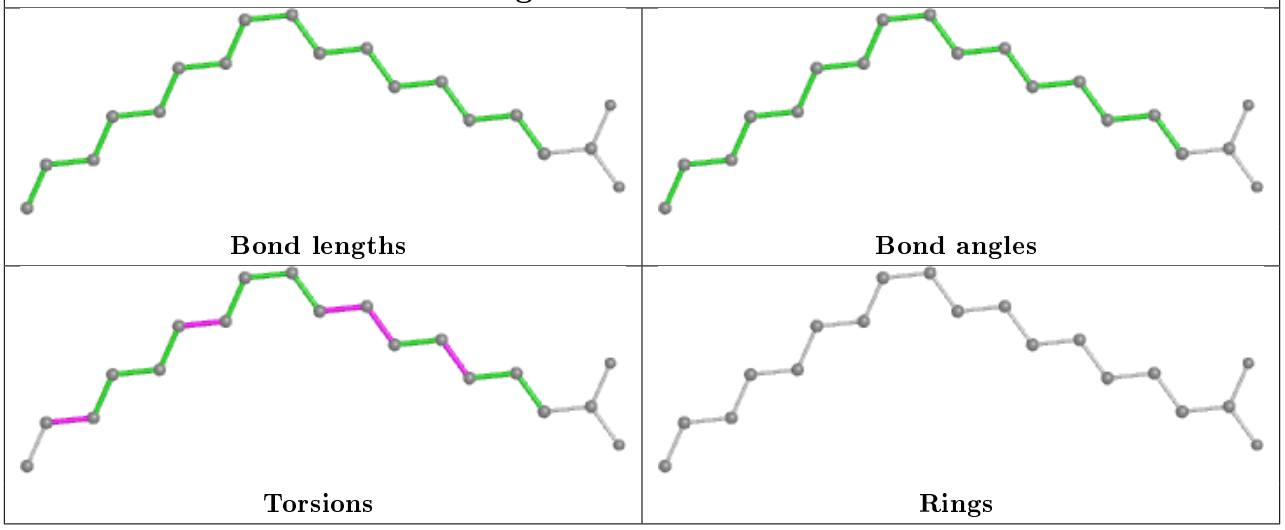

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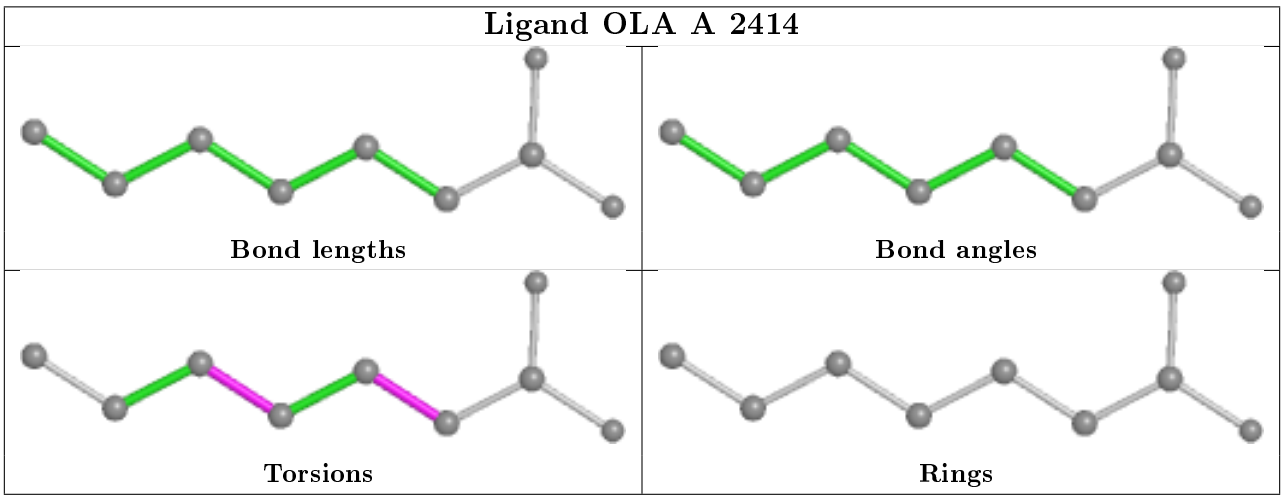

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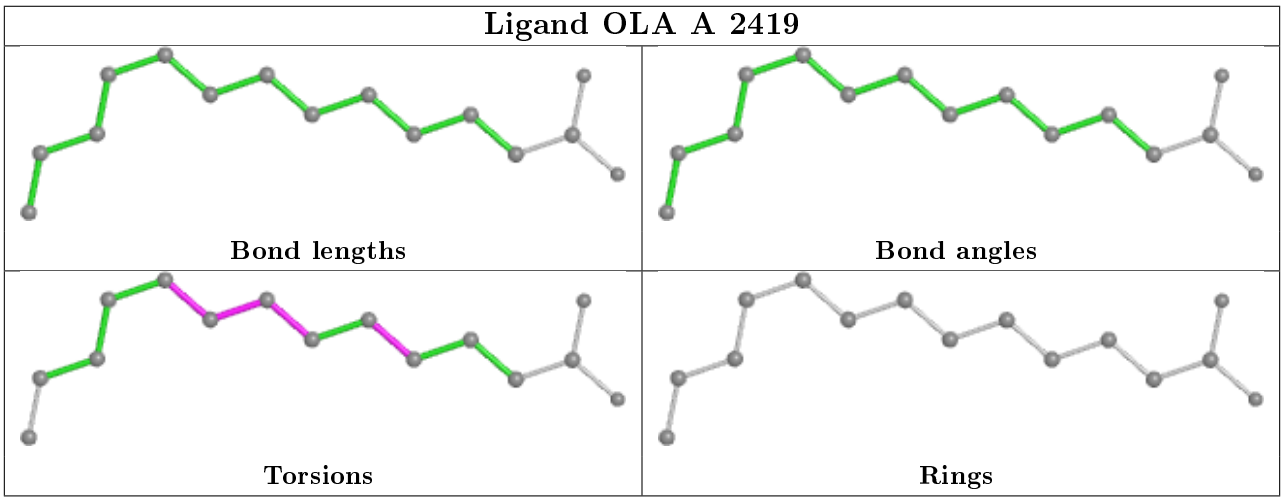

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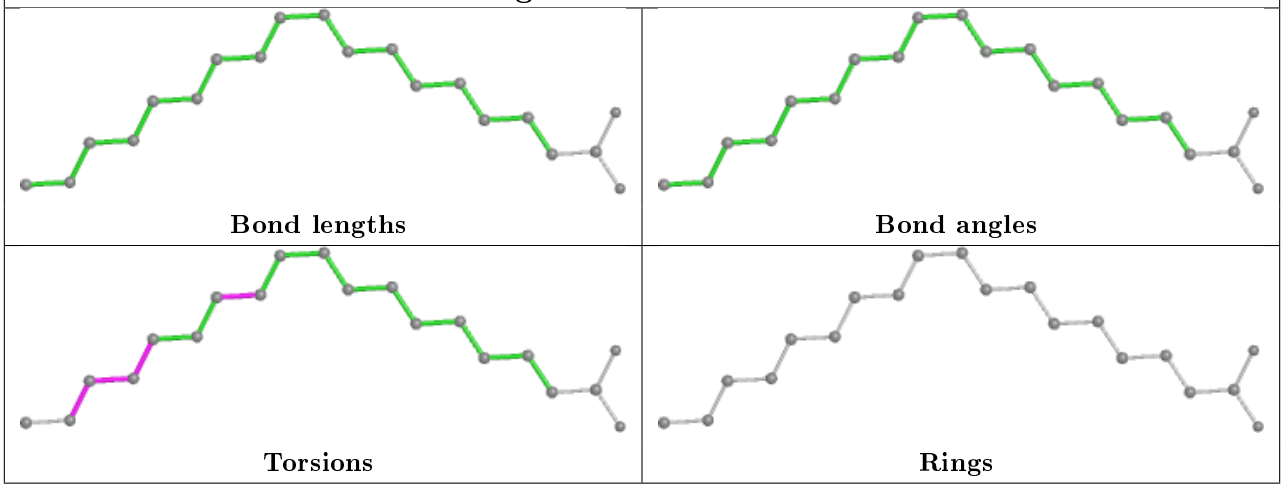

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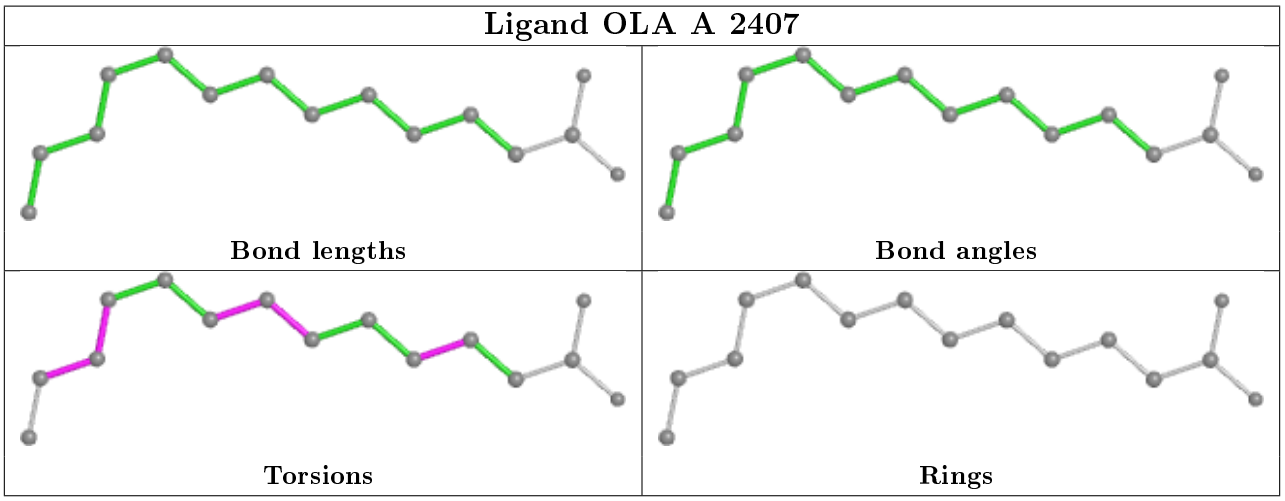

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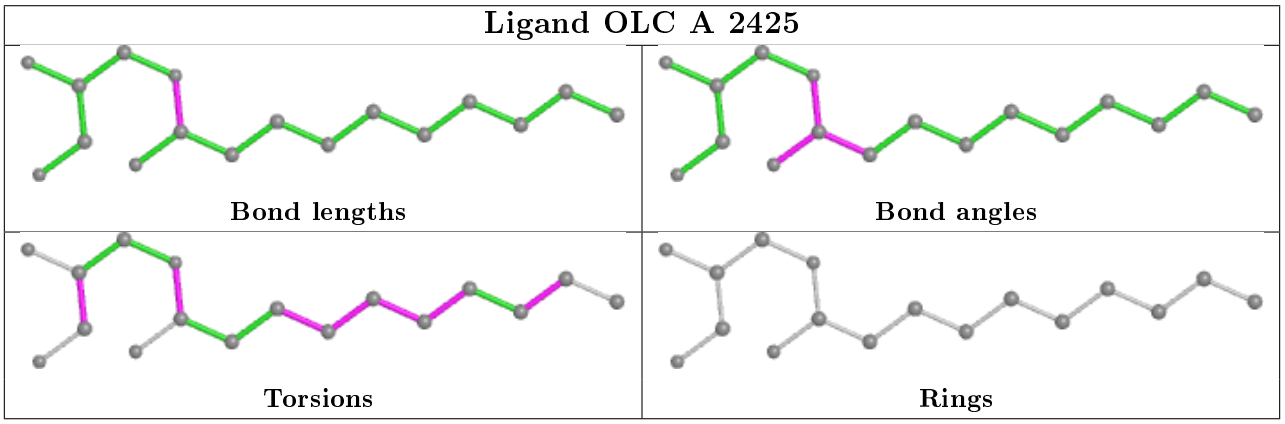

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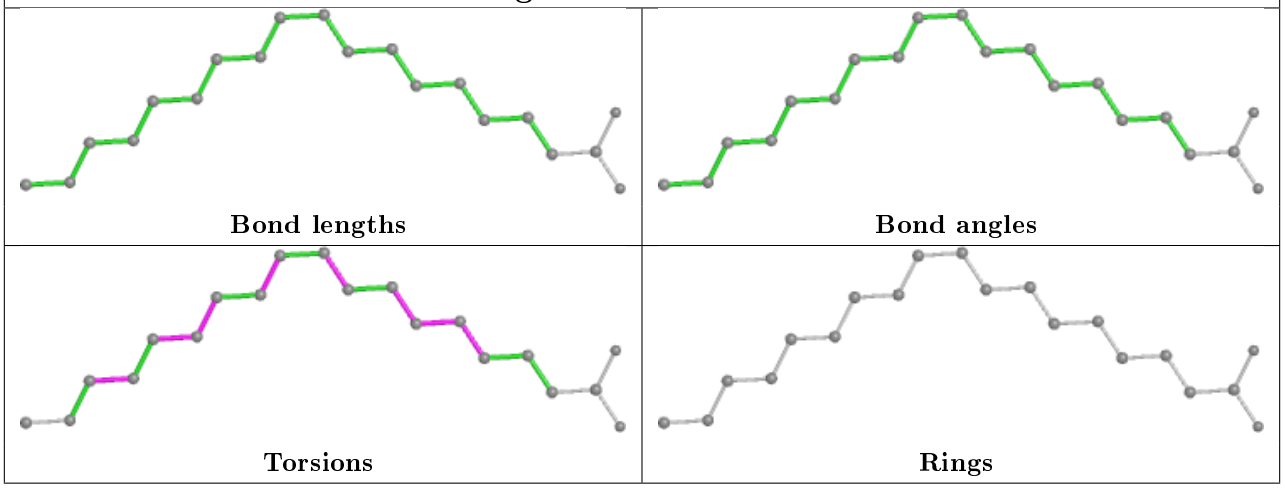

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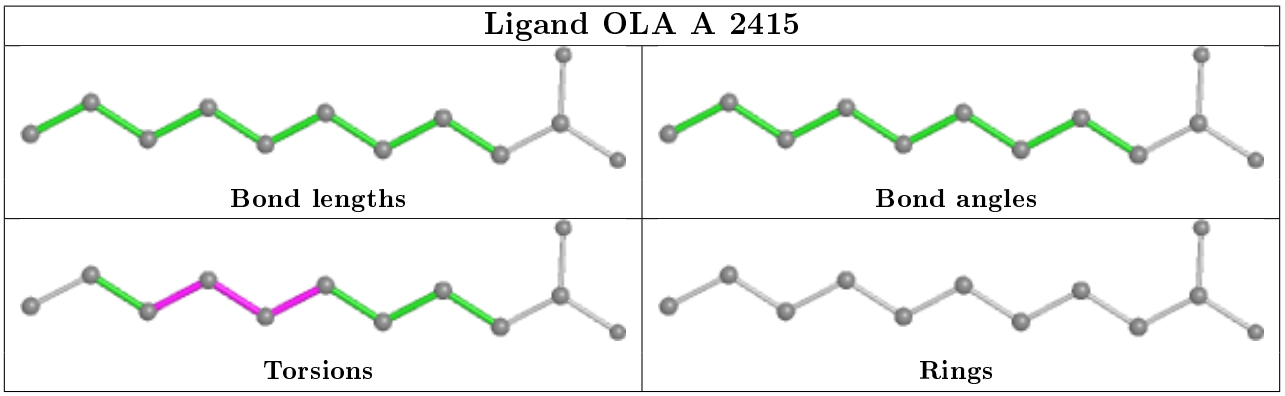

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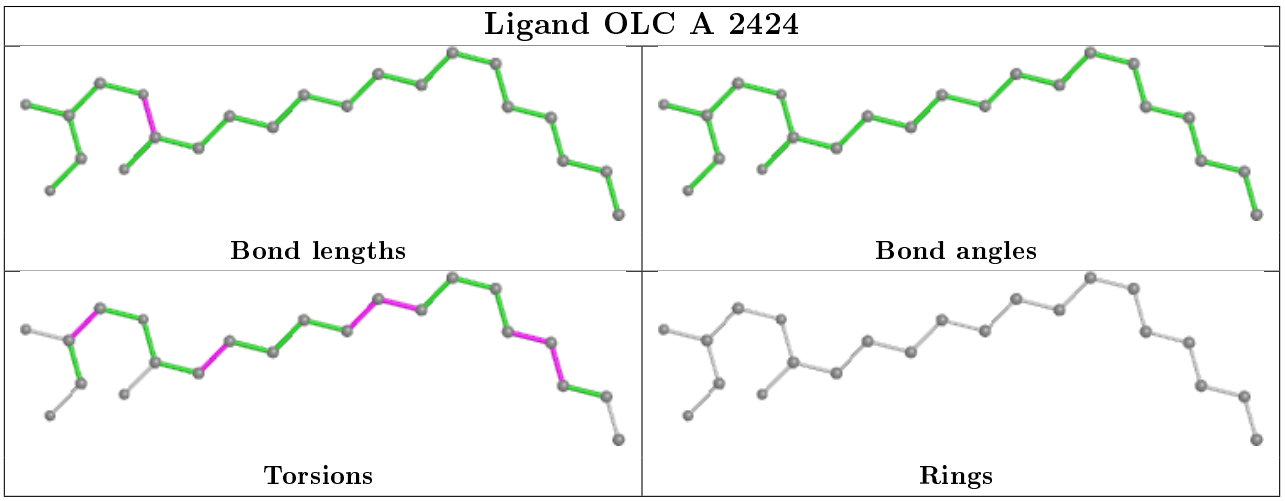

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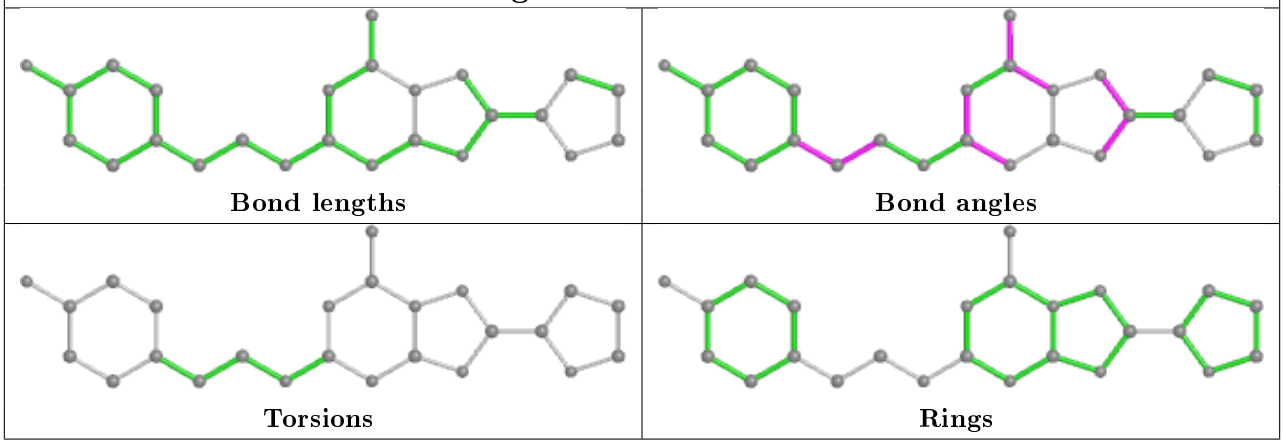

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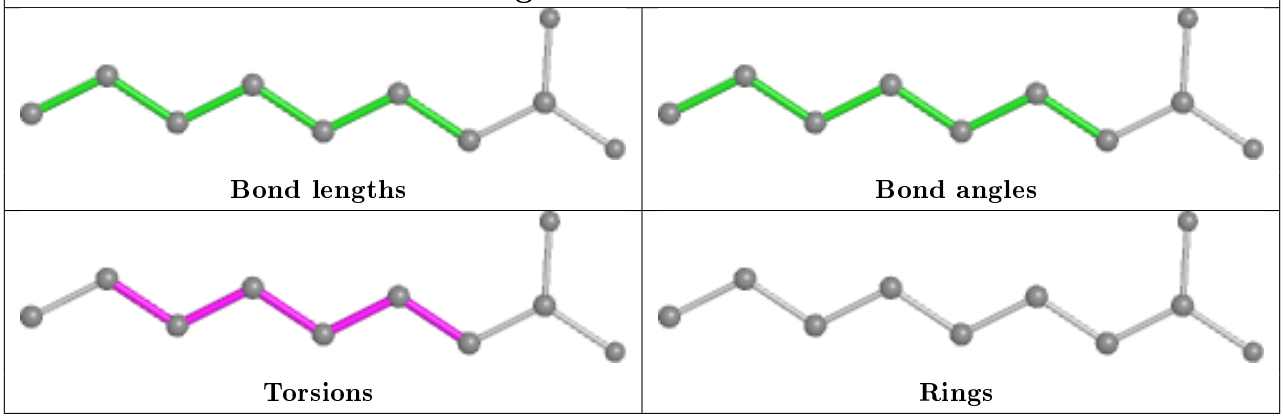

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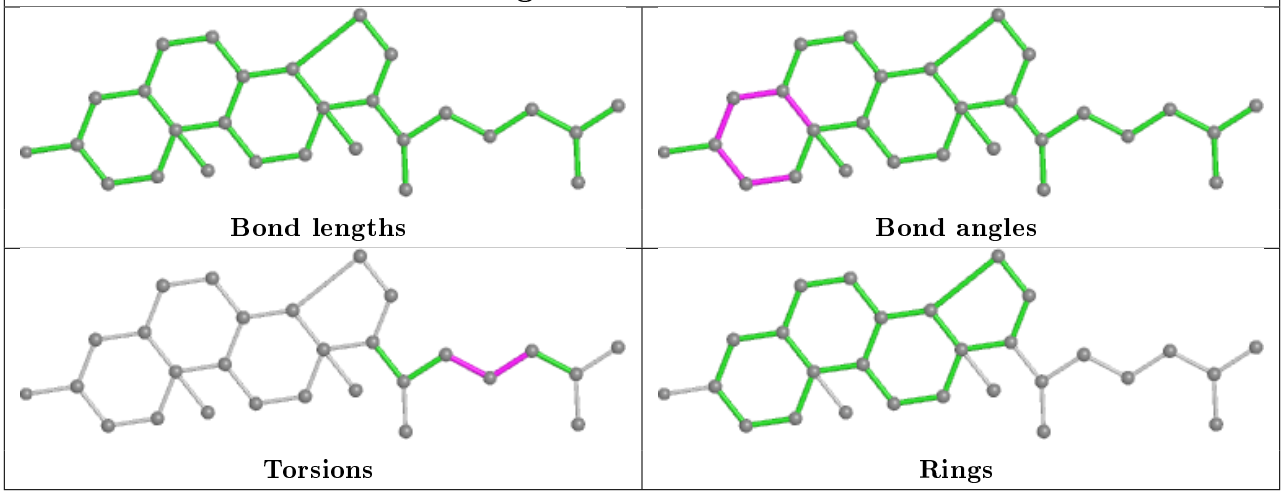

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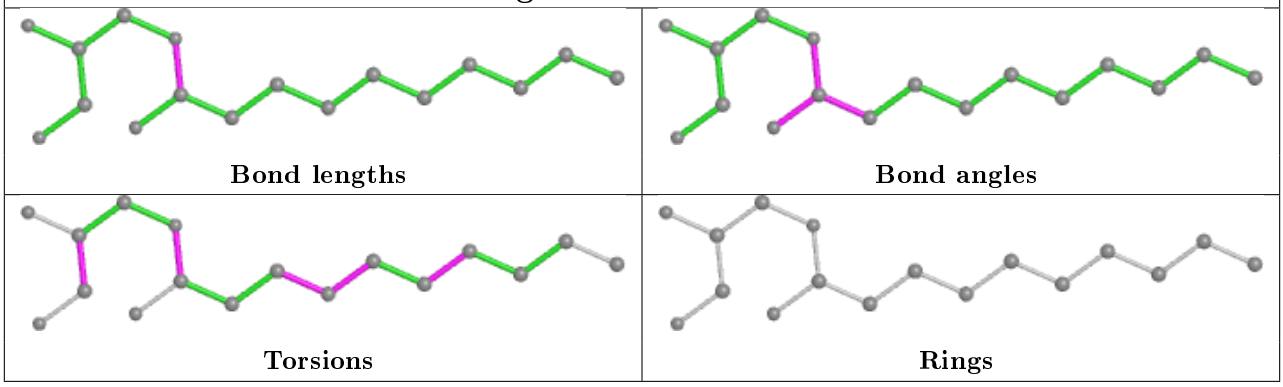

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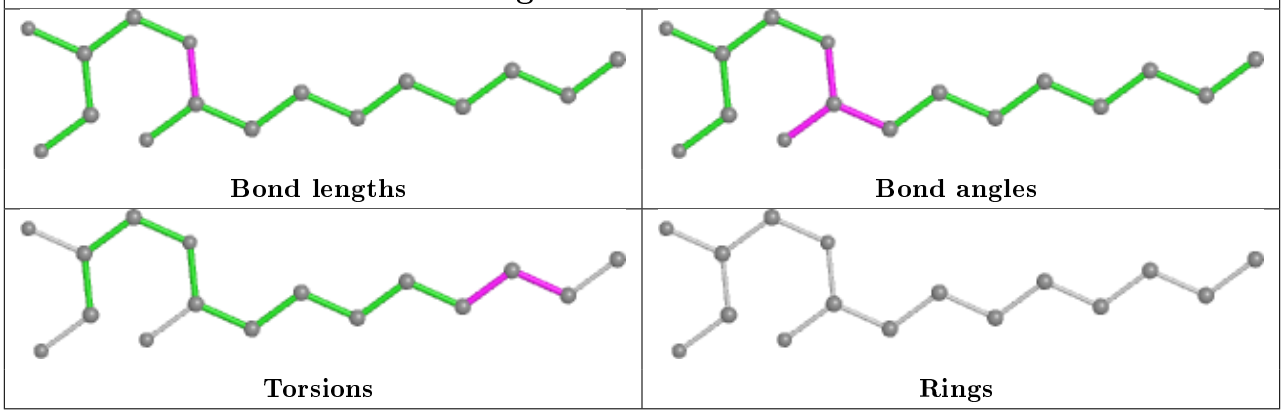
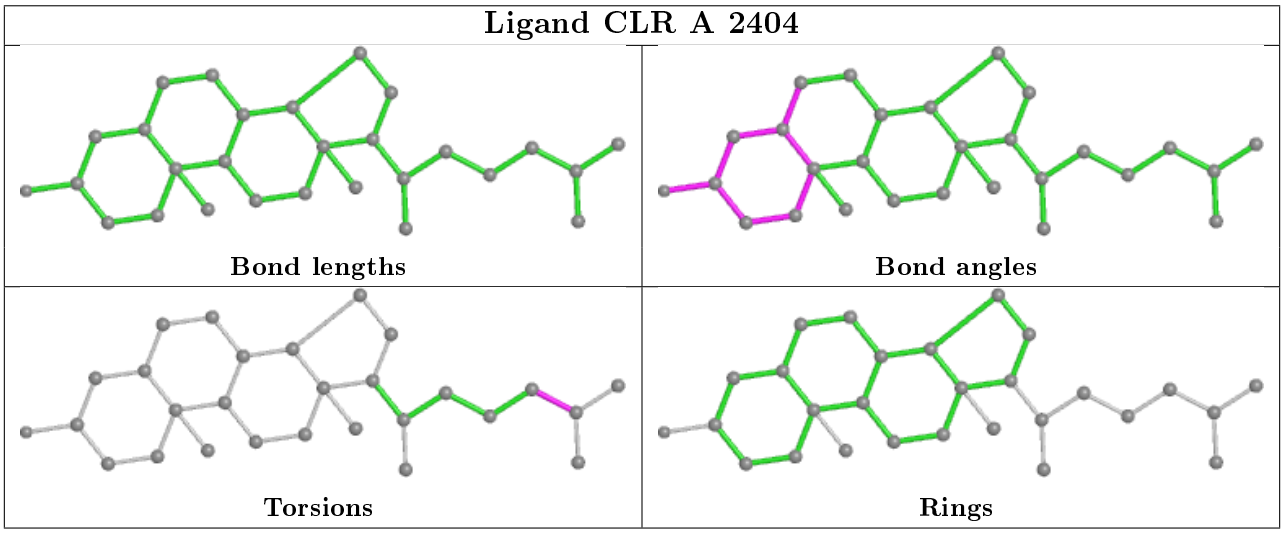
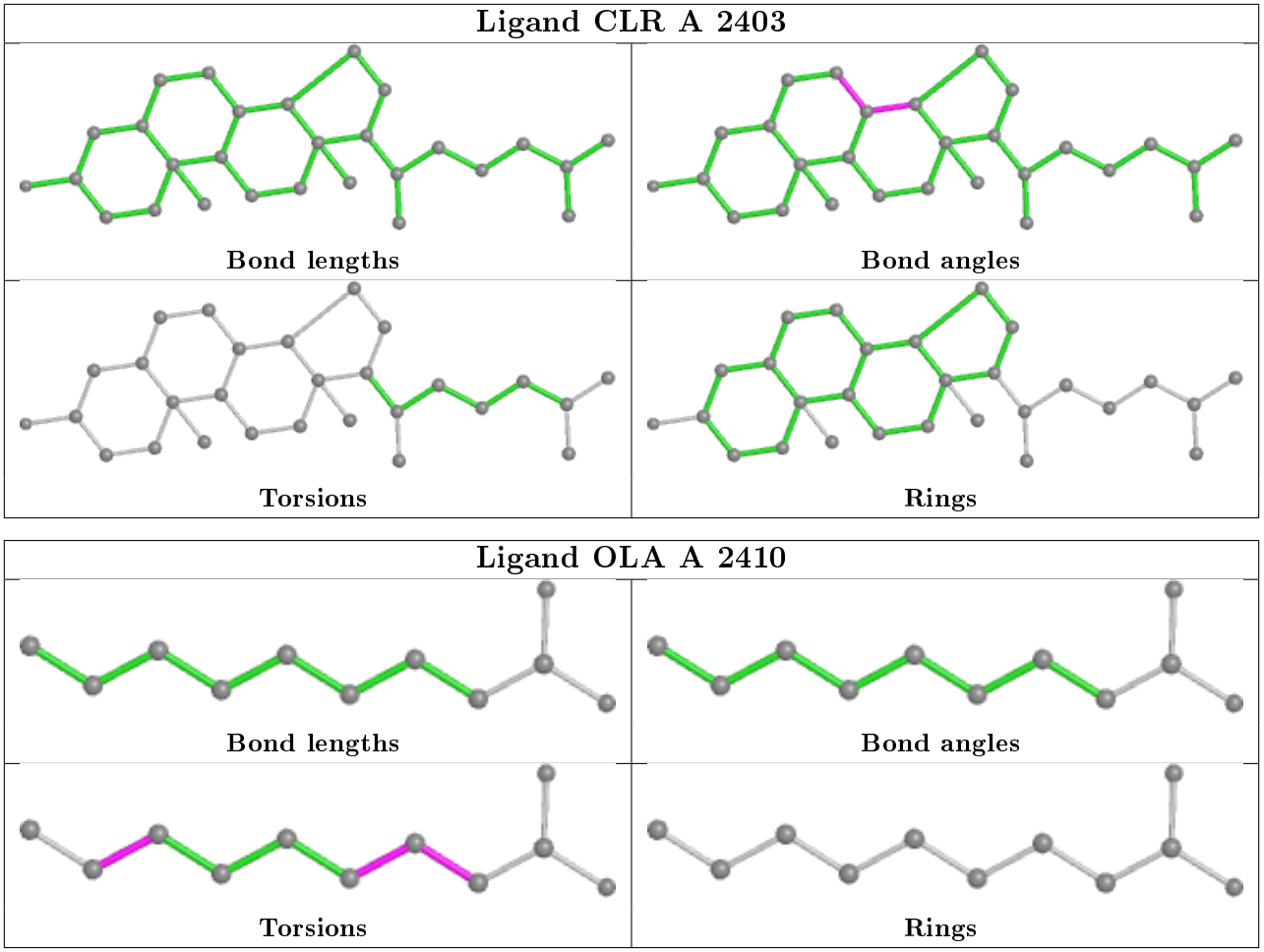


Ligand CLR A 2404





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	390/447 (87%)	-0.02	13 (3%) 46 40	13, 24, 66, 109	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	VAL	7.5
1	A	1058	MET	5.8
1	A	1061	PHE	4.9
1	A	306	HIS	4.4
1	A	1059	LYS	4.2
1	A	1023	ALA	4.0
1	A	1024	ALA	3.7
1	A	1062	ARG	3.3
1	A	1021	ASP	3.0
1	A	1063	HIS	2.9
1	A	1020	ALA	2.8
1	A	1105	TYR	2.2
1	A	1060	ASP	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

There are no carbohydrates in this entry.

6.4 Ligands (i)

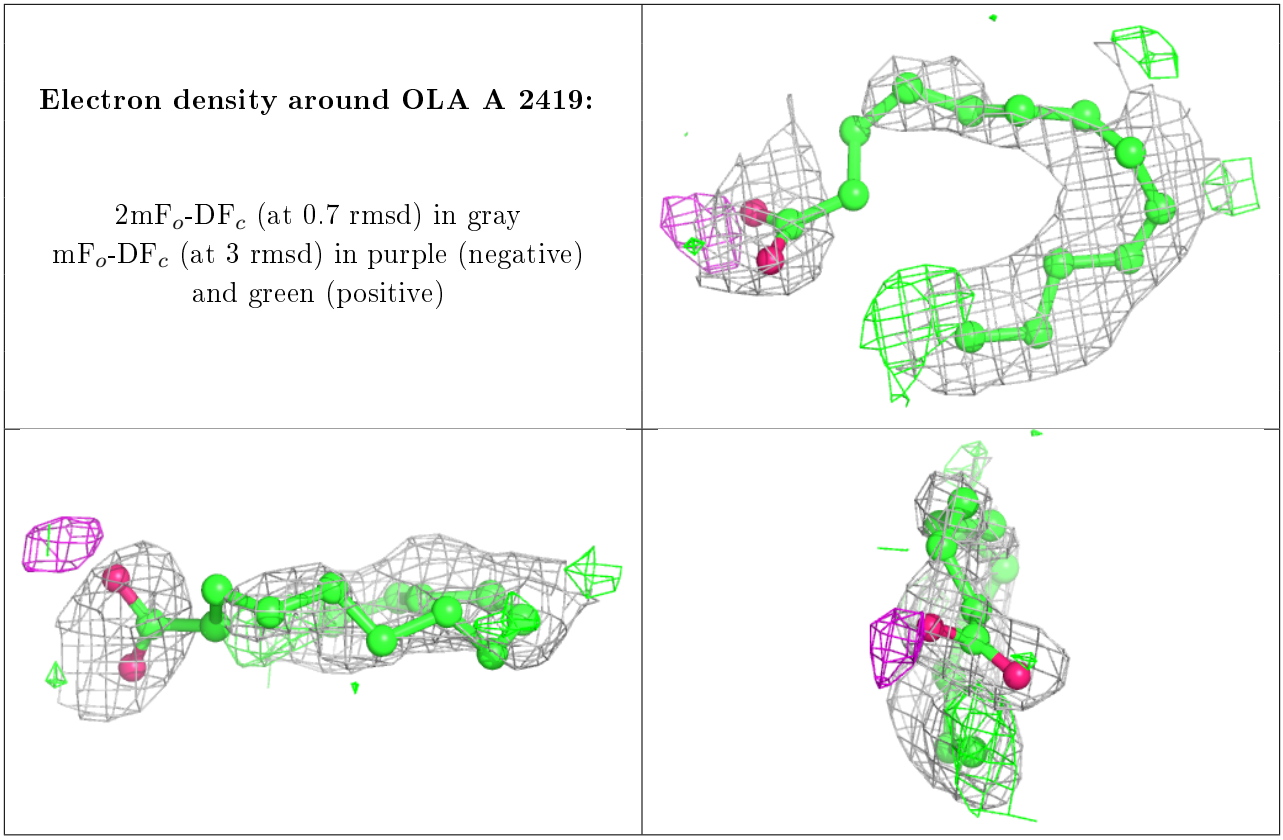
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	2419	15/20	0.50	0.34	47,61,68,69	0
5	OLA	A	2417	20/20	0.58	0.21	45,53,64,65	0
5	OLA	A	2410	11/20	0.59	0.22	34,45,60,61	0
6	OLC	A	2423	15/25	0.64	0.18	46,55,60,60	0
5	OLA	A	2415	12/20	0.68	0.29	38,45,56,57	0
5	OLA	A	2408	11/20	0.71	0.15	49,52,66,69	0
5	OLA	A	2412	8/20	0.72	0.19	46,50,55,57	0
5	OLA	A	2420	15/20	0.72	0.18	41,52,58,63	0
5	OLA	A	2413	10/20	0.75	0.25	55,58,62,63	0
6	OLC	A	2424	22/25	0.77	0.18	24,44,60,66	0
8	PEG	A	2429	7/7	0.78	0.18	49,52,60,61	0
5	OLA	A	2407	15/20	0.78	0.19	49,53,60,60	0
5	OLA	A	2416	18/20	0.81	0.18	41,50,58,59	0
5	OLA	A	2406	20/20	0.81	0.15	30,48,59,59	0
6	OLC	A	2428	21/25	0.81	0.17	41,51,59,60	0
6	OLC	A	2425	17/25	0.82	0.16	37,42,49,54	0
5	OLA	A	2418	20/20	0.83	0.19	39,54,60,60	0
5	OLA	A	2414	9/20	0.84	0.15	34,40,56,63	0
5	OLA	A	2409	19/20	0.84	0.16	35,39,51,53	0
7	OLB	A	2426	18/25	0.84	0.15	40,51,63,67	0
5	OLA	A	2421	19/20	0.85	0.15	40,44,57,59	0
6	OLC	A	2422	17/25	0.85	0.14	42,48,58,64	0
5	OLA	A	2411	9/20	0.85	0.21	33,39,49,54	0
8	PEG	A	2430	7/7	0.85	0.15	49,53,56,61	0
6	OLC	A	2427	16/25	0.88	0.14	28,38,54,57	0
4	CLR	A	2404	28/28	0.92	0.09	22,25,31,41	0
4	CLR	A	2403	28/28	0.94	0.09	18,22,48,54	0
4	CLR	A	2405	28/28	0.94	0.10	17,23,38,44	0
2	ZMA	A	2401	25/25	0.95	0.13	12,16,32,44	0
3	NA	A	2402	1/1	0.97	0.11	27,27,27,27	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.

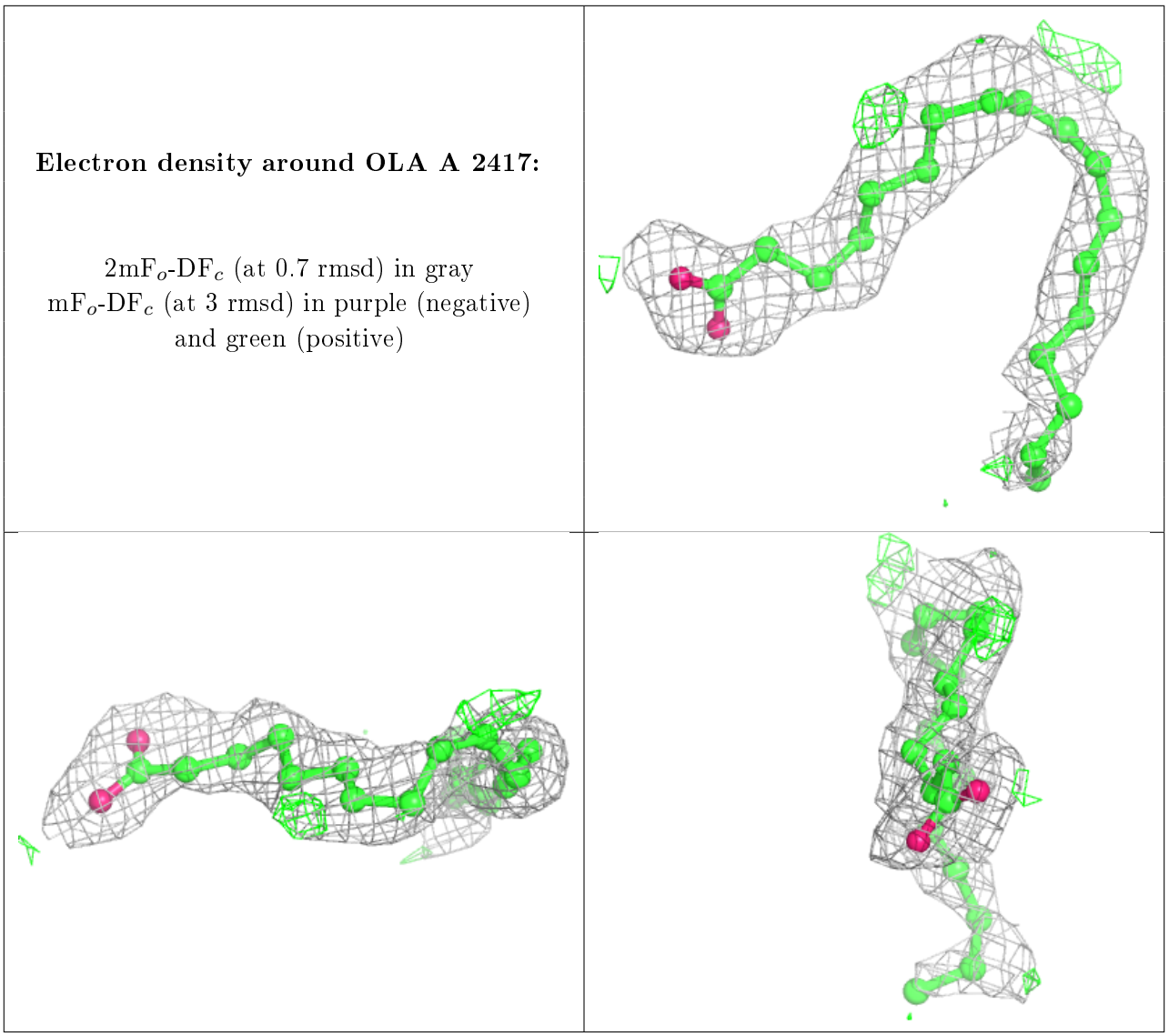
Electron density around OLA A 2419:

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



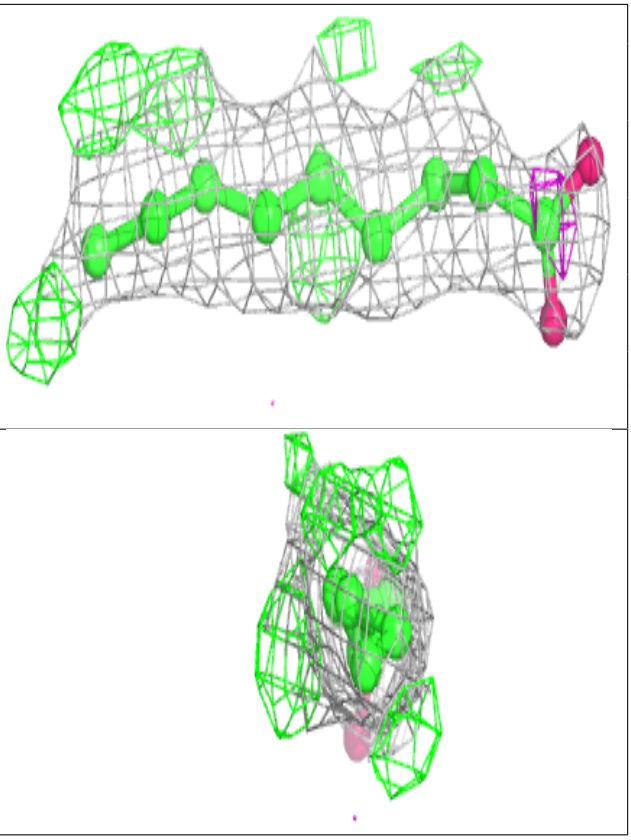
Electron density around OLA A 2417:

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



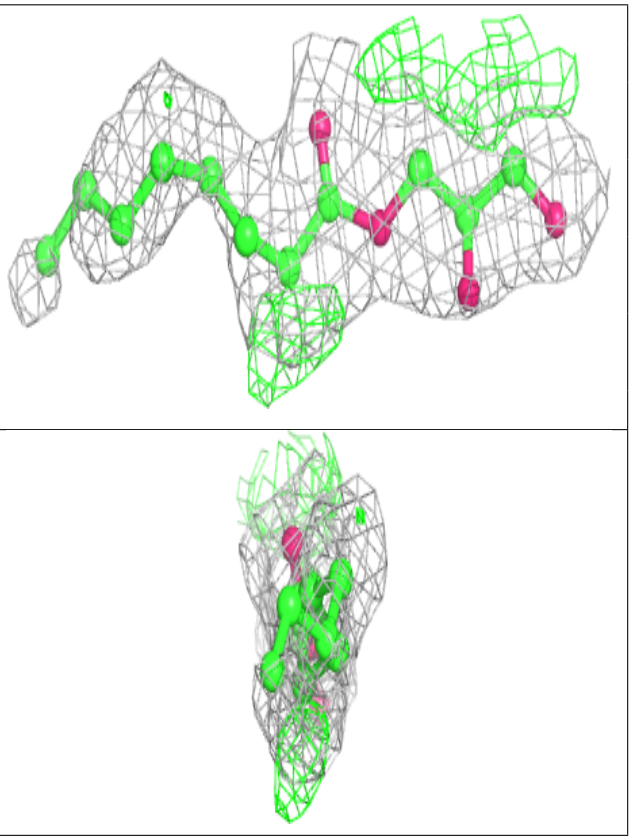
Electron density around OLA A 2410:

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



Electron density around OLC 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 2415:

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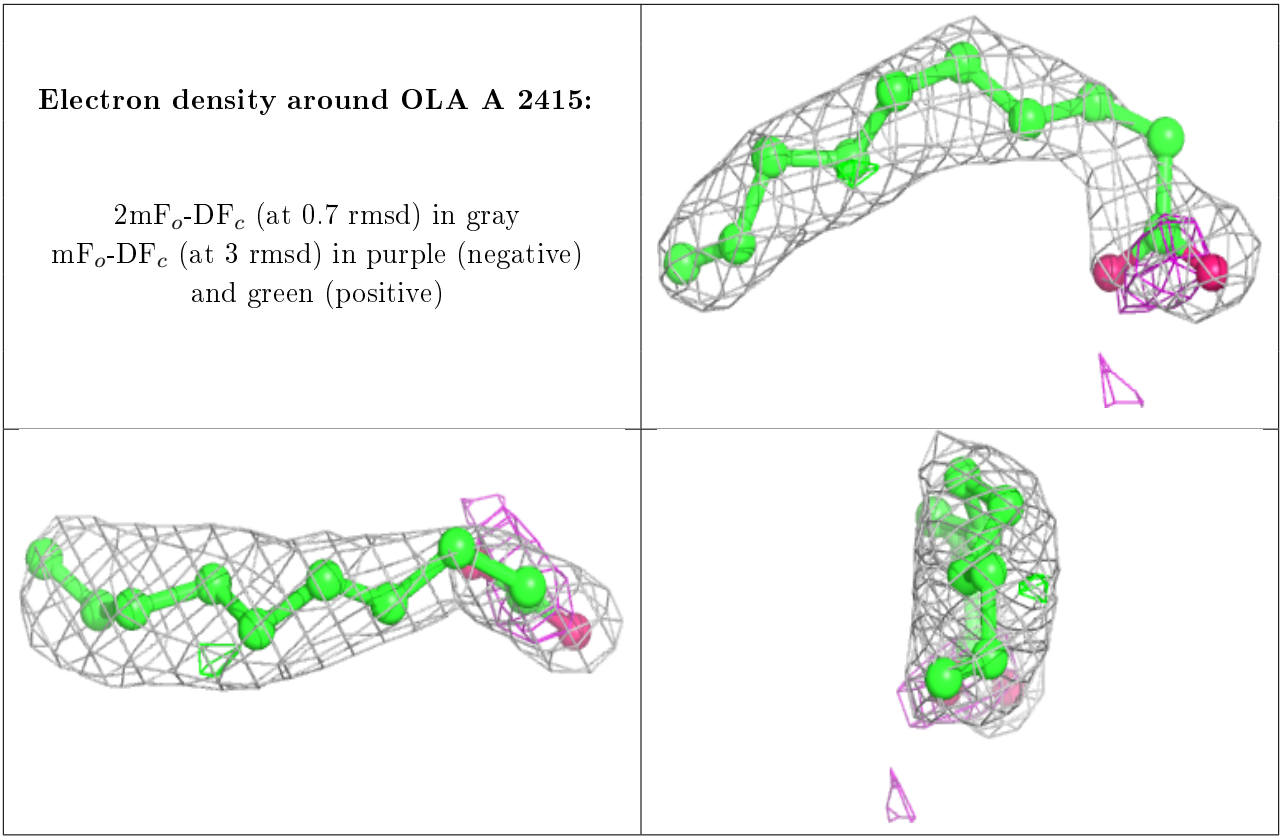

Electron density around OLA A 2408:

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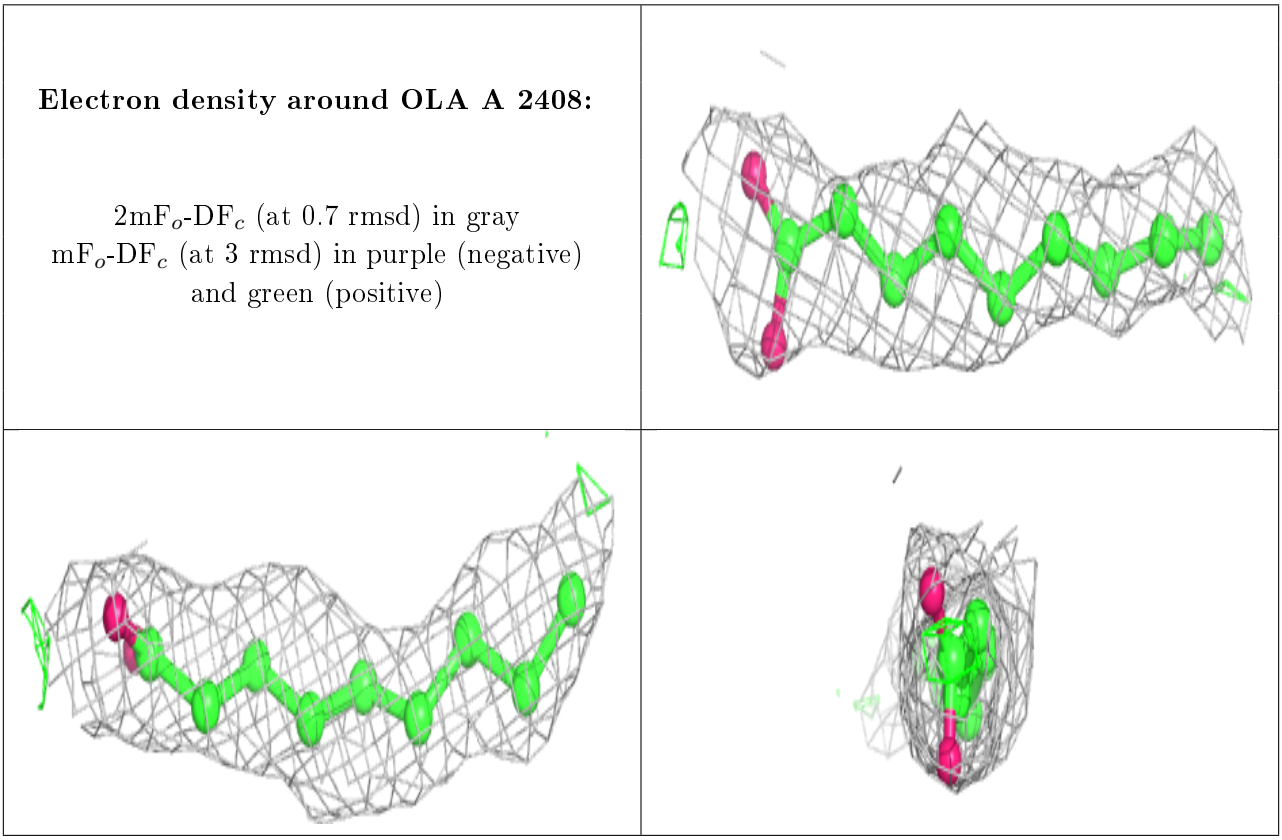
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA A 2420:

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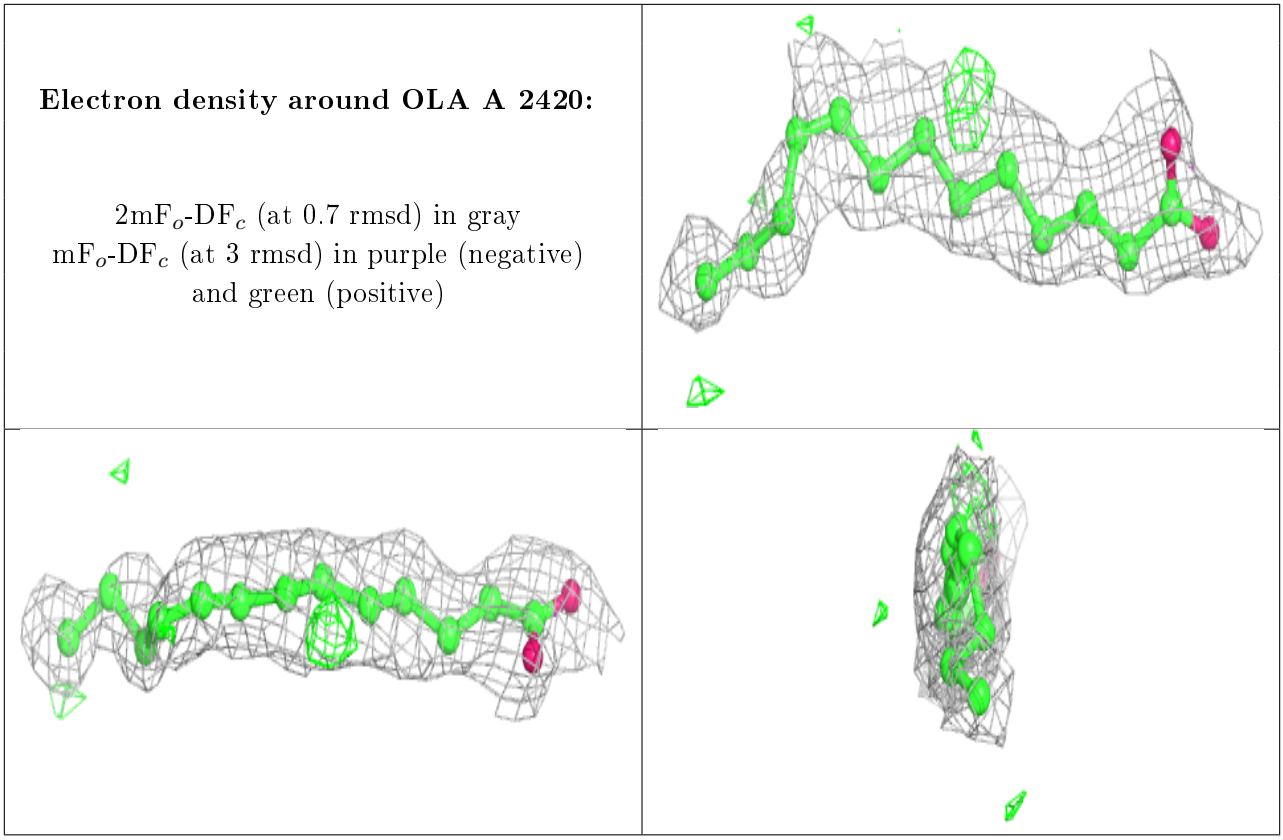
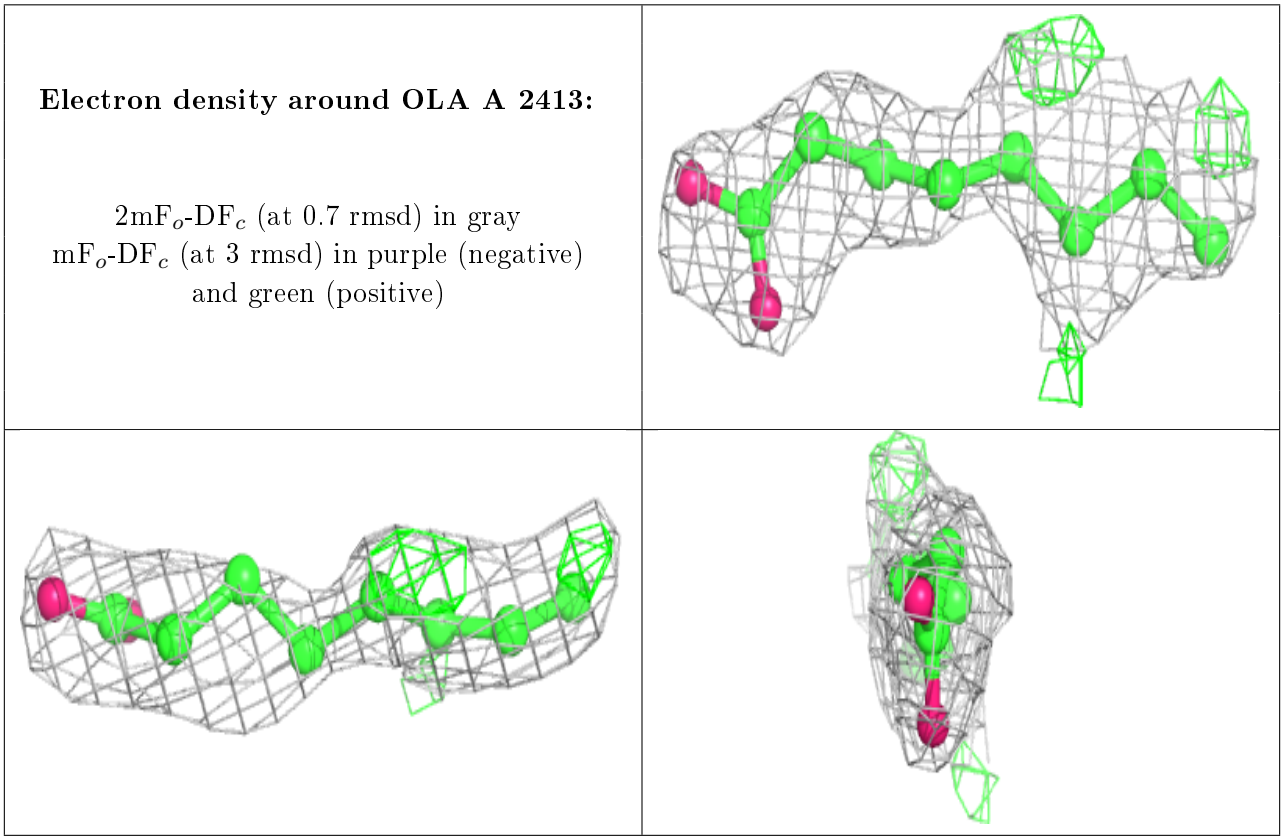
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



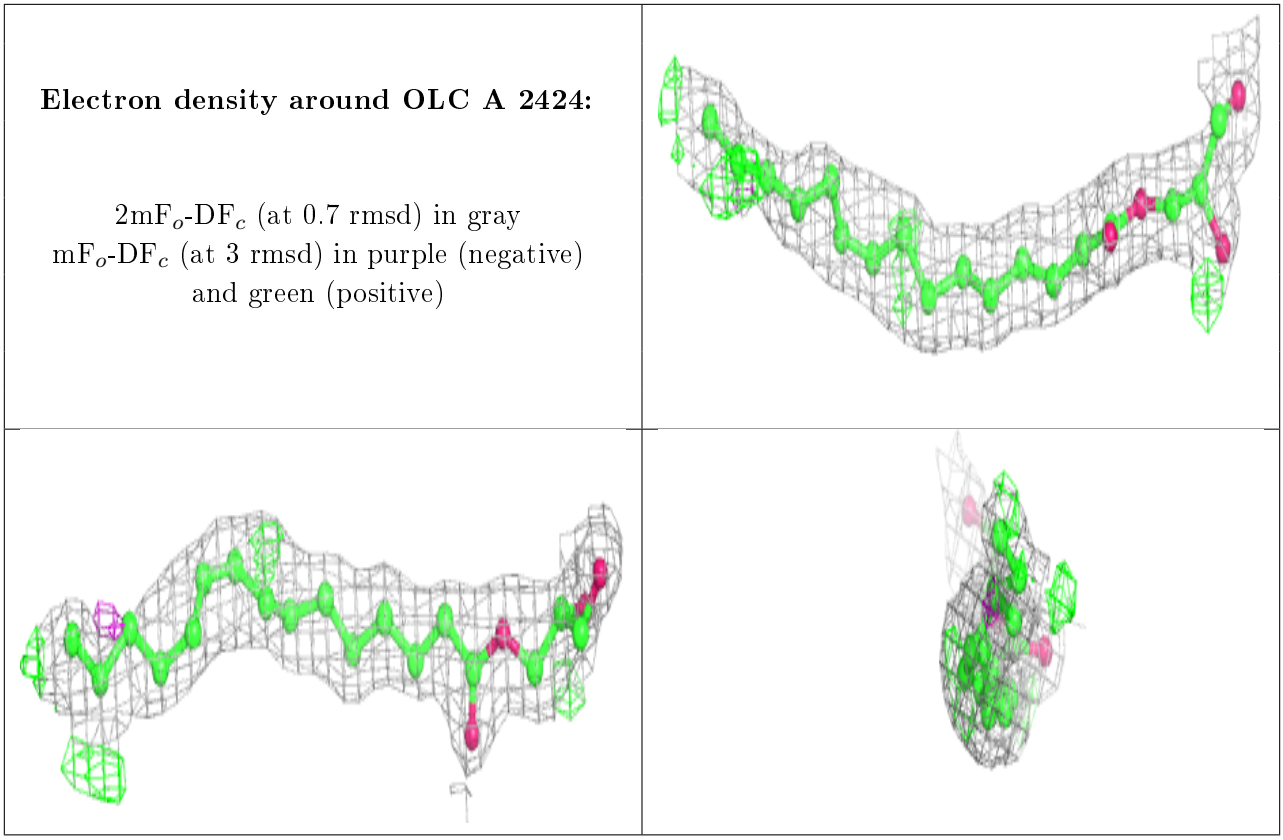
Electron density around OLA A 2413:

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



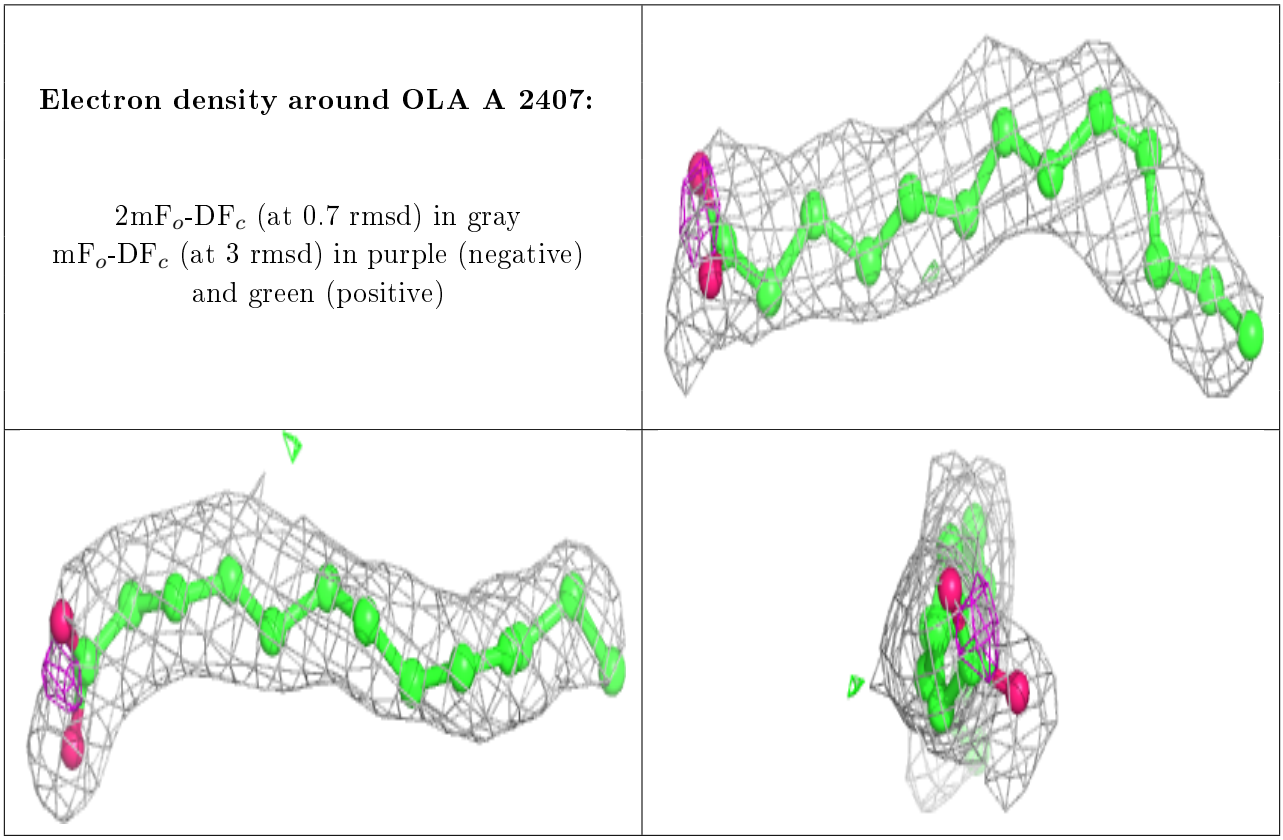
Electron density around OLC A 2424:

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



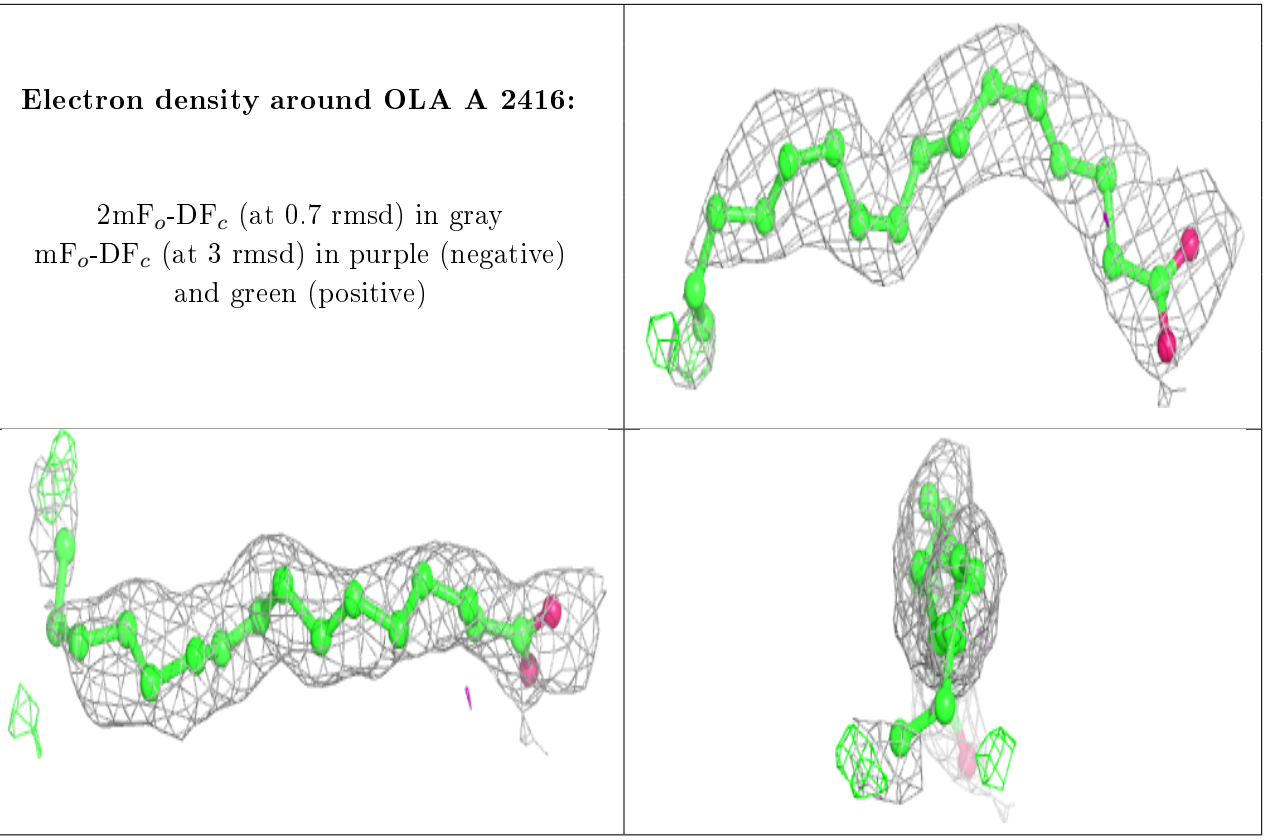
Electron density around OLA A 2407:

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



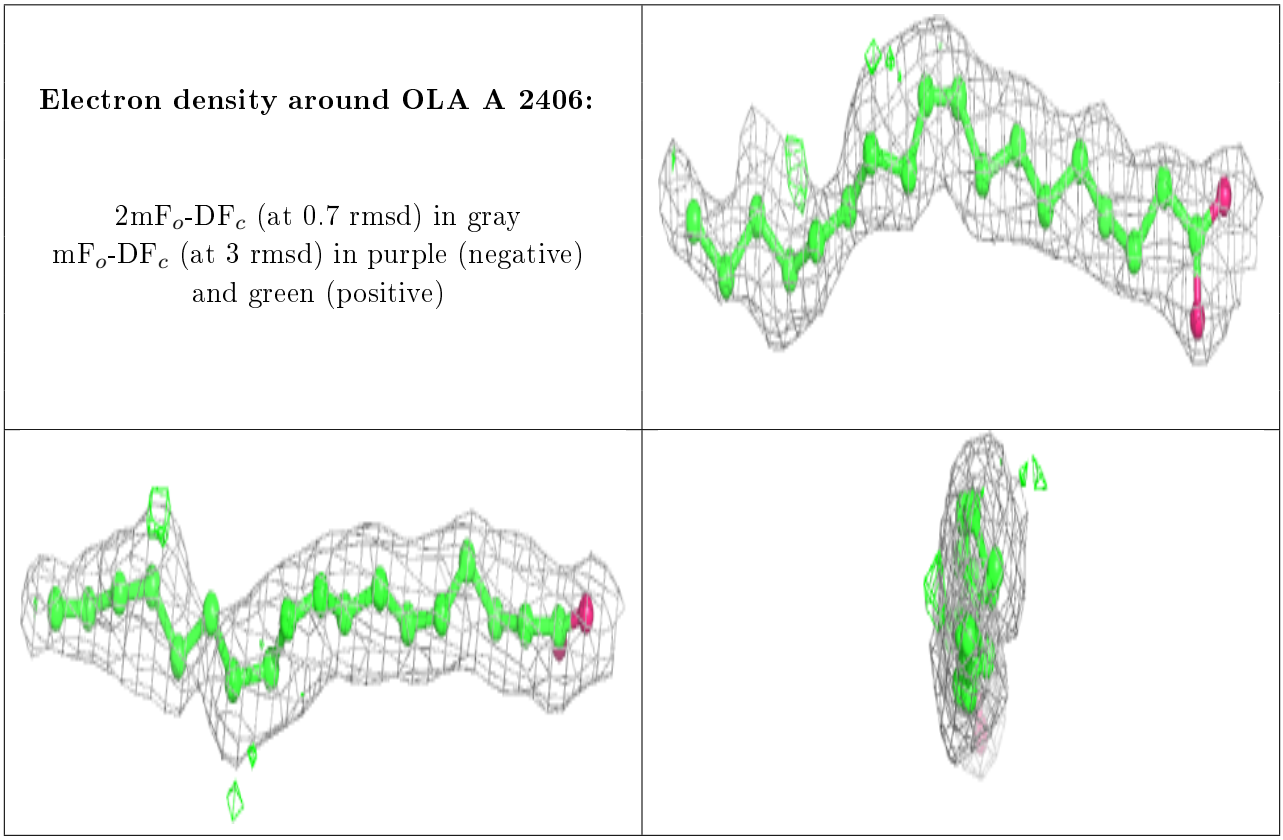
Electron density around OLA A 2416:

$2mF_o$-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 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 OLC A 2428:

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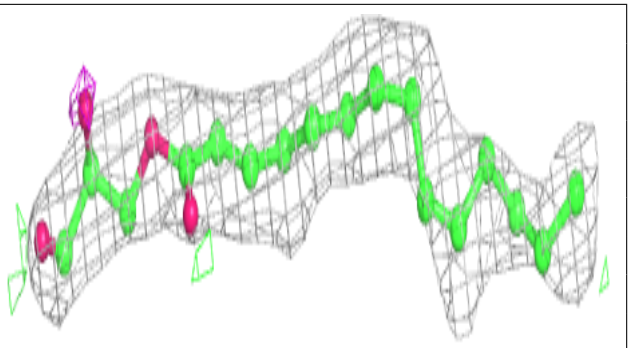
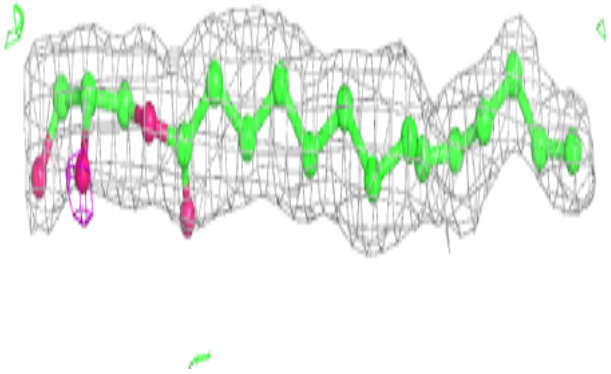
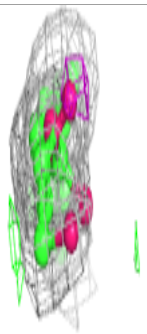
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

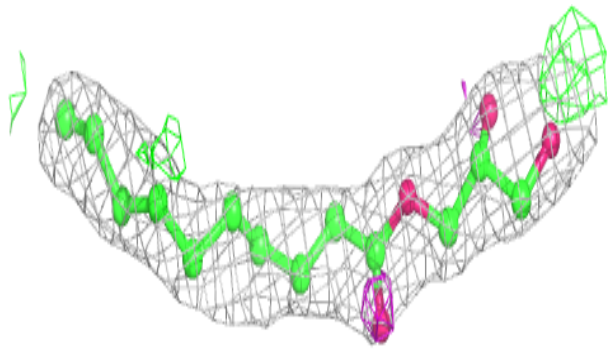


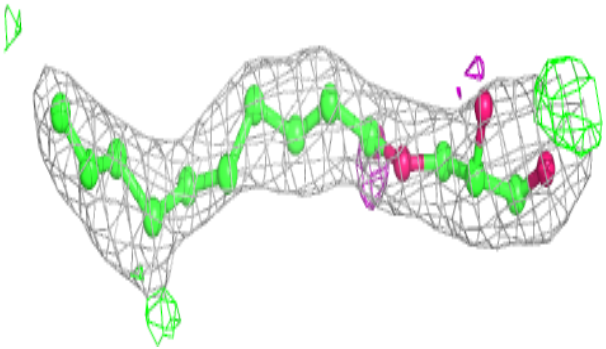


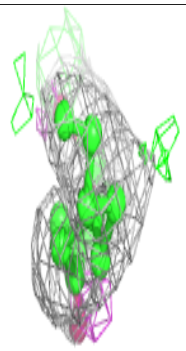


Electron density around OLC A 2425:

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

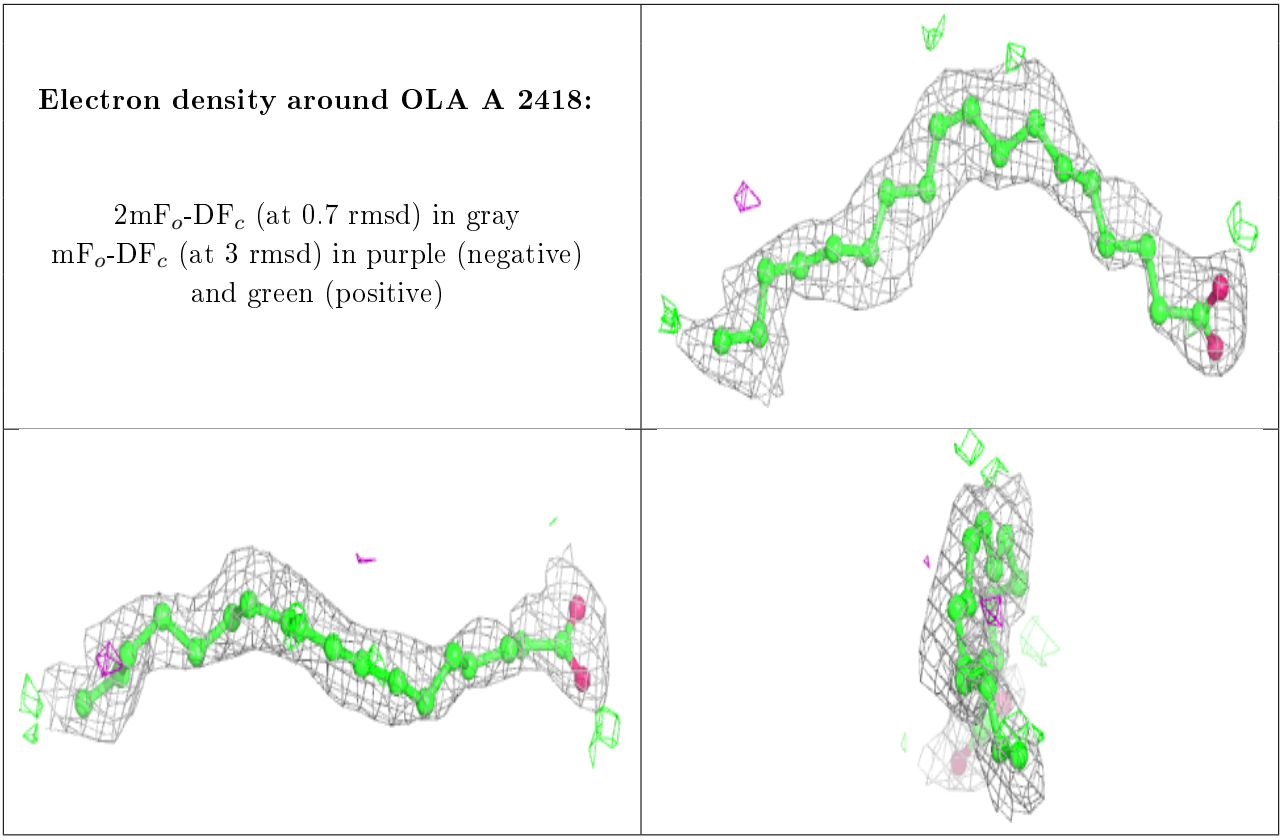






Electron density around OLA A 2418:

$2mF_o$-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 2414:

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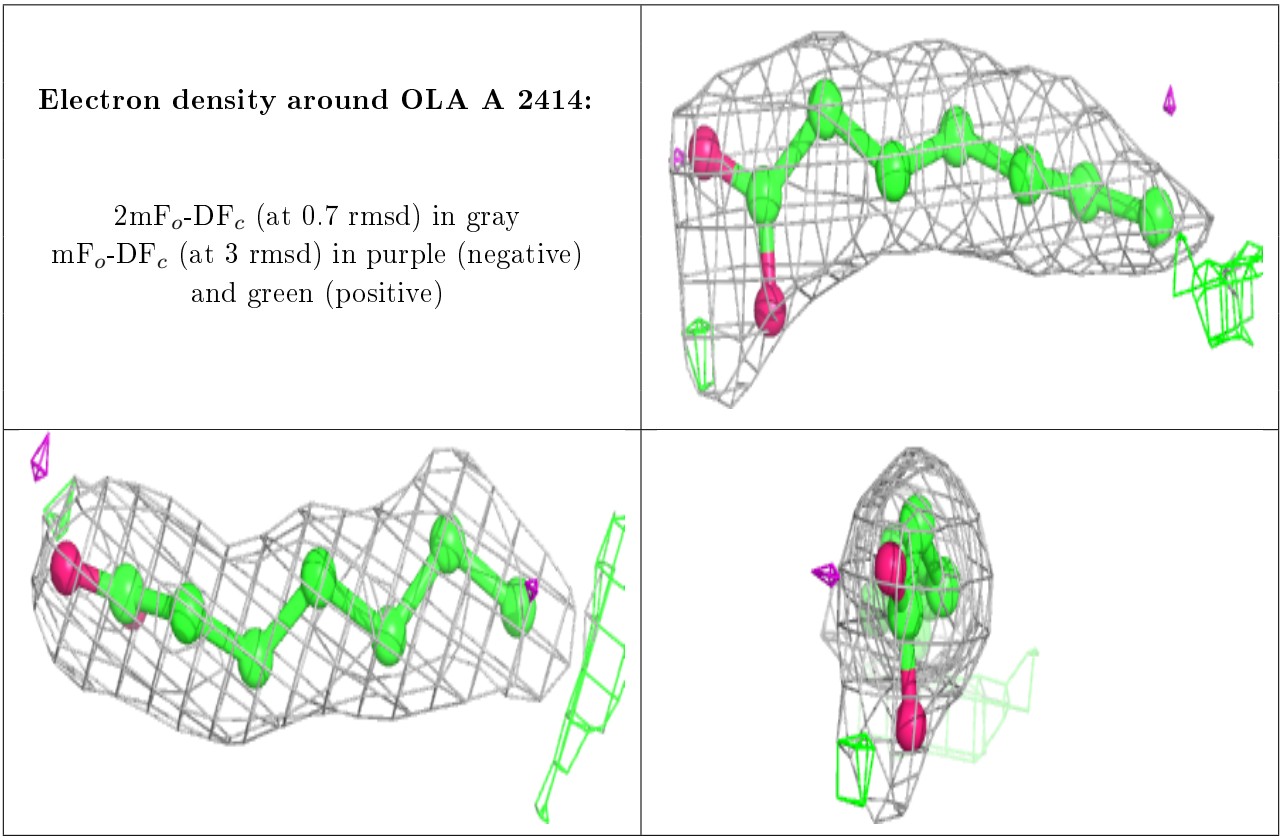
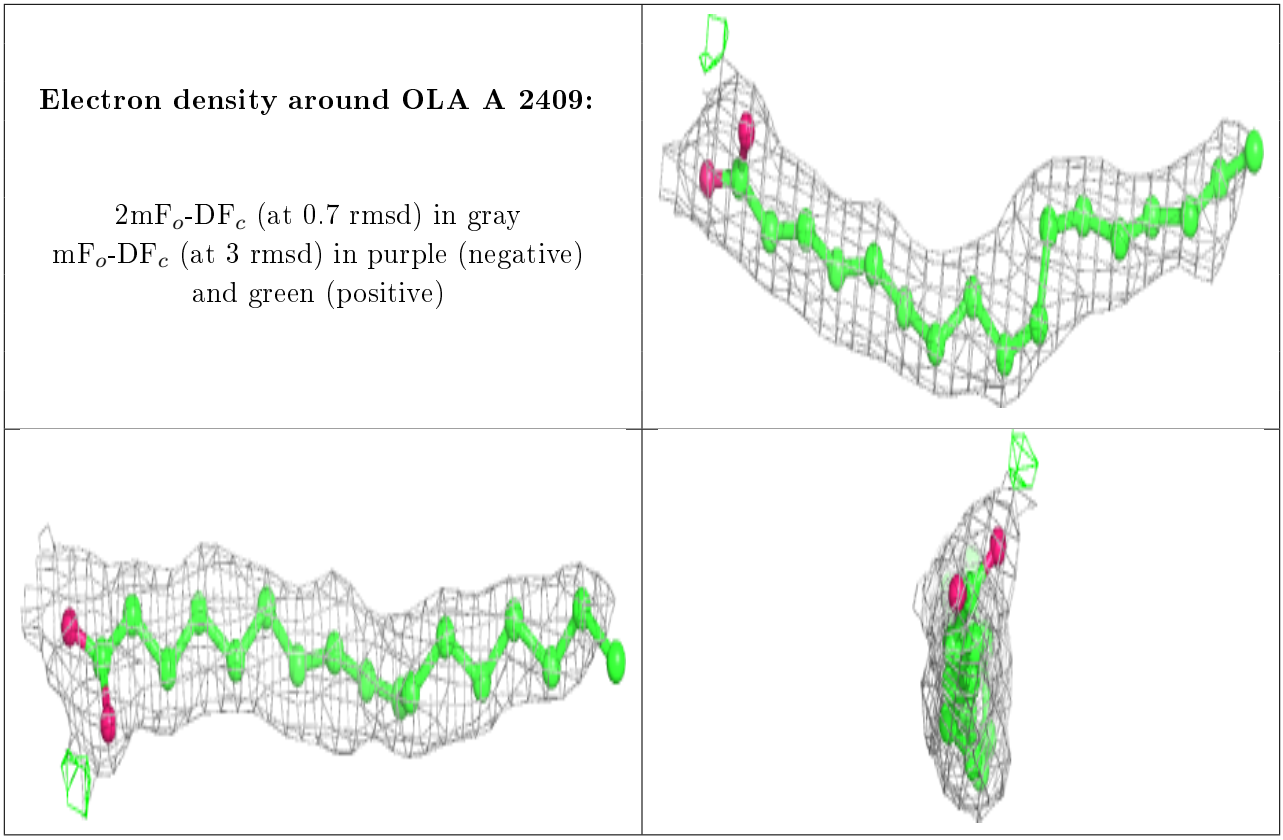
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



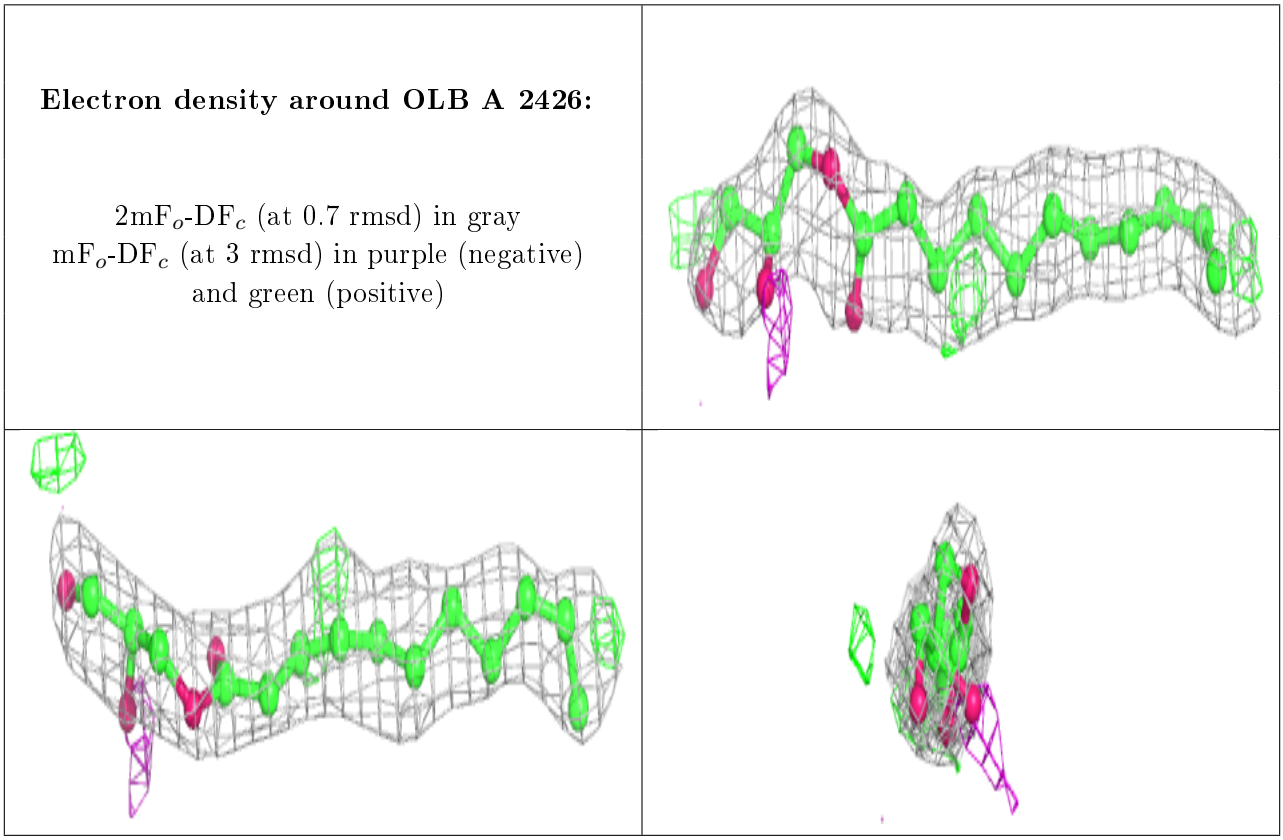
Electron density around OLA A 2409:

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



Electron density around 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 2421:

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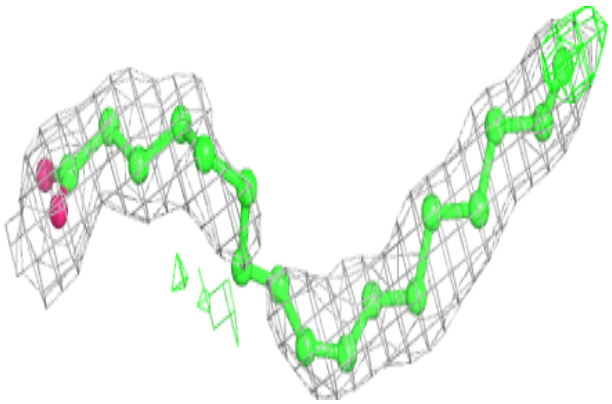
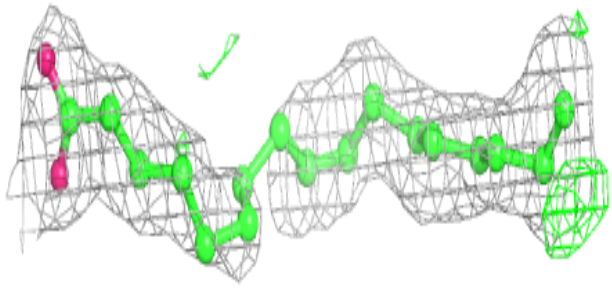
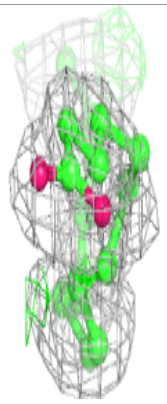
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

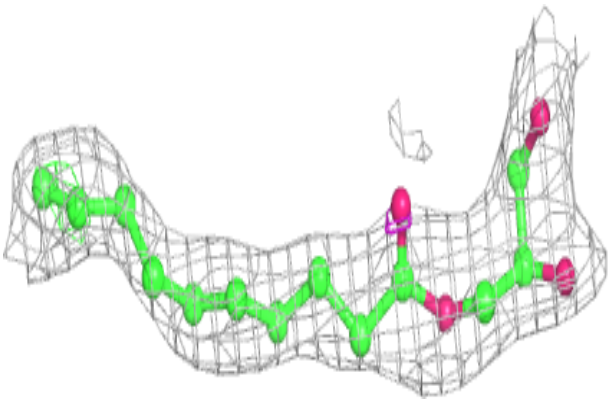


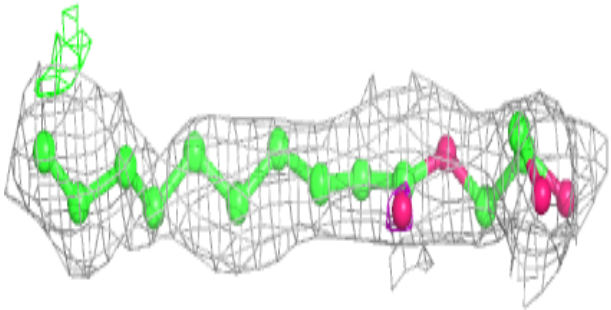


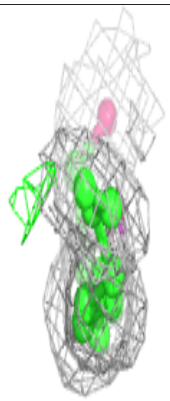


Electron density around OLC A 2422:

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







Electron density around OLC A 2427:

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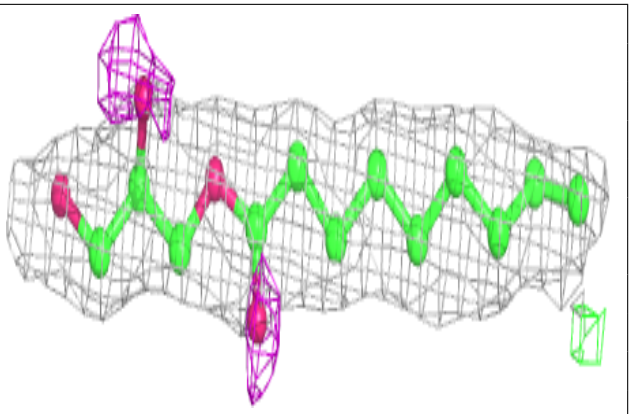
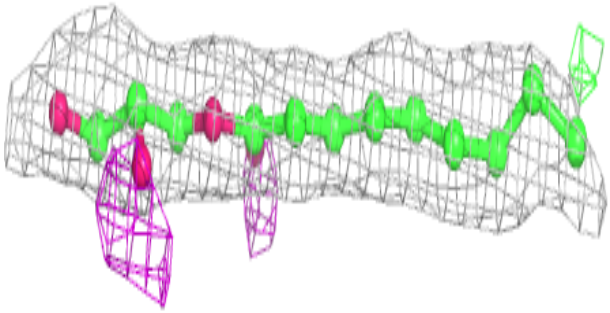
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around CLR A 2404:

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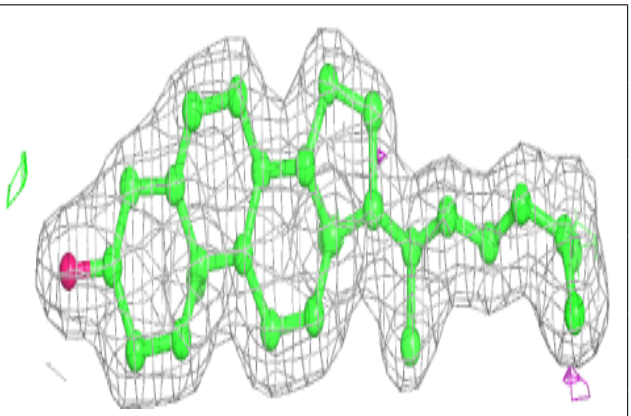
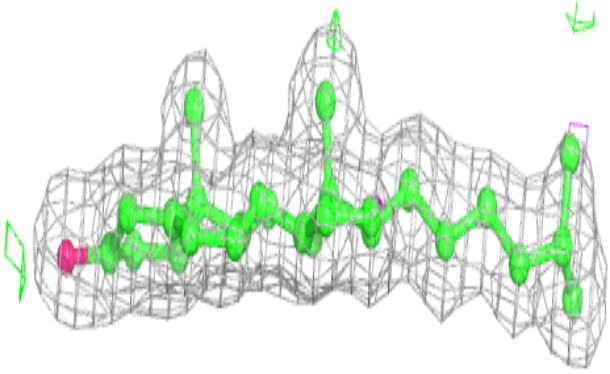
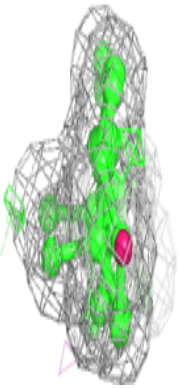
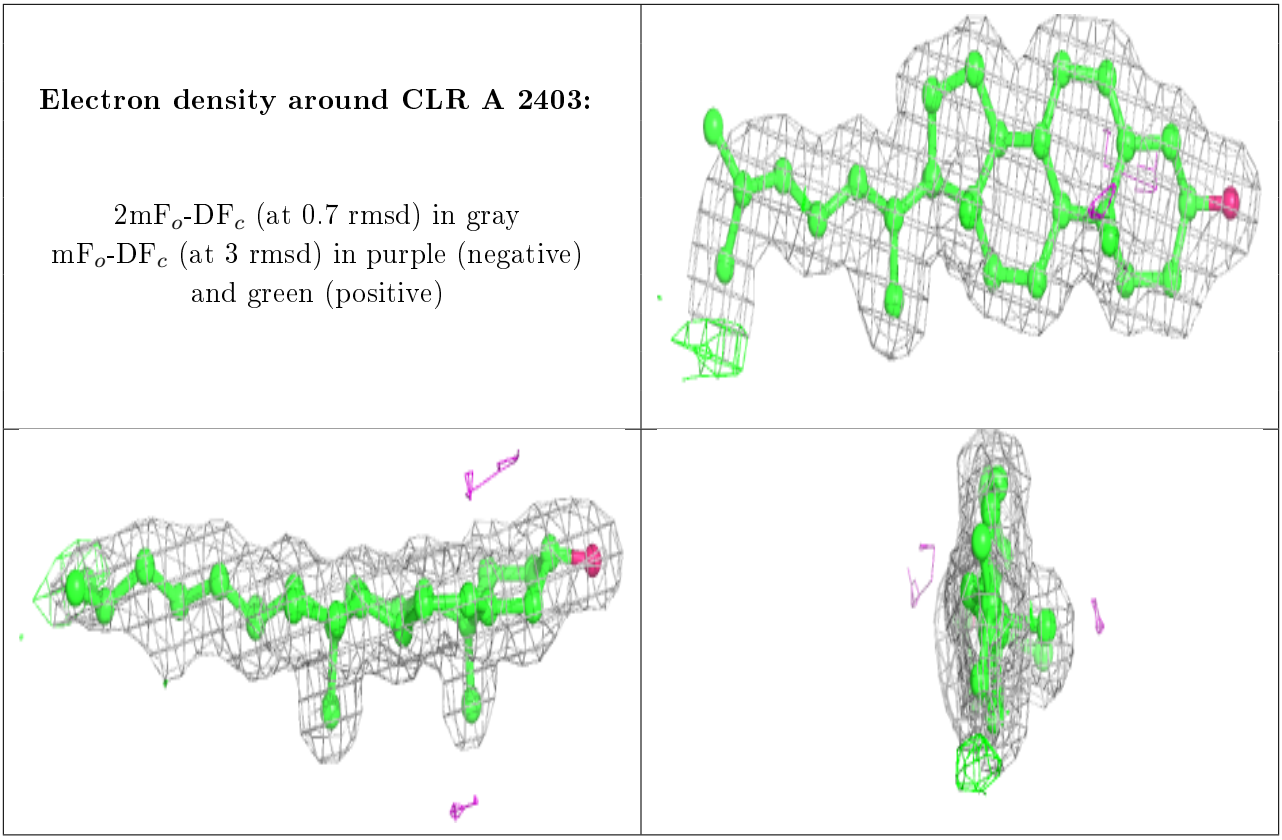






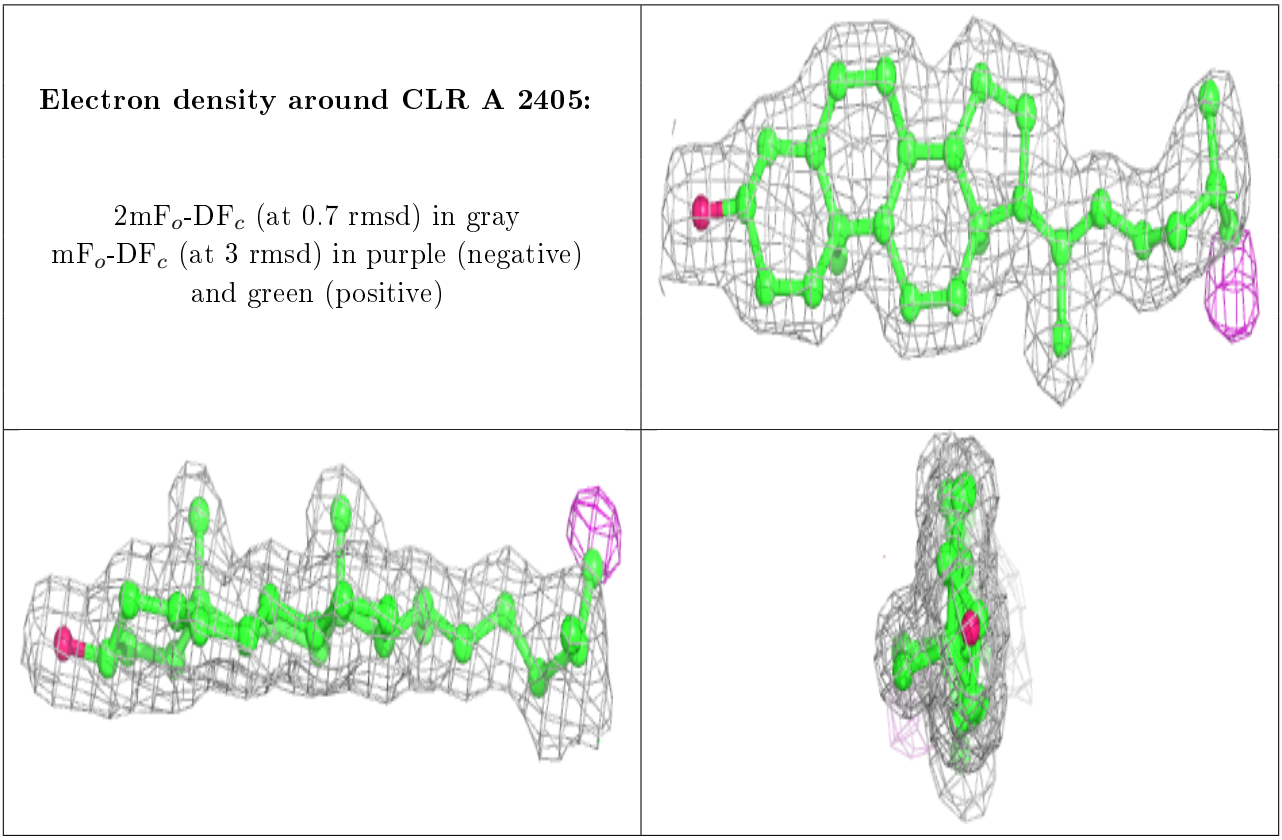
Electron density around CLR A 2403:

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



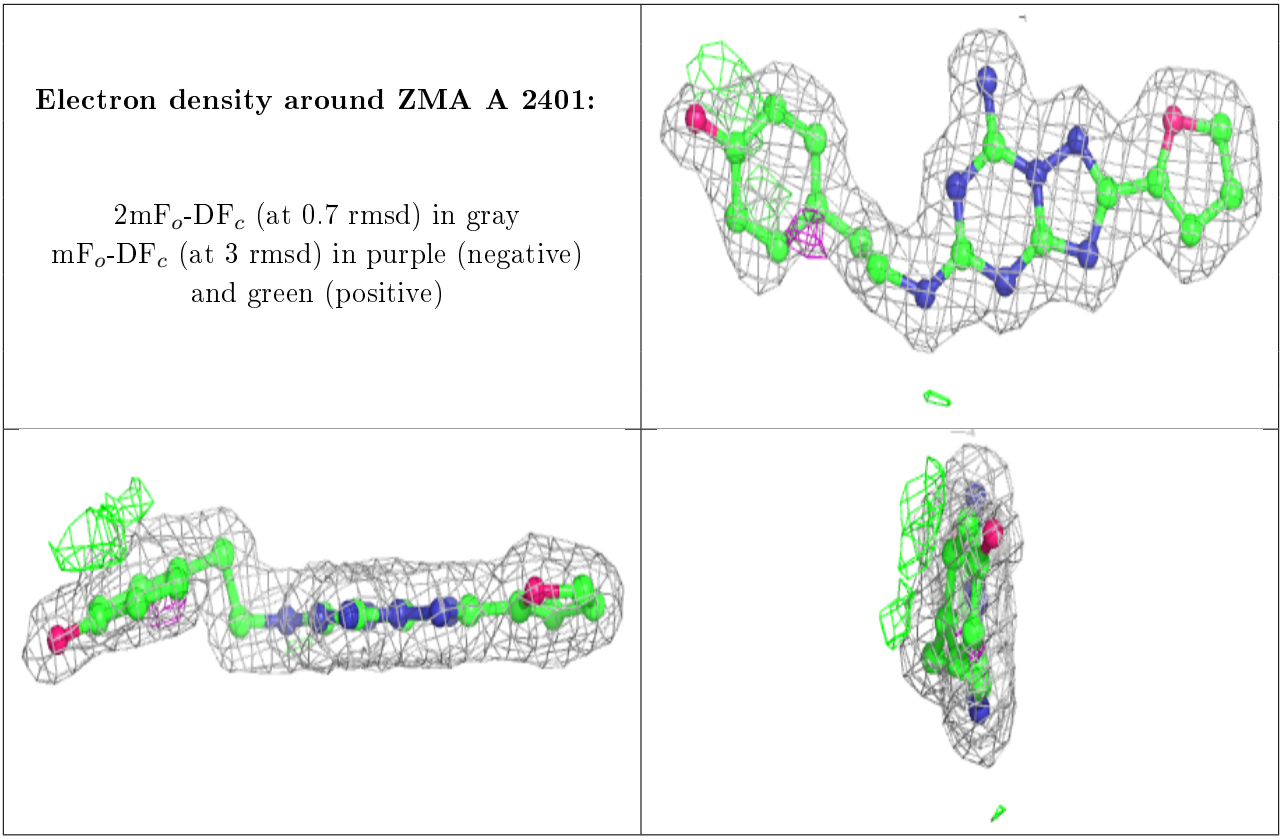
Electron density around CLR A 2405:

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



Electron density around 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.