



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:13 pm BST

PDB ID : 5VRA
Title : 2.35-Angstrom In situ Mylar structure of human A2A adenosine receptor at 100 K
Authors : Broecker, J.; Morizumi, T.; Ou, W.-L.; Klingel, V.; Kuo, A.; Kissick, D.J.; Ishchenko, A.; Lee, M.-Y.; Xu, S.; Makarov, O.; Cherezov, V.; Ogata, C.M.; Ernst, O.P.
Deposited on : 2017-05-10
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

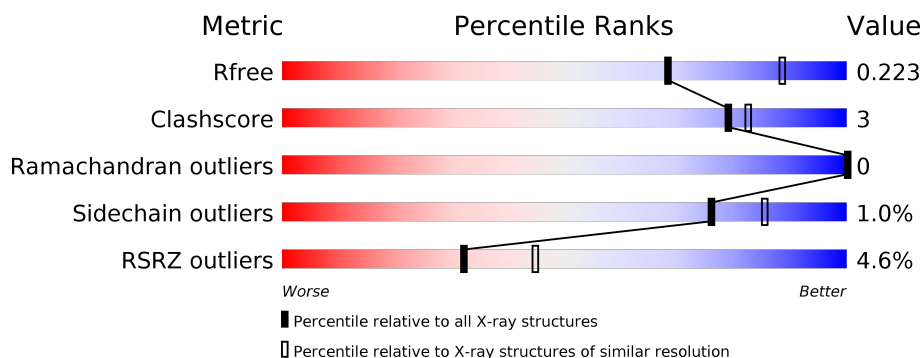
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	<div> <div>4%</div> <div>84%</div> <div>13%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OLA	A	2421	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6760 atoms, of which 3187 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	H	N	O	S			
1	A	390	6295	2026	3187	522	538	22	0	25	0

There are 39 discrepancies between the modelled and reference sequences:

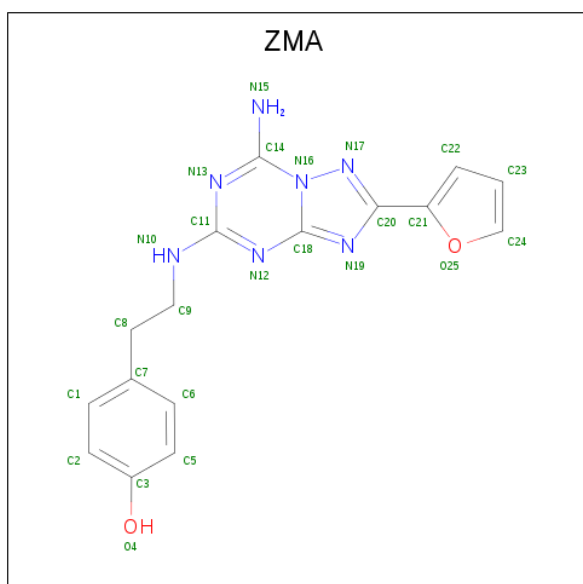
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression 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: C₁₆H₁₅N₇O₂).

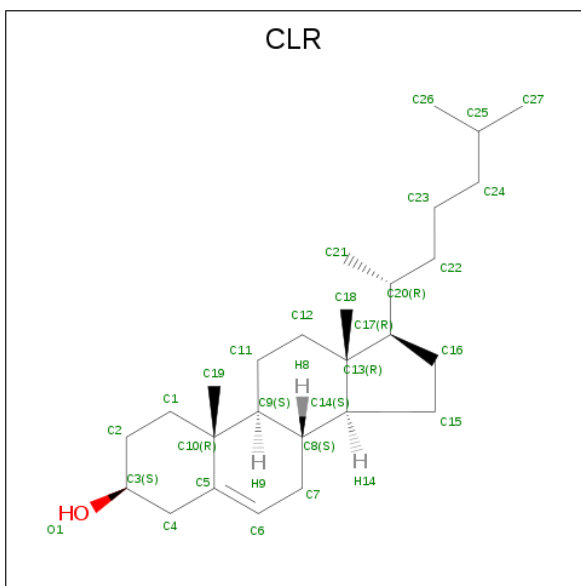


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	16	7	2		

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

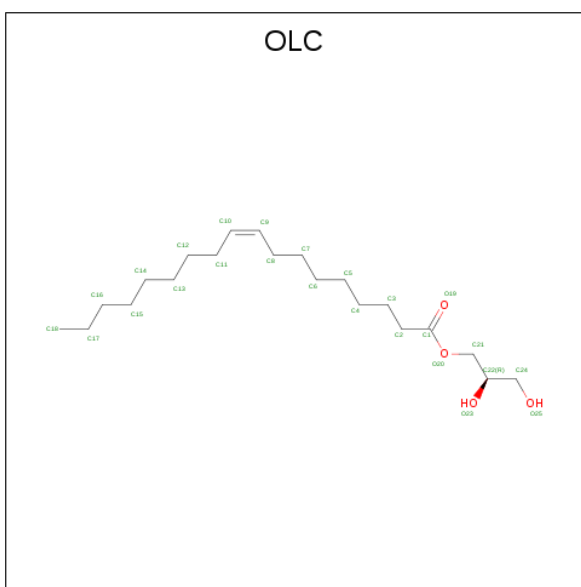
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

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



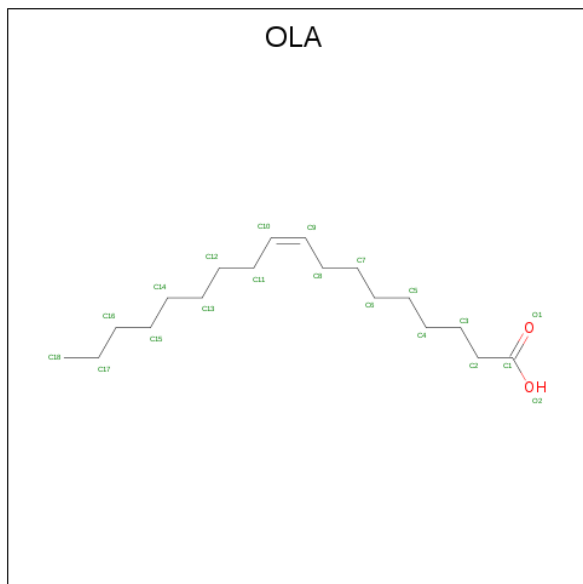
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 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
5	A	1	Total	C	O	0	0
			16	12	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			21	17	4		
5	A	1	Total	C	O	0	0
			15	11	4		
5	A	1	Total	C	O	0	0
			17	13	4		
5	A	1	Total	C	O	0	0
			16	12	4		

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



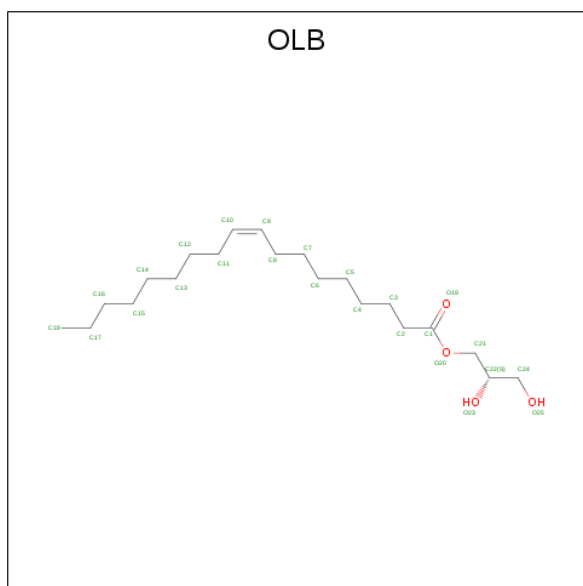
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			19	17	2		
6	A	1	Total	C	O	0	0
			20	18	2		
6	A	1	Total	C	O	0	0
			15	13	2		
6	A	1	Total	C	O	0	0
			11	9	2		
6	A	1	Total	C	O	0	0
			15	13	2		
6	A	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 7 2	0	0
6	A	1	Total C O 9 7 2	0	0
6	A	1	Total C O 12 10 2	0	0
6	A	1	Total C 8 8	0	0

- Molecule 7 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 18 14 4	0	0

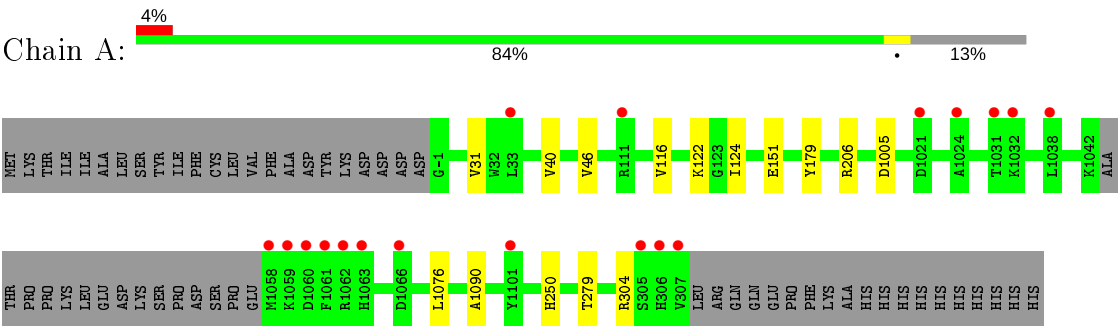
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	94	Total O 94 94	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Adenosine receptor A2a,Soluble cytochrome b562 chimera



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	39.82Å 178.90Å 140.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.42 – 2.35 41.42 – 2.35	Depositor EDS
% Data completeness (in resolution range)	90.3 (41.42-2.35) 85.2 (41.42-2.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.198 , 0.223 0.198 , 0.223	Depositor DCC
R_{free} test set	982 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6760	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLB, OLC, NA, ZMA, CLR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/3269	0.41	0/4446

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	3108	3187	3083	11	0
2	A	25	0	15	1	0
3	A	1	0	0	0	0
4	A	84	0	138	4	0
5	A	107	0	143	5	0
6	A	136	0	188	6	0
7	A	18	0	23	2	0
8	A	94	0	0	4	0
All	All	3573	3187	3590	20	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 (20) 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:2407:OLC:H13A	6:A:2412:OLA:H142	1.65	0.77
1:A:206:ARG:NH1	8:A:2503:HOH:O	2.23	0.71
1:A:1005[A]:ASP:OD1	8:A:2501:HOH:O	2.09	0.69
1:A:250:HIS:CE1	2:A:2401:ZMA:H24	2.39	0.57
5:A:2406:OLC:H21	5:A:2410:OLC:H24A	1.87	0.56
5:A:2407:OLC:H2A	6:A:2413:OLA:H32	1.88	0.56
1:A:31:VAL:HG12	7:A:2422:OLB:H24A	1.91	0.53
6:A:2412:OLA:H52	6:A:2414:OLA:H21	1.92	0.50
1:A:124:ILE:HD13	6:A:2418:OLA:H31	1.94	0.50
4:A:2404:CLR:H121	4:A:2404:CLR:H212	1.94	0.49
6:A:2412:OLA:H131	6:A:2412:OLA:H10	1.49	0.48
1:A:279[A]:THR:HG23	6:A:2419:OLA:H41	1.95	0.47
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.97	0.47
4:A:2405:CLR:H121	4:A:2405:CLR:H212	1.97	0.46
4:A:2405:CLR:H272	5:A:2407:OLC:H14A	1.99	0.45
1:A:122:LYS:HE3	8:A:2586:HOH:O	2.17	0.45
1:A:179:TYR:CD1	5:A:2411:OLC:H2	2.53	0.44
4:A:2403:CLR:H212	4:A:2403:CLR:H121	2.00	0.43
1:A:1090:ALA:O	8:A:2502:HOH:O	2.21	0.43
1:A:46:VAL:HG11	7:A:2422:OLB:H21	2.01	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/447 (92%)	406 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	338/374 (90%)	335 (99%)	3 (1%)	78	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	1076	LEU
1	A	304	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	OLC	A	2409	-	14,14,24	0.88	1 (7%)	15,15,25	0.95	1 (6%)
6	OLA	A	2417	-	14,17,19	0.26	0	13,17,19	0.50	0
6	OLA	A	2418	-	5,8,19	0.23	0	4,8,19	0.61	0
6	OLA	A	2413	-	16,19,19	0.27	0	15,19,19	0.48	0
5	OLC	A	2408	-	20,20,24	0.74	1 (5%)	21,21,25	1.01	1 (4%)
6	OLA	A	2414	-	11,14,19	0.26	0	10,14,19	0.56	0
2	ZMA	A	2401	-	21,28,28	0.89	1 (4%)	22,39,39	1.46	4 (18%)
4	CLR	A	2403	-	31,31,31	0.65	0	48,48,48	0.94	2 (4%)
4	CLR	A	2404	-	31,31,31	0.68	0	48,48,48	1.02	4 (8%)
6	OLA	A	2419	-	5,8,19	0.24	0	4,8,19	0.61	0
5	OLC	A	2410	-	16,16,24	0.85	1 (6%)	17,17,25	1.17	1 (5%)
7	OLB	A	2422	-	17,17,24	0.84	1 (5%)	18,18,25	1.00	1 (5%)
6	OLA	A	2415	-	7,10,19	0.22	0	6,10,19	0.60	0
6	OLA	A	2421	-	7,7,19	0.25	0	6,6,19	0.50	0
6	OLA	A	2416	-	11,14,19	0.25	0	10,14,19	0.57	0
5	OLC	A	2406	-	15,15,24	0.84	1 (6%)	16,16,25	1.08	1 (6%)
4	CLR	A	2405	-	31,31,31	0.65	0	48,48,48	1.09	3 (6%)
6	OLA	A	2412	-	15,18,19	0.26	0	14,18,19	0.54	0
5	OLC	A	2407	-	21,21,24	0.75	1 (4%)	22,22,25	0.96	1 (4%)
5	OLC	A	2411	-	15,15,24	0.85	1 (6%)	16,16,25	1.12	1 (6%)
6	OLA	A	2420	-	8,11,19	0.33	0	7,11,19	0.76	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	OLC	A	2409	-	-	2/14/14/24	-
6	OLA	A	2417	-	-	4/13/15/17	-
6	OLA	A	2418	-	-	1/4/6/17	-
6	OLA	A	2413	-	-	8/15/17/17	-
5	OLC	A	2408	-	-	9/20/20/24	-
6	OLA	A	2414	-	-	4/10/12/17	-
2	ZMA	A	2401	-	-	0/6/10/10	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	A	2403	-	-	3/10/68/68	0/4/4/4
4	CLR	A	2404	-	-	7/10/68/68	0/4/4/4
6	OLA	A	2419	-	-	2/4/6/17	-
5	OLC	A	2410	-	-	11/16/16/24	-
7	OLB	A	2422	-	-	4/17/17/24	-
6	OLA	A	2415	-	-	4/6/8/17	-
6	OLA	A	2421	-	-	3/5/5/17	-
6	OLA	A	2416	-	-	5/10/12/17	-
5	OLC	A	2406	-	-	3/15/15/24	-
4	CLR	A	2405	-	-	2/10/68/68	0/4/4/4
6	OLA	A	2412	-	-	9/14/16/17	-
5	OLC	A	2407	-	-	12/21/21/24	-
5	OLC	A	2411	-	-	6/15/15/24	-
6	OLA	A	2420	-	-	4/7/9/17	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2411	OLC	O20-C1	2.74	1.41	1.33
7	A	2422	OLB	O20-C1	2.73	1.41	1.33
5	A	2407	OLC	O20-C1	2.71	1.41	1.33
5	A	2409	OLC	O20-C1	2.65	1.41	1.33
5	A	2406	OLC	O20-C1	2.59	1.40	1.33
5	A	2408	OLC	O20-C1	2.59	1.40	1.33
5	A	2410	OLC	O20-C1	2.57	1.40	1.33
2	A	2401	ZMA	C11-N10	2.32	1.38	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2401	ZMA	N15-C14-N16	4.84	121.23	117.97
4	A	2404	CLR	C13-C17-C20	-3.46	114.06	119.49
4	A	2405	CLR	C4-C5-C10	3.03	120.45	116.42
5	A	2411	OLC	O20-C1-C2	2.96	121.21	111.91
4	A	2405	CLR	C4-C5-C6	-2.90	116.43	120.61
5	A	2410	OLC	O20-C1-C2	2.89	120.98	111.91
4	A	2403	CLR	C4-C5-C10	2.80	120.14	116.42
5	A	2408	OLC	O20-C1-C2	2.76	120.58	111.91
5	A	2406	OLC	O20-C1-C2	2.75	120.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2407	OLC	O20-C1-C2	2.56	119.95	111.91
7	A	2422	OLB	O20-C1-C2	2.50	119.75	111.91
4	A	2403	CLR	C4-C5-C6	-2.42	117.13	120.61
5	A	2409	OLC	O20-C1-C2	2.39	119.40	111.91
4	A	2404	CLR	C11-C12-C13	-2.28	108.88	112.78
2	A	2401	ZMA	N15-C14-N13	2.24	119.98	117.03
2	A	2401	ZMA	N12-C11-N13	-2.23	122.70	126.23
4	A	2404	CLR	C4-C5-C10	2.09	119.19	116.42
4	A	2405	CLR	C7-C8-C14	-2.03	107.96	110.91
4	A	2404	CLR	C4-C5-C6	-2.02	117.70	120.61
2	A	2401	ZMA	C21-C20-N19	-2.01	121.04	123.61

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2407	OLC	C21-C22-C24-O25
6	A	2415	OLA	C1-C2-C3-C4
6	A	2420	OLA	C1-C2-C3-C4
6	A	2413	OLA	C1-C2-C3-C4
5	A	2408	OLC	C21-C22-C24-O25
6	A	2412	OLA	C1-C2-C3-C4
6	A	2414	OLA	C1-C2-C3-C4
6	A	2419	OLA	C1-C2-C3-C4
4	A	2404	CLR	C21-C20-C22-C23
5	A	2410	OLC	C2-C1-O20-C21
5	A	2408	OLC	C2-C1-O20-C21
5	A	2411	OLC	C2-C1-O20-C21
7	A	2422	OLB	C2-C1-O20-C21
5	A	2410	OLC	O20-C21-C22-O23
5	A	2408	OLC	O19-C1-O20-C21
5	A	2411	OLC	O19-C1-O20-C21
5	A	2410	OLC	C1-C2-C3-C4
5	A	2408	OLC	O23-C22-C24-O25
7	A	2422	OLB	O19-C1-O20-C21
5	A	2410	OLC	O19-C1-O20-C21
6	A	2412	OLA	C10-C11-C12-C13
4	A	2404	CLR	C17-C20-C22-C23
4	A	2404	CLR	C20-C22-C23-C24
6	A	2420	OLA	C4-C5-C6-C7
5	A	2409	OLC	C4-C5-C6-C7
5	A	2410	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
6	A	2416	OLA	C3-C4-C5-C6
6	A	2419	OLA	C3-C4-C5-C6
6	A	2415	OLA	C4-C5-C6-C7
4	A	2405	CLR	C23-C24-C25-C27
5	A	2410	OLC	C3-C4-C5-C6
6	A	2413	OLA	C3-C4-C5-C6
6	A	2413	OLA	C4-C5-C6-C7
6	A	2416	OLA	C5-C6-C7-C8
5	A	2407	OLC	O20-C21-C22-O23
6	A	2412	OLA	C12-C13-C14-C15
6	A	2417	OLA	C4-C5-C6-C7
4	A	2405	CLR	C23-C24-C25-C26
5	A	2407	OLC	O23-C22-C24-O25
6	A	2420	OLA	C3-C4-C5-C6
5	A	2407	OLC	C6-C7-C8-C9
5	A	2407	OLC	O20-C21-C22-C24
5	A	2406	OLC	C2-C1-O20-C21
6	A	2421	OLA	C4-C5-C6-C7
6	A	2413	OLA	C5-C6-C7-C8
4	A	2403	CLR	C23-C24-C25-C26
4	A	2404	CLR	C23-C24-C25-C27
6	A	2412	OLA	C11-C12-C13-C14
5	A	2411	OLC	C1-C2-C3-C4
6	A	2417	OLA	C12-C13-C14-C15
6	A	2412	OLA	C3-C4-C5-C6
5	A	2410	OLC	C6-C7-C8-C9
5	A	2411	OLC	O20-C21-C22-O23
5	A	2408	OLC	C11-C12-C13-C14
6	A	2421	OLA	C5-C6-C7-C8
5	A	2410	OLC	C2-C3-C4-C5
5	A	2406	OLC	O19-C1-O20-C21
4	A	2403	CLR	C20-C22-C23-C24
6	A	2413	OLA	C11-C12-C13-C14
6	A	2421	OLA	C1-C2-C3-C4
4	A	2404	CLR	C22-C23-C24-C25
5	A	2407	OLC	C4-C5-C6-C7
6	A	2412	OLA	C4-C5-C6-C7
5	A	2407	OLC	C3-C4-C5-C6
6	A	2415	OLA	C3-C4-C5-C6
5	A	2410	OLC	O23-C22-C24-O25
5	A	2411	OLC	O23-C22-C24-O25
4	A	2404	CLR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	A	2409	OLC	C3-C4-C5-C6
6	A	2420	OLA	C5-C6-C7-C8
4	A	2403	CLR	C23-C24-C25-C27
6	A	2413	OLA	C2-C3-C4-C5
6	A	2414	OLA	C3-C4-C5-C6
5	A	2406	OLC	O20-C21-C22-O23
6	A	2416	OLA	C1-C2-C3-C4
5	A	2407	OLC	C5-C6-C7-C8
5	A	2407	OLC	C10-C11-C12-C13
5	A	2408	OLC	C7-C8-C9-C10
6	A	2418	OLA	C4-C5-C6-C7
6	A	2412	OLA	C2-C3-C4-C5
6	A	2412	OLA	C5-C6-C7-C8
5	A	2407	OLC	C7-C8-C9-C10
6	A	2416	OLA	C2-C3-C4-C5
5	A	2408	OLC	C6-C7-C8-C9
7	A	2422	OLB	C7-C8-C9-C10
5	A	2411	OLC	C21-C22-C24-O25
6	A	2412	OLA	C9-C10-C11-C12
6	A	2413	OLA	C10-C11-C12-C13
4	A	2404	CLR	C13-C17-C20-C21
5	A	2407	OLC	O19-C1-O20-C21
6	A	2416	OLA	C7-C8-C9-C10
6	A	2414	OLA	C7-C8-C9-C10
7	A	2422	OLB	C6-C7-C8-C9
6	A	2414	OLA	C5-C6-C7-C8
5	A	2408	OLC	C5-C6-C7-C8
5	A	2407	OLC	C2-C1-O20-C21
5	A	2408	OLC	C9-C10-C11-C12
6	A	2417	OLA	C9-C10-C11-C12
6	A	2417	OLA	C6-C7-C8-C9
5	A	2410	OLC	C21-C22-C24-O25
6	A	2413	OLA	C7-C8-C9-C10
6	A	2415	OLA	C5-C6-C7-C8
5	A	2410	OLC	C7-C8-C9-C10

There are no ring outliers.

14 monomers are involved in 15 short contacts:

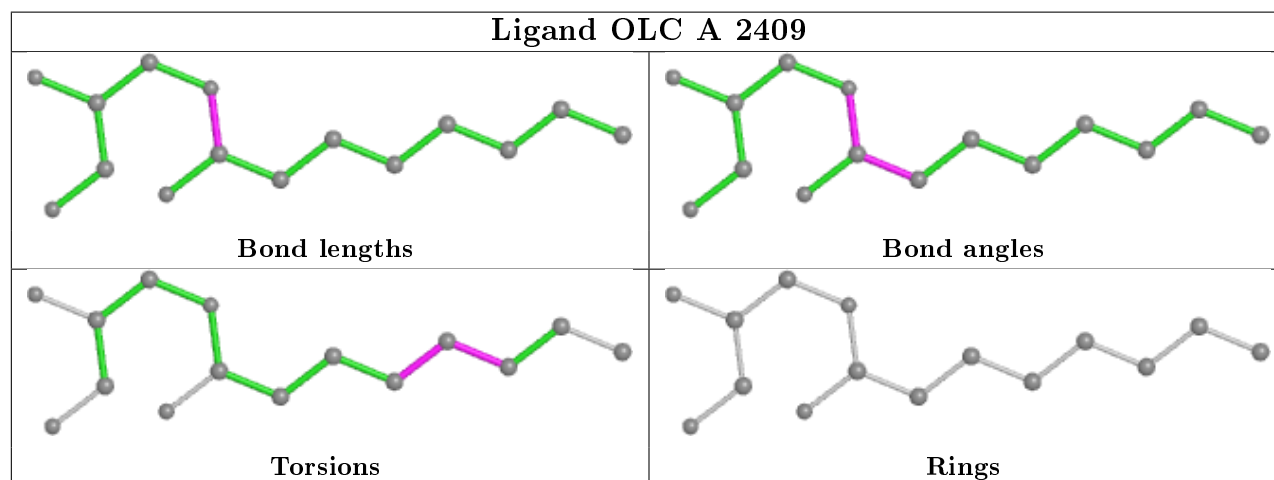
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2418	OLA	1	0
6	A	2413	OLA	1	0

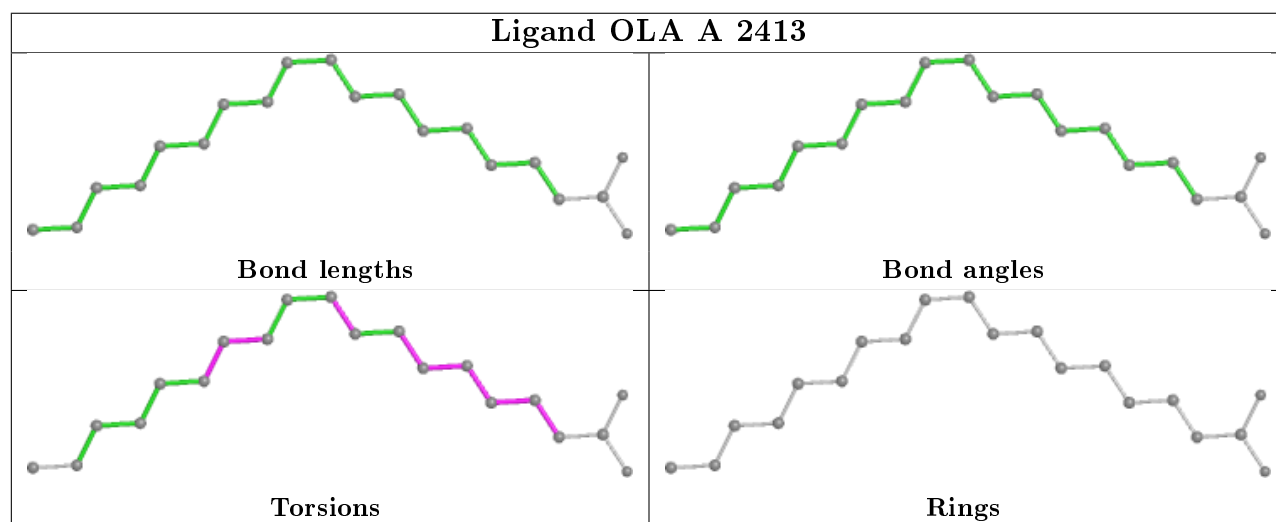
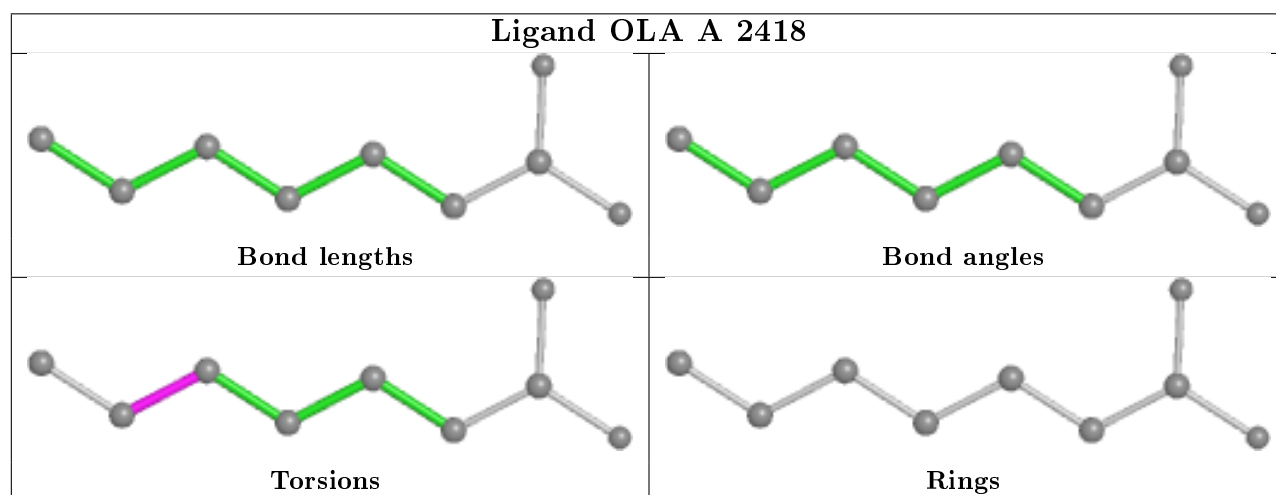
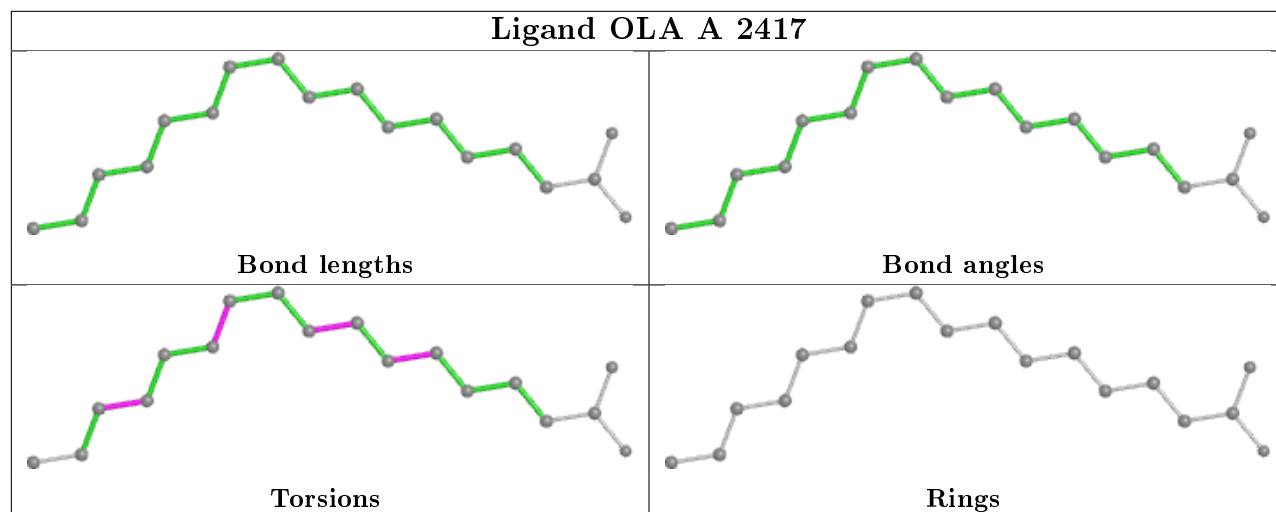
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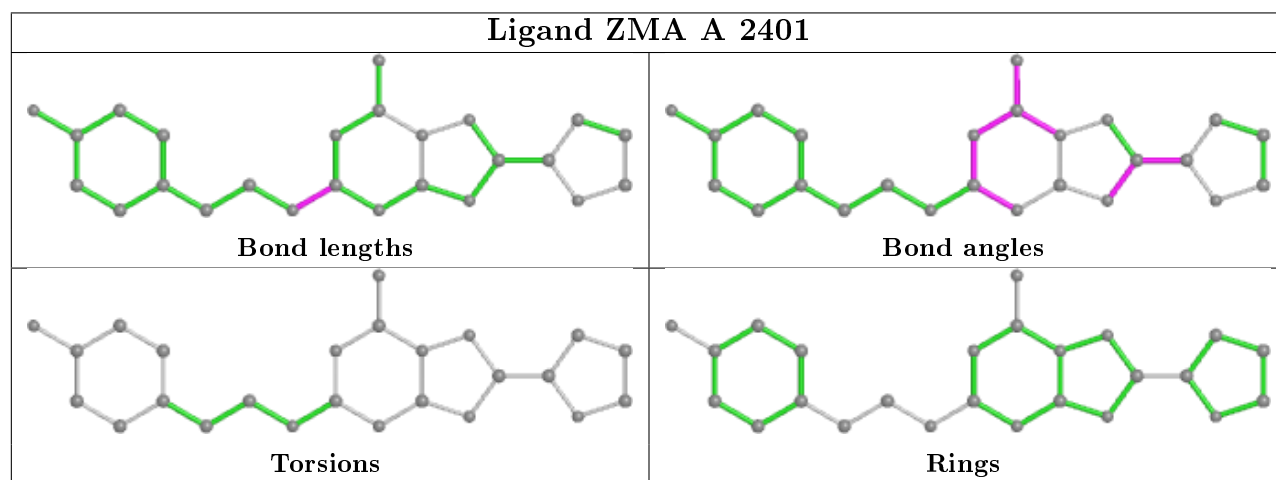
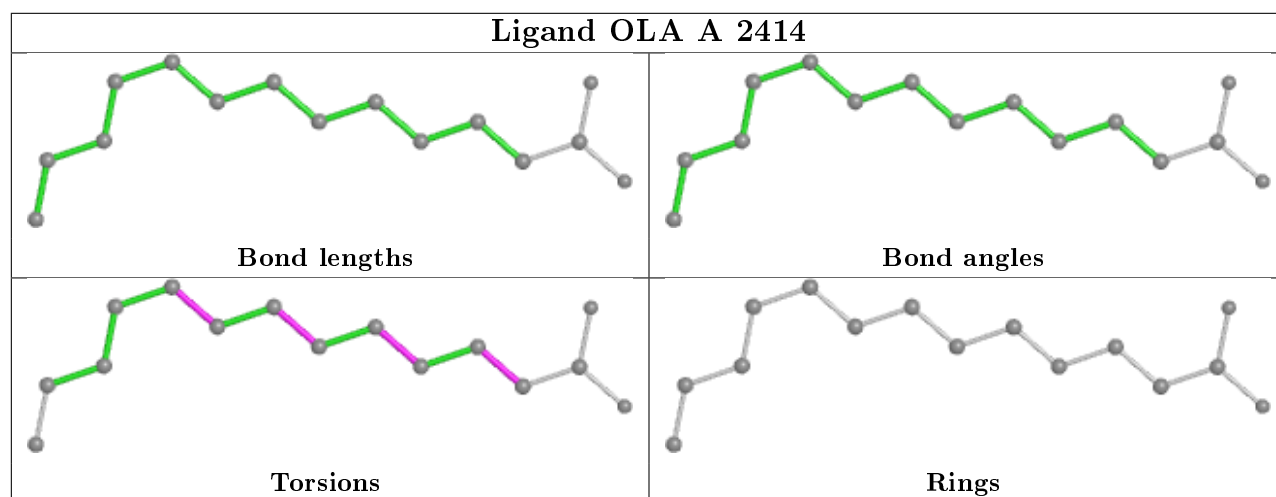
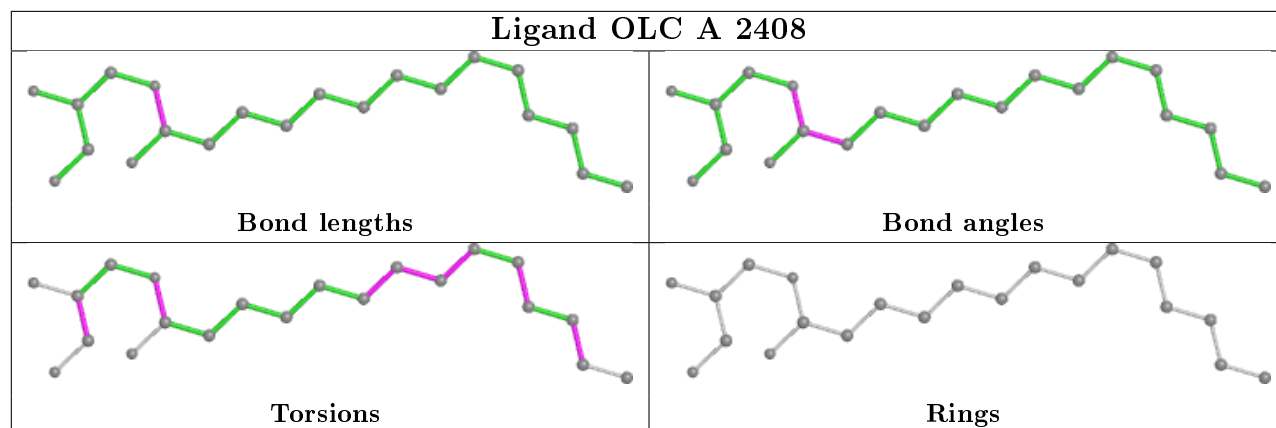
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2414	OLA	1	0
2	A	2401	ZMA	1	0
4	A	2403	CLR	1	0
4	A	2404	CLR	1	0
6	A	2419	OLA	1	0
5	A	2410	OLC	1	0
7	A	2422	OLB	2	0
5	A	2406	OLC	1	0
4	A	2405	CLR	2	0
6	A	2412	OLA	3	0
5	A	2407	OLC	3	0
5	A	2411	OLC	1	0

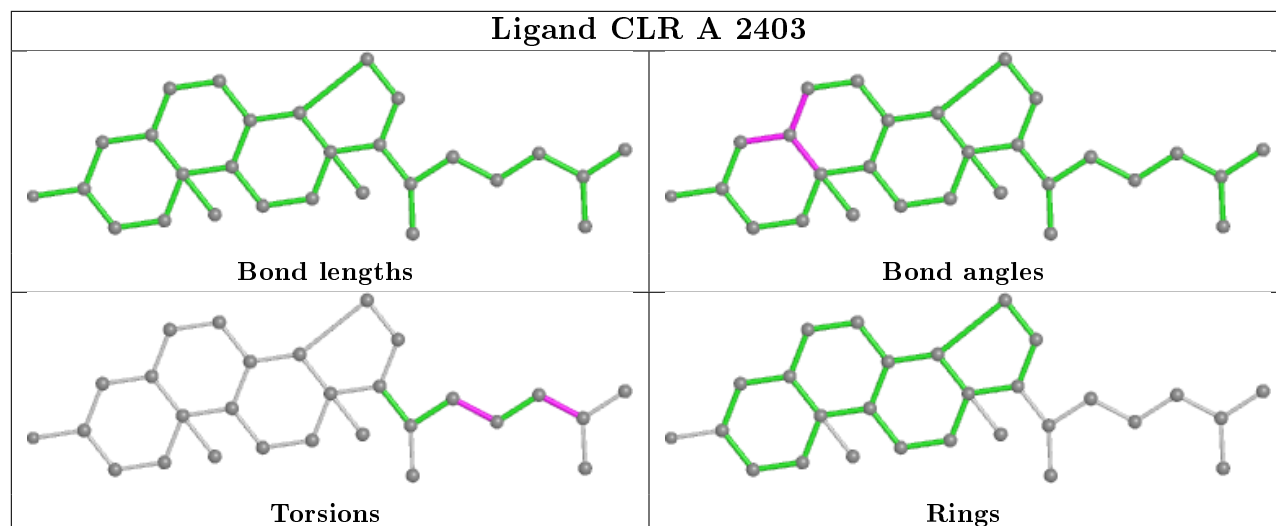
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



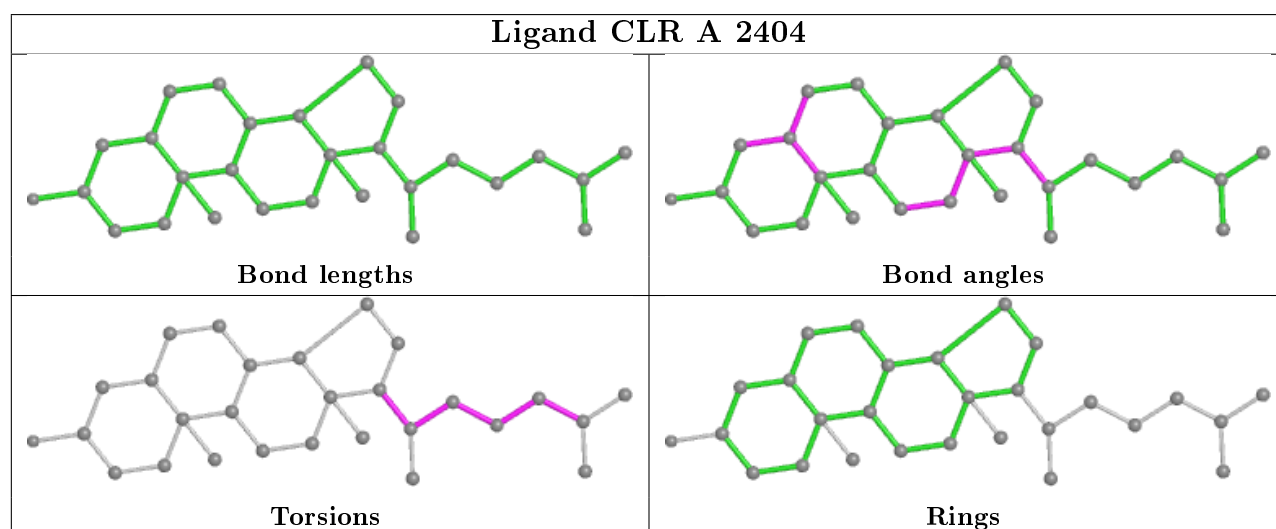




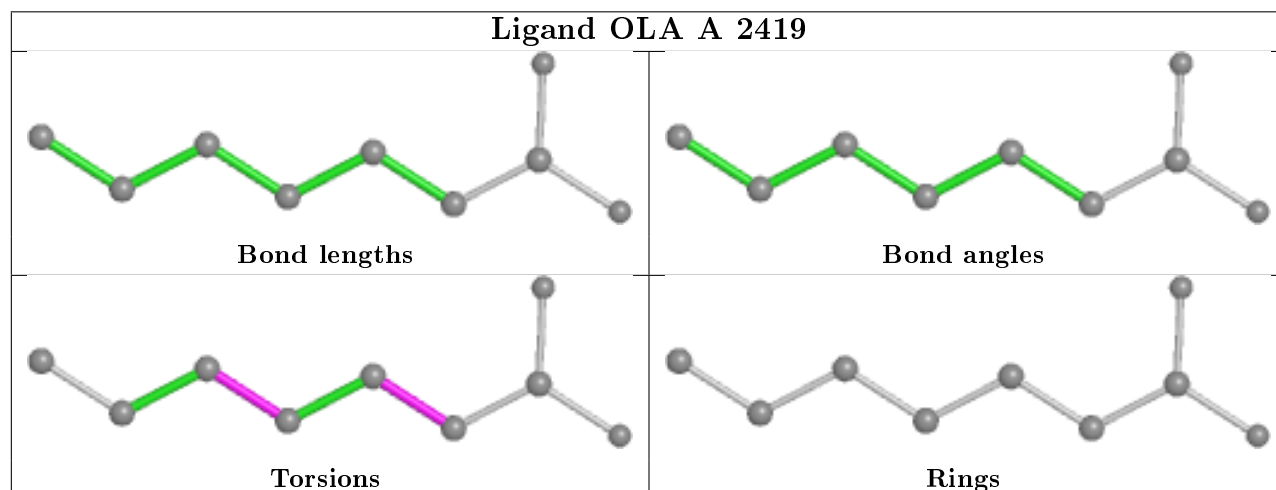
Ligand CLR A 2403

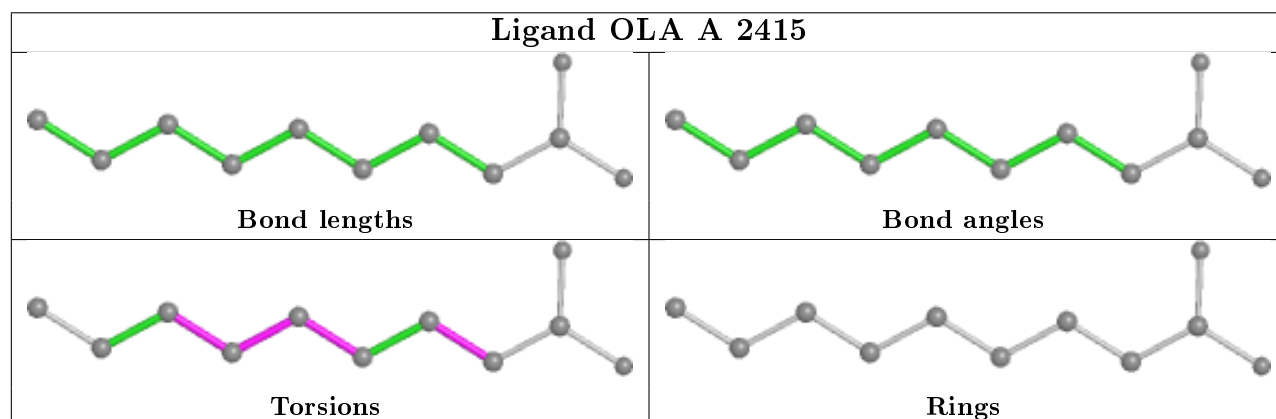
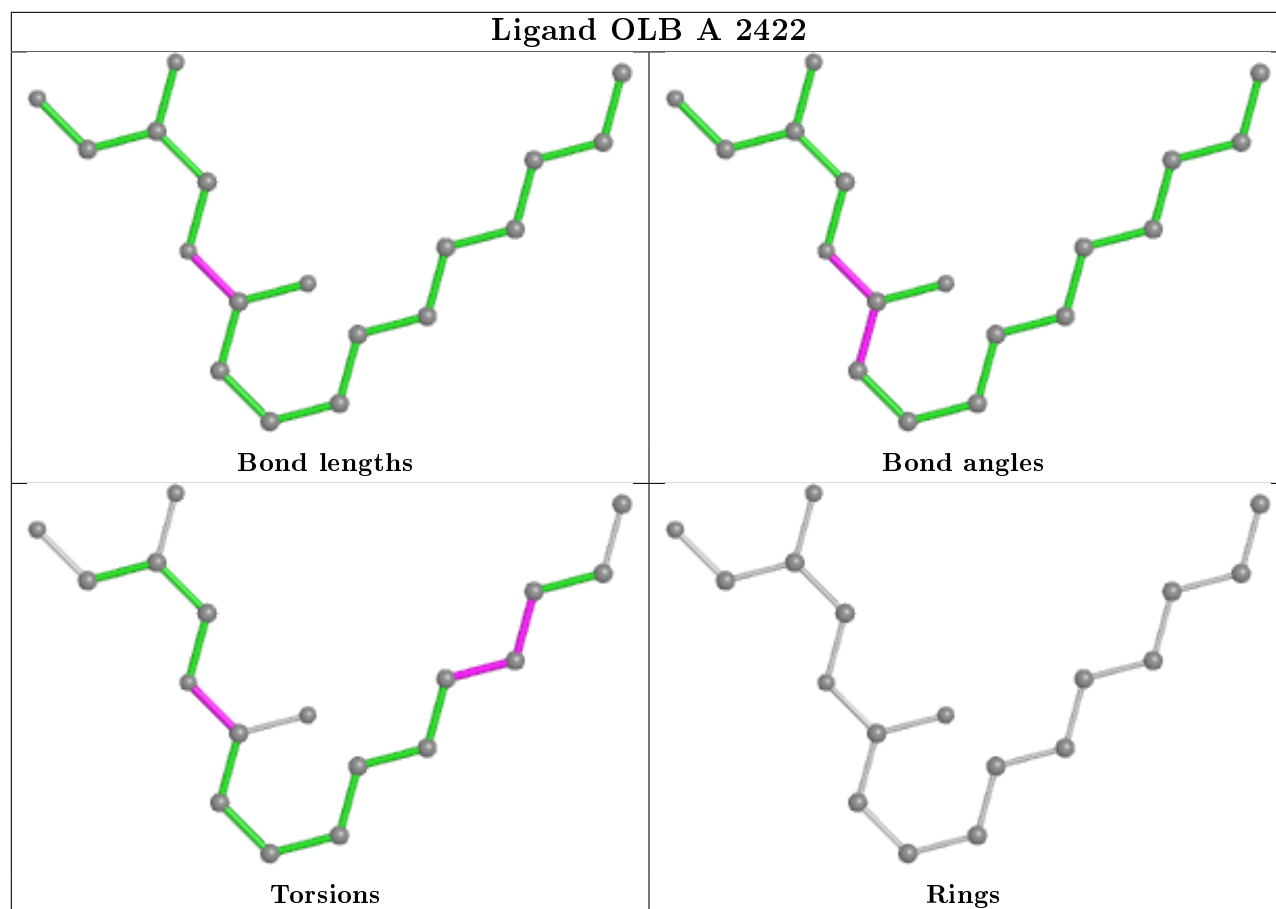
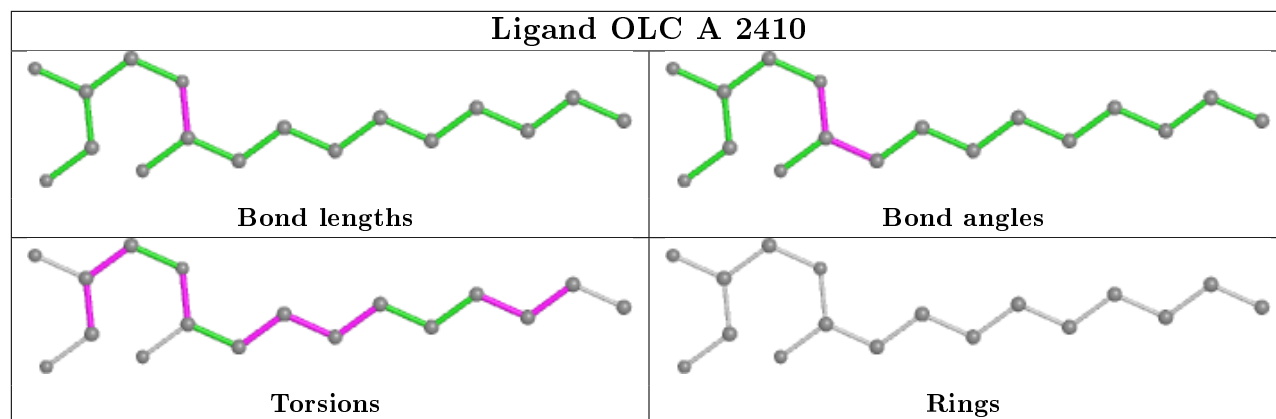


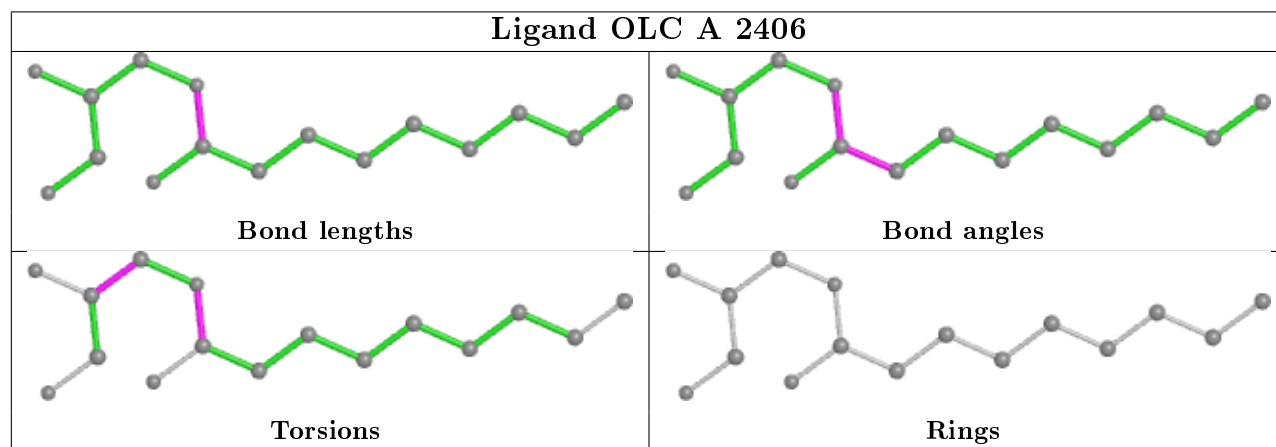
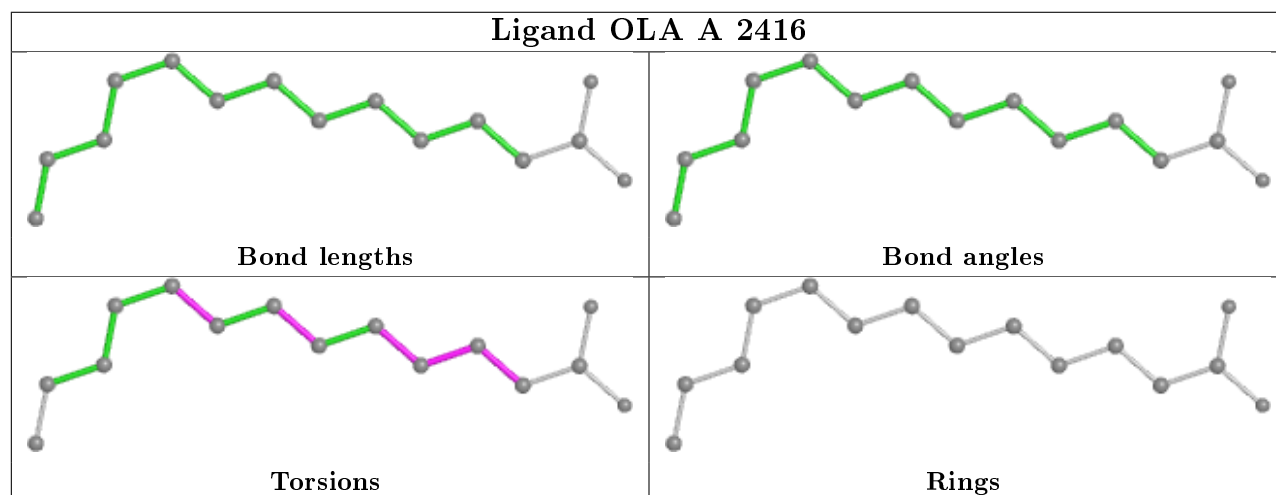
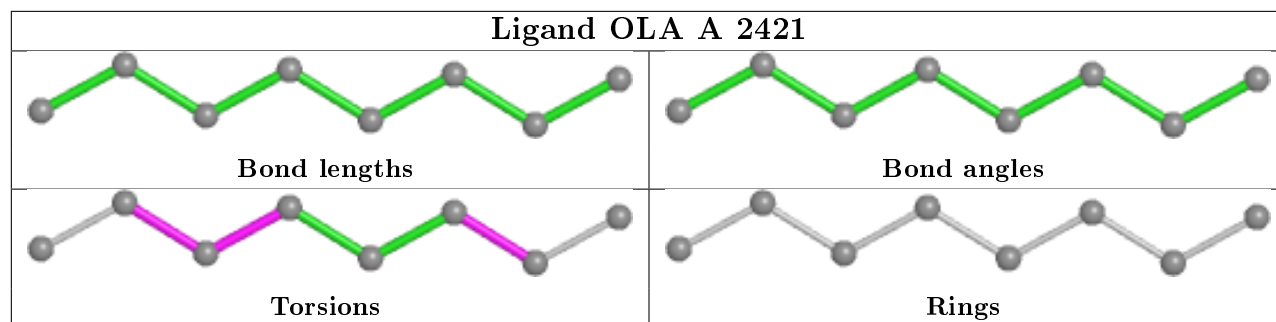
Ligand CLR A 2404

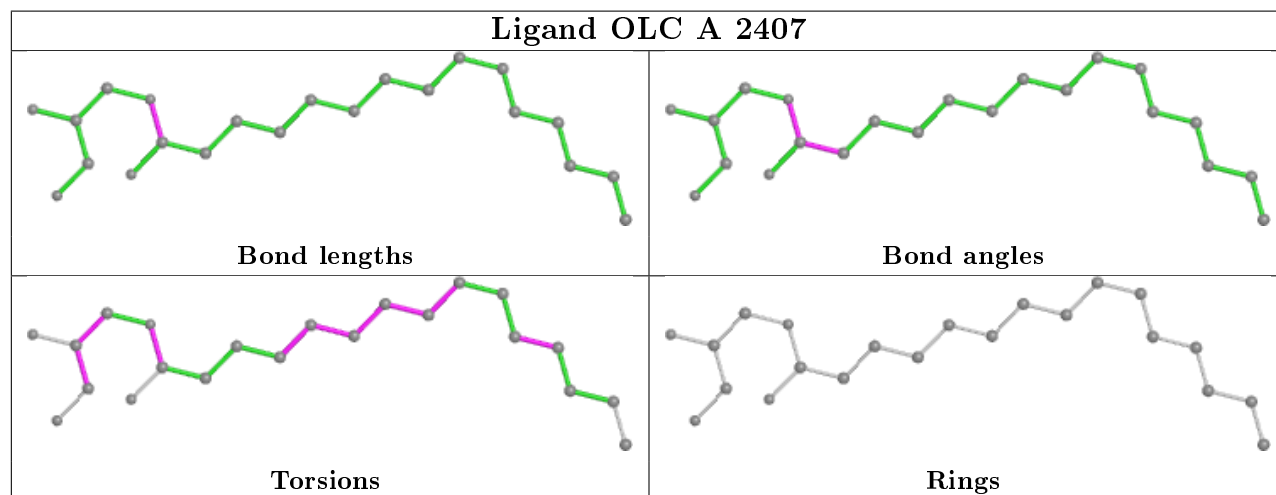
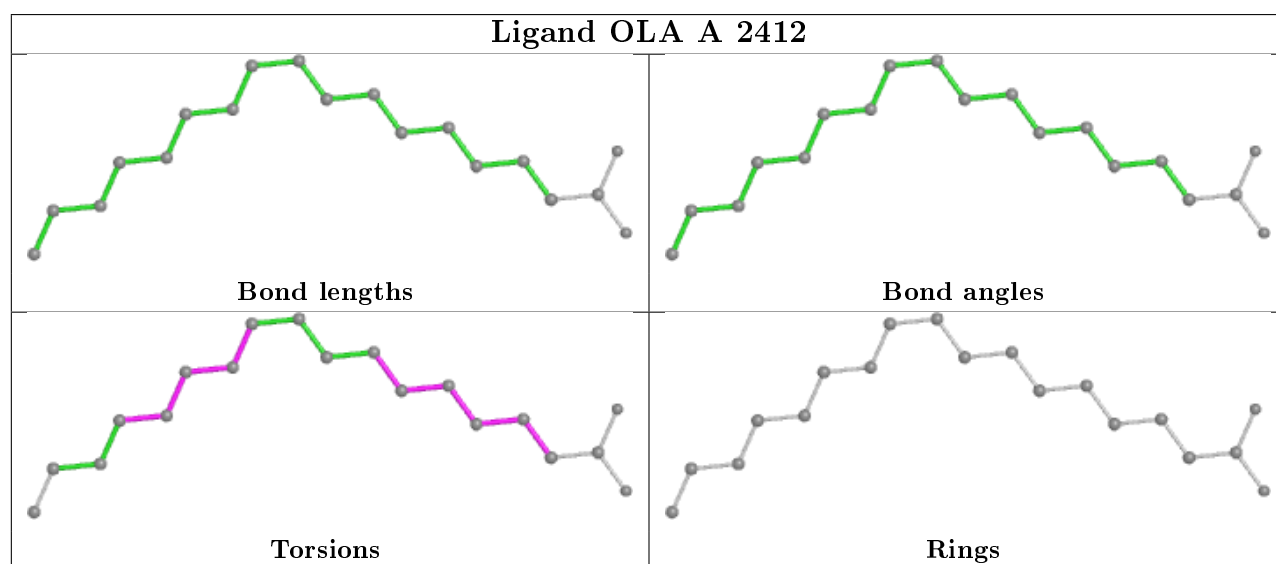
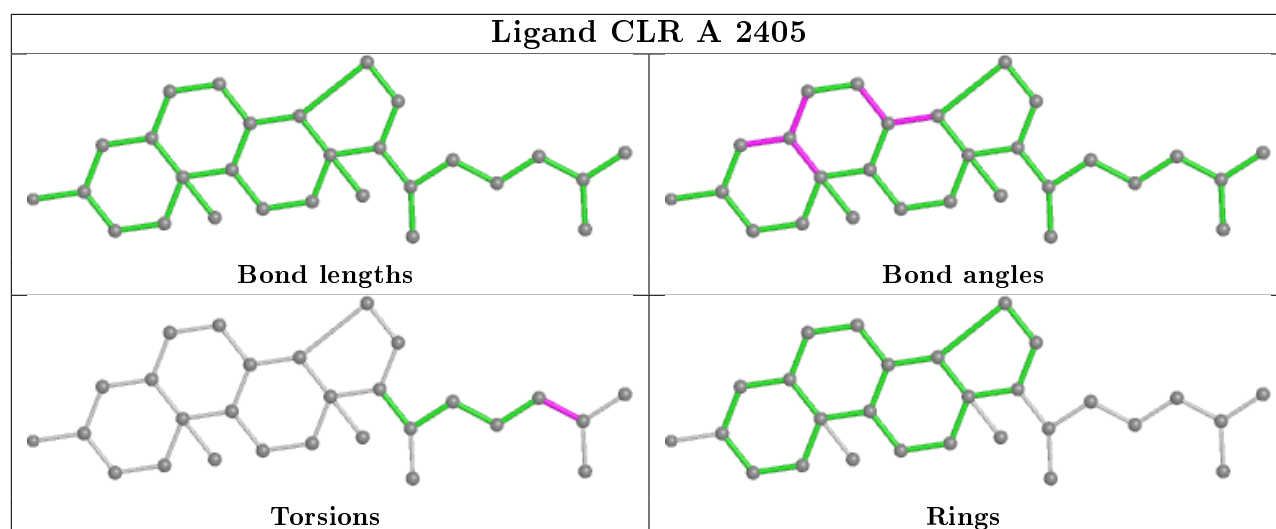


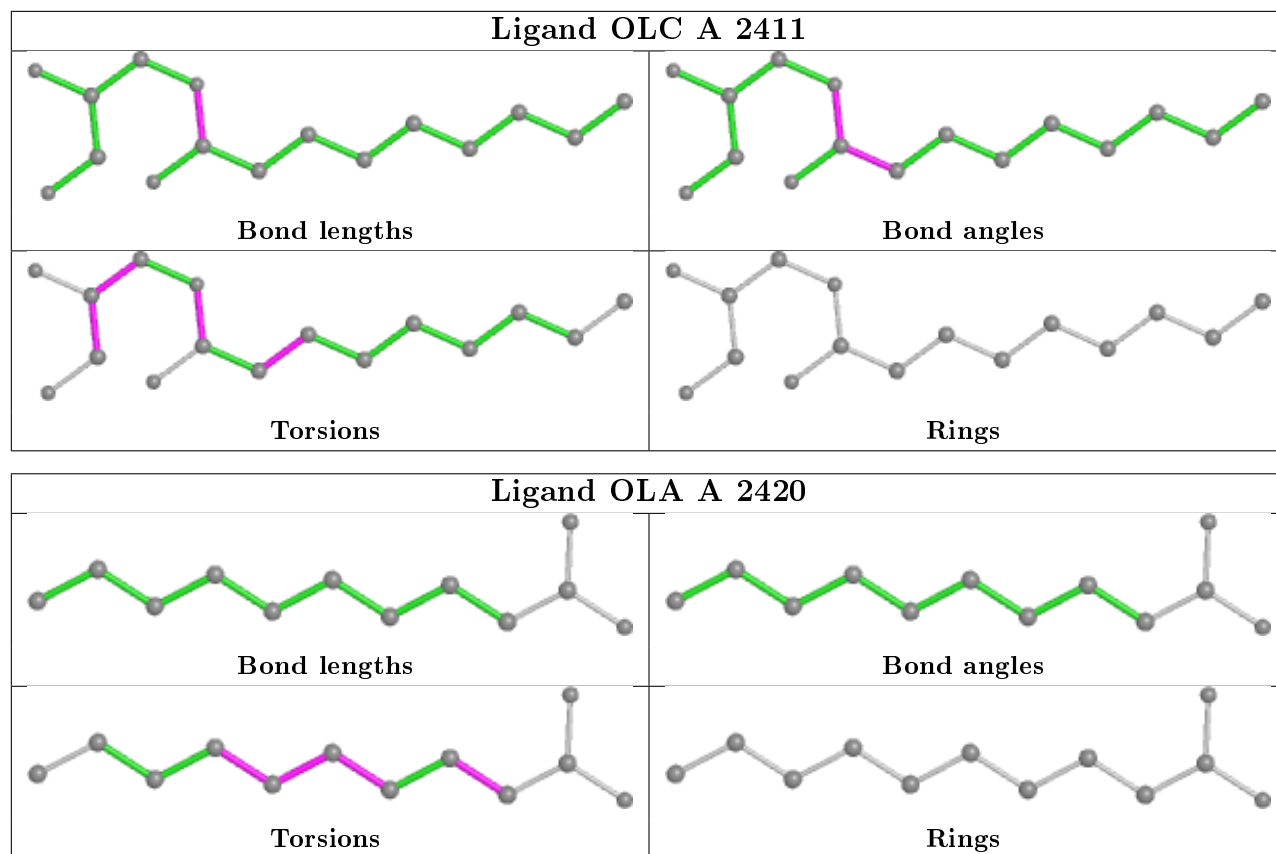
Ligand OLA A 2419











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	390/447 (87%)	0.28	18 (4%)	32 45	16, 28, 69, 99	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1062	ARG	4.8
1	A	307	VAL	3.8
1	A	1063	HIS	3.6
1	A	1024	ALA	3.3
1	A	1059	LYS	3.1
1	A	1061	PHE	3.0
1	A	1101	TYR	2.9
1	A	33[A]	LEU	2.8
1	A	1058	MET	2.8
1	A	306	HIS	2.7
1	A	1038	LEU	2.7
1	A	305	SER	2.5
1	A	1021	ASP	2.5
1	A	1066	ASP	2.4
1	A	1032	LYS	2.4
1	A	1031	THR	2.2
1	A	1060	ASP	2.2
1	A	111	ARG	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 ⓘ

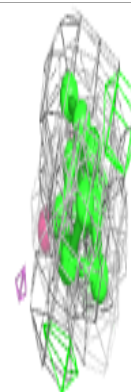
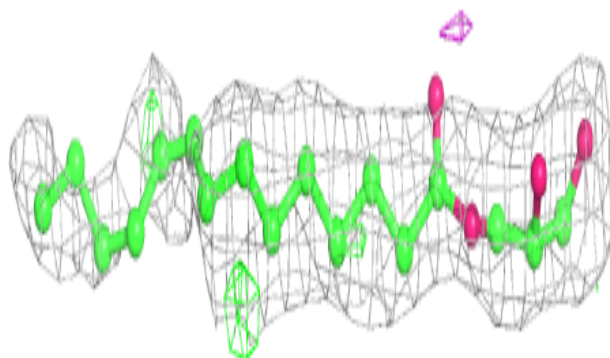
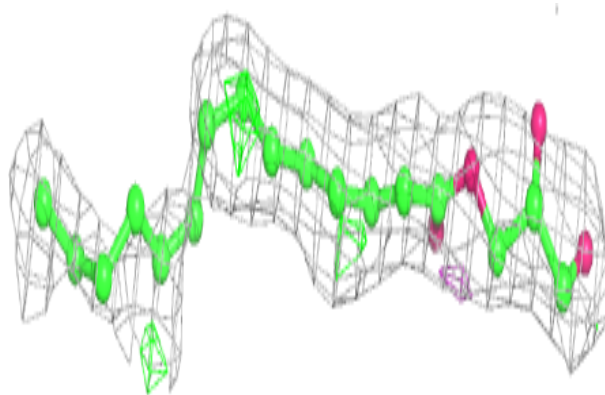
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	OLC	A	2408	21/25	0.71	0.32	62,73,75,75	0
6	OLA	A	2416	15/20	0.71	0.25	46,49,87,88	0
6	OLA	A	2414	15/20	0.71	0.29	60,69,73,73	0
5	OLC	A	2409	15/25	0.75	0.30	44,80,88,89	0
6	OLA	A	2421	8/20	0.76	0.42	54,58,78,82	0
6	OLA	A	2417	18/20	0.78	0.27	44,55,99,99	0
5	OLC	A	2410	17/25	0.78	0.27	65,66,67,67	0
7	OLB	A	2422	18/25	0.80	0.26	46,55,108,109	0
5	OLC	A	2411	16/25	0.81	0.26	45,49,64,66	0
6	OLA	A	2415	11/20	0.82	0.27	53,58,86,86	0
6	OLA	A	2420	12/20	0.82	0.22	53,65,68,68	0
6	OLA	A	2413	20/20	0.82	0.33	45,64,90,92	0
5	OLC	A	2406	16/25	0.82	0.43	65,73,96,98	0
4	CLR	A	2403	28/28	0.83	0.25	22,60,97,101	0
6	OLA	A	2412	19/20	0.85	0.24	42,46,61,63	0
5	OLC	A	2407	22/25	0.85	0.27	33,61,94,105	0
6	OLA	A	2418	9/20	0.89	0.25	38,53,78,78	0
3	NA	A	2402	1/1	0.90	0.10	35,35,35,35	0
4	CLR	A	2404	28/28	0.92	0.16	19,23,114,119	0
6	OLA	A	2419	9/20	0.93	0.23	43,57,91,91	0
4	CLR	A	2405	28/28	0.93	0.17	23,29,86,92	0
2	ZMA	A	2401	25/25	0.97	0.18	15,17,83,87	0

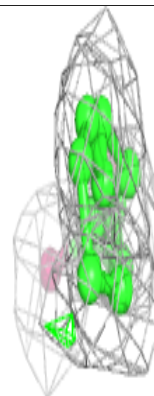
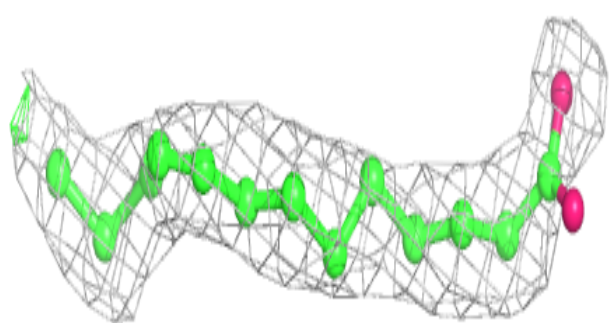
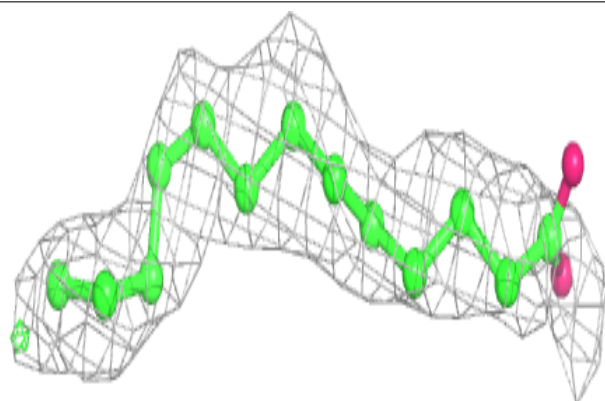
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 2408:

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

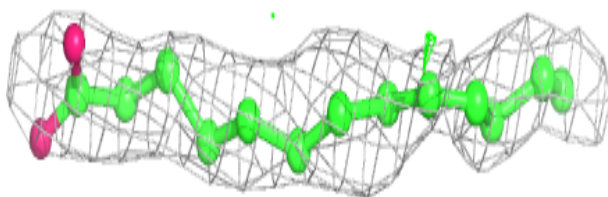
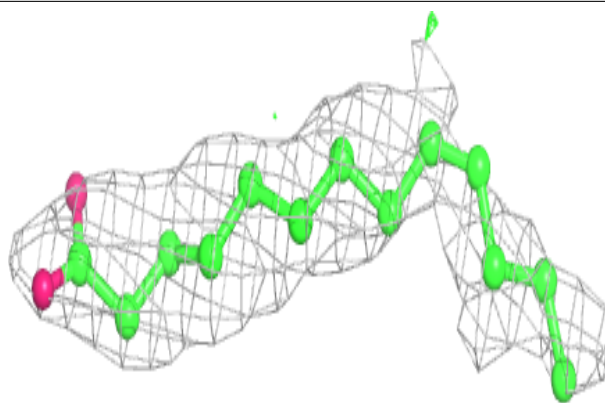
**Electron density around OLA A 2416:**

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

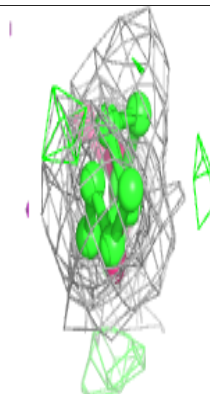
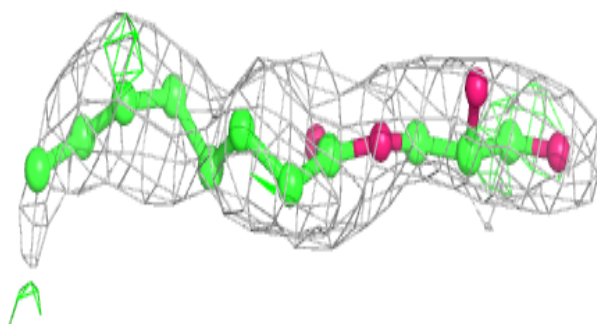
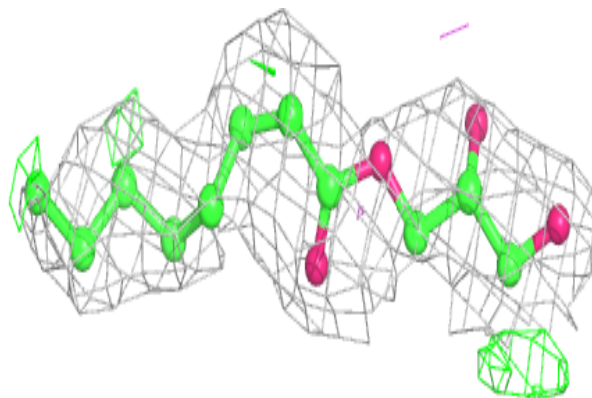


Electron density around OLA A 2414:

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

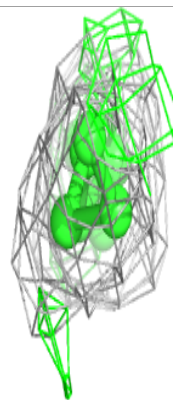
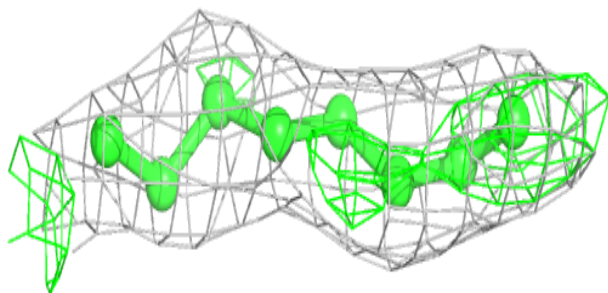
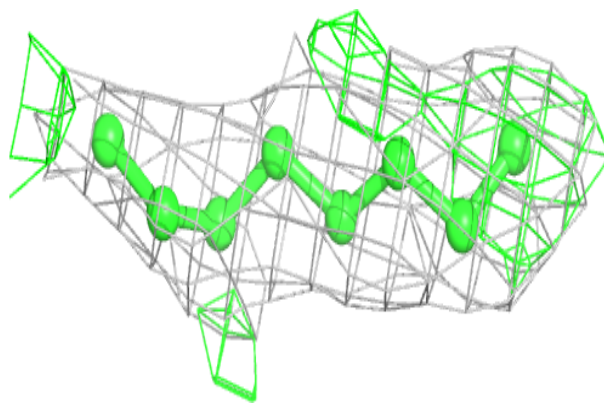
**Electron density around OLC A 2409:**

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

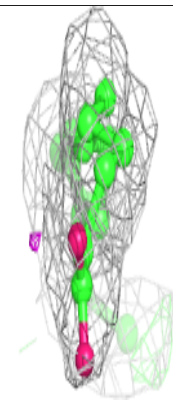
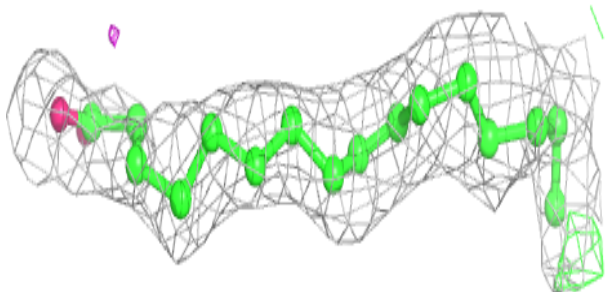
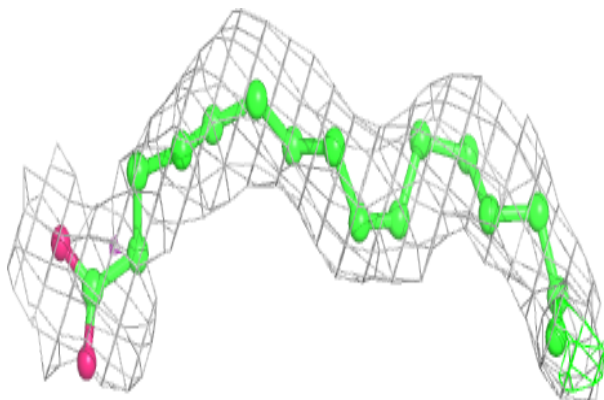


Electron density around OLA A 2421:

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

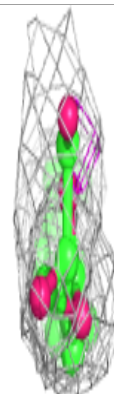
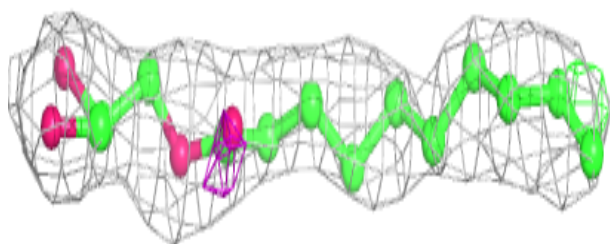
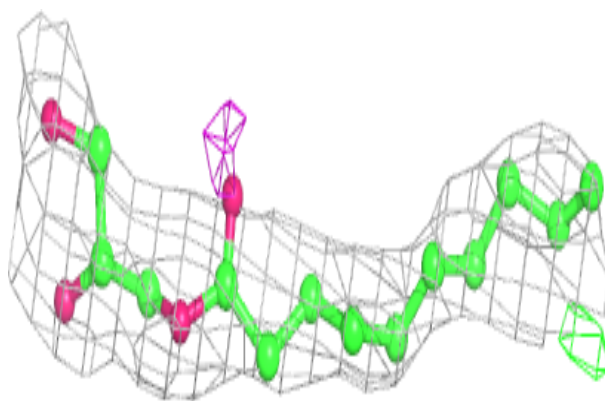
**Electron density around OLA A 2417:**

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

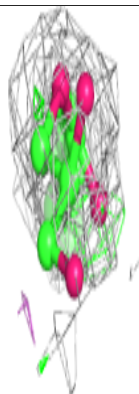
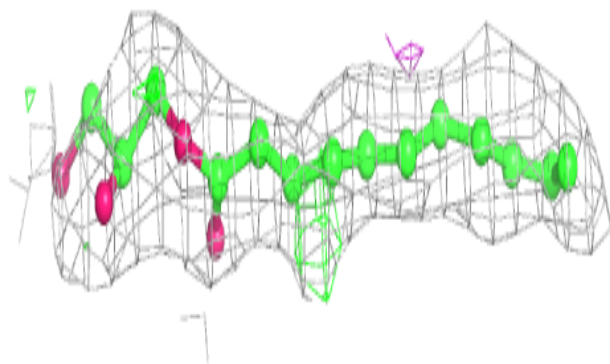
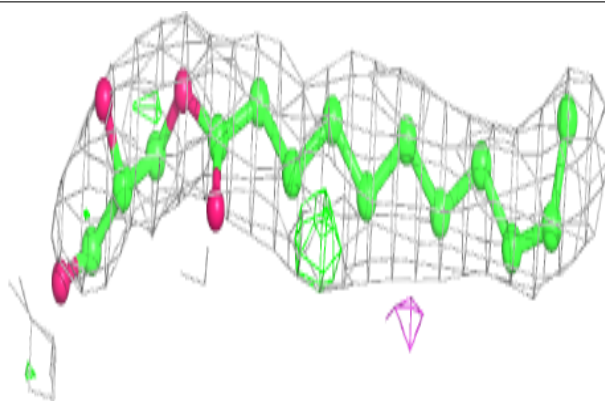


Electron density around OLC A 2410:

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

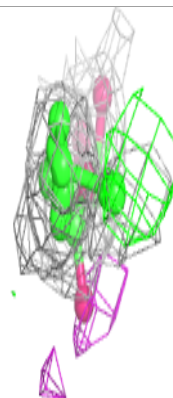
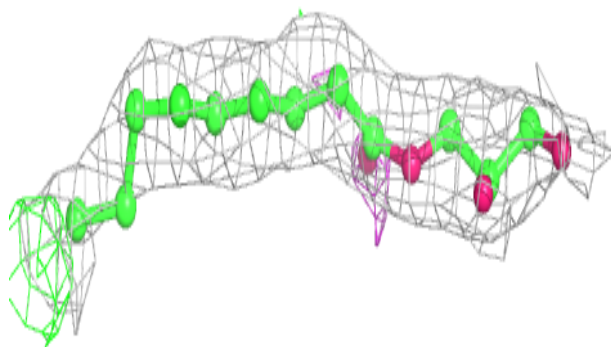
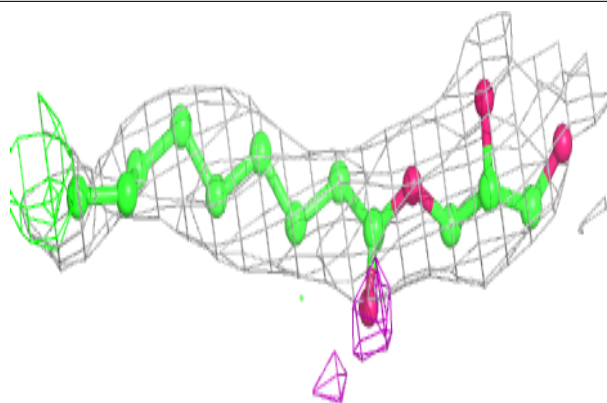
**Electron density around OLB A 2422:**

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

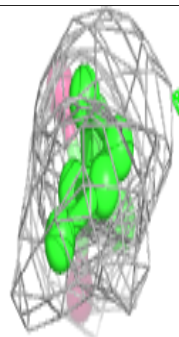
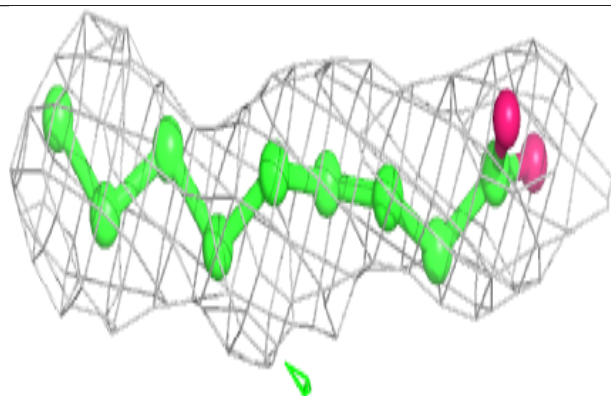
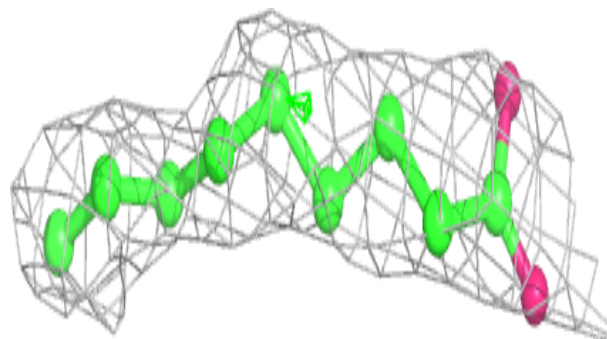


Electron density around OLC A 2411:

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

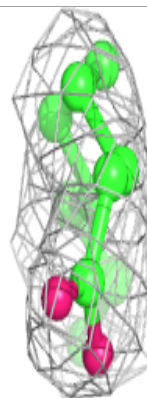
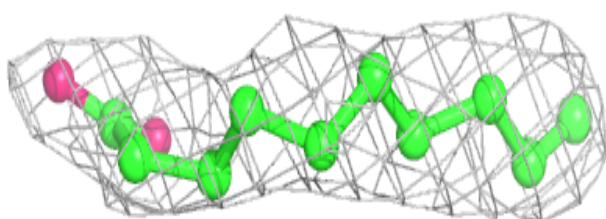
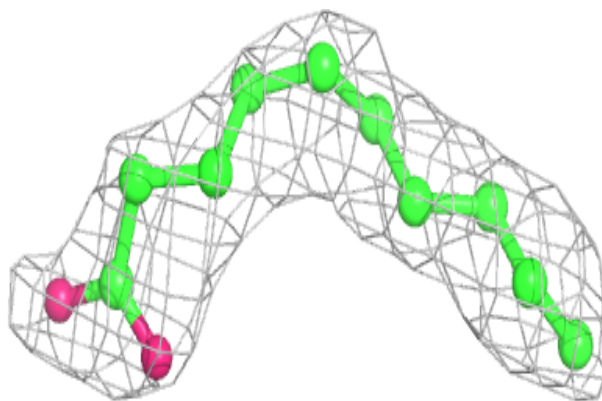
**Electron density around OLA A 2415:**

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

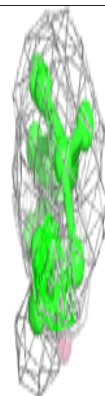
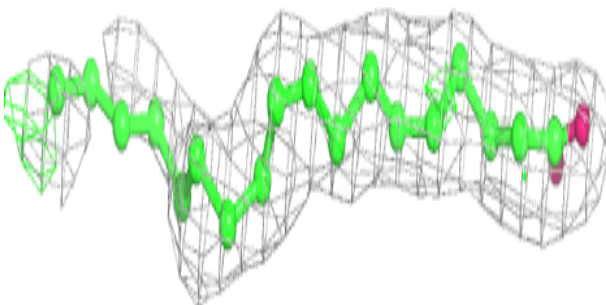
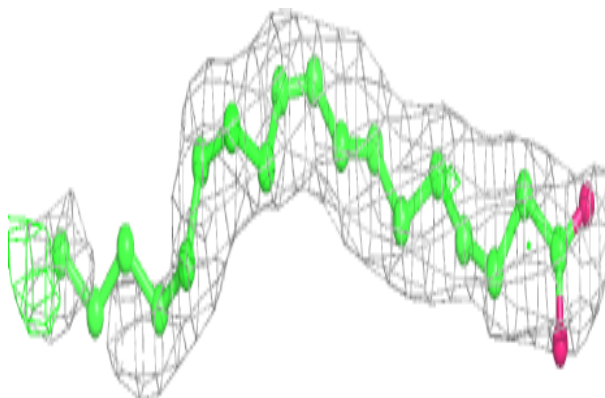


Electron density around OLA A 2420:

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

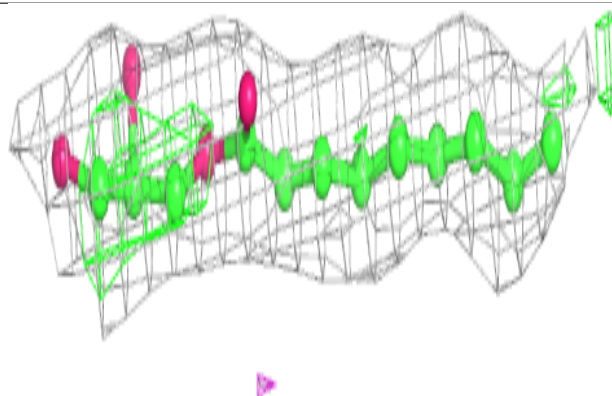
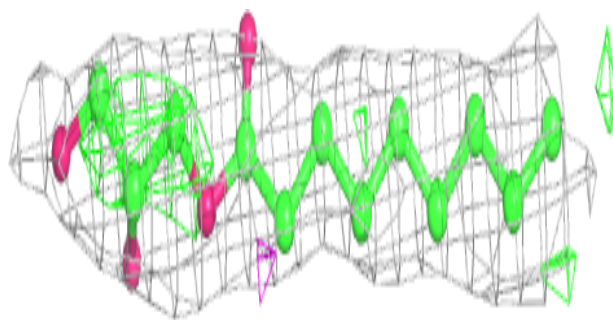
**Electron density around OLA A 2413:**

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

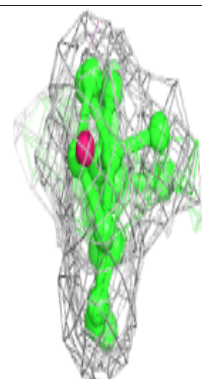
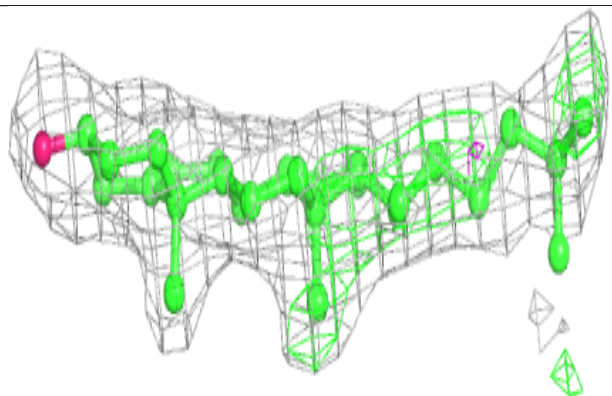
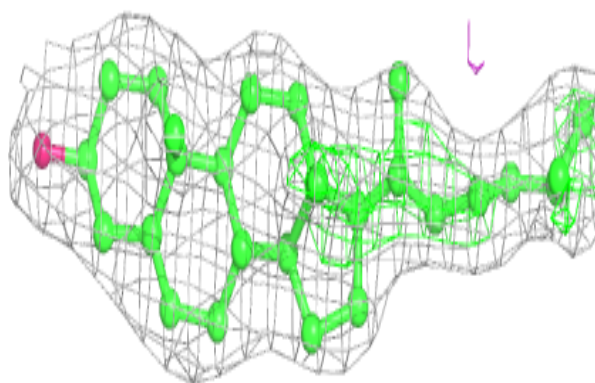


Electron density around OLC A 2406:

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

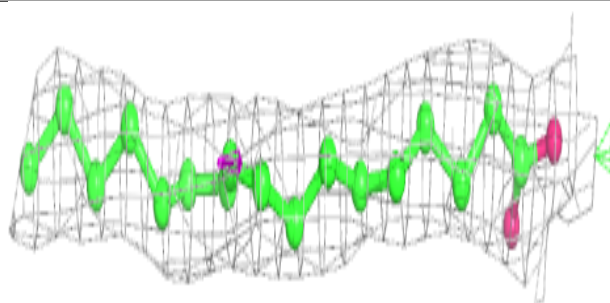
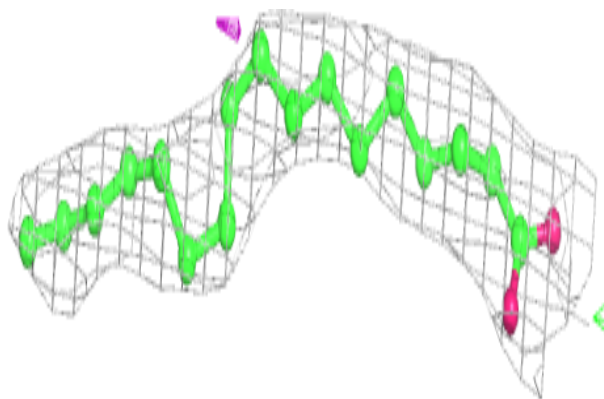
**Electron density around CLR A 2403:**

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

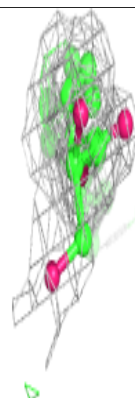
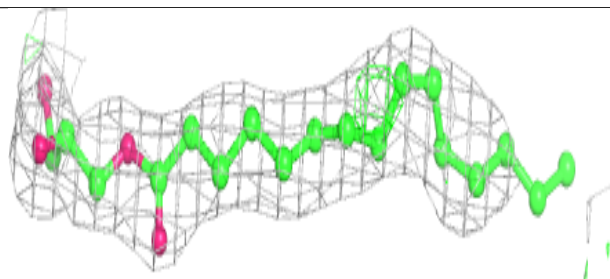
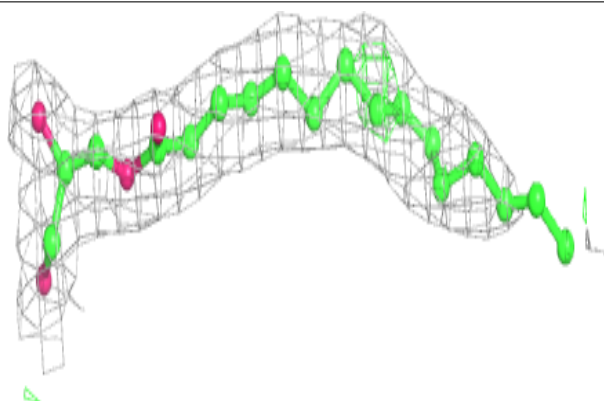


Electron density around OLA A 2412:

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

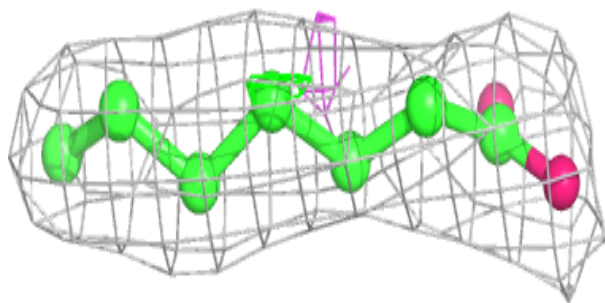
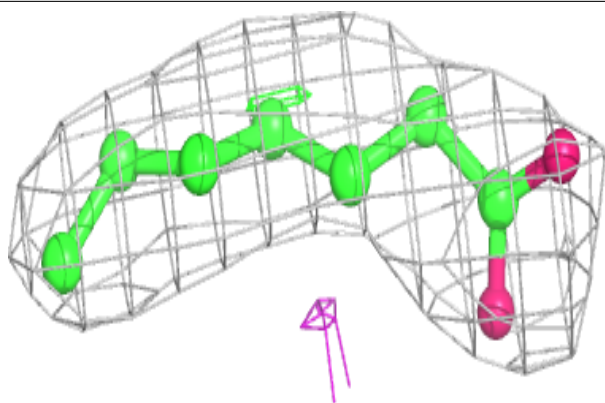
**Electron density around OLC A 2407:**

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

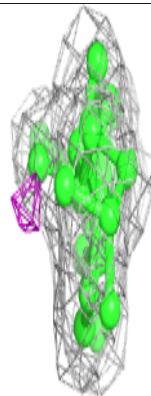
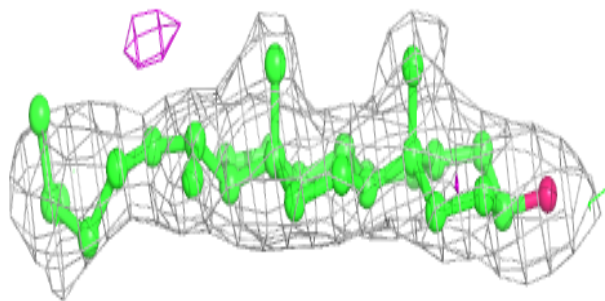
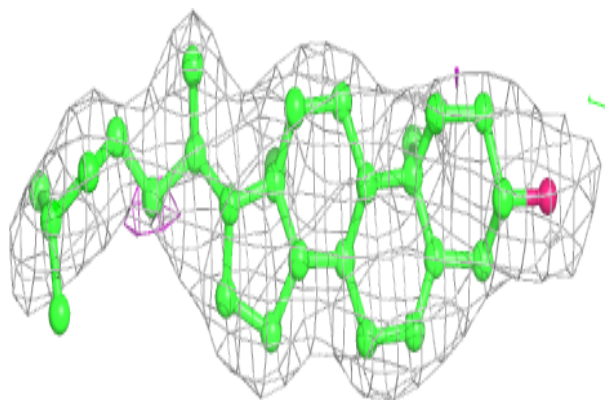


Electron density around OLA A 2418:

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

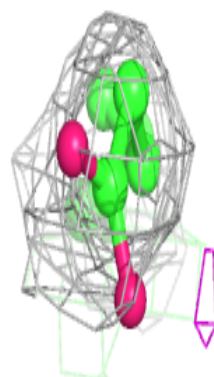
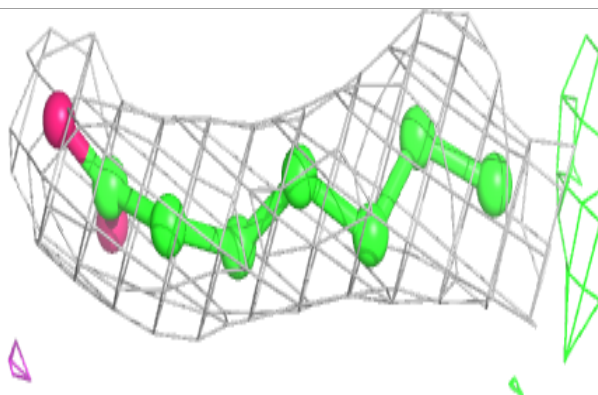
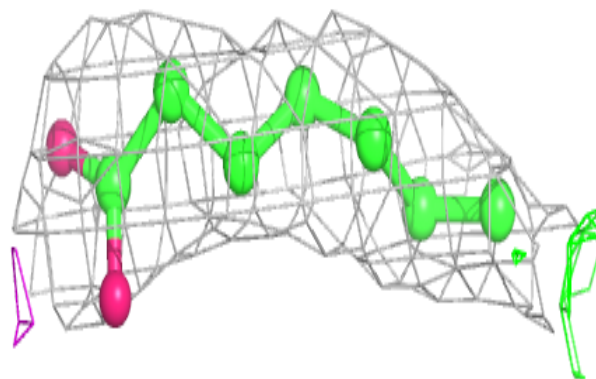
**Electron density around CLR A 2404:**

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

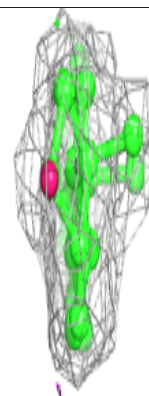
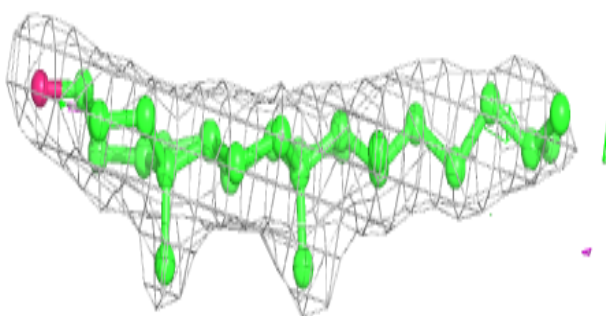
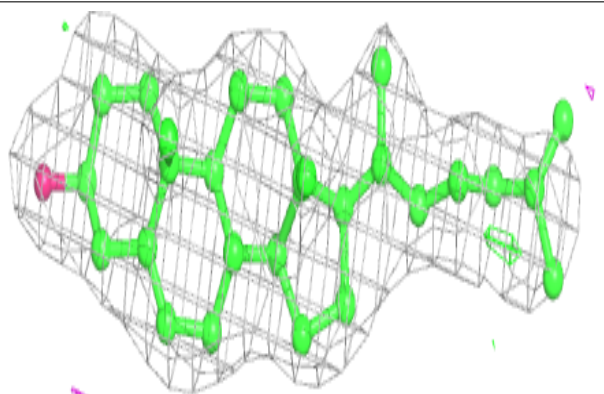


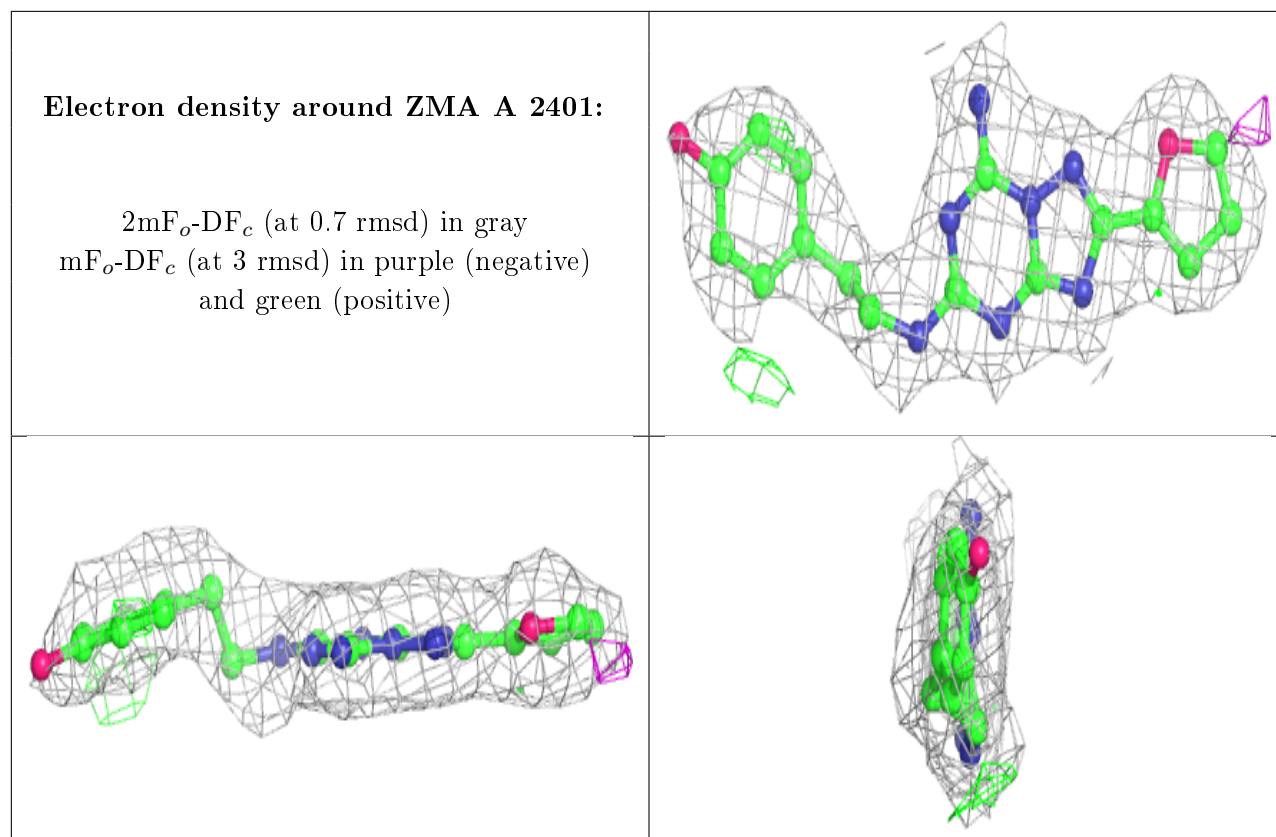
Electron density around OLA A 2419:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.