



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 11:20 am BST

PDB ID : 6JZH
Title : Structure of human A2A adenosine receptor in complex with ZM241385 obtained from SFX experiments under atmospheric pressure
Authors : Nango, E.; Shimamura, T.; Nakane, T.; Yamanaka, Y.; Mori, C.; Kimura, K.T.; Fujiwara, T.; Tanaka, T.; Iwata, S.
Deposited on : 2019-05-02
Resolution : 2.25 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

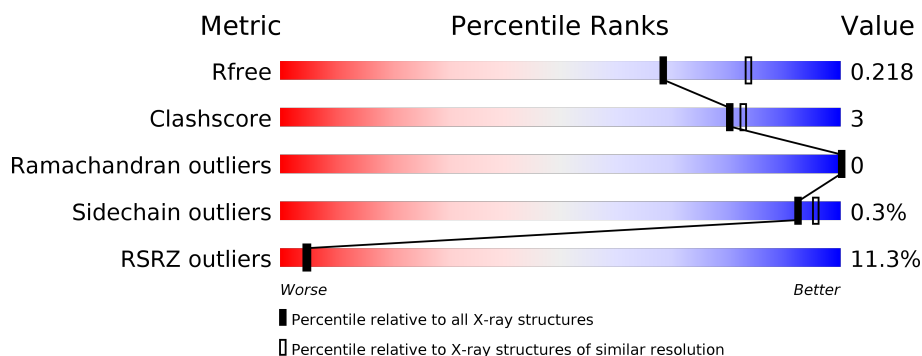
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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>10%</div> <div>82%</div> <div>5%</div> <div>13%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6884 atoms, of which 3511 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	390	Total	C	H	N	O	S	0	2	0
			5877	1919	2949	475	512	22			

There are 40 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

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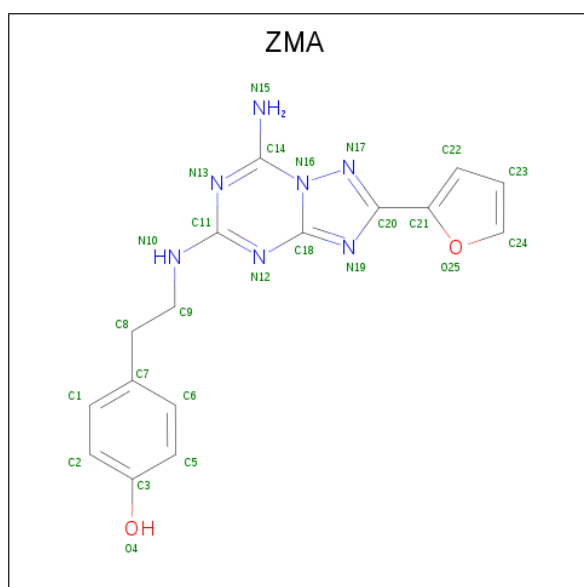
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Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLN	ASN	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression 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 SODIUM ION (three-letter code: NA) (formula: Na).

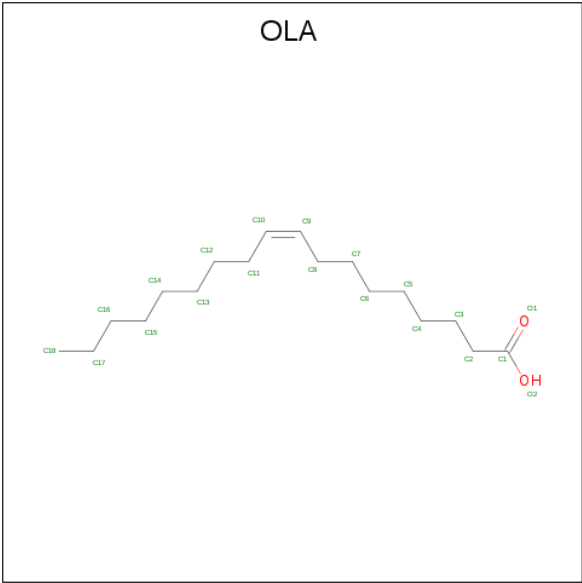
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is 4-{2-[(7-amino-2-furan-2-yl)[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl} phenol (three-letter code: ZMA) (formula: C₁₆H₁₅N₇O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			40	16	15	7	2		

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



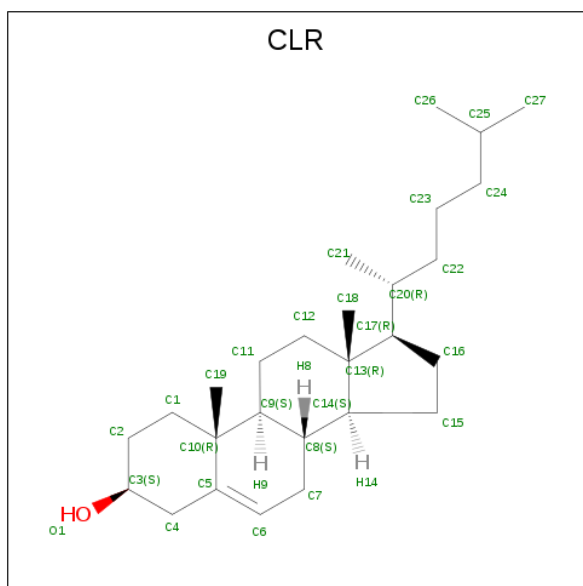
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			34	12	20	2		
4	A	1	Total	C	H	O	0	0
			21	7	12	2		
4	A	1	Total	C	H		0	0
			23	8	15			
4	A	1	Total	C	H	O	0	0
			31	11	18	2		
4	A	1	Total	C	H	O	0	0
			43	15	26	2		
4	A	1	Total	C	H	O	0	0
			43	15	26	2		
4	A	1	Total	C	H	O	0	0
			43	15	26	2		
4	A	1	Total	C	H	O	0	0
			37	13	22	2		
4	A	1	Total	C	H	O	0	0
			43	15	26	2		
4	A	1	Total	C	H	O	0	0
			43	15	26	2		
4	A	1	Total	C	H	O	0	0
			43	15	26	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 46 16 28 2	0	0
4	A	1	Total C H O 34 12 20 2	0	0
4	A	1	Total C H 21 7 14	0	0
4	A	1	Total C H O 18 6 10 2	0	0
4	A	1	Total C H O 28 10 16 2	0	0
4	A	1	Total C H 46 16 30	0	0
4	A	1	Total C H O 53 18 33 2	0	0
4	A	1	Total C H O 28 11 15 2	0	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 74 27 46 1	0	0
5	A	1	Total C H O 74 27 46 1	0	0
5	A	1	Total C H O 74 27 46 1	0	0

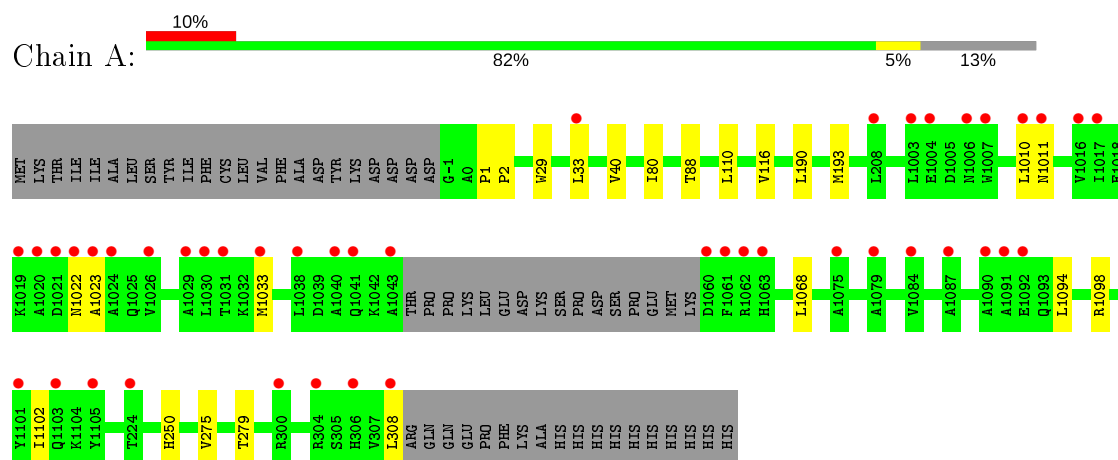
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		

3 Residue-property plots [i](#)

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

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	40.17Å 179.59Å 142.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.36 – 2.25 44.90 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.36-2.25) 93.4 (44.90-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.183 , 0.218 0.183 , 0.218	Depositor DCC
R_{free} test set	1916 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 86.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6884	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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, ZMA, CLR, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/2997	0.41	0/4094

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	2928	2949	2899	15	0
2	A	1	0	0	0	0
3	A	25	15	14	1	0
4	A	269	409	372	0	0
5	A	84	138	138	5	0
6	A	66	0	0	1	0
All	All	3373	3511	3423	18	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 (18) 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:THR:HG23	1.93	0.69
1:A:1022:ASN:OD1	1:A:1023:ALA:N	2.27	0.67
1:A:250:HIS:CE1	3:A:2002:ZMA:H24	2.41	0.55
1:A:190:LEU:HD23	1:A:193:MET:CE	2.38	0.53
1:A:1068:LEU:HD12	1:A:1094:LEU:HD22	1.91	0.52
5:A:2022:CLR:H121	5:A:2022:CLR:H212	1.93	0.51
1:A:110:LEU:HD23	1:A:110:LEU:H	1.77	0.50
1:A:1011:ASN:HD21	1:A:1098:ARG:HD2	1.76	0.49
5:A:2024:CLR:H212	5:A:2024:CLR:H121	1.98	0.46
1:A:80:ILE:HD11	5:A:2022:CLR:C18	2.45	0.46
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.46	0.46
1:A:1068:LEU:HD22	1:A:1102:ILE:HG13	1.99	0.43
5:A:2023:CLR:H121	5:A:2023:CLR:H212	2.00	0.43
1:A:80:ILE:HD11	5:A:2022:CLR:H182	2.01	0.43
1:A:1010:LEU:HD23	1:A:1033:MET:HB3	2.01	0.42
1:A:1:PRO:HA	1:A:2:PRO:HD3	1.97	0.42
1:A:29:TRP:NE1	1:A:33:LEU:HD11	2.35	0.42
1:A:88:THR:HG21	6:A:2141:HOH:O	2.20	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	388/447 (87%)	382 (98%)	6 (2%)	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	292/374 (78%)	291 (100%)	1 (0%)	92	95

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

Mol	Chain	Res	Type
1	A	308	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	1011	ASN
1	A	1013	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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
4	OLA	A	2010	-	11,14,19	0.29	0	10,14,19	0.75	0
4	OLA	A	2021	-	9,12,19	0.31	0	8,12,19	0.96	0
4	OLA	A	2017	-	4,7,19	0.34	0	3,7,19	0.77	0
4	OLA	A	2013	-	13,16,19	0.29	0	12,16,19	0.78	0
4	OLA	A	2015	-	10,13,19	0.34	0	8,13,19	0.79	0
4	OLA	A	2018	-	8,11,19	0.35	0	7,11,19	0.92	0
4	OLA	A	2016	-	6,6,19	0.35	0	5,5,19	0.66	0
4	OLA	A	2011	-	13,16,19	0.30	0	12,16,19	0.73	0
4	OLA	A	2019	-	15,15,19	0.33	0	14,14,19	0.67	0
5	CLR	A	2023	-	31,31,31	0.76	1 (3%)	48,48,48	1.19	3 (6%)
4	OLA	A	2014	-	14,17,19	0.30	0	13,17,19	0.80	0
4	OLA	A	2004	-	5,8,19	0.33	0	4,8,19	0.75	0
4	OLA	A	2006	-	9,12,19	0.32	0	8,12,19	0.92	0
5	CLR	A	2022	-	31,31,31	0.74	1 (3%)	48,48,48	1.21	4 (8%)
4	OLA	A	2012	-	13,16,19	0.30	0	12,16,19	0.75	0
4	OLA	A	2008	-	13,16,19	0.30	0	12,16,19	0.77	0
4	OLA	A	2005	-	7,7,19	0.30	0	6,6,19	0.71	0
5	CLR	A	2024	-	31,31,31	0.76	1 (3%)	48,48,48	1.13	2 (4%)
4	OLA	A	2003	-	10,13,19	0.33	0	8,13,19	0.87	0
4	OLA	A	2007	-	13,16,19	0.33	0	12,16,19	0.82	0
4	OLA	A	2009	-	13,16,19	0.32	0	12,16,19	0.70	0
4	OLA	A	2020	-	16,19,19	0.31	0	15,19,19	0.81	0
3	ZMA	A	2002	-	21,28,28	1.06	3 (14%)	22,39,39	2.14	7 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	2010	-	-	3/10/12/17	-
4	OLA	A	2021	-	-	3/8/10/17	-
4	OLA	A	2017	-	-	1/3/5/17	-
4	OLA	A	2013	-	-	6/12/14/17	-
4	OLA	A	2015	-	-	6/9/11/17	-
4	OLA	A	2018	-	-	3/7/9/17	-
4	OLA	A	2016	-	-	1/4/4/17	-
4	OLA	A	2011	-	-	5/12/14/17	-
4	OLA	A	2019	-	-	8/13/13/17	-
5	CLR	A	2023	-	-	1/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	2014	-	-	5/13/15/17	-
4	OLA	A	2004	-	-	1/4/6/17	-
4	OLA	A	2006	-	-	2/8/10/17	-
5	CLR	A	2022	-	-	3/10/68/68	0/4/4/4
4	OLA	A	2012	-	-	5/12/14/17	-
4	OLA	A	2008	-	-	8/12/14/17	-
4	OLA	A	2005	-	-	2/5/5/17	-
5	CLR	A	2024	-	-	1/10/68/68	0/4/4/4
4	OLA	A	2003	-	-	3/9/11/17	-
4	OLA	A	2007	-	-	3/12/14/17	-
4	OLA	A	2009	-	-	4/12/14/17	-
4	OLA	A	2020	-	-	10/15/17/17	-
3	ZMA	A	2002	-	-	0/6/10/10	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002	ZMA	C11-N10	2.32	1.38	1.34
3	A	2002	ZMA	C18-N19	-2.31	1.32	1.35
5	A	2023	CLR	C10-C9	-2.27	1.52	1.56
3	A	2002	ZMA	C14-N13	-2.27	1.32	1.34
5	A	2022	CLR	C10-C9	-2.24	1.52	1.56
5	A	2024	CLR	C10-C9	-2.07	1.52	1.56

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	ZMA	N17-C20-N19	-6.74	110.10	114.56
5	A	2022	CLR	C21-C20-C17	-4.04	106.74	112.92
3	A	2002	ZMA	N15-C14-N16	3.69	120.45	117.97
3	A	2002	ZMA	N15-C14-N13	2.82	120.74	117.03
3	A	2002	ZMA	N12-C11-N13	-2.67	122.00	126.23
5	A	2023	CLR	C13-C17-C20	-2.50	115.57	119.49
3	A	2002	ZMA	C21-C20-N19	2.49	126.81	123.61
3	A	2002	ZMA	C9-N10-C11	-2.49	119.45	123.75
3	A	2002	ZMA	C9-C8-C7	-2.39	107.33	112.87
5	A	2022	CLR	C15-C14-C13	-2.24	101.15	103.84
5	A	2024	CLR	C21-C20-C17	-2.16	109.62	112.92
5	A	2024	CLR	C19-C10-C9	-2.12	109.15	111.68
5	A	2023	CLR	C4-C5-C6	-2.11	117.57	120.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2022	CLR	C4-C5-C6	-2.05	117.65	120.61
5	A	2023	CLR	C19-C10-C9	-2.04	109.25	111.68
5	A	2022	CLR	C3-C4-C5	-2.01	108.62	112.03

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2015	OLA	C9-C10-C11-C12
4	A	2003	OLA	C9-C10-C11-C12
4	A	2009	OLA	C11-C10-C9-C8
4	A	2019	OLA	C11-C10-C9-C8
5	A	2022	CLR	C22-C23-C24-C25
4	A	2010	OLA	C5-C6-C7-C8
4	A	2016	OLA	C4-C5-C6-C7
4	A	2015	OLA	C2-C3-C4-C5
4	A	2018	OLA	C7-C8-C9-C10
4	A	2019	OLA	C11-C12-C13-C14
4	A	2006	OLA	C4-C5-C6-C7
4	A	2020	OLA	C5-C6-C7-C8
4	A	2018	OLA	C5-C6-C7-C8
4	A	2020	OLA	C12-C13-C14-C15
4	A	2020	OLA	C4-C5-C6-C7
4	A	2019	OLA	C10-C11-C12-C13
4	A	2010	OLA	C4-C5-C6-C7
4	A	2021	OLA	C11-C10-C9-C8
4	A	2006	OLA	C11-C10-C9-C8
4	A	2020	OLA	C6-C7-C8-C9
4	A	2019	OLA	C4-C5-C6-C7
4	A	2013	OLA	C2-C3-C4-C5
4	A	2015	OLA	C5-C6-C7-C8
4	A	2008	OLA	C5-C6-C7-C8
4	A	2012	OLA	C3-C4-C5-C6
4	A	2008	OLA	C4-C5-C6-C7
4	A	2012	OLA	C6-C7-C8-C9
4	A	2013	OLA	C12-C13-C14-C15
4	A	2005	OLA	C6-C7-C8-C9
4	A	2008	OLA	C2-C3-C4-C5
4	A	2008	OLA	C12-C13-C14-C15
4	A	2015	OLA	C6-C7-C8-C9
4	A	2021	OLA	C3-C4-C5-C6
4	A	2014	OLA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	A	2003	OLA	C11-C10-C9-C8
4	A	2004	OLA	C4-C5-C6-C7
4	A	2015	OLA	C11-C10-C9-C8
4	A	2012	OLA	C11-C10-C9-C8
4	A	2008	OLA	C11-C10-C9-C8
4	A	2020	OLA	C11-C10-C9-C8
5	A	2022	CLR	C21-C20-C22-C23
4	A	2010	OLA	C11-C10-C9-C8
4	A	2013	OLA	C3-C4-C5-C6
4	A	2011	OLA	C5-C6-C7-C8
4	A	2012	OLA	C2-C3-C4-C5
4	A	2017	OLA	C1-C2-C3-C4
4	A	2013	OLA	C1-C2-C3-C4
4	A	2020	OLA	C1-C2-C3-C4
5	A	2022	CLR	C20-C22-C23-C24
4	A	2008	OLA	C6-C7-C8-C9
4	A	2007	OLA	C11-C10-C9-C8
4	A	2011	OLA	C11-C10-C9-C8
4	A	2005	OLA	C2-C3-C4-C5
4	A	2019	OLA	C2-C3-C4-C5
4	A	2020	OLA	C11-C12-C13-C14
4	A	2020	OLA	C15-C16-C17-C18
4	A	2009	OLA	C5-C6-C7-C8
4	A	2013	OLA	C4-C5-C6-C7
4	A	2020	OLA	C2-C3-C4-C5
4	A	2018	OLA	C4-C5-C6-C7
4	A	2019	OLA	C12-C13-C14-C15
4	A	2008	OLA	C3-C4-C5-C6
4	A	2019	OLA	C9-C10-C11-C12
5	A	2023	CLR	C22-C23-C24-C25
4	A	2014	OLA	C4-C5-C6-C7
4	A	2020	OLA	C14-C15-C16-C17
4	A	2014	OLA	C9-C10-C11-C12
4	A	2003	OLA	C7-C8-C9-C10
4	A	2019	OLA	C3-C4-C5-C6
4	A	2011	OLA	C10-C11-C12-C13
4	A	2021	OLA	C7-C8-C9-C10
4	A	2013	OLA	C7-C8-C9-C10
4	A	2007	OLA	C9-C10-C11-C12
4	A	2011	OLA	C11-C12-C13-C14
5	A	2024	CLR	C20-C22-C23-C24
4	A	2014	OLA	C7-C8-C9-C10

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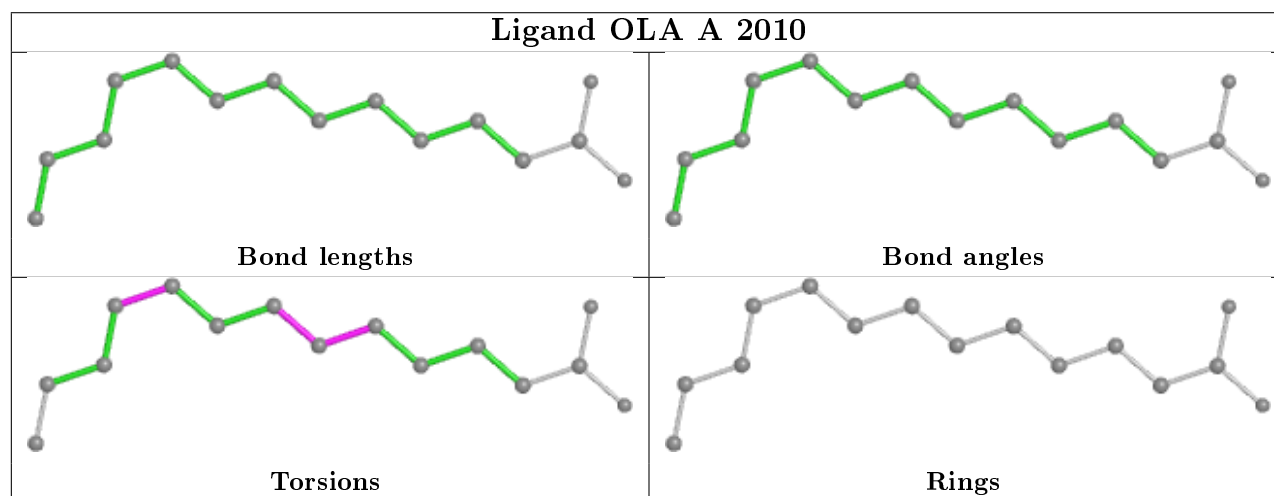
Mol	Chain	Res	Type	Atoms
4	A	2015	OLA	C1-C2-C3-C4
4	A	2012	OLA	C12-C13-C14-C15
4	A	2008	OLA	C9-C10-C11-C12
4	A	2011	OLA	C7-C8-C9-C10
4	A	2007	OLA	C11-C12-C13-C14
4	A	2014	OLA	C12-C13-C14-C15
4	A	2009	OLA	C6-C7-C8-C9
4	A	2009	OLA	C4-C5-C6-C7

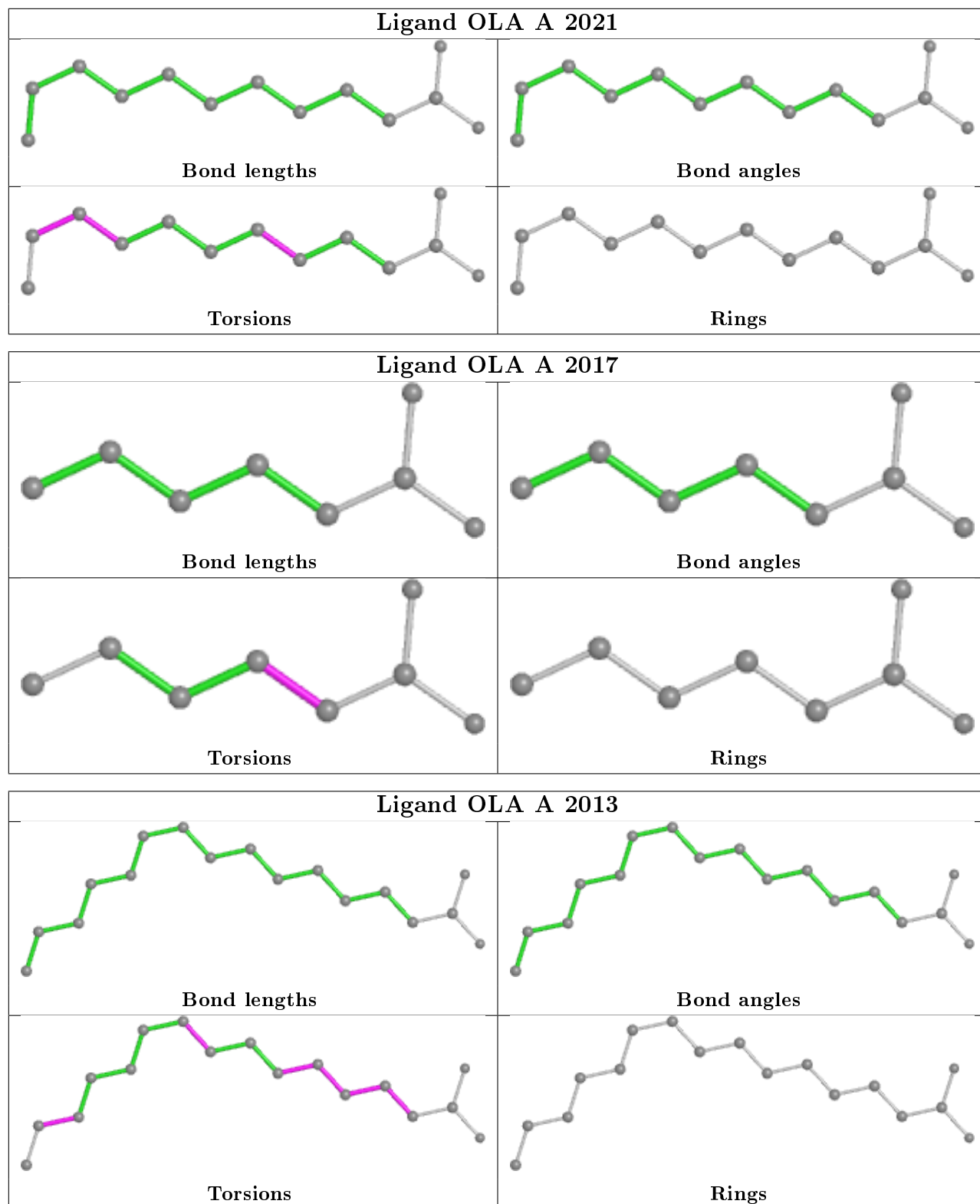
There are no ring outliers.

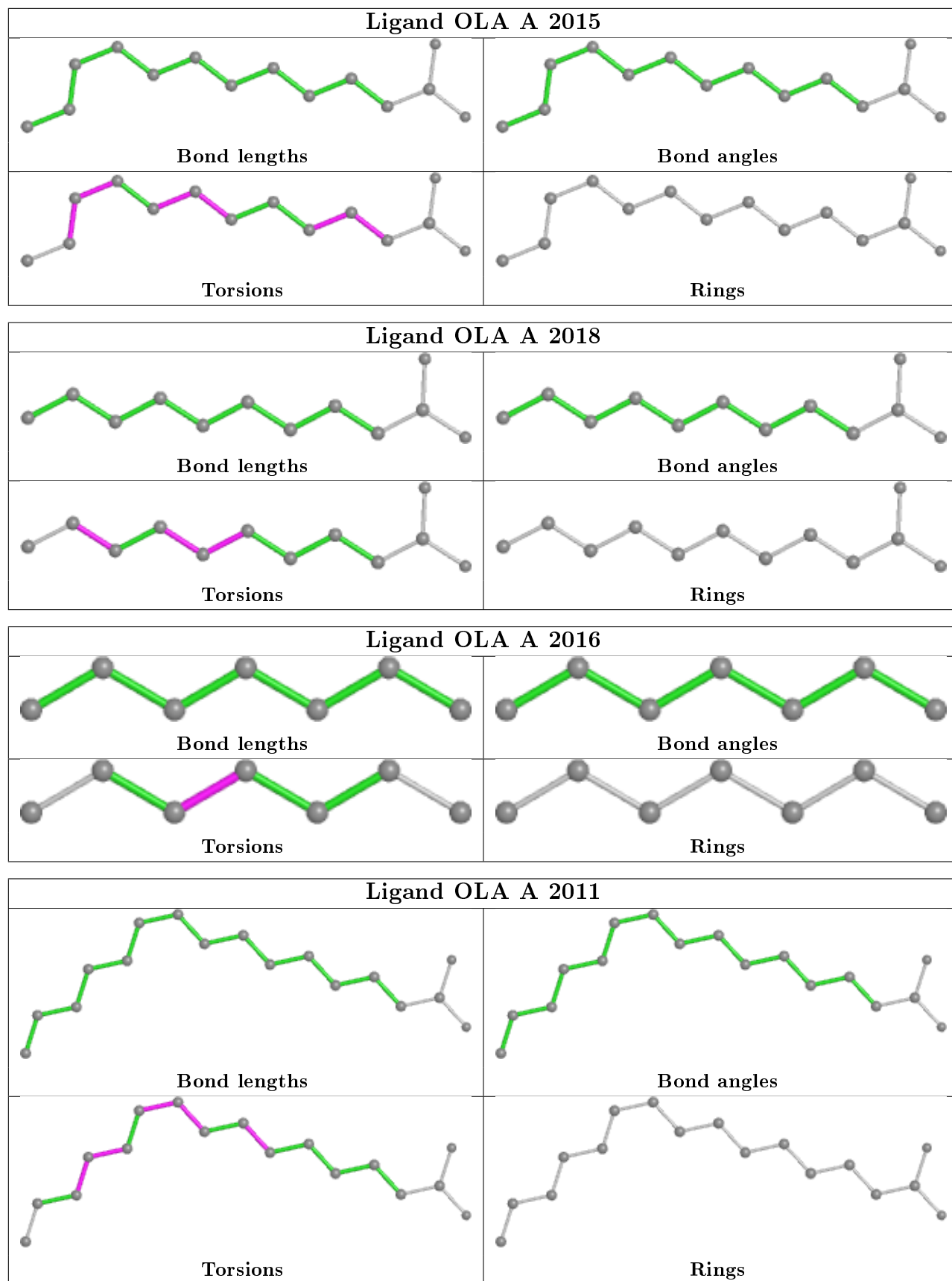
4 monomers are involved in 6 short contacts:

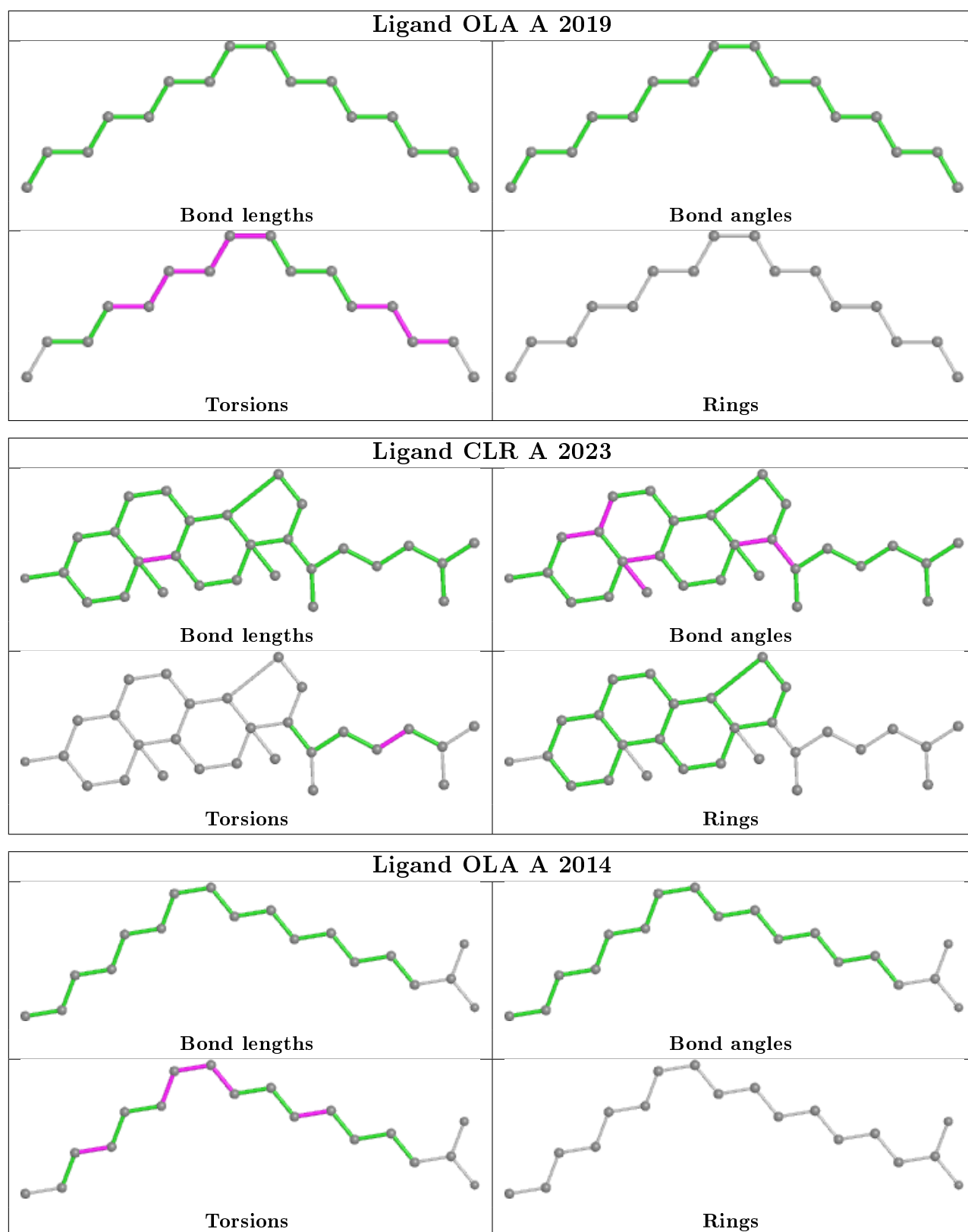
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2023	CLR	1	0
5	A	2022	CLR	3	0
5	A	2024	CLR	1	0
3	A	2002	ZMA	1	0

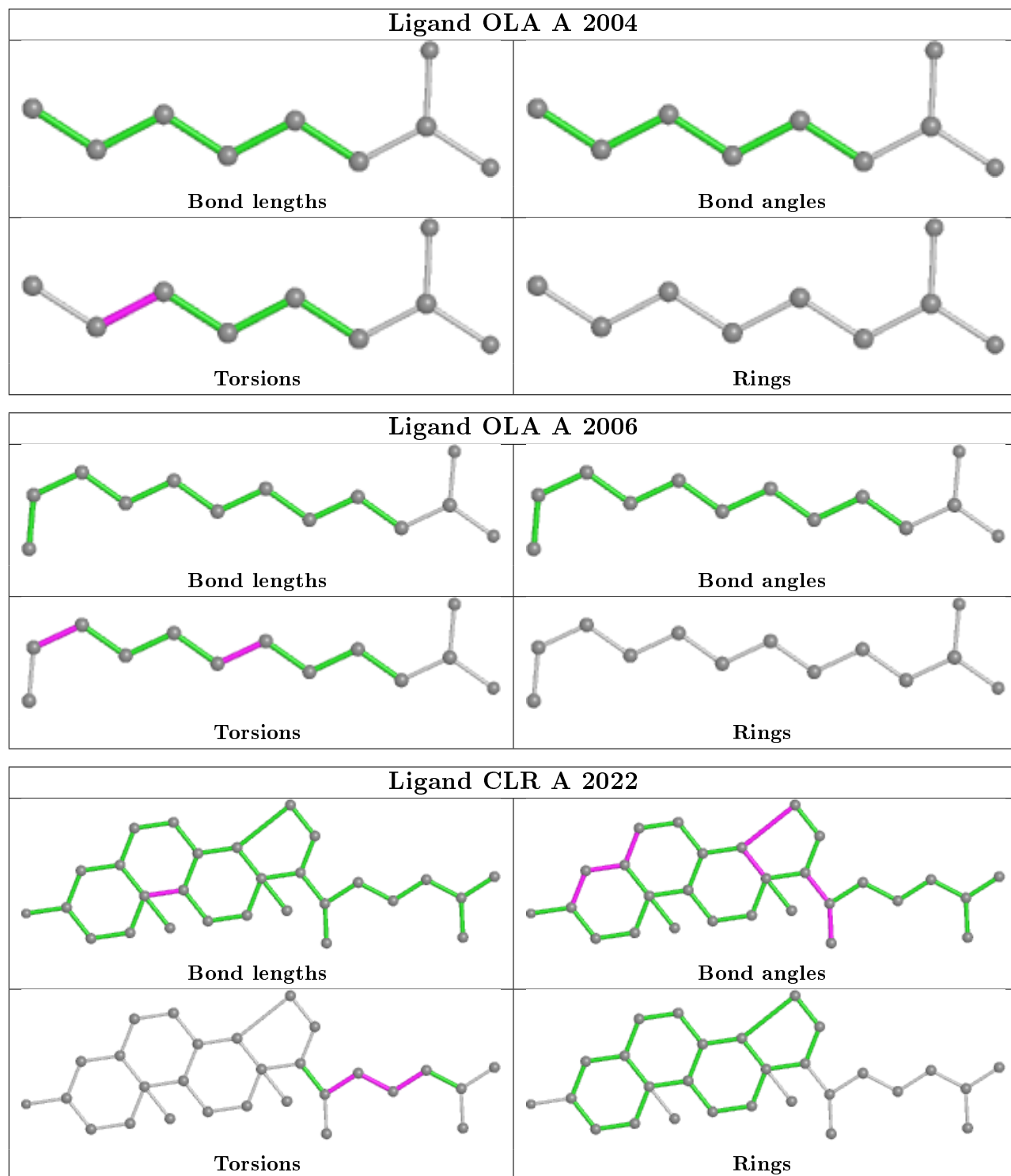
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

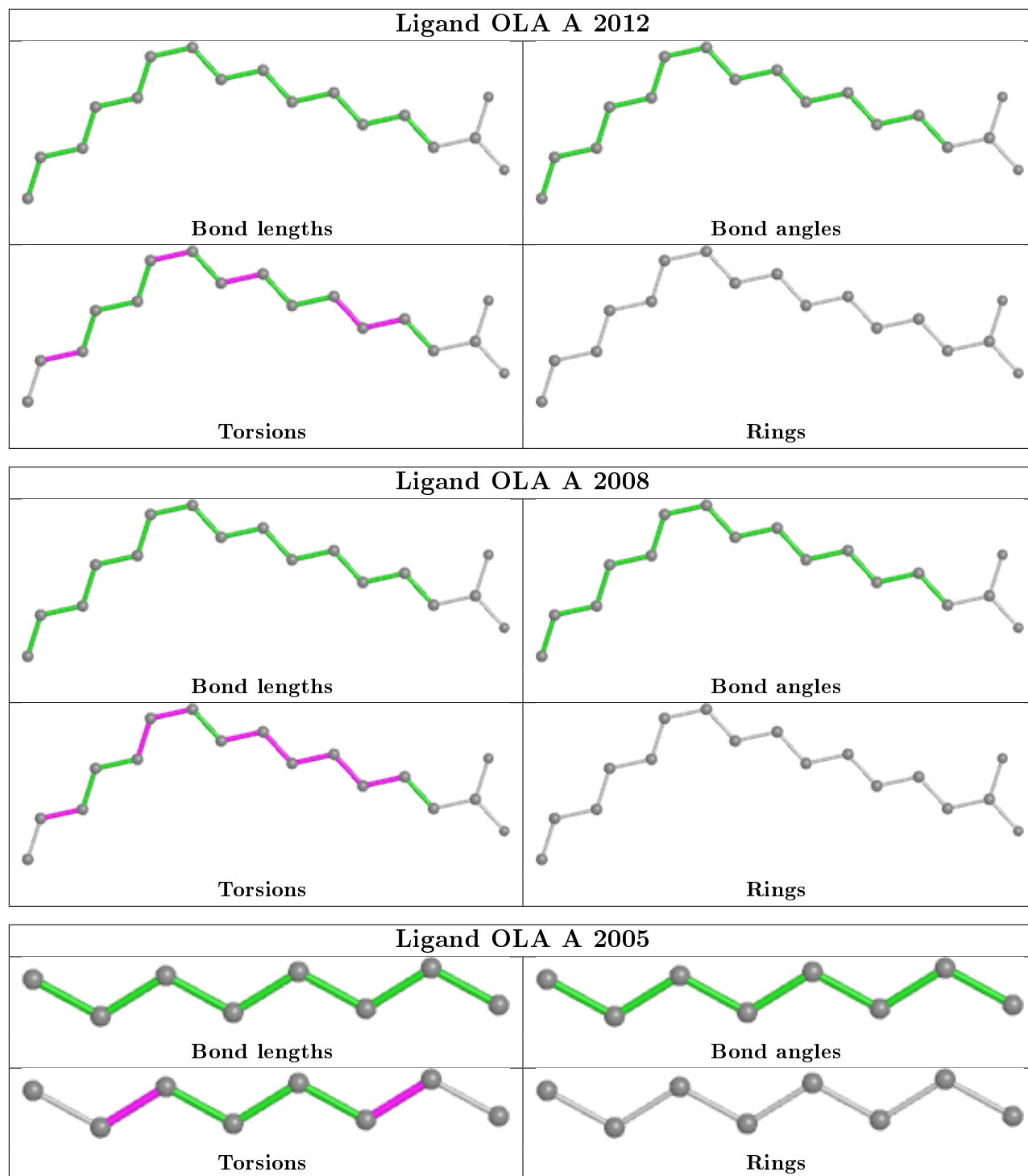


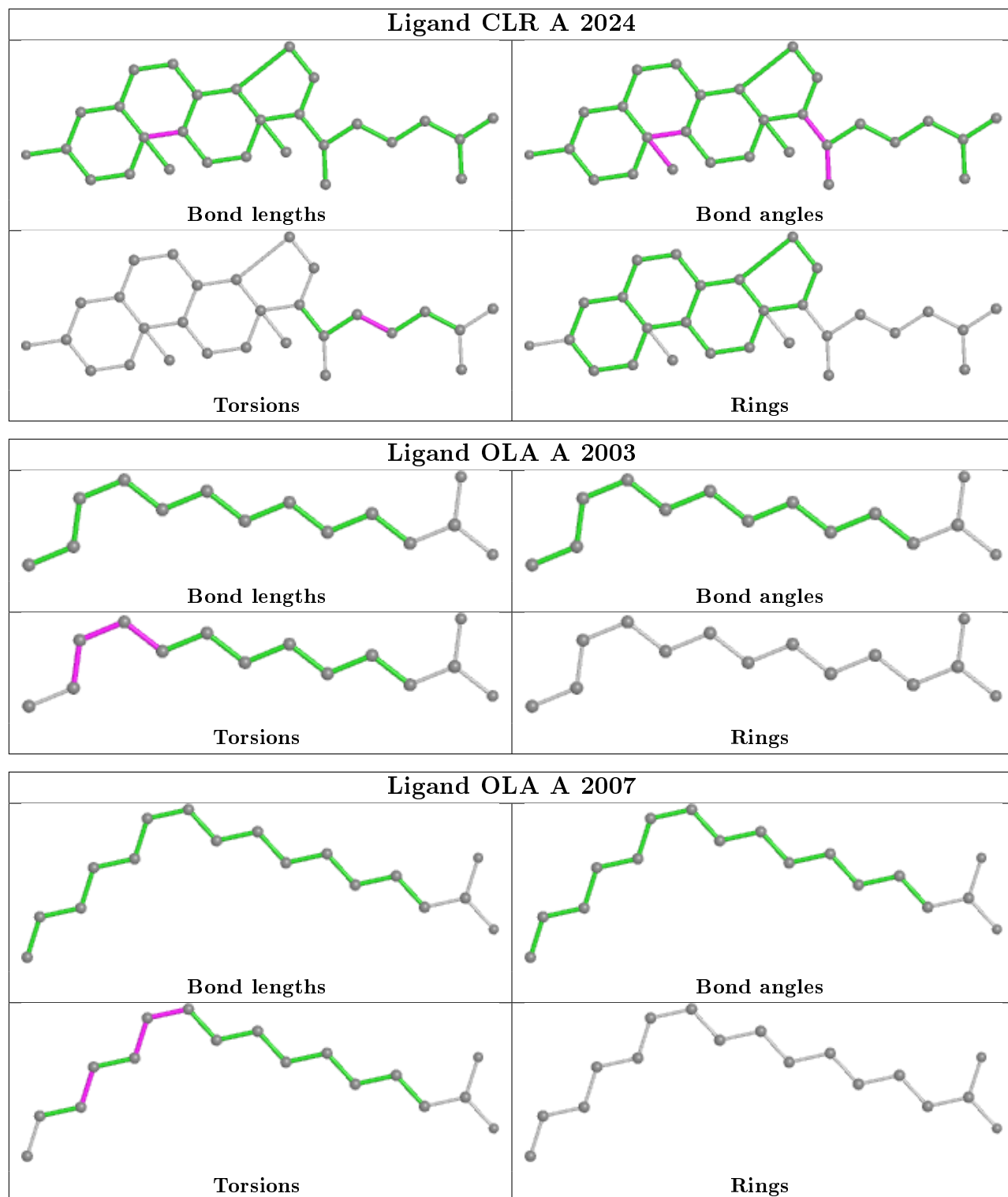


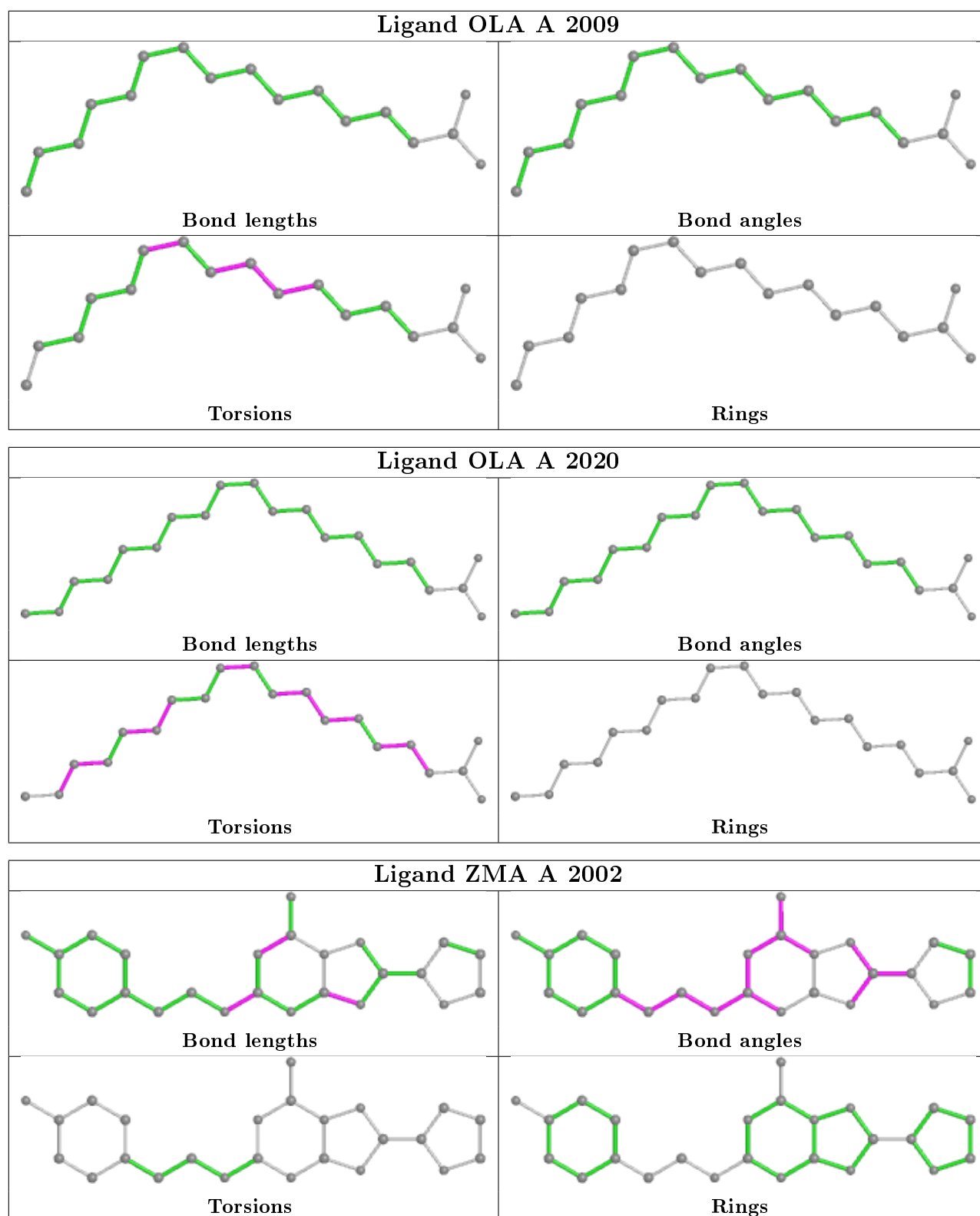












5.7 Other polymers ⓘ

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, 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%)	0.52	44 (11%) 5 4	30, 50, 106, 128	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	7.4
1	A	1020	ALA	6.7
1	A	1090	ALA	4.7
1	A	1029	ALA	4.7
1	A	304	ARG	4.6
1	A	1026	VAL	4.0
1	A	1011	ASN	3.8
1	A	1101	TYR	3.7
1	A	1023	ALA	3.6
1	A	1024	ALA	3.5
1	A	1079	ALA	3.4
1	A	1016	VAL	3.4
1	A	306	HIS	3.4
1	A	1062	ARG	3.3
1	A	1063	HIS	3.2
1	A	1007	TRP	3.1
1	A	1041	GLN	3.0
1	A	208	LEU	3.0
1	A	224	THR	2.9
1	A	33	LEU	2.8
1	A	308	LEU	2.7
1	A	1003	LEU	2.7
1	A	1043	ALA	2.7
1	A	1022	ASN	2.6
1	A	1060	ASP	2.6
1	A	1033	MET	2.6
1	A	1105	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1091	ALA	2.5
1	A	1040	ALA	2.5
1	A	1031	THR	2.4
1	A	1017	ILE	2.4
1	A	1004	GLU	2.4
1	A	1038	LEU	2.4
1	A	1087	ALA	2.4
1	A	1006	ASN	2.3
1	A	1030	LEU	2.3
1	A	1075	ALA	2.2
1	A	1092	GLU	2.2
1	A	1103	GLN	2.2
1	A	1010	LEU	2.1
1	A	1021	ASP	2.1
1	A	300	ARG	2.1
1	A	1019	LYS	2.0
1	A	1084	VAL	2.0

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(\AA^2)	Q<0.9
4	OLA	A	2021	13/20	0.57	0.28	75,95,108,117	0
4	OLA	A	2018	12/20	0.64	0.20	65,87,100,100	0
4	OLA	A	2019	16/20	0.69	0.17	77,101,116,121	0
4	OLA	A	2007	17/20	0.69	0.26	72,90,101,104	0
4	OLA	A	2008	17/20	0.72	0.33	62,89,130,131	0
4	OLA	A	2013	17/20	0.73	0.20	60,87,110,125	0

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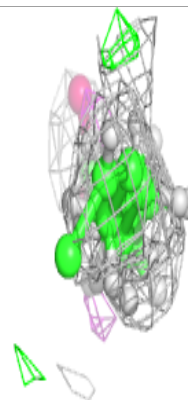
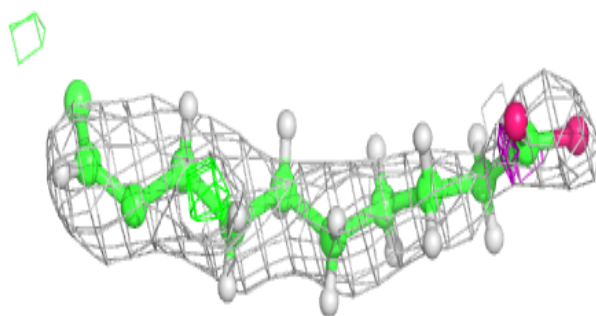
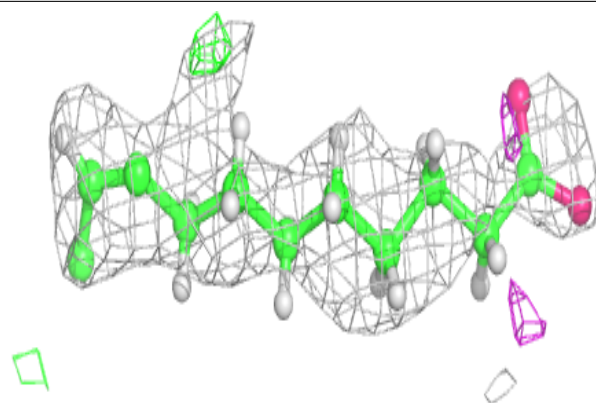
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	OLA	A	2015	14/20	0.73	0.21	71,97,119,120	0
4	OLA	A	2005	8/20	0.74	0.26	64,80,87,90	0
4	OLA	A	2003	14/20	0.75	0.25	63,81,94,96	0
4	OLA	A	2014	18/20	0.76	0.21	62,82,110,118	0
4	OLA	A	2012	17/20	0.77	0.27	76,108,136,140	0
4	OLA	A	2006	13/20	0.81	0.14	73,93,116,128	0
4	OLA	A	2009	17/20	0.81	0.24	65,85,109,126	0
4	OLA	A	2011	17/20	0.81	0.18	62,81,98,108	0
4	OLA	A	2010	15/20	0.82	0.17	58,75,83,86	0
5	CLR	A	2022	28/28	0.84	0.17	58,75,111,114	0
4	OLA	A	2020	20/20	0.84	0.21	63,80,100,100	0
5	CLR	A	2023	28/28	0.86	0.15	54,74,105,138	0
4	OLA	A	2004	9/20	0.87	0.17	54,65,78,79	0
4	OLA	A	2017	8/20	0.88	0.24	72,87,100,100	0
5	CLR	A	2024	28/28	0.89	0.14	50,69,101,105	0
4	OLA	A	2016	7/20	0.93	0.16	54,66,76,79	0
3	ZMA	A	2002	25/25	0.97	0.15	29,42,66,86	0
2	NA	A	2001	1/1	0.98	0.09	41,41,41,41	0

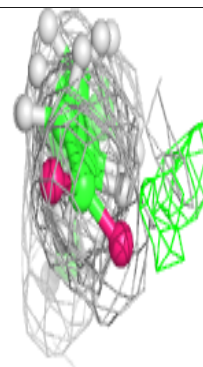
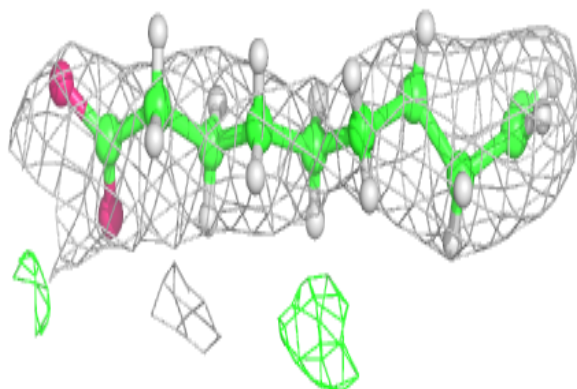
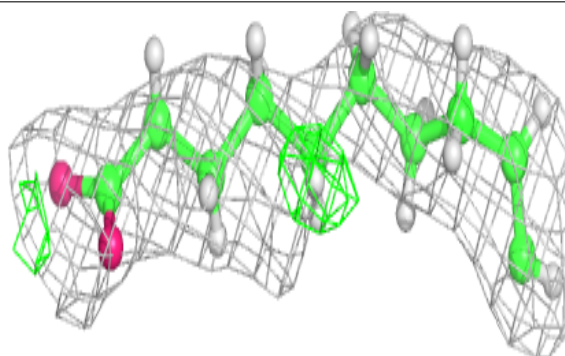
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 2021:

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

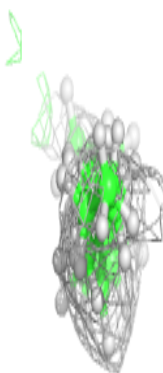
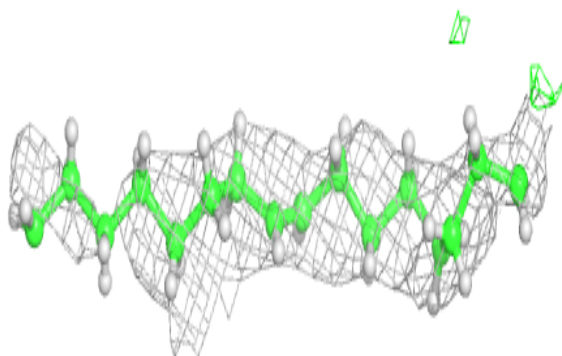
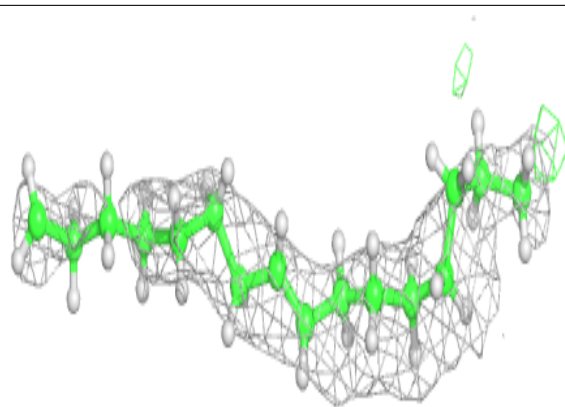
**Electron density around OLA A 2018:**

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

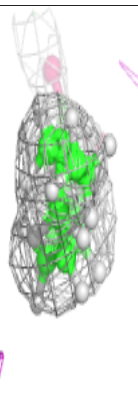
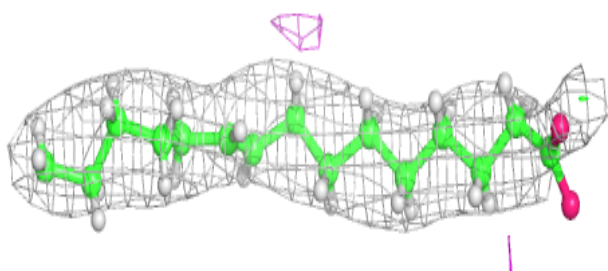
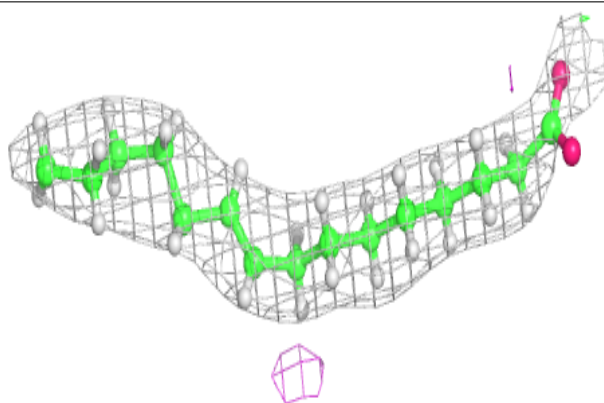


Electron density around OLA A 2019:

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

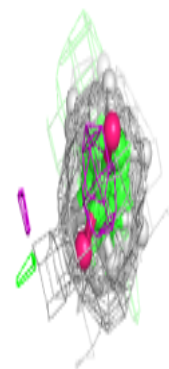
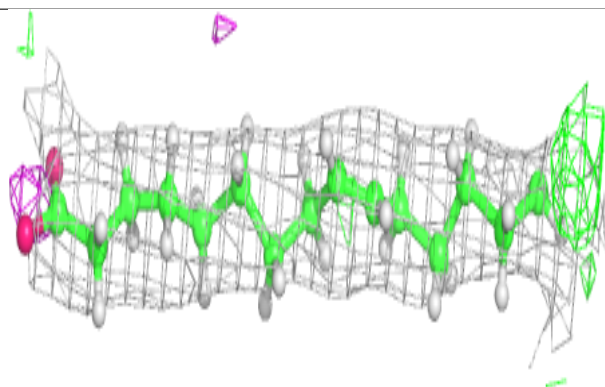
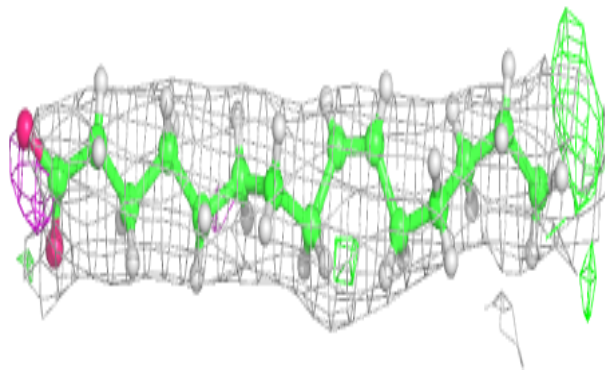
**Electron density around OLA A 2007:**

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

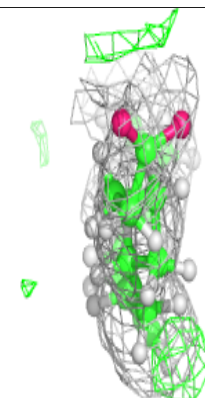
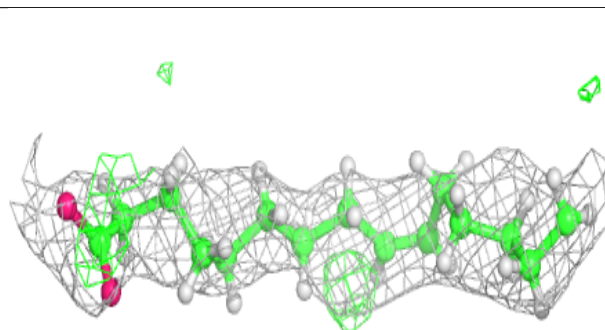
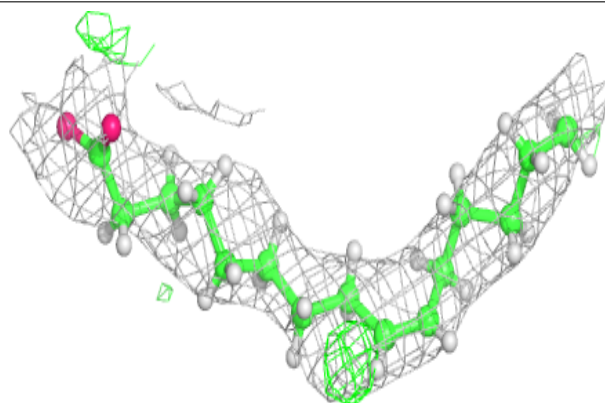


Electron density around OLA A 2008:

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

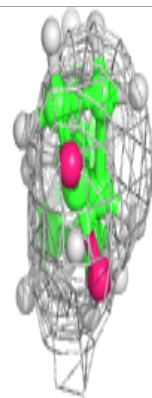
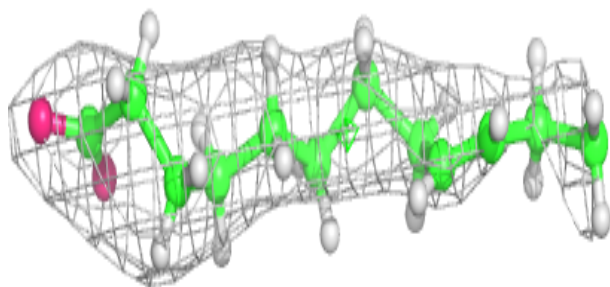
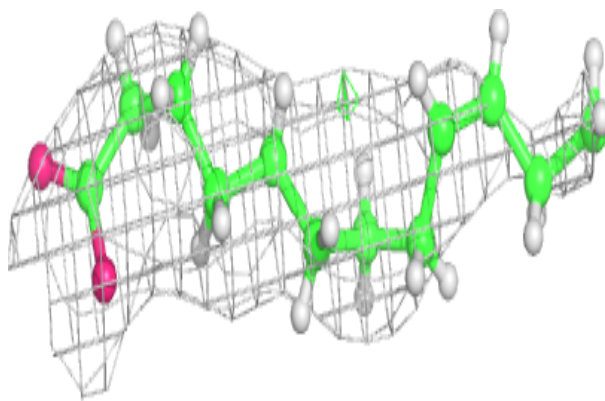
**Electron density around OLA A 2013:**

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

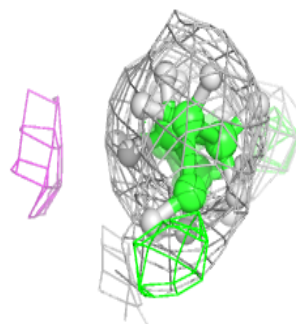
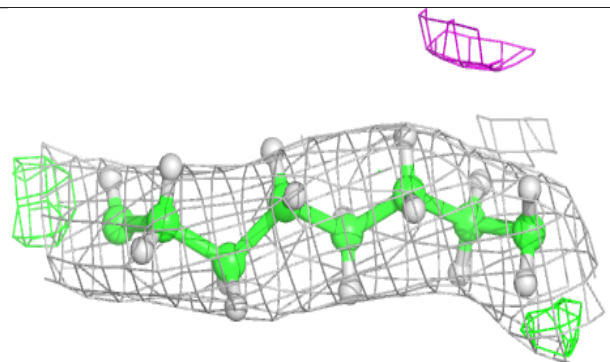
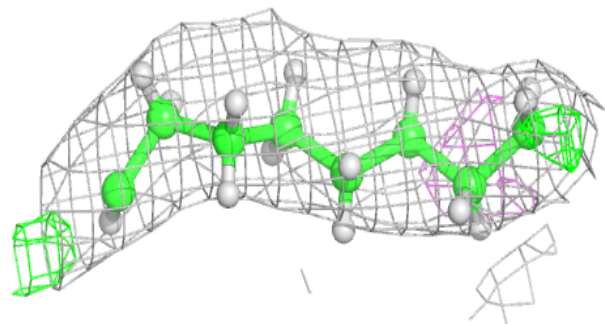


Electron density around OLA A 2015:

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

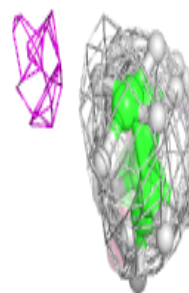
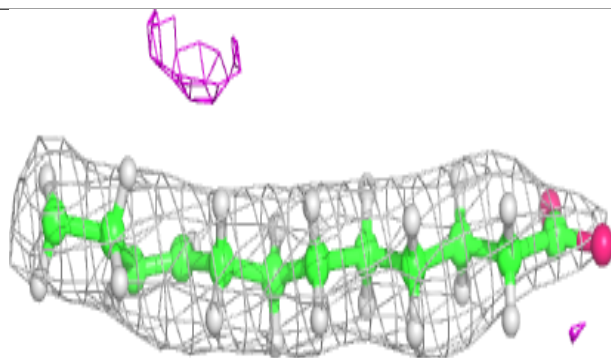
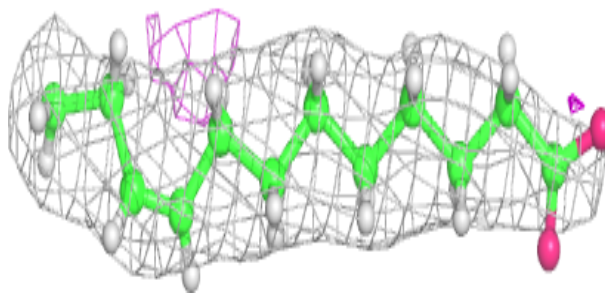
**Electron density around OLA A 2005:**

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

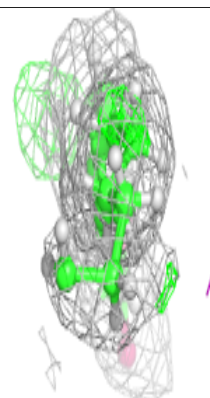
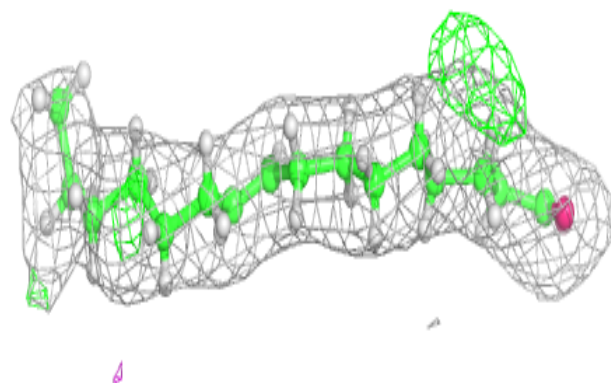
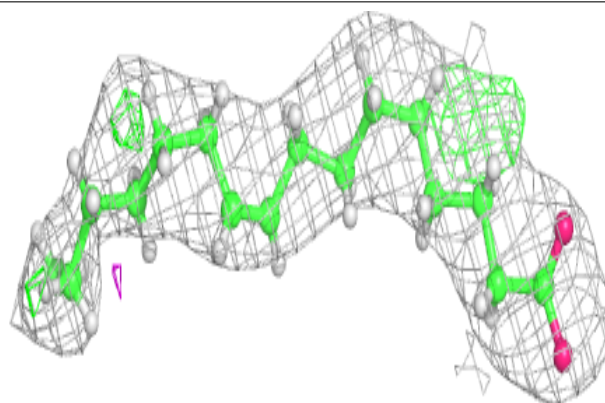


Electron density around OLA A 2003:

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

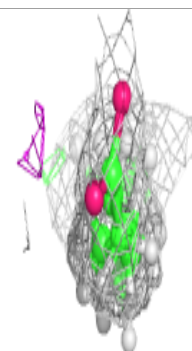
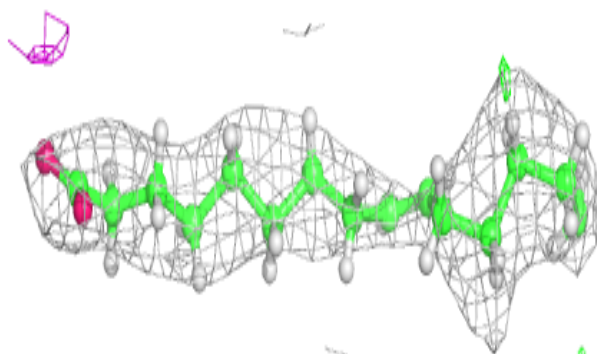
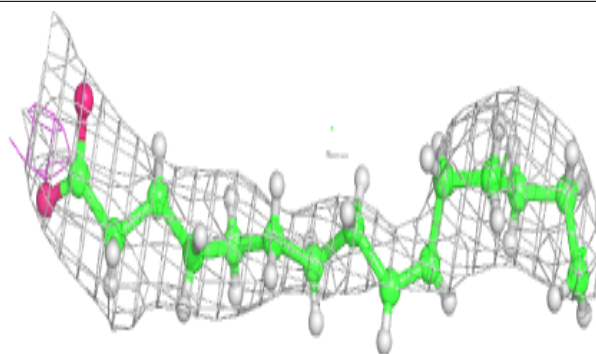
**Electron density around OLA A 2014:**

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

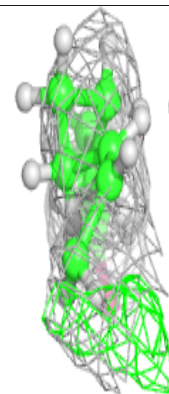
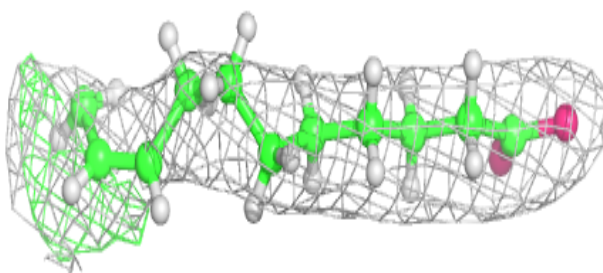
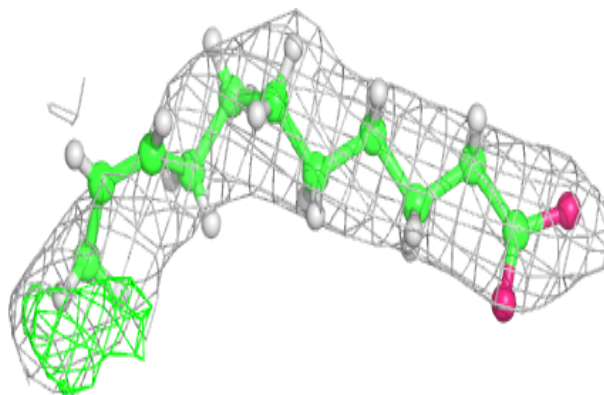


Electron density around OLA A 2012:

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

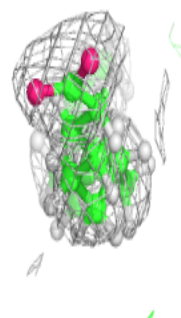
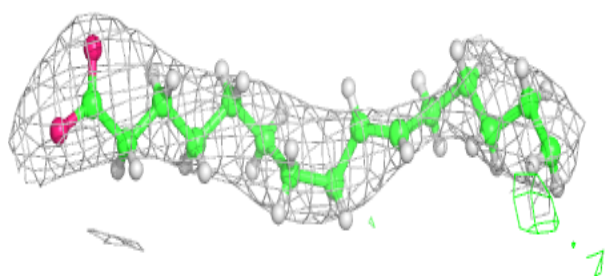
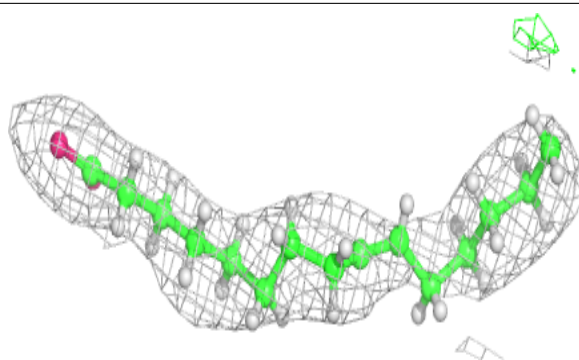
**Electron density around OLA A 2006:**

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

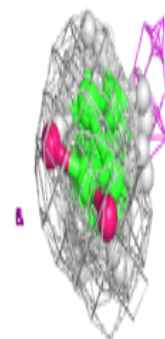
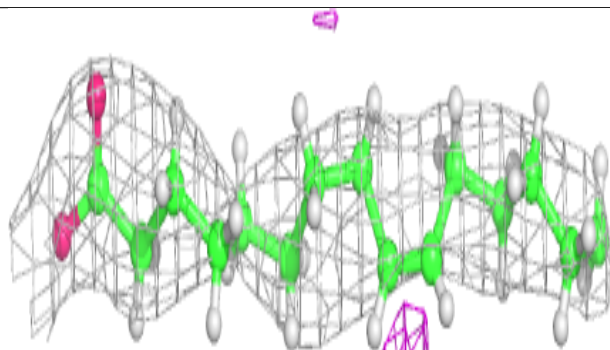
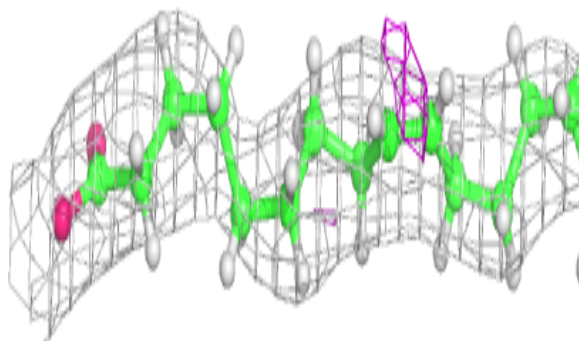


Electron density around OLA A 2009:

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

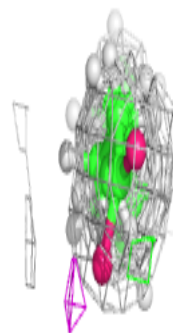
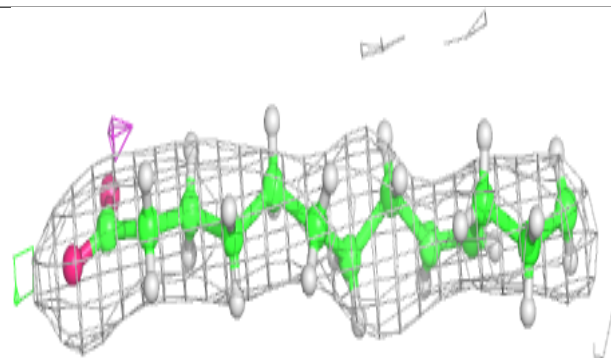
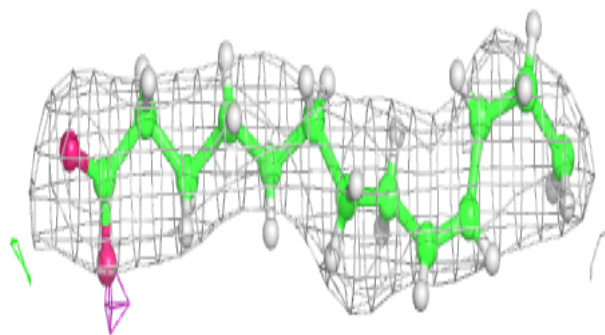
**Electron density around OLA A 2011:**

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

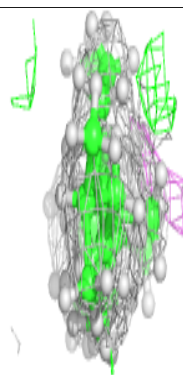
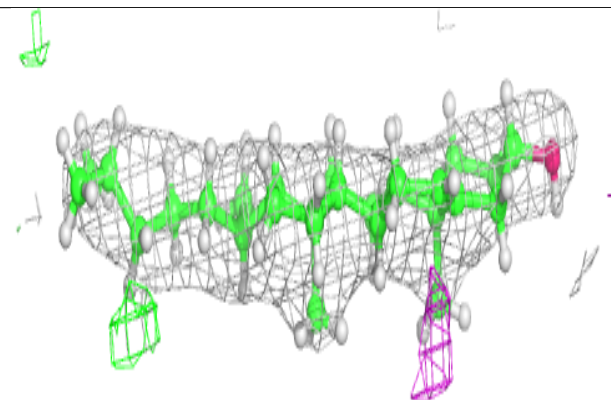
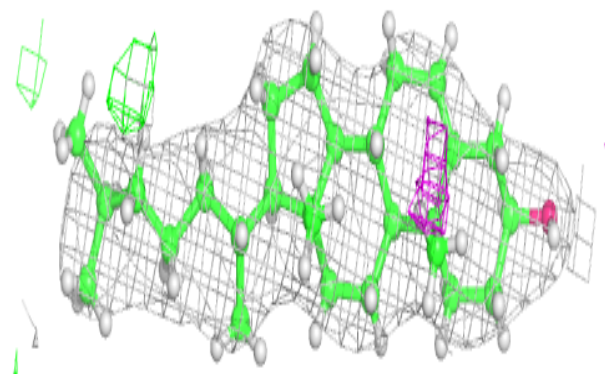


Electron density around OLA A 2010:

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

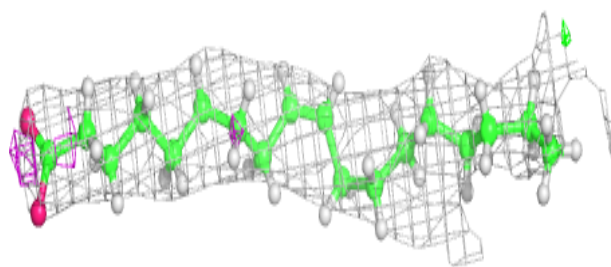
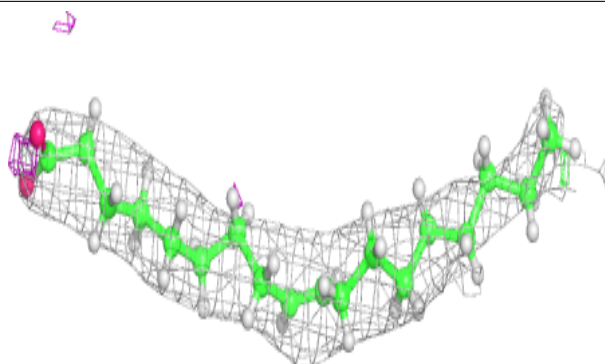
**Electron density around CLR A 2022:**

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

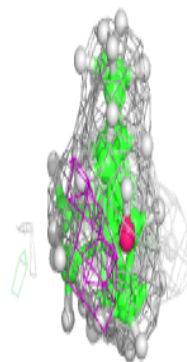
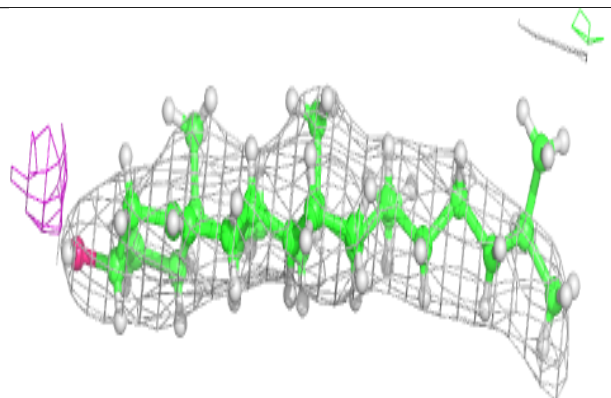
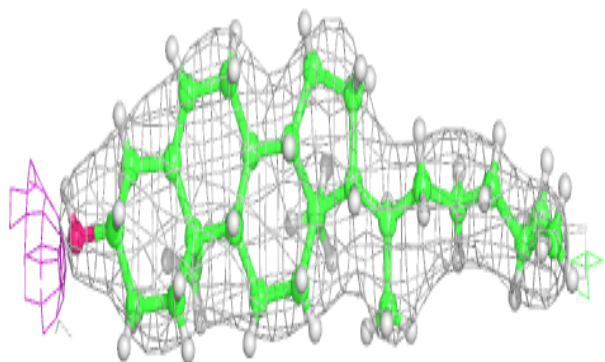


Electron density around OLA A 2020:

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

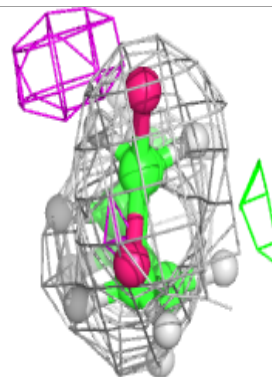
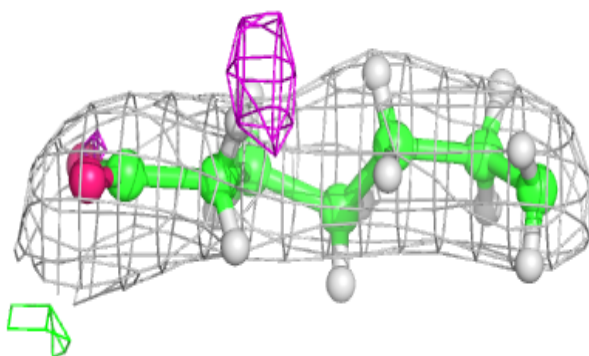
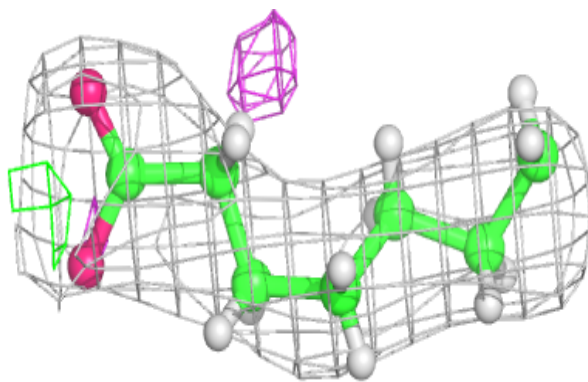
**Electron density around CLR A 2023:**

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

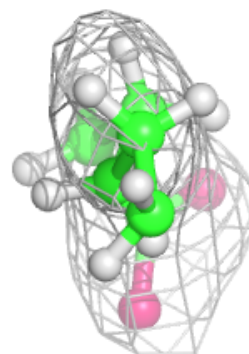
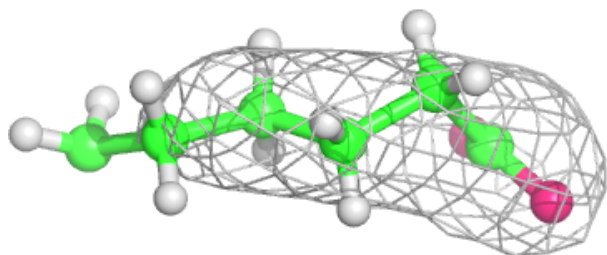
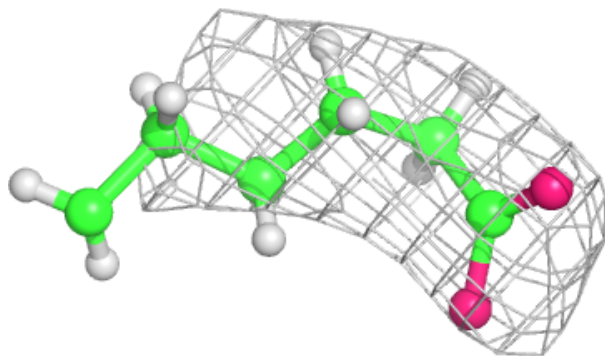


Electron density around OLA A 2004:

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

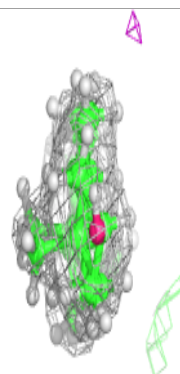
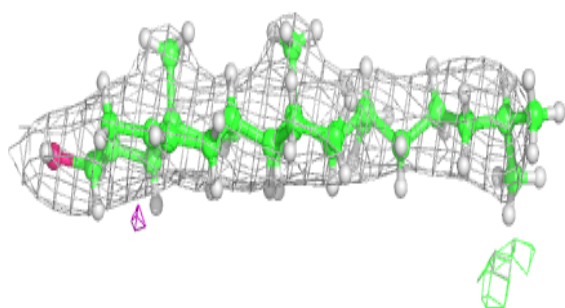
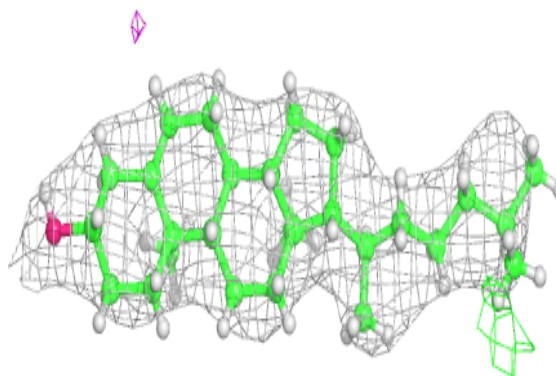
**Electron density around OLA A 2017:**

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

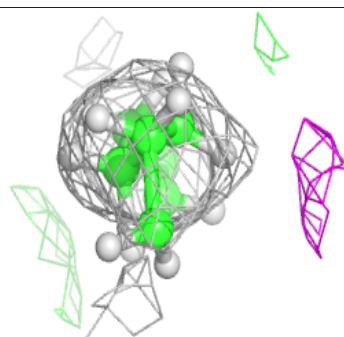
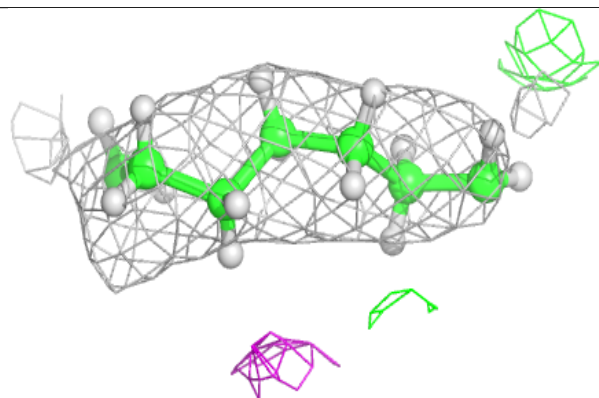
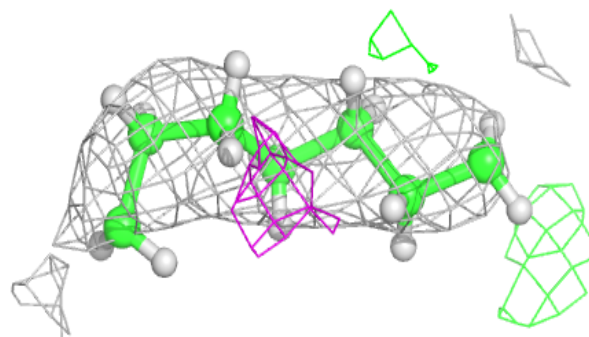


Electron density around CLR A 2024:

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

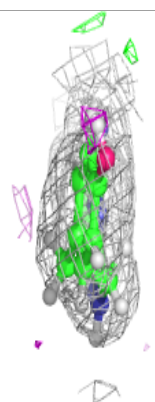
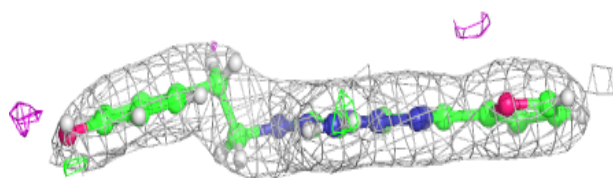
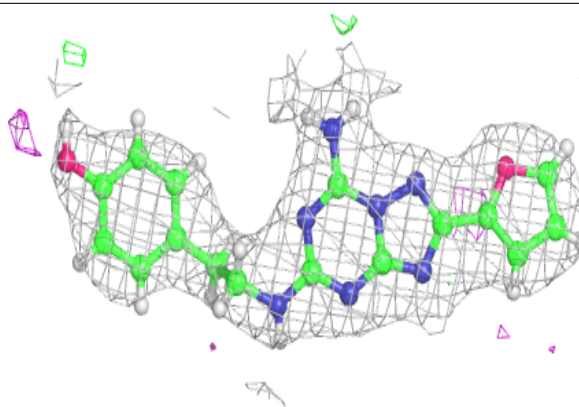
**Electron density around OLA A 2016:**

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



Electron density around ZMA A 2002:

$2mF_o-DF_c$ (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.