



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2022 – 04:27 PM EDT

PDB ID : 8DU3
Title : Crystal structure of A2AAR-StaR2-bRIL in complex with compound 21a
Authors : Shiriaeva, A.; Stauch, B.; Han, G.W.; Cherezov, V.
Deposited on : 2022-07-26
Resolution : 2.50 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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.29
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) : 2.29

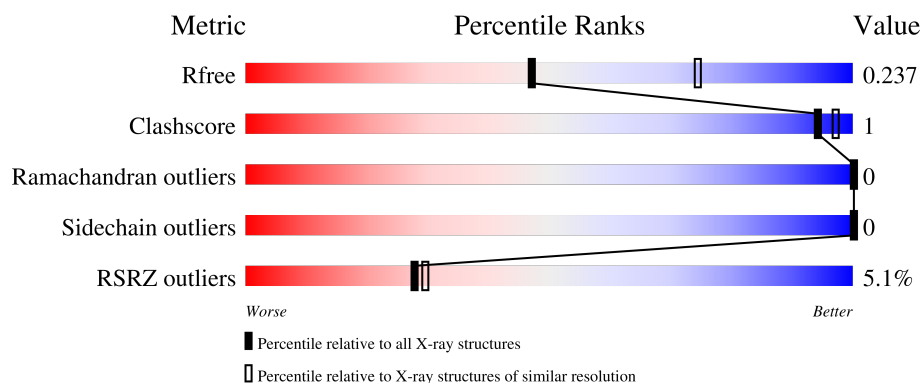
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of 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	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3466 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2984	1946	496	521	21			

There are 48 discrepancies between the modelled and reference sequences:

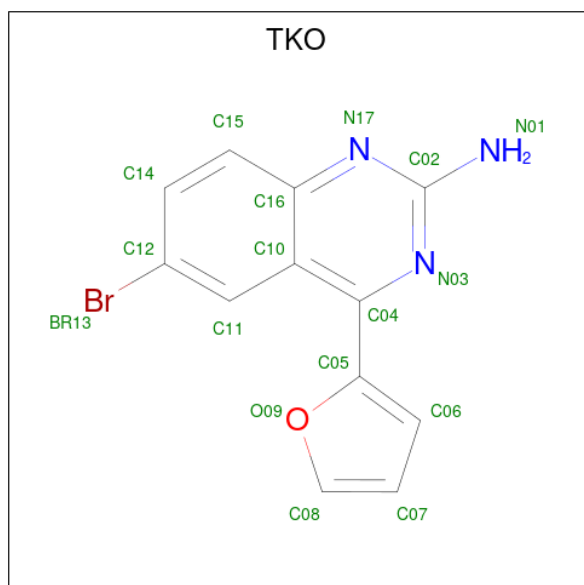
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression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

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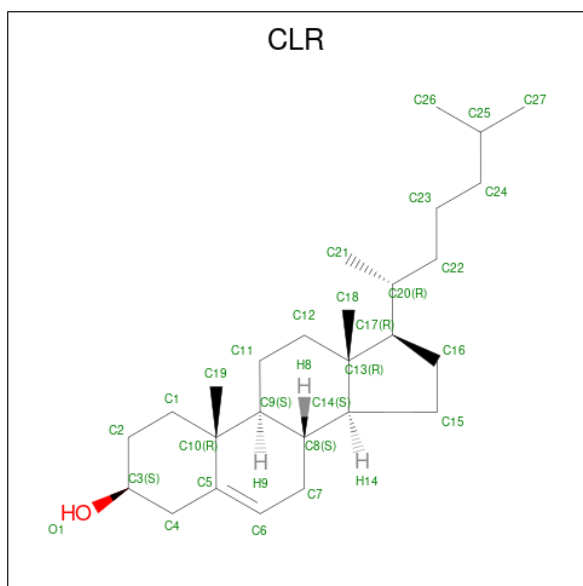
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	LEU	ALA	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	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 (4M)-6-bromo-4-(furan-2-yl)quinazolin-2-amine (three-letter code: TKO) (formula: C₁₂H₈BrN₃O) (labeled as "Ligand of Interest" by depositor).



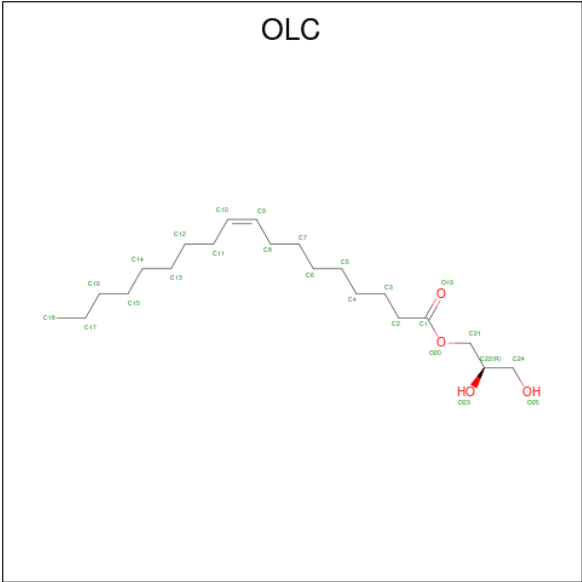
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			17	1	12	3	1		

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



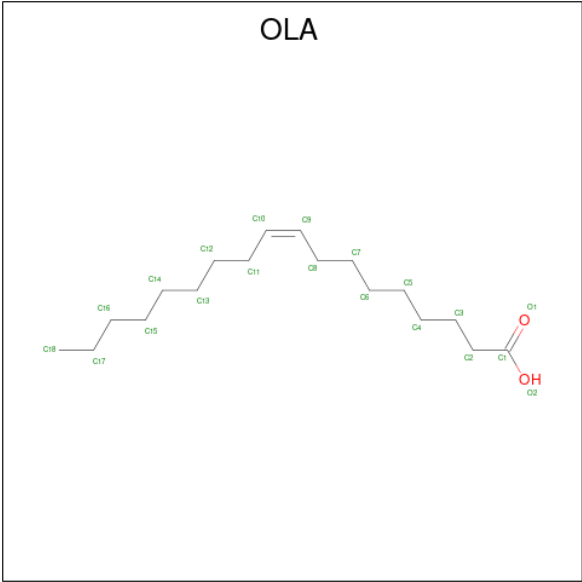
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			23	19	4		
4	A	1	Total	C	O	0	0
			16	12	4		
4	A	1	Total	C	O	0	0
			21	17	4		
4	A	1	Total	C	O	0	0
			20	16	4		

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



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

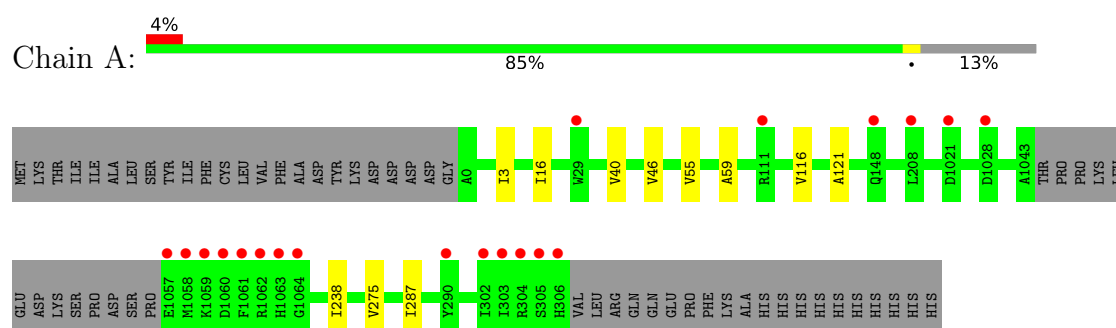
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	51	Total O 51 51	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Adenosine receptor A2a, soluble cytochrome b562 chimera, 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	39.60Å 179.80Å 141.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.83 – 2.50 42.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.83-2.50) 98.9 (42.83-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.189 , 0.232 0.196 , 0.237	Depositor DCC
R_{free} test set	896 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	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	0.94	EDS
Total number of atoms	3466	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: OLC, TKO, OLA, 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	0.24	0/3049	0.41	0/4155

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	2984	0	3008	7	0
2	A	17	0	0	0	0
3	A	84	0	138	2	0
4	A	80	0	110	1	0
5	A	250	0	370	1	0
6	A	51	0	0	0	0
All	All	3466	0	3626	9	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 1.

All (9) 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:40:VAL:HG11	1:A:116:VAL:CG1	2.43	0.49
1:A:40:VAL:HG13	1:A:121:ALA:HB2	1.97	0.47
3:A:3004:CLR:H212	3:A:3004:CLR:H121	1.97	0.46
1:A:238:ILE:HD11	1:A:287:ILE:HB	1.97	0.45
1:A:3:ILE:HD11	5:A:3023:OLA:O2	2.17	0.45
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.98	0.44
3:A:3003:CLR:H212	3:A:3003:CLR:H121	2.00	0.44
1:A:16:ILE:HD11	1:A:275:VAL:HG13	2.00	0.42
1:A:46:VAL:HG11	4:A:3006:OLC:H3A	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	386/447 (86%)	384 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/367 (84%)	307 (100%)	0	100	100

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

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	OLA	A	3023	-	12,12,19	0.70	0	12,12,19	1.08	0
5	OLA	A	3019	-	19,19,19	0.57	0	19,19,19	0.87	1 (5%)
4	OLC	A	3007	-	20,20,24	0.66	0	21,21,25	0.94	1 (4%)
5	OLA	A	3017	-	6,6,19	0.92	0	6,6,19	1.30	1 (16%)
5	OLA	A	3012	-	8,8,19	0.81	0	8,8,19	1.15	0
5	OLA	A	3025	-	13,13,19	0.26	0	12,12,19	0.49	0
5	OLA	A	3021	-	19,19,19	0.55	0	19,19,19	0.91	0
5	OLA	A	3009	-	17,17,19	0.60	0	17,17,19	0.88	1 (5%)
5	OLA	A	3015	-	10,10,19	0.29	0	8,9,19	0.54	0
5	OLA	A	3022	-	16,16,19	0.61	0	16,16,19	0.86	1 (6%)
2	TKO	A	3001	-	15,19,19	2.29	5 (33%)	22,27,27	1.35	3 (13%)
3	CLR	A	3002	-	31,31,31	0.57	0	48,48,48	0.75	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLA	A	3014	-	19,19,19	0.59	0	19,19,19	0.81	0
5	OLA	A	3011	-	10,10,19	0.74	0	10,10,19	1.07	0
4	OLC	A	3008	-	19,19,24	0.66	0	20,20,25	0.98	1 (5%)
5	OLA	A	3010	-	19,19,19	0.59	0	19,19,19	0.82	0
3	CLR	A	3004	-	31,31,31	0.57	0	48,48,48	0.89	3 (6%)
5	OLA	A	3024	-	19,19,19	0.58	0	19,19,19	0.87	1 (5%)
5	OLA	A	3013	-	19,19,19	0.59	0	19,19,19	0.81	0
4	OLC	A	3005	-	22,22,24	0.67	0	23,23,25	0.86	0
5	OLA	A	3018	-	10,10,19	0.28	0	8,9,19	0.54	0
5	OLA	A	3016	-	7,7,19	0.93	0	7,7,19	1.24	1 (14%)
5	OLA	A	3020	-	10,10,19	0.73	0	10,10,19	1.07	1 (10%)
3	CLR	A	3003	-	31,31,31	0.57	0	48,48,48	0.87	1 (2%)
4	OLC	A	3006	-	15,15,24	0.72	0	16,16,25	1.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	3023	-	-	4/10/10/17	-
5	OLA	A	3019	-	-	9/17/17/17	-
4	OLC	A	3007	-	-	8/20/20/24	-
5	OLA	A	3017	-	-	0/4/4/17	-
5	OLA	A	3012	-	-	1/6/6/17	-
5	OLA	A	3025	-	-	7/11/11/17	-
5	OLA	A	3021	-	-	7/17/17/17	-
5	OLA	A	3009	-	-	11/15/15/17	-
5	OLA	A	3015	-	-	4/8/8/17	-
5	OLA	A	3022	-	-	7/14/14/17	-
2	TKO	A	3001	-	-	0/0/4/4	0/3/3/3
3	CLR	A	3002	-	-	4/10/68/68	0/4/4/4
5	OLA	A	3014	-	-	10/17/17/17	-
5	OLA	A	3011	-	-	4/8/8/17	-
4	OLC	A	3008	-	-	8/19/19/24	-
5	OLA	A	3010	-	-	8/17/17/17	-
3	CLR	A	3004	-	-	2/10/68/68	0/4/4/4
5	OLA	A	3024	-	-	7/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	3013	-	-	7/17/17/17	-
4	OLC	A	3005	-	-	7/22/22/24	-
5	OLA	A	3018	-	-	6/8/8/17	-
5	OLA	A	3016	-	-	2/5/5/17	-
5	OLA	A	3020	-	-	4/8/8/17	-
3	CLR	A	3003	-	-	2/10/68/68	0/4/4/4
4	OLC	A	3006	-	-	7/15/15/24	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	TKO	C02-N03	4.99	1.44	1.35
2	A	3001	TKO	C02-N01	4.63	1.43	1.33
2	A	3001	TKO	BR13-C12	2.99	1.96	1.90
2	A	3001	TKO	C04-C10	2.21	1.47	1.43
2	A	3001	TKO	C04-C05	2.21	1.53	1.49

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	TKO	N17-C02-N03	-3.32	122.80	127.22
2	A	3001	TKO	C04-N03-C02	2.84	119.98	117.31
3	A	3004	CLR	C7-C8-C9	2.73	113.02	109.71
3	A	3004	CLR	C4-C5-C10	2.43	119.65	116.42
3	A	3004	CLR	C4-C5-C6	-2.28	117.32	120.61
5	A	3016	OLA	O2-C1-C2	2.23	121.18	114.03
4	A	3008	OLC	C3-C2-C1	-2.22	105.55	113.62
5	A	3017	OLA	O2-C1-C2	2.20	121.09	114.03
2	A	3001	TKO	C06-C07-C08	-2.18	105.15	112.92
5	A	3022	OLA	O2-C1-C2	2.09	120.75	114.03
4	A	3007	OLC	C3-C2-C1	-2.08	106.06	113.62
3	A	3002	CLR	C4-C5-C6	-2.08	117.61	120.61
5	A	3009	OLA	O2-C1-C2	2.07	120.68	114.03
5	A	3024	OLA	O2-C1-C2	2.05	120.62	114.03
5	A	3020	OLA	O2-C1-C2	2.04	120.57	114.03
3	A	3003	CLR	C4-C5-C6	-2.01	117.71	120.61
5	A	3019	OLA	O2-C1-C2	2.00	120.46	114.03

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	OLC	O20-C21-C22-C24
4	A	3006	OLC	O20-C21-C22-C24
4	A	3006	OLC	O20-C21-C22-O23
4	A	3008	OLC	O20-C21-C22-O23
4	A	3008	OLC	C2-C1-O20-C21
3	A	3002	CLR	C21-C20-C22-C23
4	A	3008	OLC	O19-C1-O20-C21
4	A	3007	OLC	C2-C1-O20-C21
5	A	3019	OLA	C6-C7-C8-C9
4	A	3007	OLC	O19-C1-O20-C21
4	A	3005	OLC	O20-C21-C22-O23
5	A	3024	OLA	C1-C2-C3-C4
5	A	3022	OLA	C1-C2-C3-C4
4	A	3007	OLC	O20-C21-C22-O23
5	A	3020	OLA	C2-C3-C4-C5
4	A	3008	OLC	O20-C21-C22-C24
5	A	3022	OLA	C4-C5-C6-C7
5	A	3014	OLA	C3-C4-C5-C6
5	A	3021	OLA	C11-C12-C13-C14
5	A	3019	OLA	C3-C4-C5-C6
5	A	3019	OLA	C10-C11-C12-C13
5	A	3025	OLA	C10-C11-C12-C13
4	A	3007	OLC	C3-C4-C5-C6
4	A	3007	OLC	C5-C6-C7-C8
5	A	3024	OLA	C12-C13-C14-C15
5	A	3019	OLA	C2-C3-C4-C5
5	A	3019	OLA	C4-C5-C6-C7
5	A	3022	OLA	C6-C7-C8-C9
5	A	3010	OLA	C11-C12-C13-C14
4	A	3006	OLC	C4-C5-C6-C7
4	A	3008	OLC	C4-C5-C6-C7
5	A	3011	OLA	C5-C6-C7-C8
5	A	3013	OLA	C12-C13-C14-C15
4	A	3008	OLC	C6-C7-C8-C9
5	A	3015	OLA	C10-C11-C12-C13
5	A	3023	OLA	C5-C6-C7-C8
5	A	3014	OLA	C5-C6-C7-C8
5	A	3009	OLA	C11-C12-C13-C14
5	A	3018	OLA	C12-C13-C14-C15
5	A	3010	OLA	C3-C4-C5-C6
5	A	3013	OLA	C2-C3-C4-C5
5	A	3012	OLA	C3-C4-C5-C6
5	A	3015	OLA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	3005	OLC	C6-C7-C8-C9
5	A	3025	OLA	C12-C13-C14-C15
5	A	3022	OLA	C2-C3-C4-C5
4	A	3005	OLC	C1-C2-C3-C4
4	A	3006	OLC	C6-C7-C8-C9
4	A	3005	OLC	C2-C3-C4-C5
5	A	3014	OLA	C12-C13-C14-C15
5	A	3021	OLA	C14-C15-C16-C17
4	A	3006	OLC	C1-C2-C3-C4
5	A	3025	OLA	C4-C5-C6-C7
5	A	3024	OLA	C3-C4-C5-C6
5	A	3010	OLA	C14-C15-C16-C17
5	A	3025	OLA	C5-C6-C7-C8
5	A	3016	OLA	C1-C2-C3-C4
5	A	3019	OLA	C15-C16-C17-C18
4	A	3005	OLC	C5-C6-C7-C8
5	A	3016	OLA	C3-C4-C5-C6
5	A	3020	OLA	C5-C6-C7-C8
5	A	3009	OLA	C12-C13-C14-C15
5	A	3025	OLA	C14-C15-C16-C17
5	A	3015	OLA	C7-C8-C9-C10
5	A	3018	OLA	C7-C8-C9-C10
3	A	3003	CLR	C20-C22-C23-C24
5	A	3024	OLA	C14-C15-C16-C17
5	A	3018	OLA	C14-C15-C16-C17
5	A	3018	OLA	C13-C14-C15-C16
5	A	3023	OLA	C2-C3-C4-C5
5	A	3009	OLA	C10-C11-C12-C13
5	A	3011	OLA	C2-C3-C4-C5
3	A	3002	CLR	C23-C24-C25-C26
5	A	3015	OLA	C11-C12-C13-C14
5	A	3013	OLA	C14-C15-C16-C17
3	A	3002	CLR	C23-C24-C25-C27
5	A	3014	OLA	C15-C16-C17-C18
4	A	3008	OLC	C1-C2-C3-C4
5	A	3021	OLA	C7-C8-C9-C10
5	A	3019	OLA	C14-C15-C16-C17
3	A	3004	CLR	C23-C24-C25-C26
5	A	3021	OLA	C4-C5-C6-C7
5	A	3023	OLA	C3-C4-C5-C6
5	A	3009	OLA	C9-C10-C11-C12
5	A	3025	OLA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
5	A	3009	OLA	C5-C6-C7-C8
5	A	3009	OLA	C3-C4-C5-C6
5	A	3010	OLA	O1-C1-C2-C3
4	A	3008	OLC	C9-C10-C11-C12
5	A	3013	OLA	C9-C10-C11-C12
5	A	3023	OLA	C6-C7-C8-C9
5	A	3010	OLA	O2-C1-C2-C3
5	A	3014	OLA	O1-C1-C2-C3
3	A	3004	CLR	C23-C24-C25-C27
5	A	3013	OLA	C6-C7-C8-C9
5	A	3014	OLA	C10-C11-C12-C13
5	A	3024	OLA	O1-C1-C2-C3
5	A	3020	OLA	C6-C7-C8-C9
5	A	3024	OLA	O2-C1-C2-C3
5	A	3019	OLA	C11-C12-C13-C14
5	A	3013	OLA	O2-C1-C2-C3
5	A	3025	OLA	C7-C8-C9-C10
5	A	3014	OLA	O2-C1-C2-C3
5	A	3022	OLA	C7-C8-C9-C10
5	A	3013	OLA	O1-C1-C2-C3
5	A	3019	OLA	C7-C8-C9-C10
5	A	3021	OLA	O2-C1-C2-C3
3	A	3002	CLR	C17-C20-C22-C23
4	A	3005	OLC	C9-C10-C11-C12
5	A	3014	OLA	C7-C8-C9-C10
5	A	3018	OLA	C9-C10-C11-C12
5	A	3022	OLA	C9-C10-C11-C12
5	A	3009	OLA	C4-C5-C6-C7
5	A	3021	OLA	O1-C1-C2-C3
5	A	3009	OLA	O2-C1-C2-C3
4	A	3007	OLC	C9-C10-C11-C12
5	A	3010	OLA	C7-C8-C9-C10
5	A	3010	OLA	C9-C10-C11-C12
5	A	3014	OLA	C9-C10-C11-C12
5	A	3021	OLA	C9-C10-C11-C12
5	A	3024	OLA	C7-C8-C9-C10
4	A	3007	OLC	C6-C7-C8-C9
5	A	3018	OLA	C10-C11-C12-C13
5	A	3009	OLA	O1-C1-C2-C3
5	A	3010	OLA	C15-C16-C17-C18
4	A	3007	OLC	C7-C8-C9-C10
5	A	3009	OLA	C7-C8-C9-C10

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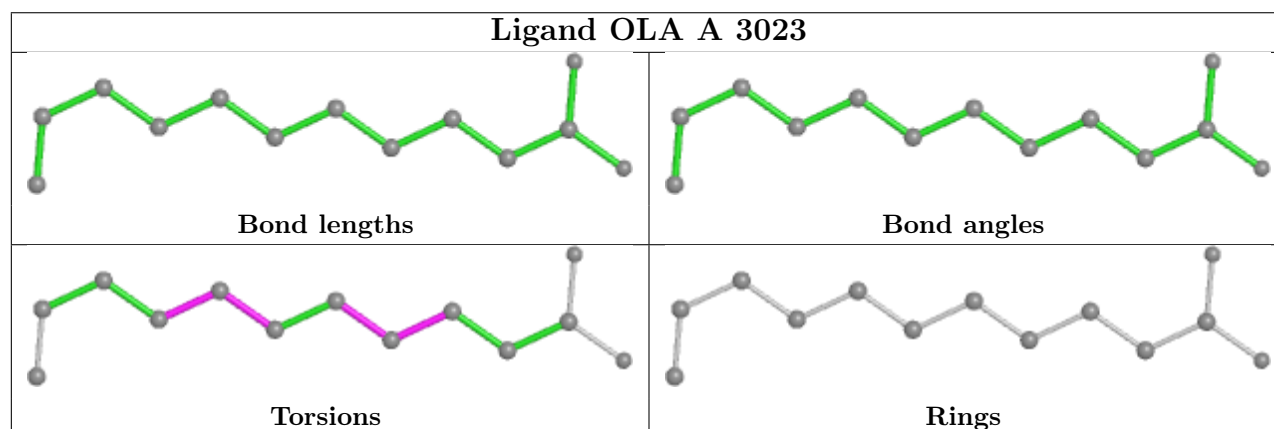
Mol	Chain	Res	Type	Atoms
5	A	3009	OLA	C13-C14-C15-C16
5	A	3011	OLA	O2-C1-C2-C3
4	A	3006	OLC	O20-C1-C2-C3
4	A	3006	OLC	O19-C1-C2-C3
5	A	3020	OLA	O2-C1-C2-C3
3	A	3003	CLR	C22-C23-C24-C25
5	A	3011	OLA	O1-C1-C2-C3
5	A	3014	OLA	C13-C14-C15-C16
5	A	3022	OLA	O1-C1-C2-C3

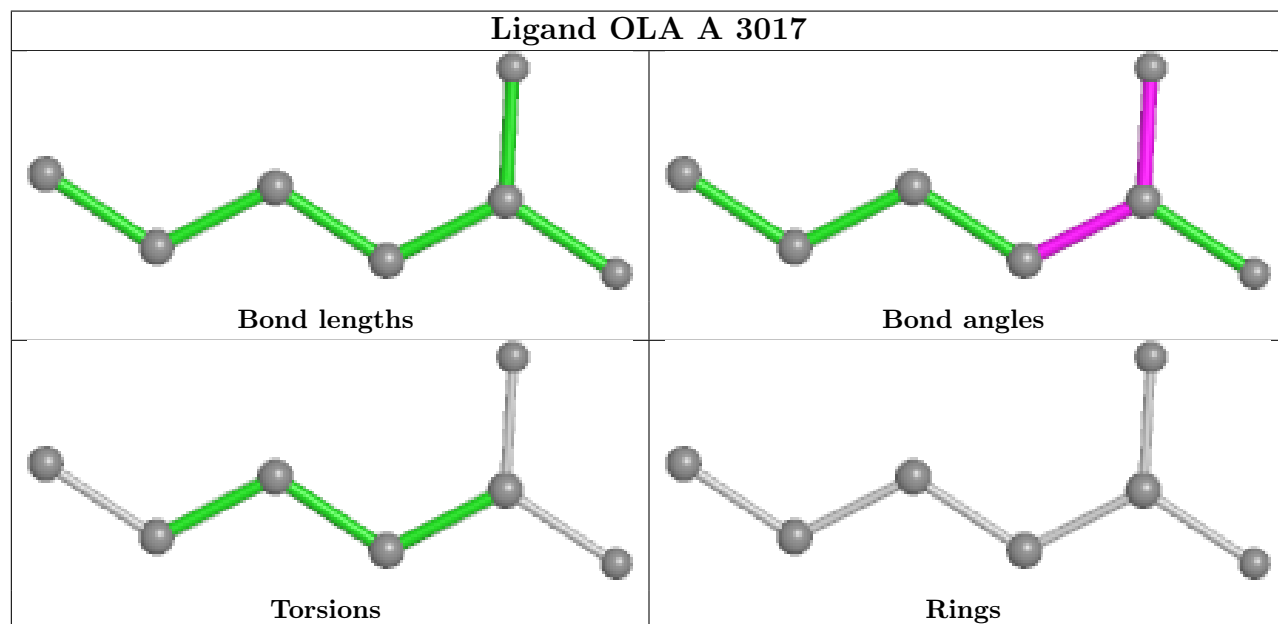
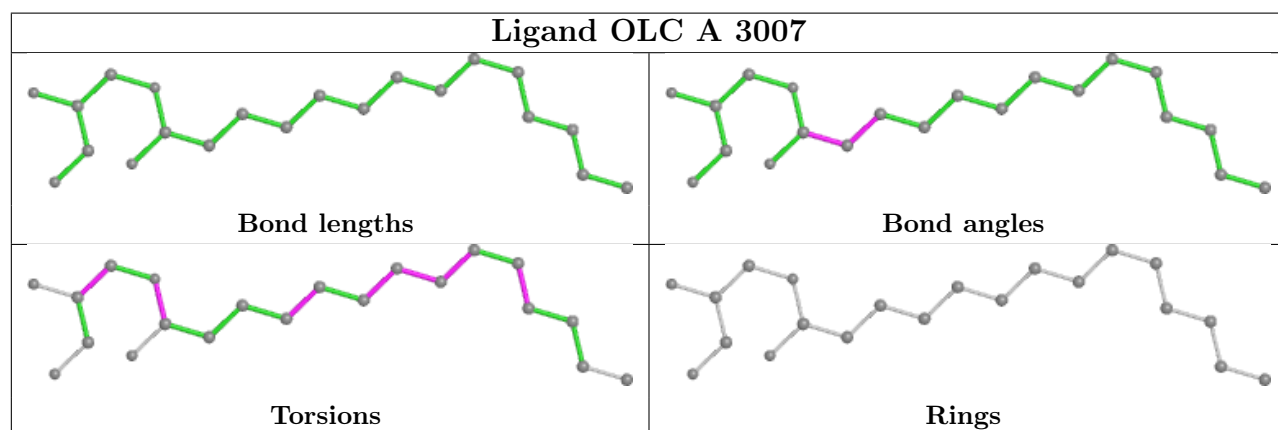
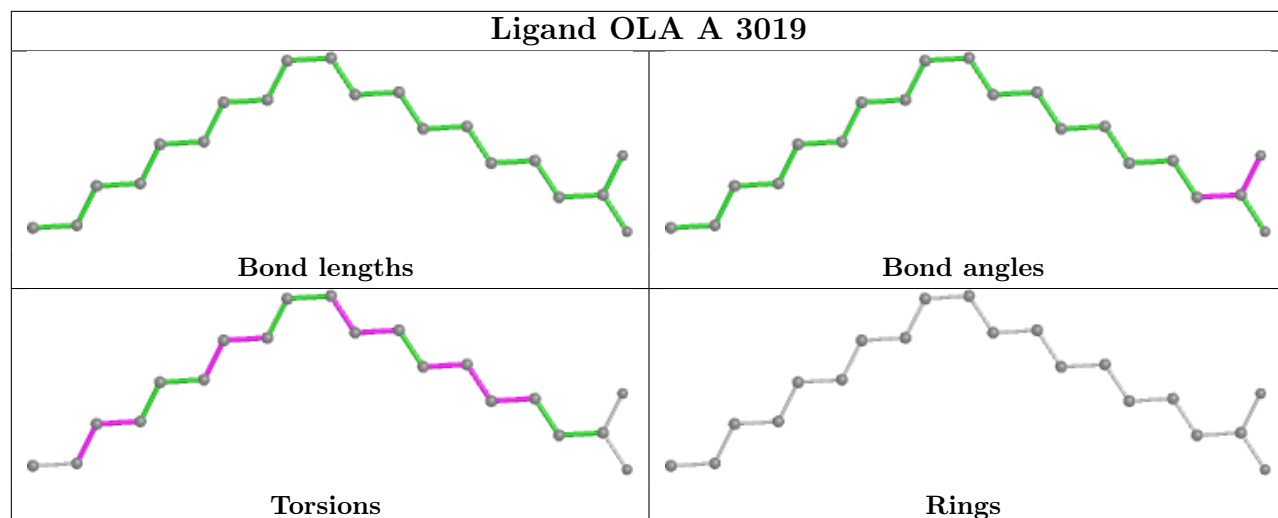
There are no ring outliers.

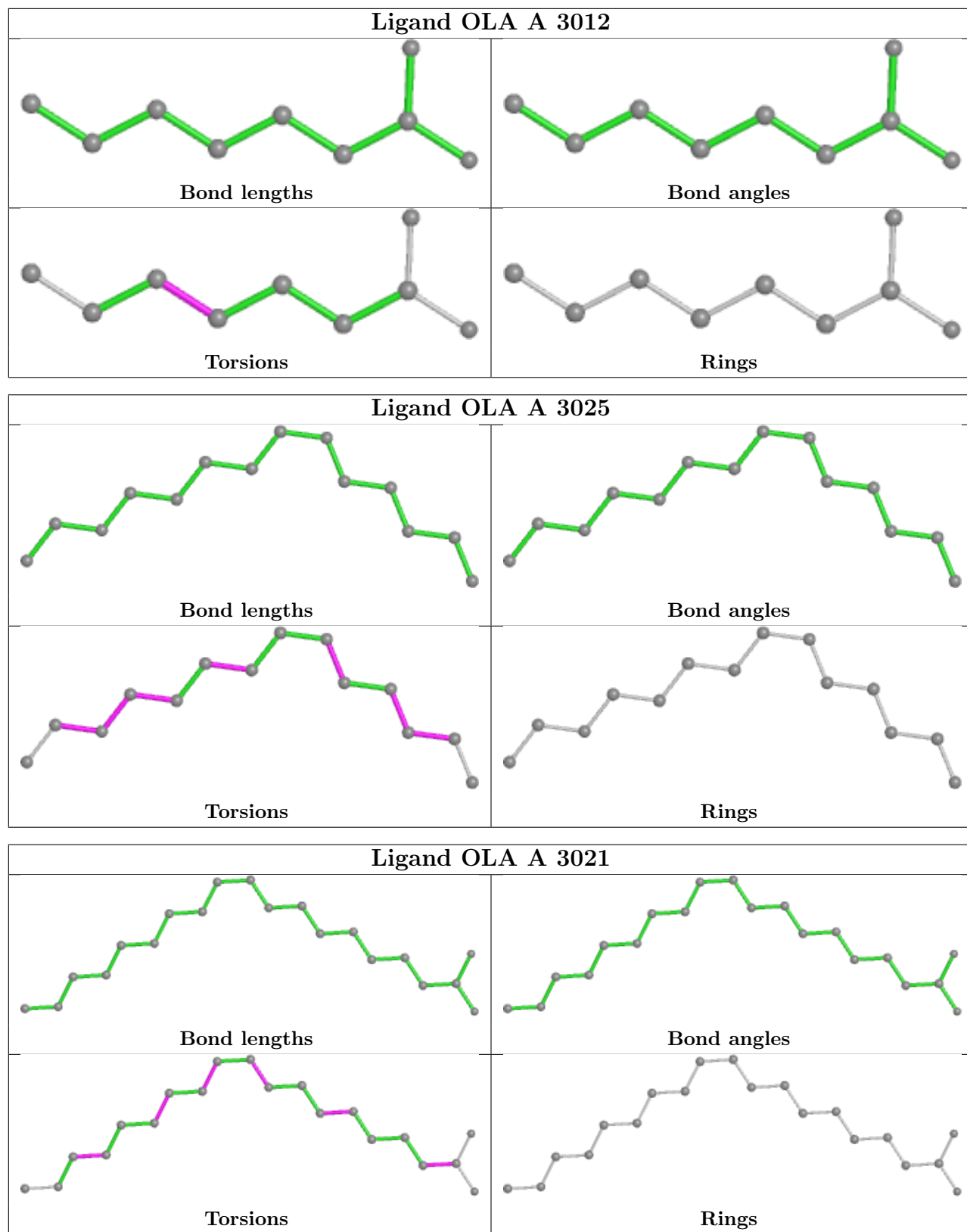
4 monomers are involved in 4 short contacts:

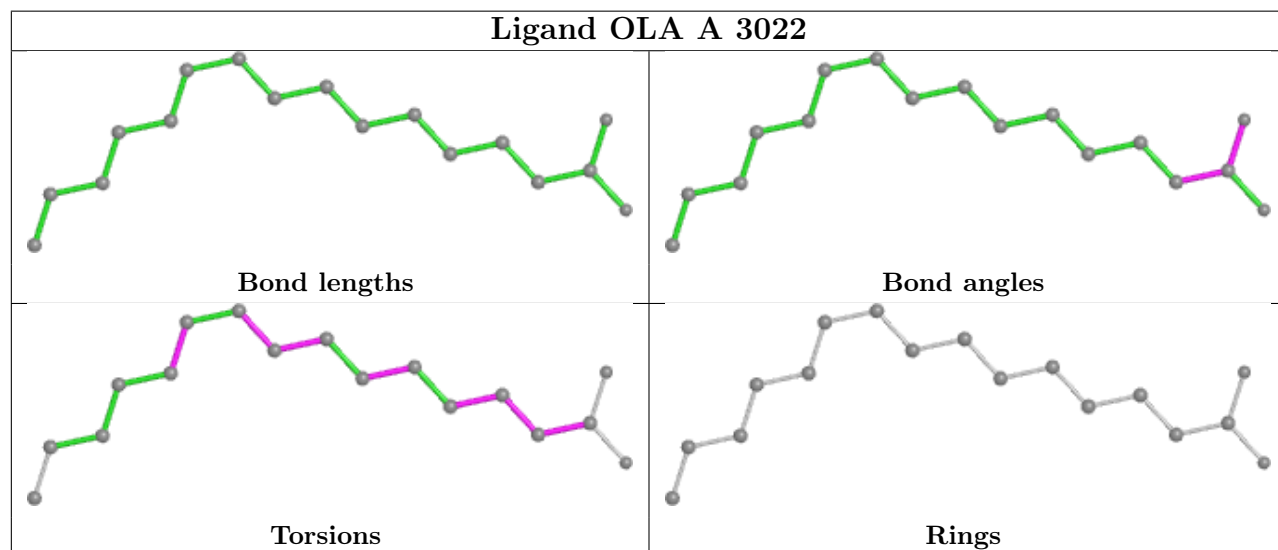
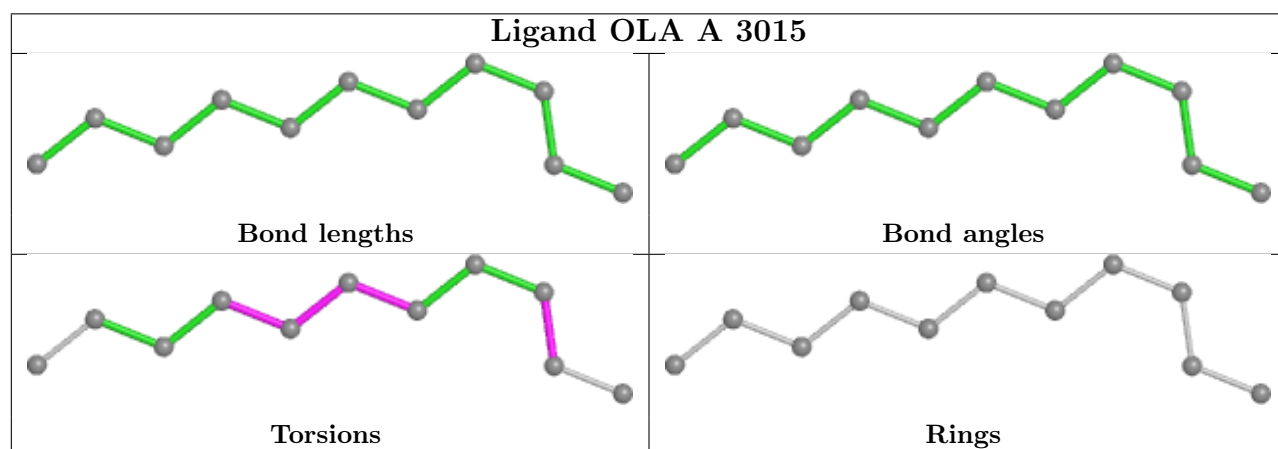
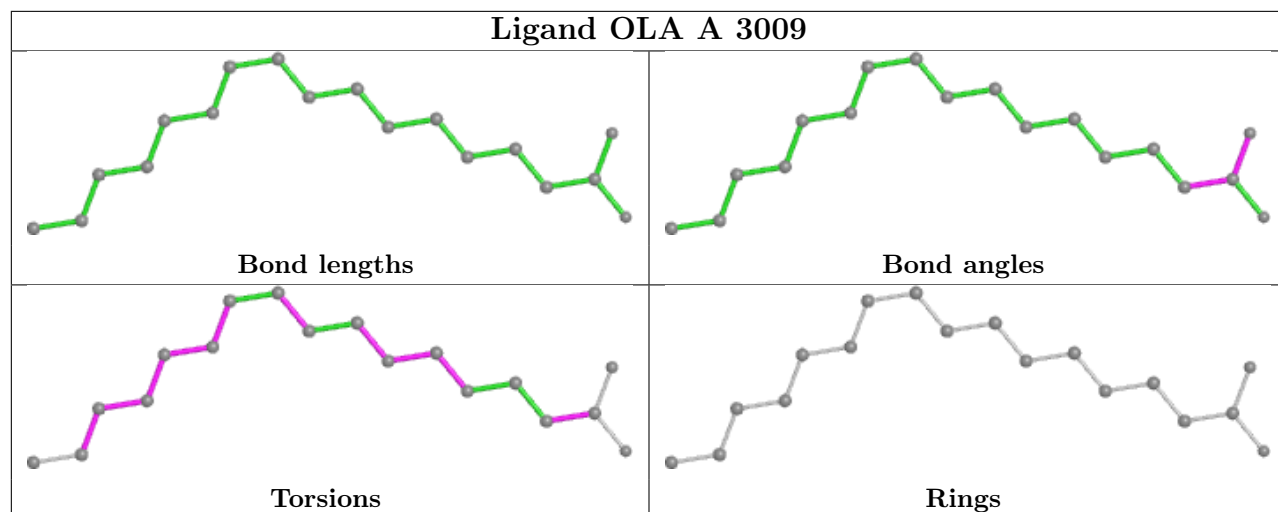
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3023	OLA	1	0
3	A	3004	CLR	1	0
3	A	3003	CLR	1	0
4	A	3006	OLC	1	0

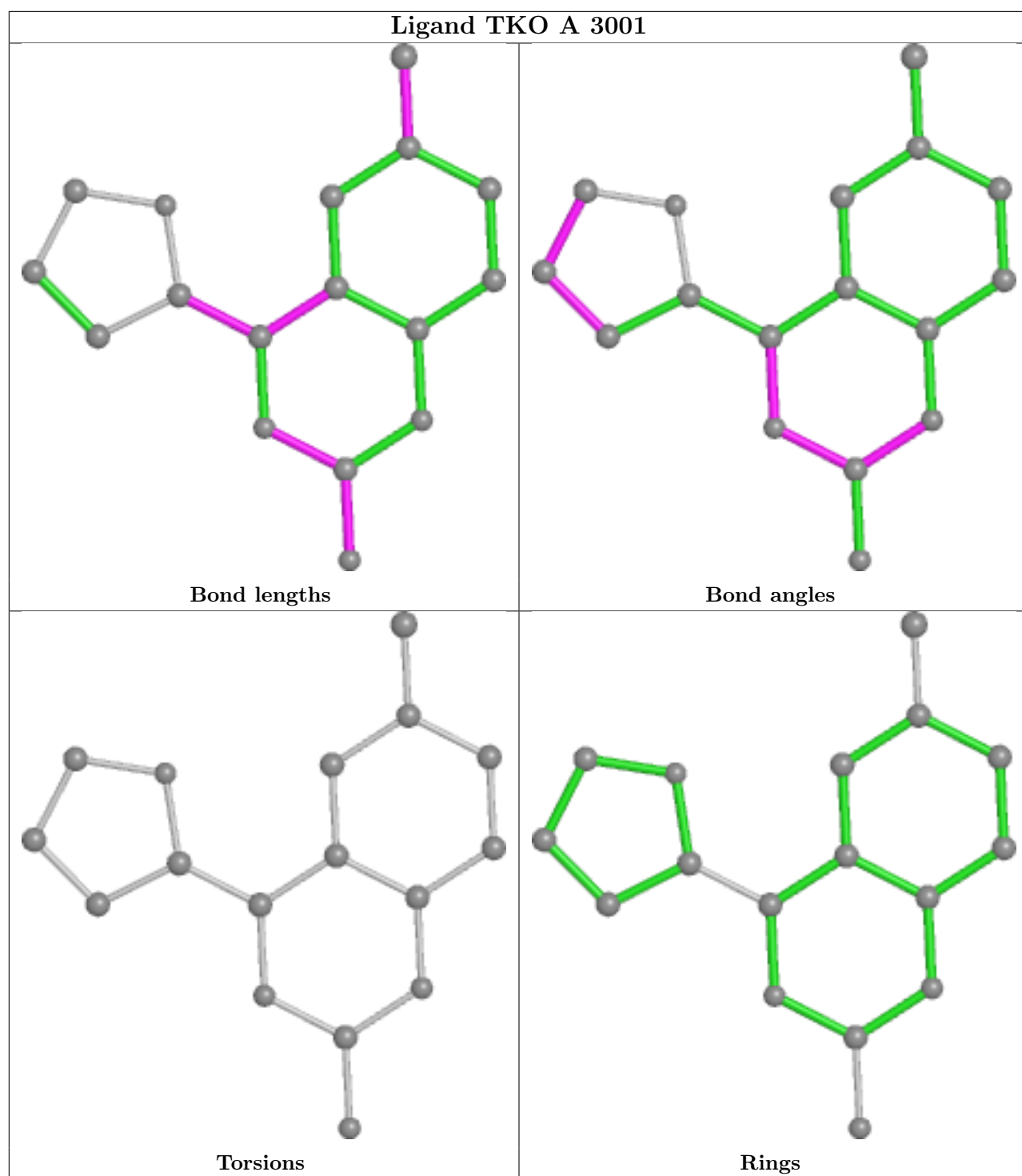
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

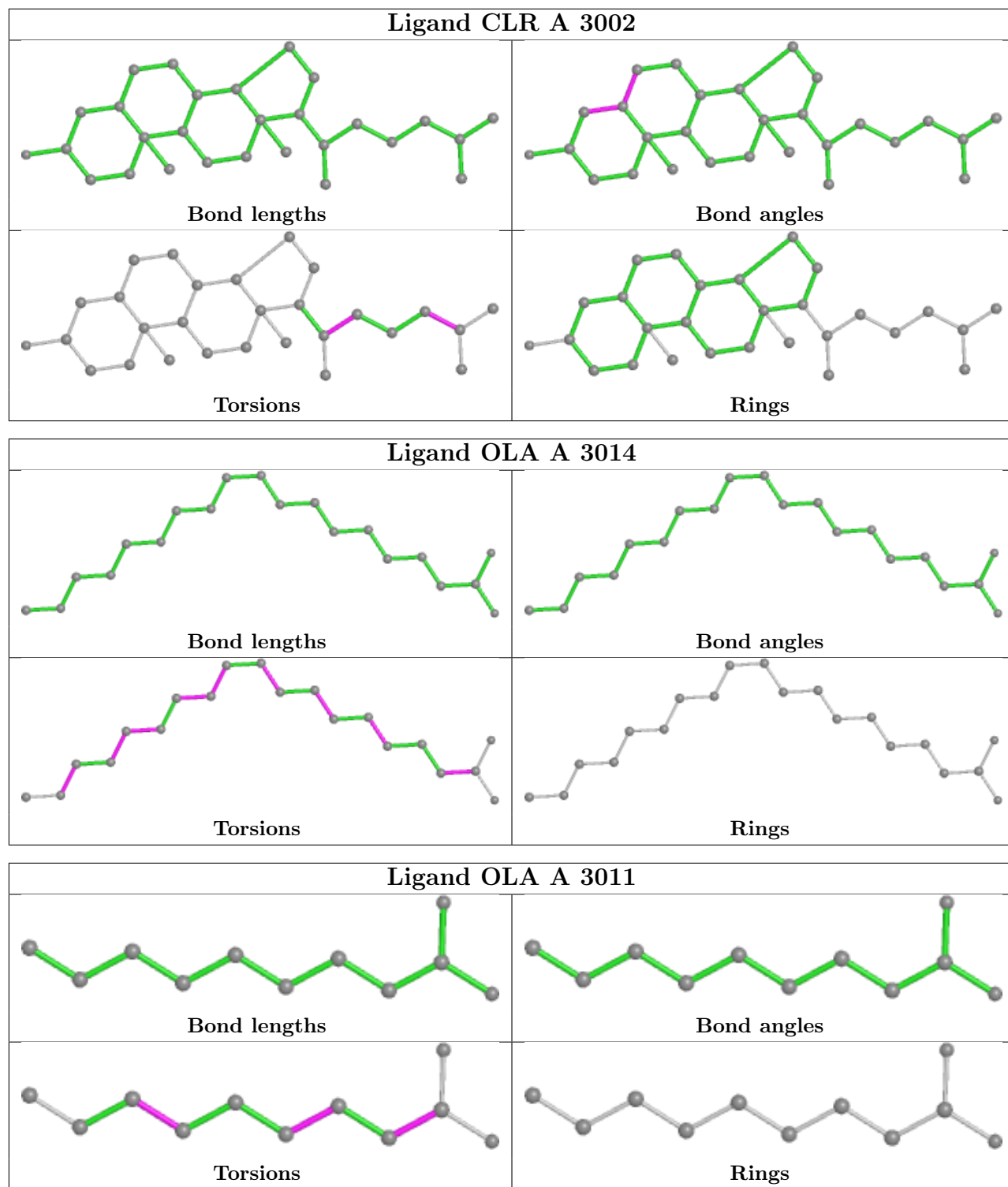


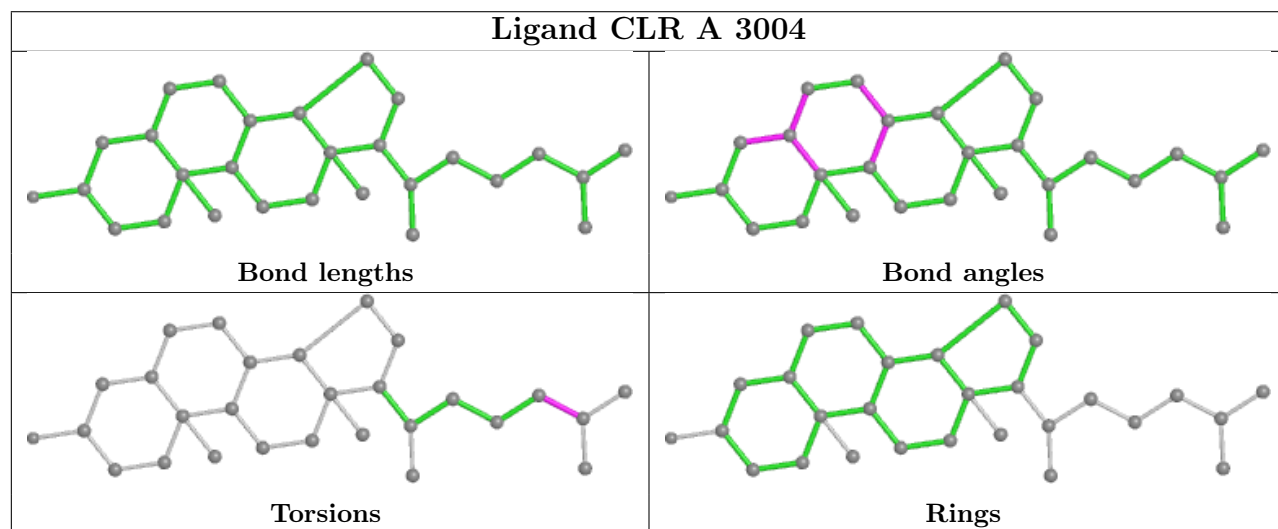
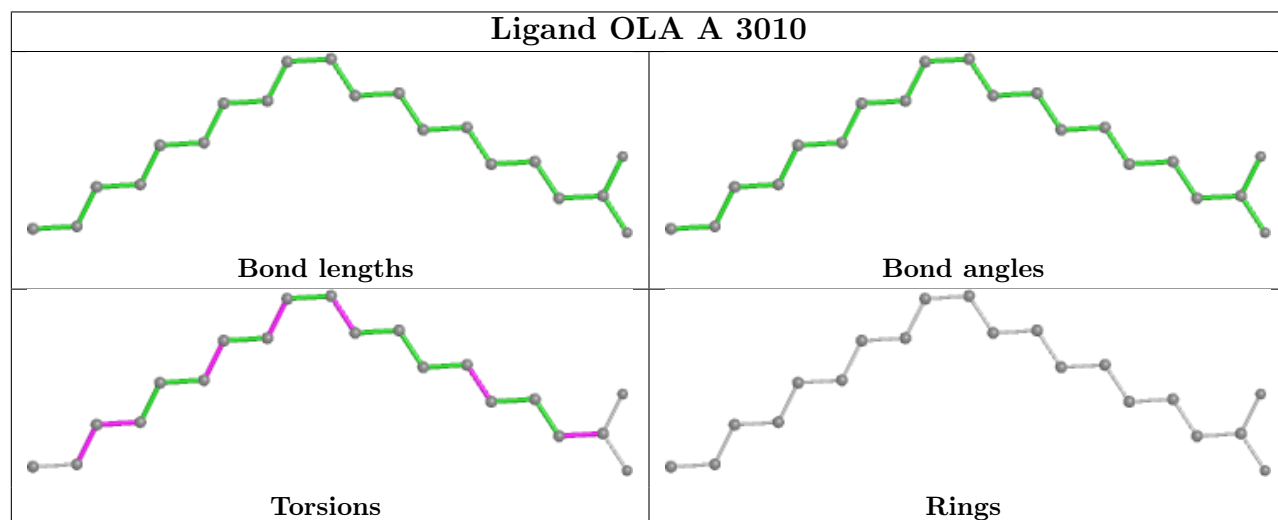
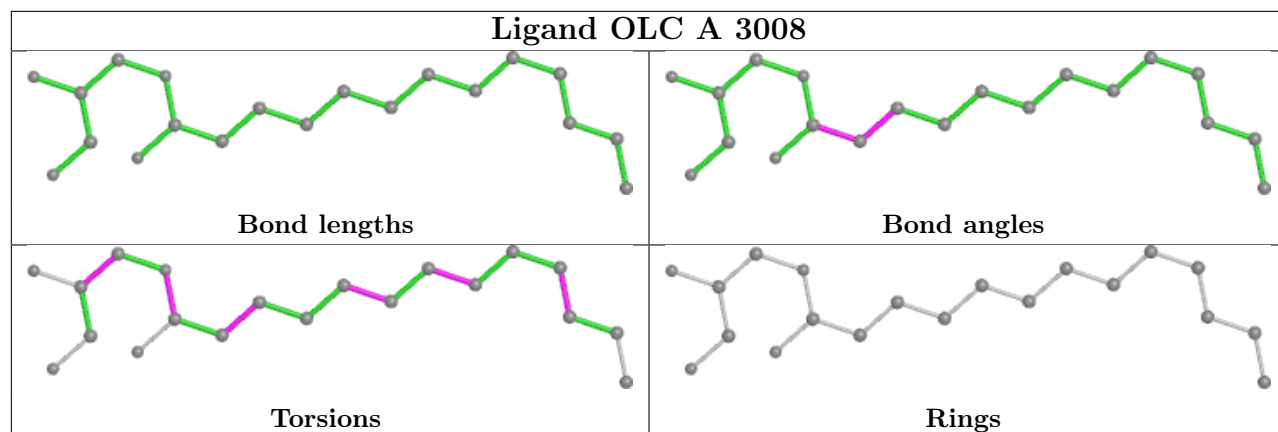


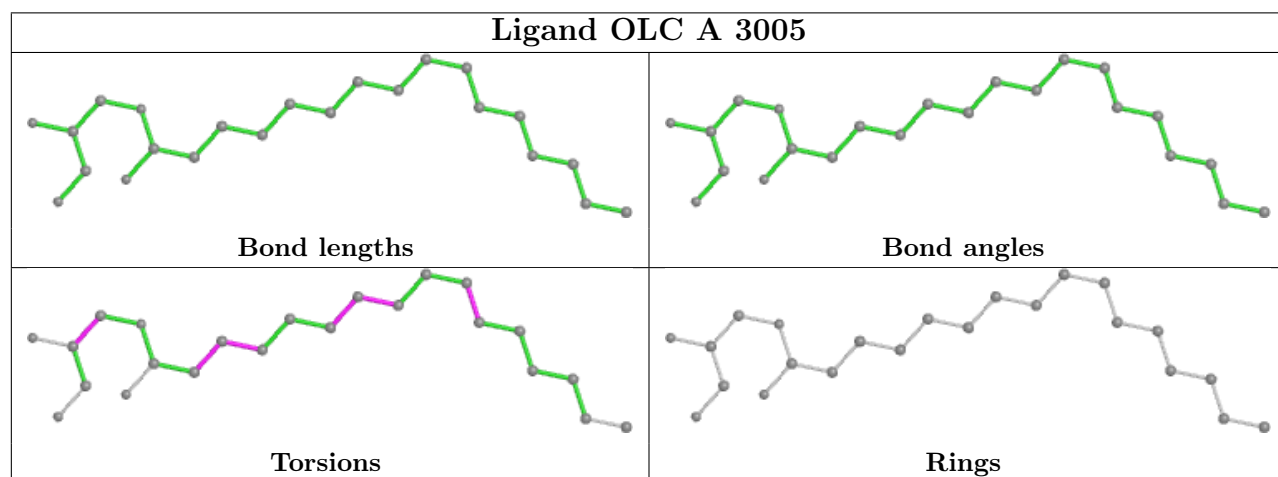
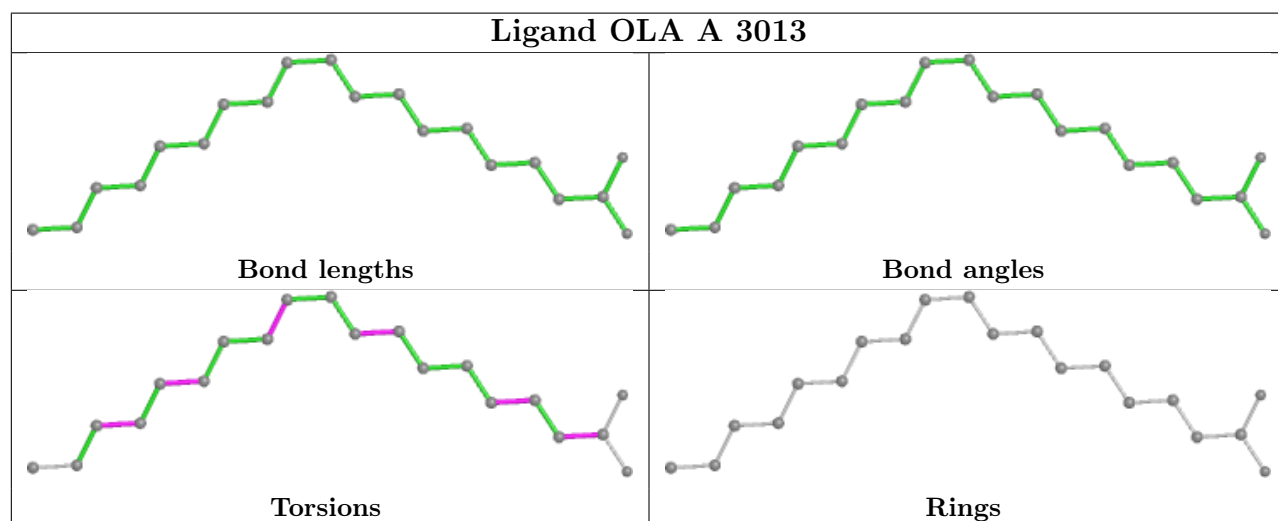
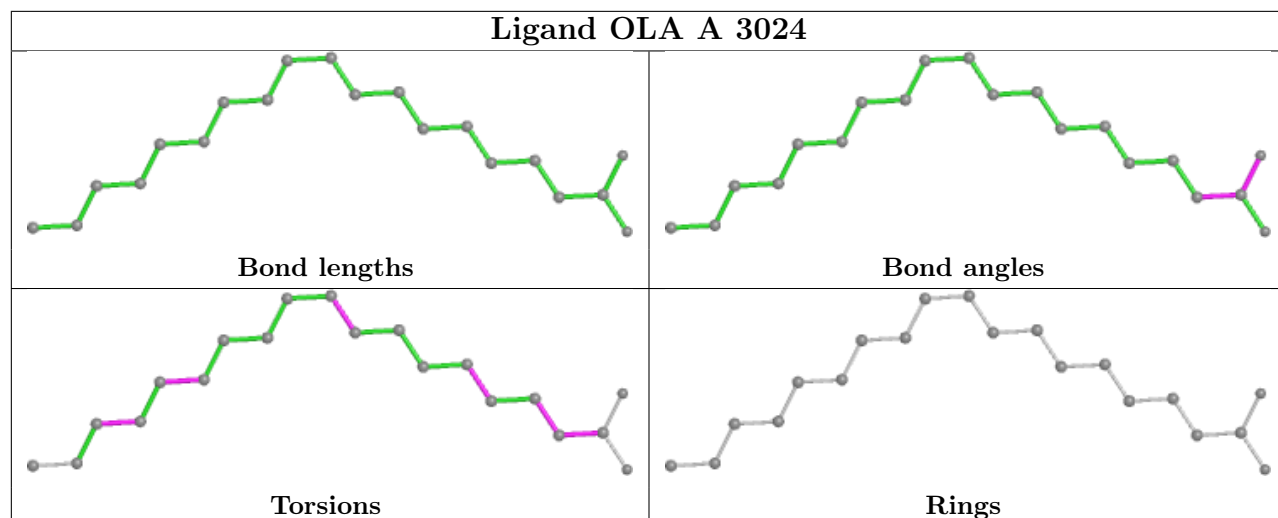


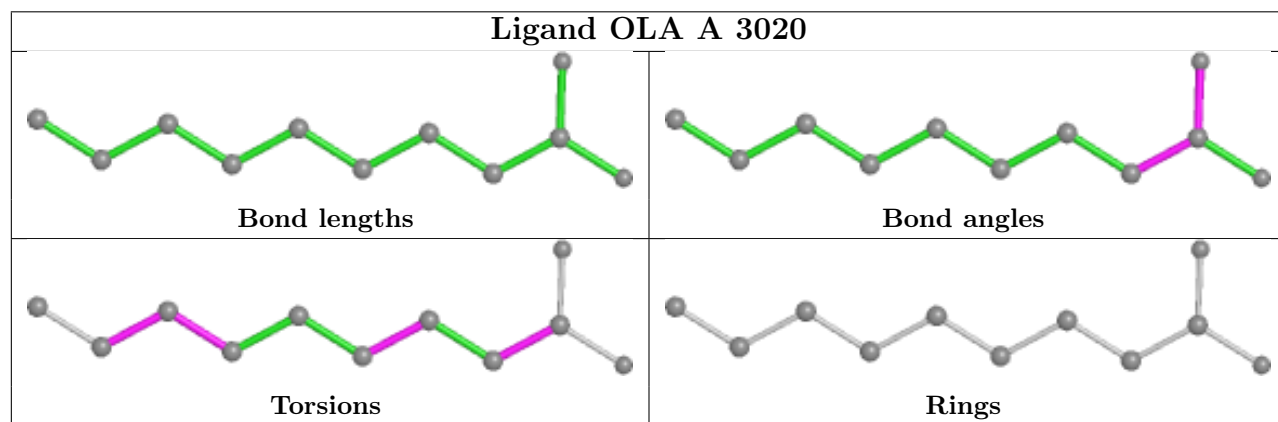
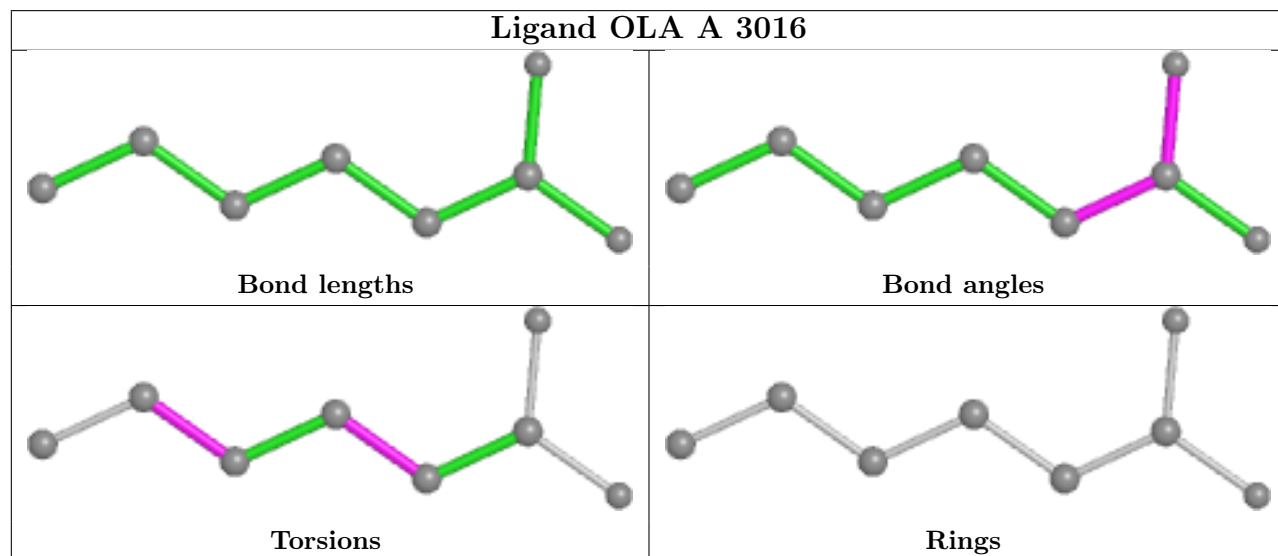
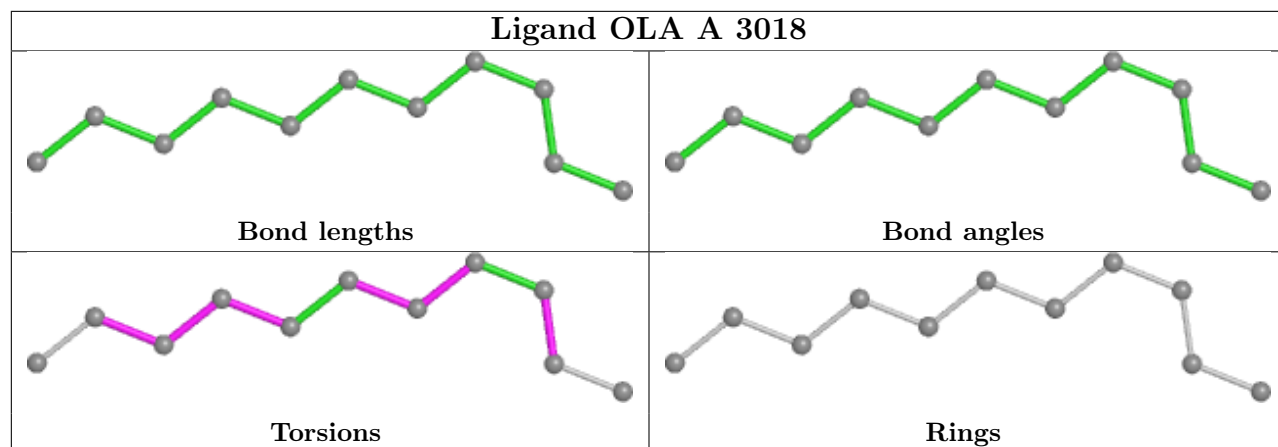


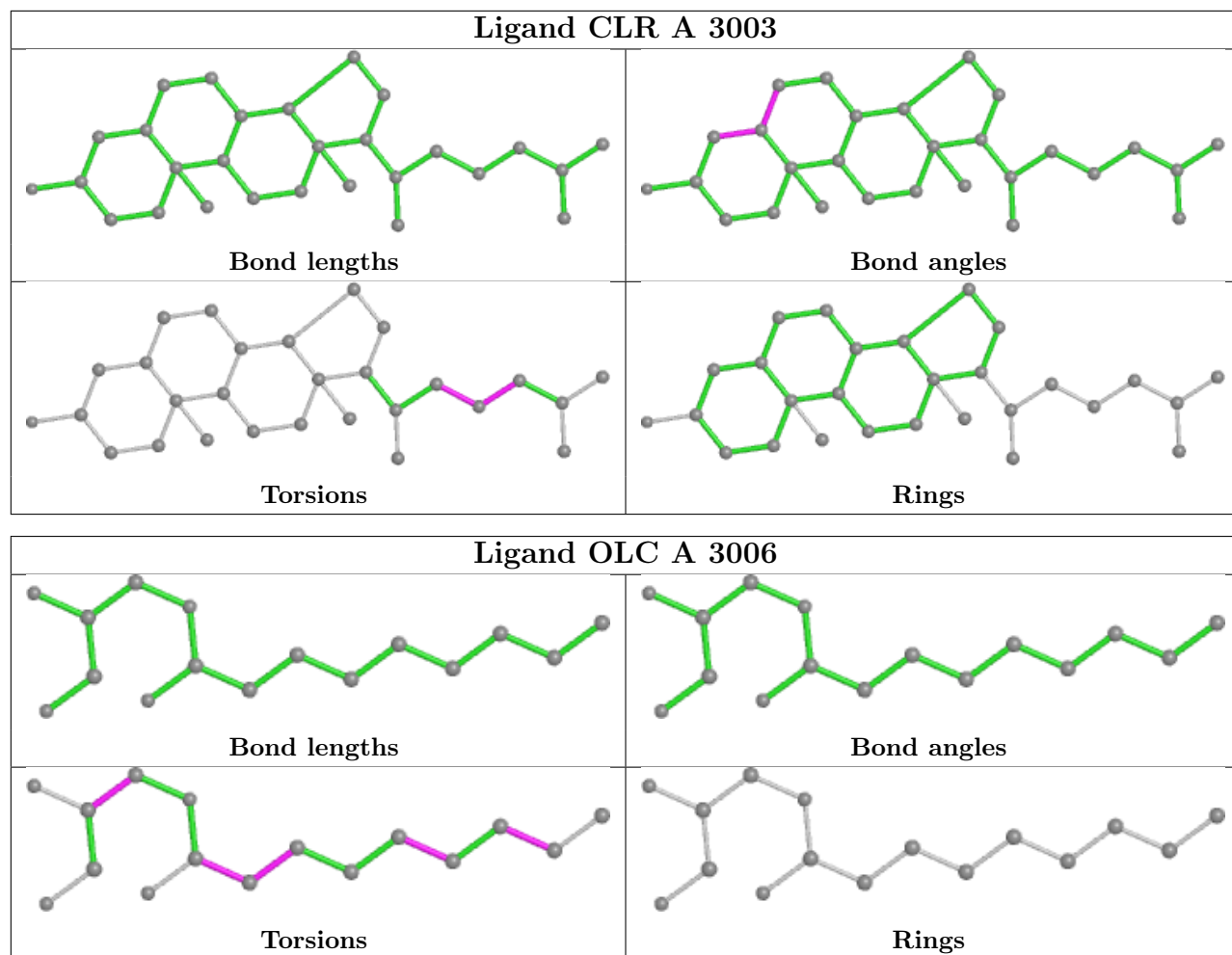












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.31	20 (5%)	28 29	27, 47, 90, 143	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1058	MET	9.0
1	A	1057	GLU	8.3
1	A	1060	ASP	7.4
1	A	1061	PHE	7.4
1	A	306	HIS	5.9
1	A	1059	LYS	5.5
1	A	304	ARG	5.3
1	A	305	SER	3.5
1	A	111	ARG	3.4
1	A	1021	ASP	3.1
1	A	1062	ARG	3.1
1	A	1063	HIS	3.0
1	A	1064	GLY	2.7
1	A	302	ILE	2.6
1	A	303	ILE	2.5
1	A	208	LEU	2.2
1	A	1028	ASP	2.1
1	A	148	GLN	2.0
1	A	29	TRP	2.0
1	A	290	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

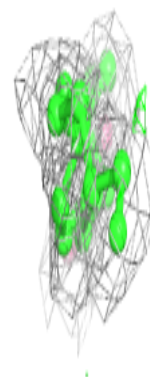
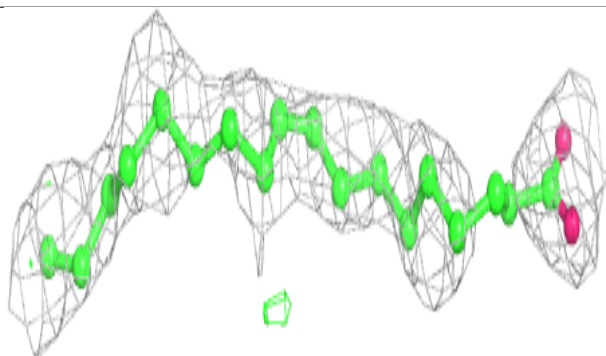
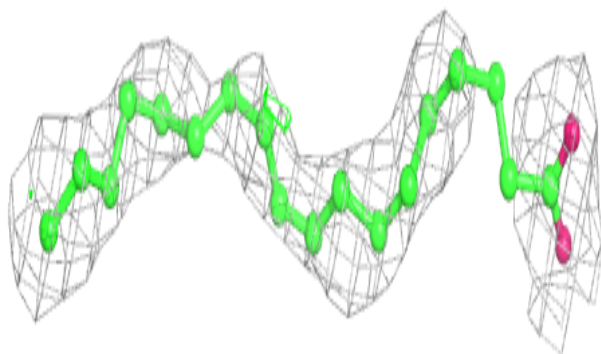
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	OLA	A	3014	20/20	0.63	0.29	50,65,80,81	0
4	OLC	A	3006	16/25	0.72	0.25	43,60,80,89	0
5	OLA	A	3021	20/20	0.72	0.29	48,77,88,90	0
4	OLC	A	3008	20/25	0.73	0.33	48,55,76,81	0
5	OLA	A	3016	8/20	0.73	0.23	58,61,64,68	0
5	OLA	A	3011	11/20	0.73	0.25	61,64,87,88	0
4	OLC	A	3007	21/25	0.74	0.28	34,59,70,81	0
5	OLA	A	3018	11/20	0.75	0.27	51,56,70,75	0
5	OLA	A	3013	20/20	0.75	0.27	49,56,70,74	0
5	OLA	A	3023	13/20	0.76	0.29	50,56,79,82	0
5	OLA	A	3024	20/20	0.78	0.26	57,72,84,85	0
5	OLA	A	3019	20/20	0.80	0.28	51,59,73,73	0
4	OLC	A	3005	23/25	0.80	0.26	44,56,76,83	0
5	OLA	A	3009	18/20	0.81	0.23	46,59,76,77	0
5	OLA	A	3010	20/20	0.82	0.24	43,59,73,75	0
5	OLA	A	3025	14/20	0.85	0.30	40,49,63,63	0
5	OLA	A	3012	9/20	0.86	0.22	42,50,60,72	0
5	OLA	A	3020	11/20	0.87	0.26	41,46,62,67	0
5	OLA	A	3015	11/20	0.88	0.20	38,51,63,68	0
3	CLR	A	3004	28/28	0.89	0.19	41,47,61,67	0
5	OLA	A	3017	7/20	0.89	0.29	60,71,73,74	0
5	OLA	A	3022	17/20	0.89	0.23	48,57,70,71	0
3	CLR	A	3002	28/28	0.92	0.17	40,47,53,62	0
3	CLR	A	3003	28/28	0.92	0.19	36,43,55,59	0
2	TKO	A	3001	17/17	0.95	0.15	25,33,44,69	0

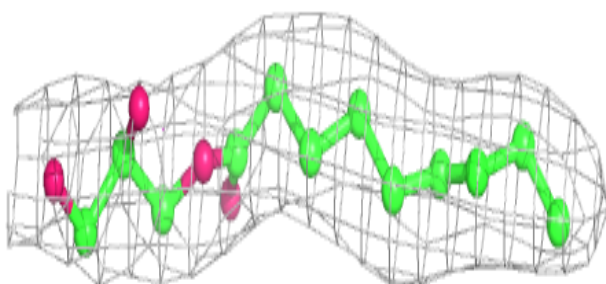
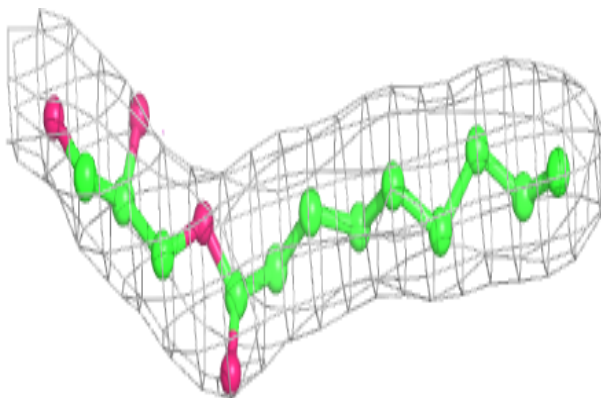
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 3014:

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

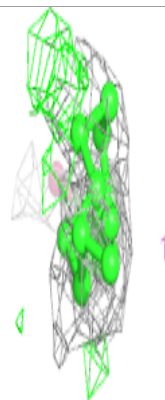
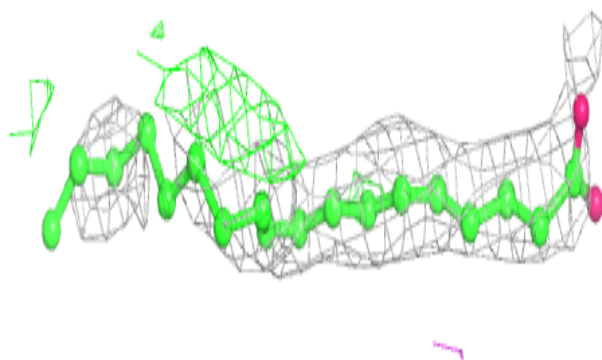
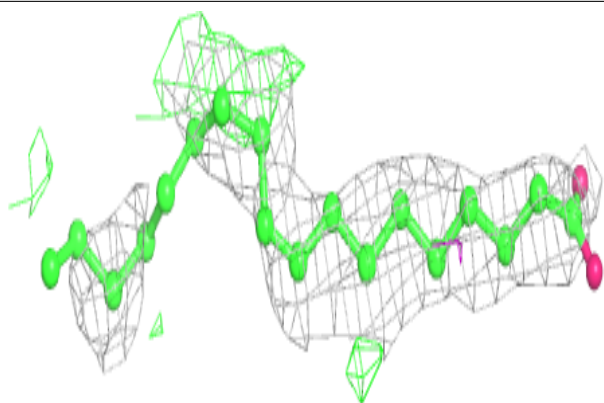
**Electron density around OLC A 3006:**

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

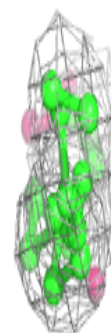
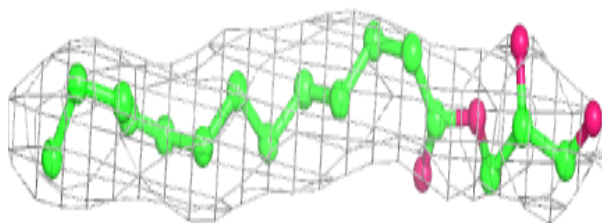
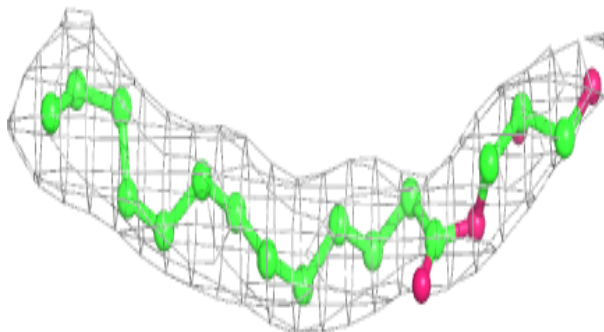


Electron density around OLA A 3021:

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

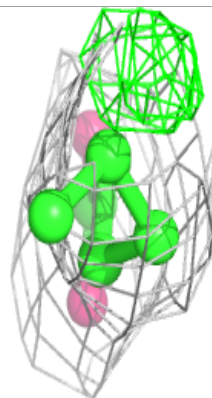
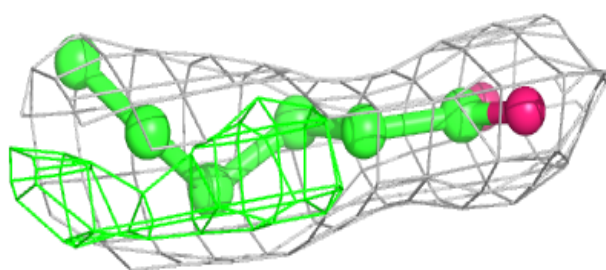
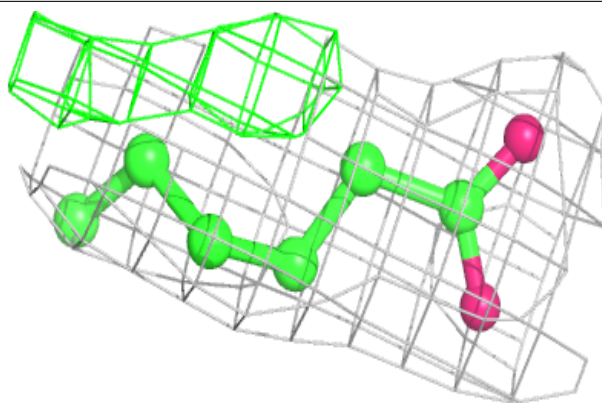
**Electron density around OLC A 3008:**

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

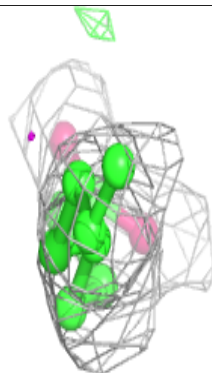
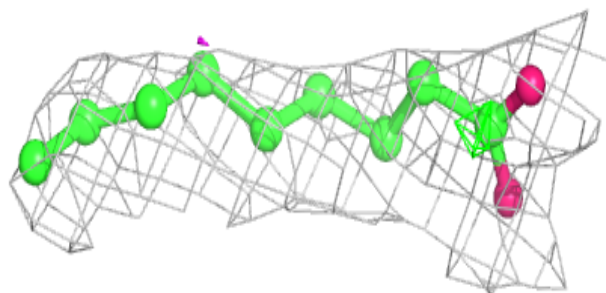
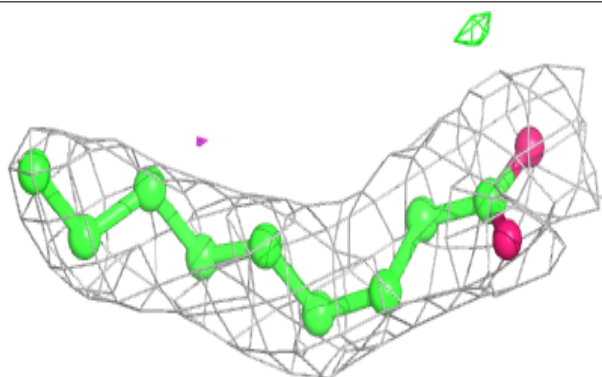


Electron density around OLA A 3016:

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

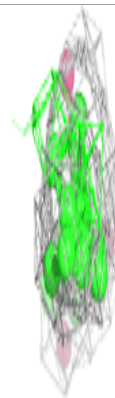
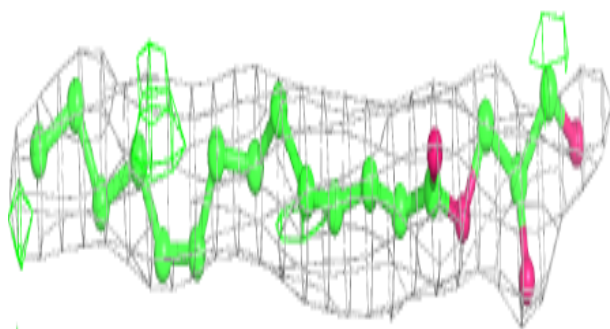
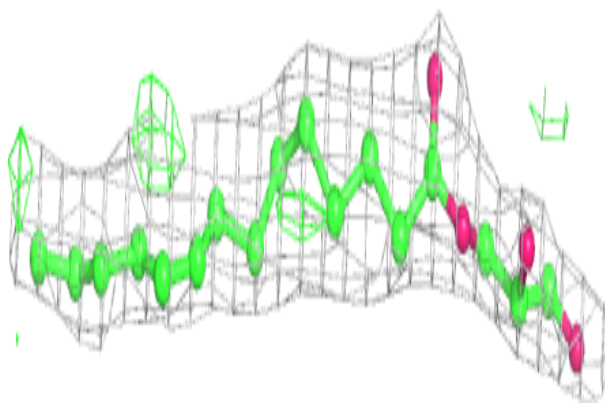
**Electron density around OLA A 3011:**

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

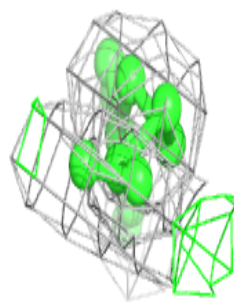
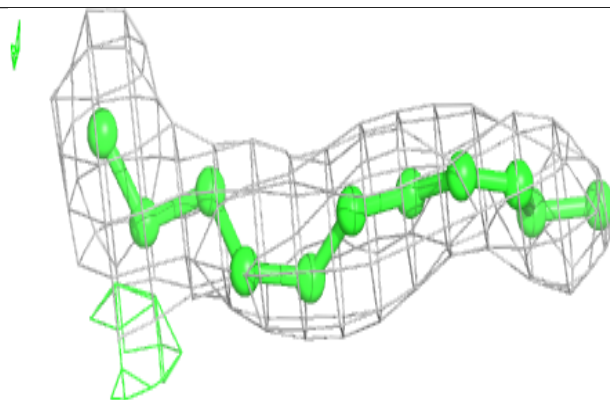
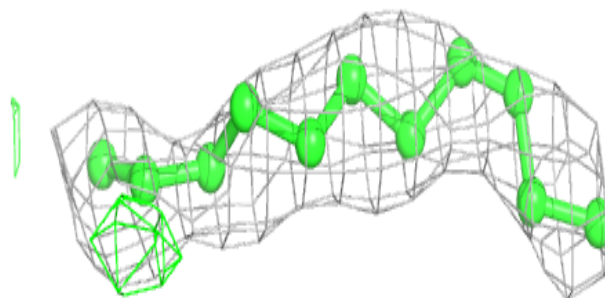


Electron density around OLC A 3007:

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

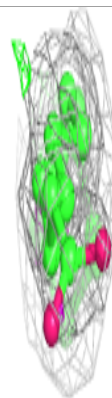
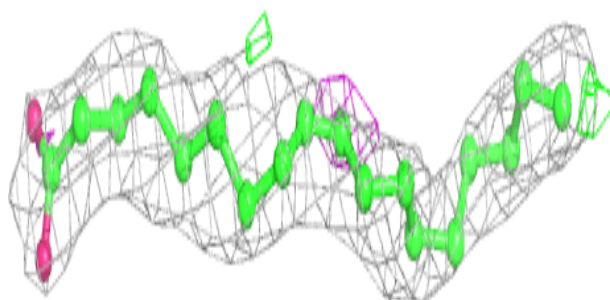
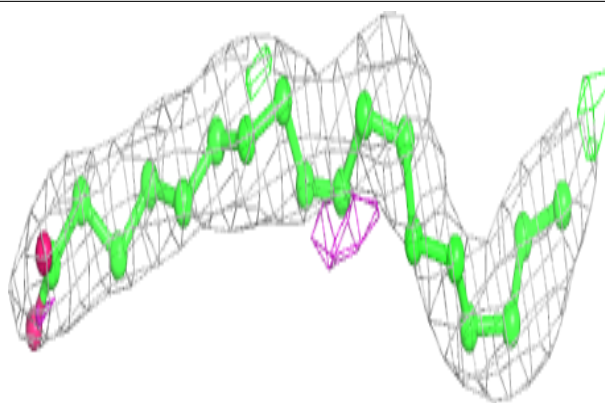
**Electron density around OLA A 3018:**

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

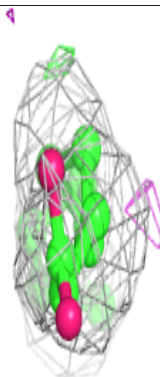
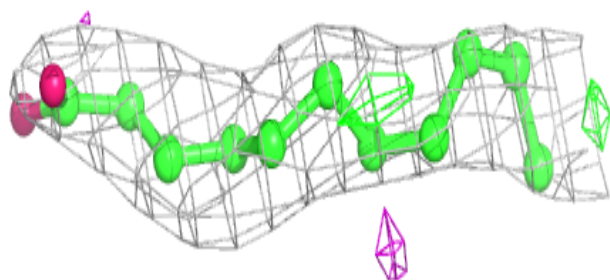
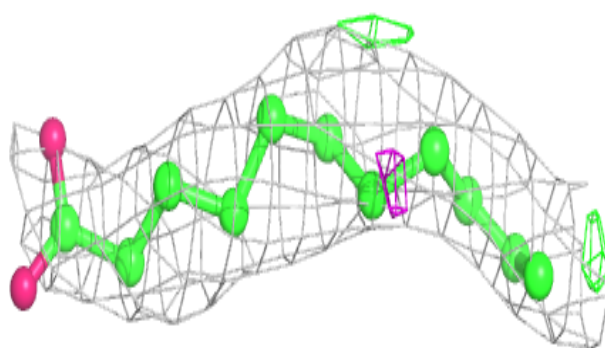


Electron density around OLA A 3013:

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

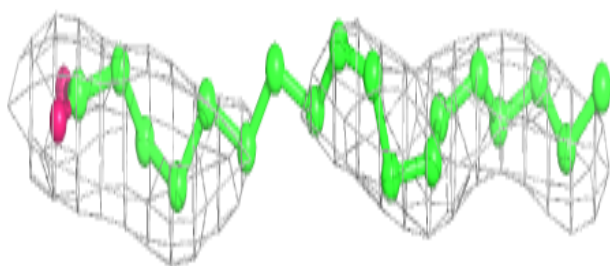
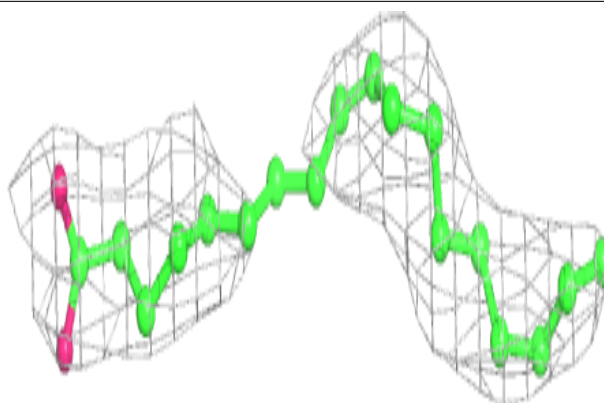
**Electron density around OLA A 3023:**

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

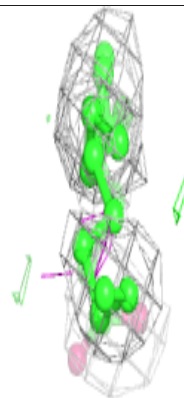
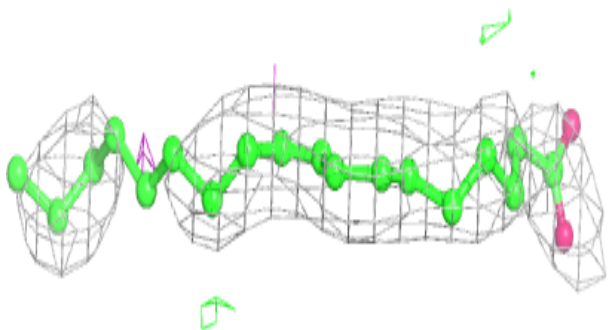
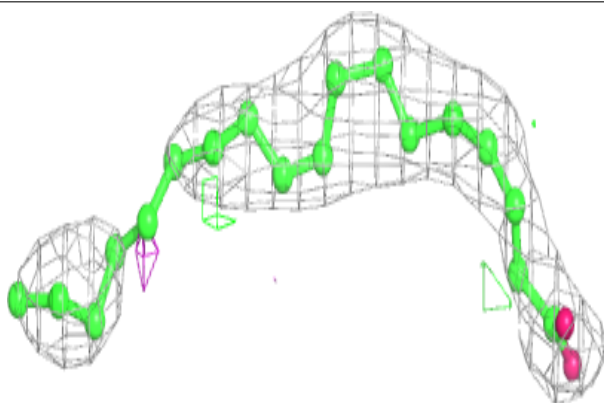


Electron density around OLA A 3024:

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

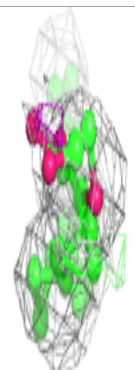
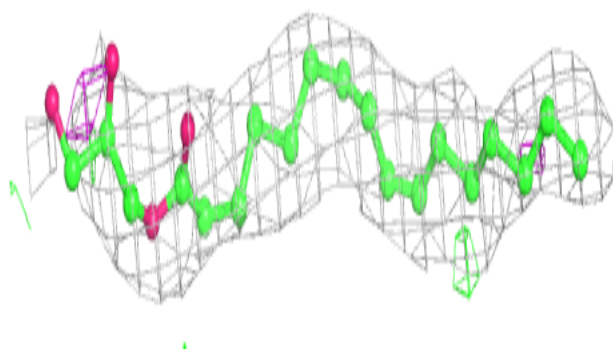
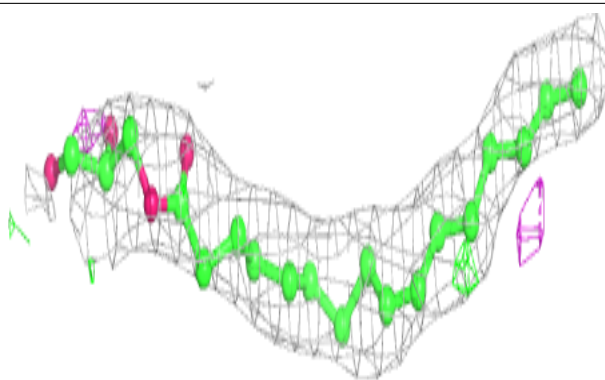
**Electron density around OLA A 3019:**

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

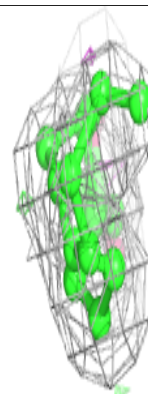
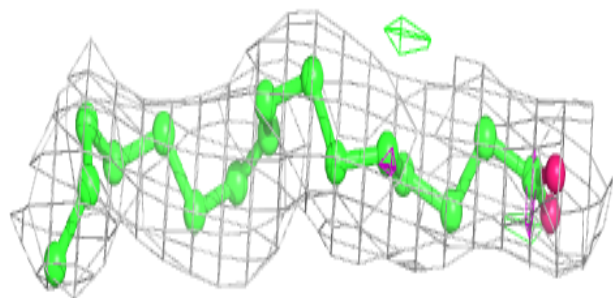
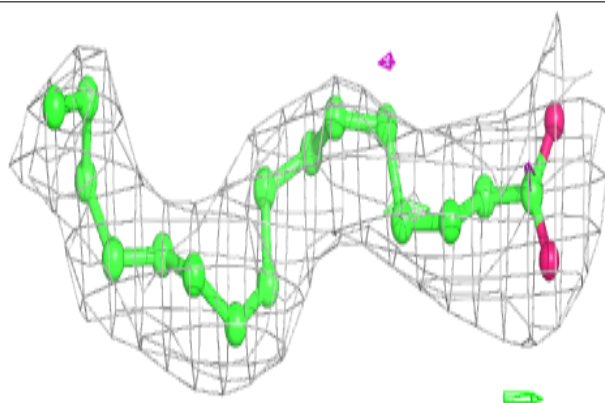


Electron density around OLC A 3005:

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

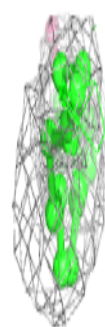
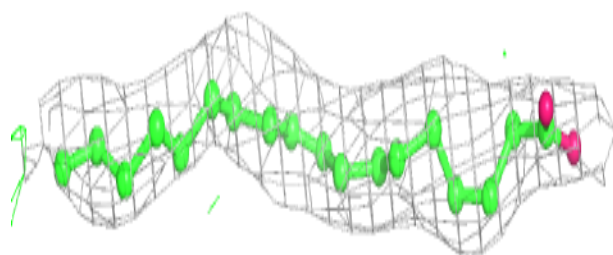
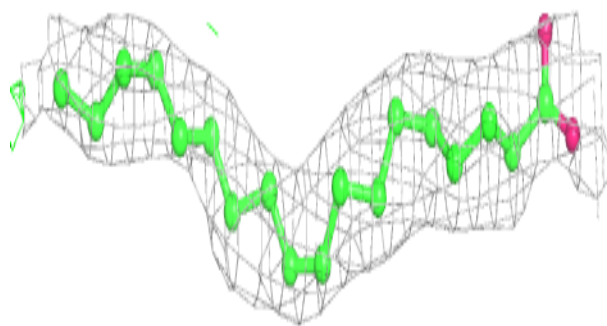
**Electron density around OLA A 3009:**

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

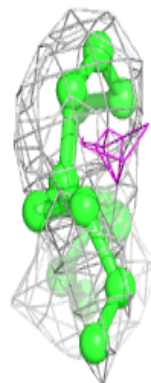
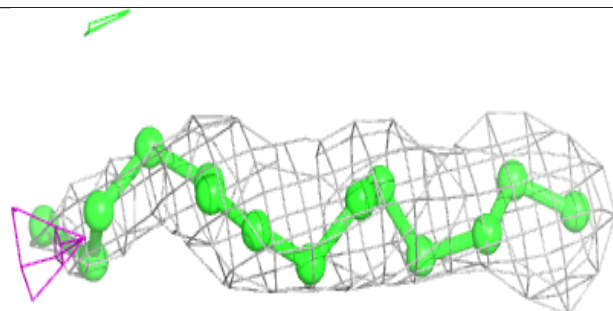
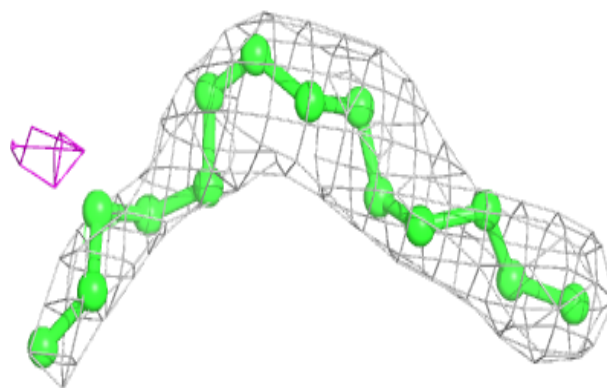


Electron density around OLA A 3010:

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

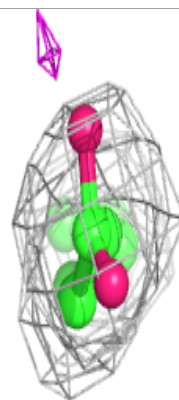
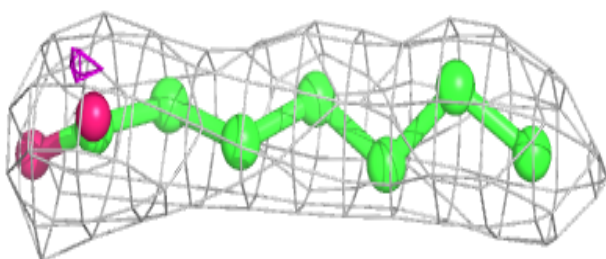
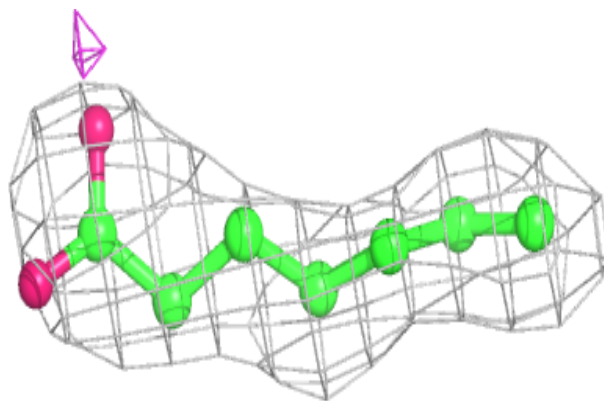
**Electron density around OLA A 3025:**

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

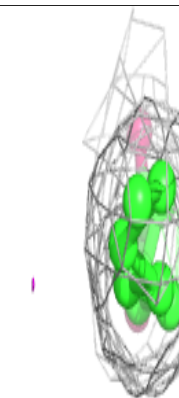
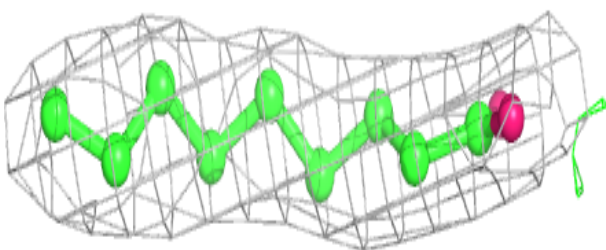
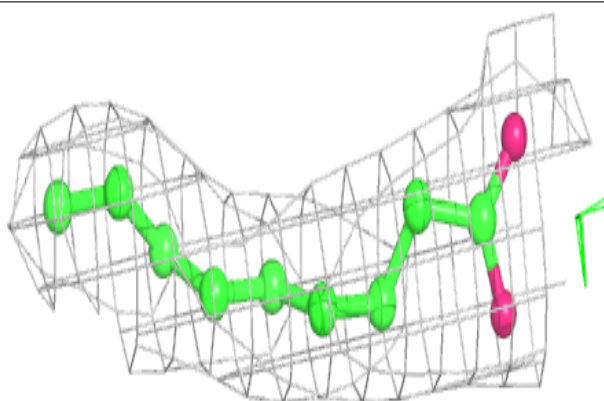


Electron density around OLA A 3012:

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

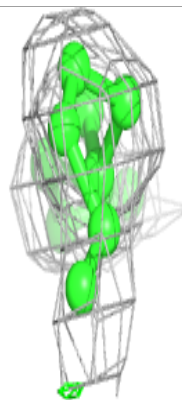
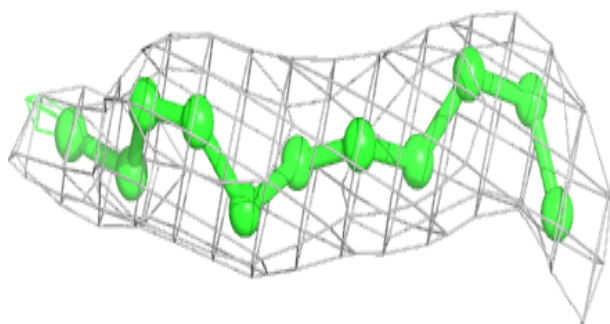
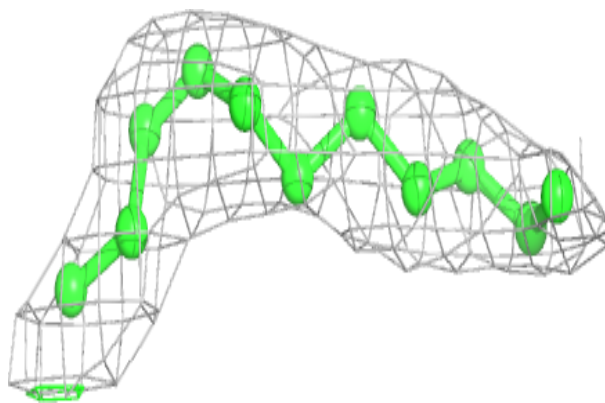
**Electron density around OLA A 3020:**

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

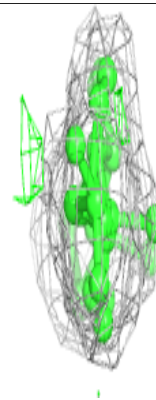
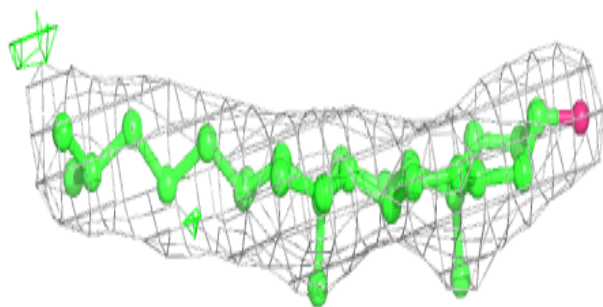
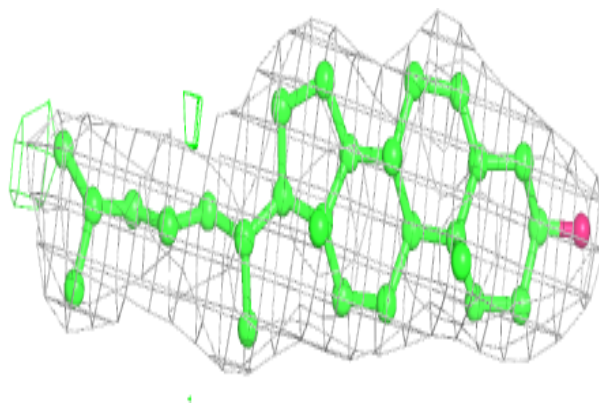


Electron density around OLA A 3015:

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

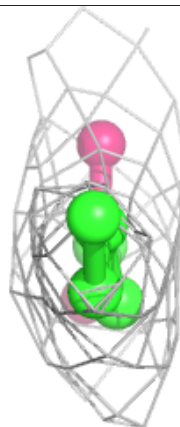
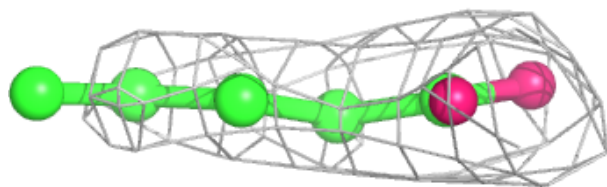
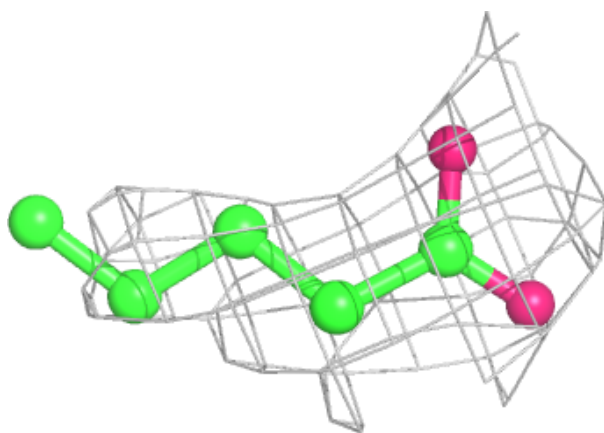
**Electron density around CLR A 3004:**

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

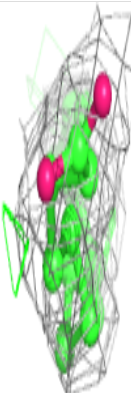
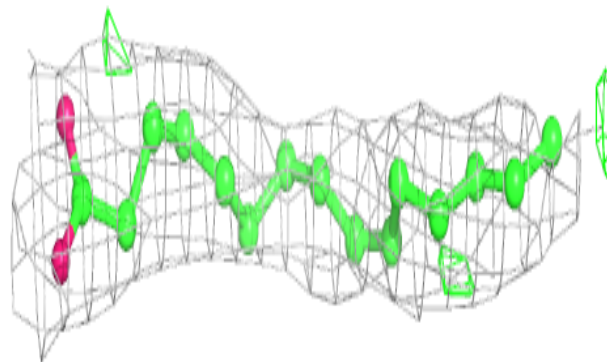
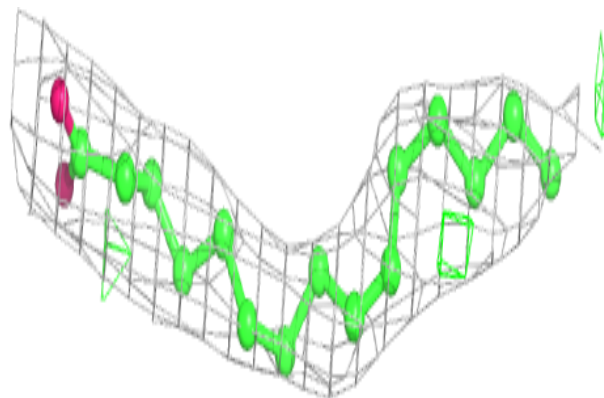


Electron density around OLA A 3017:

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

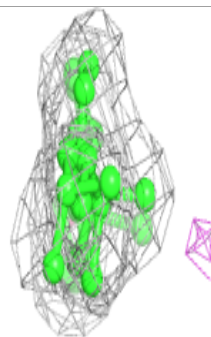
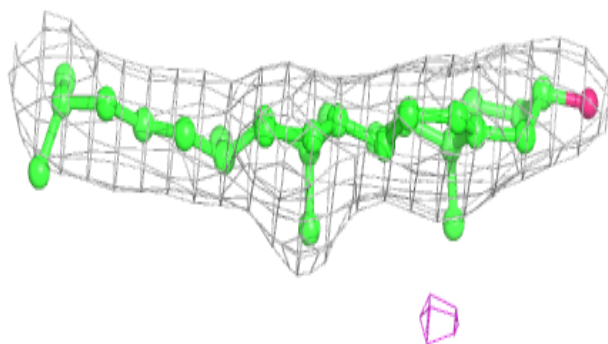
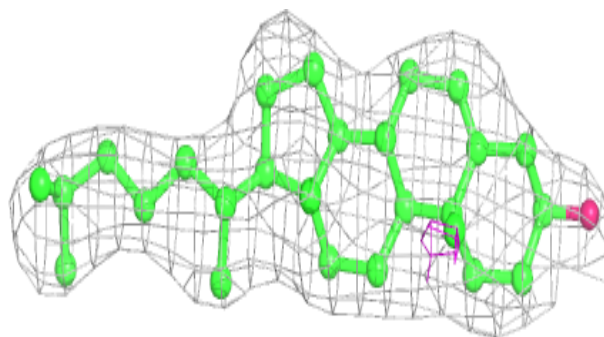
**Electron density around OLA A 3022:**

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

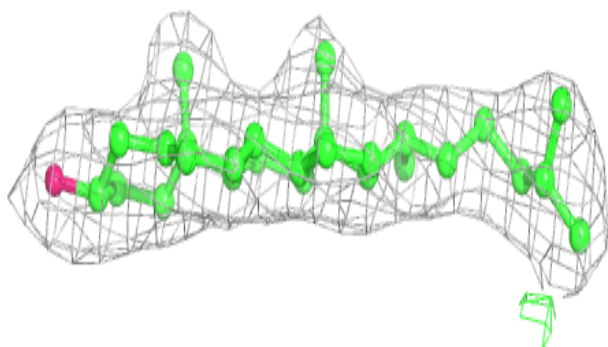
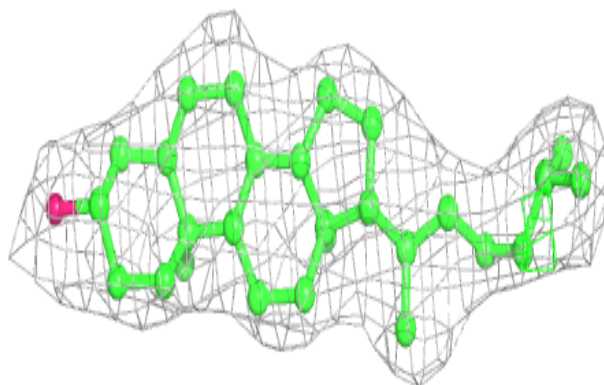


Electron density around CLR A 3002:

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

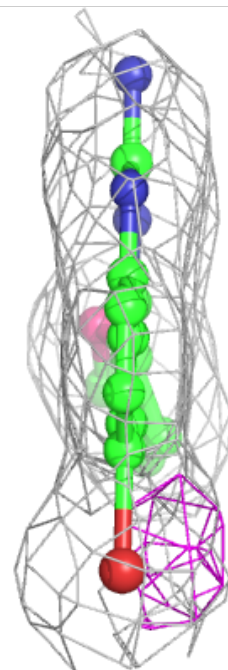
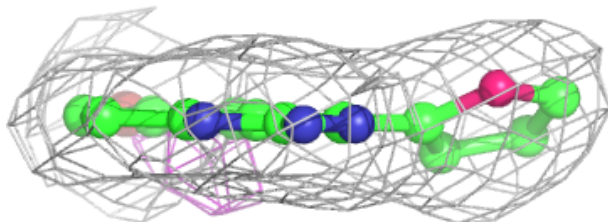
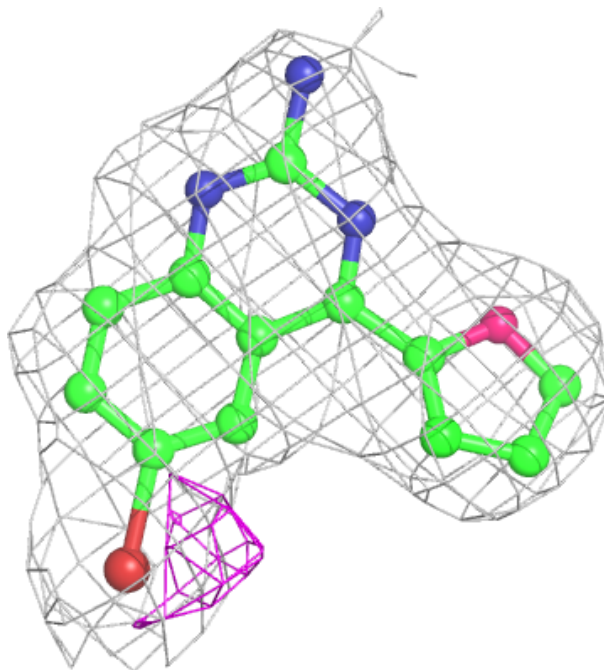
**Electron density around CLR A 3003:**

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



Electron density around TKO A 3001:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.