



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:08 AM UTC

PDB ID : 6RZ9 / pdb_00006rz9
Title : Crystal structure of the human cysteinyl leukotriene receptor 2 in complex with ONO-2770372
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Deposited on : 2019-06-12
Resolution : 2.73 Å(reported)

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

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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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12

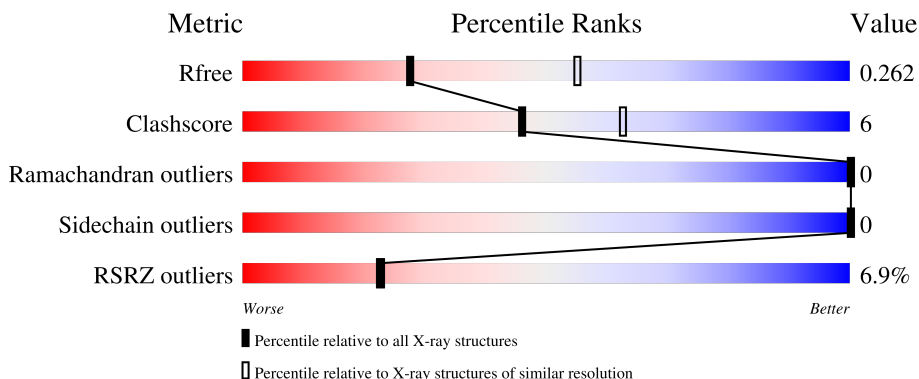
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	405	

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3106 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.

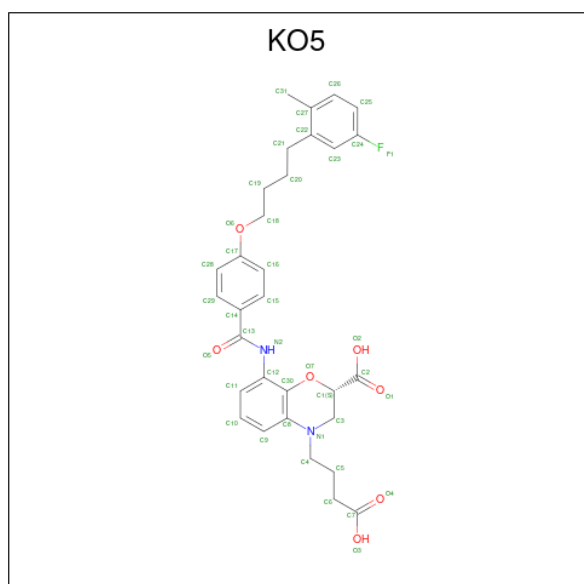
- Molecule 1 is a protein called Cysteinyl leukotriene receptor 2, Soluble cytochrome b562, Cysteinyl leukotriene receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2740	1816	441	466	17			

There are 6 discrepancies between the modelled and reference sequences:

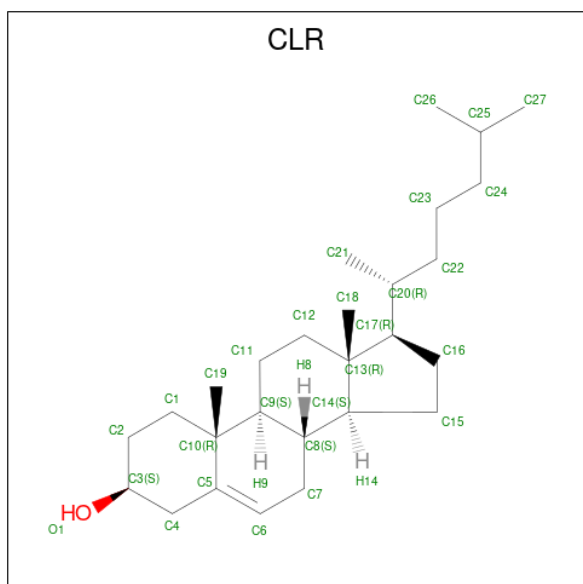
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	VAL	TRP	engineered mutation	UNP Q9NS75
A	84	ASN	ASP	engineered mutation	UNP Q9NS75
A	137	TYR	PHE	engineered mutation	UNP Q9NS75
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7

- Molecule 2 is (2 {S})-8-[[4-[4-(5-fluoranyl-2-methyl-phenyl)butoxy]phenyl]carbonylamino]-4-(4-oxidanyl-4-oxidanylidene-butyl)-2,3-dihydro-1,4-benzoxazine-2-carboxylic acid (CCD ID: KO5) (formula: C₃₁H₃₃FN₂O₇) (labeled as "Ligand of Interest" by depositor).



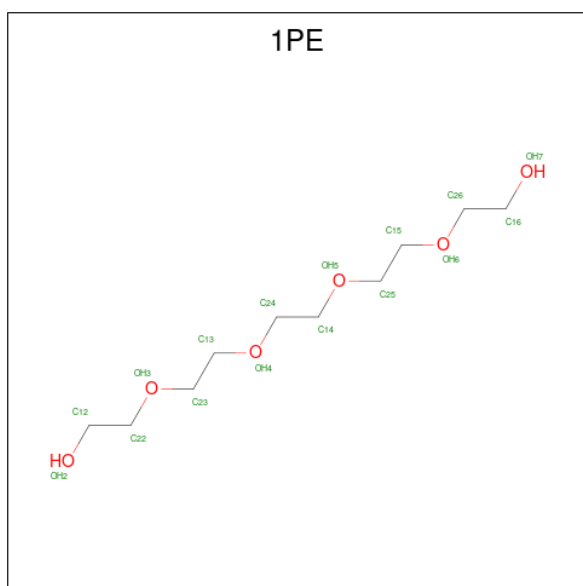
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			41	31	1	2	7		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



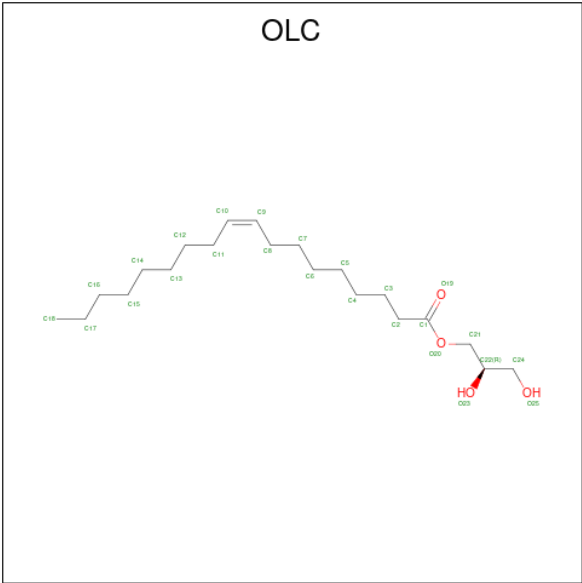
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	9	4		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



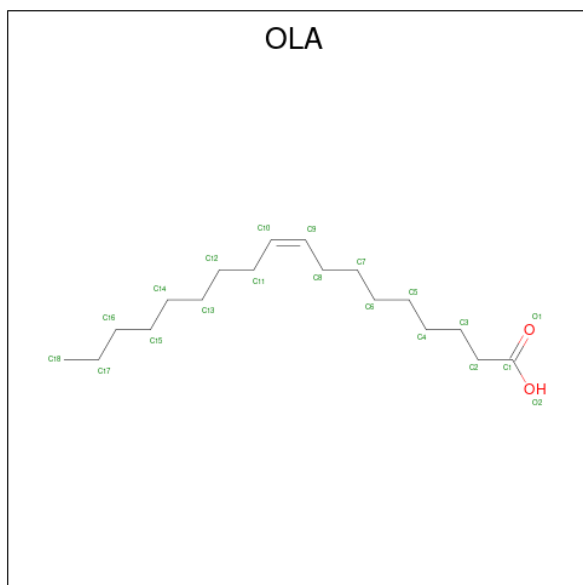
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	9	4		
5	A	1	Total	C	O	0	0
			14	10	4		
5	A	1	Total	C	O	0	0
			17	13	4		
5	A	1	Total	C		0	0
			8	8			
5	A	1	Total	C		0	0
			8	8			
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C		0	0
			6	6			
5	A	1	Total	C		0	0
			10	10			
5	A	1	Total	C	O	0	0
			17	13	4		
5	A	1	Total	C		0	0
			8	8			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 11 11	0	0
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C 14 14	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 16 14 2	0	0
6	A	1	Total C O 17 15 2	0	0
6	A	1	Total C 9 9	0	0
6	A	1	Total C O 20 18 2	0	0
6	A	1	Total C O 19 17 2	0	0
6	A	1	Total C O 20 18 2	0	0
6	A	1	Total C O 13 11 2	0	0

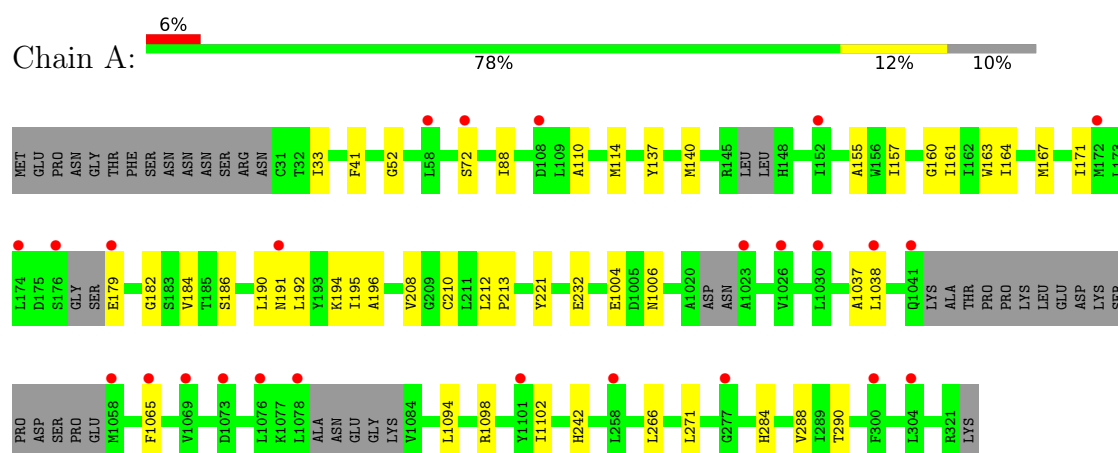
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		

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: Cysteinyl leukotriene receptor 2, Soluble cytochrome b562, Cysteinyl leukotriene receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	69.63Å 170.21Å 85.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 – 2.73 28.80 – 2.73	Depositor EDS
% Data completeness (in resolution range)	97.1 (28.80-2.73) 86.6 (28.80-2.73)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.12-2829, BUSTER 2.10.3	Depositor
R, R_{free}	0.217 , 0.254 (Not available) , 0.262	Depositor DCC
R_{free} test set	680 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.6	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	0.94	EDS
Total number of atoms	3106	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, OLC, OLA, 1PE, KO5

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	0.21	0/2794	0.46	0/3810

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 [i](#)

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	2740	0	2702	31	0
2	A	41	0	0	2	0
3	A	28	0	46	0	0
4	A	13	0	14	1	0
5	A	158	0	209	7	0
6	A	114	0	169	5	0
7	A	12	0	0	0	0
All	All	3106	0	3140	36	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 6.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2012:OLC:H8	6:A:2023:OLA:H41	1.68	0.75
1:A:1006:ASN:OD1	1:A:1098:ARG:NH1	2.29	0.66
1:A:33:ILE:HD13	1:A:284:HIS:CG	2.34	0.61
5:A:2012:OLC:H6	6:A:2023:OLA:H21	1.82	0.60
1:A:179:GLU:N	1:A:186:SER:O	2.35	0.60
2:A:2001:KO5:C25	5:A:2014:OLC:H17	2.32	0.60
1:A:1102:ILE:HG21	4:A:2003:1PE:H141	1.85	0.58
1:A:72:SER:HB2	1:A:155:ALA:HB2	1.86	0.57
1:A:208:VAL:HG11	5:A:2014:OLC:H18A	1.88	0.55
1:A:137:TYR:O	1:A:140:MET:HG2	2.07	0.55
1:A:232:GLU:O	1:A:1004:GLU:HG3	2.09	0.53
1:A:192:LEU:O	1:A:195:ILE:HG22	2.09	0.51
1:A:157:ILE:O	1:A:161:ILE:HG12	2.11	0.50
5:A:2009:OLC:H2A	6:A:2017:OLA:H81	1.93	0.50
1:A:140:MET:HE3	1:A:242:HIS:ND1	2.27	0.49
1:A:208:VAL:HG11	5:A:2014:OLC:H16A	1.93	0.49
1:A:1037:ALA:HB2	1:A:1065:PHE:HE2	1.78	0.48
1:A:167:MET:O	1:A:171:ILE:HG23	2.14	0.47
1:A:41:PHE:CZ	1:A:288:VAL:HG13	2.50	0.47
1:A:271:LEU:HD11	2:A:2001:KO5:O5	2.15	0.46
1:A:163:TRP:CE2	6:A:2022:OLA:H81	2.50	0.46
1:A:266:LEU:HD12	1:A:290:THR:HG21	1.98	0.46
1:A:52:GLY:HA3	1:A:88:ILE:HD13	1.98	0.45
1:A:221:TYR:OH	5:A:2013:OLC:H10	2.17	0.45
1:A:160:GLY:O	1:A:164:ILE:HG12	2.16	0.45
1:A:1065:PHE:CE1	1:A:1094:LEU:HD22	2.53	0.44
1:A:182:GLY:C	1:A:184:VAL:H	2.25	0.44
1:A:1038:LEU:HD23	1:A:1038:LEU:HA	1.79	0.42
1:A:1065:PHE:CD1	1:A:1094:LEU:HD22	2.54	0.42
1:A:191:ASN:OD1	1:A:194:LYS:HG2	2.20	0.42
1:A:195:ILE:HG23	1:A:196:ALA:N	2.35	0.42
6:A:2022:OLA:H152	6:A:2022:OLA:H182	1.78	0.42
1:A:210:CYS:C	1:A:213:PRO:HD2	2.44	0.42
1:A:212:LEU:HB3	1:A:213:PRO:HD3	2.02	0.41
1:A:110:ALA:O	1:A:114:MET:HG2	2.21	0.40
1:A:190:LEU:HD21	1:A:195:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	351/405 (87%)	347 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/356 (76%)	271 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	1011	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 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	OLC	A	2008	-	7,7,24	0.45	0	6,6,25	0.82	0
6	OLA	A	2019	-	8,8,19	0.35	0	7,7,19	0.64	0
5	OLC	A	2007	-	7,7,24	0.42	0	6,6,25	0.73	0
5	OLC	A	2011	-	9,9,24	0.37	0	8,8,25	0.61	0
5	OLC	A	2012	-	16,16,24	0.98	2 (12%)	17,17,25	1.08	1 (5%)
5	OLC	A	2010	-	5,5,24	0.32	0	4,4,25	0.62	0
2	KO5	A	2001	-	44,44,44	0.70	1 (2%)	53,60,60	0.77	1 (1%)
6	OLA	A	2017	-	15,15,19	0.55	0	15,15,19	0.83	0
5	OLC	A	2013	-	7,7,24	0.44	0	6,6,25	0.94	0
6	OLA	A	2018	-	16,16,19	0.54	0	16,16,19	0.89	1 (6%)
3	CLR	A	2002	-	31,31,31	0.67	1 (3%)	48,48,48	1.11	4 (8%)
6	OLA	A	2021	-	18,18,19	0.50	0	18,18,19	0.99	1 (5%)
6	OLA	A	2022	-	19,19,19	0.48	0	19,19,19	0.85	0
6	OLA	A	2020	-	19,19,19	0.49	0	19,19,19	0.88	1 (5%)
6	OLA	A	2023	-	12,12,19	0.63	0	12,12,19	1.00	0
5	OLC	A	2015	-	9,9,24	1.24	2 (22%)	10,10,25	1.22	1 (10%)
5	OLC	A	2016	-	13,13,24	0.33	0	12,12,25	0.74	0
5	OLC	A	2006	-	16,16,24	0.98	2 (12%)	17,17,25	1.07	1 (5%)
5	OLC	A	2004	-	12,12,24	1.12	2 (16%)	13,13,25	1.16	1 (7%)
4	1PE	A	2003	-	12,12,15	0.48	0	11,11,14	0.37	0
5	OLC	A	2014	-	10,10,24	0.39	0	9,9,25	0.90	0
5	OLC	A	2005	-	13,13,24	1.06	2 (15%)	14,14,25	1.07	1 (7%)
5	OLC	A	2009	-	21,21,24	0.86	2 (9%)	22,22,25	0.97	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	2008	-	-	2/5/5/24	-
6	OLA	A	2019	-	-	2/6/6/17	-
5	OLC	A	2007	-	-	3/5/5/24	-
5	OLC	A	2011	-	-	3/7/7/24	-
5	OLC	A	2012	-	-	6/16/16/24	-
5	OLC	A	2010	-	-	0/3/3/24	-
2	KO5	A	2001	-	-	2/26/38/38	0/4/4/4
6	OLA	A	2017	-	-	10/13/13/17	-
5	OLC	A	2013	-	-	0/5/5/24	-
6	OLA	A	2018	-	-	5/14/14/17	-
3	CLR	A	2002	-	-	6/10/68/68	0/4/4/4
6	OLA	A	2021	-	-	5/16/16/17	-
6	OLA	A	2022	-	-	9/17/17/17	-
6	OLA	A	2020	-	-	5/17/17/17	-
6	OLA	A	2023	-	-	2/10/10/17	-
5	OLC	A	2015	-	-	6/9/9/24	-
5	OLC	A	2016	-	-	3/11/11/24	-
5	OLC	A	2006	-	-	8/16/16/24	-
5	OLC	A	2004	-	-	1/12/12/24	-
4	1PE	A	2003	-	-	4/10/10/13	-
5	OLC	A	2014	-	-	4/8/8/24	-
5	OLC	A	2005	-	-	5/13/13/24	-
5	OLC	A	2009	-	-	5/21/21/24	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	KO5	O2-C2	-2.96	1.21	1.30
5	A	2004	OLC	O20-C1	2.50	1.40	1.33
5	A	2009	OLC	O20-C1	2.41	1.40	1.33
5	A	2006	OLC	O20-C1	2.40	1.40	1.33
5	A	2005	OLC	O20-C1	2.38	1.40	1.33
5	A	2015	OLC	O20-C1	2.37	1.40	1.33
5	A	2012	OLC	O20-C1	2.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2009	OLC	O20-C21	-2.17	1.40	1.45
5	A	2006	OLC	O20-C21	-2.17	1.40	1.45
5	A	2015	OLC	O20-C21	-2.16	1.40	1.45
5	A	2012	OLC	O20-C21	-2.16	1.40	1.45
5	A	2005	OLC	O20-C21	-2.12	1.40	1.45
5	A	2004	OLC	O20-C21	-2.09	1.40	1.45
3	A	2002	CLR	C10-C9	-2.03	1.52	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2015	OLC	O20-C1-C2	2.99	120.24	111.15
5	A	2004	OLC	O20-C1-C2	2.95	120.82	111.83
3	A	2002	CLR	C21-C20-C22	-2.81	105.98	110.34
2	A	2001	KO5	O2-C2-C1	2.72	119.78	112.71
5	A	2012	OLC	O20-C1-C2	2.72	120.11	111.83
5	A	2006	OLC	O20-C1-C2	2.71	120.11	111.83
5	A	2005	OLC	O20-C1-C2	2.70	120.08	111.83
3	A	2002	CLR	C21-C20-C17	2.64	116.85	112.88
5	A	2009	OLC	O20-C1-C2	2.64	119.89	111.83
6	A	2021	OLA	C3-C2-C1	-2.49	108.02	114.51
6	A	2020	OLA	C3-C2-C1	-2.39	108.28	114.51
3	A	2002	CLR	C4-C5-C10	2.36	119.45	116.42
3	A	2002	CLR	C11-C9-C10	-2.23	110.33	113.08
6	A	2018	OLA	C3-C2-C1	-2.10	109.02	114.51

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2005	OLC	C21-C22-C24-O25
5	A	2009	OLC	C21-C22-C24-O25
5	A	2011	OLC	C10-C11-C12-C13
5	A	2015	OLC	C21-C22-C24-O25
5	A	2015	OLC	O23-C22-C24-O25
5	A	2006	OLC	O19-C1-O20-C21
5	A	2006	OLC	C2-C1-O20-C21
4	A	2003	1PE	OH4-C13-C23-OH3
5	A	2012	OLC	C2-C1-O20-C21
5	A	2012	OLC	O19-C1-O20-C21
3	A	2002	CLR	C17-C20-C22-C23
6	A	2018	OLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	2002	CLR	C21-C20-C22-C23
3	A	2002	CLR	C22-C23-C24-C25
5	A	2015	OLC	O20-C21-C22-O23
6	A	2017	OLA	C1-C2-C3-C4
5	A	2014	OLC	C12-C13-C14-C15
5	A	2014	OLC	C14-C15-C16-C17
6	A	2020	OLA	C14-C15-C16-C17
5	A	2005	OLC	O23-C22-C24-O25
5	A	2009	OLC	O23-C22-C24-O25
5	A	2005	OLC	C1-C2-C3-C4
6	A	2022	OLA	C3-C4-C5-C6
6	A	2020	OLA	C11-C12-C13-C14
6	A	2017	OLA	C5-C6-C7-C8
6	A	2022	OLA	C2-C3-C4-C5
6	A	2017	OLA	C3-C4-C5-C6
5	A	2015	OLC	O20-C21-C22-C24
6	A	2018	OLA	C2-C3-C4-C5
5	A	2014	OLC	C13-C14-C15-C16
6	A	2020	OLA	C1-C2-C3-C4
6	A	2017	OLA	C2-C3-C4-C5
6	A	2018	OLA	C3-C4-C5-C6
6	A	2021	OLA	C1-C2-C3-C4
5	A	2011	OLC	C6-C7-C8-C9
5	A	2014	OLC	C10-C11-C12-C13
5	A	2006	OLC	C5-C6-C7-C8
5	A	2007	OLC	C10-C11-C12-C13
5	A	2006	OLC	C2-C3-C4-C5
3	A	2002	CLR	C20-C22-C23-C24
6	A	2017	OLA	C6-C7-C8-C9
6	A	2017	OLA	C4-C5-C6-C7
6	A	2021	OLA	C4-C5-C6-C7
6	A	2017	OLA	C11-C12-C13-C14
5	A	2009	OLC	C12-C13-C14-C15
6	A	2019	OLA	C3-C4-C5-C6
6	A	2022	OLA	C4-C5-C6-C7
5	A	2005	OLC	C3-C4-C5-C6
5	A	2008	OLC	C11-C12-C13-C14
5	A	2007	OLC	C11-C12-C13-C14
5	A	2006	OLC	C3-C4-C5-C6
6	A	2022	OLA	C12-C13-C14-C15
3	A	2002	CLR	C16-C17-C20-C22
5	A	2011	OLC	C5-C6-C7-C8

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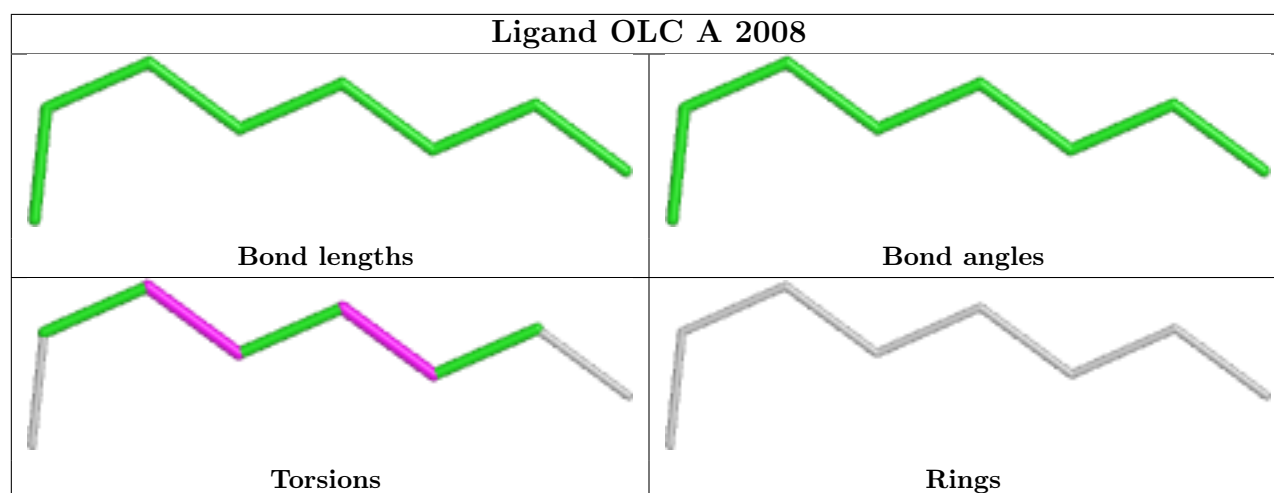
Mol	Chain	Res	Type	Atoms
5	A	2006	OLC	C4-C5-C6-C7
4	A	2003	1PE	C14-C24-OH4-C13
5	A	2015	OLC	C2-C1-O20-C21
5	A	2012	OLC	O23-C22-C24-O25
4	A	2003	1PE	C24-C14-OH5-C25
6	A	2019	OLA	C2-C3-C4-C5
5	A	2015	OLC	O19-C1-O20-C21
5	A	2016	OLC	C6-C7-C8-C9
4	A	2003	1PE	OH5-C14-C24-OH4
6	A	2023	OLA	C6-C7-C8-C9
5	A	2012	OLC	C7-C8-C9-C10
5	A	2012	OLC	C21-C22-C24-O25
6	A	2018	OLA	C12-C13-C14-C15
6	A	2021	OLA	C7-C8-C9-C10
6	A	2017	OLA	O1-C1-C2-C3
6	A	2020	OLA	C12-C13-C14-C15
5	A	2005	OLC	C4-C5-C6-C7
2	A	2001	KO5	C5-C6-C7-O3
6	A	2017	OLA	O2-C1-C2-C3
6	A	2022	OLA	C6-C7-C8-C9
5	A	2012	OLC	C1-C2-C3-C4
6	A	2018	OLA	C9-C10-C11-C12
6	A	2021	OLA	O2-C1-C2-C3
6	A	2020	OLA	C7-C8-C9-C10
6	A	2022	OLA	C9-C10-C11-C12
5	A	2004	OLC	C3-C4-C5-C6
5	A	2007	OLC	C9-C10-C11-C12
5	A	2008	OLC	C9-C10-C11-C12
6	A	2022	OLA	C5-C6-C7-C8
6	A	2021	OLA	O1-C1-C2-C3
5	A	2006	OLC	O20-C1-C2-C3
2	A	2001	KO5	C5-C6-C7-O4
5	A	2009	OLC	C9-C10-C11-C12
5	A	2016	OLC	C9-C10-C11-C12
6	A	2023	OLA	C4-C5-C6-C7
6	A	2022	OLA	C15-C16-C17-C18
6	A	2022	OLA	C13-C14-C15-C16
6	A	2017	OLA	C9-C10-C11-C12
5	A	2009	OLC	C2-C3-C4-C5
3	A	2002	CLR	C13-C17-C20-C21
5	A	2006	OLC	O19-C1-C2-C3
5	A	2016	OLC	C4-C5-C6-C7

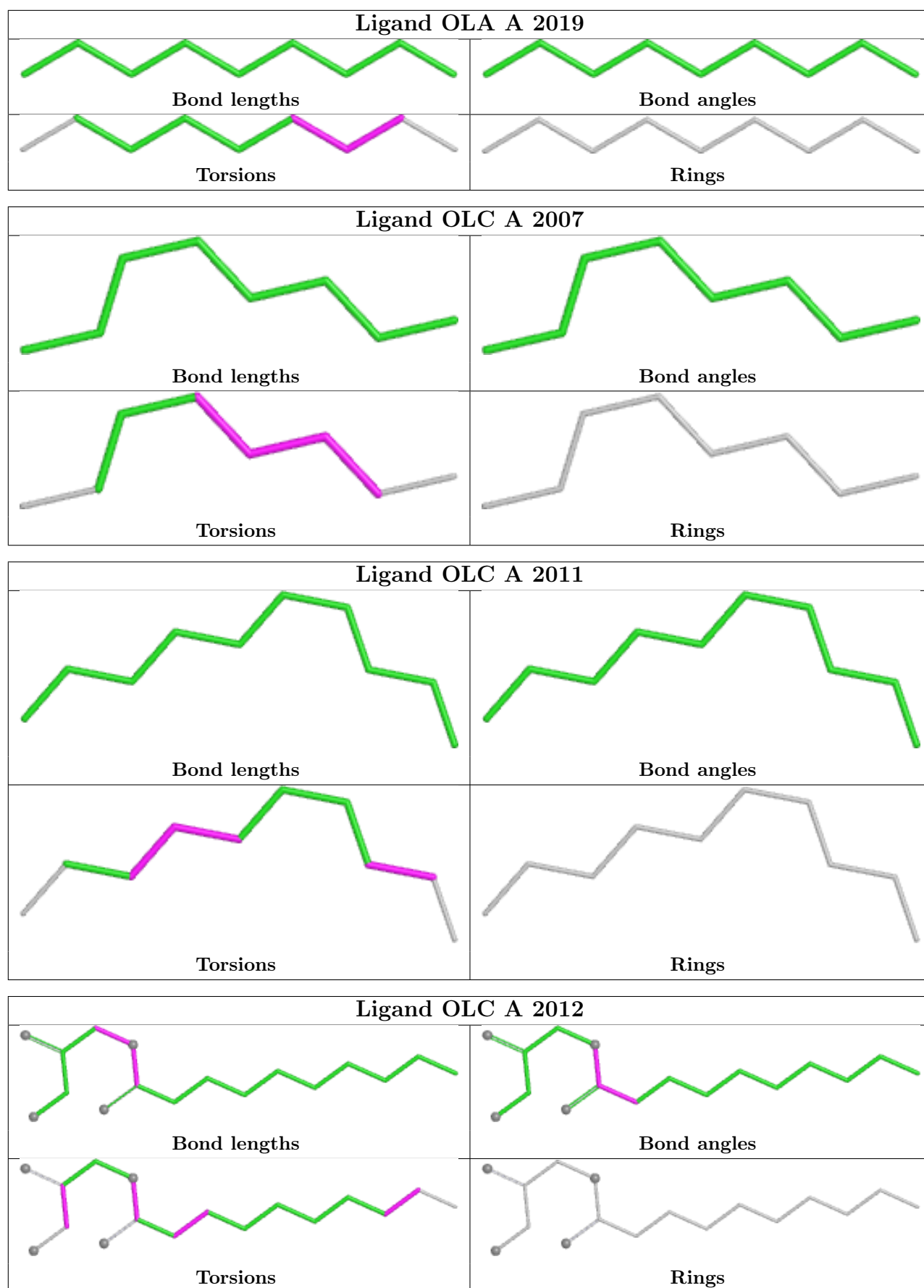
There are no ring outliers.

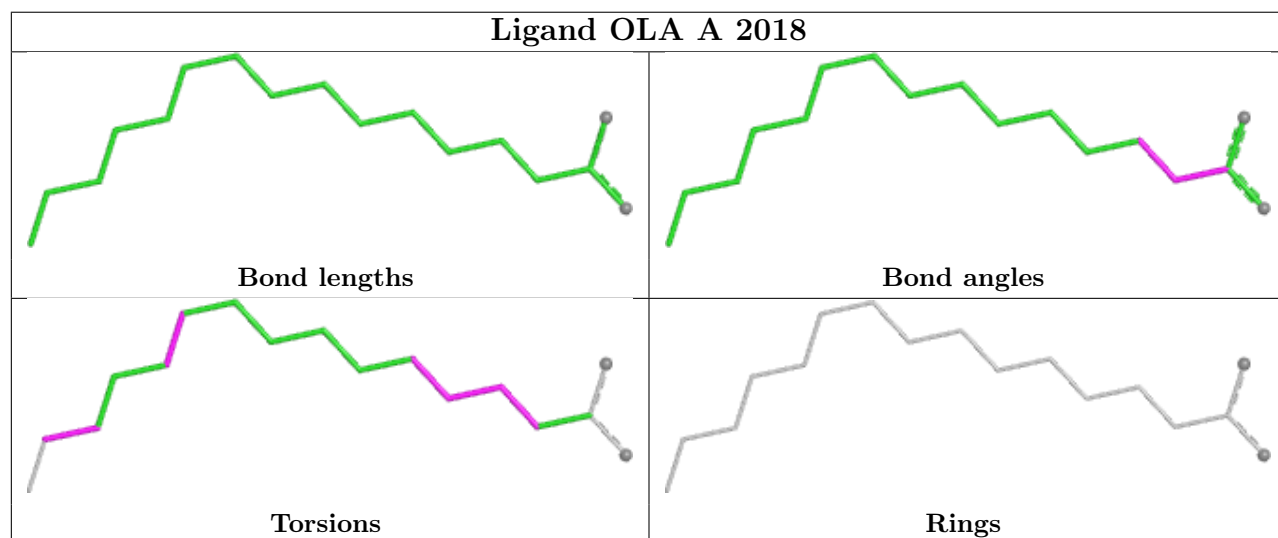
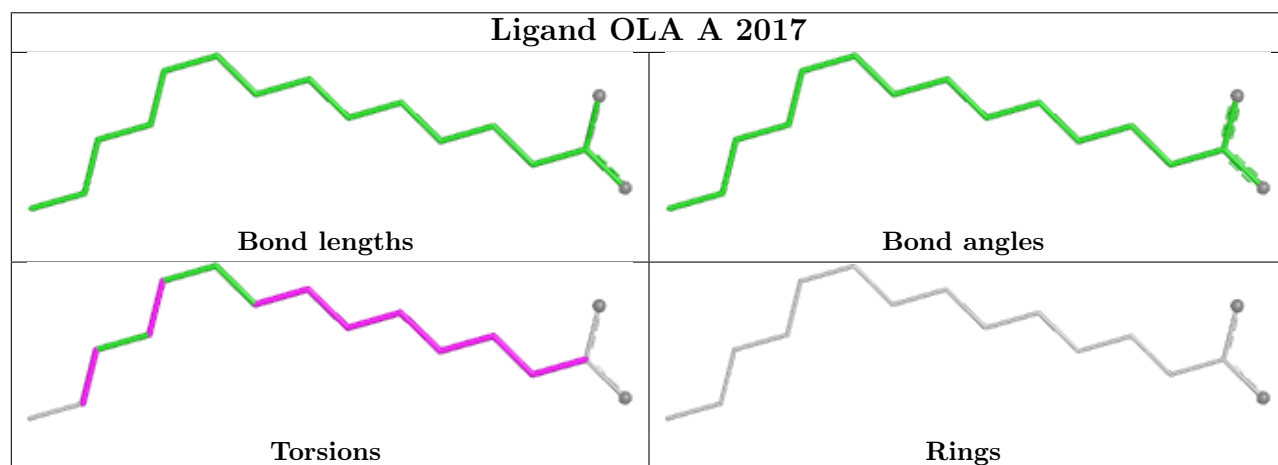
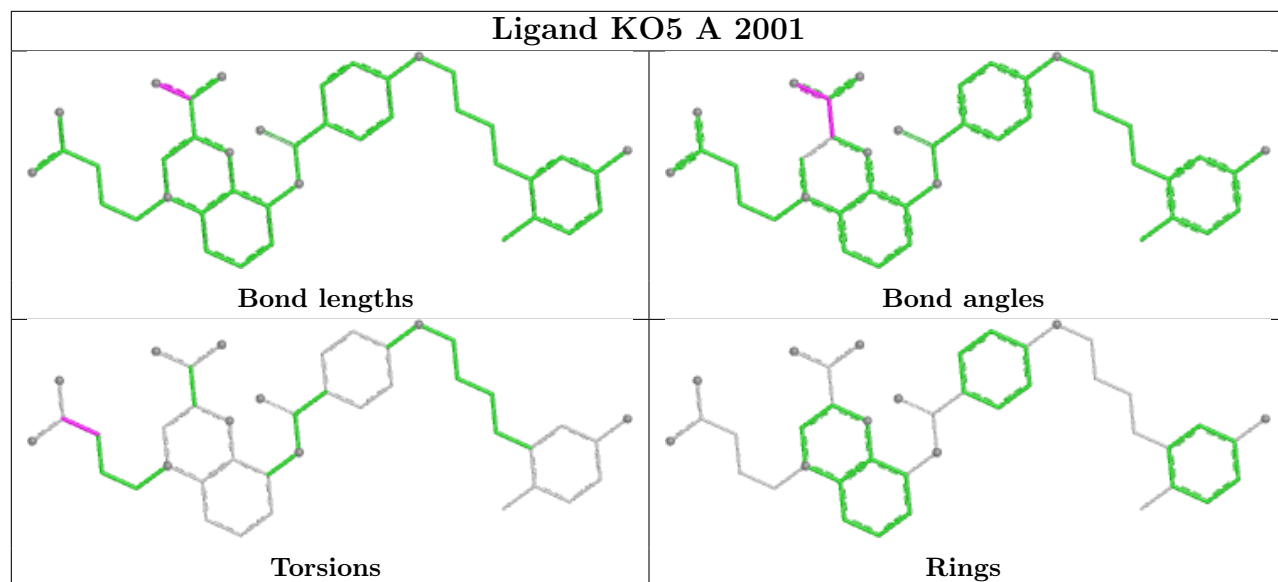
9 monomers are involved in 11 short contacts:

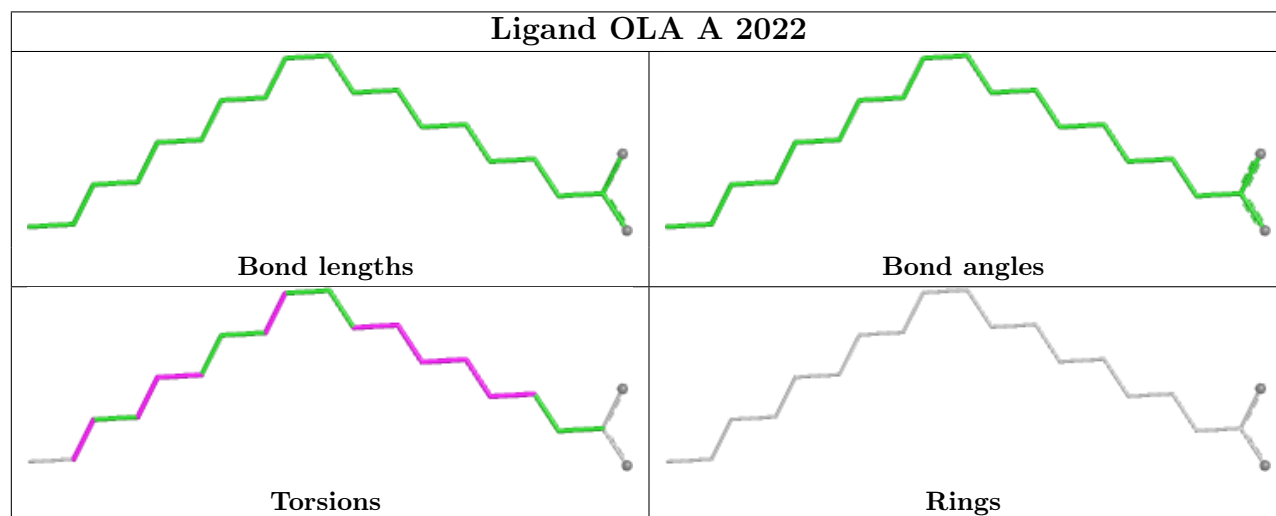
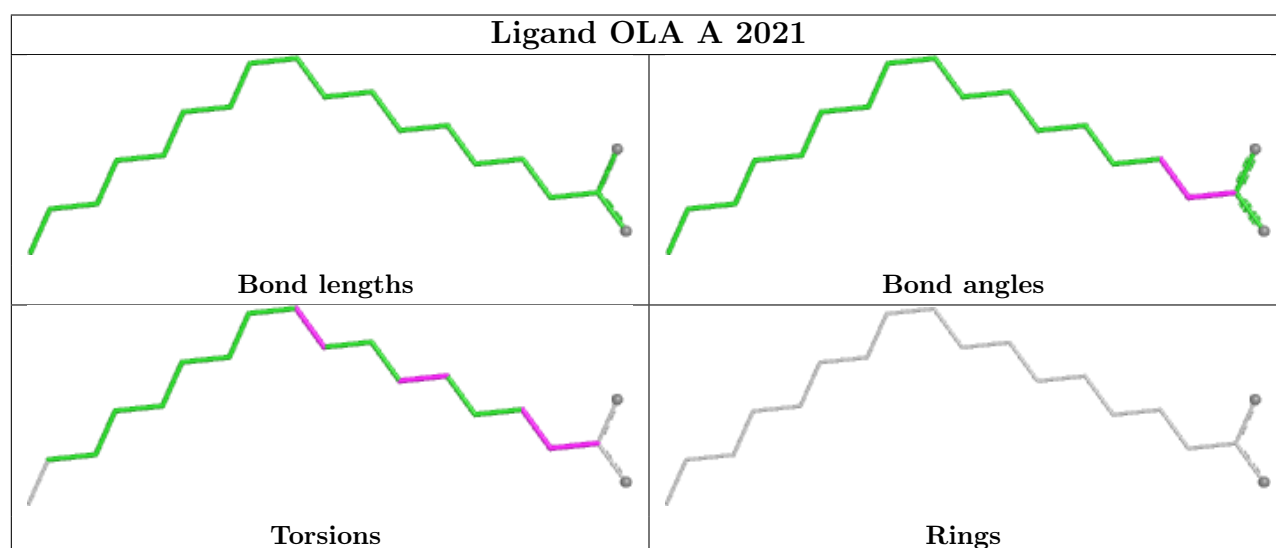
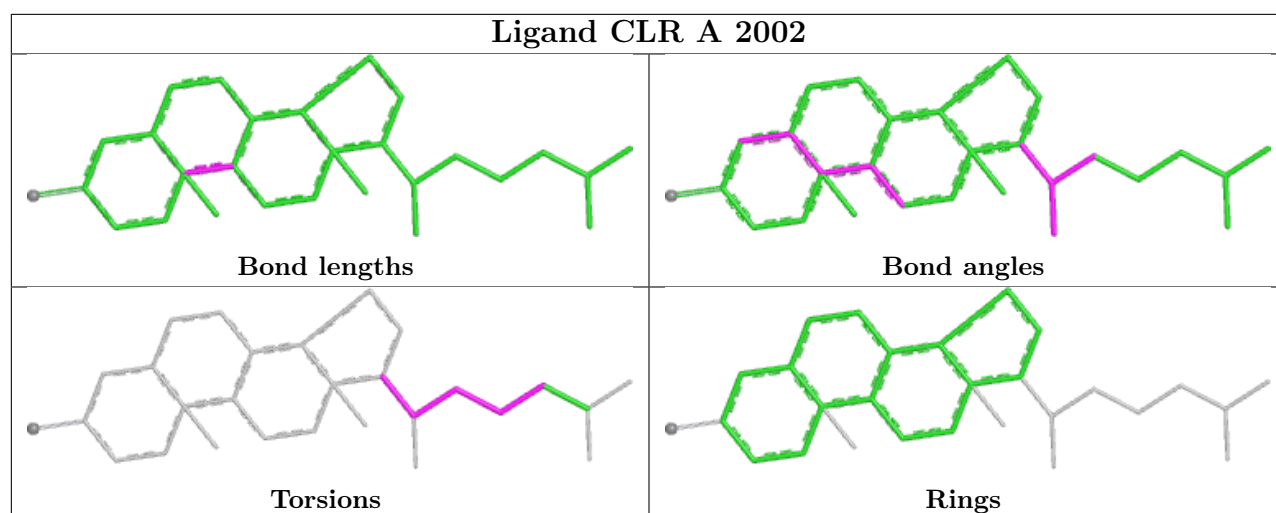
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2012	OLC	2	0
2	A	2001	KO5	2	0
6	A	2017	OLA	1	0
5	A	2013	OLC	1	0
6	A	2022	OLA	2	0
6	A	2023	OLA	2	0
4	A	2003	1PE	1	0
5	A	2014	OLC	3	0
5	A	2009	OLC	1	0

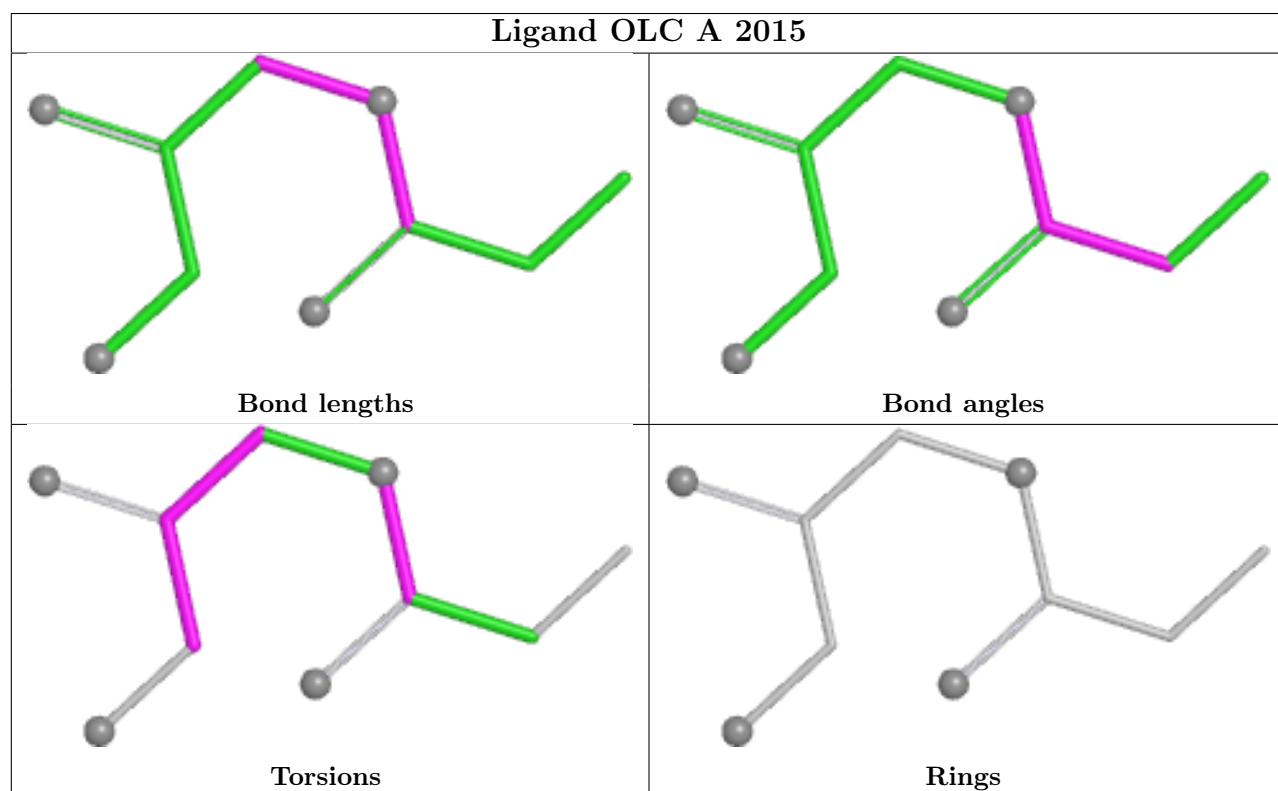
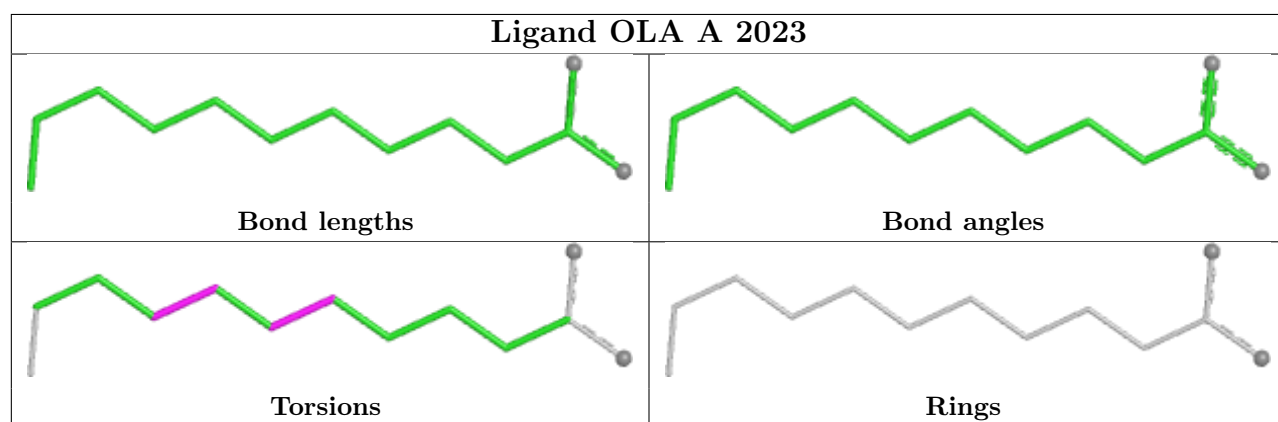
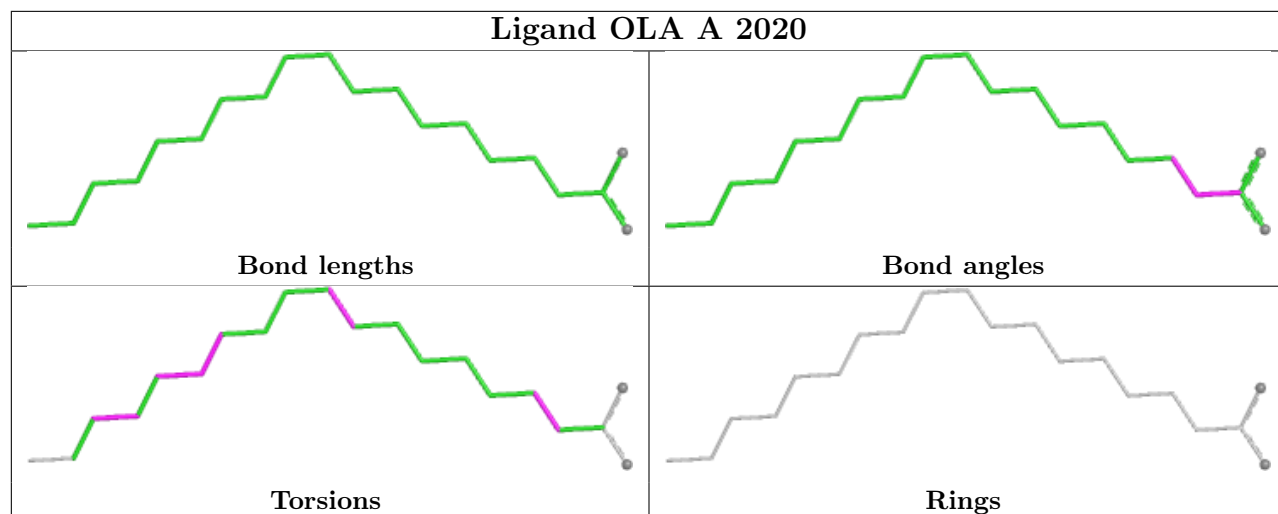
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

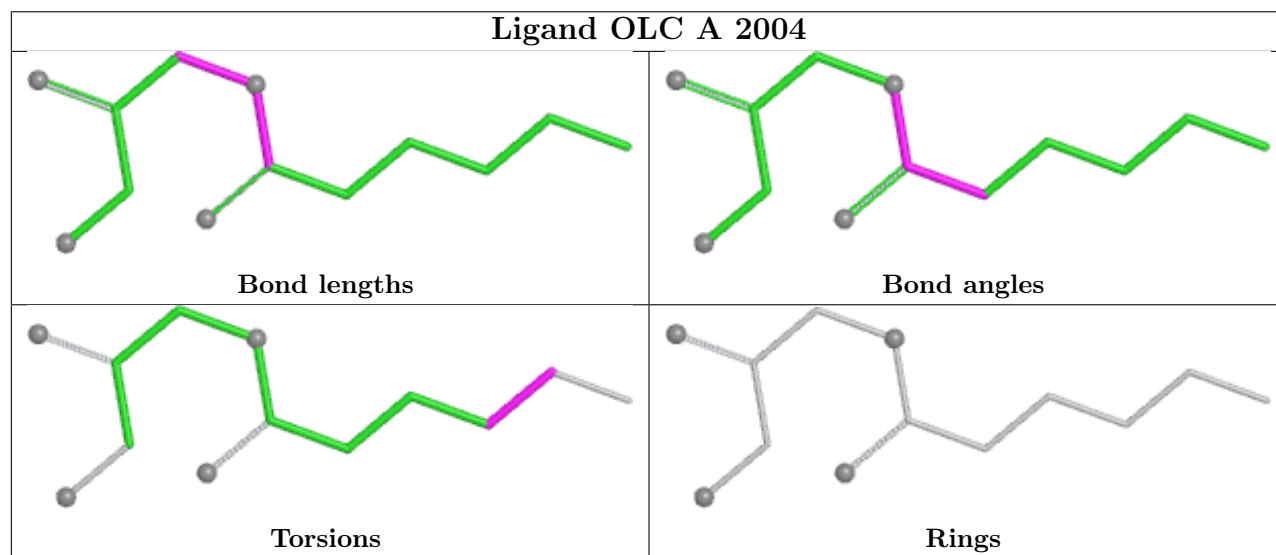
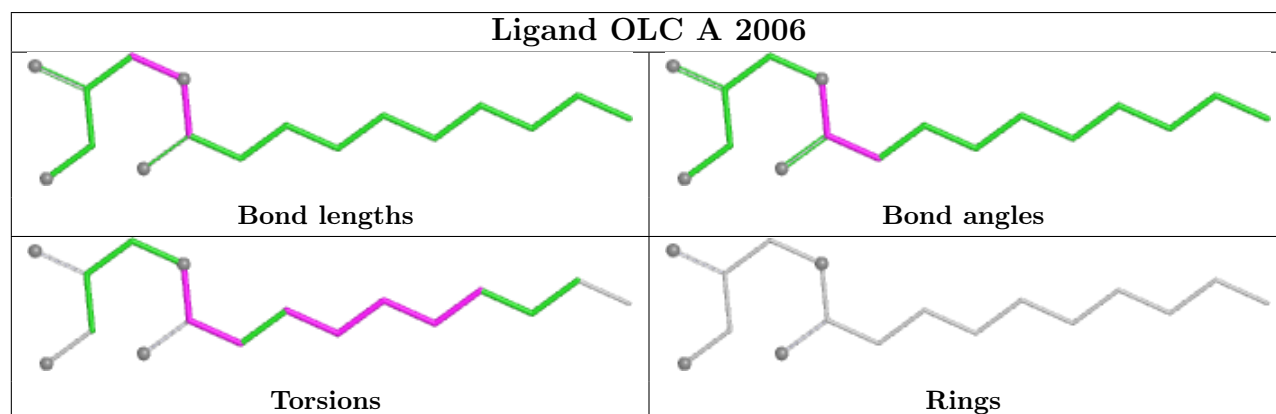
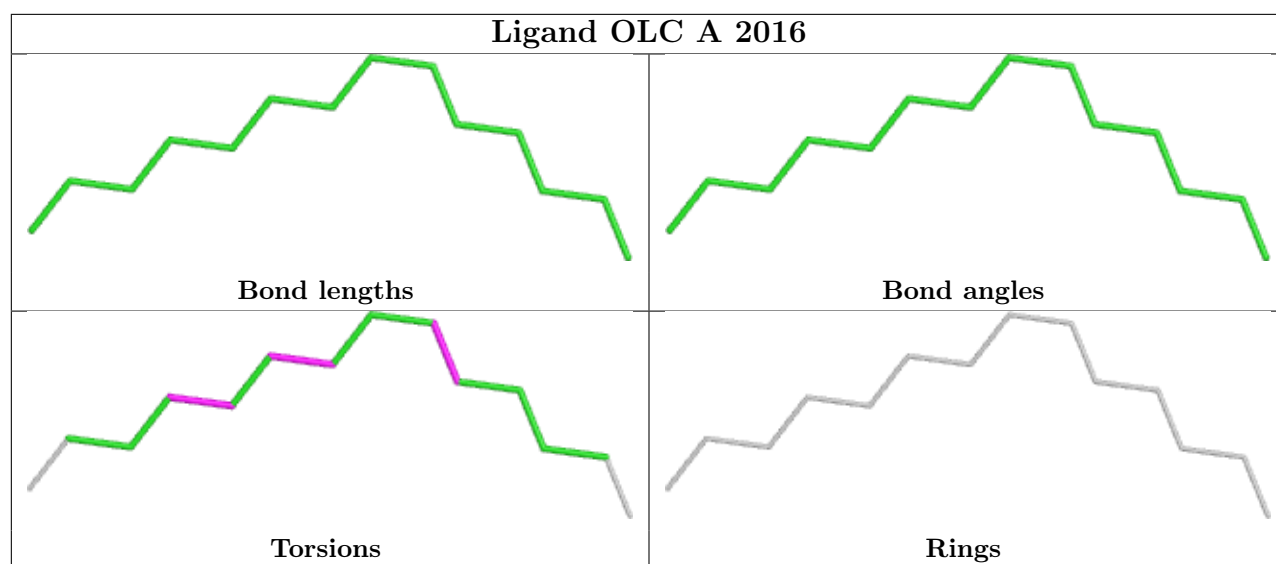


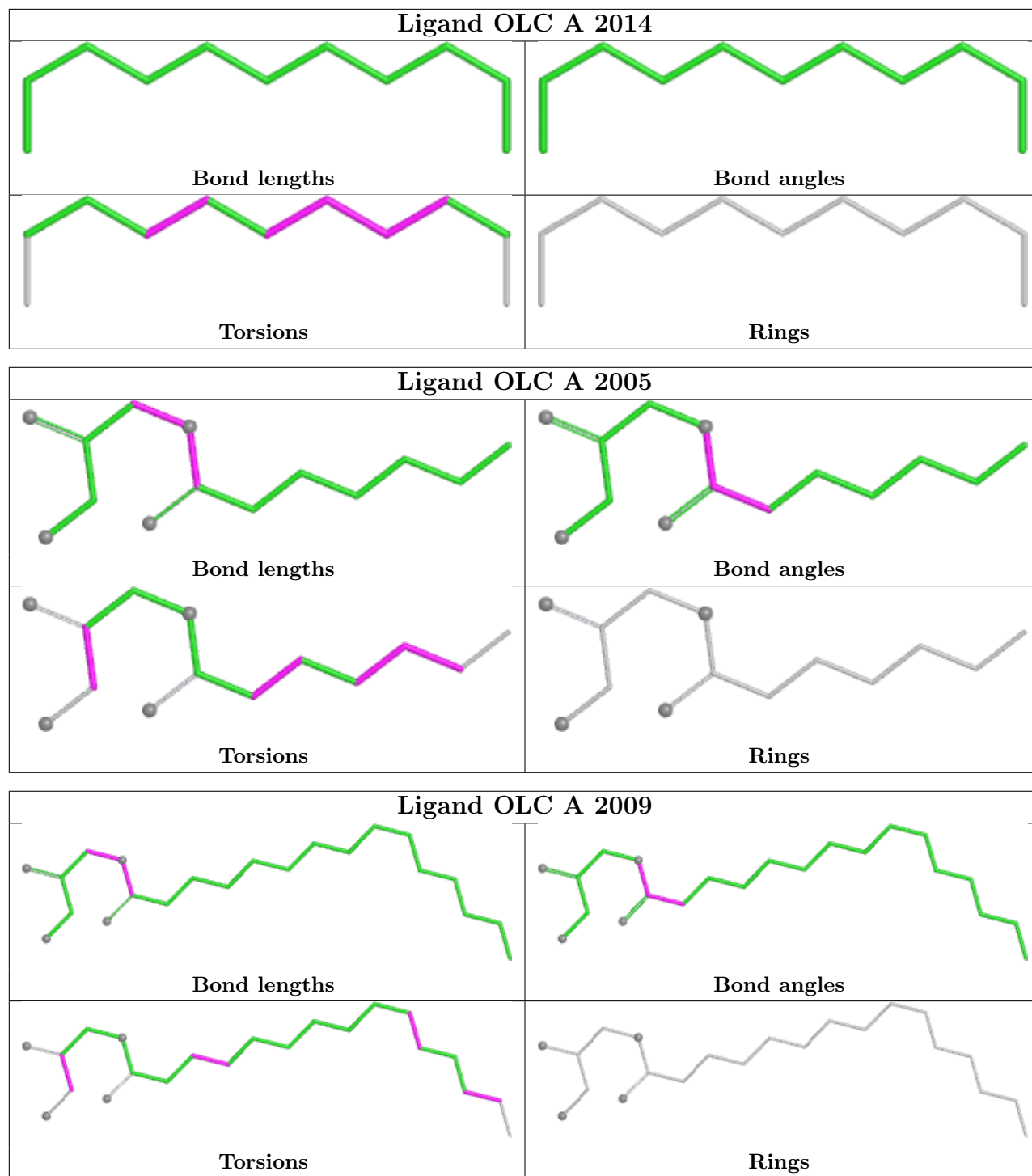












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	363/405 (89%)	0.55	25 (6%)	23 22	48, 74, 162, 200	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1041	GLN	3.7
1	A	1065	PHE	3.4
1	A	179	GLU	3.2
1	A	176	SER	3.1
1	A	1030	LEU	3.0
1	A	1073	ASP	2.8
1	A	1038	LEU	2.7
1	A	277	GLY	2.7
1	A	258	LEU	2.7
1	A	1058	MET	2.6
1	A	1076	LEU	2.6
1	A	191	ASN	2.4
1	A	1069	VAL	2.4
1	A	58	LEU	2.3
1	A	174	LEU	2.3
1	A	1101	TYR	2.3
1	A	304	LEU	2.3
1	A	1078	LEU	2.2
1	A	1023	ALA	2.2
1	A	1026	VAL	2.2
1	A	172	MET	2.1
1	A	300	PHE	2.1
1	A	108	ASP	2.0
1	A	72	SER	2.0
1	A	152	ILE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

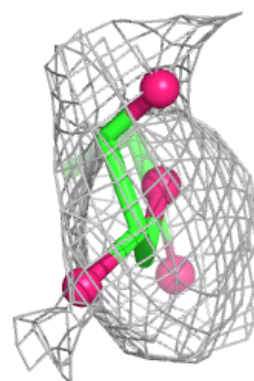
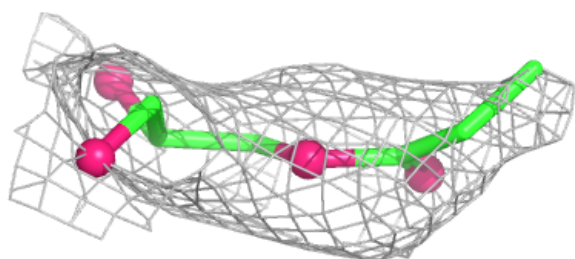
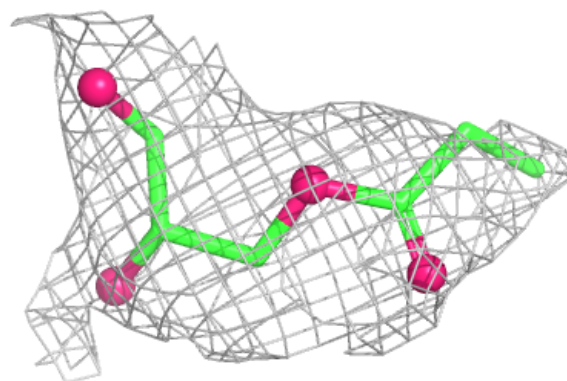
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	1PE	A	2003	13/16	0.78	0.21	96,114,133,134	0
5	OLC	A	2015	10/25	0.79	0.14	94,102,119,126	0
5	OLC	A	2012	17/25	0.80	0.15	80,90,120,121	0
5	OLC	A	2010	6/25	0.80	0.19	79,83,84,89	0
6	OLA	A	2018	17/20	0.80	0.14	82,99,122,123	0
6	OLA	A	2023	13/20	0.81	0.13	87,102,116,116	0
6	OLA	A	2019	9/20	0.83	0.16	77,87,115,120	0
5	OLC	A	2014	11/25	0.83	0.27	63,83,119,123	0
6	OLA	A	2022	20/20	0.84	0.17	56,97,106,117	0
6	OLA	A	2021	19/20	0.84	0.14	82,103,131,138	0
5	OLC	A	2006	17/25	0.86	0.15	76,99,140,140	0
5	OLC	A	2011	10/25	0.86	0.14	77,82,101,104	0
5	OLC	A	2009	22/25	0.87	0.12	70,97,115,131	0
5	OLC	A	2007	8/25	0.87	0.16	84,94,98,105	0
6	OLA	A	2017	16/20	0.87	0.16	70,94,123,123	0
5	OLC	A	2013	8/25	0.87	0.15	82,96,101,102	0
5	OLC	A	2004	13/25	0.88	0.13	60,90,116,123	0
5	OLC	A	2005	14/25	0.88	0.12	83,92,110,112	0
6	OLA	A	2020	20/20	0.88	0.20	57,93,106,112	0
5	OLC	A	2016	14/25	0.89	0.12	71,81,101,103	0
5	OLC	A	2008	8/25	0.89	0.13	81,90,97,98	0
3	CLR	A	2002	28/28	0.93	0.11	55,72,87,95	0
2	KO5	A	2001	41/41	0.94	0.13	69,79,106,113	0

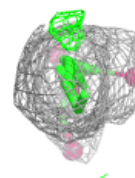
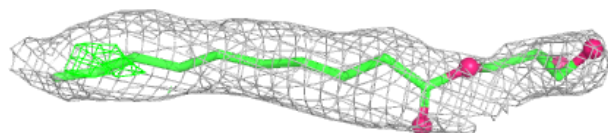
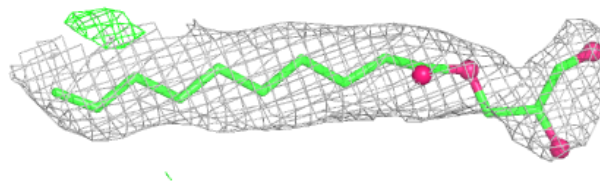
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 2015:

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

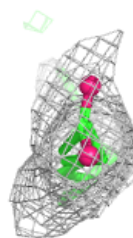
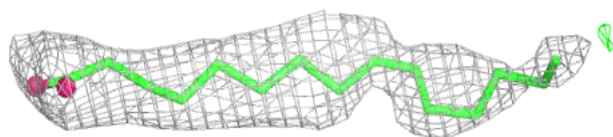
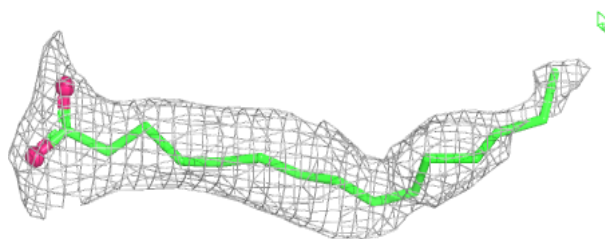
**Electron density around OLC A 2012:**

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

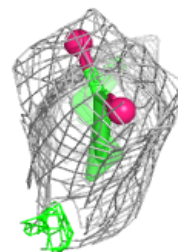
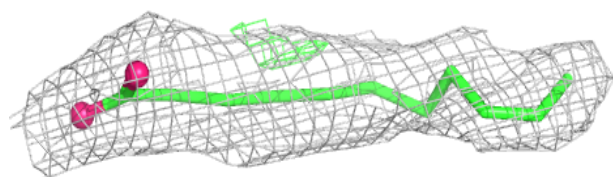
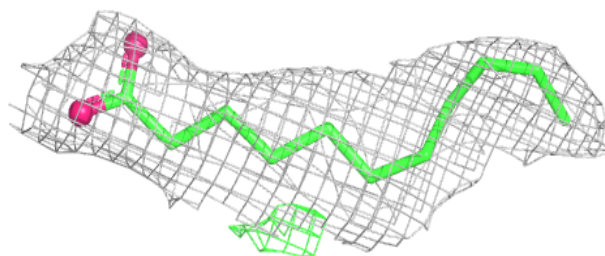


Electron density around OLA A 2018:

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

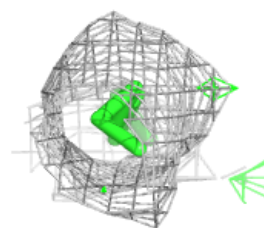
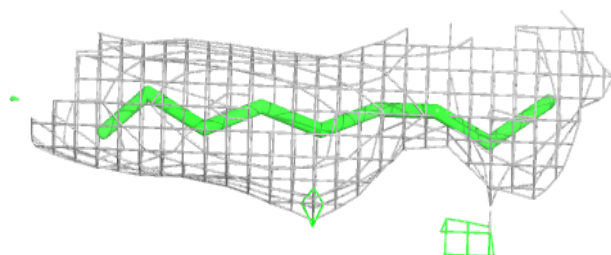
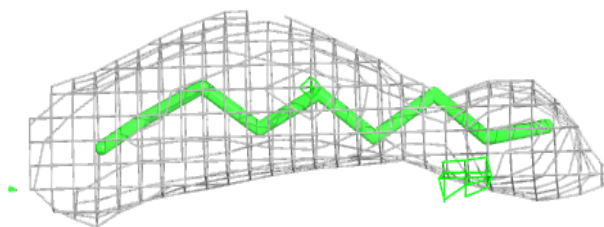
**Electron density around OLA A 2023:**

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

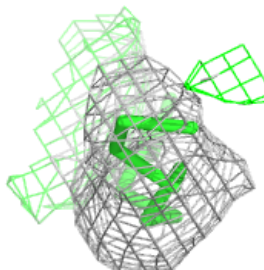
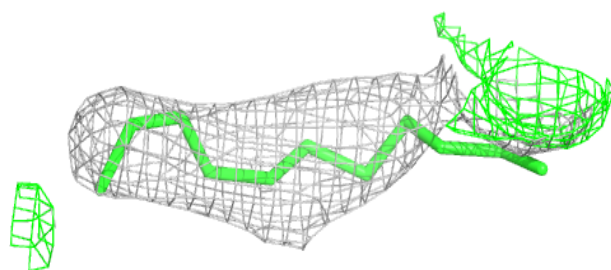
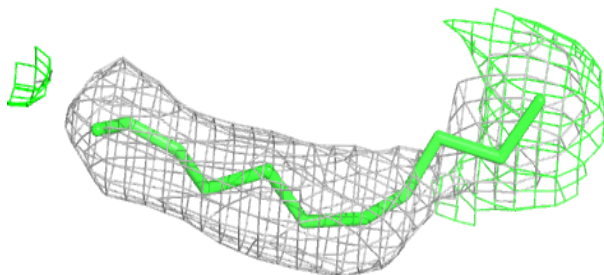


Electron density around OLA A 2019:

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

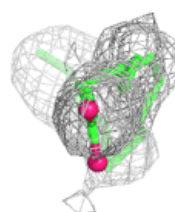
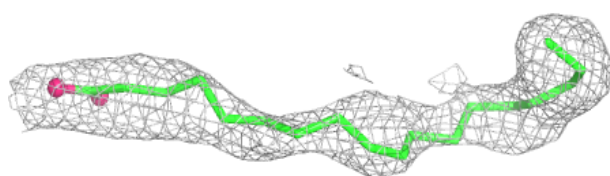
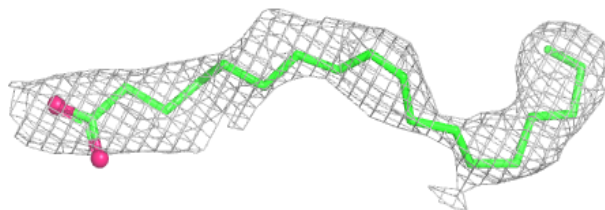
**Electron density around OLC A 2014:**

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

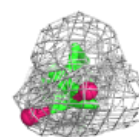
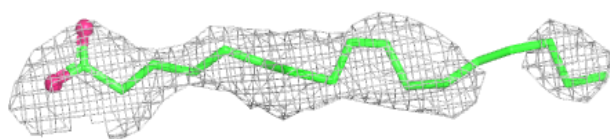
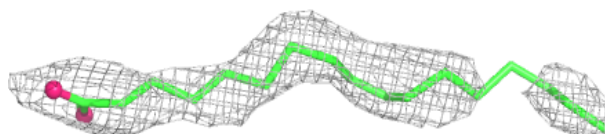


Electron density around OLA A 2022:

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

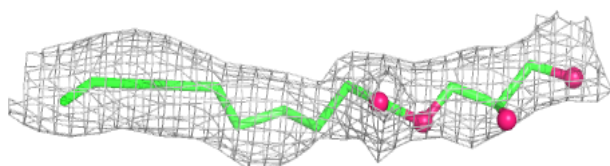
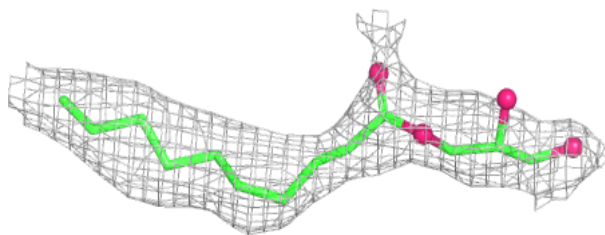
**Electron density around OLA A 2021:**

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

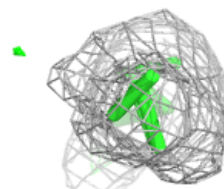
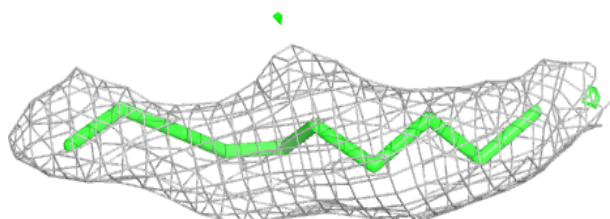
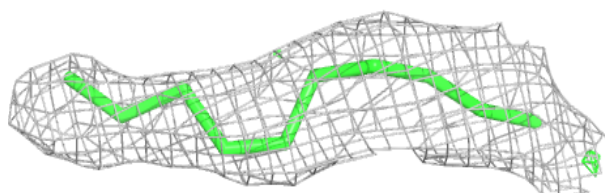


Electron density around OLC A 2006:

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

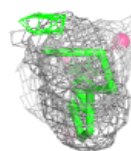
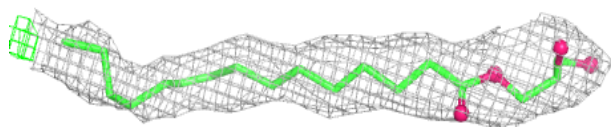
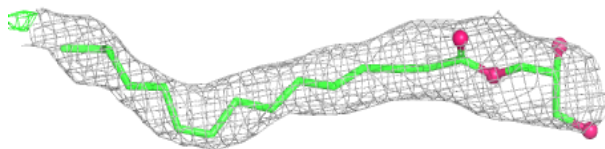
**Electron density around OLC A 2011:**

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

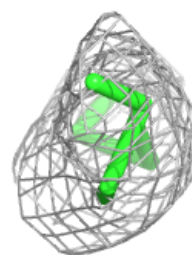
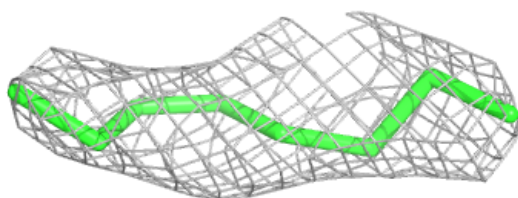
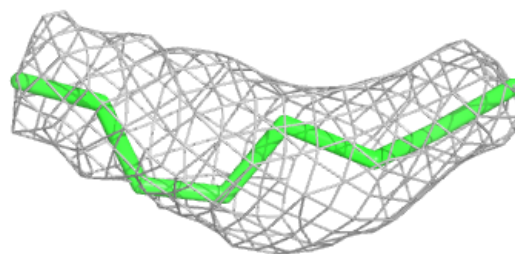


Electron density around OLC A 2009:

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

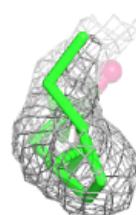
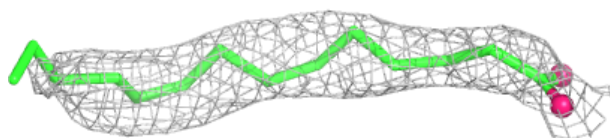
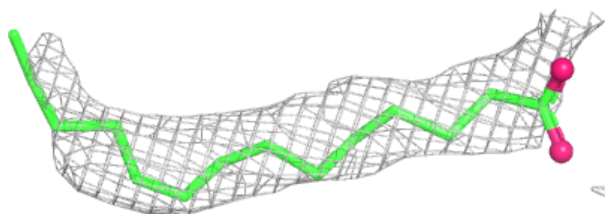
**Electron density around OLC A 2007:**

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

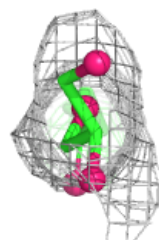
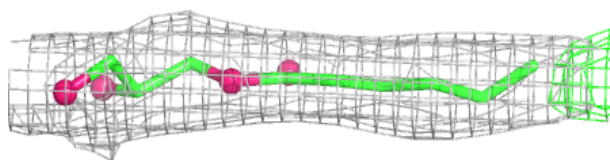
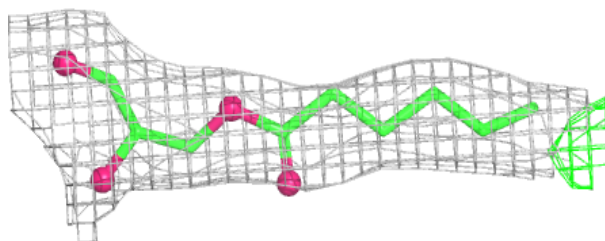


Electron density around OLA A 2017:

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

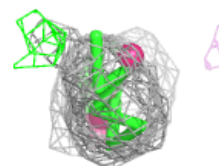
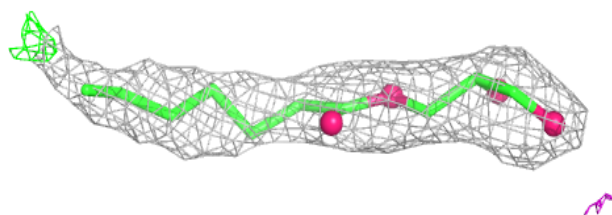
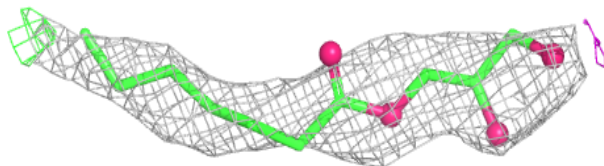
**Electron density around OLC A 2004:**

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

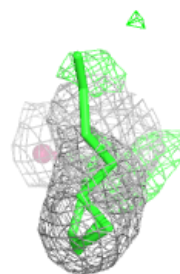
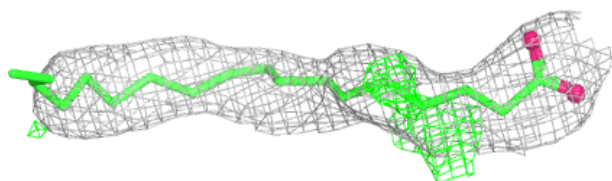
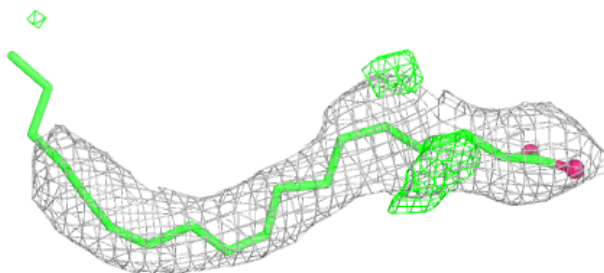


Electron density around OLC A 2005:

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

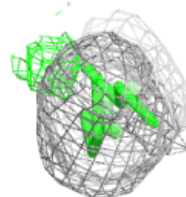
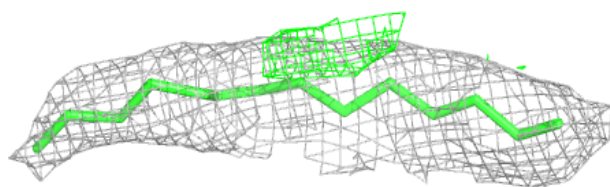
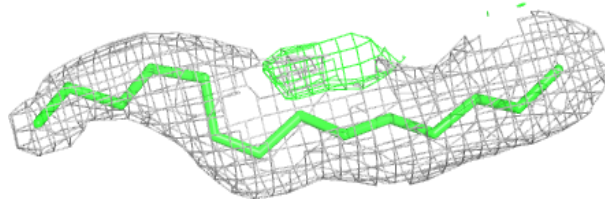
**Electron density around OLA A 2020:**

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

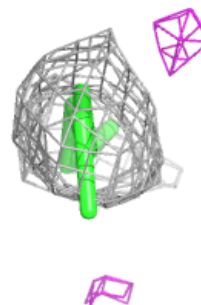
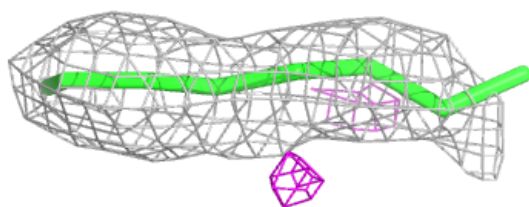
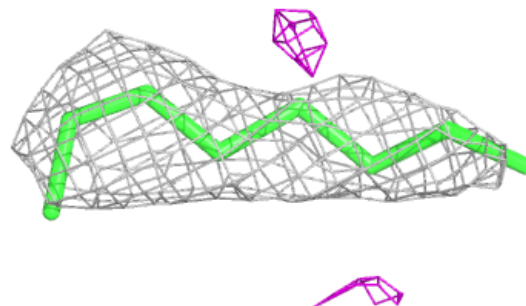


Electron density around OLC A 2016:

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

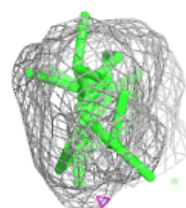
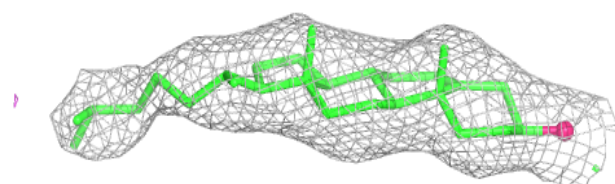
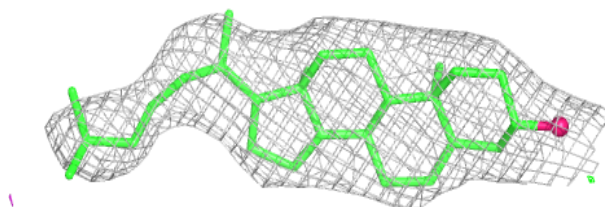
**Electron density around OLC A 2008:**

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

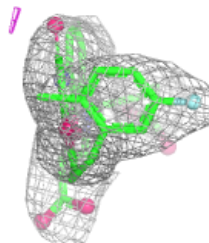
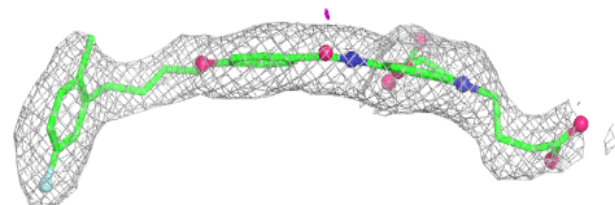
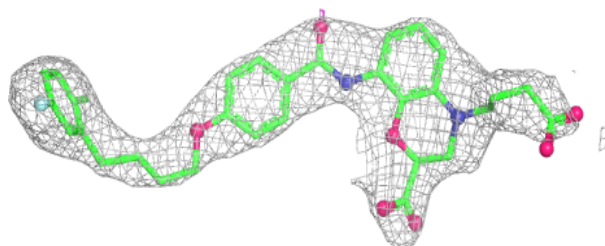


Electron density around CLR A 2002:

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

**Electron density around KO5 A 2001:**

$2mF_o-DF_c$ (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.