



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:01 PM UTC

PDB ID : 8CU7 / pdb_00008cu7
Title : Crystal structure of A2AAR-StaR2-bRIL in complex with a novel A2a antagonist, LJ-4517
Authors : Shiriaeva, A.; Park, D.-J.; Kim, G.; Lee, Y.; Hou, X.; Jarhad, D.B.; Kim, G.; Yu, J.; Hyun, Y.E.; Kim, W.; Gao, Z.-G.; Jacobson, K.A.; Han, G.W.; Stevens, R.C.; Jeong, L.S.; Choi, S.; Cherezov, V.
Deposited on : 2022-05-16
Resolution : 2.05 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (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
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

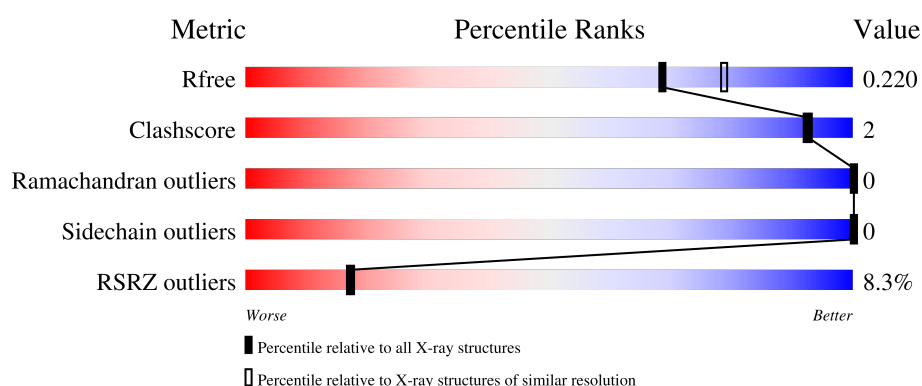
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	7% 87% 11%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3919 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3116	2028	523	542	23	0	8	0

There are 48 discrepancies between the modelled and reference sequences:

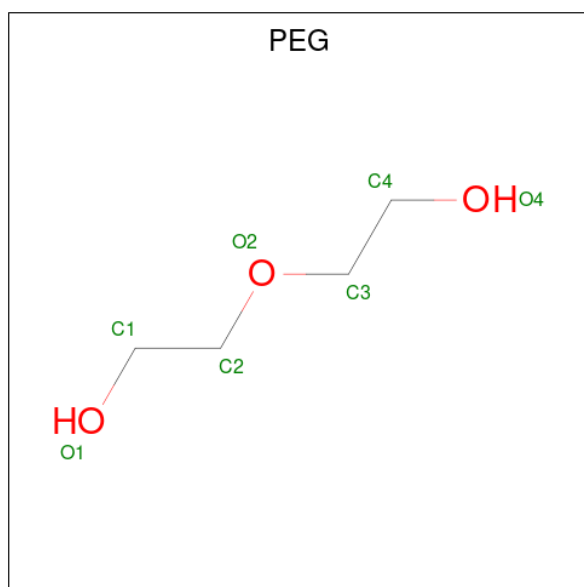
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	54	LEU	ALA	engineered mutation	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	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 DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



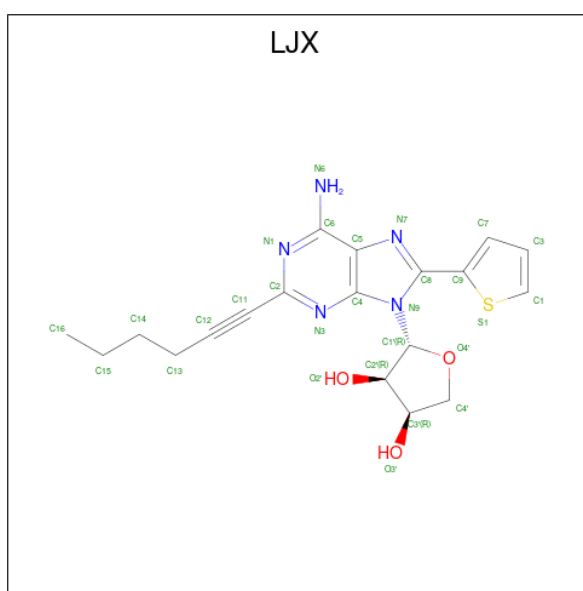
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 3 is (2R,3R,4R)-2-[(8P)-6-amino-2-(hex-1-yn-1-yl)-8-(thiophen-2-yl)-9H-purin-9-yl]oxolane-3,4-diol (CCD ID: LJX) (formula: C₁₉H₂₁N₅O₃S) (labeled as "Ligand of Interest" by depositor).

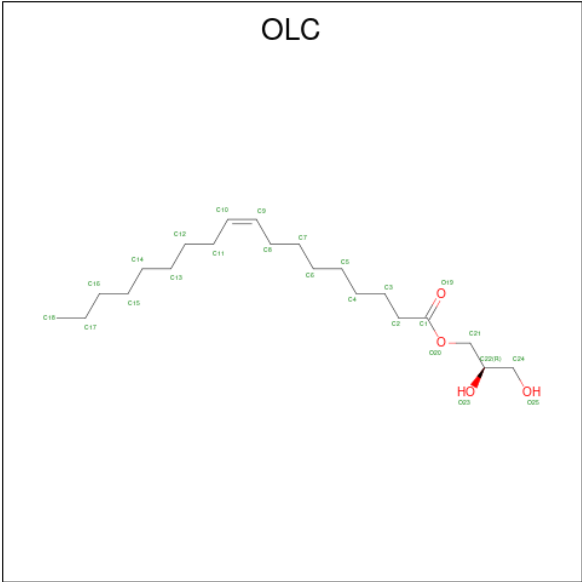


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	5	3	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

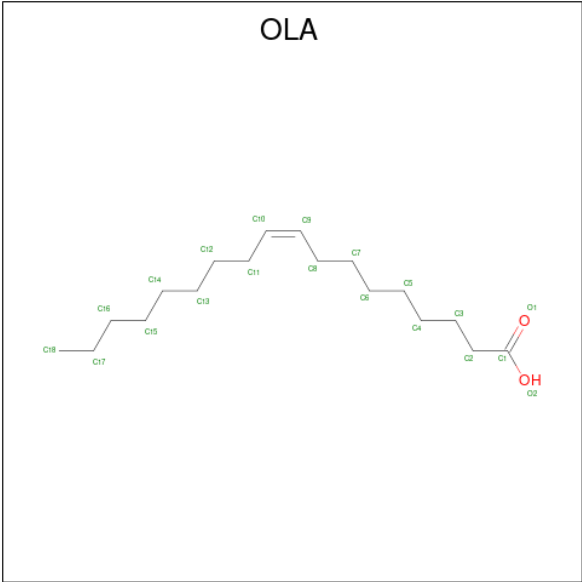
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- 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
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			15	11	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 6 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



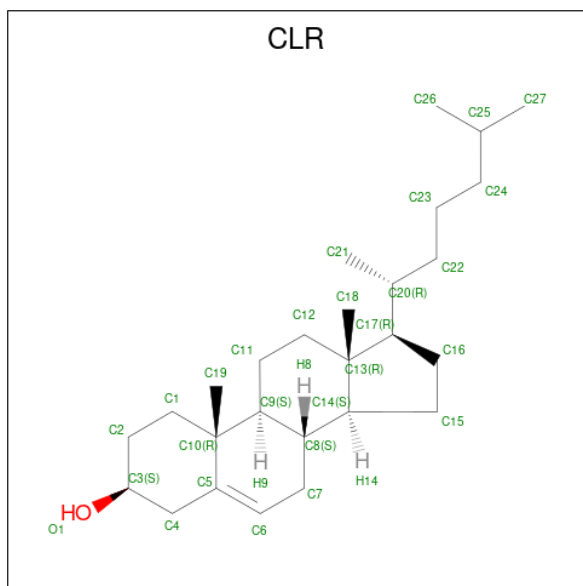
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			18	16	2		
6	A	1	Total	C	O	0	0
			20	18	2		
6	A	1	Total	C	O	0	0
			20	18	2		
6	A	1	Total	C	O	0	0
			20	18	2		
6	A	1	Total	C		0	0
			14	14			
6	A	1	Total	C	O	0	0
			9	7	2		
6	A	1	Total	C	O	0	0
			17	15	2		
6	A	1	Total	C	O	0	0
			12	10	2		
6	A	1	Total	C	O	0	0
			15	13	2		
6	A	1	Total	C	O	0	0
			11	9	2		
6	A	1	Total	C		0	0
			11	11			
6	A	1	Total	C		0	0
			12	12			
6	A	1	Total	C	O	0	0
			15	13	2		
6	A	1	Total	C	O	0	0
			19	17	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 15 13 2	0	0
6	A	1	Total C 11 11	0	0
6	A	1	Total C 10 10	0	0
6	A	1	Total C 13 13	0	0
6	A	1	Total C O 9 7 2	0	0
6	A	1	Total C O 7 5 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
6	A	1	Total C O 18 16 2	0	0

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



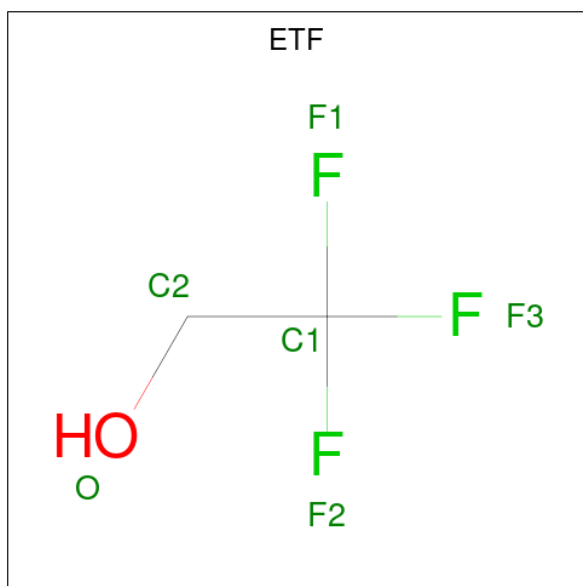
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 28 27 1	0	0
7	A	1	Total C O 28 27 1	0	0

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

- Molecule 8 is TRIFLUOROETHANOL (CCD ID: ETF) (formula: $C_2H_3F_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	F	O	0	0
			6	2	3	1		

- Molecule 9 is water.

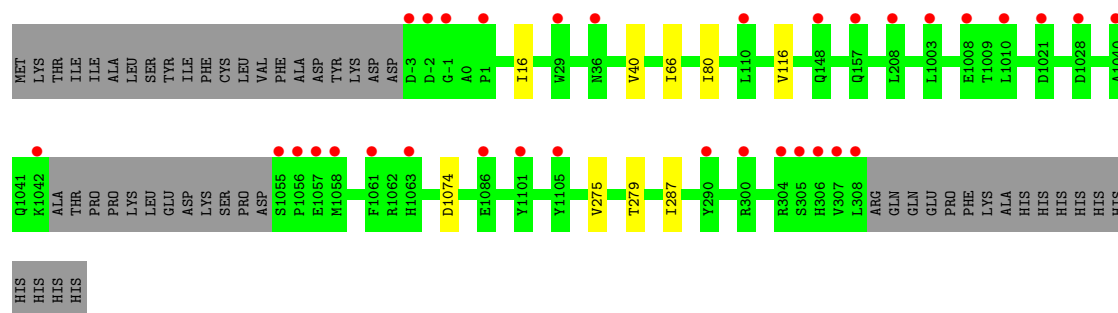
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	177	Total	O	0	0
			177	177		

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

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	39.46Å 179.58Å 140.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.89 – 2.05 44.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	87.3 (44.89-2.05) 87.7 (44.89-2.05)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.177 , 0.211 0.184 , 0.220	Depositor DCC
R_{free} test set	1445 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3919	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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: OLA, OLC, NA, CLR, LJX, PEG, ETF

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	0.09	0/3182	0.22	0/4331

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	3116	0	3173	9	0
2	A	28	0	40	0	0
3	A	28	0	0	0	0
4	A	1	0	0	0	0
5	A	150	0	228	2	0
6	A	329	0	476	4	0
7	A	84	0	138	1	0
8	A	6	0	3	0	0
9	A	177	0	0	2	0
All	All	3919	0	4058	12	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 2.

All (12) 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:279[A]:THR:HG21	5:A:1206:OLC:H16A	1.76	0.66
1:A:287:ILE:HD13	6:A:1207:OLA:H42	1.83	0.61
1:A:1074:ASP:OD1	9:A:1301:HOH:O	2.19	0.52
1:A:275[B]:VAL:O	1:A:279[B]:THR:HG23	2.12	0.50
1:A:66:ILE:HD11	1:A:80:ILE:HG13	1.97	0.47
1:A:16:ILE:HD11	1:A:275[A]:VAL:HG13	1.96	0.46
1:A:287:ILE:HD13	6:A:1207:OLA:C4	2.45	0.46
1:A:279[A]:THR:HG23	6:A:1207:OLA:H142	1.98	0.46
7:A:1211:CLR:H212	7:A:1211:CLR:H121	1.99	0.45
5:A:1239:OLC:O25	9:A:1302:HOH:O	2.20	0.44
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.50	0.42
6:A:1215:OLA:H10	6:A:1228:OLA:H72	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/447 (90%)	395 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/367 (89%)	327 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	1088	GLN
1	A	280	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 1 is monoatomic - leaving 39 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	CLR	A	1209	-	31,31,31	0.63	0	48,48,48	0.95	3 (6%)
5	OLC	A	1240	-	24,24,24	0.61	0	25,25,25	0.97	2 (8%)
6	OLA	A	1227	-	9,9,19	0.30	0	8,8,19	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLC	A	1238	-	24,24,24	0.62	0	25,25,25	0.95	1 (4%)
5	OLC	A	1204	-	24,24,24	0.61	0	25,25,25	0.94	1 (4%)
6	OLA	A	1208	-	19,19,19	0.58	0	19,19,19	0.85	1 (5%)
5	OLC	A	1223	-	9,9,24	0.95	0	10,10,25	1.18	0
5	OLC	A	1222	-	14,14,24	0.79	0	15,15,25	1.11	1 (6%)
6	OLA	A	1232	-	12,12,19	0.73	0	12,12,19	0.99	1 (8%)
2	PEG	A	1237	-	6,6,6	0.65	0	5,5,5	0.85	0
6	OLA	A	1231	-	19,19,19	0.57	0	19,19,19	0.85	1 (5%)
6	OLA	A	1207	-	19,19,19	0.57	0	19,19,19	0.87	1 (5%)
6	OLA	A	1225	-	14,14,19	0.65	0	14,14,19	0.92	1 (7%)
6	OLA	A	1229	-	8,8,19	0.84	0	8,8,19	1.14	1 (12%)
7	CLR	A	1211	-	31,31,31	0.63	0	48,48,48	0.81	1 (2%)
2	PEG	A	1201	-	6,6,6	0.54	0	5,5,5	0.80	0
6	OLA	A	1213	-	13,13,19	0.28	0	12,12,19	0.47	0
6	OLA	A	1217	-	14,14,19	0.65	0	14,14,19	0.92	1 (7%)
6	OLA	A	1221	-	14,14,19	0.66	0	14,14,19	0.92	1 (7%)
6	OLA	A	1216	-	11,11,19	0.75	0	11,11,19	1.06	1 (9%)
6	OLA	A	1219	-	10,10,19	0.30	0	9,9,19	0.51	0
6	OLA	A	1224	-	18,18,19	0.59	0	18,18,19	0.87	1 (5%)
6	OLA	A	1233	-	17,17,19	0.59	0	17,17,19	0.89	1 (5%)
6	OLA	A	1212	-	19,19,19	0.56	0	19,19,19	0.88	1 (5%)
5	OLC	A	1206	-	24,24,24	0.62	0	25,25,25	0.94	1 (4%)
6	OLA	A	1215	-	16,16,19	0.60	0	16,16,19	0.89	1 (6%)
6	OLA	A	1220	-	11,11,19	0.30	0	10,10,19	0.54	0
8	ETF	A	1234	-	5,5,5	0.46	0	7,7,7	0.28	0
6	OLA	A	1230	-	6,6,19	0.95	0	6,6,19	1.31	1 (16%)
5	OLC	A	1239	-	24,24,24	0.60	0	25,25,25	0.95	1 (4%)
6	OLA	A	1218	-	10,10,19	0.74	0	10,10,19	1.07	1 (10%)
6	OLA	A	1228	-	12,12,19	0.25	0	11,11,19	0.52	0
2	PEG	A	1235	-	6,6,6	0.65	0	5,5,5	0.90	0
6	OLA	A	1205	-	17,17,19	0.60	0	17,17,19	0.85	1 (5%)
2	PEG	A	1236	-	6,6,6	0.65	0	5,5,5	0.89	0
6	OLA	A	1214	-	8,8,19	0.84	0	8,8,19	1.16	1 (12%)
6	OLA	A	1226	-	10,10,19	0.27	0	9,9,19	0.43	0
7	CLR	A	1210	-	31,31,31	0.61	0	48,48,48	0.79	2 (4%)
3	LJX	A	1202	-	31,31,31	0.83	0	40,44,44	2.02	10 (25%)

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
7	CLR	A	1209	-	-	2/10/68/68	0/4/4/4
5	OLC	A	1240	-	-	11/24/24/24	-
6	OLA	A	1227	-	-	3/7/7/17	-
5	OLC	A	1238	-	-	14/24/24/24	-
5	OLC	A	1204	-	-	11/24/24/24	-
6	OLA	A	1208	-	-	9/17/17/17	-
5	OLC	A	1223	-	-	2/9/9/24	-
5	OLC	A	1222	-	-	8/14/14/24	-
6	OLA	A	1232	-	-	6/10/10/17	-
2	PEG	A	1237	-	-	3/4/4/4	-
6	OLA	A	1231	-	-	8/17/17/17	-
6	OLA	A	1207	-	-	10/17/17/17	-
6	OLA	A	1225	-	-	4/12/12/17	-
6	OLA	A	1229	-	-	3/6/6/17	-
7	CLR	A	1211	-	-	3/10/68/68	0/4/4/4
2	PEG	A	1201	-	-	3/4/4/4	-
6	OLA	A	1213	-	-	5/11/11/17	-
6	OLA	A	1217	-	-	4/12/12/17	-
6	OLA	A	1221	-	-	8/12/12/17	-
6	OLA	A	1216	-	-	3/9/9/17	-
6	OLA	A	1219	-	-	3/8/8/17	-
6	OLA	A	1224	-	-	4/16/16/17	-
6	OLA	A	1233	-	-	9/15/15/17	-
6	OLA	A	1212	-	-	8/17/17/17	-
5	OLC	A	1206	-	-	11/24/24/24	-
6	OLA	A	1215	-	-	7/14/14/17	-
6	OLA	A	1220	-	-	5/9/9/17	-
8	ETF	A	1234	-	-	0/3/3/3	-
6	OLA	A	1230	-	-	4/4/4/17	-
5	OLC	A	1239	-	-	13/24/24/24	-
6	OLA	A	1218	-	-	5/8/8/17	-
6	OLA	A	1228	-	-	5/10/10/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	1235	-	-	2/4/4/4	-
6	OLA	A	1205	-	-	6/15/15/17	-
2	PEG	A	1236	-	-	1/4/4/4	-
6	OLA	A	1214	-	-	2/6/6/17	-
6	OLA	A	1226	-	-	1/8/8/17	-
7	CLR	A	1210	-	-	2/10/68/68	0/4/4/4
3	LJX	A	1202	-	-	2/11/27/27	0/4/4/4

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	LJX	C5-C4-N3	-7.53	119.25	127.18
3	A	1202	LJX	C5-C4-N9	4.24	108.29	105.63
3	A	1202	LJX	C5-N7-C8	3.60	107.40	104.12
3	A	1202	LJX	N3-C2-N1	-3.42	120.57	127.62
3	A	1202	LJX	C4-N3-C2	3.21	120.91	116.16
3	A	1202	LJX	C4-C5-N7	-2.86	107.99	110.91
7	A	1209	CLR	C4-C5-C10	2.58	119.73	116.42
3	A	1202	LJX	C4-N9-C8	2.55	107.25	105.87
7	A	1209	CLR	C4-C5-C6	-2.54	117.13	120.57
3	A	1202	LJX	C6-N1-C2	2.45	119.78	116.16
7	A	1210	CLR	C4-C5-C6	-2.41	117.30	120.57
7	A	1209	CLR	C7-C8-C9	2.29	112.36	109.72
5	A	1222	OLC	C3-C2-C1	-2.22	105.55	113.69
5	A	1240	OLC	C3-C2-C1	-2.19	105.67	113.69
7	A	1211	CLR	C4-C5-C6	-2.14	117.66	120.57
3	A	1202	LJX	C9-C8-N7	2.13	124.71	121.99
6	A	1232	OLA	O2-C1-C2	2.13	120.73	114.00
6	A	1214	OLA	O2-C1-C2	2.11	120.67	114.00
6	A	1224	OLA	O2-C1-C2	2.11	120.67	114.00
6	A	1225	OLA	O2-C1-C2	2.11	120.66	114.00
6	A	1218	OLA	O2-C1-C2	2.11	120.66	114.00
6	A	1231	OLA	O2-C1-C2	2.10	120.62	114.00
7	A	1210	CLR	C4-C5-C10	2.10	119.11	116.42
6	A	1208	OLA	O2-C1-C2	2.09	120.59	114.00
5	A	1238	OLC	C3-C2-C1	-2.08	106.07	113.69
6	A	1212	OLA	O2-C1-C2	2.08	120.57	114.00
6	A	1229	OLA	O2-C1-C2	2.07	120.54	114.00
6	A	1233	OLA	O2-C1-C2	2.06	120.51	114.00
6	A	1230	OLA	O2-C1-C2	2.05	120.48	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1207	OLA	O2-C1-C2	2.05	120.48	114.00
5	A	1206	OLC	O20-C1-O19	-2.05	118.50	123.63
6	A	1205	OLA	O2-C1-C2	2.05	120.47	114.00
3	A	1202	LJX	N6-C6-N1	2.04	119.78	117.03
6	A	1215	OLA	O2-C1-C2	2.04	120.45	114.00
5	A	1204	OLC	O20-C1-O19	-2.04	118.53	123.63
6	A	1216	OLA	O2-C1-C2	2.03	120.41	114.00
5	A	1240	OLC	O20-C1-O19	-2.03	118.56	123.63
5	A	1239	OLC	C3-C2-C1	-2.02	106.28	113.69
6	A	1217	OLA	O2-C1-C2	2.01	120.36	114.00
6	A	1221	OLA	O2-C1-C2	2.01	120.36	114.00

There are no chirality outliers.

All (210) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1204	OLC	C21-C22-C24-O25
5	A	1238	OLC	O20-C21-C22-C24
5	A	1238	OLC	O20-C21-C22-O23
5	A	1240	OLC	O20-C21-C22-C24
5	A	1222	OLC	C2-C1-O20-C21
5	A	1240	OLC	C2-C1-O20-C21
5	A	1238	OLC	O19-C1-O20-C21
5	A	1240	OLC	O19-C1-O20-C21
5	A	1240	OLC	O20-C21-C22-O23
5	A	1222	OLC	O19-C1-O20-C21
5	A	1238	OLC	C2-C1-O20-C21
2	A	1201	PEG	O2-C3-C4-O4
5	A	1204	OLC	C2-C1-O20-C21
5	A	1206	OLC	C2-C1-O20-C21
5	A	1239	OLC	C2-C1-O20-C21
5	A	1204	OLC	O19-C1-O20-C21
5	A	1206	OLC	O19-C1-O20-C21
5	A	1239	OLC	O19-C1-O20-C21
5	A	1204	OLC	O23-C22-C24-O25
6	A	1230	OLA	C1-C2-C3-C4
5	A	1222	OLC	O20-C21-C22-O23
6	A	1208	OLA	C1-C2-C3-C4
6	A	1231	OLA	C1-C2-C3-C4
6	A	1215	OLA	C1-C2-C3-C4
5	A	1222	OLC	O20-C21-C22-C24
5	A	1206	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
5	A	1222	OLC	C21-C22-C24-O25
5	A	1223	OLC	C21-C22-C24-O25
5	A	1238	OLC	C21-C22-C24-O25
5	A	1206	OLC	C11-C12-C13-C14
5	A	1240	OLC	C13-C14-C15-C16
6	A	1213	OLA	C11-C12-C13-C14
6	A	1229	OLA	C3-C4-C5-C6
6	A	1208	OLA	C11-C12-C13-C14
5	A	1222	OLC	C4-C5-C6-C7
6	A	1205	OLA	C11-C12-C13-C14
6	A	1219	OLA	C13-C14-C15-C16
6	A	1231	OLA	C11-C12-C13-C14
5	A	1239	OLC	C4-C5-C6-C7
2	A	1235	PEG	O1-C1-C2-O2
6	A	1208	OLA	C13-C14-C15-C16
6	A	1215	OLA	C4-C5-C6-C7
6	A	1205	OLA	C12-C13-C14-C15
6	A	1232	OLA	C1-C2-C3-C4
5	A	1239	OLC	C13-C14-C15-C16
5	A	1204	OLC	C4-C5-C6-C7
5	A	1204	OLC	C12-C13-C14-C15
6	A	1205	OLA	C4-C5-C6-C7
6	A	1205	OLA	C10-C11-C12-C13
6	A	1213	OLA	C10-C11-C12-C13
6	A	1224	OLA	C10-C11-C12-C13
6	A	1212	OLA	C11-C12-C13-C14
6	A	1224	OLA	C1-C2-C3-C4
5	A	1206	OLC	C12-C13-C14-C15
6	A	1225	OLA	C4-C5-C6-C7
5	A	1239	OLC	O20-C21-C22-O23
5	A	1240	OLC	C2-C3-C4-C5
6	A	1220	OLA	C3-C4-C5-C6
7	A	1211	CLR	C22-C23-C24-C25
6	A	1213	OLA	C13-C14-C15-C16
5	A	1206	OLC	C6-C7-C8-C9
6	A	1227	OLA	C10-C11-C12-C13
6	A	1233	OLA	C10-C11-C12-C13
5	A	1240	OLC	C5-C6-C7-C8
2	A	1201	PEG	O1-C1-C2-O2
5	A	1206	OLC	C4-C5-C6-C7
6	A	1232	OLA	C3-C4-C5-C6
6	A	1227	OLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
5	A	1238	OLC	C5-C6-C7-C8
6	A	1212	OLA	C3-C4-C5-C6
6	A	1212	OLA	C10-C11-C12-C13
6	A	1212	OLA	C4-C5-C6-C7
6	A	1225	OLA	C3-C4-C5-C6
5	A	1204	OLC	C14-C15-C16-C17
6	A	1233	OLA	C4-C5-C6-C7
5	A	1238	OLC	C3-C4-C5-C6
5	A	1239	OLC	C6-C7-C8-C9
6	A	1215	OLA	C6-C7-C8-C9
6	A	1221	OLA	C6-C7-C8-C9
6	A	1232	OLA	C6-C7-C8-C9
5	A	1206	OLC	C1-C2-C3-C4
2	A	1237	PEG	O1-C1-C2-O2
5	A	1240	OLC	C15-C16-C17-C18
6	A	1221	OLA	C4-C5-C6-C7
6	A	1228	OLA	C14-C15-C16-C17
6	A	1232	OLA	C4-C5-C6-C7
6	A	1226	OLA	C12-C13-C14-C15
5	A	1238	OLC	C11-C12-C13-C14
6	A	1218	OLA	C6-C7-C8-C9
5	A	1222	OLC	O23-C22-C24-O25
6	A	1233	OLA	C13-C14-C15-C16
5	A	1239	OLC	C11-C12-C13-C14
6	A	1228	OLA	C13-C14-C15-C16
6	A	1216	OLA	C2-C3-C4-C5
5	A	1238	OLC	C4-C5-C6-C7
5	A	1240	OLC	C11-C12-C13-C14
6	A	1230	OLA	C2-C3-C4-C5
6	A	1214	OLA	C2-C3-C4-C5
6	A	1231	OLA	C13-C14-C15-C16
6	A	1205	OLA	C13-C14-C15-C16
7	A	1210	CLR	C23-C24-C25-C26
5	A	1238	OLC	C15-C16-C17-C18
5	A	1239	OLC	C5-C6-C7-C8
6	A	1218	OLA	C4-C5-C6-C7
6	A	1212	OLA	C15-C16-C17-C18
6	A	1233	OLA	C5-C6-C7-C8
6	A	1207	OLA	C10-C11-C12-C13
6	A	1218	OLA	C1-C2-C3-C4
6	A	1212	OLA	C13-C14-C15-C16
6	A	1208	OLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
5	A	1239	OLC	C2-C3-C4-C5
6	A	1221	OLA	C2-C3-C4-C5
6	A	1207	OLA	C12-C13-C14-C15
6	A	1207	OLA	C5-C6-C7-C8
7	A	1210	CLR	C23-C24-C25-C27
6	A	1219	OLA	C12-C13-C14-C15
2	A	1201	PEG	C1-C2-O2-C3
6	A	1207	OLA	C13-C14-C15-C16
5	A	1238	OLC	C12-C13-C14-C15
2	A	1236	PEG	O1-C1-C2-O2
6	A	1213	OLA	C14-C15-C16-C17
6	A	1214	OLA	C4-C5-C6-C7
2	A	1235	PEG	C1-C2-O2-C3
3	A	1202	LJX	C13-C14-C15-C16
7	A	1209	CLR	C23-C24-C25-C26
5	A	1206	OLC	C3-C4-C5-C6
6	A	1228	OLA	C7-C8-C9-C10
6	A	1207	OLA	C1-C2-C3-C4
6	A	1221	OLA	C5-C6-C7-C8
6	A	1220	OLA	C9-C10-C11-C12
6	A	1231	OLA	C12-C13-C14-C15
6	A	1208	OLA	C6-C7-C8-C9
6	A	1231	OLA	C6-C7-C8-C9
6	A	1205	OLA	C7-C8-C9-C10
5	A	1238	OLC	C9-C10-C11-C12
5	A	1238	OLC	C7-C8-C9-C10
6	A	1208	OLA	C9-C10-C11-C12
6	A	1225	OLA	C9-C10-C11-C12
7	A	1209	CLR	C23-C24-C25-C27
5	A	1206	OLC	C7-C8-C9-C10
6	A	1217	OLA	C9-C10-C11-C12
2	A	1237	PEG	C4-C3-O2-C2
5	A	1239	OLC	C15-C16-C17-C18
6	A	1221	OLA	O1-C1-C2-C3
5	A	1204	OLC	C13-C14-C15-C16
6	A	1215	OLA	C3-C4-C5-C6
5	A	1223	OLC	O23-C22-C24-O25
5	A	1238	OLC	O23-C22-C24-O25
6	A	1232	OLA	O1-C1-C2-C3
6	A	1208	OLA	C3-C4-C5-C6
6	A	1228	OLA	C11-C12-C13-C14
5	A	1240	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
5	A	1240	OLC	C7-C8-C9-C10
6	A	1215	OLA	C10-C11-C12-C13
6	A	1221	OLA	O2-C1-C2-C3
6	A	1231	OLA	O1-C1-C2-C3
6	A	1232	OLA	O2-C1-C2-C3
6	A	1225	OLA	C5-C6-C7-C8
6	A	1227	OLA	C12-C13-C14-C15
6	A	1224	OLA	C7-C8-C9-C10
6	A	1216	OLA	O1-C1-C2-C3
6	A	1220	OLA	C2-C3-C4-C5
6	A	1233	OLA	O2-C1-C2-C3
6	A	1221	OLA	C1-C2-C3-C4
5	A	1206	OLC	C13-C14-C15-C16
6	A	1233	OLA	O1-C1-C2-C3
5	A	1222	OLC	C5-C6-C7-C8
6	A	1213	OLA	C7-C8-C9-C10
6	A	1221	OLA	C9-C10-C11-C12
6	A	1229	OLA	O2-C1-C2-C3
6	A	1216	OLA	O2-C1-C2-C3
6	A	1230	OLA	O2-C1-C2-C3
6	A	1231	OLA	C9-C10-C11-C12
6	A	1233	OLA	C7-C8-C9-C10
6	A	1231	OLA	O2-C1-C2-C3
5	A	1204	OLC	C3-C4-C5-C6
6	A	1212	OLA	C9-C10-C11-C12
6	A	1217	OLA	C7-C8-C9-C10
6	A	1218	OLA	O2-C1-C2-C3
5	A	1204	OLC	C6-C7-C8-C9
6	A	1207	OLA	O2-C1-C2-C3
6	A	1207	OLA	C4-C5-C6-C7
3	A	1202	LJX	C2'-C1'-N9-C4
6	A	1229	OLA	O1-C1-C2-C3
6	A	1230	OLA	O1-C1-C2-C3
6	A	1224	OLA	C4-C5-C6-C7
6	A	1215	OLA	C11-C12-C13-C14
6	A	1207	OLA	O1-C1-C2-C3
6	A	1218	OLA	O1-C1-C2-C3
5	A	1204	OLC	C9-C10-C11-C12
5	A	1239	OLC	C9-C10-C11-C12
6	A	1220	OLA	C7-C8-C9-C10
6	A	1217	OLA	C6-C7-C8-C9
7	A	1211	CLR	C21-C20-C22-C23

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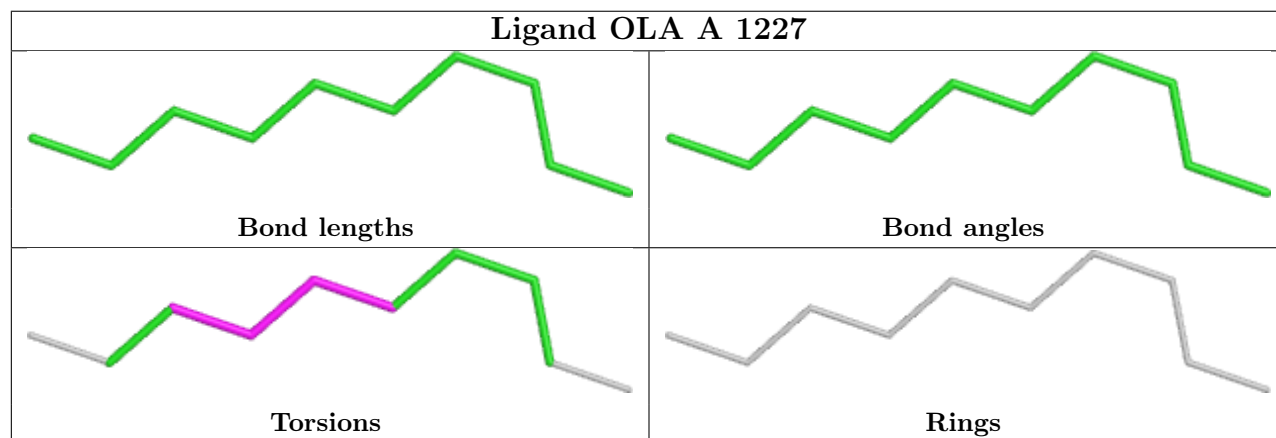
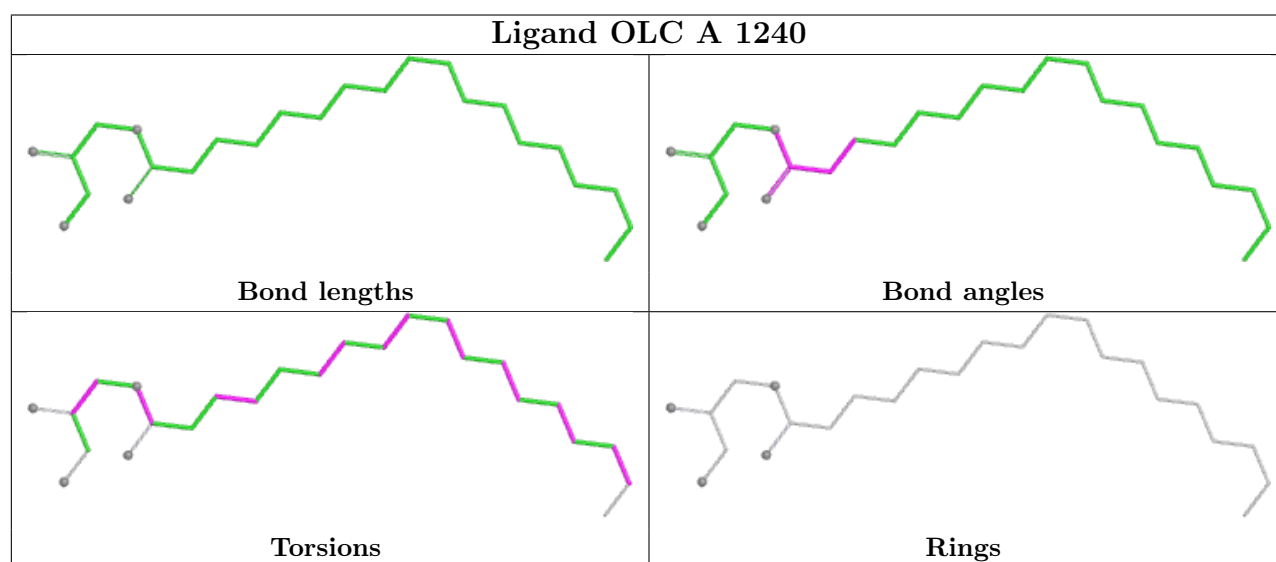
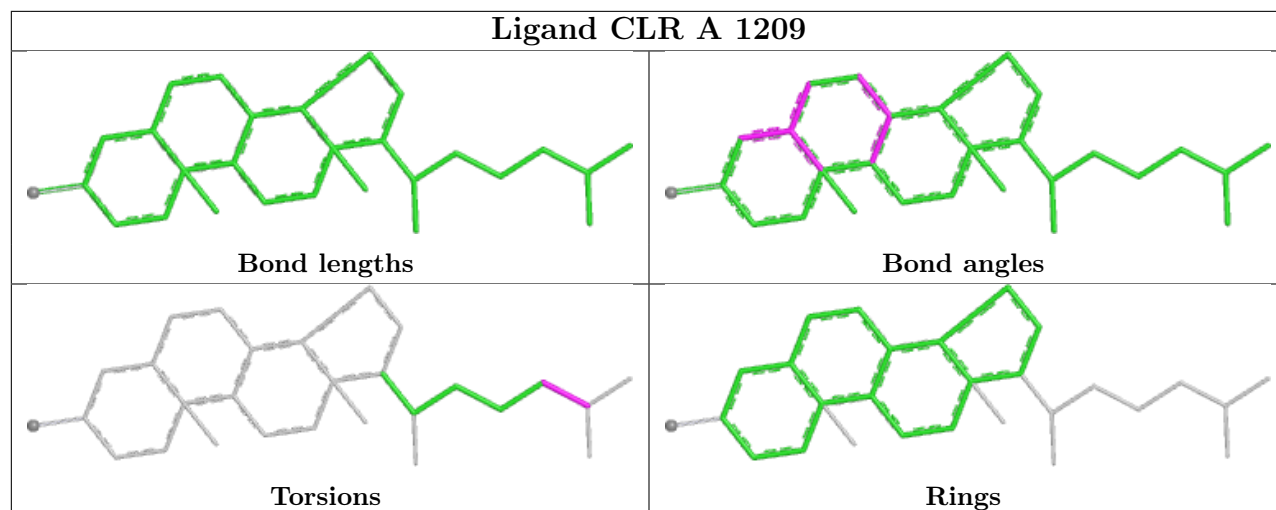
Mol	Chain	Res	Type	Atoms
2	A	1237	PEG	O2-C3-C4-O4
6	A	1207	OLA	C7-C8-C9-C10
6	A	1228	OLA	C9-C10-C11-C12
6	A	1208	OLA	O1-C1-C2-C3
6	A	1233	OLA	C3-C4-C5-C6
5	A	1239	OLC	O20-C21-C22-C24
7	A	1211	CLR	C17-C20-C22-C23
6	A	1207	OLA	C3-C4-C5-C6
6	A	1233	OLA	C2-C3-C4-C5
6	A	1219	OLA	C7-C8-C9-C10
6	A	1215	OLA	C7-C8-C9-C10
6	A	1208	OLA	O2-C1-C2-C3
6	A	1217	OLA	O2-C1-C2-C3
5	A	1239	OLC	O23-C22-C24-O25
6	A	1220	OLA	C1-C2-C3-C4
6	A	1212	OLA	O2-C1-C2-C3

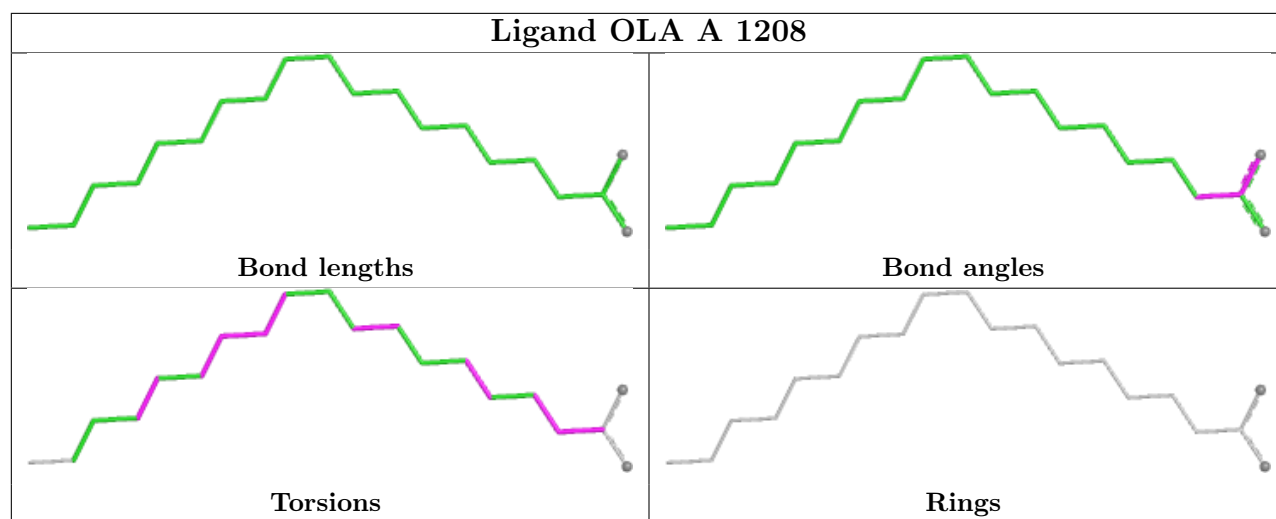
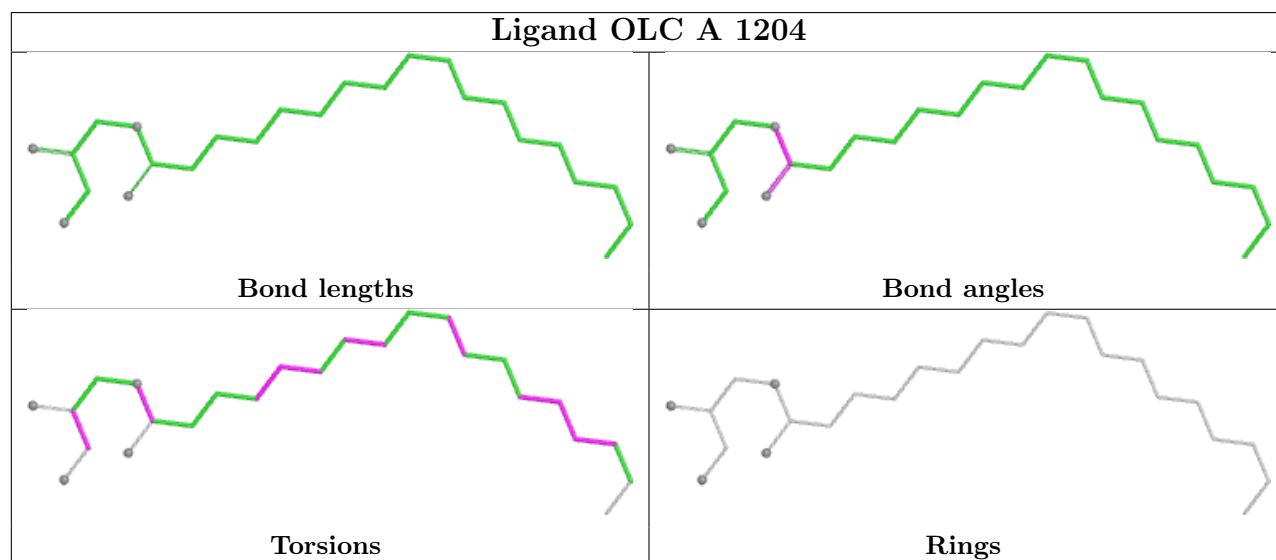
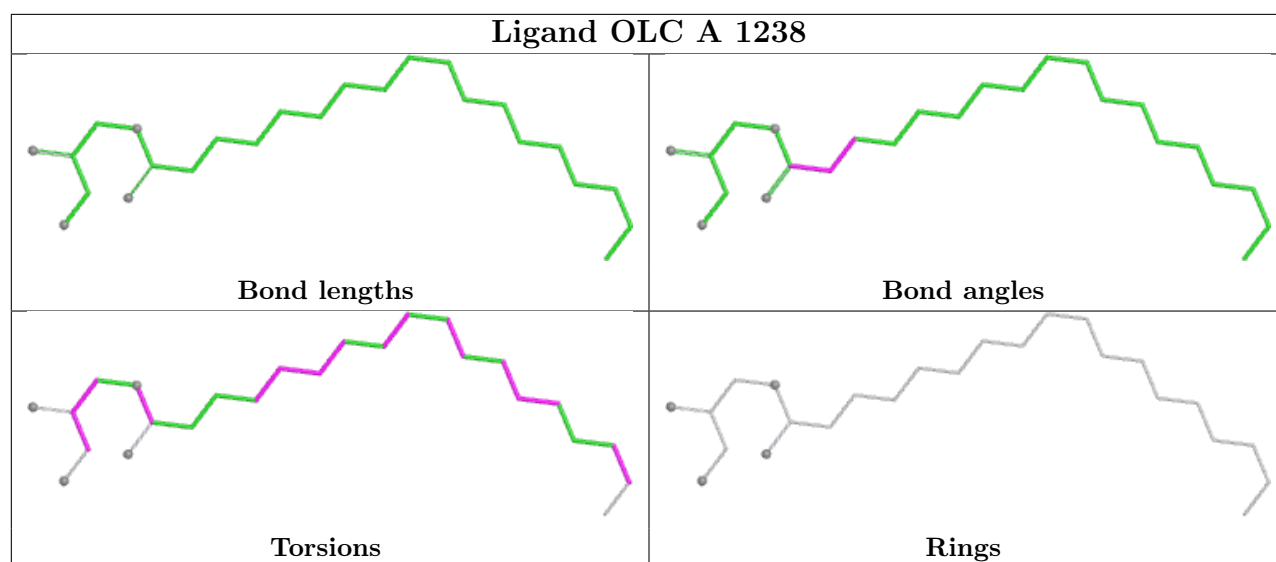
There are no ring outliers.

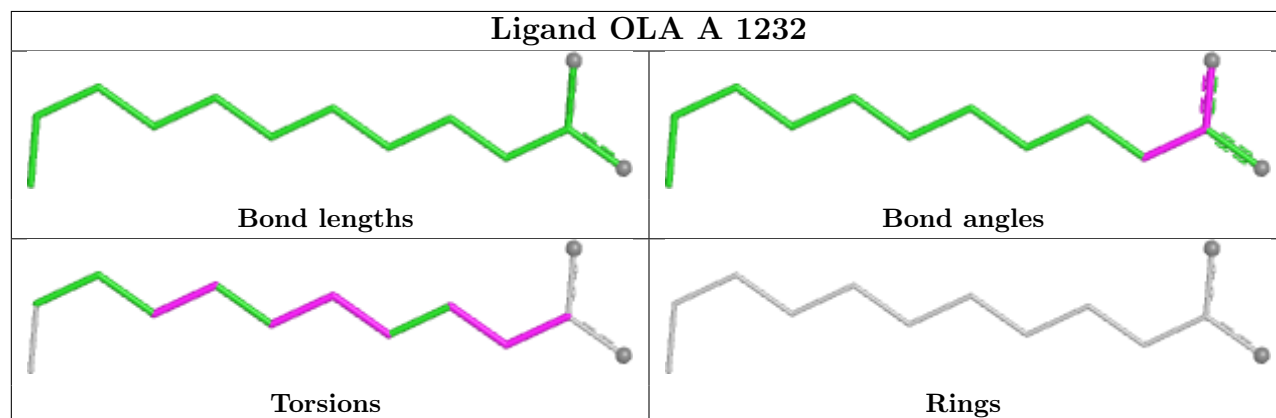
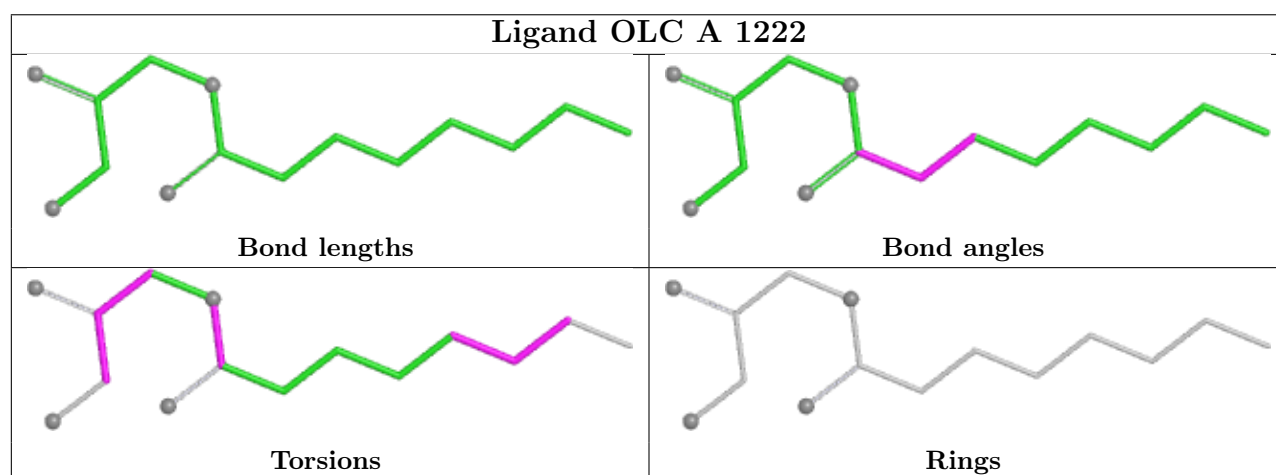
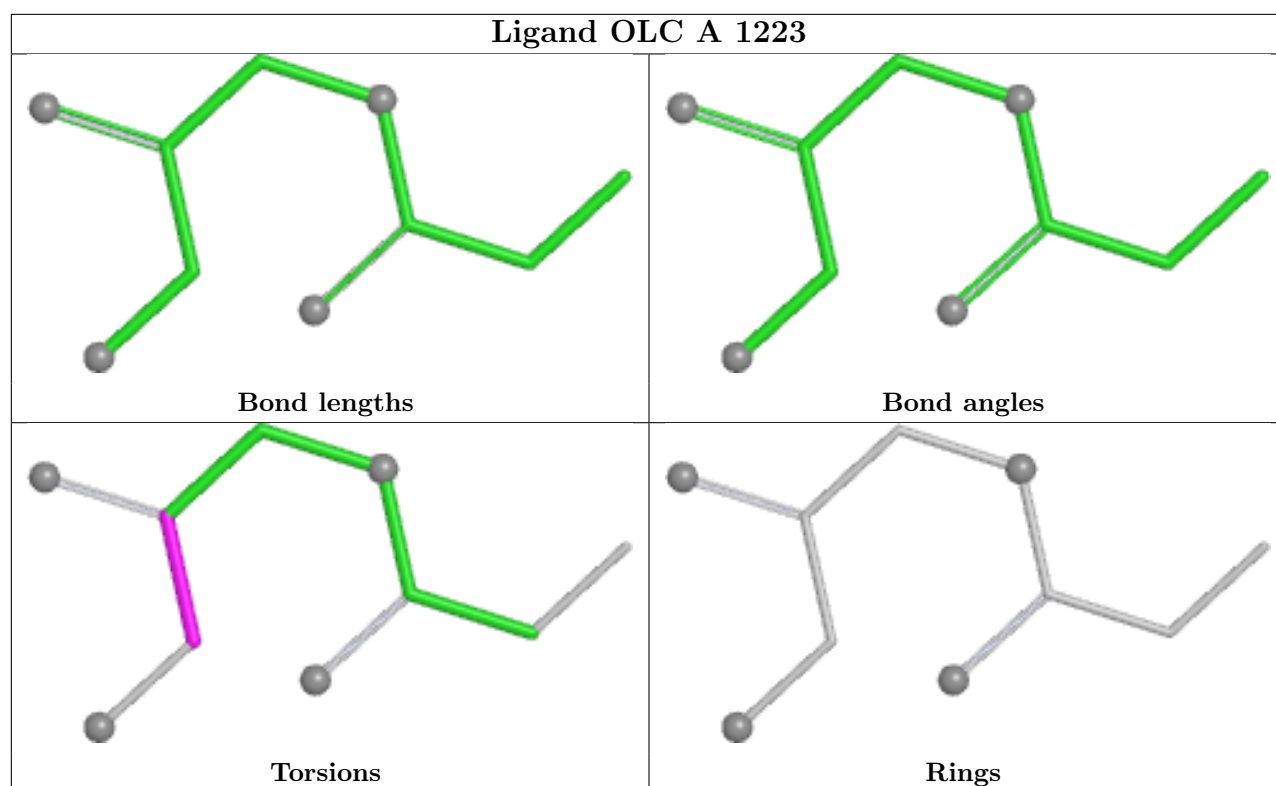
6 monomers are involved in 7 short contacts:

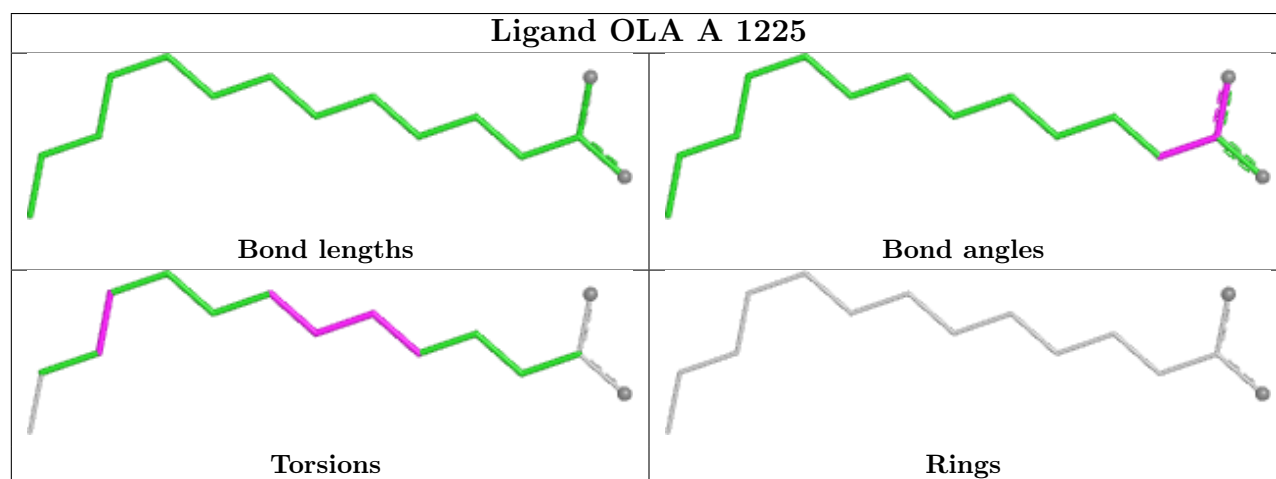
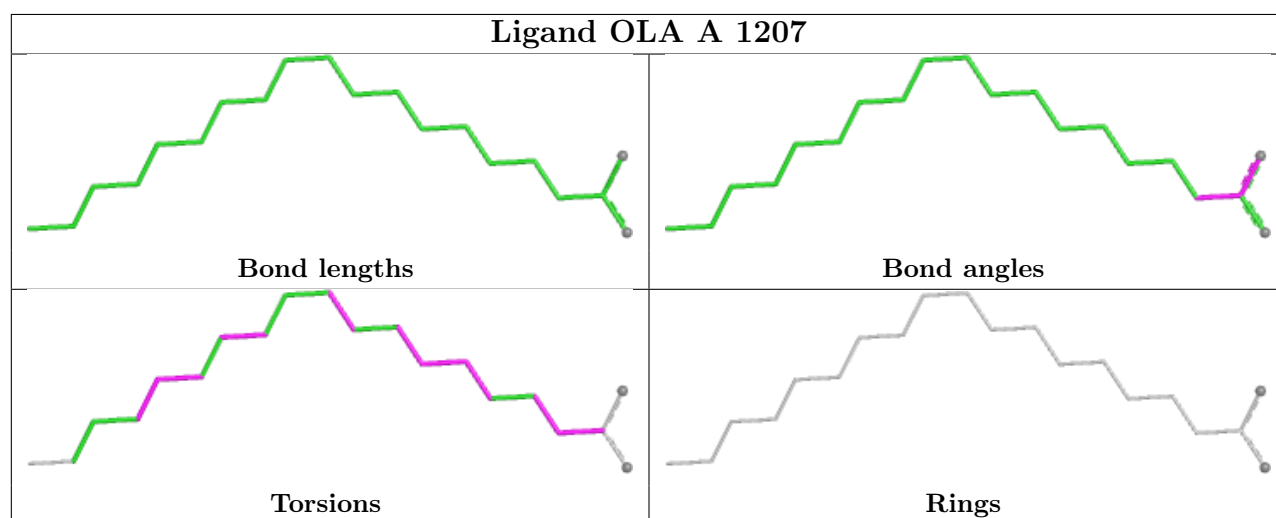
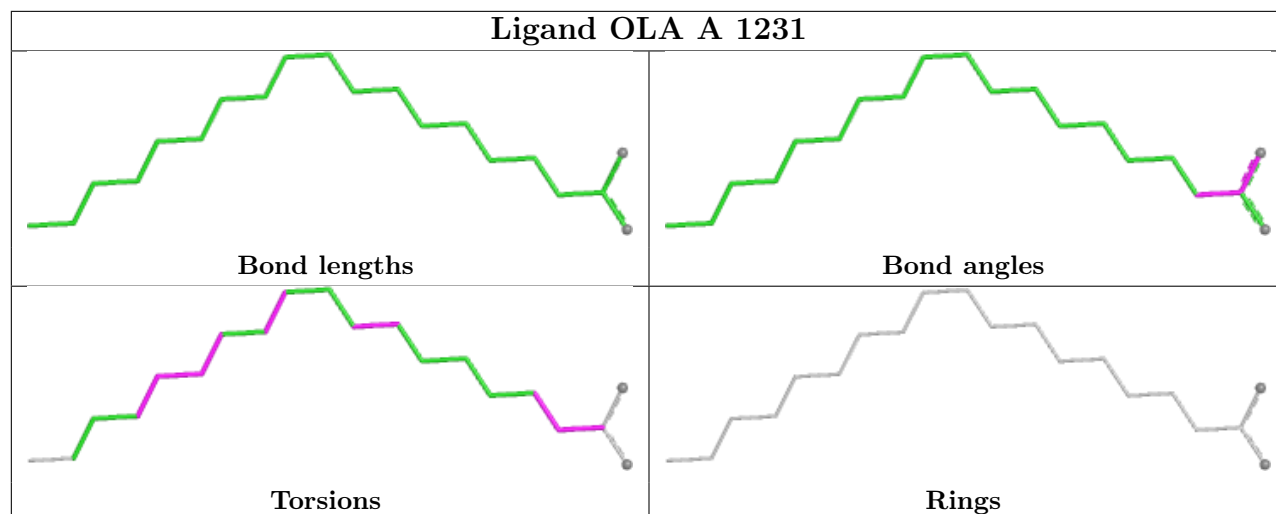
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1207	OLA	3	0
7	A	1211	CLR	1	0
5	A	1206	OLC	1	0
6	A	1215	OLA	1	0
5	A	1239	OLC	1	0
6	A	1228	OLA	1	0

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

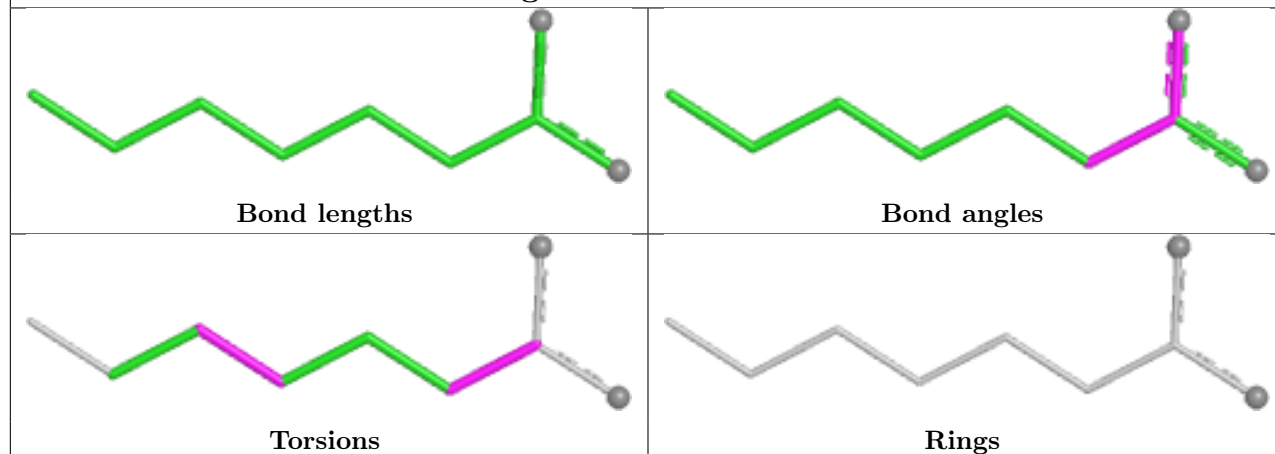




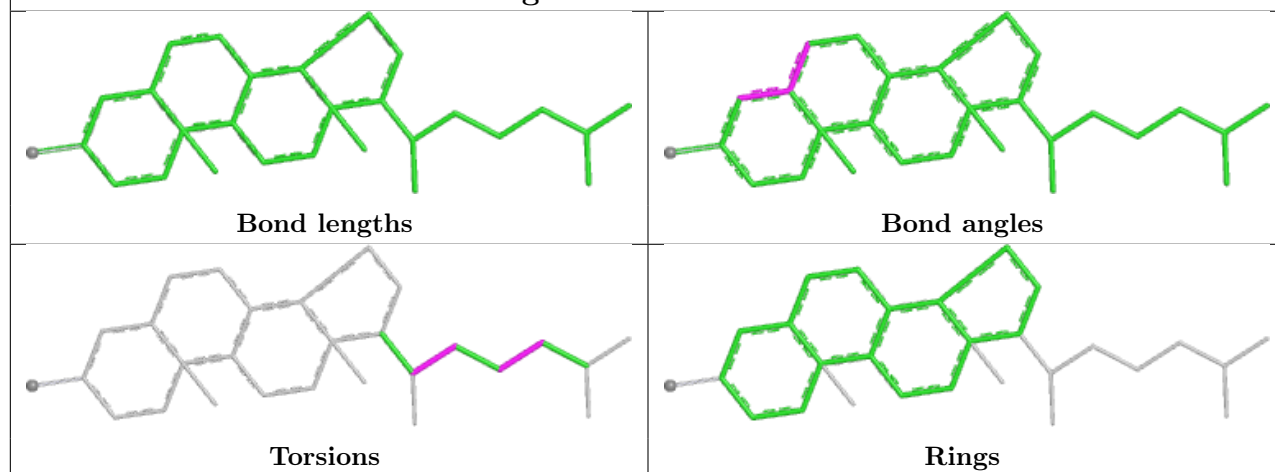




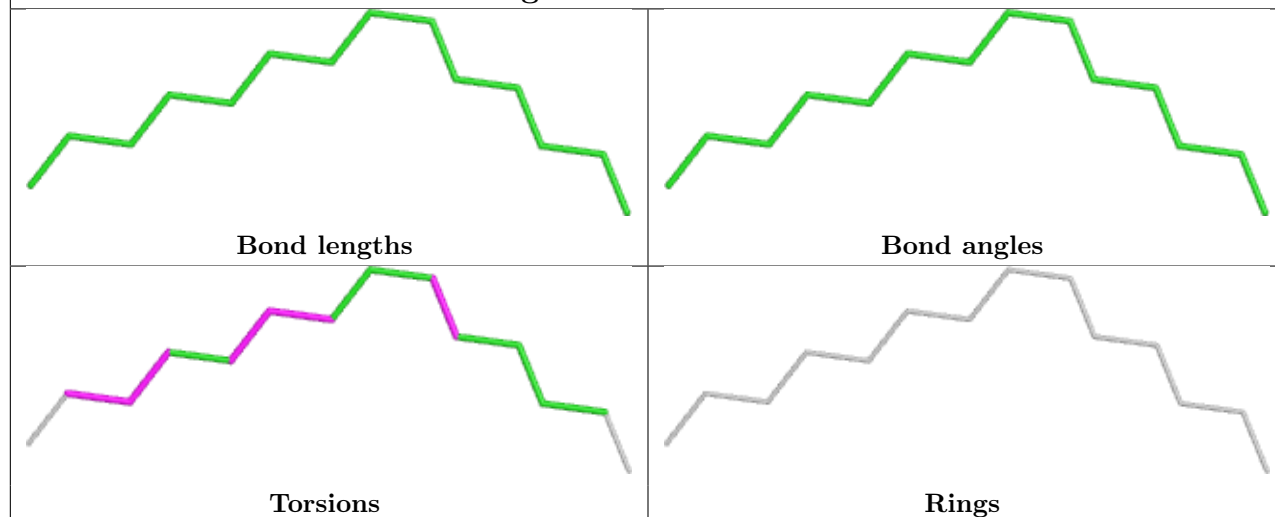
Ligand OLA A 1229

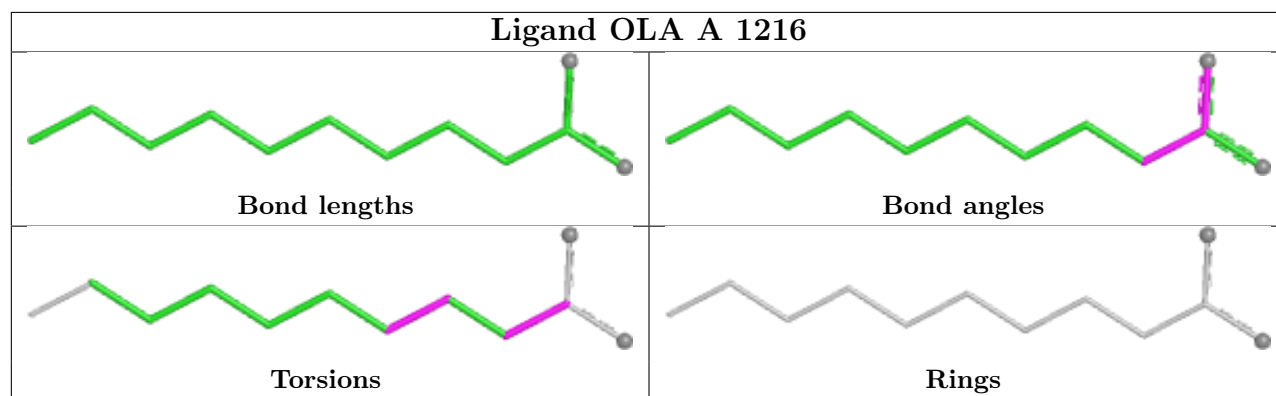
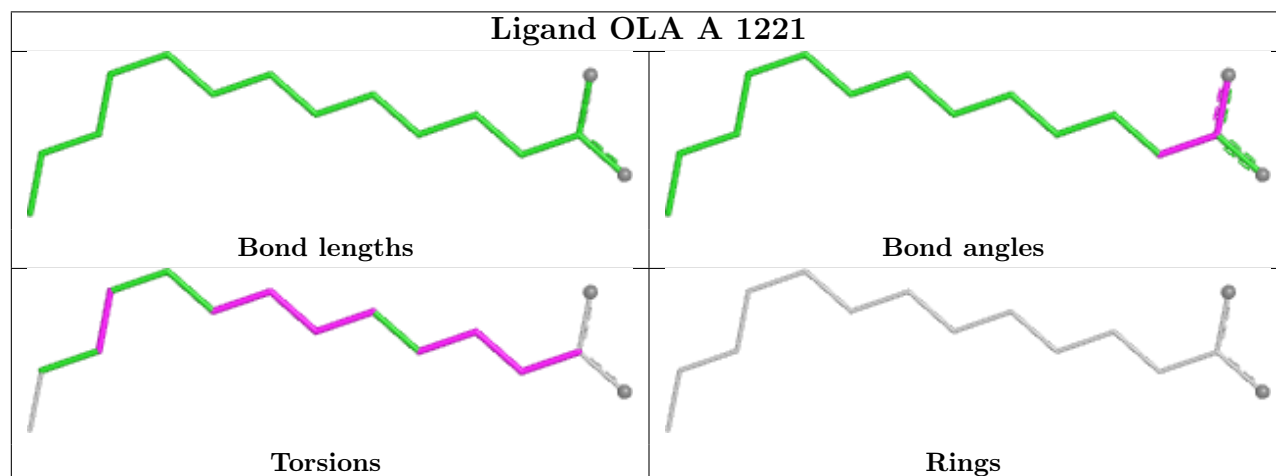
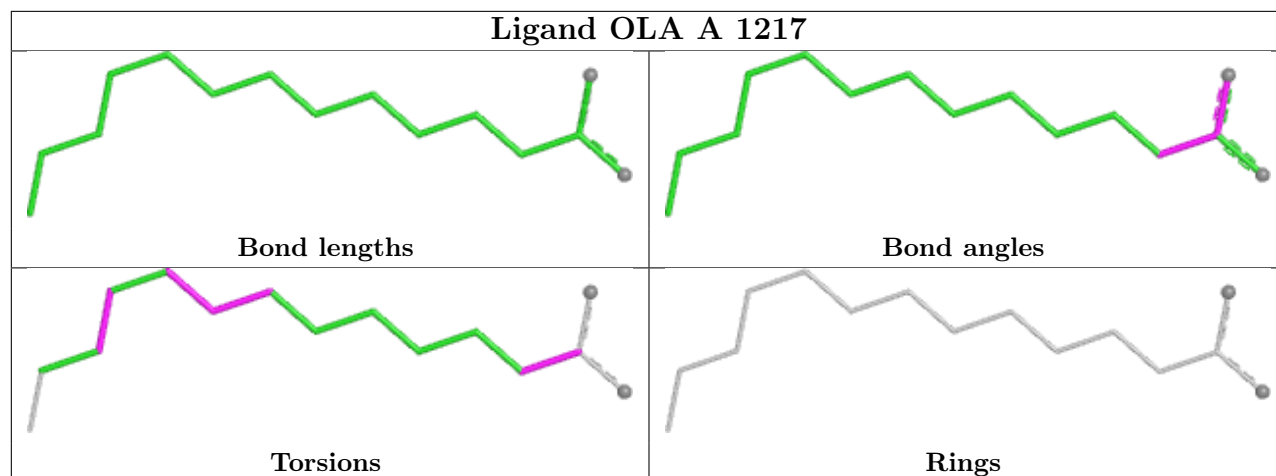


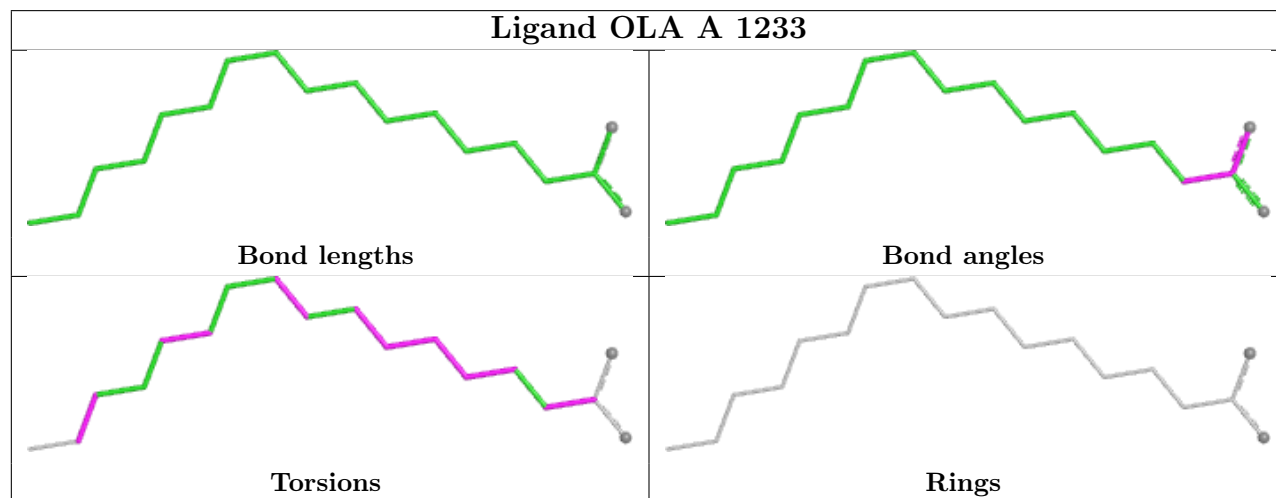
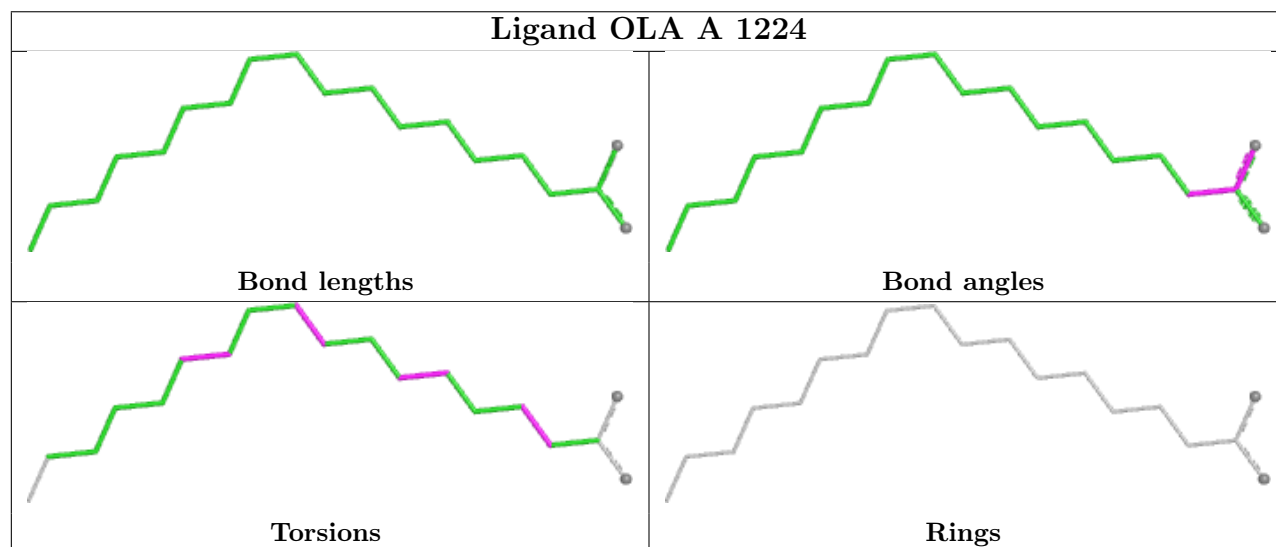
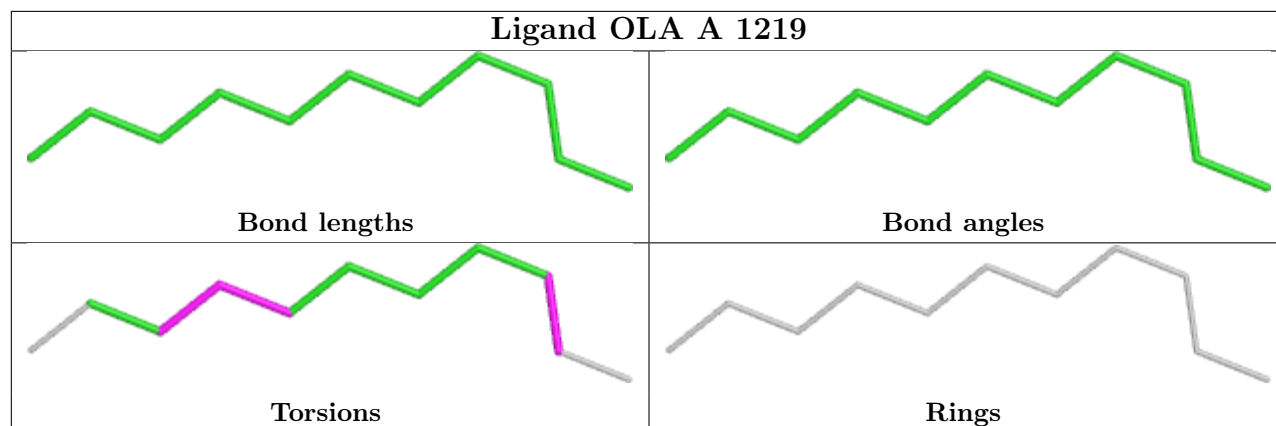
Ligand CLR A 1211

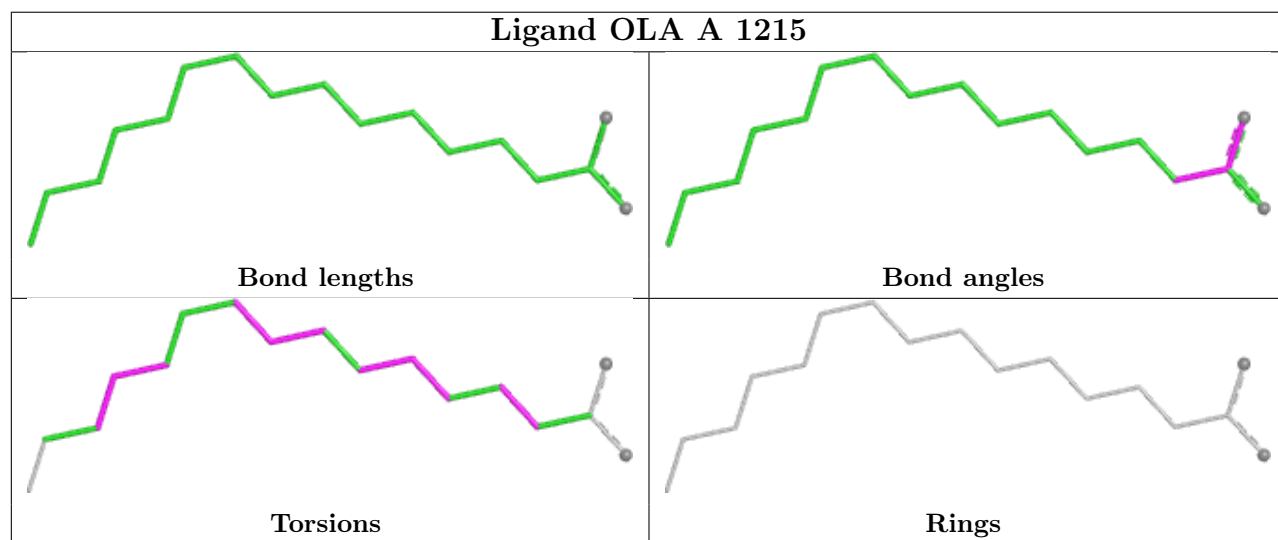
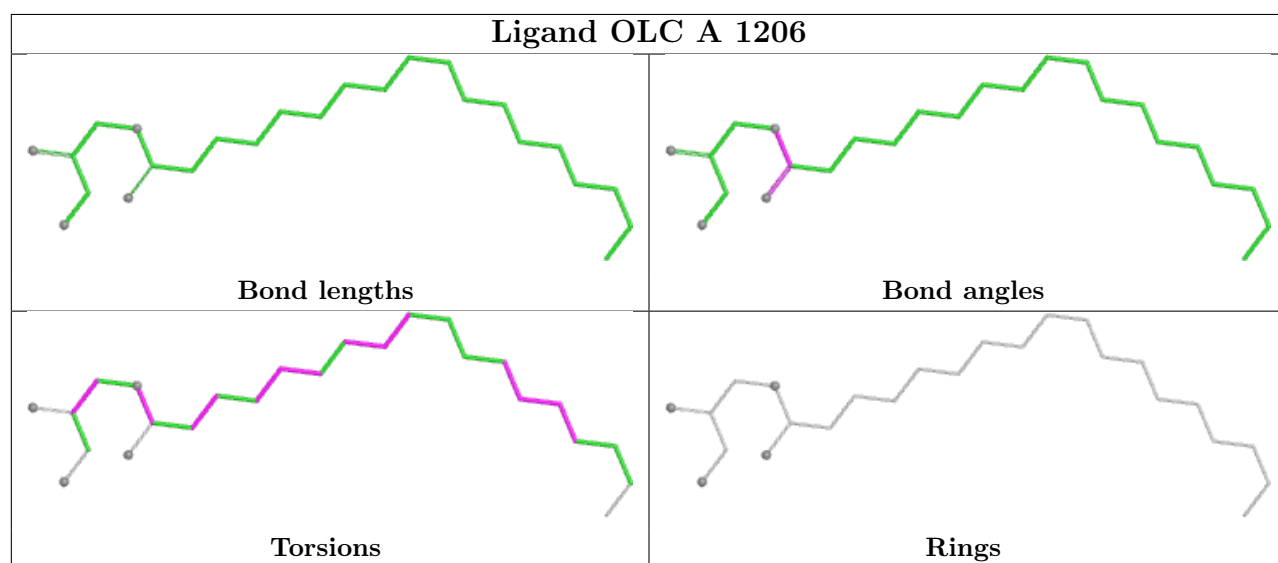
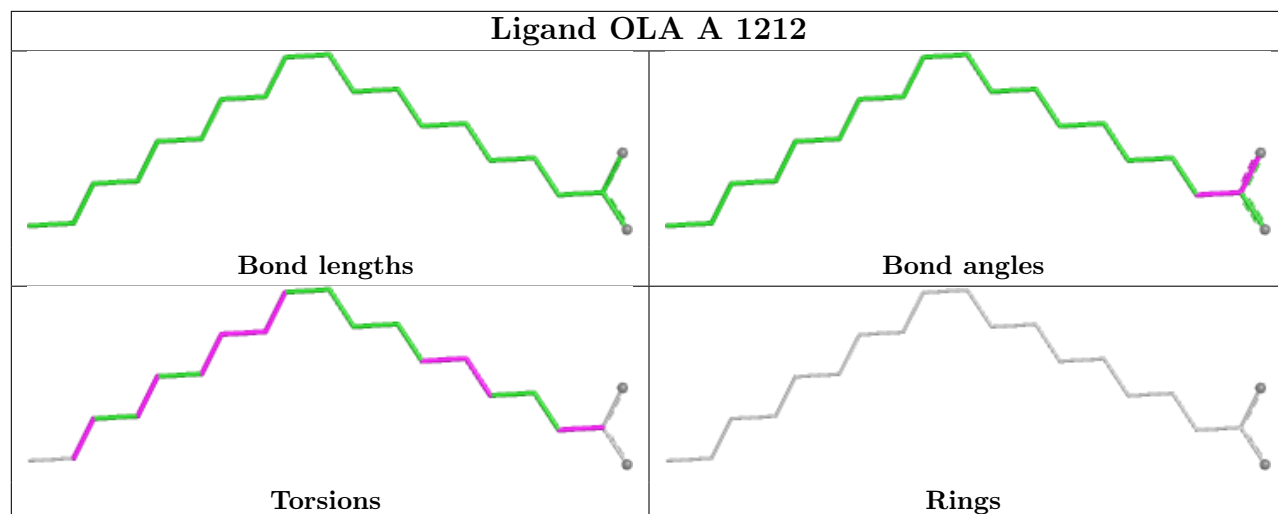


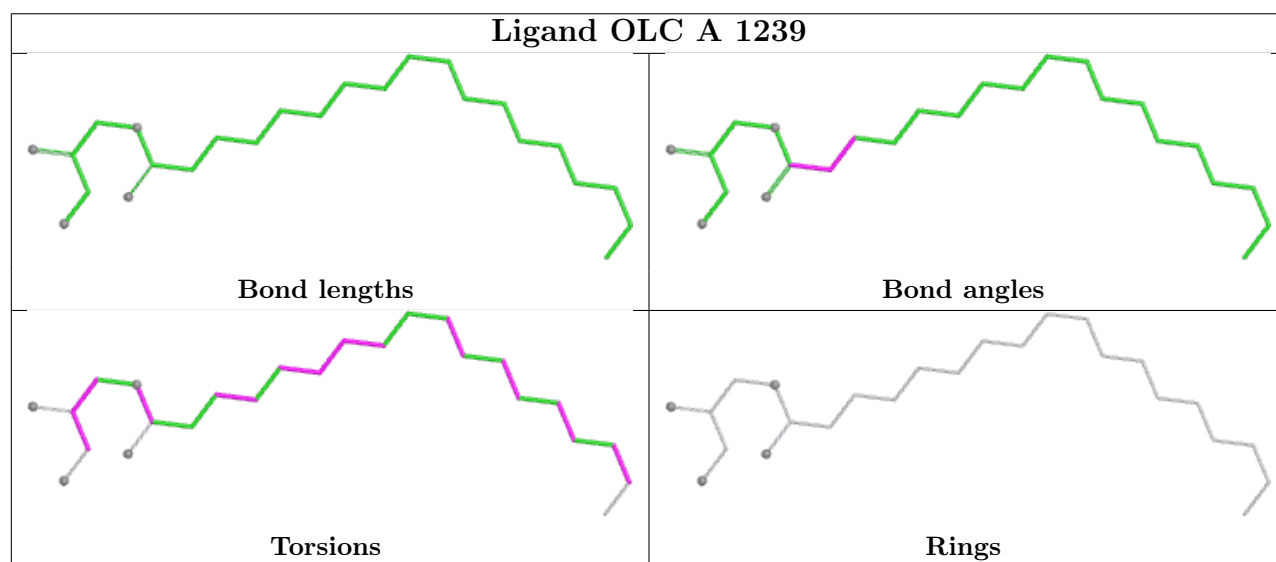
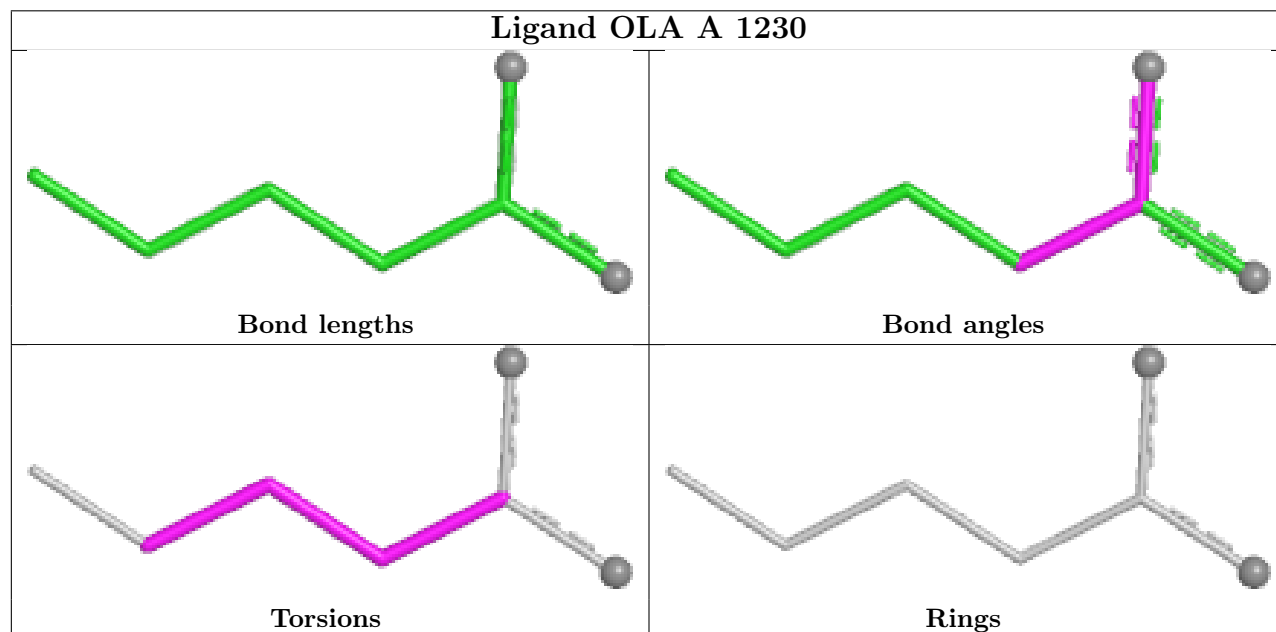
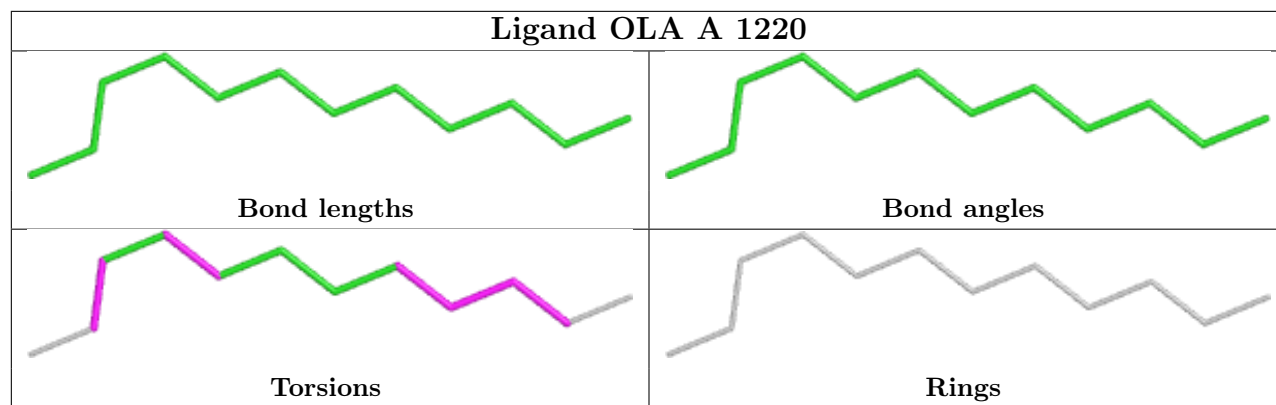
Ligand OLA A 1213

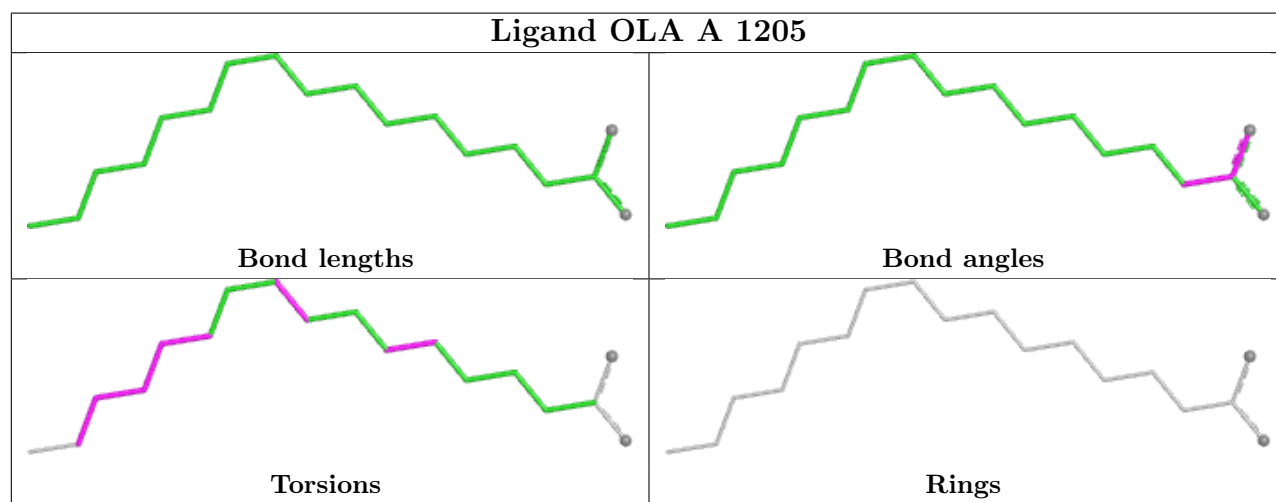
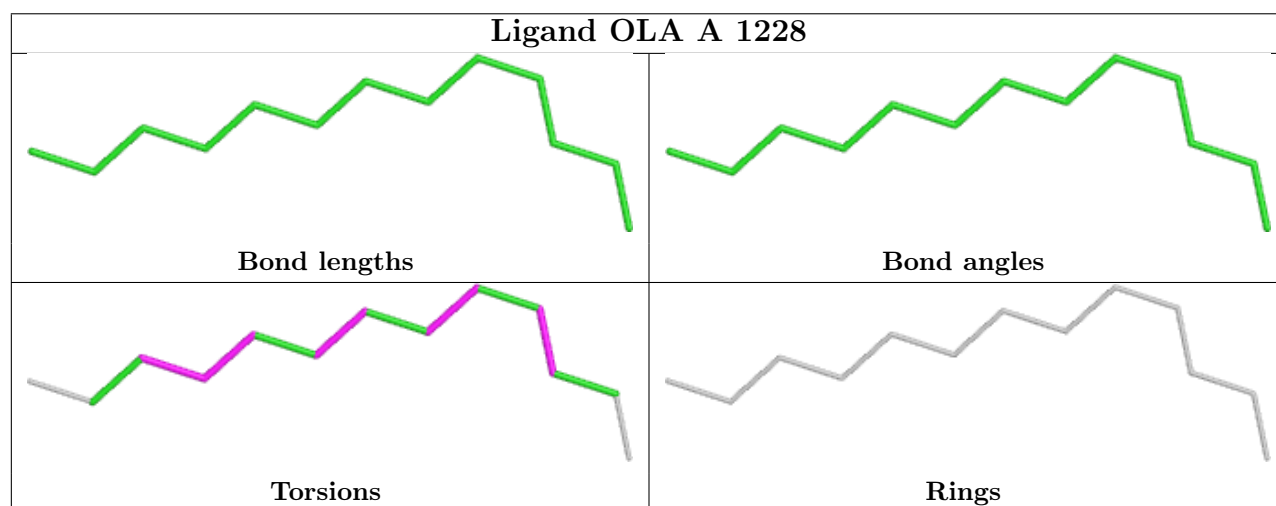
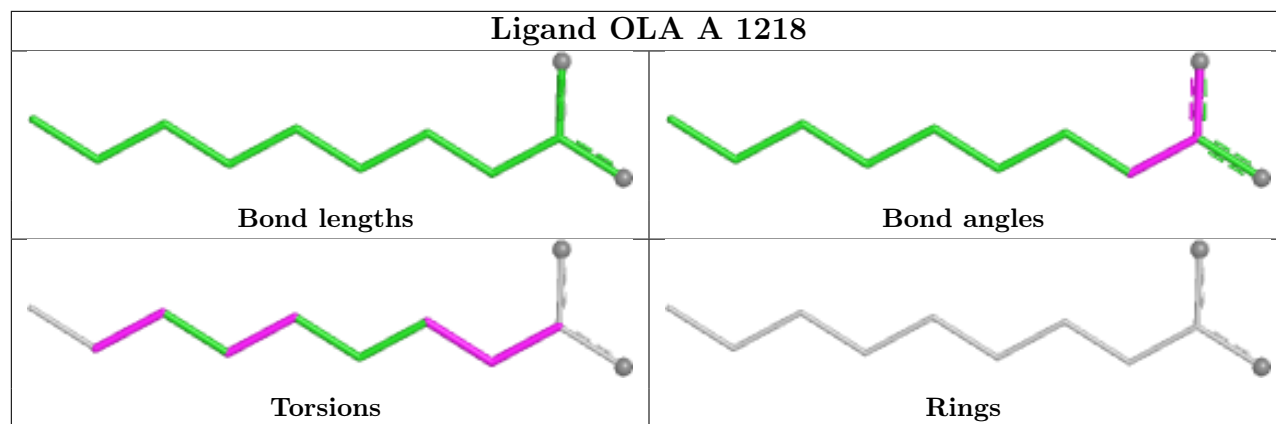


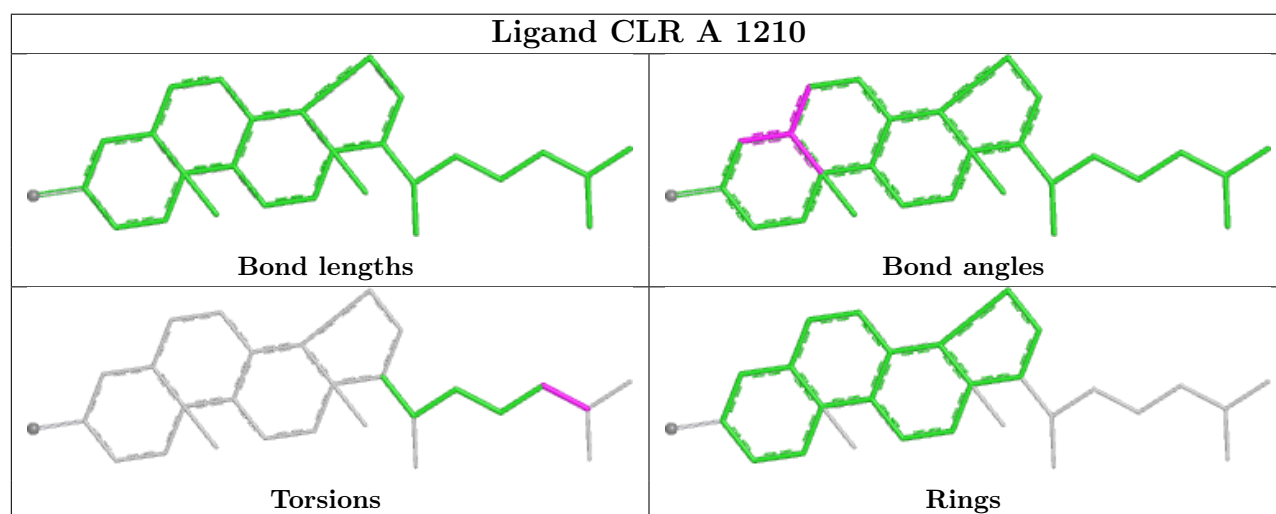
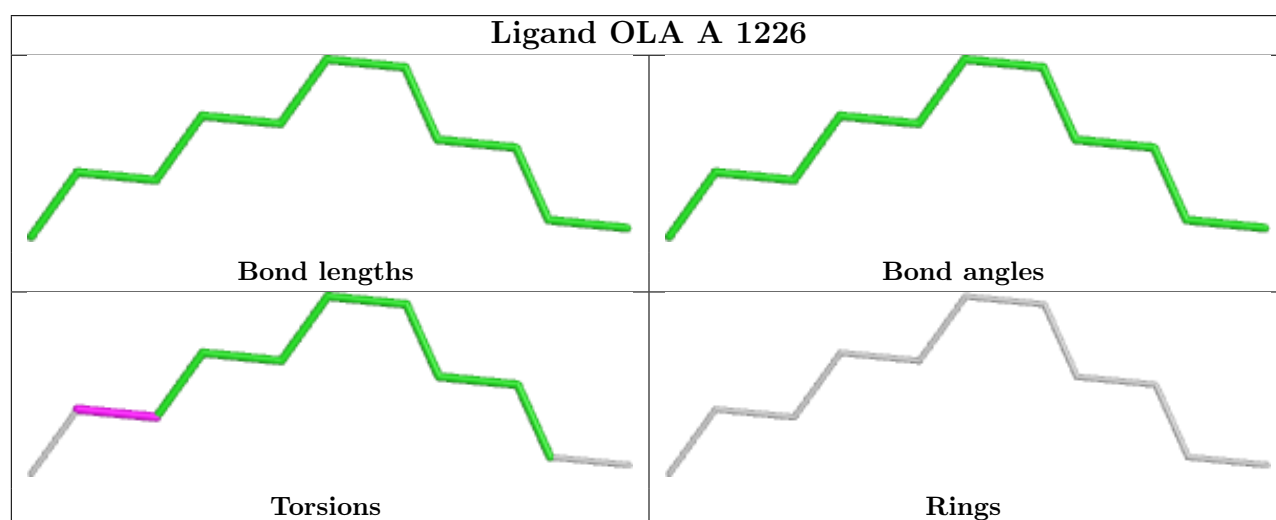
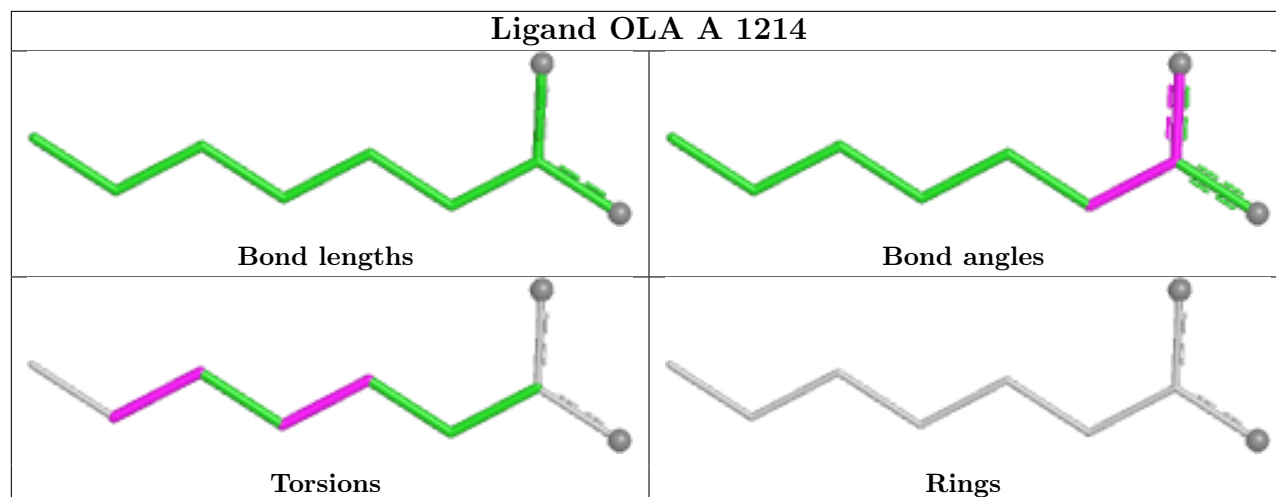


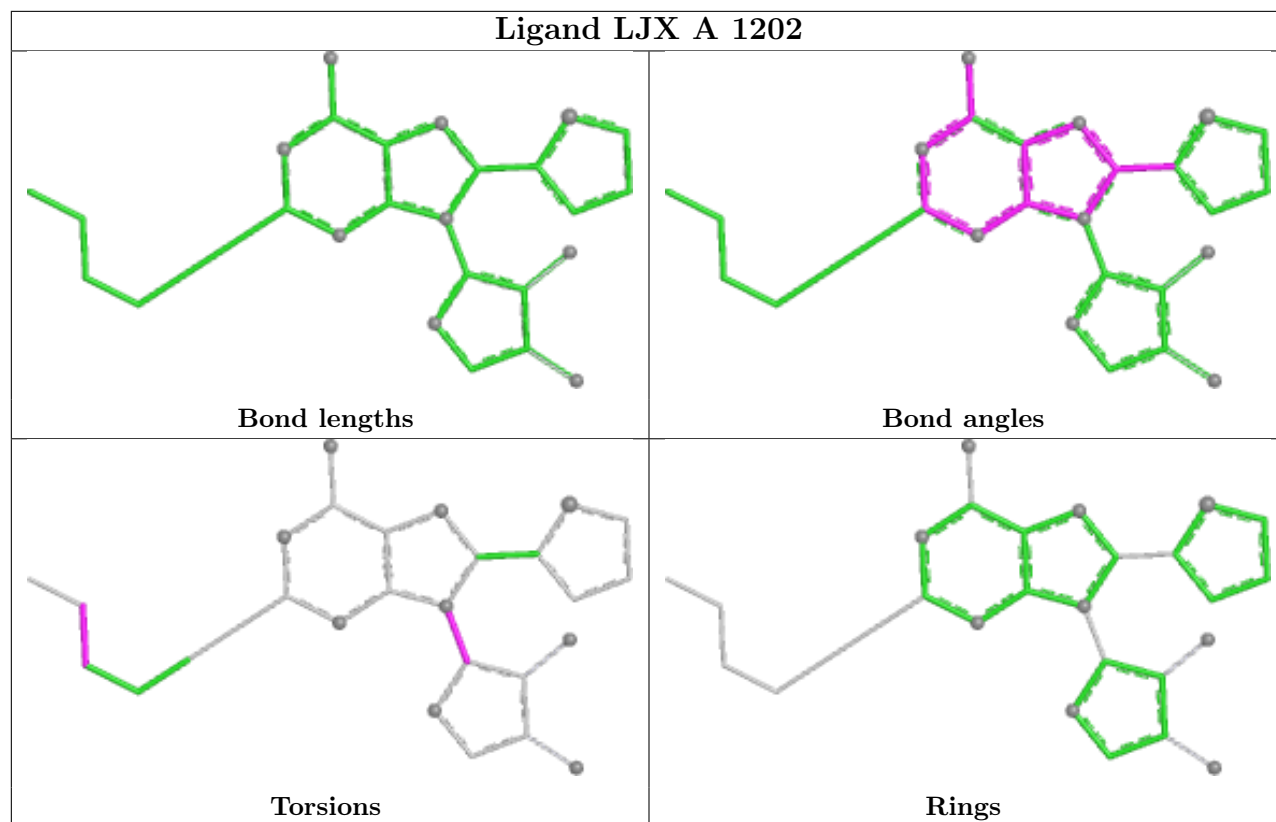












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/447 (88%)	0.34	33 (8%) 17 17	8, 28, 74, 108	8 (2%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	VAL	5.2
1	A	1010[A]	LEU	4.1
1	A	-3	ASP	3.9
1	A	1061	PHE	3.4
1	A	110	LEU	3.3
1	A	305	SER	3.3
1	A	29	TRP	3.2
1	A	290	TYR	3.2
1	A	-1	GLY	3.1
1	A	1021	ASP	2.9
1	A	1057	GLU	2.8
1	A	148	GLN	2.8
1	A	1003	LEU	2.7
1	A	1042	LYS	2.6
1	A	1055	SER	2.6
1	A	1058	MET	2.5
1	A	308	LEU	2.4
1	A	1105	TYR	2.4
1	A	208	LEU	2.4
1	A	157	GLN	2.3
1	A	1008	GLU	2.3
1	A	-2	ASP	2.3
1	A	1086	GLU	2.3
1	A	1056	PRO	2.3
1	A	1101	TYR	2.3
1	A	1	PRO	2.2
1	A	36	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	304	ARG	2.2
1	A	1063	HIS	2.1
1	A	1040	ALA	2.1
1	A	1028	ASP	2.0
1	A	300	ARG	2.0
1	A	306	HIS	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(Å ²)	Q<0.9
2	PEG	A	1236	7/7	0.63	0.19	71,72,78,78	0
6	OLA	A	1228	13/20	0.64	0.19	34,58,68,69	0
6	OLA	A	1230	7/20	0.69	0.16	62,65,74,77	0
2	PEG	A	1237	7/7	0.70	0.19	49,50,71,72	0
6	OLA	A	1215	17/20	0.70	0.19	50,55,68,71	0
6	OLA	A	1218	11/20	0.71	0.17	35,47,60,69	0
5	OLC	A	1204	25/25	0.72	0.16	43,49,67,84	0
6	OLA	A	1207	20/20	0.72	0.20	37,48,73,73	0
2	PEG	A	1201	7/7	0.72	0.16	58,69,81,85	0
5	OLC	A	1238	25/25	0.73	0.17	58,73,103,107	0
6	OLA	A	1208	20/20	0.75	0.16	56,65,80,82	0
5	OLC	A	1206	25/25	0.75	0.17	41,51,62,63	0
6	OLA	A	1217	15/20	0.75	0.16	61,66,80,81	0
6	OLA	A	1212	20/20	0.76	0.18	38,53,65,71	0
5	OLC	A	1240	25/25	0.76	0.17	54,71,81,88	0
2	PEG	A	1235	7/7	0.77	0.17	48,51,56,62	0
6	OLA	A	1219	11/20	0.78	0.16	37,44,49,52	0

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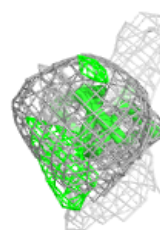
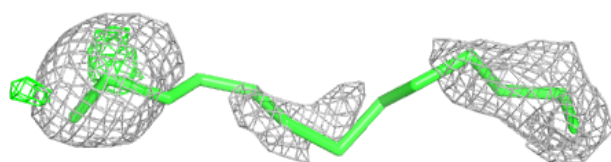
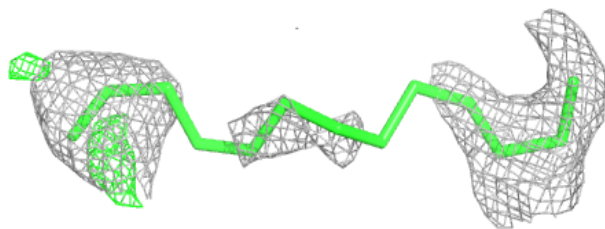
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OLC	A	1222	15/25	0.78	0.16	47,56,66,66	0
5	OLC	A	1223	10/25	0.78	0.15	45,55,62,63	0
6	OLA	A	1221	15/20	0.79	0.17	50,55,74,76	0
6	OLA	A	1225	15/20	0.79	0.14	49,59,65,68	0
6	OLA	A	1213	14/20	0.79	0.16	32,46,56,60	0
6	OLA	A	1229	9/20	0.79	0.14	47,54,61,62	0
6	OLA	A	1220	12/20	0.79	0.16	32,41,48,52	0
6	OLA	A	1216	12/20	0.80	0.18	30,55,73,75	0
6	OLA	A	1233	18/20	0.80	0.18	31,45,61,67	0
6	OLA	A	1224	19/20	0.81	0.15	31,41,58,61	0
5	OLC	A	1239	25/25	0.83	0.15	39,51,79,86	0
6	OLA	A	1227	10/20	0.83	0.16	52,57,62,74	0
6	OLA	A	1205	18/20	0.84	0.17	31,43,68,73	0
6	OLA	A	1231	20/20	0.85	0.15	36,46,59,61	0
6	OLA	A	1226	11/20	0.86	0.12	31,32,47,50	0
6	OLA	A	1214	9/20	0.88	0.10	34,40,43,52	0
6	OLA	A	1232	13/20	0.89	0.12	36,39,49,51	0
8	ETF	A	1234	6/6	0.89	0.11	36,41,43,43	0
7	CLR	A	1210	28/28	0.90	0.10	25,32,49,57	0
7	CLR	A	1209	28/28	0.93	0.09	23,27,55,66	0
7	CLR	A	1211	28/28	0.94	0.08	21,25,44,49	0
3	LJX	A	1202	28/28	0.95	0.08	11,16,29,30	0
4	NA	A	1203	1/1	0.99	0.14	27,27,27,27	0

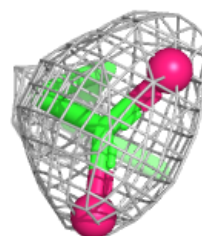
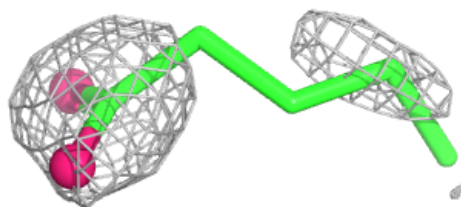
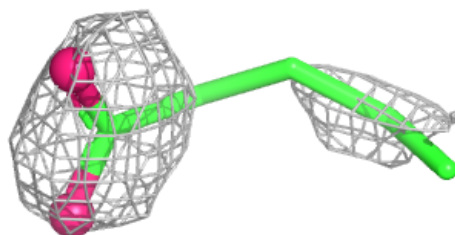
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1228:

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

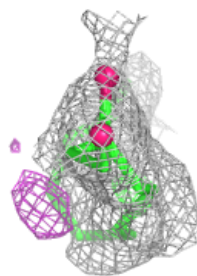
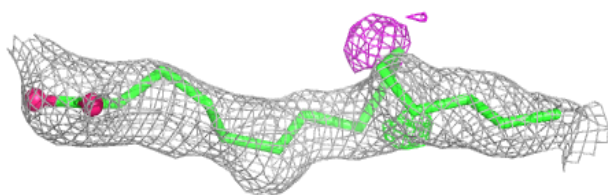
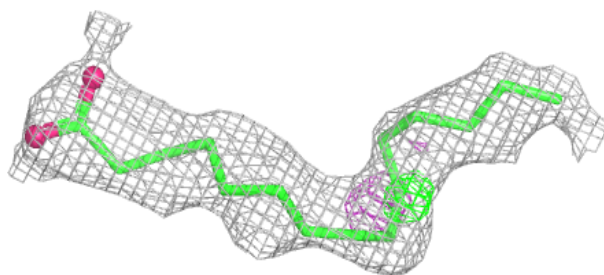
**Electron density around OLA A 1230:**

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and green (positive)

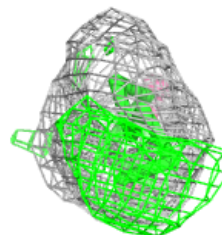
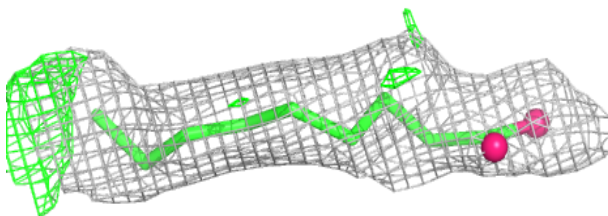
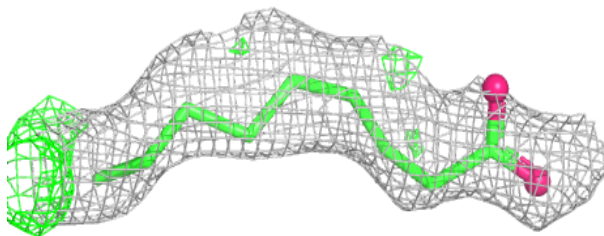


Electron density around OLA A 1215:

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and green (positive)

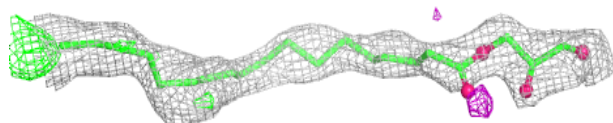
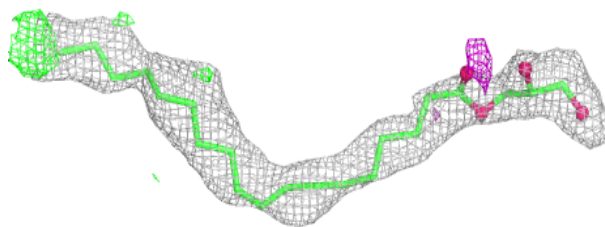
**Electron density around OLA A 1218:**

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and green (positive)

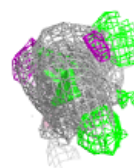
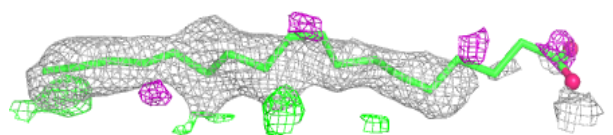
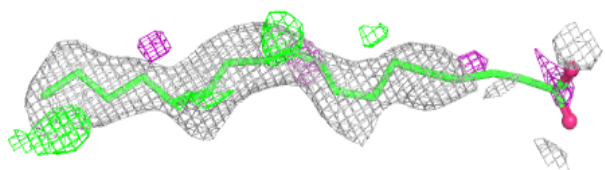


Electron density around OLC A 1204:

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and green (positive)

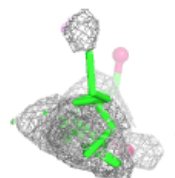
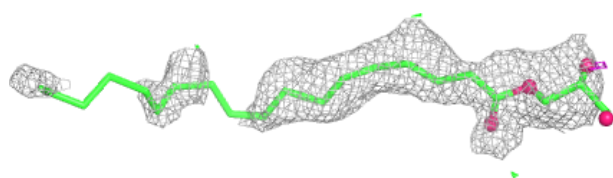
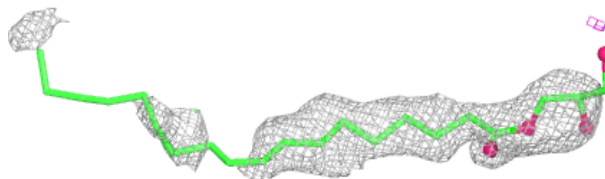
**Electron density around OLA A 1207:**

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and green (positive)

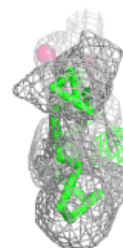
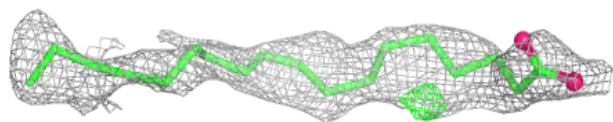
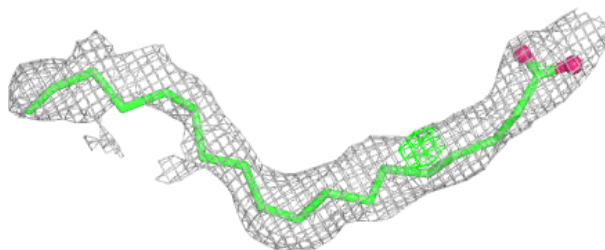


Electron density around OLC A 1238:

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and green (positive)

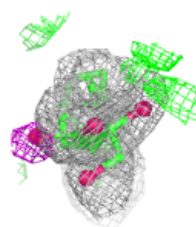
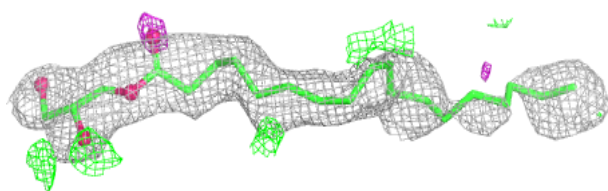
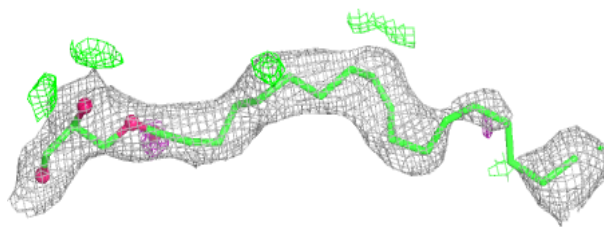
**Electron density around OLA A 1208:**

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

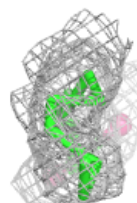
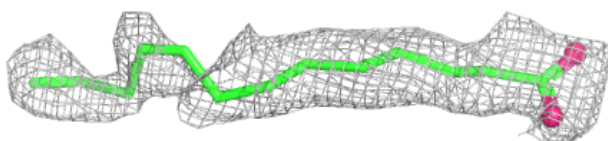
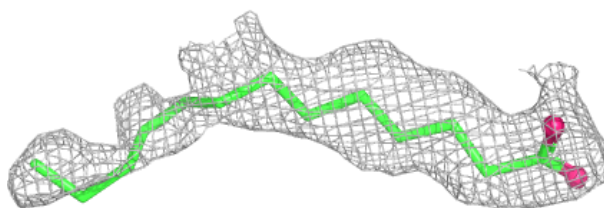


Electron density around OLC A 1206:

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

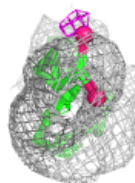
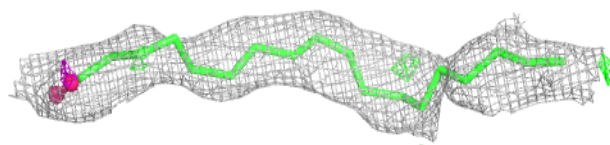
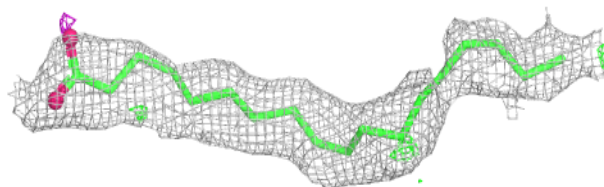
**Electron density around OLA A 1217:**

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

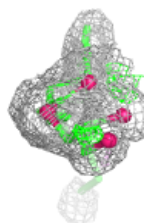
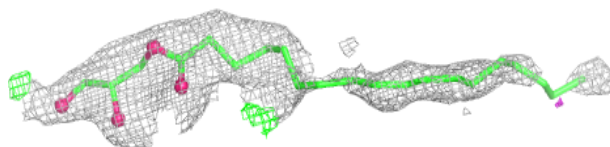
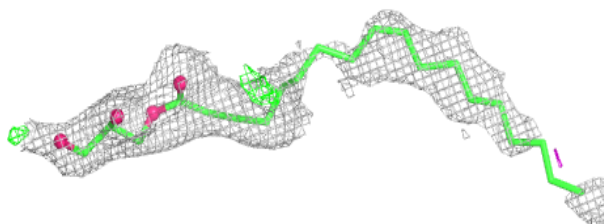


Electron density around OLA A 1212:

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

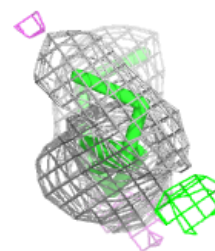
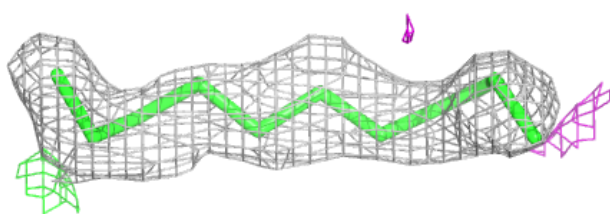
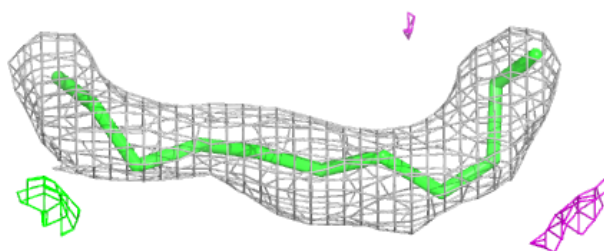
**Electron density around OLC A 1240:**

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

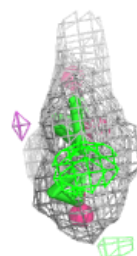
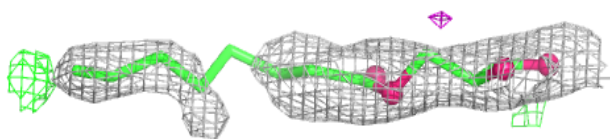
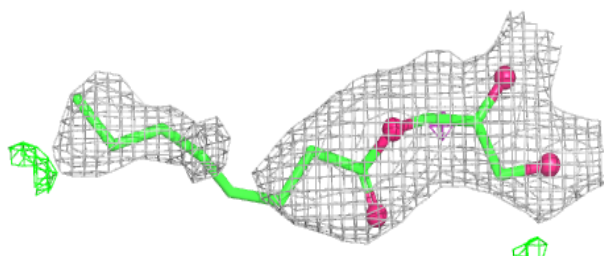


Electron density around OLA A 1219:

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

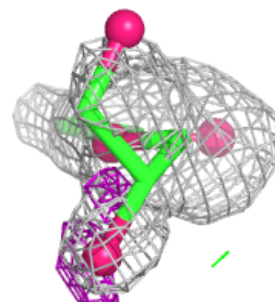
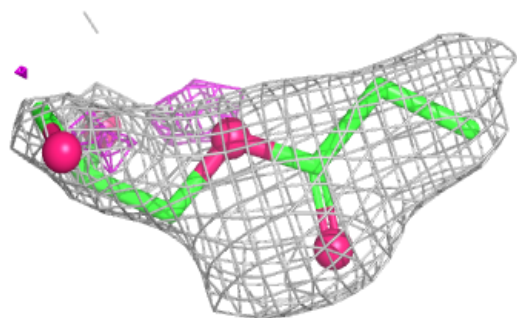
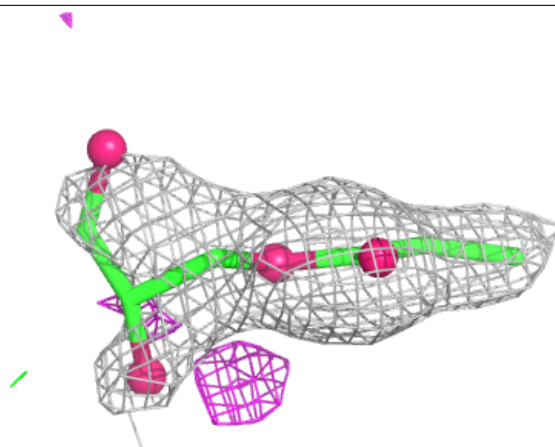
**Electron density around OLC A 1222:**

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

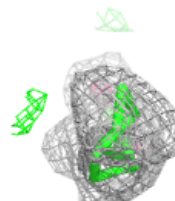
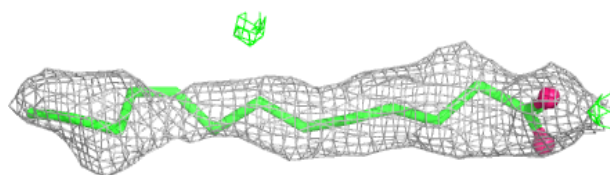
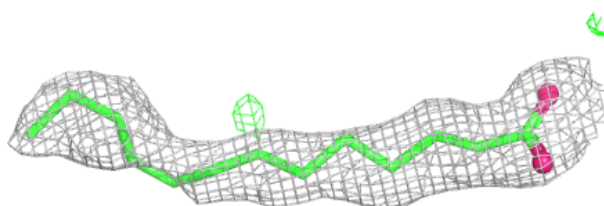


Electron density around OLC A 1223:

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

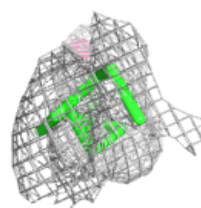
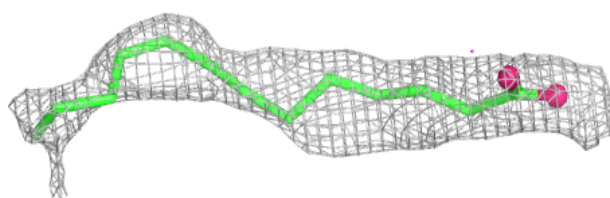
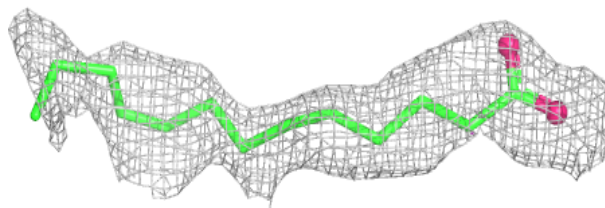
**Electron density around OLA A 1221:**

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

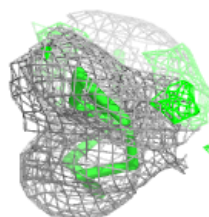
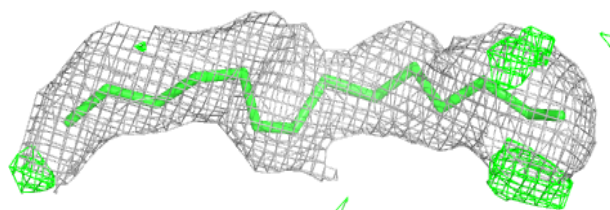
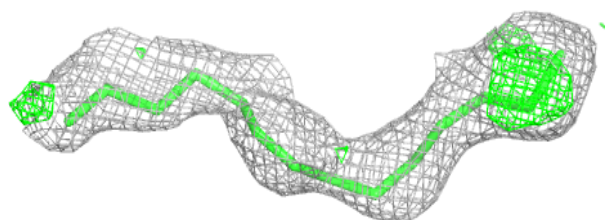


Electron density around OLA A 1225:

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

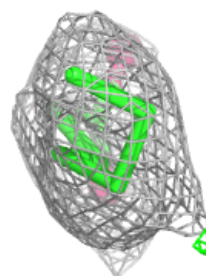
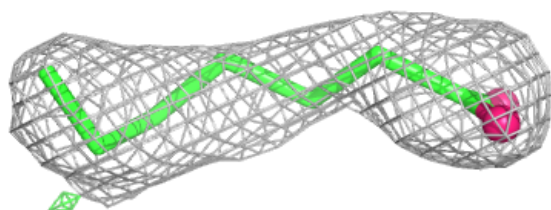
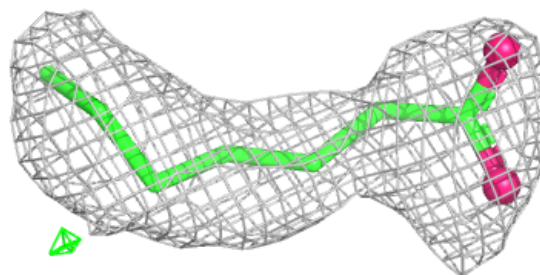
**Electron density around OLA A 1213:**

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

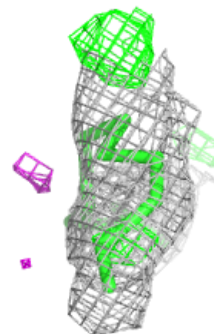
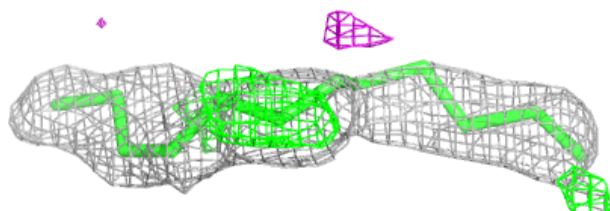
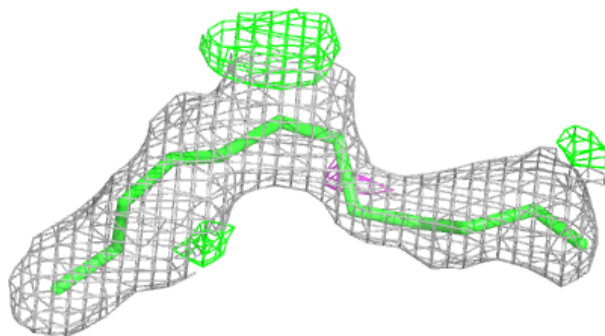


Electron density around OLA A 1229:

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

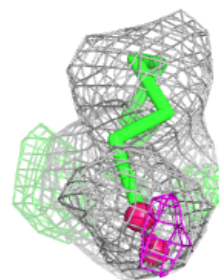
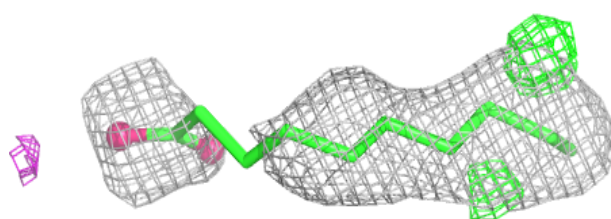
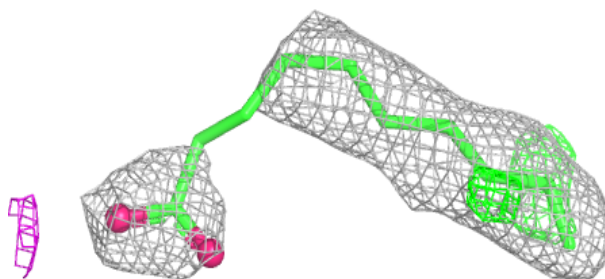
**Electron density around OLA A 1220:**

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

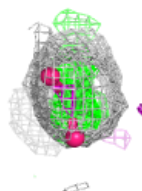
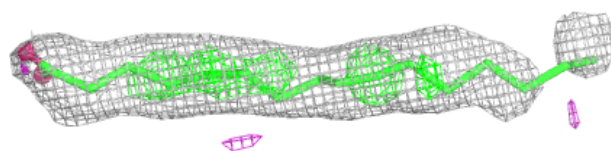
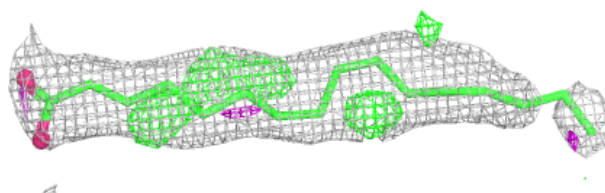


Electron density around OLA A 1216:

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

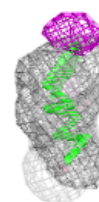
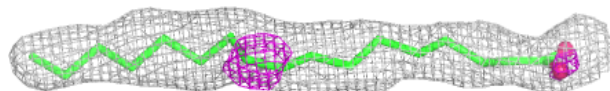
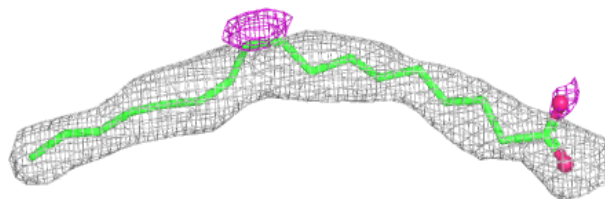
**Electron density around OLA A 1233:**

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

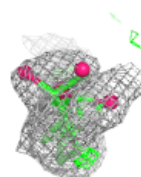
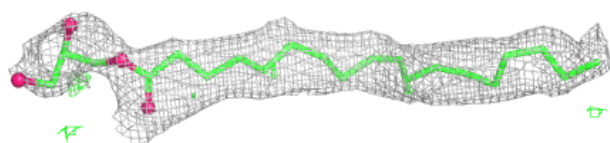
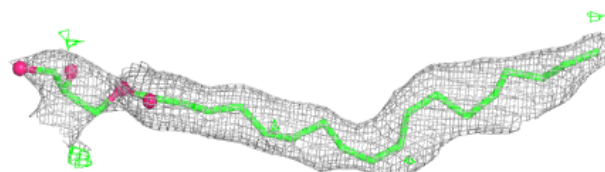


Electron density around OLA A 1224:

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

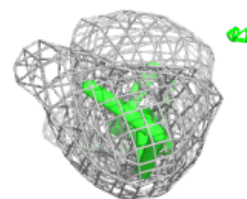
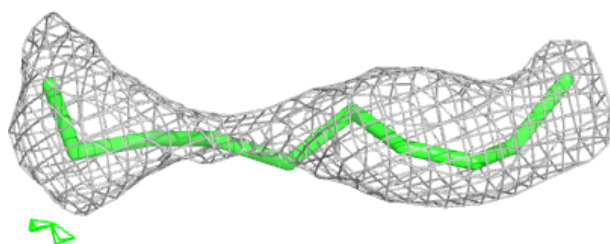
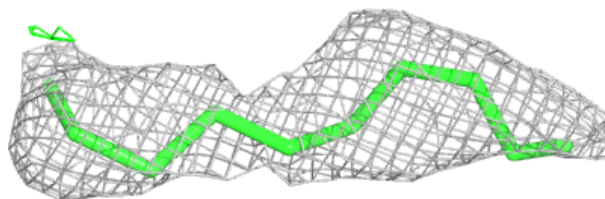
**Electron density around OLC A 1239:**

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

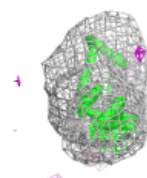
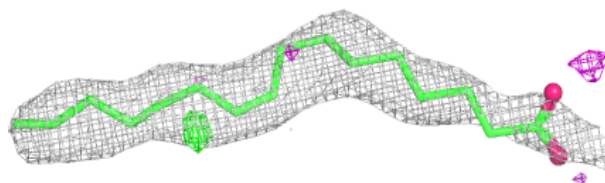


Electron density around OLA A 1227:

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

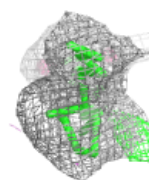
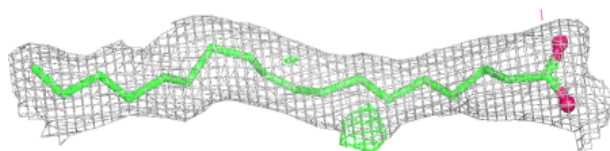
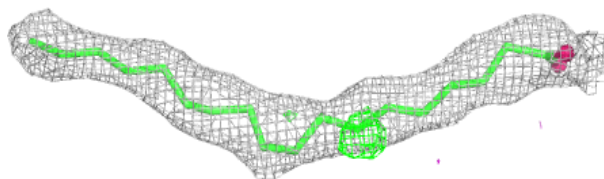
**Electron density around OLA A 1205:**

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

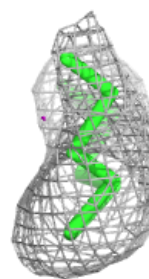
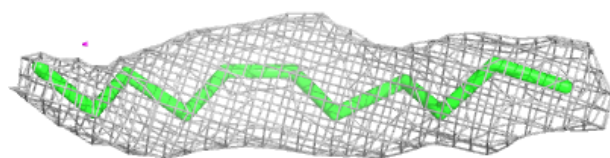
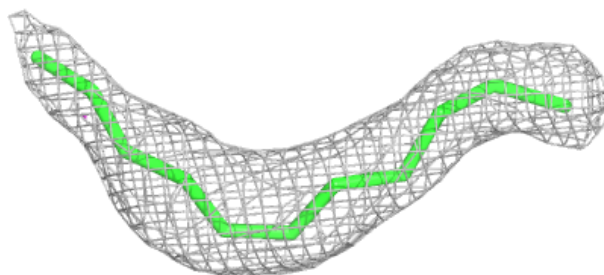


Electron density around OLA A 1231:

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

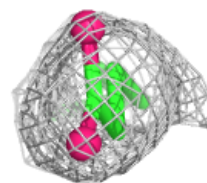
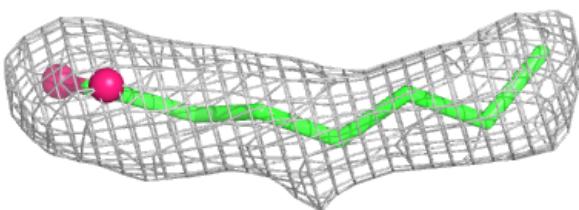
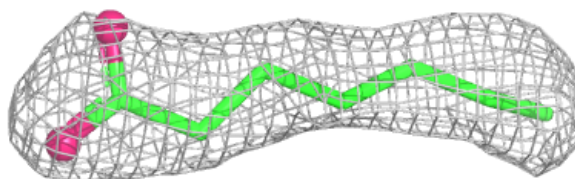
**Electron density around OLA A 1226:**

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

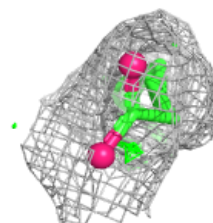
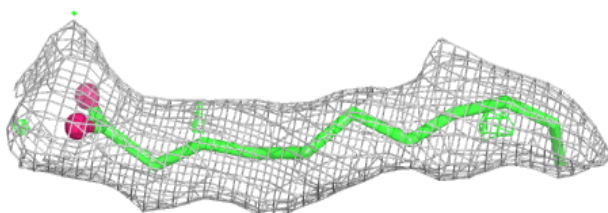
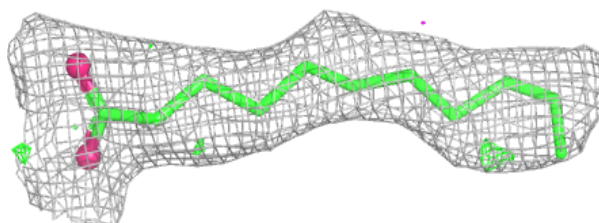


Electron density around OLA A 1214:

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

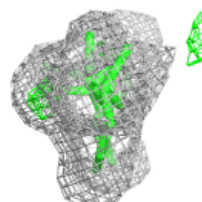
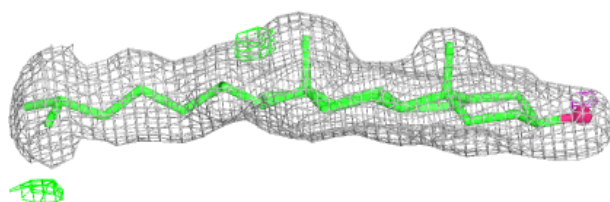
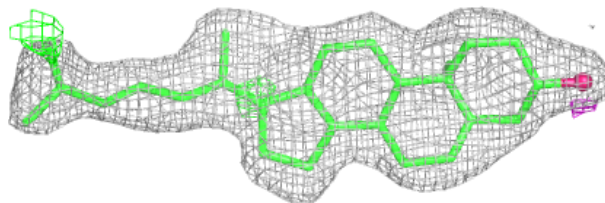
**Electron density around OLA A 1232:**

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

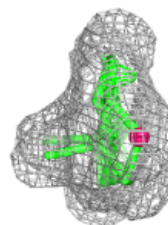
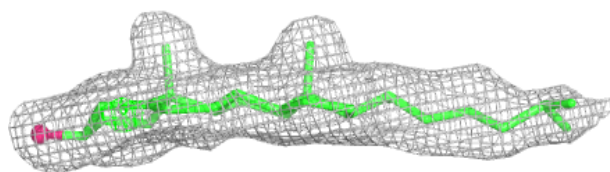
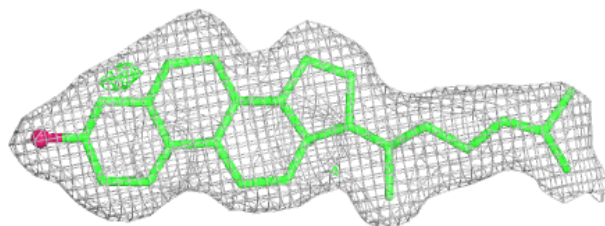


Electron density around CLR A 1210:

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

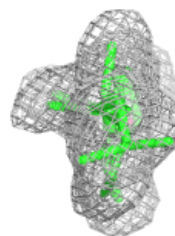
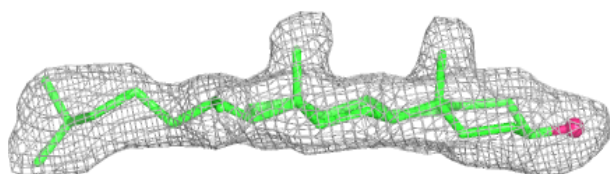
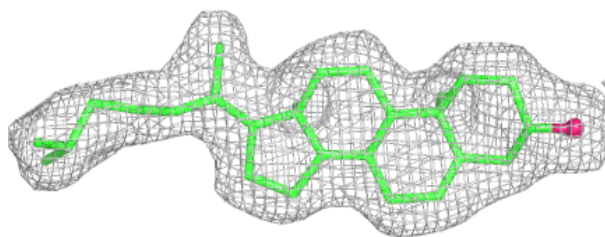
**Electron density around CLR A 1209:**

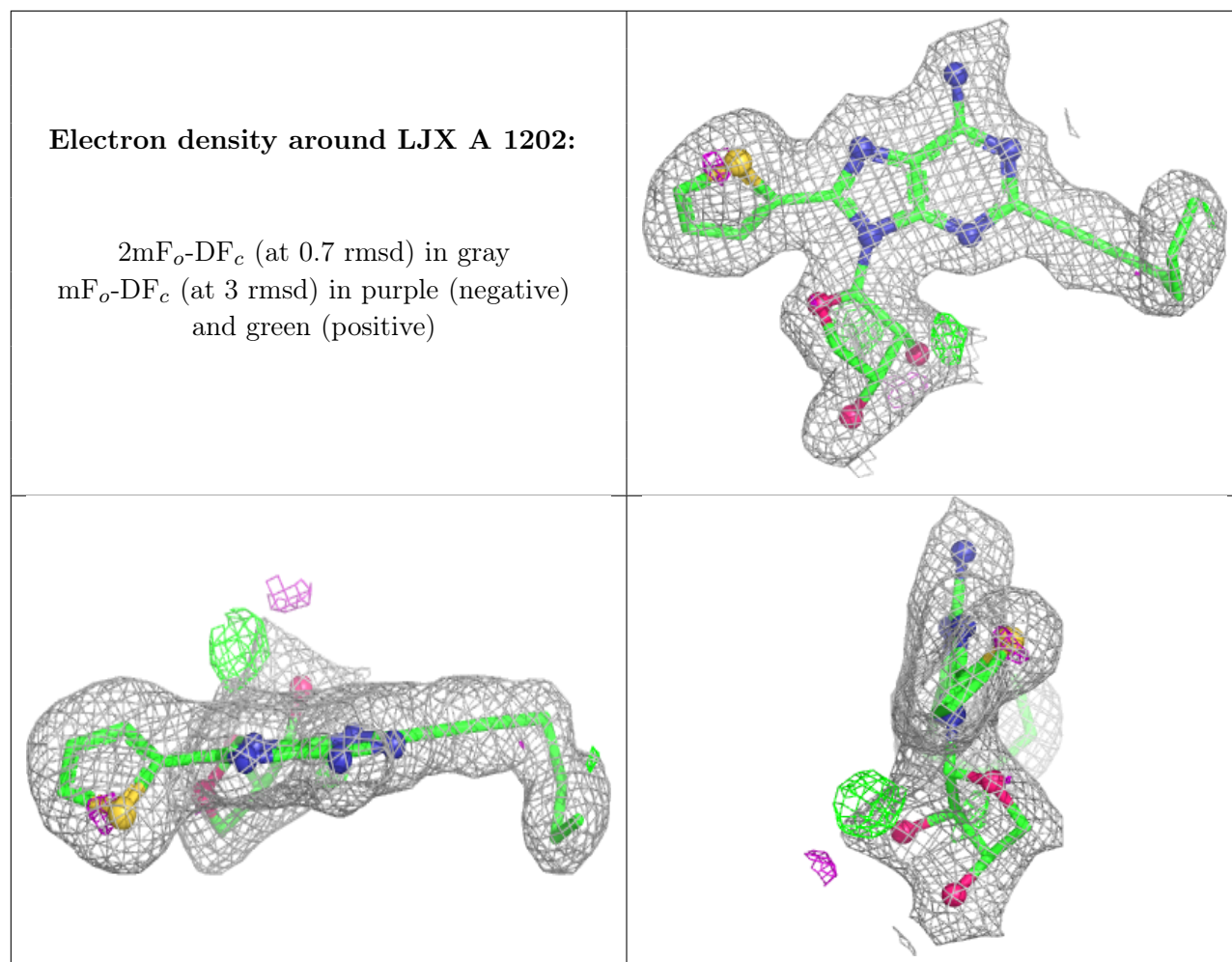
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLR A 1211:

$2mF_o-DF_c$ (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.