



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:21 am BST

PDB ID : 5OM4  
Title : Structure of the A2A-StaR2-bRIL562-Compound 4e complex at 1.86Å obtained from in meso soaking experiments (24 hour soak).  
Authors : Rucktooa, P.; Cheng, R.K.Y.; Segala, E.; Geng, T.; Errey, J.C.; Brown, G.A.; Cooke, R.; Marshall, F.H.; Dore, A.S.  
Deposited on : 2017-07-28  
Resolution : 2.00 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.

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

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

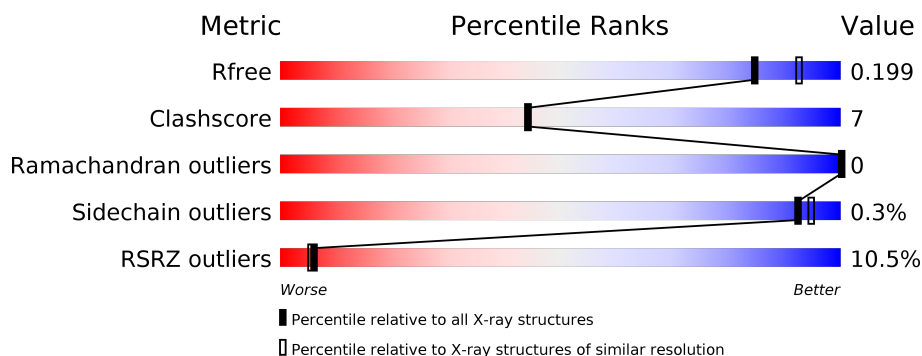
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	434	<div> <div>9%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CLR	A	1203	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3824 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,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	9	0
			3076	2005	521	528	22			

There are 34 discrepancies between the modelled and reference sequences:

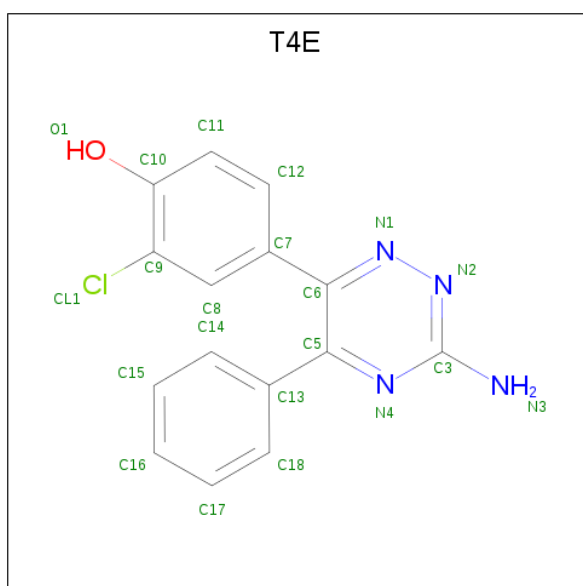
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
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
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-(3-amino-5-phenyl-1,2,4-triazin-6-yl)-2-chlorophenol (three-letter code: T4E) (formula: C<sub>15</sub>H<sub>11</sub>ClN<sub>4</sub>O).

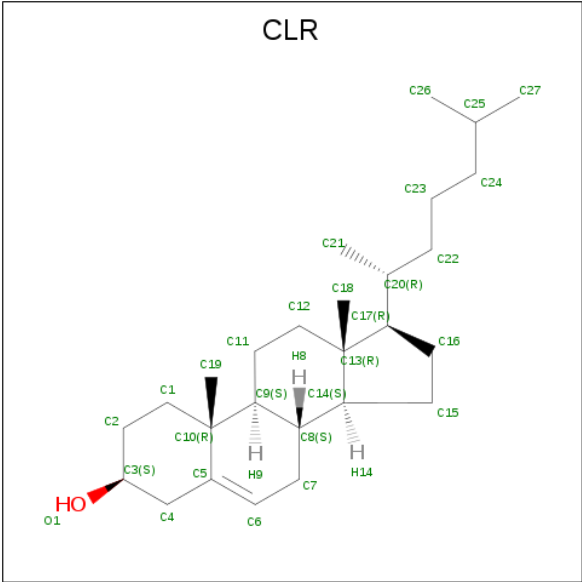


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	
			21	15	1	4	1	

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

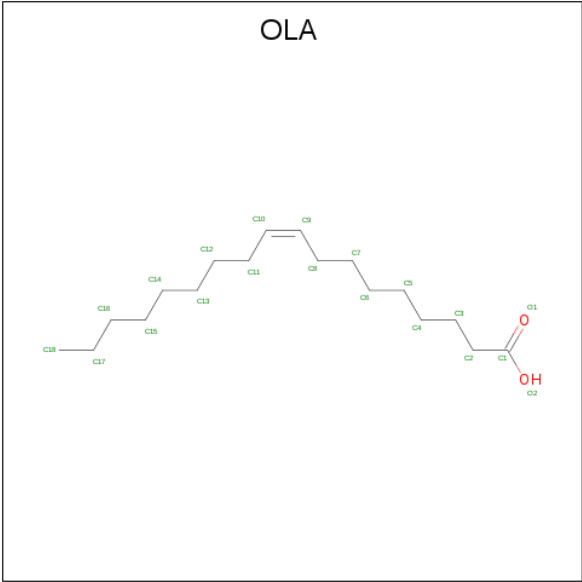
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na		
			1	1	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



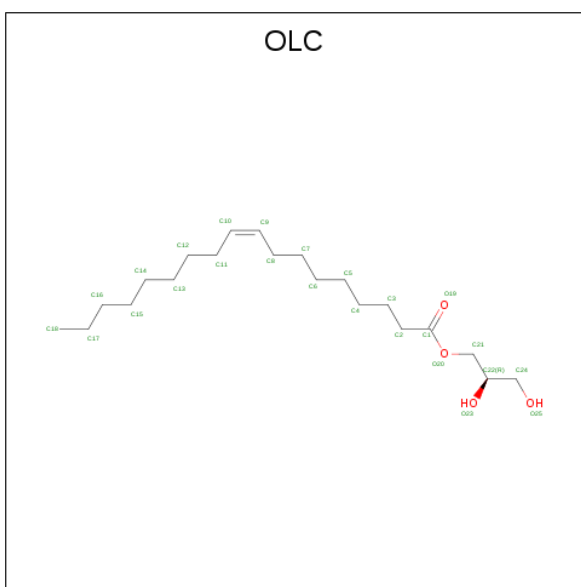
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



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

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 19	C 15	O 4	0	0
6	A	1	Total 16	C 12	O 4	0	0
6	A	1	Total 22	C 18	O 4	0	0
6	A	1	Total 25	C 21	O 4	0	0
6	A	1	Total 25	C 21	O 4	0	0
6	A	1	Total 24	C 20	O 4	0	0
6	A	1	Total 17	C 13	O 4	0	0
6	A	1	Total 14	C 14		0	0
6	A	1	Total 25	C 21	O 4	0	0
6	A	1	Total 17	C 13	O 4	0	0
6	A	1	Total 17	C 13	O 4	0	0

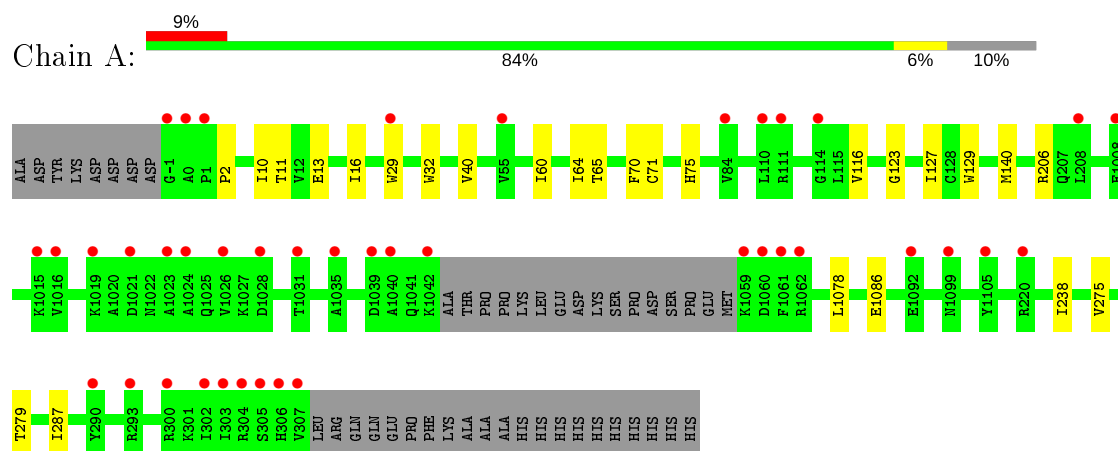
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	156	Total O 156 156	0	0

### 3 Residue-property plots [i](#)

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

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.47Å 179.11Å 140.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.92 – 2.00 32.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (32.92-2.00) 98.3 (32.92-2.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.12rc2_2821: ???)	Depositor
R, $R_{free}$	0.183 , 0.205 0.181 , 0.199	Depositor DCC
$R_{free}$ test set	1679 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLC, CLR, T4E, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/3143	0.39	0/4276

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3076	0	3140	28	0
2	A	21	0	10	0	0
3	A	1	0	0	0	0
4	A	112	0	184	9	0
5	A	237	0	362	20	0
6	A	221	0	320	28	0
7	A	156	0	0	2	0
All	All	3824	0	4016	51	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 7.

All (51) 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)
4:A:1203:CLR:C19	6:A:1232:OLC:H2	2.08	0.82
1:A:71:CYS:O	6:A:1227:OLC:H24A	1.85	0.77
4:A:1203:CLR:H191	6:A:1232:OLC:H2	1.68	0.76
1:A:65:THR:HG21	6:A:1227:OLC:H5	1.74	0.70
1:A:29[B]:TRP:HZ3	5:A:1219:OLA:H61	1.57	0.70
1:A:127:ILE:HG12	5:A:1210:OLA:H82	1.75	0.68
1:A:140[A]:MET:HE2	6:A:1232:OLC:H4	1.77	0.64
1:A:2:PRO:HB2	6:A:1231:OLC:H2	1.86	0.58
1:A:140[A]:MET:CE	6:A:1232:OLC:H4	2.33	0.58
1:A:75:HIS:ND1	6:A:1232:OLC:H21A	2.18	0.58
5:A:1210:OLA:C14	6:A:1226:OLC:H12	2.33	0.57
4:A:1203:CLR:H191	6:A:1232:OLC:C2	2.34	0.57
1:A:70:PHE:HD2	6:A:1227:OLC:H24A	1.70	0.57
1:A:123:GLY:HA3	5:A:1210:OLA:H22	1.89	0.54
5:A:1207:OLA:H22	5:A:1217:OLA:C2	2.37	0.53
1:A:70:PHE:HD2	6:A:1227:OLC:C24	2.23	0.52
4:A:1203:CLR:H42	6:A:1232:OLC:O20	2.11	0.51
1:A:16:ILE:HD11	1:A:275[A]:VAL:HG13	1.92	0.51
1:A:75:HIS:CG	6:A:1232:OLC:H21A	2.46	0.51
5:A:1210:OLA:H142	6:A:1226:OLC:H12	1.93	0.51
4:A:1203:CLR:H192	6:A:1232:OLC:H2	1.93	0.50
1:A:279[A]:THR:HG23	5:A:1213:OLA:H131	1.94	0.50
5:A:1207:OLA:H22	5:A:1217:OLA:H22	1.92	0.49
5:A:1217:OLA:H61	6:A:1225:OLC:H5A	1.96	0.48
1:A:32:TRP:CE3	5:A:1219:OLA:H71	2.49	0.48
1:A:1078:LEU:HD13	1:A:1086:GLU:HG2	1.96	0.48
4:A:1203:CLR:H162	4:A:1203:CLR:H222	1.61	0.47
1:A:40:VAL:HG11	1:A:116:VAL:HG12	1.96	0.47
5:A:1221:OLA:H141	5:A:1221:OLA:H171	1.72	0.46
1:A:127:ILE:HD13	6:A:1226:OLC:H6	1.97	0.45
5:A:1210:OLA:H151	6:A:1226:OLC:H12	1.98	0.45
1:A:70:PHE:CD2	6:A:1227:OLC:H24A	2.49	0.45
1:A:238:ILE:HD11	1:A:287:ILE:HB	1.99	0.45
4:A:1206:CLR:H263	4:A:1206:CLR:H231	1.84	0.45
4:A:1203:CLR:H191	6:A:1232:OLC:H3A	2.01	0.43
4:A:1203:CLR:H12	4:A:1204:CLR:H6	2.01	0.43
1:A:275[B]:VAL:HG21	5:A:1211:OLA:H82	2.00	0.43
6:A:1225:OLC:H4	6:A:1227:OLC:H2	2.00	0.43
1:A:129:TRP:CE2	6:A:1228:OLC:H7A	2.54	0.43
5:A:1210:OLA:H131	6:A:1226:OLC:H11A	2.00	0.42
6:A:1225:OLC:H21A	7:A:1338:HOH:O	2.18	0.42
6:A:1232:OLC:H2A	7:A:1329:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1207:OLA:H22	5:A:1217:OLA:H21	2.02	0.42
5:A:1210:OLA:H122	6:A:1226:OLC:H8	2.02	0.42
1:A:11:THR:HG23	5:A:1208:OLA:H72	2.02	0.42
5:A:1217:OLA:H152	6:A:1225:OLC:H14A	2.02	0.42
1:A:29[A]:TRP:CD1	5:A:1219:OLA:H112	2.55	0.41
1:A:29[A]:TRP:NE1	5:A:1219:OLA:H112	2.36	0.41
1:A:10:ILE:HG12	1:A:64:ILE:HG23	2.03	0.41
1:A:13:GLU:HB3	1:A:60:ILE:HG23	2.03	0.40
1:A:65:THR:HG22	1:A:70:PHE:CE1	2.56	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	393/434 (91%)	391 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/353 (91%)	320 (100%)	1 (0%)	92	95

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

Mol	Chain	Res	Type
1	A	206	ARG

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 1 is monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	OLA	A	1214	-	8,11,19	0.47	0	7,11,19	0.44	0
5	OLA	A	1218	-	8,8,19	0.48	0	7,7,19	0.49	0
4	CLR	A	1203	-	31,31,31	0.69	0	48,48,48	1.16	4 (8%)
5	OLA	A	1221	-	8,8,19	0.46	0	7,7,19	0.17	0
5	OLA	A	1219	-	15,18,19	0.43	0	14,18,19	0.24	0
6	OLC	A	1223	-	18,18,24	1.01	2 (11%)	18,19,25	1.17	2 (11%)
4	CLR	A	1205	-	31,31,31	0.71	0	48,48,48	0.80	0
5	OLA	A	1217	-	16,19,19	0.41	0	15,19,19	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	OLC	A	1225	-	21,21,24	0.93	1 (4%)	22,22,25	1.03	2 (9%)
6	OLC	A	1228	-	23,23,24	0.98	1 (4%)	24,24,25	1.05	1 (4%)
6	OLC	A	1233	-	16,16,24	1.15	2 (12%)	17,17,25	1.54	2 (11%)
4	CLR	A	1204	-	31,31,31	0.68	0	48,48,48	1.06	5 (10%)
5	OLA	A	1209	-	5,8,19	0.25	0	4,8,19	0.19	0
6	OLC	A	1227	-	24,24,24	0.87	1 (4%)	25,25,25	1.27	2 (8%)
2	T4E	A	1201	-	23,23,23	2.14	8 (34%)	32,32,32	2.82	8 (25%)
6	OLC	A	1232	-	16,16,24	1.06	1 (6%)	17,17,25	1.56	2 (11%)
5	OLA	A	1208	-	16,19,19	0.41	0	15,19,19	0.27	0
4	CLR	A	1206	-	31,31,31	0.73	0	48,48,48	0.89	0
5	OLA	A	1207	-	16,19,19	0.41	0	15,19,19	0.25	0
5	OLA	A	1211	-	14,17,19	0.41	0	13,17,19	0.26	0
6	OLC	A	1224	-	15,15,24	1.13	2 (13%)	16,16,25	0.91	1 (6%)
5	OLA	A	1220	-	11,11,19	0.41	0	9,10,19	0.28	0
5	OLA	A	1215	-	8,11,19	0.49	0	7,11,19	0.46	0
6	OLC	A	1231	-	24,24,24	0.93	1 (4%)	25,25,25	1.24	2 (8%)
5	OLA	A	1213	-	12,12,19	0.47	0	11,11,19	0.27	0
6	OLC	A	1229	-	16,16,24	1.09	1 (6%)	17,17,25	1.16	1 (5%)
5	OLA	A	1210	-	16,19,19	0.43	0	15,19,19	0.25	0
5	OLA	A	1222	-	16,19,19	0.41	0	15,19,19	0.28	0
6	OLC	A	1230	-	13,13,24	0.18	0	12,12,25	0.61	0
6	OLC	A	1226	-	24,24,24	0.91	1 (4%)	25,25,25	0.80	1 (4%)
5	OLA	A	1212	-	10,13,19	0.41	0	8,13,19	0.32	0
5	OLA	A	1216	-	9,9,19	0.44	0	7,8,19	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	1214	-	-	4/7/9/17	-
5	OLA	A	1218	-	-	2/6/6/17	-
4	CLR	A	1203	-	-	8/10/68/68	0/4/4/4
5	OLA	A	1221	-	-	3/6/6/17	-
5	OLA	A	1219	-	-	2/14/16/17	-
6	OLC	A	1223	-	-	12/18/18/24	-
4	CLR	A	1205	-	-	1/10/68/68	0/4/4/4
5	OLA	A	1217	-	-	11/15/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLC	A	1225	-	-	8/21/21/24	-
6	OLC	A	1228	-	-	7/23/23/24	-
6	OLC	A	1233	-	-	8/16/16/24	-
4	CLR	A	1204	-	-	0/10/68/68	0/4/4/4
5	OLA	A	1209	-	-	1/4/6/17	-
6	OLC	A	1227	-	-	11/24/24/24	-
2	T4E	A	1201	-	-	0/8/8/8	0/3/3/3
6	OLC	A	1232	-	-	6/16/16/24	-
5	OLA	A	1208	-	-	6/15/17/17	-
4	CLR	A	1206	-	-	1/10/68/68	0/4/4/4
5	OLA	A	1207	-	-	9/15/17/17	-
5	OLA	A	1211	-	-	9/13/15/17	-
6	OLC	A	1224	-	-	7/15/15/24	-
5	OLA	A	1220	-	-	7/9/9/17	-
5	OLA	A	1215	-	-	5/7/9/17	-
6	OLC	A	1231	-	-	9/24/24/24	-
5	OLA	A	1213	-	-	4/10/10/17	-
6	OLC	A	1229	-	-	5/16/16/24	-
5	OLA	A	1210	-	-	7/15/17/17	-
5	OLA	A	1222	-	-	12/15/17/17	-
6	OLC	A	1230	-	-	6/11/11/24	-
6	OLC	A	1226	-	-	8/24/24/24	-
5	OLA	A	1212	-	-	4/9/11/17	-
5	OLA	A	1216	-	-	4/7/7/17	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	T4E	C3-N2	5.07	1.41	1.35
6	A	1231	OLC	O20-C1	4.40	1.46	1.33
6	A	1228	OLC	O20-C1	4.24	1.45	1.33
6	A	1226	OLC	O20-C1	4.04	1.45	1.33
6	A	1232	OLC	O20-C1	3.78	1.44	1.33
6	A	1229	OLC	O20-C1	3.75	1.44	1.33
6	A	1225	OLC	O20-C1	3.72	1.44	1.33
6	A	1233	OLC	O20-C1	3.66	1.44	1.33
6	A	1224	OLC	O20-C1	3.46	1.43	1.33
6	A	1227	OLC	O20-C1	3.45	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	T4E	C6-N1	3.38	1.39	1.33
6	A	1223	OLC	O20-C1	3.32	1.43	1.33
2	A	1201	T4E	C12-C11	3.06	1.44	1.38
2	A	1201	T4E	N1-N2	-2.96	1.26	1.34
2	A	1201	T4E	C3-N3	2.82	1.39	1.33
2	A	1201	T4E	C13-C5	2.80	1.52	1.49
2	A	1201	T4E	C5-N4	2.42	1.38	1.34
6	A	1224	OLC	O20-C21	-2.31	1.39	1.45
2	A	1201	T4E	C3-N4	2.26	1.39	1.35
6	A	1223	OLC	O20-C21	-2.13	1.40	1.45
6	A	1233	OLC	O20-C21	-2.01	1.40	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	T4E	N4-C3-N2	-8.69	119.64	125.57
2	A	1201	T4E	C5-C6-N1	-7.48	115.44	119.87
2	A	1201	T4E	C8-C9-C10	5.69	124.21	120.91
2	A	1201	T4E	C3-N2-N1	5.10	121.08	117.38
6	A	1232	OLC	O20-C1-C2	4.50	126.04	111.91
6	A	1227	OLC	O20-C1-C2	4.19	125.06	111.91
6	A	1231	OLC	O20-C1-C2	4.17	125.00	111.91
6	A	1233	OLC	O20-C1-C2	4.16	124.95	111.91
2	A	1201	T4E	C6-N1-N2	3.98	124.77	120.43
6	A	1232	OLC	O20-C1-O19	-3.93	113.69	123.59
2	A	1201	T4E	C7-C6-N1	3.83	119.54	114.44
6	A	1233	OLC	O20-C1-O19	-3.42	114.97	123.59
2	A	1201	T4E	N3-C3-N2	3.35	120.43	117.26
6	A	1228	OLC	O20-C1-C2	3.32	122.32	111.91
6	A	1223	OLC	O20-C1-C2	3.14	121.77	111.91
6	A	1229	OLC	O20-C1-C2	2.96	121.19	111.91
6	A	1223	OLC	O20-C1-O19	-2.88	116.32	123.59
6	A	1227	OLC	O20-C1-O19	-2.88	116.33	123.59
4	A	1203	CLR	C1-C2-C3	2.84	114.11	110.47
6	A	1225	OLC	O20-C1-C2	2.82	120.75	111.91
6	A	1231	OLC	O20-C1-O19	-2.71	116.74	123.59
4	A	1204	CLR	C18-C13-C17	-2.60	106.87	111.71
4	A	1204	CLR	C12-C13-C17	2.33	120.06	116.57
4	A	1203	CLR	C12-C13-C17	2.20	119.87	116.57
6	A	1226	OLC	O20-C1-C2	2.20	118.81	111.91
4	A	1204	CLR	C7-C8-C14	-2.17	107.76	110.91
2	A	1201	T4E	C11-C10-C9	-2.15	116.46	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1204	CLR	C4-C5-C10	2.15	119.27	116.42
4	A	1204	CLR	C4-C5-C6	-2.09	117.59	120.61
4	A	1203	CLR	C1-C10-C9	2.08	111.64	108.73
6	A	1225	OLC	O20-C1-O19	-2.07	118.37	123.59
6	A	1224	OLC	O20-C1-C2	2.05	118.34	111.91
4	A	1203	CLR	C8-C7-C6	-2.02	109.84	112.73

There are no chirality outliers.

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1203	CLR	C13-C17-C20-C21
4	A	1203	CLR	C16-C17-C20-C22
6	A	1223	OLC	C9-C10-C11-C12
5	A	1217	OLA	C1-C2-C3-C4
6	A	1233	OLC	O20-C21-C22-C24
6	A	1232	OLC	O20-C21-C22-O23
5	A	1220	OLA	C9-C10-C11-C12
5	A	1211	OLA	C1-C2-C3-C4
6	A	1224	OLC	C21-C22-C24-O25
5	A	1215	OLA	C1-C2-C3-C4
5	A	1222	OLA	C1-C2-C3-C4
5	A	1212	OLA	C1-C2-C3-C4
6	A	1229	OLC	O19-C1-O20-C21
4	A	1203	CLR	C16-C17-C20-C21
4	A	1203	CLR	C13-C17-C20-C22
6	A	1229	OLC	C2-C1-O20-C21
6	A	1232	OLC	C2-C1-O20-C21
5	A	1213	OLA	C14-C15-C16-C17
5	A	1219	OLA	C3-C4-C5-C6
6	A	1231	OLC	C14-C15-C16-C17
5	A	1222	OLA	C13-C14-C15-C16
6	A	1232	OLC	O19-C1-O20-C21
6	A	1231	OLC	O20-C21-C22-C24
5	A	1221	OLA	C14-C15-C16-C17
6	A	1224	OLC	O23-C22-C24-O25
6	A	1223	OLC	C1-C2-C3-C4
6	A	1227	OLC	C1-C2-C3-C4
6	A	1233	OLC	O20-C21-C22-O23
6	A	1231	OLC	O20-C21-C22-O23
6	A	1229	OLC	C1-C2-C3-C4
4	A	1205	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
5	A	1214	OLA	C2-C3-C4-C5
5	A	1208	OLA	C14-C15-C16-C17
5	A	1211	OLA	C5-C6-C7-C8
5	A	1220	OLA	C5-C6-C7-C8
5	A	1207	OLA	C14-C15-C16-C17
5	A	1208	OLA	C12-C13-C14-C15
5	A	1217	OLA	C11-C12-C13-C14
6	A	1227	OLC	C12-C13-C14-C15
5	A	1215	OLA	C2-C3-C4-C5
4	A	1206	CLR	C22-C23-C24-C25
5	A	1217	OLA	C13-C14-C15-C16
6	A	1226	OLC	C5-C6-C7-C8
5	A	1221	OLA	C13-C14-C15-C16
5	A	1220	OLA	C3-C4-C5-C6
5	A	1207	OLA	C13-C14-C15-C16
5	A	1222	OLA	C4-C5-C6-C7
5	A	1212	OLA	C3-C4-C5-C6
6	A	1223	OLC	C21-C22-C24-O25
6	A	1227	OLC	C21-C22-C24-O25
5	A	1222	OLA	C10-C11-C12-C13
6	A	1226	OLC	C10-C11-C12-C13
5	A	1218	OLA	C5-C6-C7-C8
5	A	1217	OLA	C4-C5-C6-C7
5	A	1215	OLA	C3-C4-C5-C6
6	A	1223	OLC	C2-C3-C4-C5
5	A	1210	OLA	C3-C4-C5-C6
5	A	1209	OLA	C3-C4-C5-C6
6	A	1227	OLC	C14-C15-C16-C17
5	A	1207	OLA	C2-C3-C4-C5
5	A	1207	OLA	C4-C5-C6-C7
5	A	1214	OLA	C4-C5-C6-C7
5	A	1211	OLA	C2-C3-C4-C5
5	A	1210	OLA	C11-C12-C13-C14
6	A	1223	OLC	O23-C22-C24-O25
6	A	1227	OLC	O23-C22-C24-O25
5	A	1220	OLA	C2-C3-C4-C5
5	A	1222	OLA	C12-C13-C14-C15
5	A	1214	OLA	C6-C7-C8-C9
5	A	1207	OLA	C10-C11-C12-C13
5	A	1214	OLA	C3-C4-C5-C6
4	A	1203	CLR	C22-C23-C24-C25
5	A	1215	OLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	A	1223	OLC	C2-C1-O20-C21
6	A	1233	OLC	C2-C1-O20-C21
6	A	1228	OLC	C11-C12-C13-C14
6	A	1233	OLC	C5-C6-C7-C8
5	A	1216	OLA	C5-C6-C7-C8
6	A	1232	OLC	O20-C21-C22-C24
6	A	1223	OLC	C3-C4-C5-C6
6	A	1224	OLC	C3-C4-C5-C6
5	A	1222	OLA	C2-C3-C4-C5
5	A	1222	OLA	C11-C12-C13-C14
5	A	1208	OLA	C13-C14-C15-C16
6	A	1226	OLC	O20-C21-C22-O23
4	A	1203	CLR	C23-C24-C25-C27
6	A	1223	OLC	C6-C7-C8-C9
5	A	1217	OLA	C10-C11-C12-C13
6	A	1229	OLC	C6-C7-C8-C9
5	A	1212	OLA	C6-C7-C8-C9
6	A	1225	OLC	C5-C6-C7-C8
5	A	1217	OLA	C14-C15-C16-C17
6	A	1223	OLC	O19-C1-O20-C21
6	A	1231	OLC	C4-C5-C6-C7
6	A	1233	OLC	O19-C1-O20-C21
5	A	1217	OLA	C6-C7-C8-C9
5	A	1220	OLA	C6-C7-C8-C9
5	A	1208	OLA	C10-C11-C12-C13
5	A	1222	OLA	C15-C16-C17-C18
5	A	1211	OLA	C13-C14-C15-C16
5	A	1210	OLA	C15-C16-C17-C18
6	A	1228	OLC	C2-C1-O20-C21
5	A	1222	OLA	C6-C7-C8-C9
6	A	1223	OLC	C4-C5-C6-C7
6	A	1228	OLC	C12-C13-C14-C15
6	A	1231	OLC	C2-C3-C4-C5
5	A	1211	OLA	C12-C13-C14-C15
6	A	1225	OLC	O20-C21-C22-O23
5	A	1213	OLA	C6-C7-C8-C9
5	A	1222	OLA	C3-C4-C5-C6
6	A	1224	OLC	C2-C1-O20-C21
5	A	1207	OLA	C11-C12-C13-C14
6	A	1232	OLC	C1-C2-C3-C4
6	A	1223	OLC	C5-C6-C7-C8
5	A	1219	OLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
6	A	1227	OLC	C15-C16-C17-C18
6	A	1228	OLC	O19-C1-O20-C21
4	A	1203	CLR	C23-C24-C25-C26
5	A	1208	OLA	C5-C6-C7-C8
5	A	1216	OLA	C9-C10-C11-C12
6	A	1233	OLC	C4-C5-C6-C7
6	A	1225	OLC	C2-C3-C4-C5
5	A	1213	OLA	C11-C12-C13-C14
6	A	1226	OLC	O20-C21-C22-C24
6	A	1232	OLC	C4-C5-C6-C7
5	A	1216	OLA	C3-C4-C5-C6
5	A	1210	OLA	C6-C7-C8-C9
6	A	1224	OLC	O19-C1-O20-C21
6	A	1226	OLC	C11-C12-C13-C14
6	A	1228	OLC	C2-C3-C4-C5
5	A	1220	OLA	C1-C2-C3-C4
6	A	1233	OLC	C7-C8-C9-C10
5	A	1217	OLA	C2-C3-C4-C5
6	A	1231	OLC	C1-C2-C3-C4
5	A	1207	OLA	C12-C13-C14-C15
6	A	1230	OLC	C6-C7-C8-C9
6	A	1229	OLC	C5-C6-C7-C8
6	A	1226	OLC	C14-C15-C16-C17
5	A	1215	OLA	C5-C6-C7-C8
6	A	1226	OLC	C3-C4-C5-C6
6	A	1230	OLC	C11-C12-C13-C14
6	A	1224	OLC	C2-C3-C4-C5
4	A	1203	CLR	C20-C22-C23-C24
5	A	1207	OLA	C3-C4-C5-C6
6	A	1230	OLC	C5-C6-C7-C8
5	A	1217	OLA	C3-C4-C5-C6
5	A	1212	OLA	C2-C3-C4-C5
6	A	1224	OLC	C4-C5-C6-C7
5	A	1210	OLA	C5-C6-C7-C8
5	A	1220	OLA	C7-C8-C9-C10
5	A	1210	OLA	C7-C8-C9-C10
5	A	1211	OLA	C3-C4-C5-C6
5	A	1213	OLA	C15-C16-C17-C18
6	A	1225	OLC	C9-C10-C11-C12
6	A	1231	OLC	C10-C11-C12-C13
5	A	1221	OLA	C10-C11-C12-C13
5	A	1211	OLA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
6	A	1225	OLC	C11-C12-C13-C14
5	A	1216	OLA	C6-C7-C8-C9
6	A	1227	OLC	C11-C12-C13-C14
6	A	1226	OLC	C7-C8-C9-C10
5	A	1208	OLA	C11-C12-C13-C14
6	A	1225	OLC	C1-C2-C3-C4
5	A	1210	OLA	C13-C14-C15-C16
6	A	1231	OLC	C5-C6-C7-C8
6	A	1233	OLC	C6-C7-C8-C9
5	A	1211	OLA	C11-C12-C13-C14
6	A	1225	OLC	C12-C13-C14-C15
5	A	1222	OLA	C9-C10-C11-C12
6	A	1227	OLC	C13-C14-C15-C16
6	A	1225	OLC	C10-C11-C12-C13
6	A	1228	OLC	C7-C8-C9-C10
6	A	1227	OLC	C9-C10-C11-C12
6	A	1228	OLC	C9-C10-C11-C12
5	A	1222	OLA	C7-C8-C9-C10
6	A	1230	OLC	C9-C10-C11-C12
6	A	1227	OLC	C6-C7-C8-C9
6	A	1230	OLC	C12-C13-C14-C15
6	A	1227	OLC	C7-C8-C9-C10
5	A	1211	OLA	C7-C8-C9-C10
5	A	1217	OLA	C7-C8-C9-C10
5	A	1218	OLA	C2-C3-C4-C5
5	A	1217	OLA	C9-C10-C11-C12
6	A	1231	OLC	C9-C10-C11-C12
6	A	1230	OLC	C7-C8-C9-C10
6	A	1223	OLC	C7-C8-C9-C10
5	A	1207	OLA	C5-C6-C7-C8

There are no ring outliers.

17 monomers are involved in 44 short contacts:

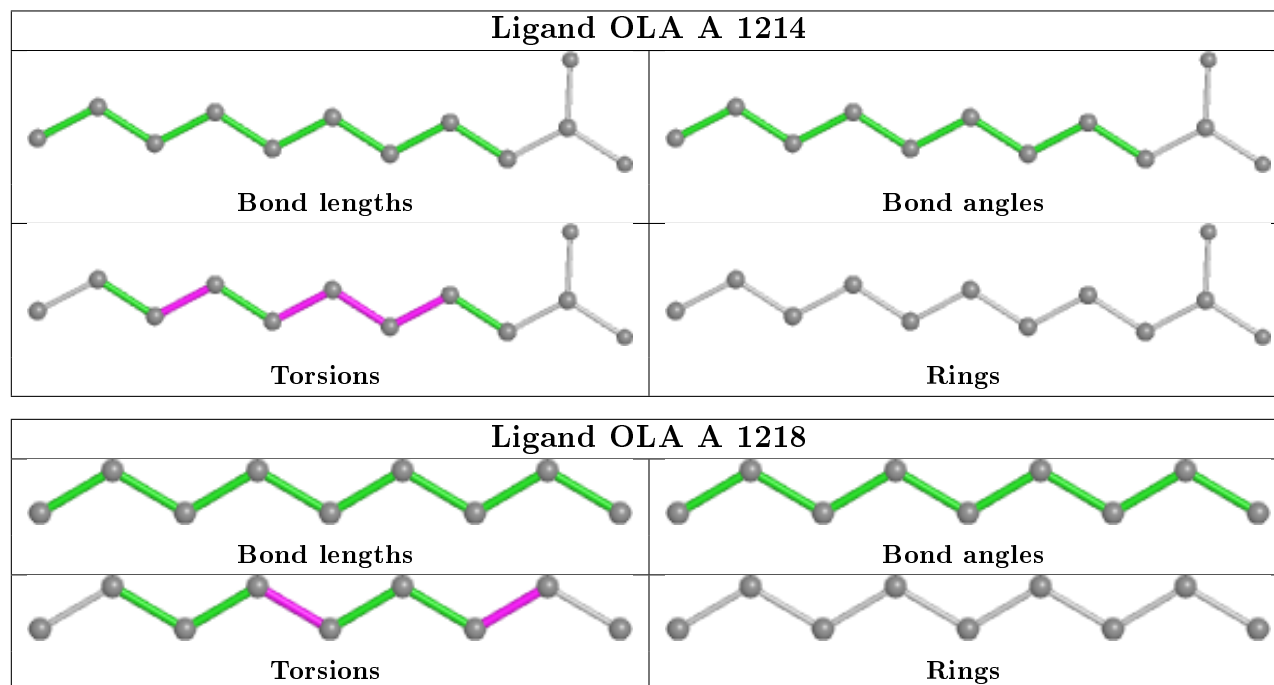
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1203	CLR	8	0
5	A	1221	OLA	1	0
5	A	1219	OLA	4	0
5	A	1217	OLA	5	0
6	A	1225	OLC	4	0
6	A	1228	OLC	1	0
4	A	1204	CLR	1	0

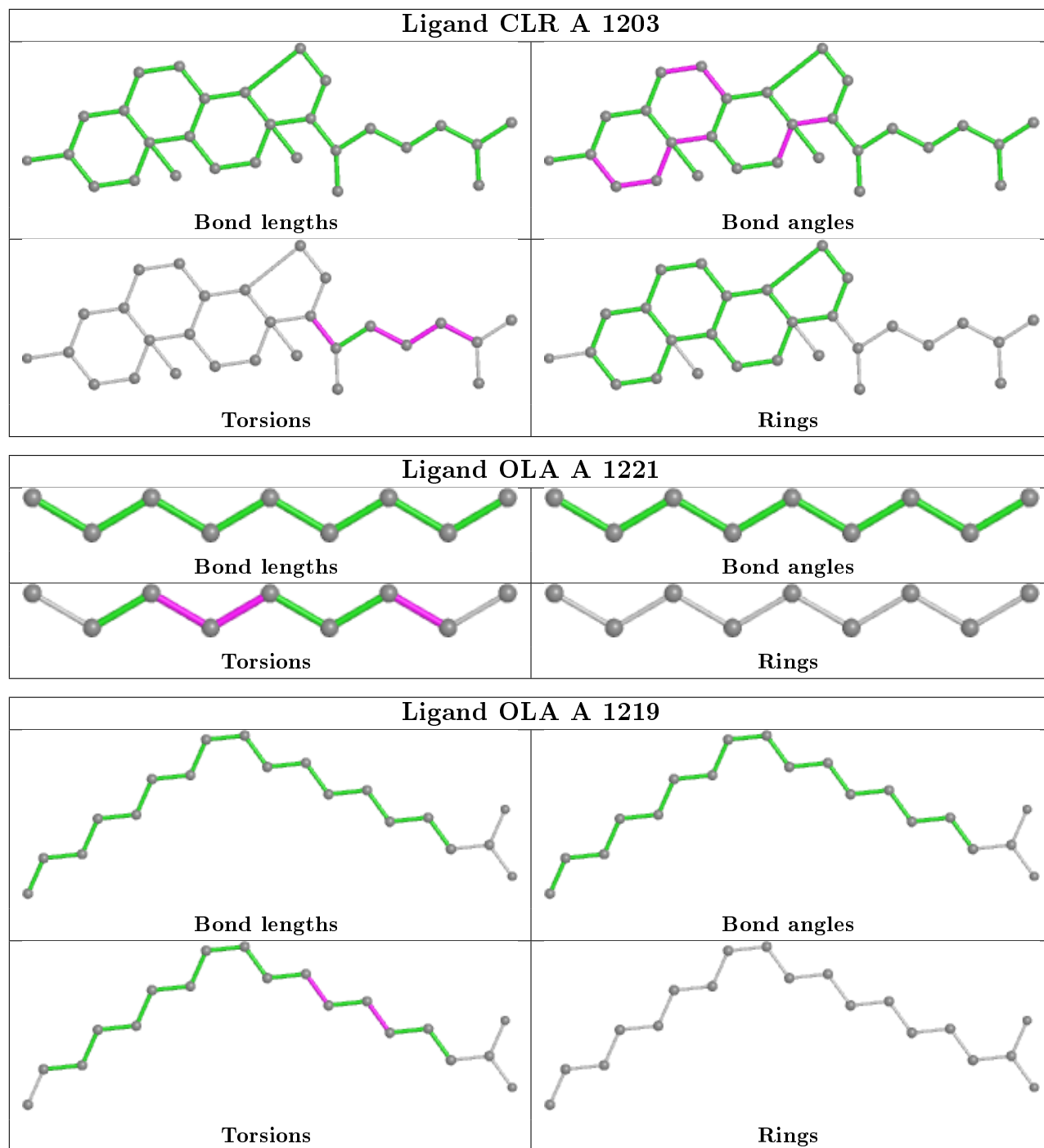
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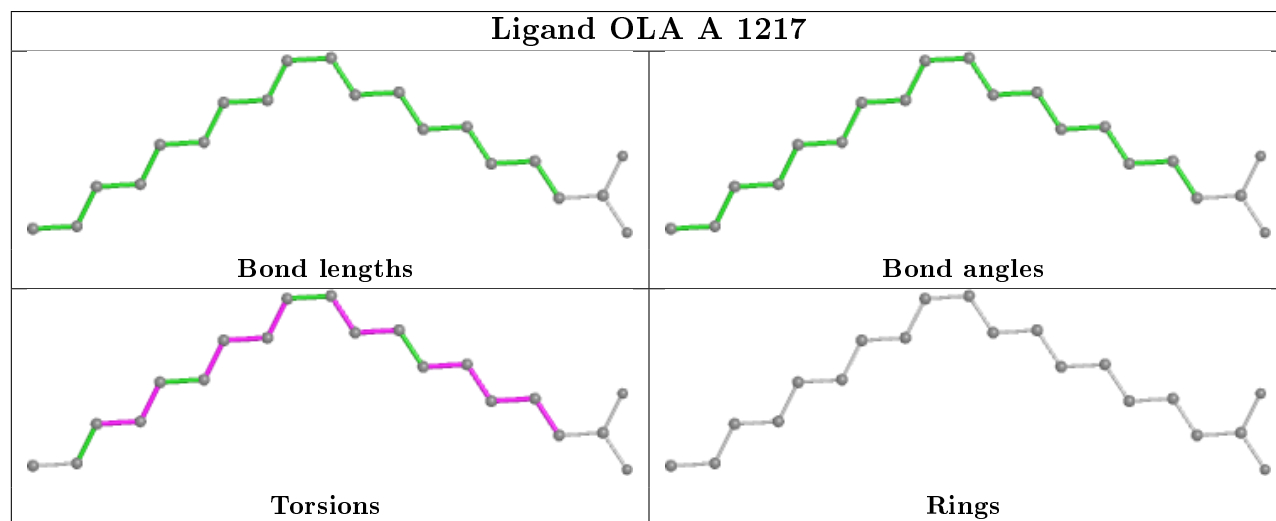
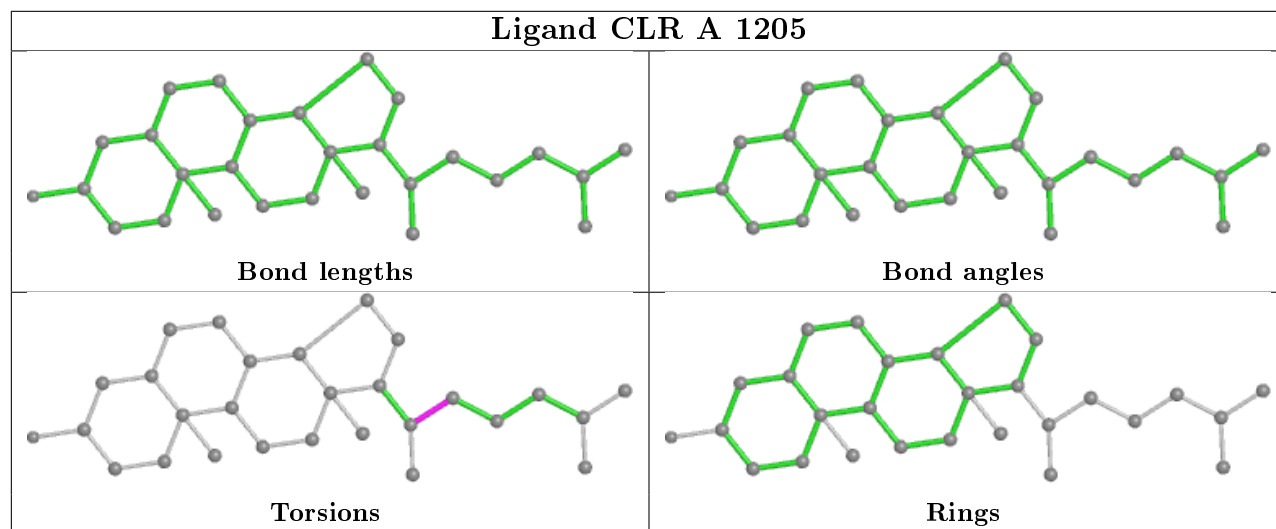
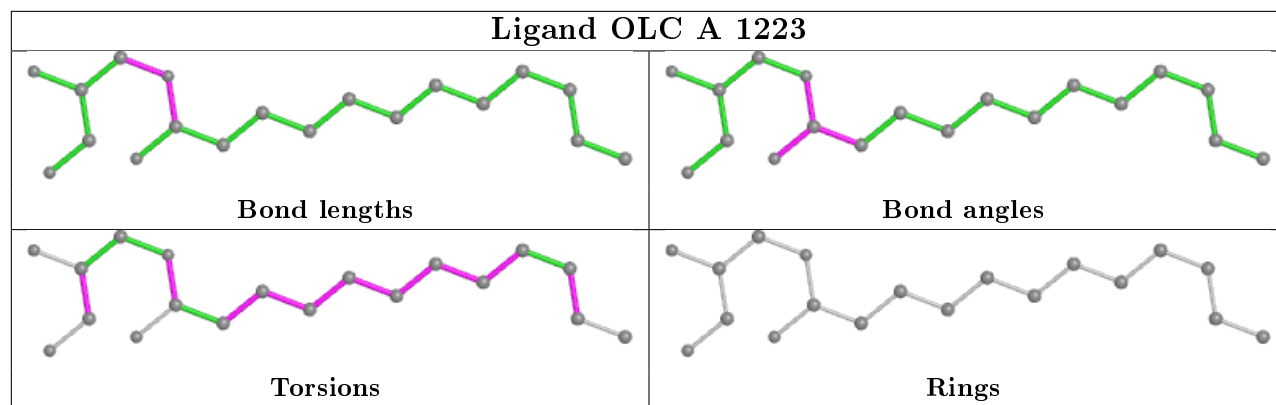
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1227	OLC	6	0
6	A	1232	OLC	11	0
5	A	1208	OLA	1	0
4	A	1206	CLR	1	0
5	A	1207	OLA	3	0
5	A	1211	OLA	1	0
6	A	1231	OLC	1	0
5	A	1213	OLA	1	0
5	A	1210	OLA	7	0
6	A	1226	OLC	6	0

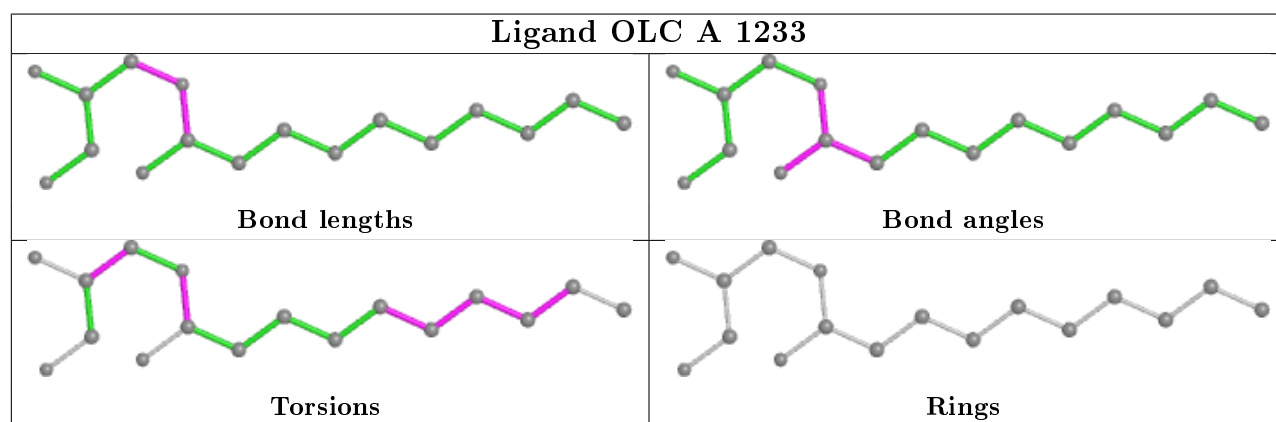
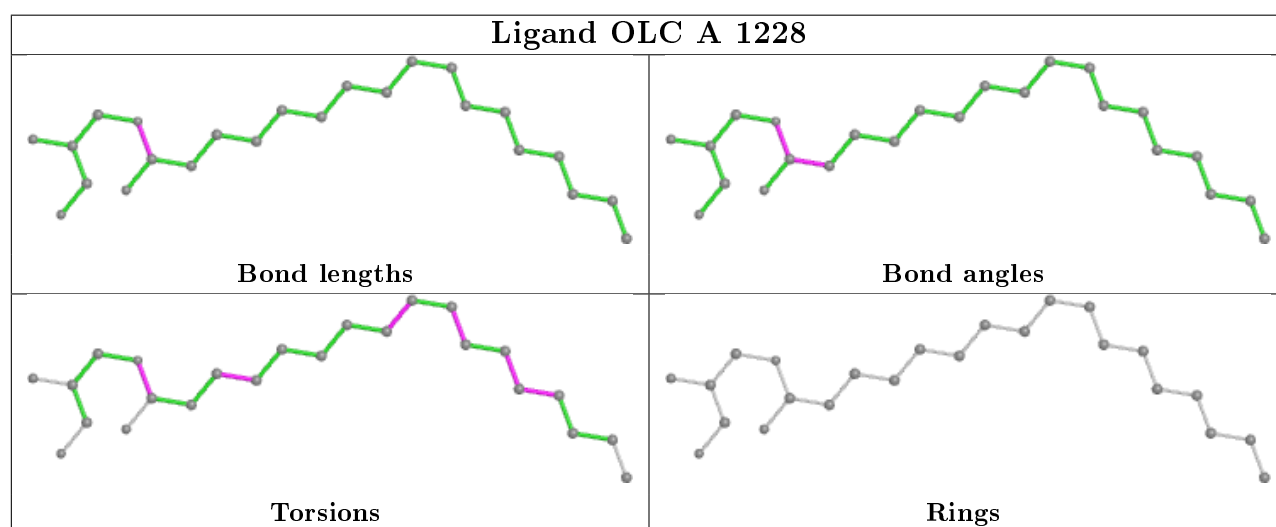
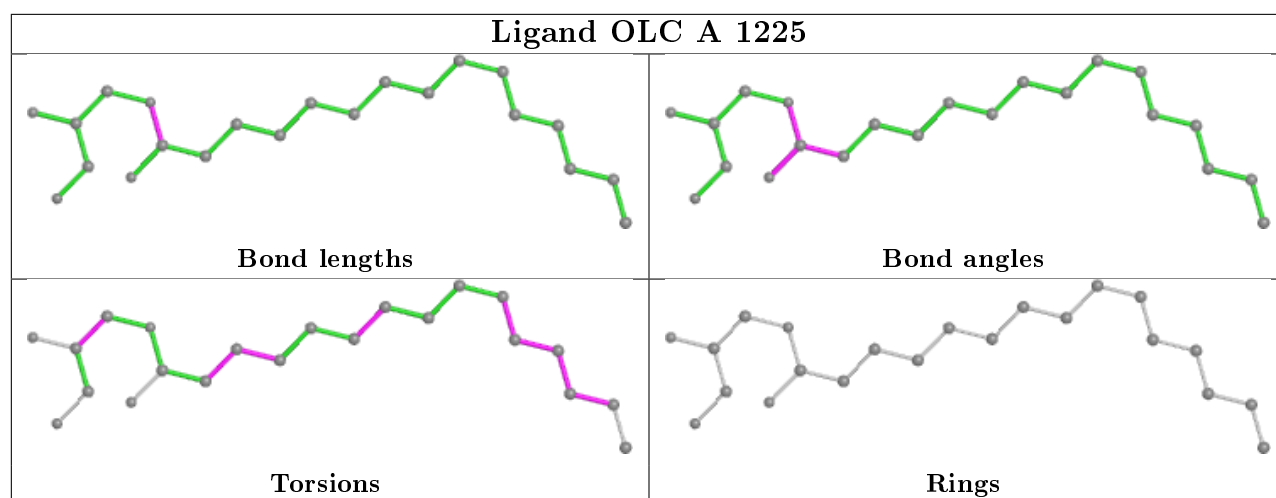
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



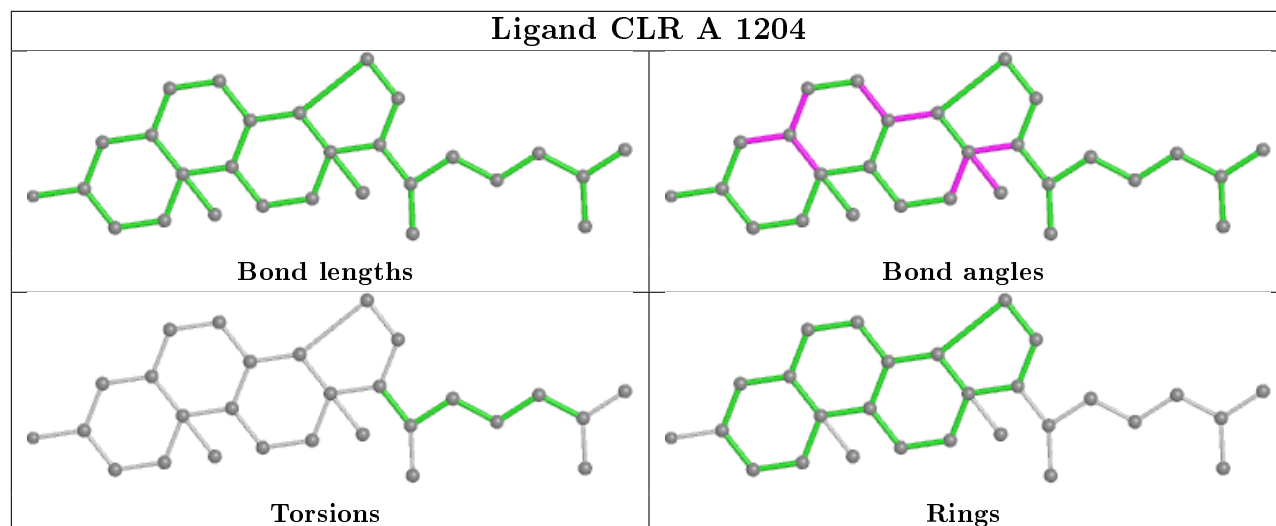




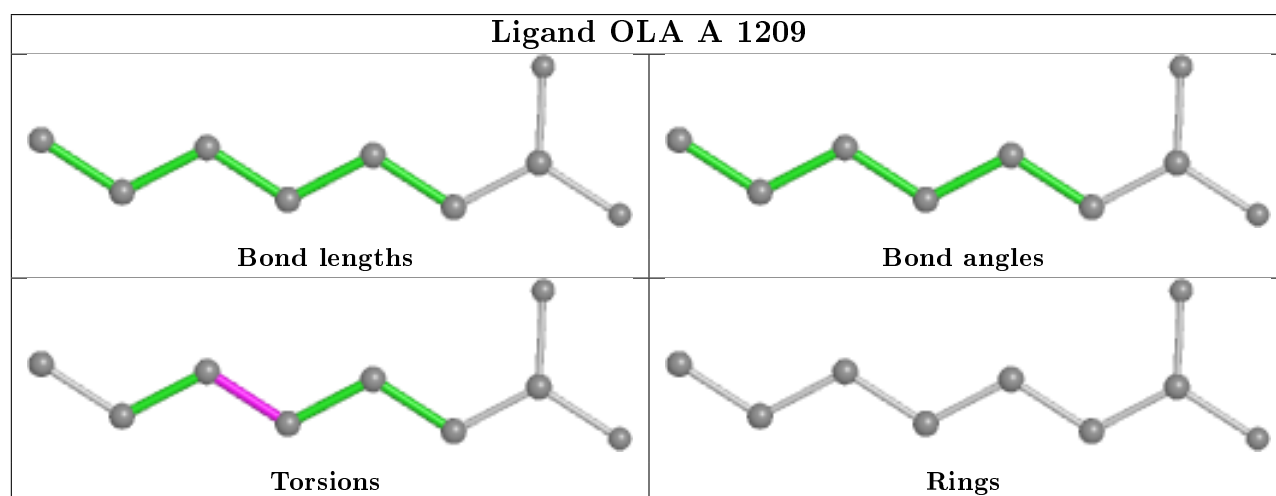




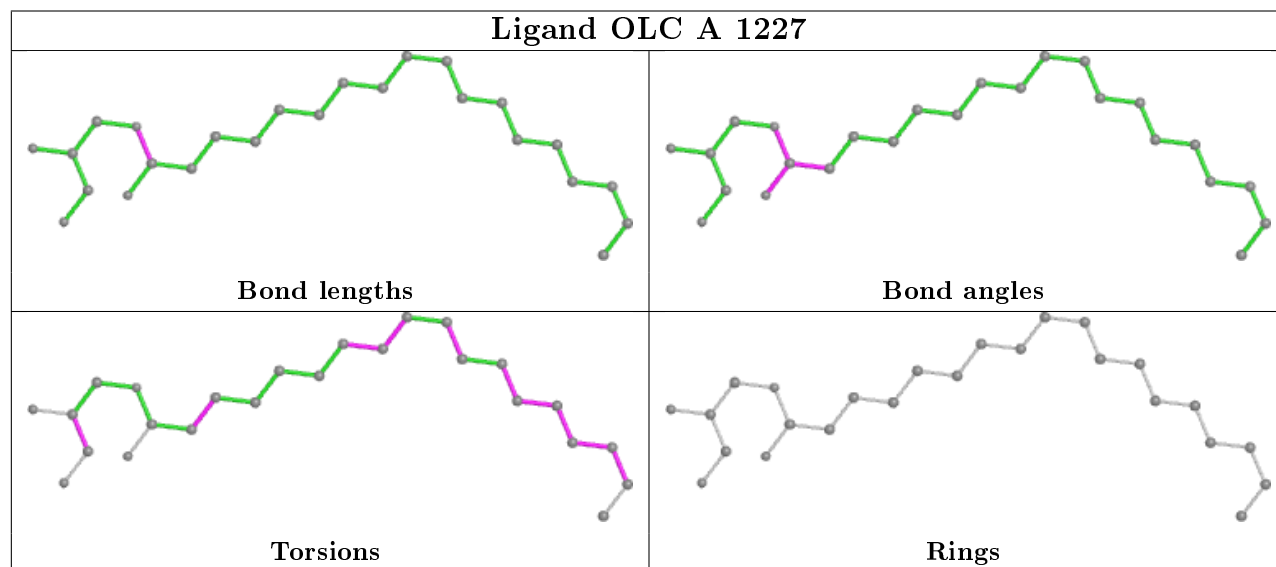
## Ligand CLR A 1204

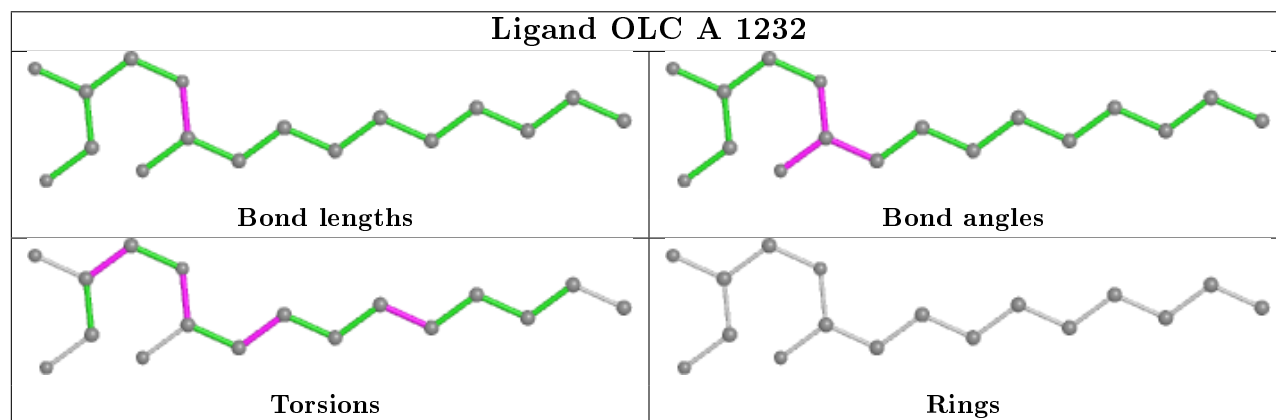
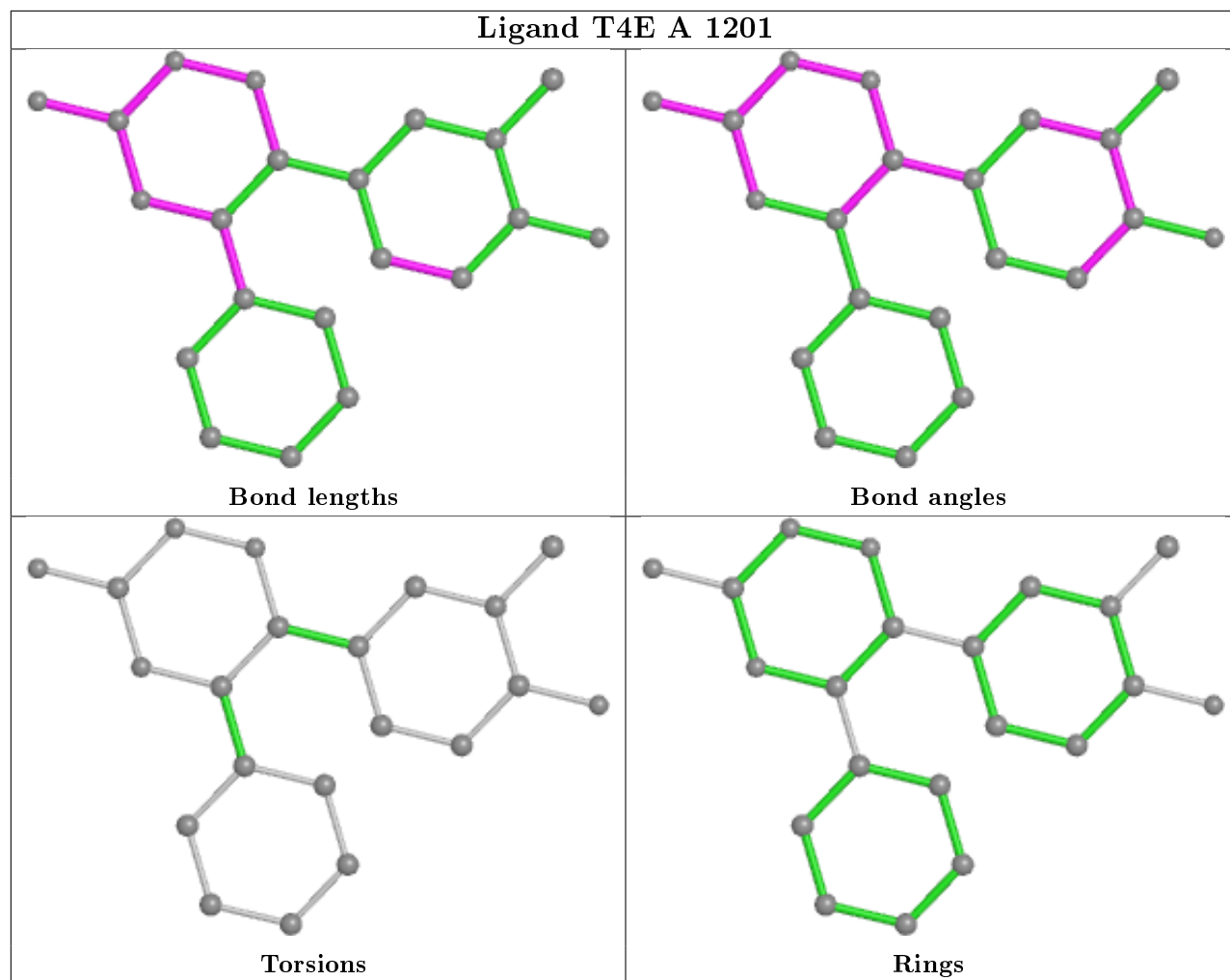


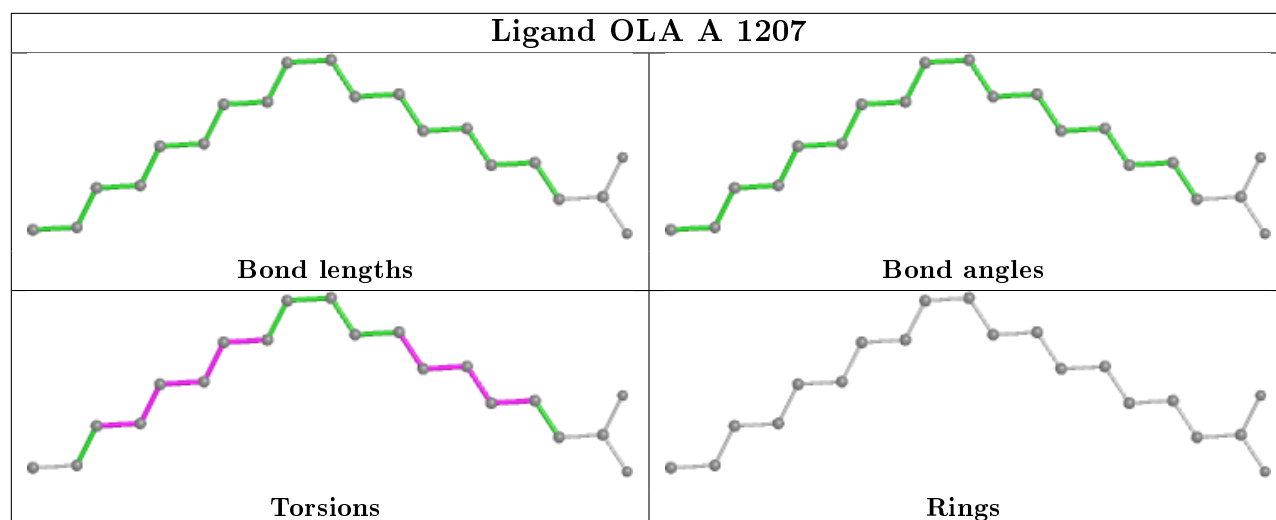
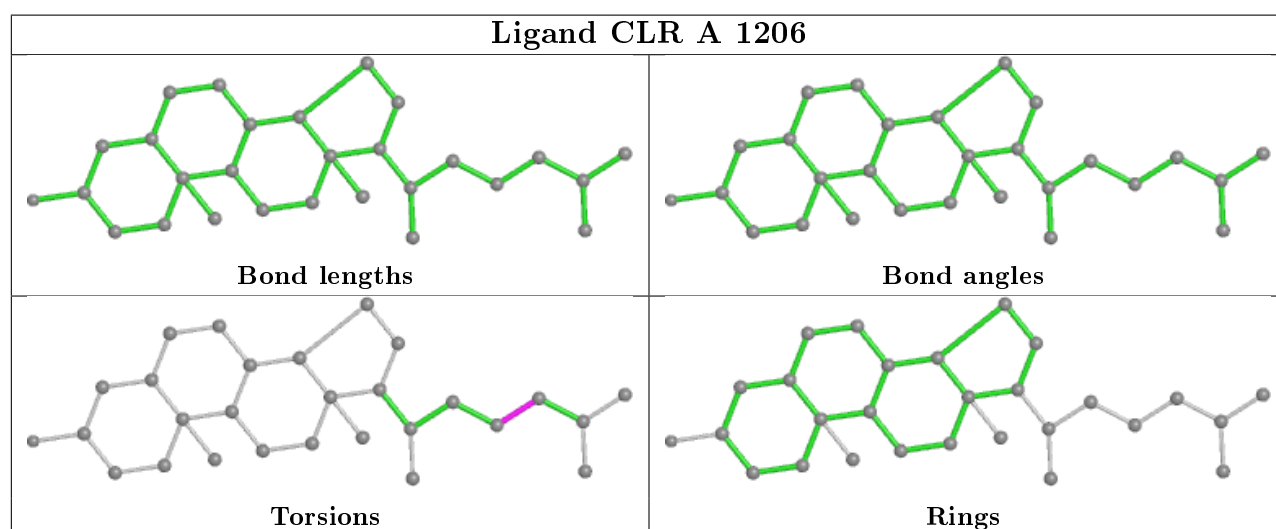
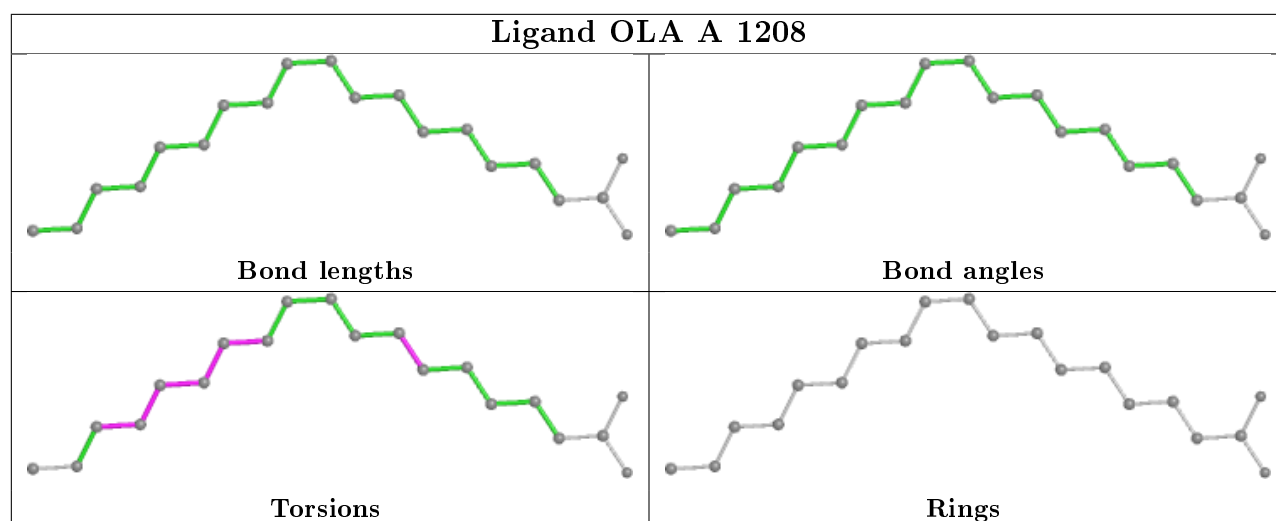
## Ligand OLA A 1209

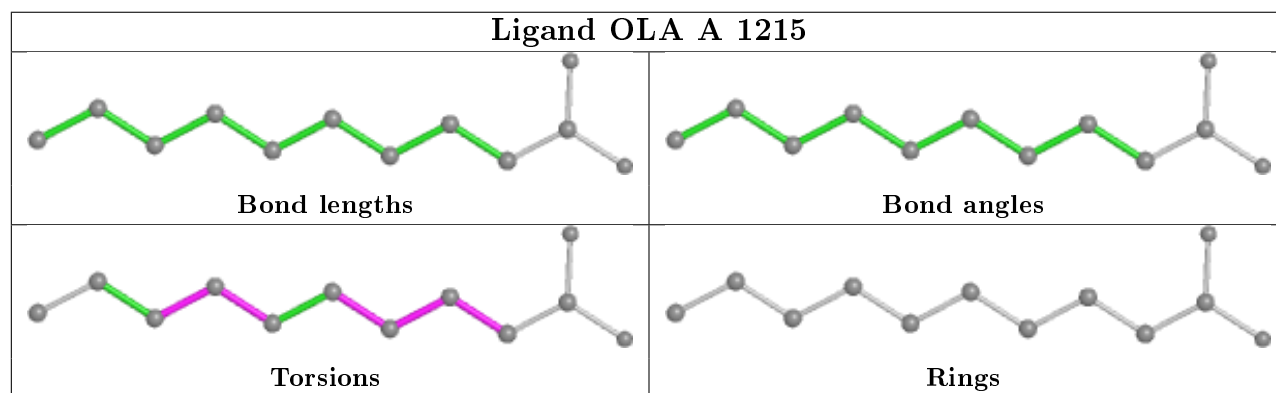
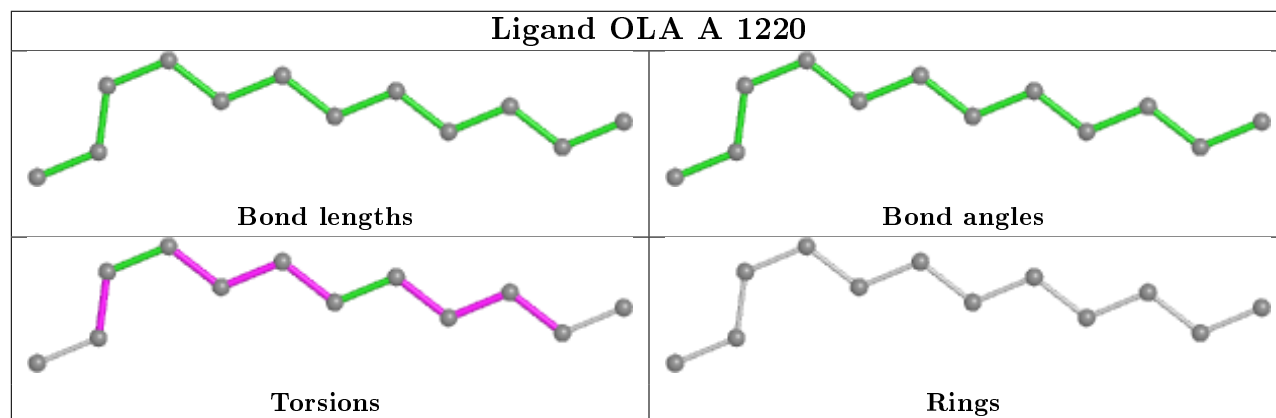
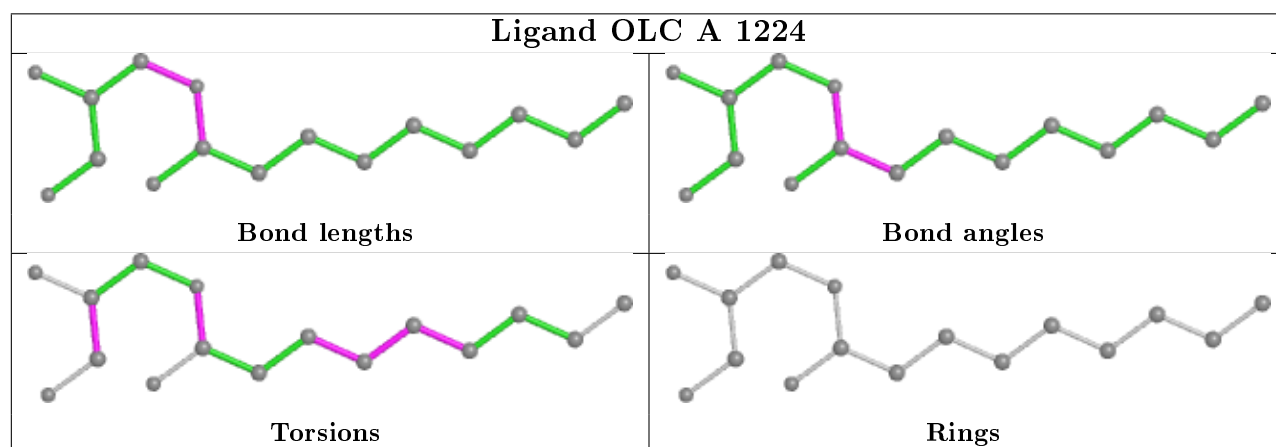
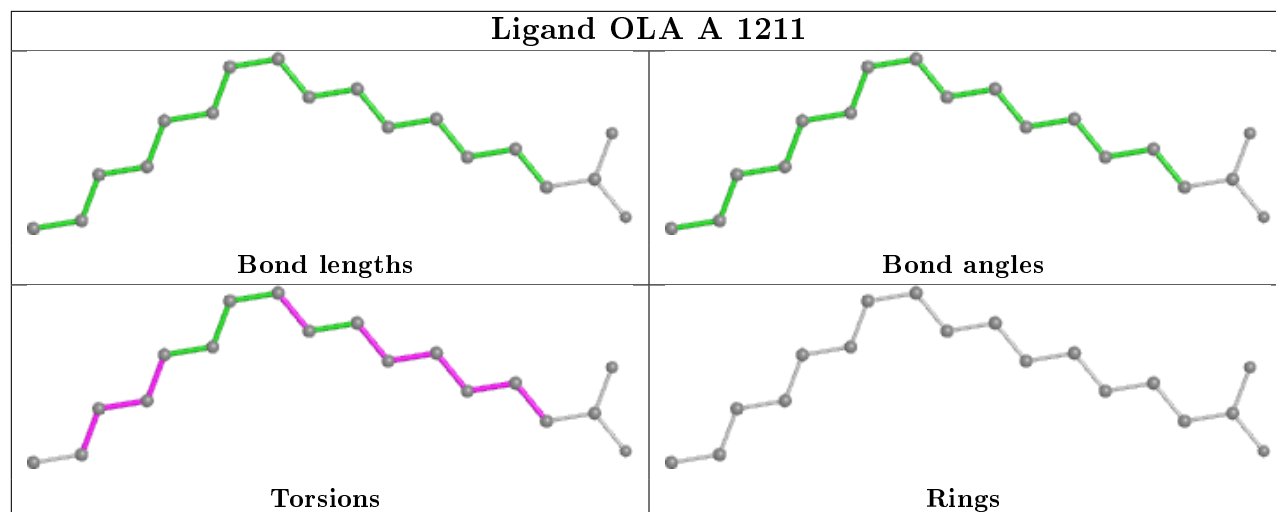


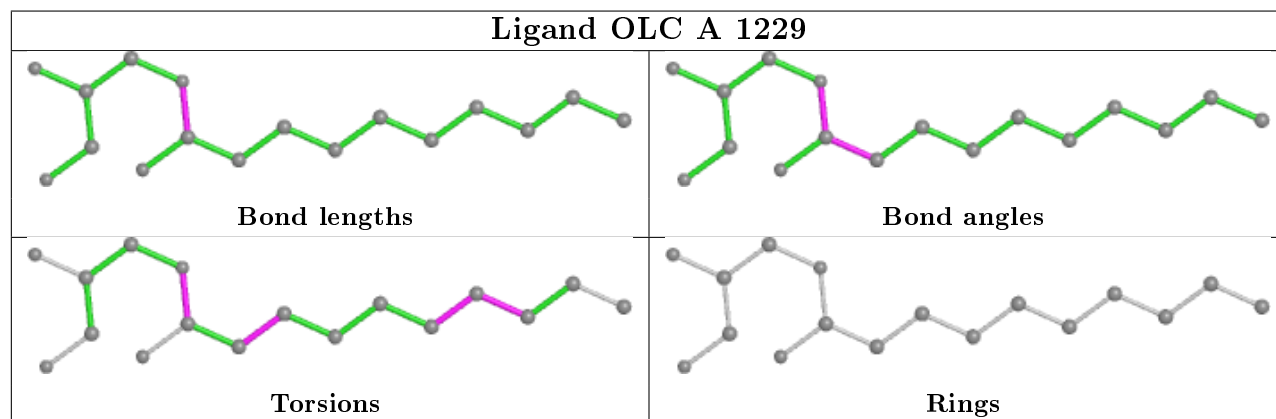
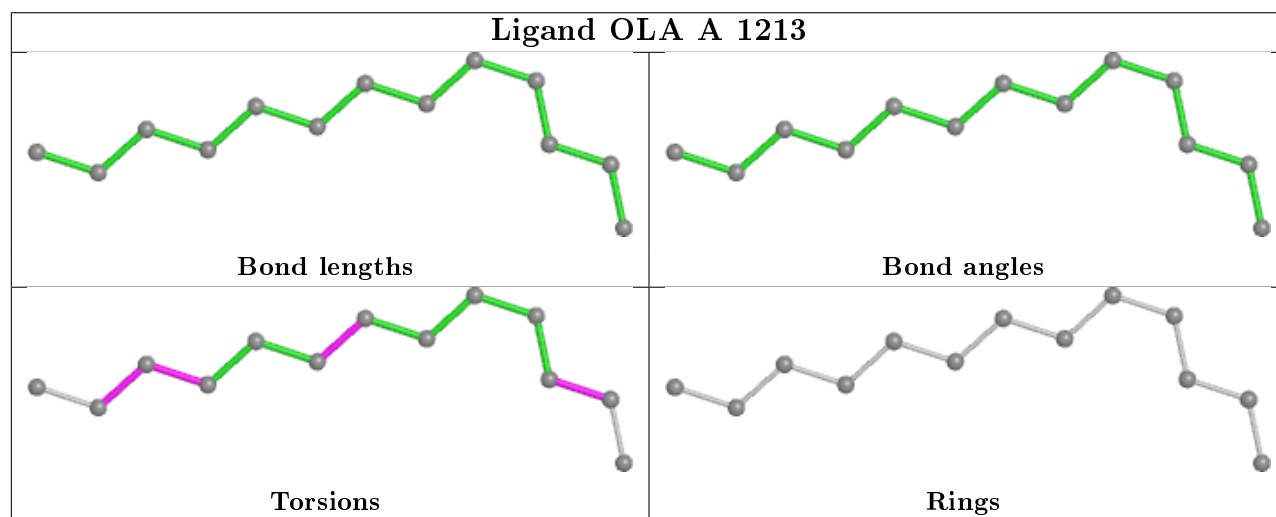
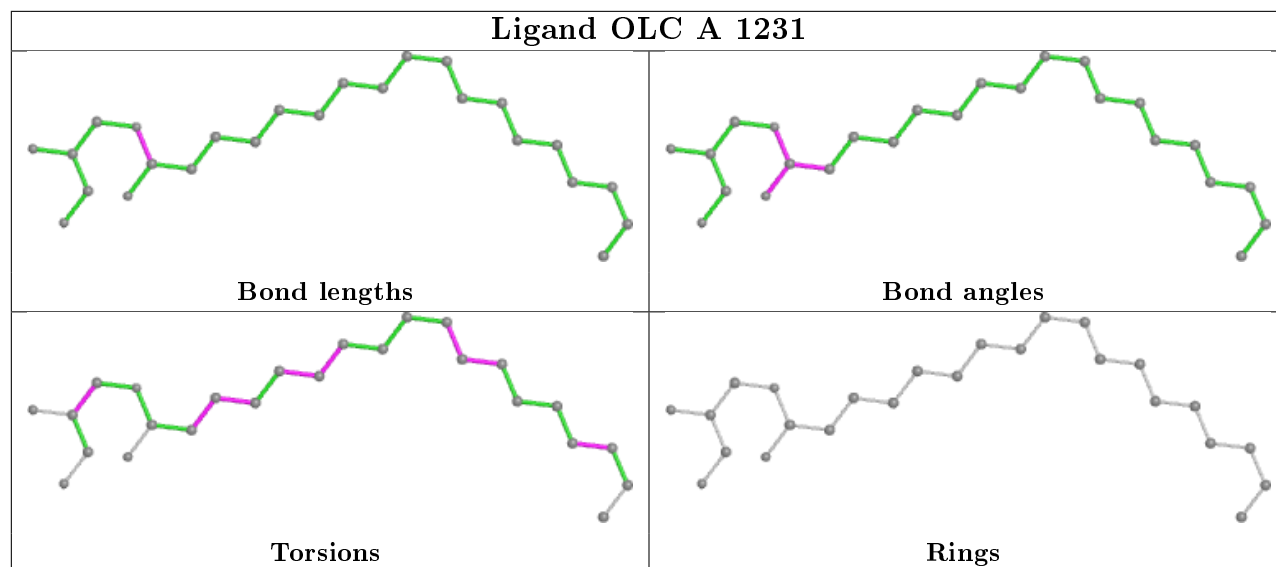
## Ligand OLC A 1227

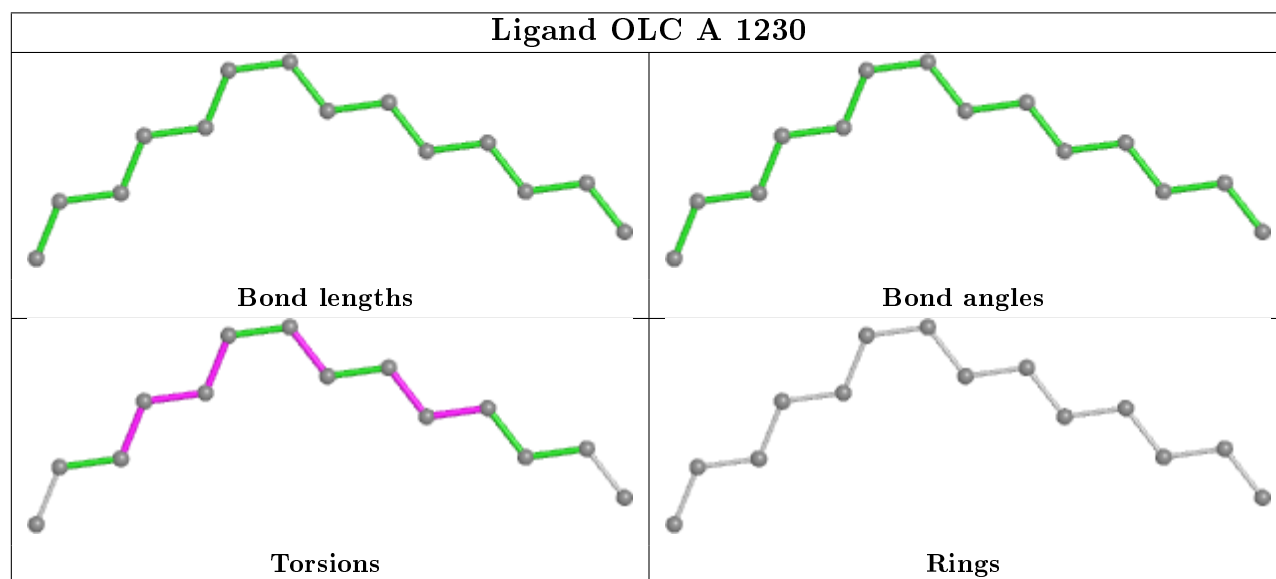
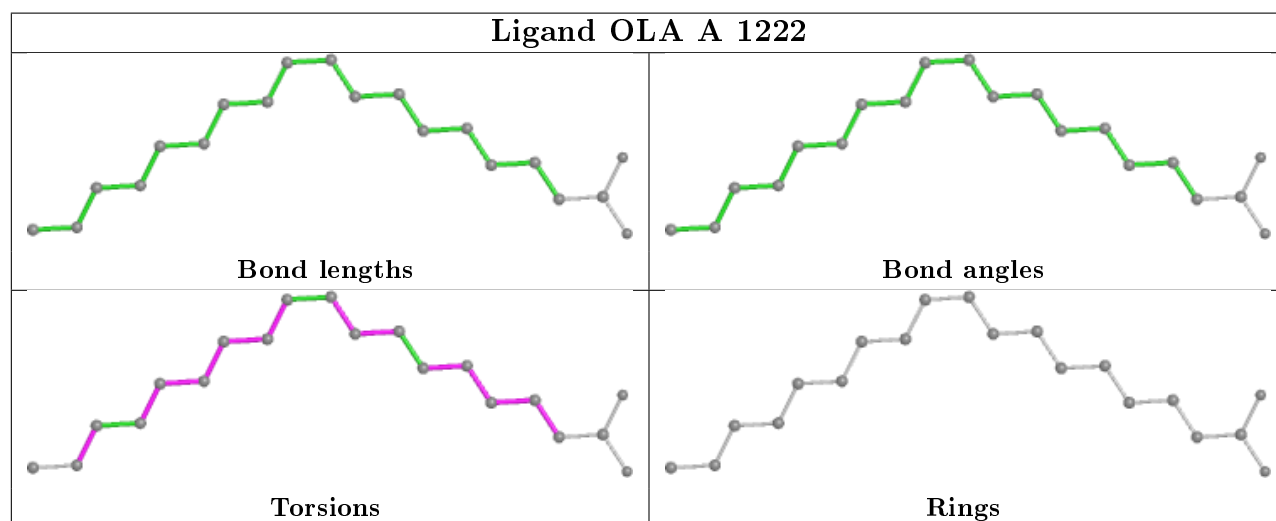
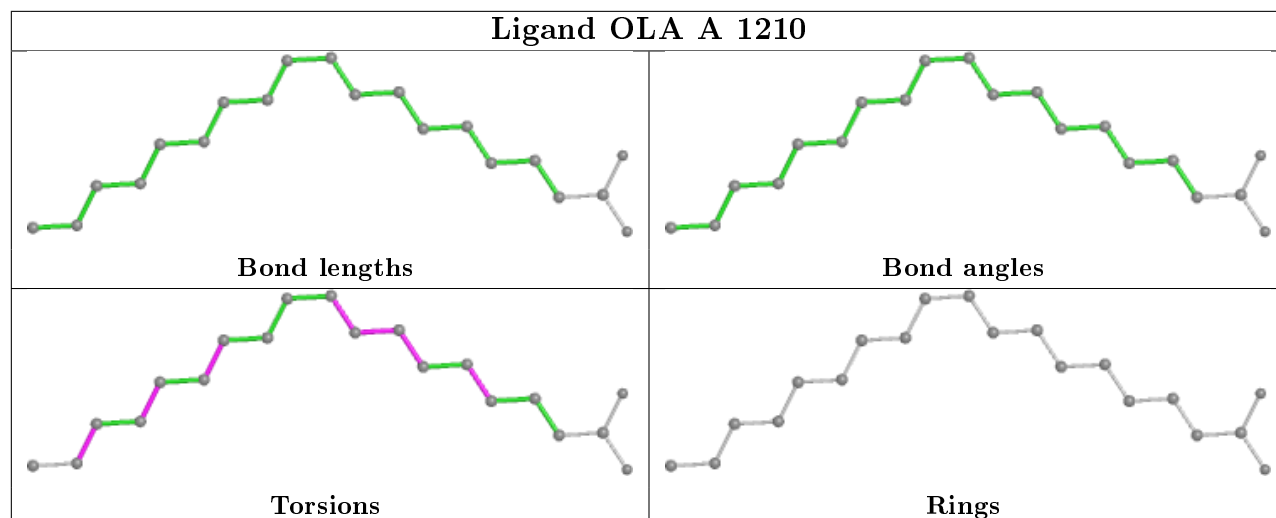


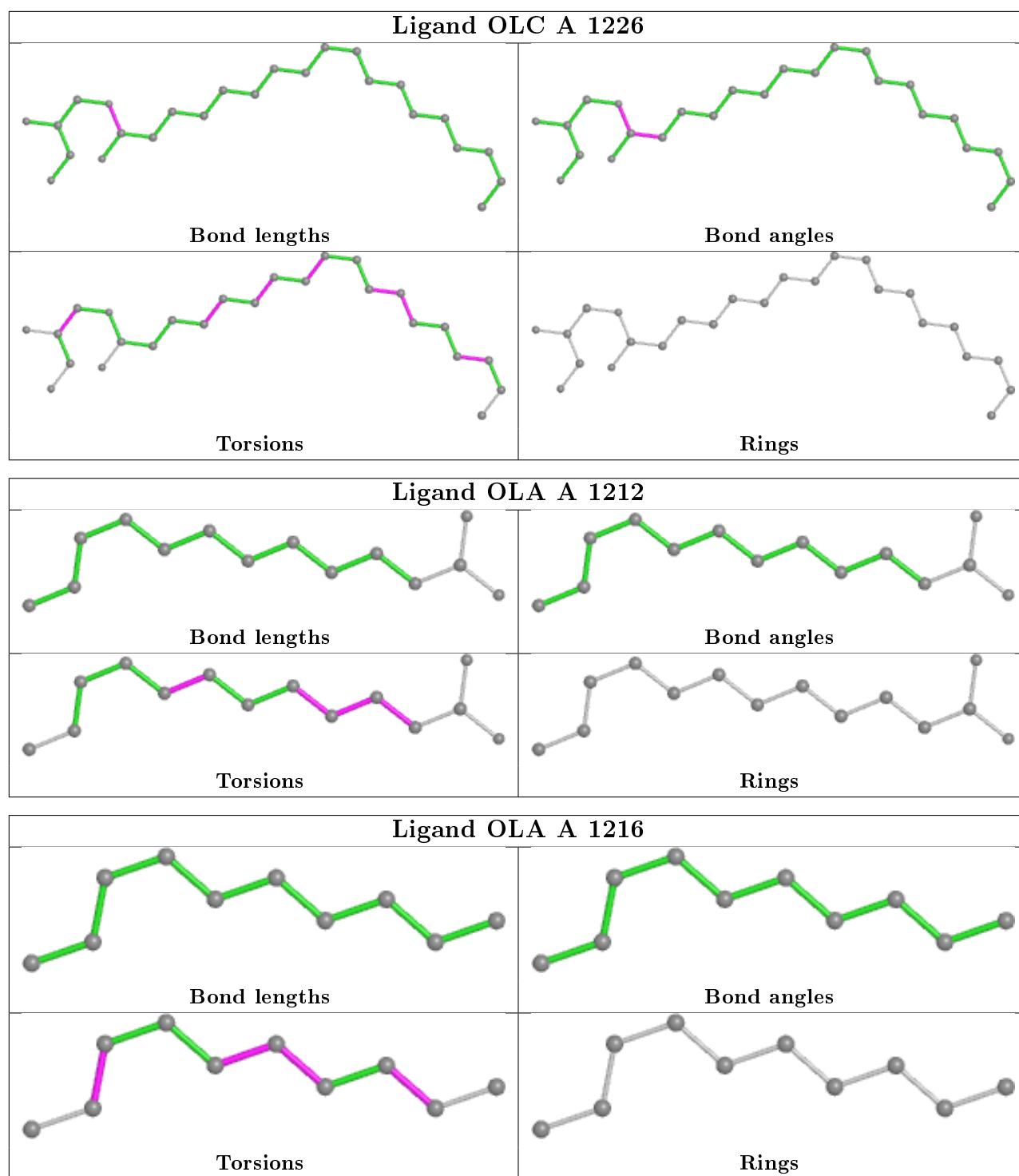












## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	389/434 (89%)	0.49	41 (10%) 6 5	16, 32, 75, 100	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	5.7
1	A	306	HIS	5.5
1	A	-1	GLY	5.3
1	A	1059	LYS	4.8
1	A	111	ARG	4.5
1	A	1062	ARG	4.3
1	A	0	ALA	4.0
1	A	307	VAL	4.0
1	A	1105	TYR	3.8
1	A	304	ARG	3.7
1	A	305	SER	3.7
1	A	290	TYR	3.6
1	A	1021	ASP	3.6
1	A	1028	ASP	3.4
1	A	302	ILE	3.3
1	A	110	LEU	3.3
1	A	1019	LYS	3.2
1	A	1060	ASP	2.8
1	A	220	ARG	2.7
1	A	1092	GLU	2.7
1	A	1031	THR	2.4
1	A	1	PRO	2.4
1	A	1016	VAL	2.4
1	A	29[A]	TRP	2.3
1	A	114	GLY	2.3
1	A	300[A]	ARG	2.3
1	A	303	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1023	ALA	2.2
1	A	1040	ALA	2.2
1	A	55	VAL	2.1
1	A	1039	ASP	2.1
1	A	293	ARG	2.1
1	A	208	LEU	2.1
1	A	1008	GLU	2.1
1	A	84	VAL	2.1
1	A	1026	VAL	2.1
1	A	1024	ALA	2.1
1	A	1035	ALA	2.1
1	A	1099	ASN	2.1
1	A	1042	LYS	2.1
1	A	1015	LYS	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 carbohydrates 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, 95<sup>th</sup> 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
6	OLC	A	1226	25/25	0.53	0.27	44,69,90,92	0
4	CLR	A	1203	28/28	0.55	0.41	73,88,92,93	0
5	OLA	A	1221	9/20	0.64	0.27	47,62,64,66	0
6	OLC	A	1232	17/25	0.67	0.33	49,65,86,89	0
5	OLA	A	1210	20/20	0.67	0.29	53,74,80,80	0
5	OLA	A	1219	19/20	0.67	0.27	58,66,72,73	0
6	OLC	A	1231	25/25	0.68	0.26	72,82,91,92	0
5	OLA	A	1217	20/20	0.69	0.23	71,75,84,85	0
5	OLA	A	1215	12/20	0.71	0.17	62,63,66,66	0

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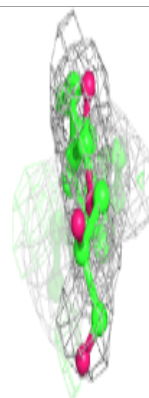
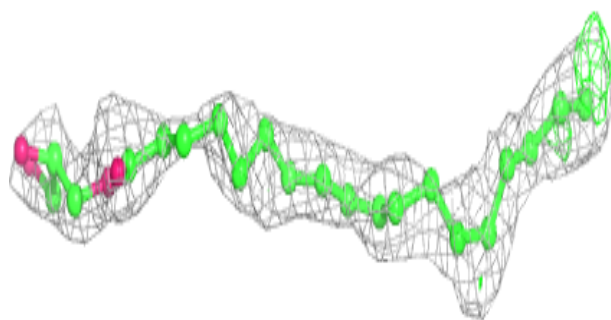
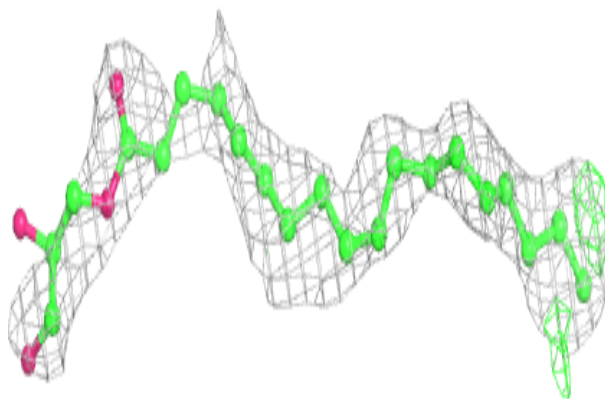
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	OLA	A	1212	14/20	0.72	0.23	67,81,95,96	0
5	OLA	A	1216	10/20	0.72	0.19	62,68,70,71	0
5	OLA	A	1220	12/20	0.77	0.20	57,60,62,64	0
6	OLC	A	1230	14/25	0.78	0.18	44,52,55,57	0
6	OLC	A	1229	17/25	0.78	0.24	51,56,72,74	0
6	OLC	A	1228	24/25	0.78	0.22	45,63,70,72	0
5	OLA	A	1222	20/20	0.78	0.21	57,68,77,77	0
5	OLA	A	1211	18/20	0.79	0.20	56,62,72,74	0
5	OLA	A	1214	12/20	0.79	0.29	38,59,74,74	0
6	OLC	A	1223	19/25	0.80	0.24	33,49,64,65	0
6	OLC	A	1233	17/25	0.80	0.26	61,66,69,71	0
6	OLC	A	1224	16/25	0.81	0.17	45,51,64,65	0
5	OLA	A	1208	20/20	0.84	0.14	57,58,61,61	20
5	OLA	A	1213	13/20	0.85	0.17	46,53,60,62	0
6	OLC	A	1225	22/25	0.85	0.19	44,50,86,94	0
5	OLA	A	1209	9/20	0.86	0.19	39,42,58,60	0
5	OLA	A	1207	20/20	0.86	0.20	41,56,66,66	0
5	OLA	A	1218	9/20	0.89	0.23	41,46,55,56	0
6	OLC	A	1227	25/25	0.90	0.20	39,56,82,84	0
4	CLR	A	1204	28/28	0.93	0.12	24,29,56,62	0
3	NA	A	1202	1/1	0.94	0.11	41,41,41,41	0
4	CLR	A	1205	28/28	0.95	0.10	27,30,35,42	0
4	CLR	A	1206	28/28	0.96	0.09	21,26,51,53	0
2	T4E	A	1201	21/21	0.98	0.20	13,16,20,24	0

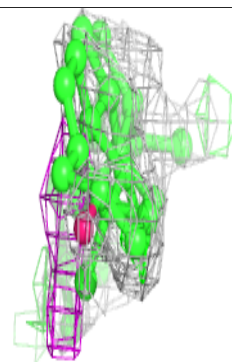
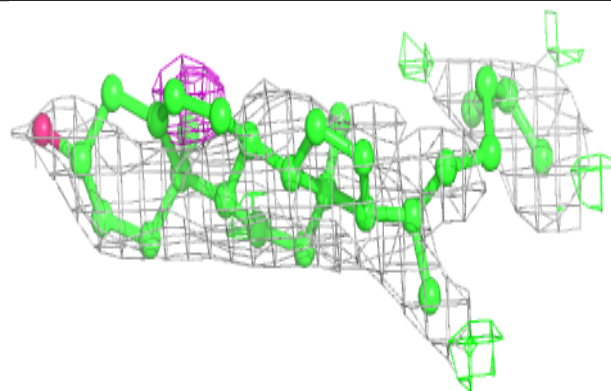
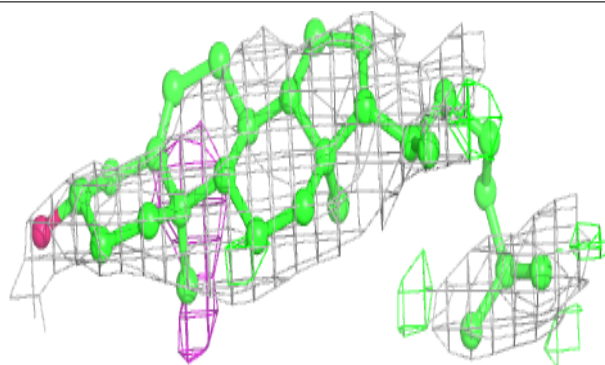
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC A 1226:**

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

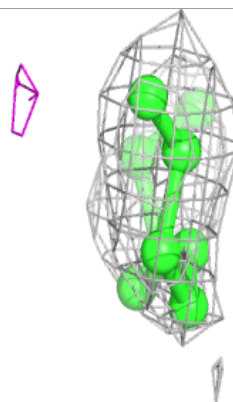
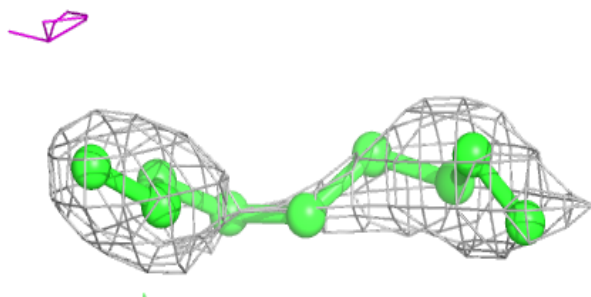
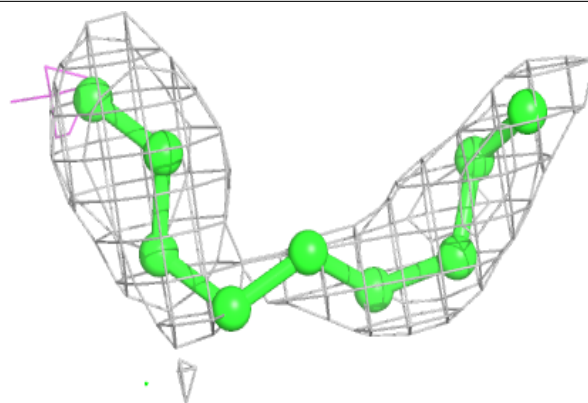
**Electron density around CLR A 1203:**

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

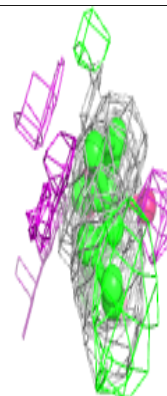
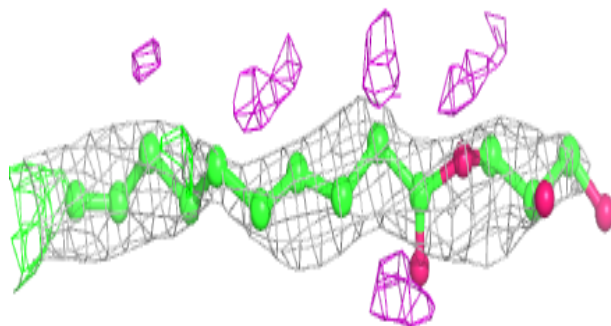
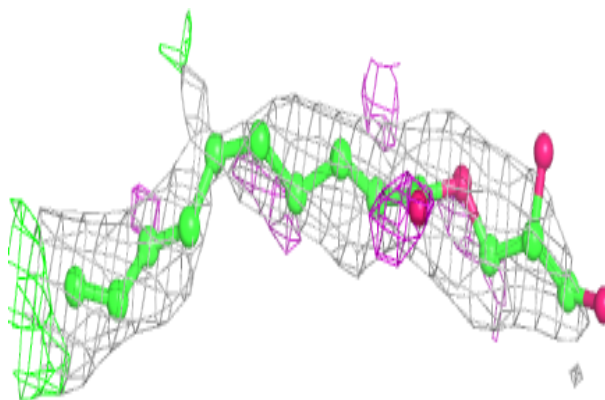


**Electron density around OLA A 1221:**

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

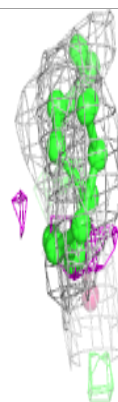
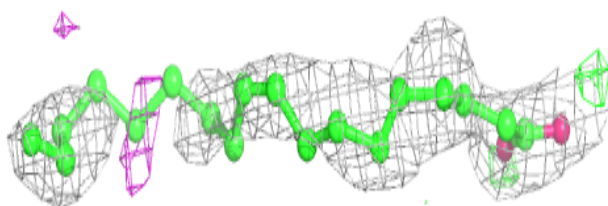
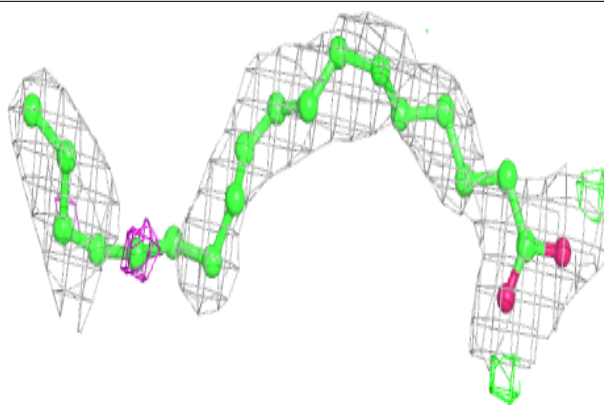
**Electron density around OLC A 1232:**

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

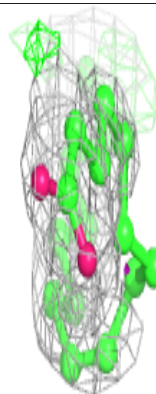
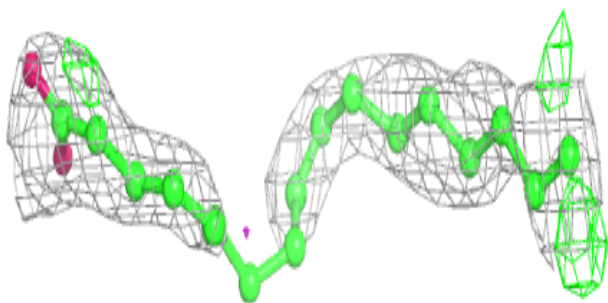
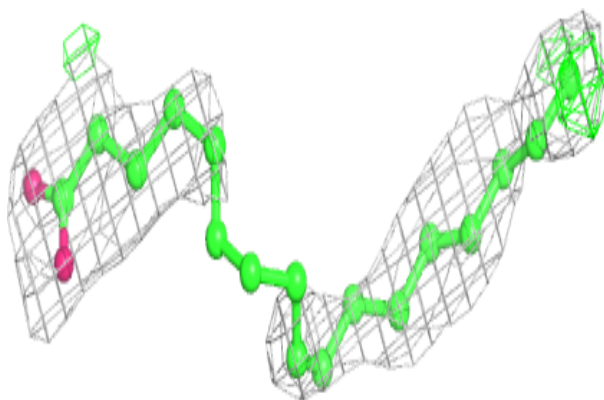


**Electron density around OLA A 1210:**

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

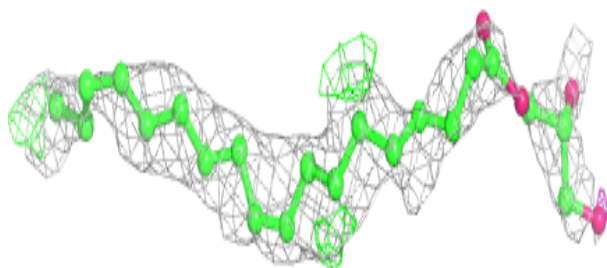
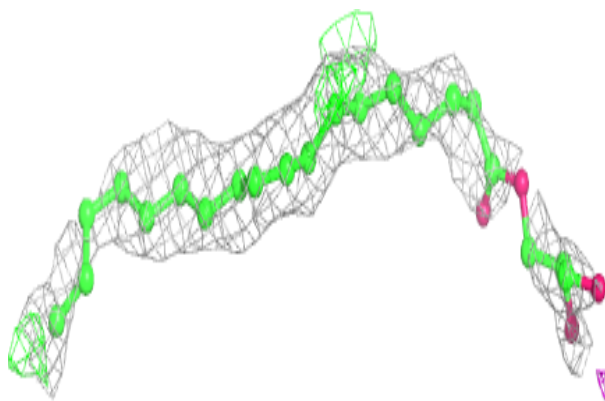
**Electron density around OLA A 1219:**

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

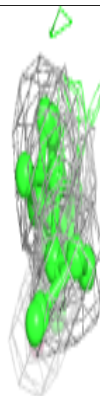
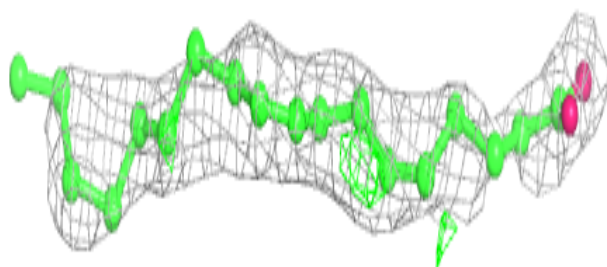
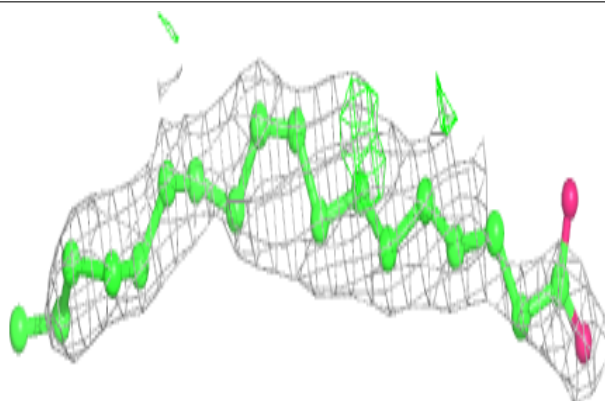


**Electron density around OLC A 1231:**

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

**Electron density around OLA A 1217:**

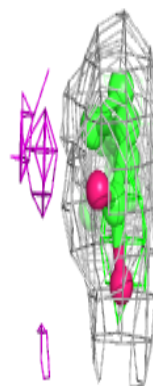
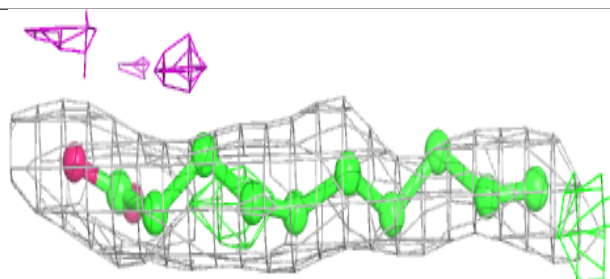
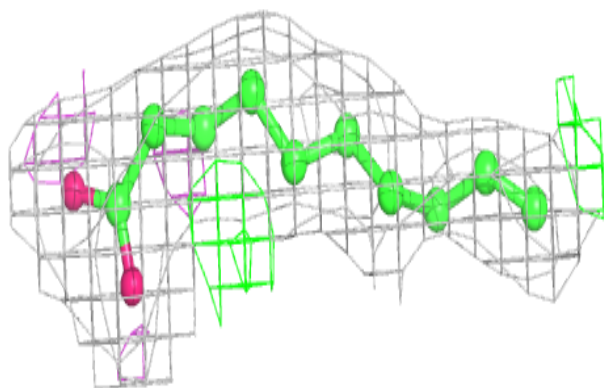
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and green (positive)



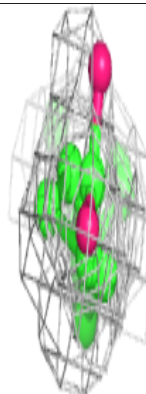
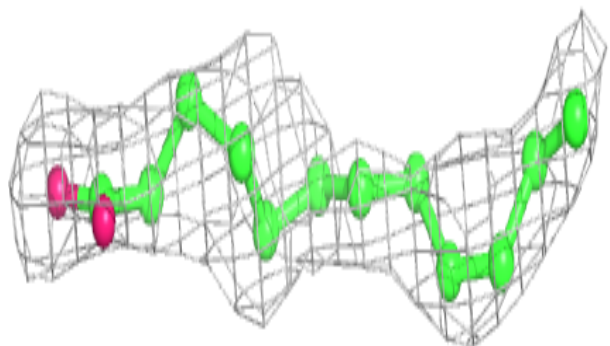
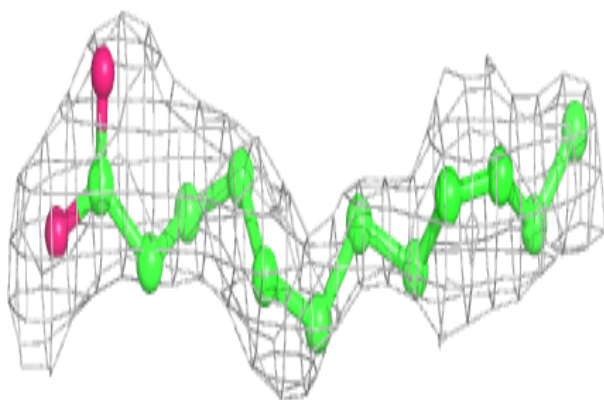


**Electron density around OLA A 1215:**

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and green (positive)

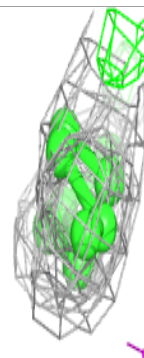
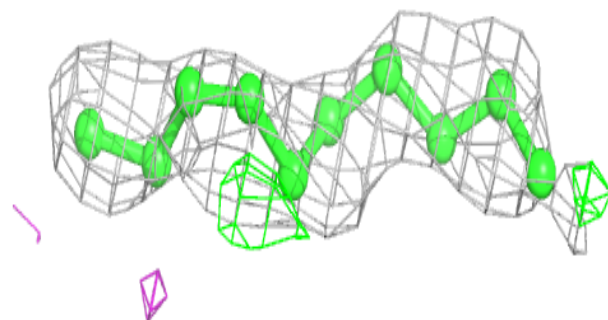
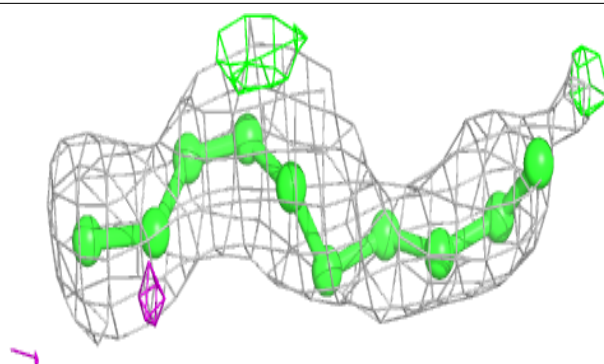
**Electron density around OLA A 1212:**

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

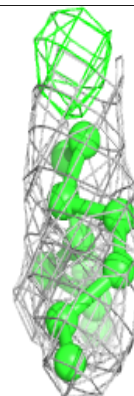
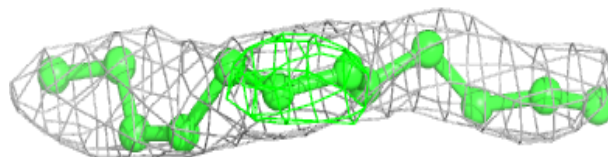
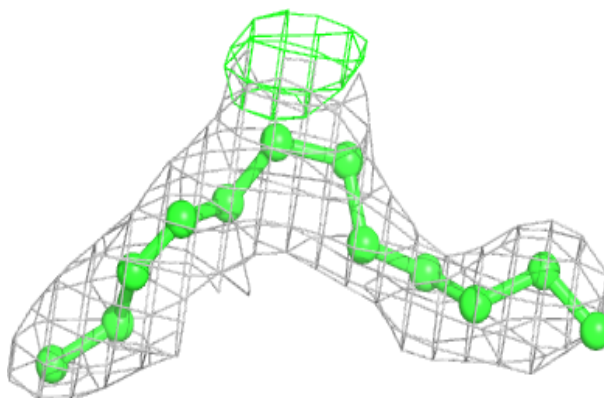


**Electron density around OLA A 1216:**

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

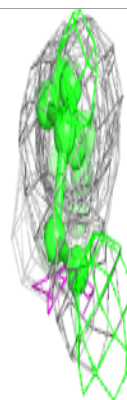
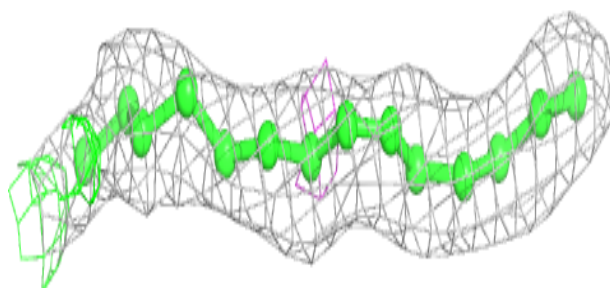
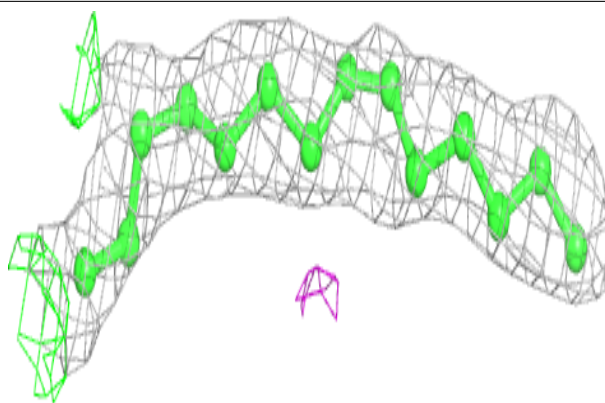
**Electron density around OLA A 1220:**

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

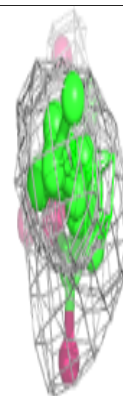
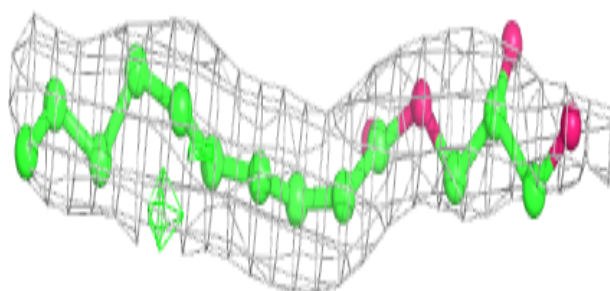
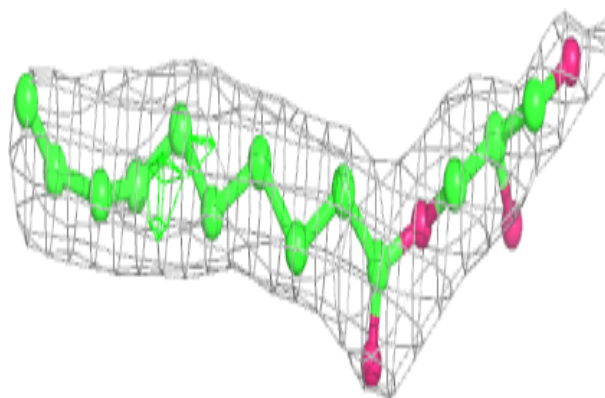


**Electron density around OLC A 1230:**

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

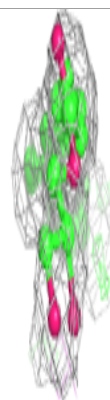
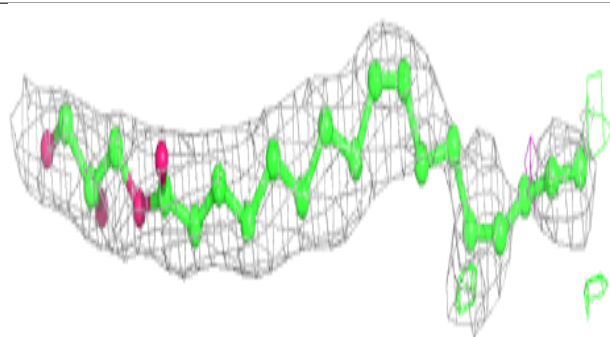
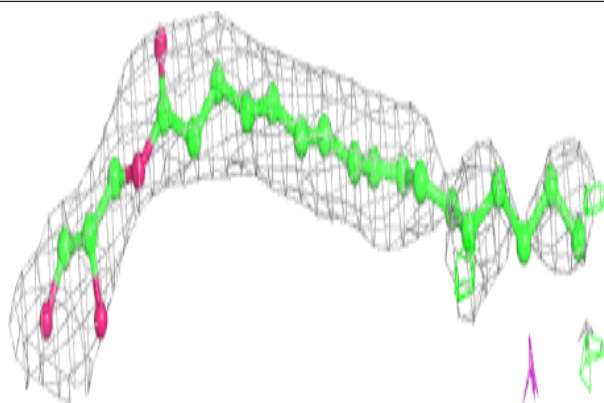
**Electron density around OLC A 1229:**

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

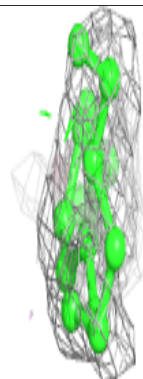
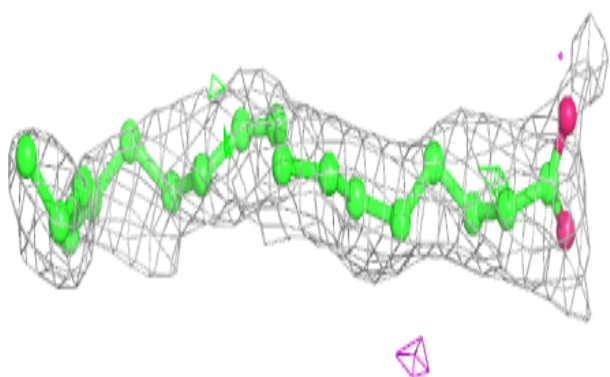
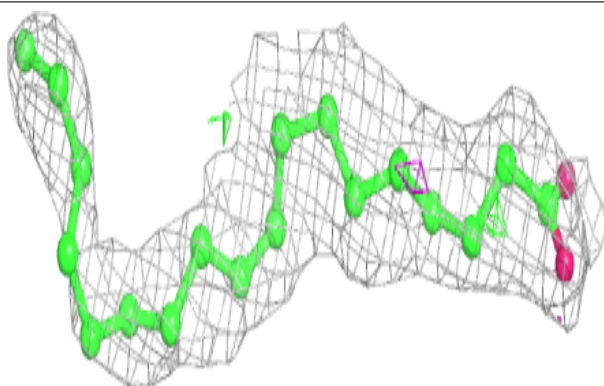


**Electron density around OLC A 1228:**

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

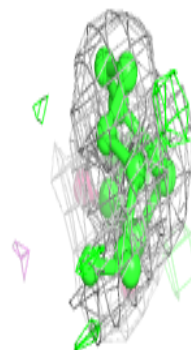
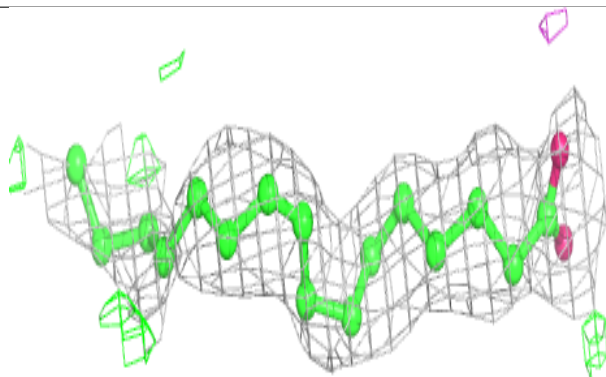
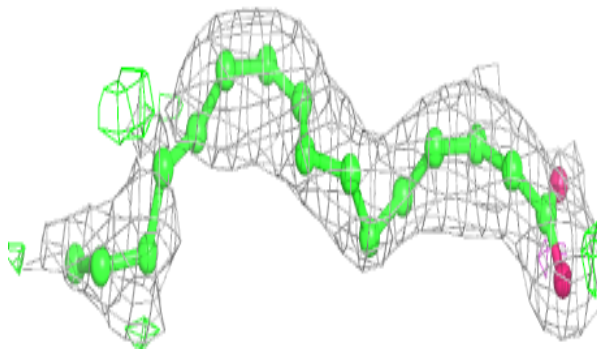
**Electron density around OLA A 1222:**

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

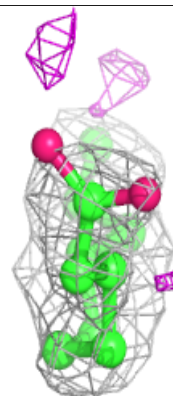
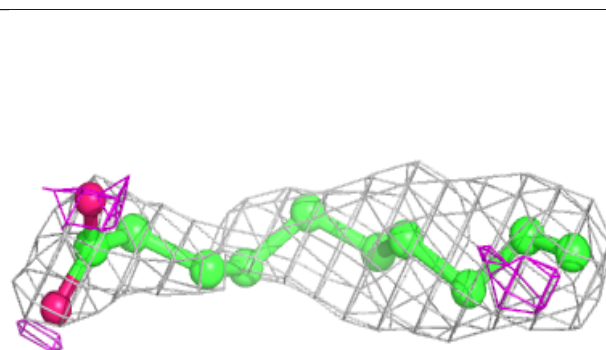
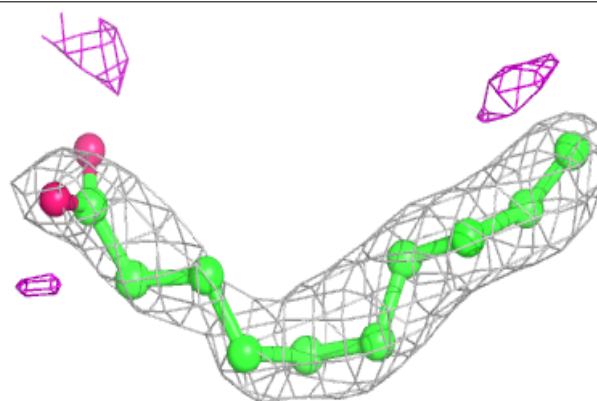


**Electron density around OLA A 1211:**

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

**Electron density around OLA A 1214:**

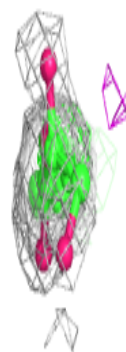
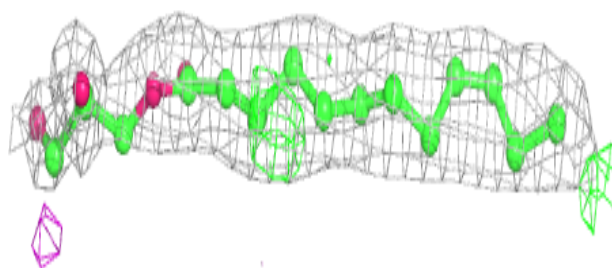
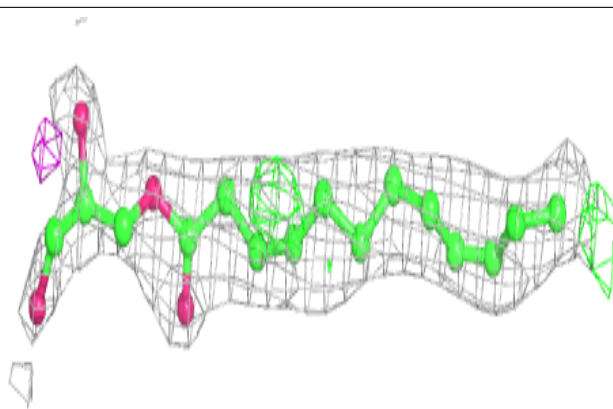
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



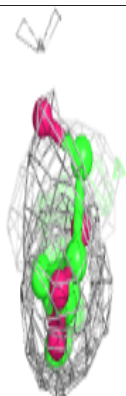
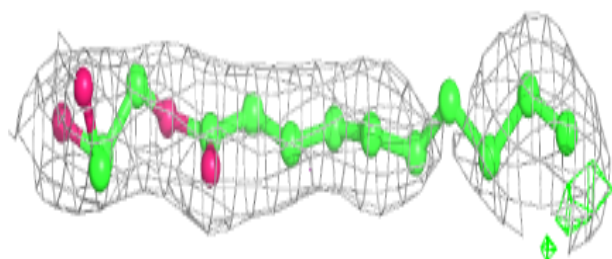
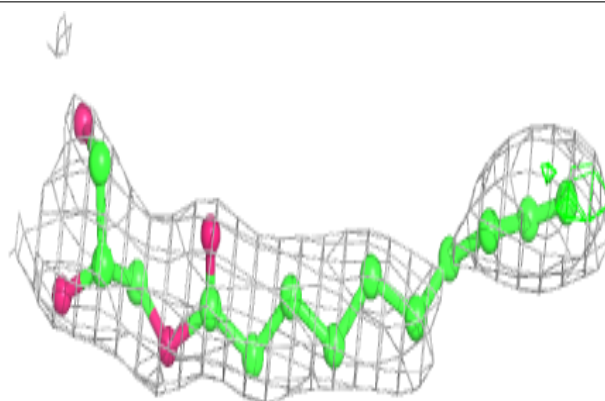


**Electron density around OLC A 1223:**

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

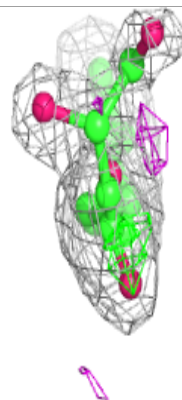
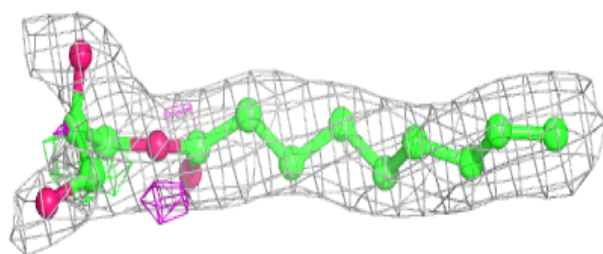
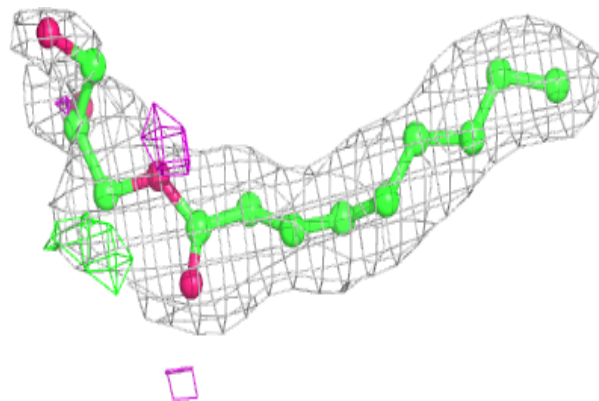
**Electron density around OLC A 1233:**

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

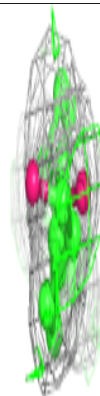
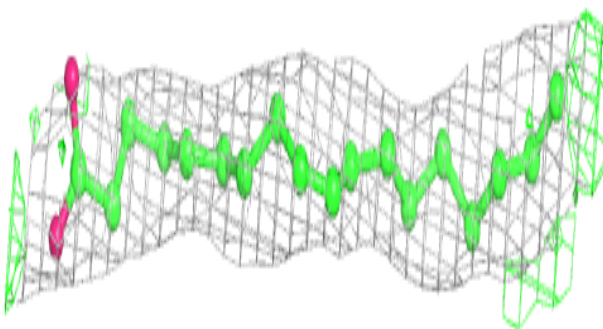
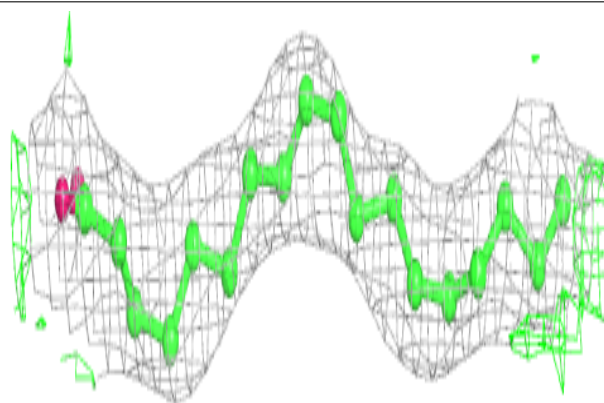


**Electron density around OLC A 1224:**

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

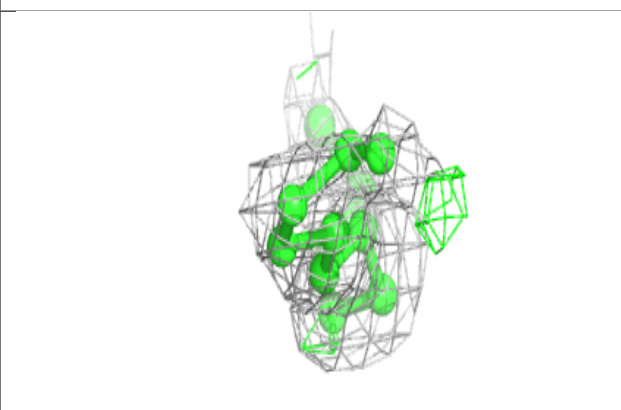
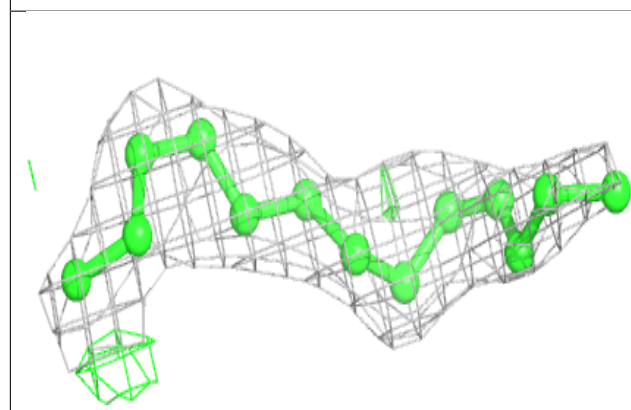
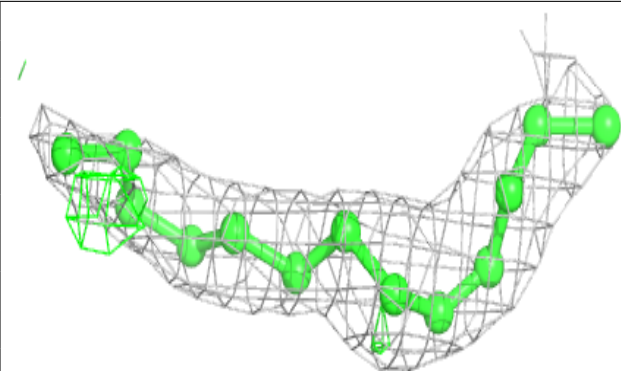
**Electron density around OLA A 1208:**

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

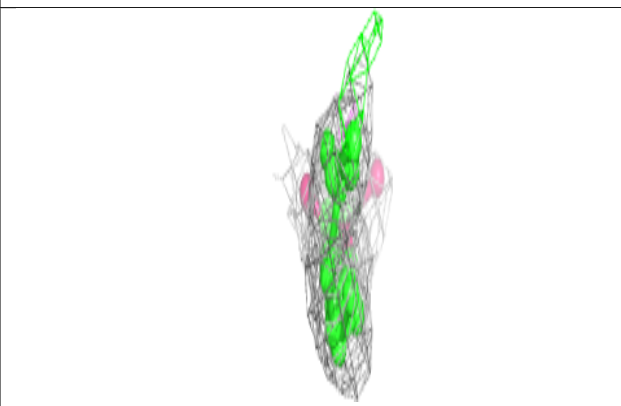
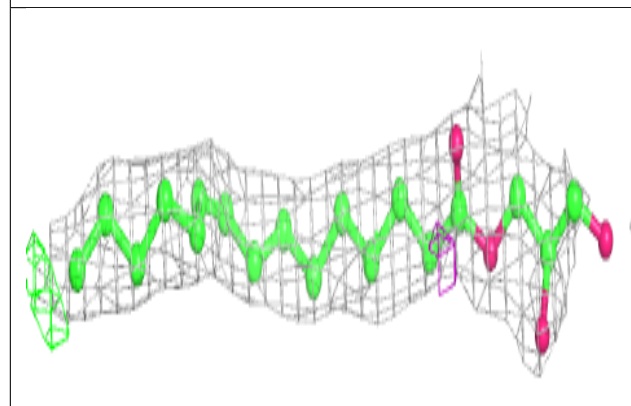
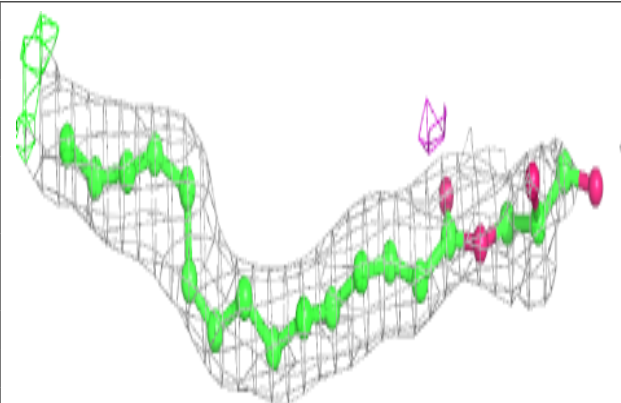


**Electron density around OLA A 1213:**

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

**Electron density around OLC A 1225:**

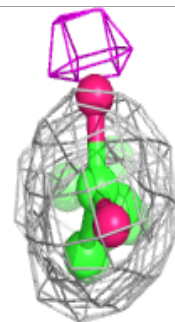
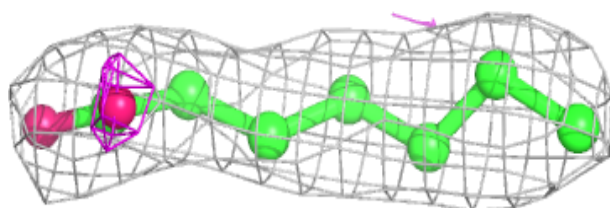
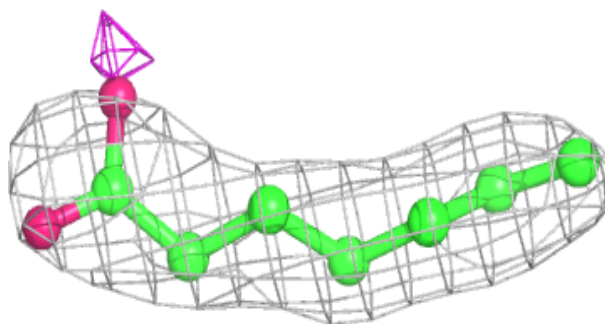
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



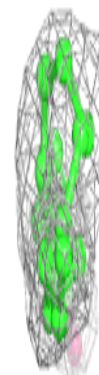
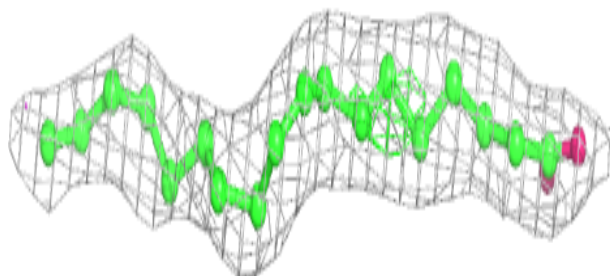
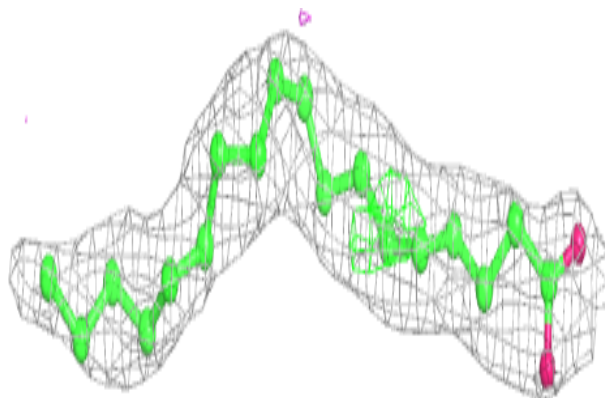


**Electron density around OLA A 1209:**

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

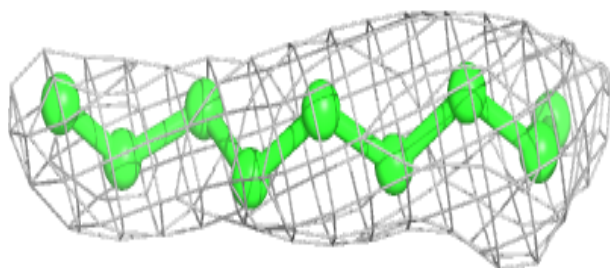
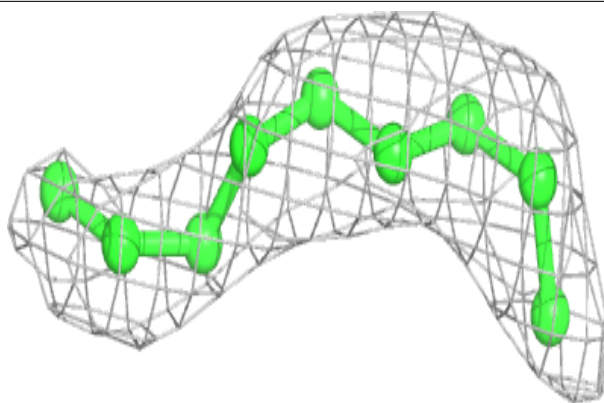
**Electron density around OLA A 1207:**

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

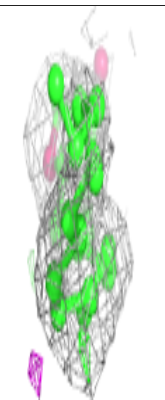
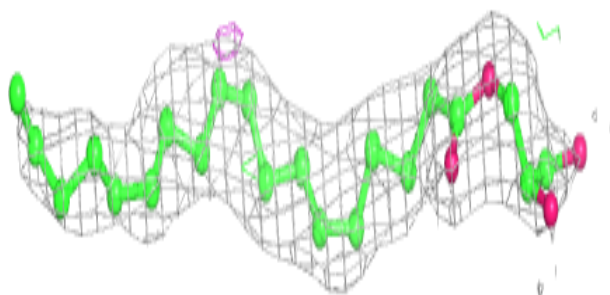
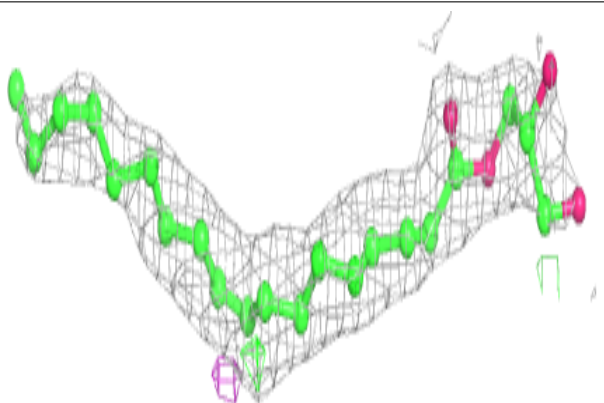


**Electron density around OLA A 1218:**

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

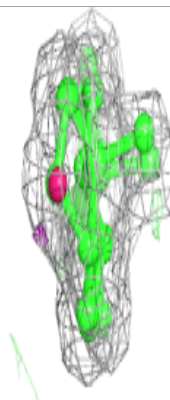
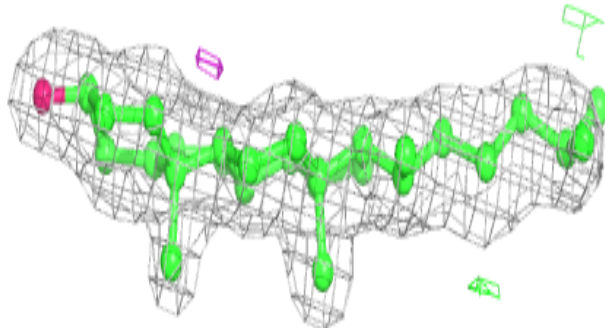
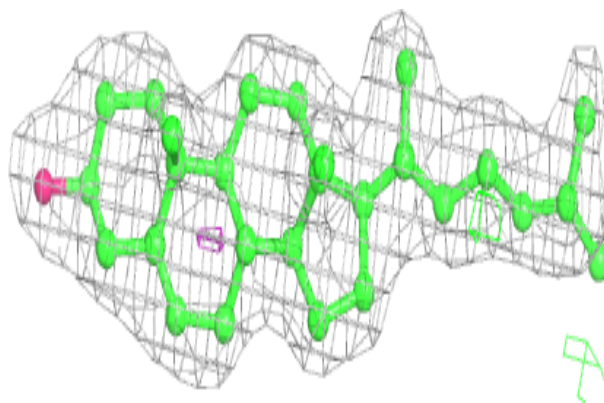
**Electron density around OLC A 1227:**

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

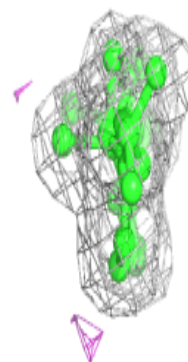
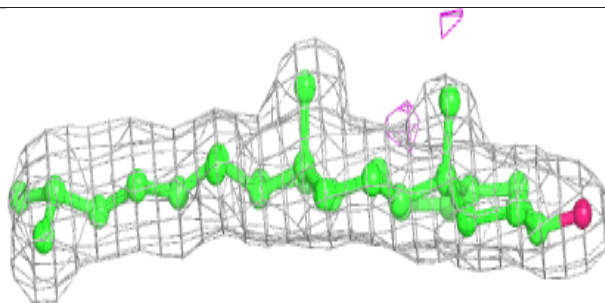
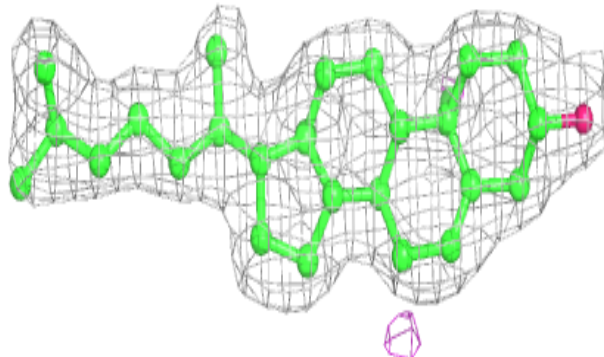


**Electron density around CLR A 1204:**

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

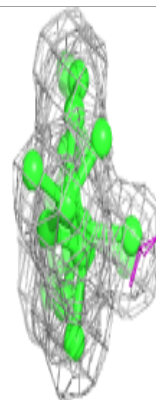
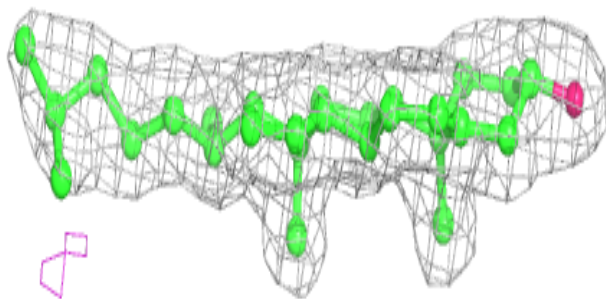
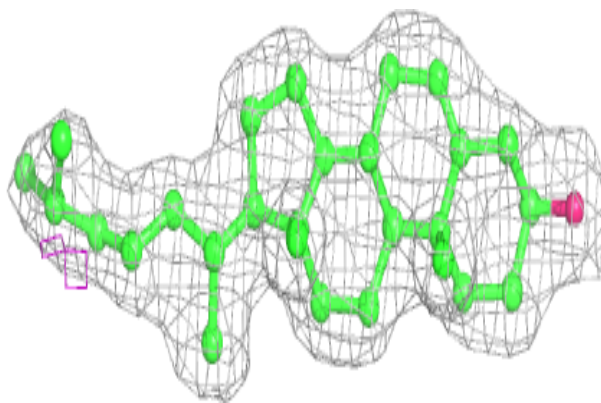
**Electron density around CLR A 1205:**

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



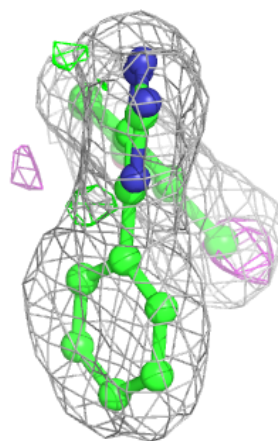
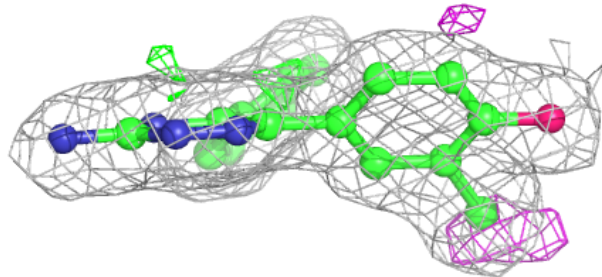
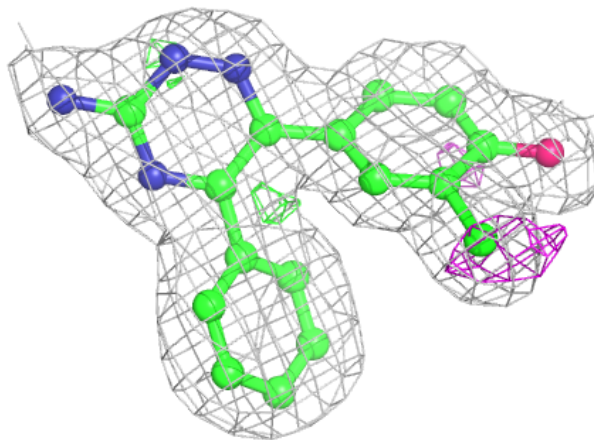
**Electron density around CLR A 1206:**

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



**Electron density around T4E A 1201:**

$2mF_o-DF_c$  (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.