



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 06:23 AM BST

PDB ID : 6PS7  
Title : XFEL A2aR structure by ligand exchange from LUF5843 to ZM241385.  
Authors : Ishchenko, A.; Stauch, B.; Han, G.W.; Batyuk, A.; Shiriaeva, A.; Li, C.;  
Zatsepin, N.A.; Weierstall, U.; Liu, W.; Nango, E.; Nakane, T.; Tanaka, R.;  
Tono, K.; Joti, Y.; Iwata, S.; Moraes, I.; Gati, C.; Cherezov, C.  
Deposited on : 2019-07-12  
Resolution : 1.85 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

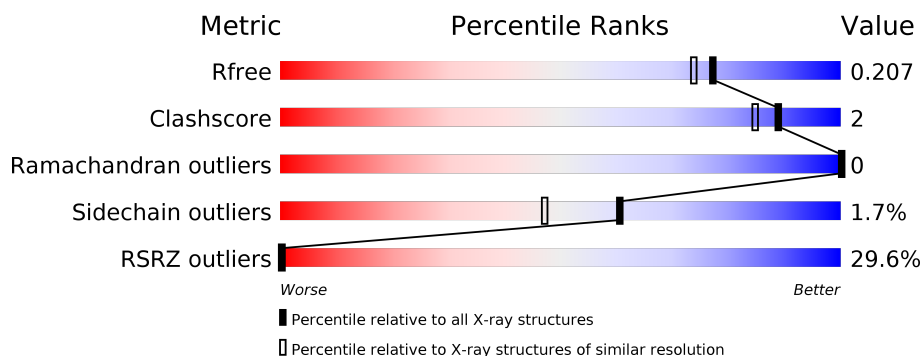
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	442	

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
3	OLC	A	1208	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3655 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	392	Total	C	N	O	S	0	20	0
			3131	2053	516	539	23			

There are 34 discrepancies between the modelled and reference sequences:

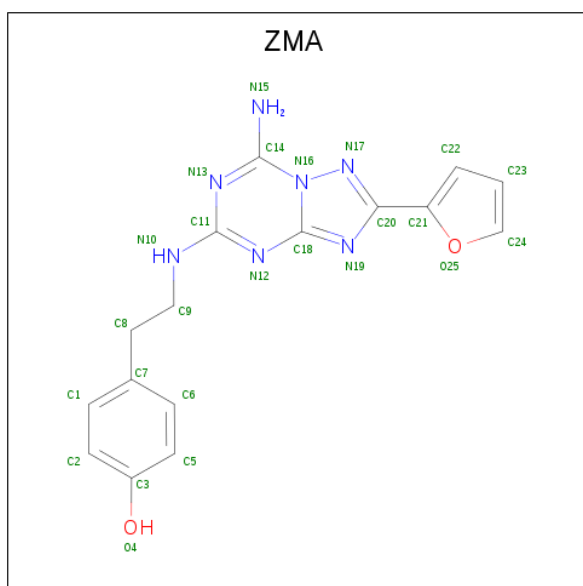
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	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	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274

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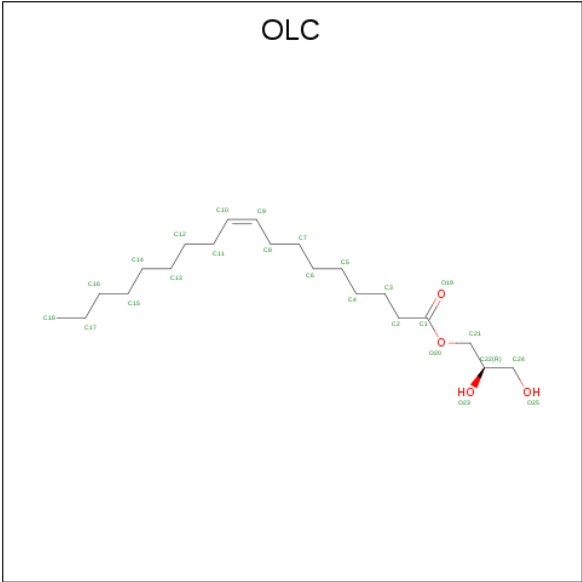
Chain	Residue	Modelled	Actual	Comment	Reference
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-{2-[(7-amino-2-furan-2-yl)[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl} phenol (three-letter code: ZMA) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>7</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by author).



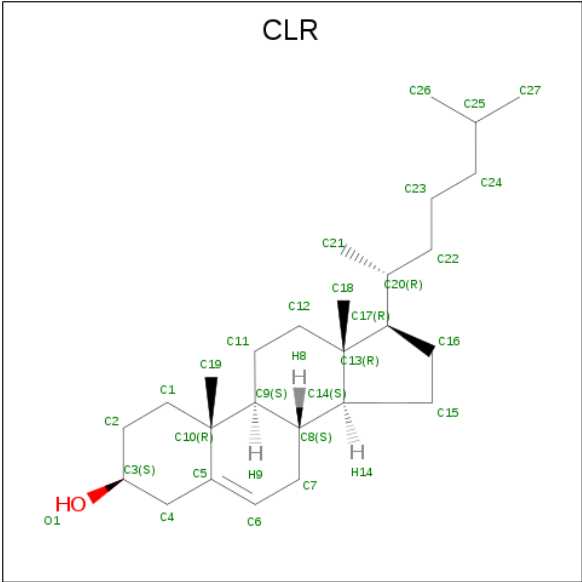
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	16	7	2		

- Molecule 3 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>).



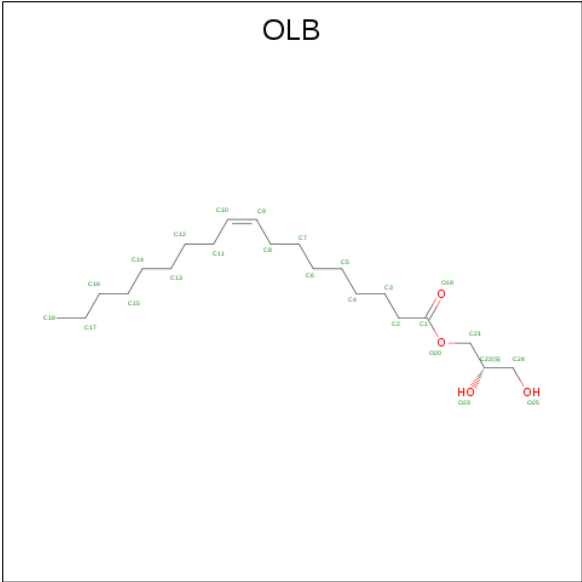
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	13	4		
3	A	1	Total	C	O	0	0
			16	12	4		
3	A	1	Total	C	O	0	0
			18	14	4		
3	A	1	Total	C	O	0	0
			17	13	4		
3	A	1	Total	C	O	0	0
			17	13	4		
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			17	13	4		

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



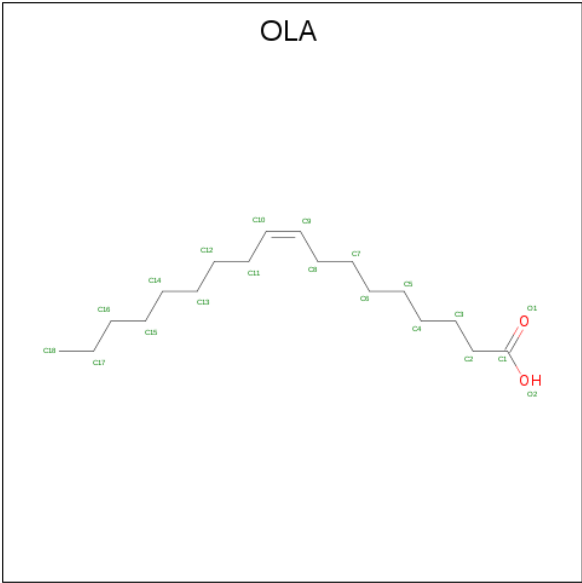
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	13	4		

- Molecule 6 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
6	A	1	Total	C	O	0	0
			16	14	2		
6	A	1	Total	C	O	0	0
			9	7	2		
6	A	1	Total	C	O	0	0
			9	7	2		
6	A	1	Total	C	O	0	0
			12	10	2		
6	A	1	Total	C	O	0	0
			11	9	2		
6	A	1	Total	C	O	0	0
			13	11	2		
6	A	1	Total	C	O	0	0
			12	10	2		
6	A	1	Total	C	O	0	0
			11	9	2		
6	A	1	Total	C		0	0
			9	9			
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	10	2		
6	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is water.

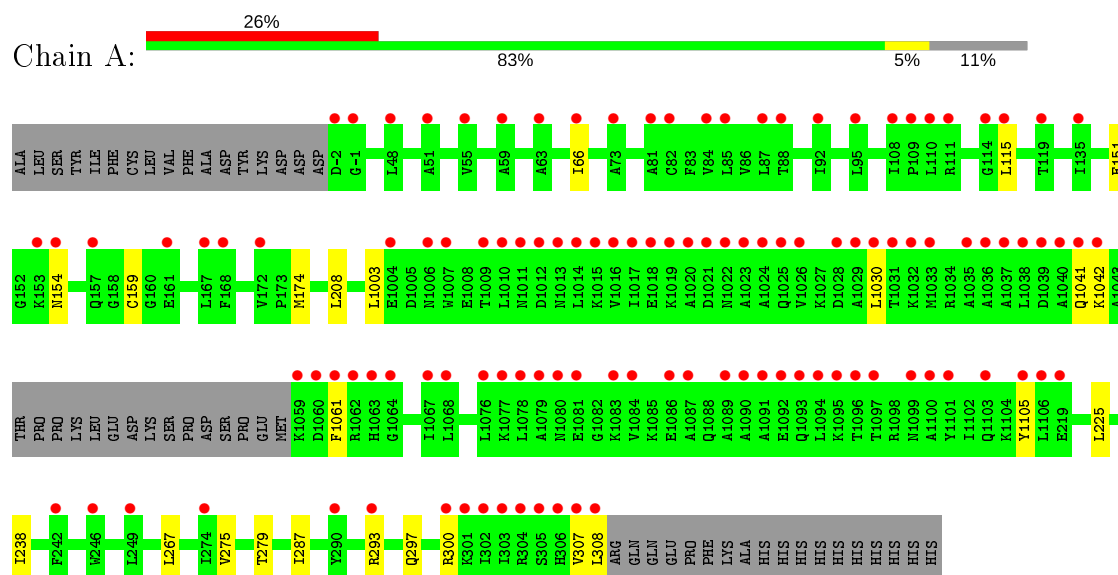
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	105	Total	O	0	0
			105	105		



### 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,Adenosine receptor A2a



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.32Å 180.49Å 142.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.49 – 1.85 33.49 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.49-1.85) 99.9 (33.49-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.175 , 0.201 0.183 , 0.207	Depositor DCC
$R_{free}$ test set	1233 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 92.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.45	0/3215	0.55	0/4381

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	3131	0	3164	14	0
2	A	25	0	14	0	0
3	A	135	0	165	1	0
4	A	84	0	138	0	0
5	A	17	0	22	0	0
6	A	157	0	202	0	0
7	A	1	0	0	0	0
8	A	105	0	0	2	0
All	All	3655	0	3705	14	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 (14) 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:297:GLN:OE1	1:A:300[B]:ARG:NH1	2.31	0.63
1:A:275[B]:VAL:O	1:A:279:THR:HG23	2.03	0.58
1:A:66[B]:ILE:HD11	8:A:1348:HOH:O	2.04	0.56
1:A:154[B]:ASN:OD1	1:A:159:CYS:HB2	2.12	0.49
1:A:1061:PHE:HA	1:A:1105[A]:TYR:CE2	2.51	0.46
1:A:275[A]:VAL:O	1:A:279:THR:HG23	2.16	0.46
1:A:293:ARG:O	1:A:297:GLN:HG2	2.17	0.45
1:A:238:ILE:HD13	1:A:287[B]:ILE:HD13	1.99	0.45
1:A:307:VAL:O	1:A:308:LEU:HD12	2.17	0.45
1:A:208:LEU:HG	1:A:225[B]:LEU:HD23	1.99	0.43
1:A:151:GLU:OE1	1:A:151:GLU:HA	2.21	0.41
1:A:174[A]:MET:HE1	8:A:1344:HOH:O	2.21	0.41
1:A:151:GLU:OE1	1:A:154[B]:ASN:ND2	2.54	0.41
1:A:267:LEU:HD21	3:A:1204:OLC:H22	2.03	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	408/442 (92%)	404 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/369 (88%)	318 (98%)	5 (2%)	65	53

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	1003	LEU
1	A	1030	LEU
1	A	1041	GLN
1	A	1042	LYS

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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
6	OLA	A	1220	-	9,12,19	0.35	0	8,12,19	0.68	0
6	OLA	A	1215	-	12,15,19	0.28	0	11,15,19	0.52	0
3	OLC	A	1203	-	15,15,24	0.56	0	16,16,25	1.06	1 (6%)
3	OLC	A	1209	-	10,10,24	0.65	0	11,11,25	1.13	1 (9%)
6	OLA	A	1219	-	7,10,19	0.21	0	6,10,19	0.51	0
4	CLR	A	1211	-	31,31,31	0.71	0	48,48,48	0.91	1 (2%)
6	OLA	A	1226	-	8,11,19	0.33	0	7,11,19	0.72	0
3	OLC	A	1202	-	16,16,24	0.62	0	17,17,25	1.02	1 (5%)
6	OLA	A	1216	-	5,8,19	0.23	0	4,8,19	0.51	0
3	OLC	A	1206	-	16,16,24	0.56	0	17,17,25	1.22	2 (11%)
3	OLC	A	1210	-	16,16,24	0.61	0	17,17,25	1.04	2 (11%)
3	OLC	A	1204	-	17,17,24	0.56	0	18,18,25	1.06	1 (5%)
6	OLA	A	1217	-	5,8,19	0.25	0	4,8,19	0.55	0
6	OLA	A	1218	-	8,11,19	0.35	0	7,11,19	0.75	0
3	OLC	A	1208	-	10,10,24	0.64	0	11,11,25	1.10	1 (9%)
4	CLR	A	1213	-	31,31,31	0.58	0	48,48,48	0.76	2 (4%)
6	OLA	A	1224	-	4,7,19	0.31	0	3,7,19	0.30	0
3	OLC	A	1207	-	10,10,24	0.64	0	11,11,25	1.10	1 (9%)
6	OLA	A	1223	-	8,8,19	0.39	0	7,7,19	0.70	0
6	OLA	A	1227	-	13,16,19	0.19	0	12,16,19	0.60	0
2	ZMA	A	1201	-	21,28,28	0.88	1 (4%)	22,39,39	1.47	2 (9%)
6	OLA	A	1221	-	8,11,19	0.33	0	7,11,19	0.75	0
6	OLA	A	1222	-	7,10,19	0.20	0	6,10,19	0.54	0
6	OLA	A	1225	-	14,17,19	0.29	0	13,17,19	0.48	0
3	OLC	A	1205	-	16,16,24	0.58	0	17,17,25	1.17	1 (5%)
5	OLB	A	1214	-	16,16,24	0.32	0	17,17,25	0.33	0
4	CLR	A	1212	-	31,31,31	0.64	0	48,48,48	0.90	1 (2%)

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
6	OLA	A	1220	-	-	5/8/10/17	-
6	OLA	A	1215	-	-	4/11/13/17	-
3	OLC	A	1203	-	-	2/15/15/24	-
3	OLC	A	1209	-	-	4/10/10/24	-
6	OLA	A	1219	-	-	1/6/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	A	1211	-	-	1/10/68/68	0/4/4/4
6	OLA	A	1226	-	-	2/7/9/17	-
3	OLC	A	1202	-	-	5/16/16/24	-
6	OLA	A	1216	-	-	1/4/6/17	-
3	OLC	A	1206	-	-	4/16/16/24	-
3	OLC	A	1210	-	-	12/16/16/24	-
3	OLC	A	1204	-	-	4/17/17/24	-
6	OLA	A	1217	-	-	3/4/6/17	-
6	OLA	A	1218	-	-	1/7/9/17	-
3	OLC	A	1208	-	-	5/10/10/24	-
4	CLR	A	1213	-	-	1/10/68/68	0/4/4/4
6	OLA	A	1224	-	-	1/3/5/17	-
3	OLC	A	1207	-	-	1/10/10/24	-
6	OLA	A	1223	-	-	1/6/6/17	-
6	OLA	A	1227	-	-	6/12/14/17	-
2	ZMA	A	1201	-	-	0/6/10/10	0/4/4/4
6	OLA	A	1221	-	-	2/7/9/17	-
6	OLA	A	1222	-	-	2/6/8/17	-
6	OLA	A	1225	-	-	7/13/15/17	-
3	OLC	A	1205	-	-	4/16/16/24	-
5	OLB	A	1214	-	-	0/16/16/24	-
4	CLR	A	1212	-	-	2/10/68/68	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ZMA	C20-N19	3.02	1.39	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ZMA	N15-C14-N16	5.67	121.78	117.97
3	A	1206	OLC	O20-C1-C2	3.18	121.89	111.91
3	A	1210	OLC	O20-C1-C2	3.04	121.46	111.91
3	A	1205	OLC	O20-C1-C2	2.99	121.30	111.91
3	A	1203	OLC	O20-C1-C2	2.88	120.95	111.91
3	A	1209	OLC	O20-C1-C2	2.74	120.51	111.91
3	A	1204	OLC	O20-C1-C2	2.63	120.15	111.91
3	A	1207	OLC	O20-C1-C2	2.60	120.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1208	OLC	O20-C1-C2	2.59	120.03	111.91
3	A	1202	OLC	O20-C1-C2	2.58	120.01	111.91
4	A	1213	CLR	C4-C5-C10	2.35	119.54	116.42
4	A	1213	CLR	C4-C5-C6	-2.34	117.23	120.61
2	A	1201	ZMA	N17-C20-N19	2.31	116.08	114.56
3	A	1206	OLC	O20-C1-O19	-2.13	118.22	123.59
4	A	1212	CLR	C4-C5-C10	2.09	119.19	116.42
4	A	1211	CLR	C4-C5-C10	2.04	119.12	116.42
3	A	1210	OLC	O20-C1-O19	-2.02	118.50	123.59

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1226	OLA	C1-C2-C3-C4
3	A	1202	OLC	C21-C22-C24-O25
6	A	1216	OLA	C1-C2-C3-C4
6	A	1217	OLA	C1-C2-C3-C4
6	A	1221	OLA	C1-C2-C3-C4
6	A	1222	OLA	C1-C2-C3-C4
3	A	1205	OLC	O20-C21-C22-O23
3	A	1204	OLC	C2-C1-O20-C21
3	A	1204	OLC	O19-C1-O20-C21
3	A	1206	OLC	O20-C21-C22-C24
3	A	1210	OLC	C1-C2-C3-C4
3	A	1209	OLC	C2-C1-O20-C21
3	A	1210	OLC	O20-C21-C22-O23
3	A	1210	OLC	O20-C21-C22-C24
3	A	1208	OLC	C21-C22-C24-O25
3	A	1206	OLC	O20-C21-C22-O23
6	A	1220	OLA	C4-C5-C6-C7
6	A	1227	OLA	C11-C12-C13-C14
3	A	1209	OLC	O19-C1-O20-C21
3	A	1202	OLC	O23-C22-C24-O25
6	A	1227	OLA	C6-C7-C8-C9
3	A	1207	OLC	O20-C21-C22-O23
6	A	1220	OLA	C5-C6-C7-C8
3	A	1203	OLC	C5-C6-C7-C8
6	A	1218	OLA	C4-C5-C6-C7
3	A	1210	OLC	C2-C3-C4-C5
6	A	1225	OLA	C12-C13-C14-C15
3	A	1210	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	A	1225	OLA	C10-C11-C12-C13
6	A	1220	OLA	C2-C3-C4-C5
6	A	1227	OLA	C2-C3-C4-C5
6	A	1225	OLA	C5-C6-C7-C8
3	A	1210	OLC	C2-C1-O20-C21
6	A	1224	OLA	C2-C3-C4-C5
3	A	1202	OLC	C2-C1-O20-C21
6	A	1217	OLA	C4-C5-C6-C7
3	A	1206	OLC	C6-C7-C8-C9
6	A	1217	OLA	C2-C3-C4-C5
3	A	1202	OLC	O19-C1-O20-C21
3	A	1210	OLC	O19-C1-O20-C21
3	A	1210	OLC	O23-C22-C24-O25
3	A	1203	OLC	C6-C7-C8-C9
6	A	1215	OLA	C6-C7-C8-C9
6	A	1221	OLA	C4-C5-C6-C7
4	A	1213	CLR	C22-C23-C24-C25
6	A	1215	OLA	C4-C5-C6-C7
6	A	1215	OLA	C1-C2-C3-C4
6	A	1225	OLA	C4-C5-C6-C7
3	A	1205	OLC	O20-C21-C22-C24
6	A	1227	OLA	C5-C6-C7-C8
3	A	1210	OLC	C5-C6-C7-C8
3	A	1209	OLC	O23-C22-C24-O25
6	A	1225	OLA	C2-C3-C4-C5
6	A	1220	OLA	C6-C7-C8-C9
6	A	1223	OLA	C10-C11-C12-C13
6	A	1219	OLA	C3-C4-C5-C6
3	A	1205	OLC	C7-C8-C9-C10
3	A	1210	OLC	C3-C4-C5-C6
6	A	1222	OLA	C4-C5-C6-C7
3	A	1205	OLC	C1-C2-C3-C4
3	A	1204	OLC	C2-C3-C4-C5
4	A	1212	CLR	C23-C24-C25-C27
3	A	1204	OLC	C7-C8-C9-C10
6	A	1225	OLA	C9-C10-C11-C12
3	A	1208	OLC	O19-C1-O20-C21
4	A	1211	CLR	C22-C23-C24-C25
3	A	1206	OLC	C7-C8-C9-C10
3	A	1210	OLC	C7-C8-C9-C10
3	A	1208	OLC	C2-C1-O20-C21
6	A	1227	OLA	C9-C10-C11-C12

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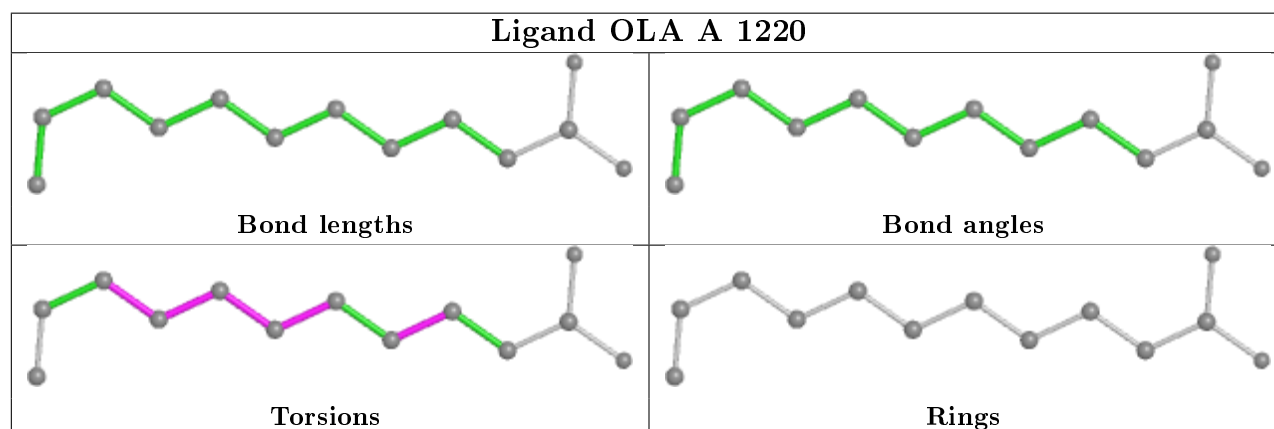
Mol	Chain	Res	Type	Atoms
3	A	1202	OLC	C7-C8-C9-C10
6	A	1215	OLA	C9-C10-C11-C12
6	A	1227	OLA	C4-C5-C6-C7
6	A	1226	OLA	C5-C6-C7-C8
3	A	1208	OLC	O23-C22-C24-O25
3	A	1208	OLC	O20-C21-C22-O23
6	A	1220	OLA	C7-C8-C9-C10
4	A	1212	CLR	C23-C24-C25-C26
3	A	1209	OLC	C21-C22-C24-O25
3	A	1210	OLC	C21-C22-C24-O25
6	A	1225	OLA	C6-C7-C8-C9

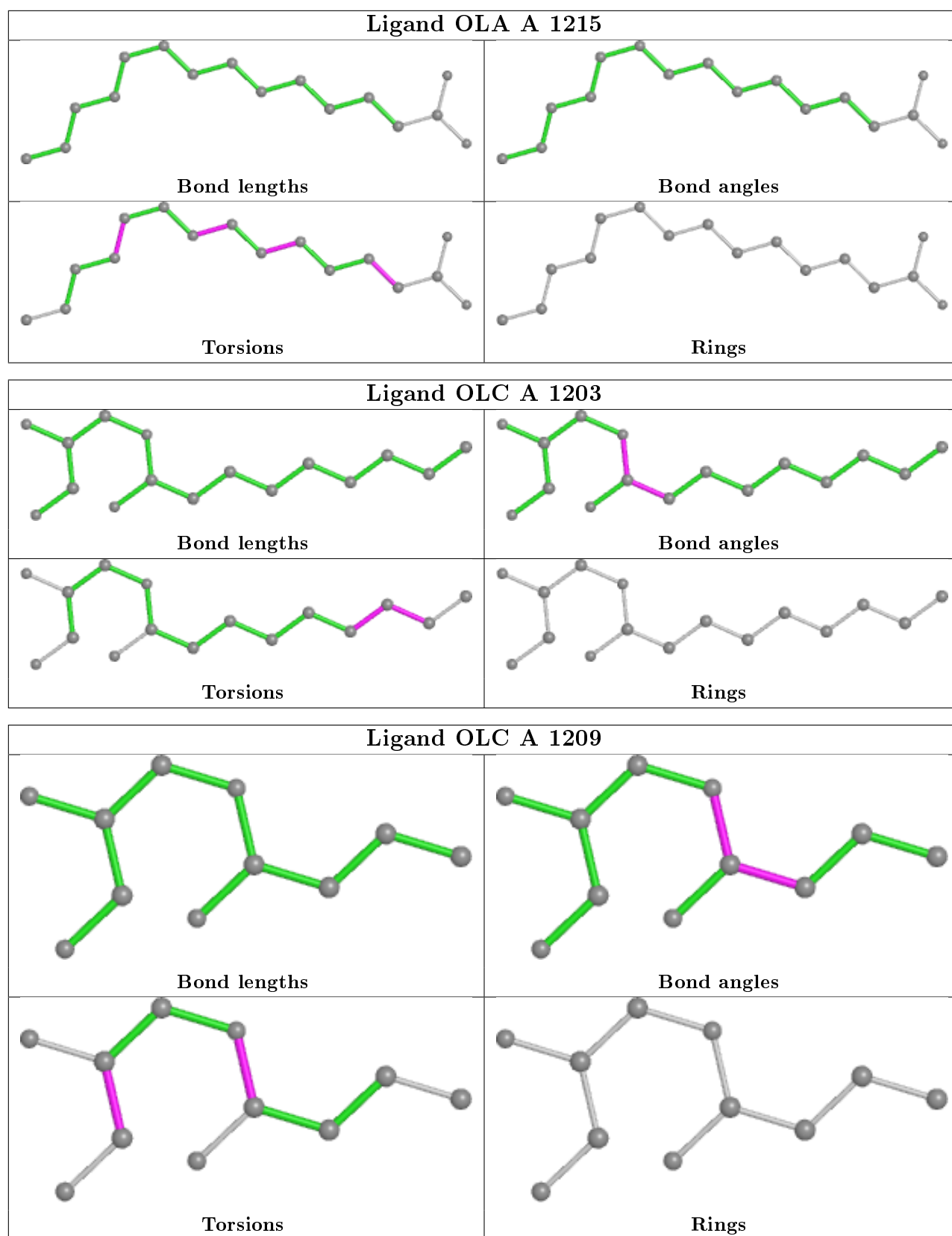
There are no ring outliers.

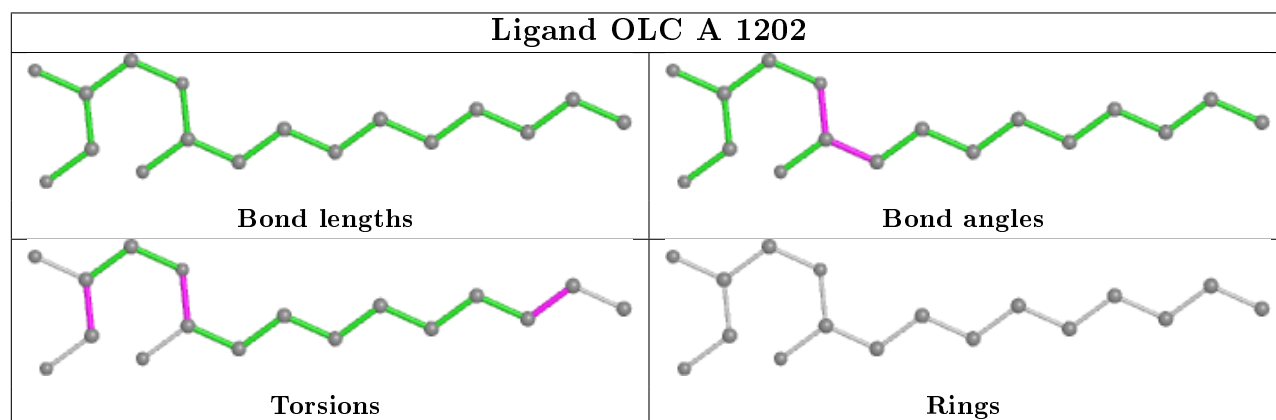
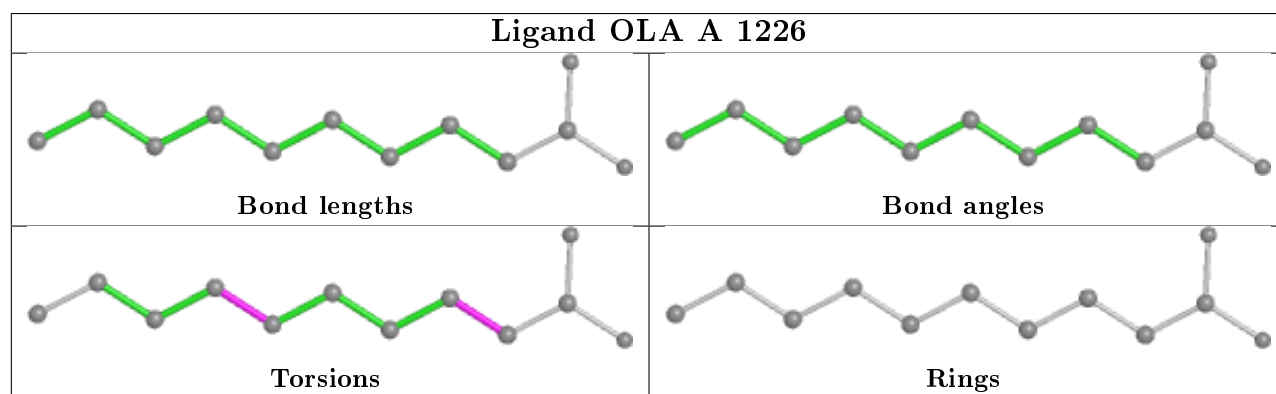
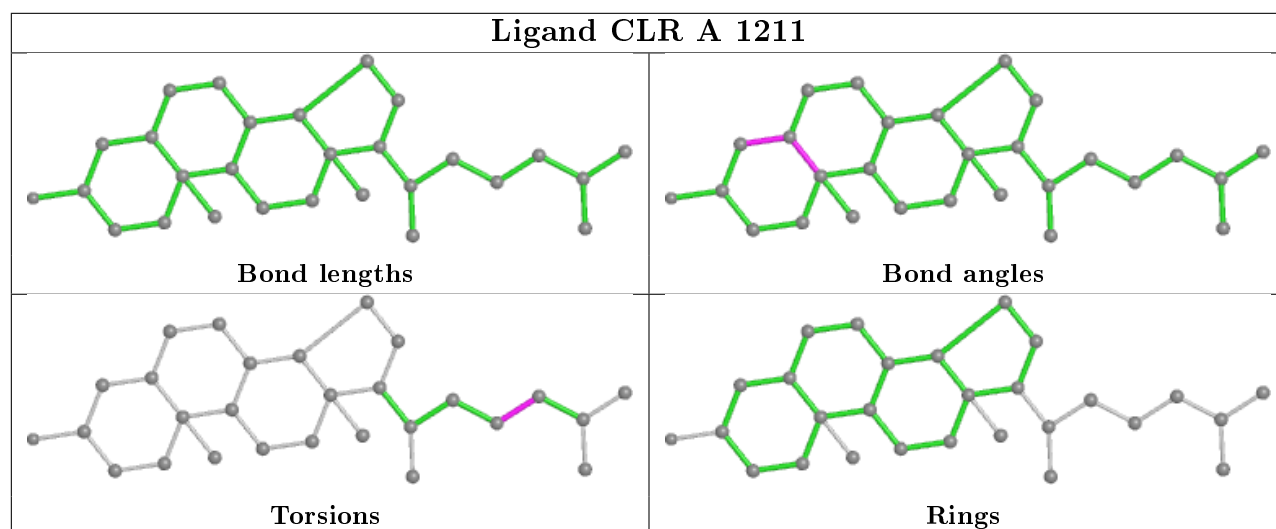
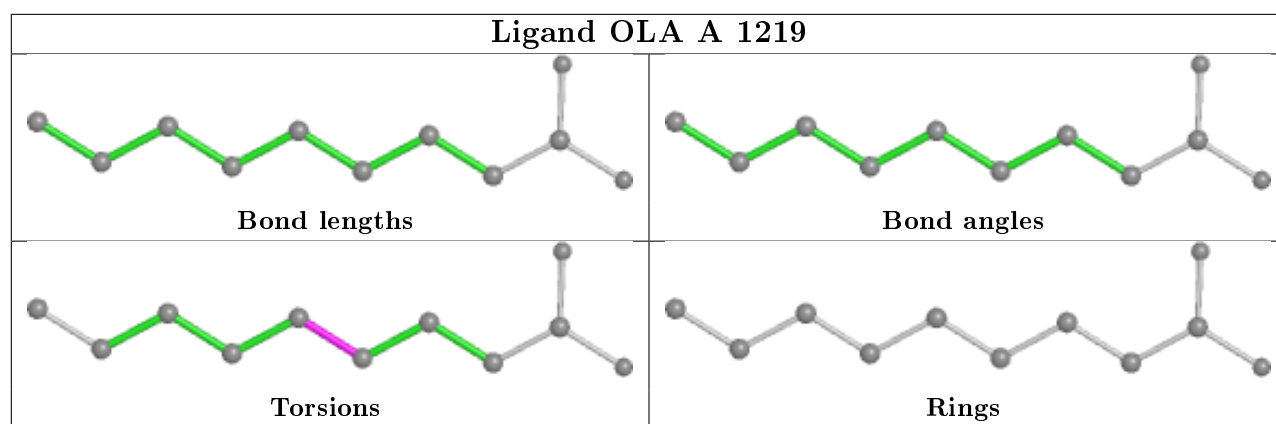
1 monomer is involved in 1 short contact:

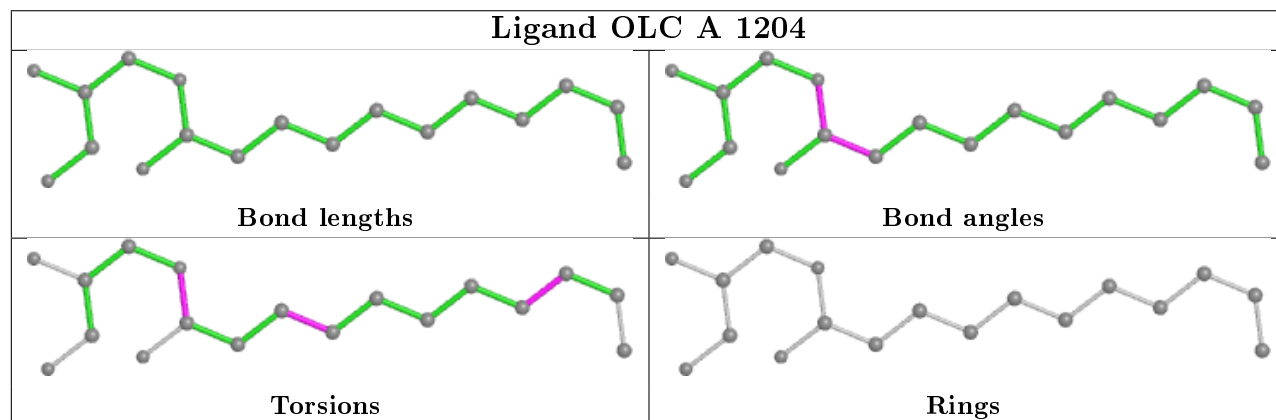
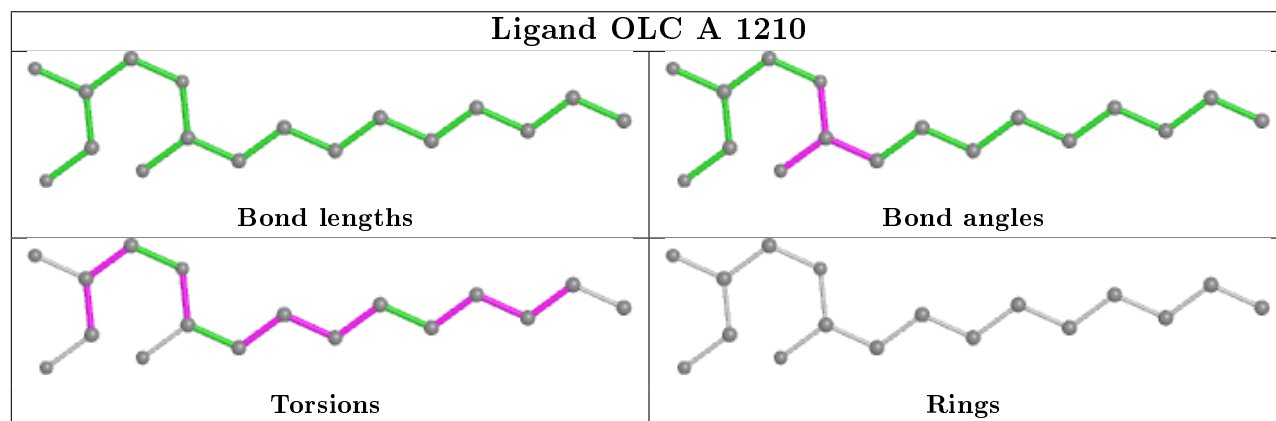
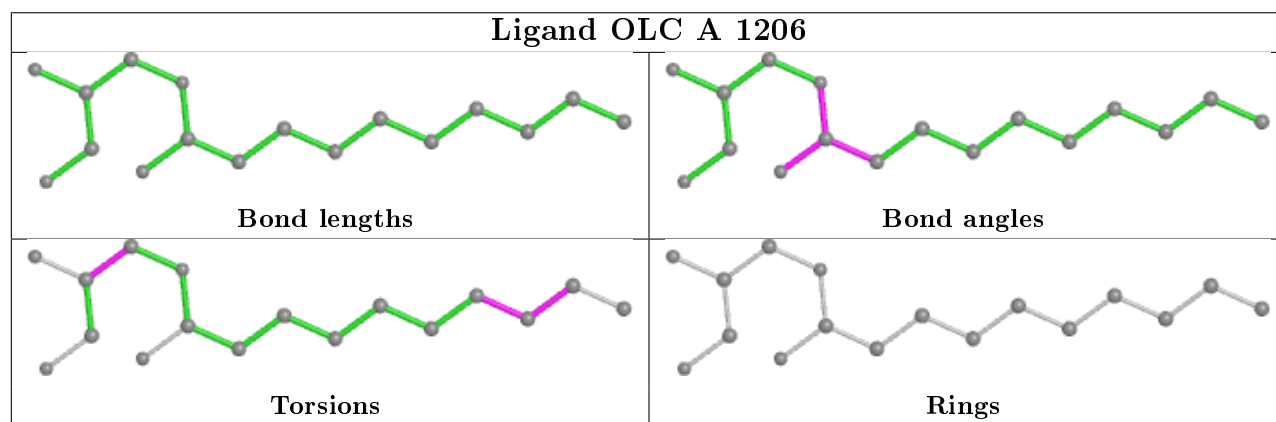
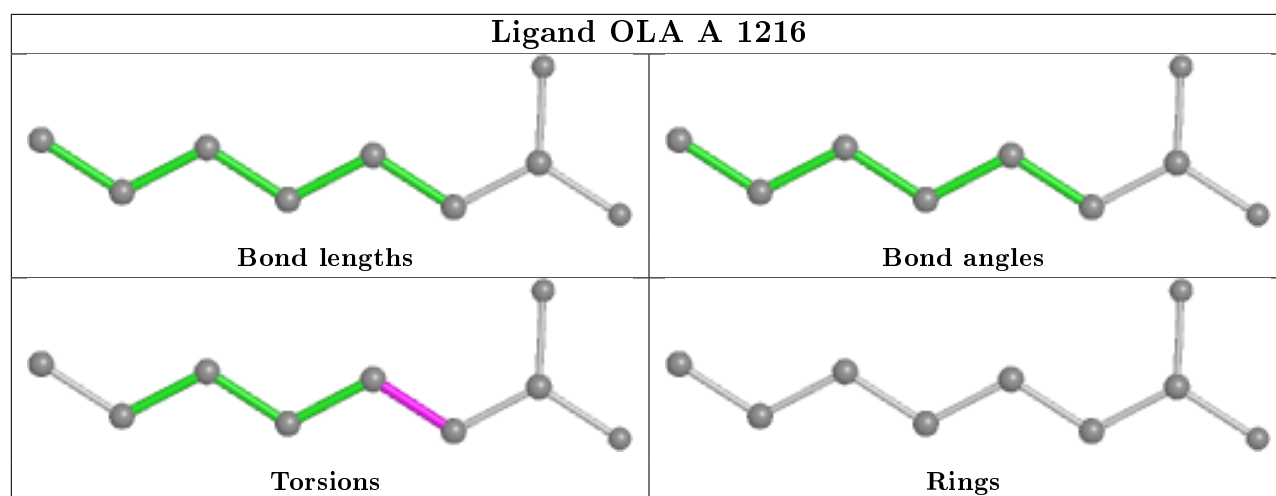
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1204	OLC	1	0

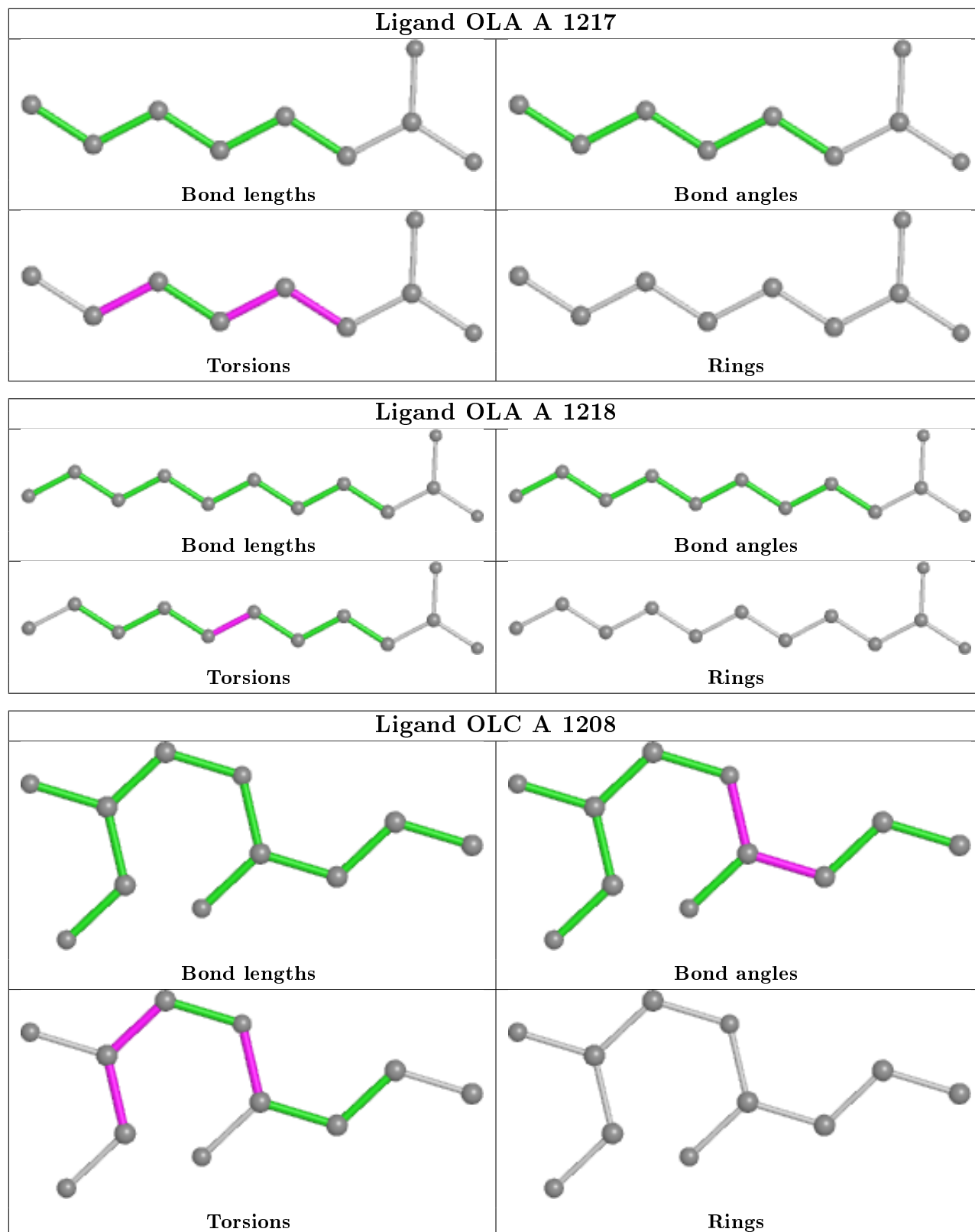
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

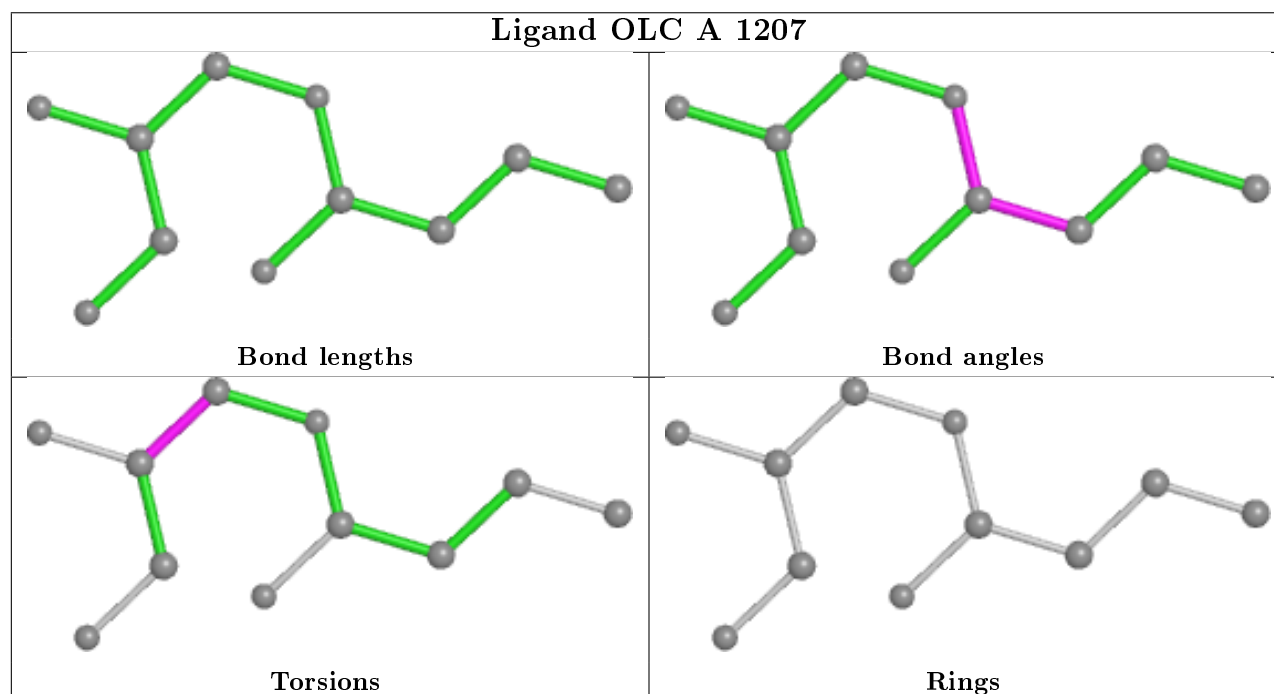
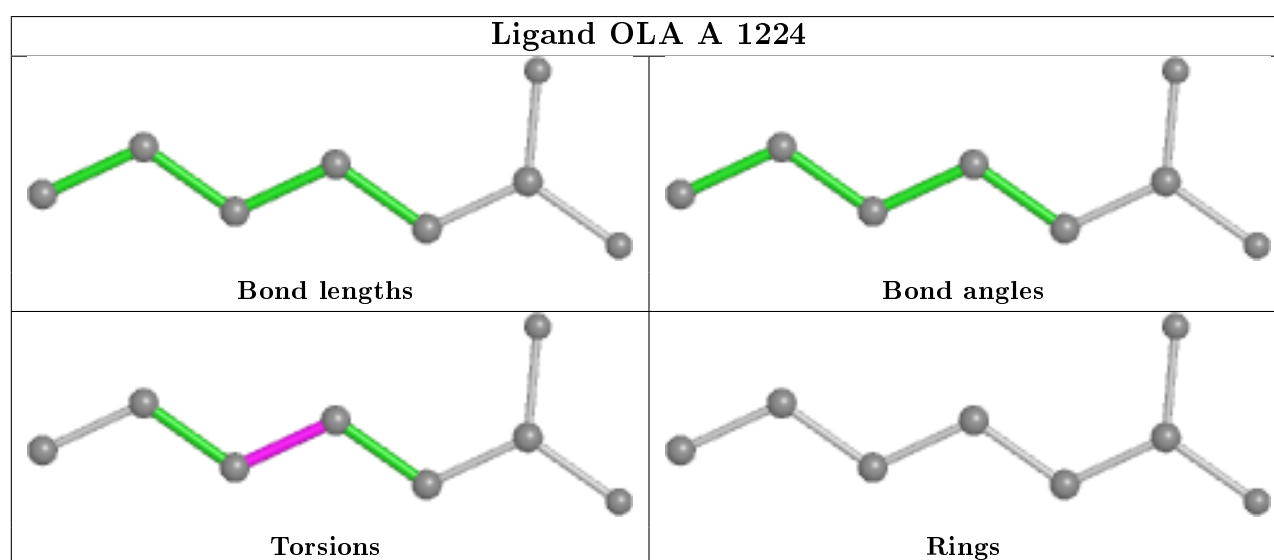
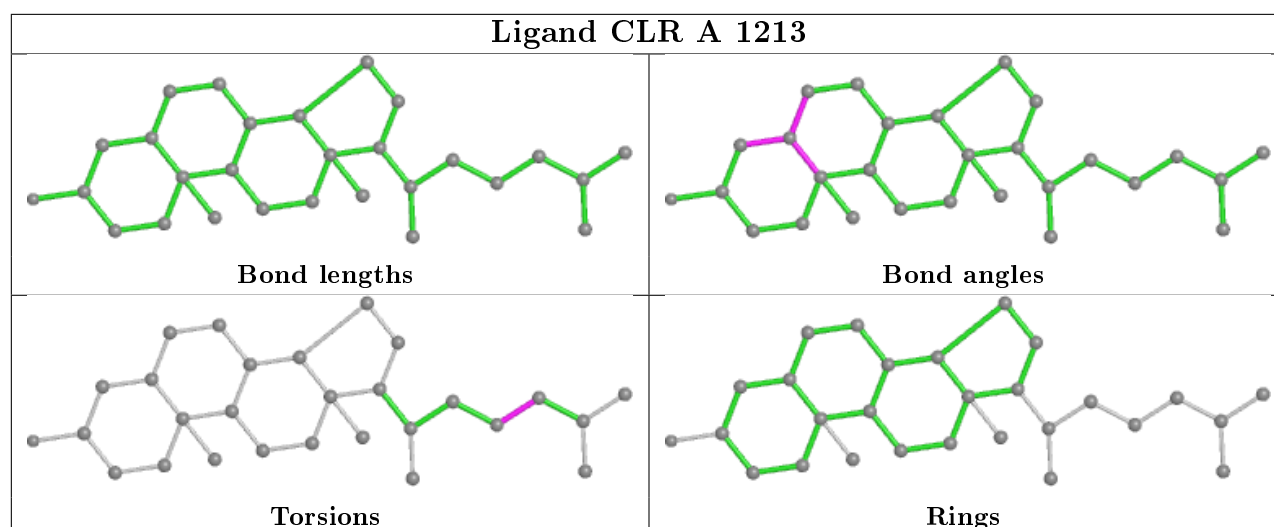


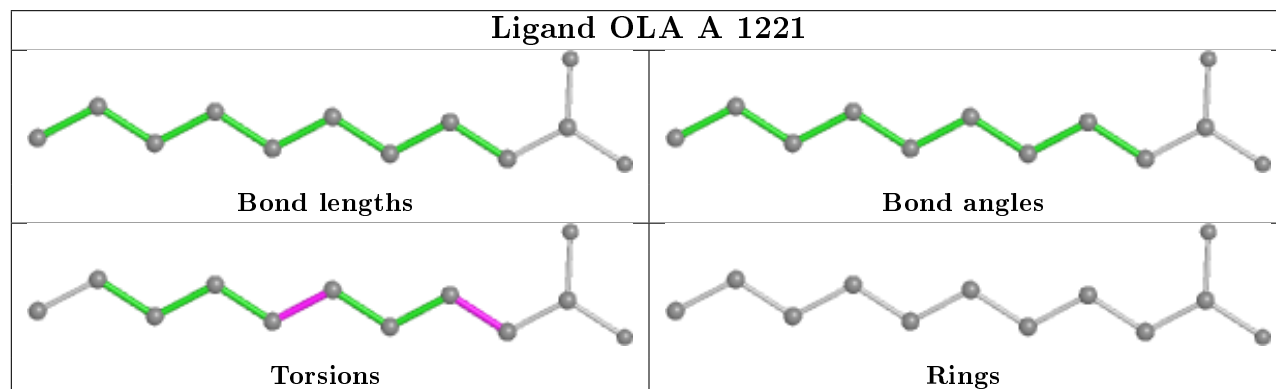
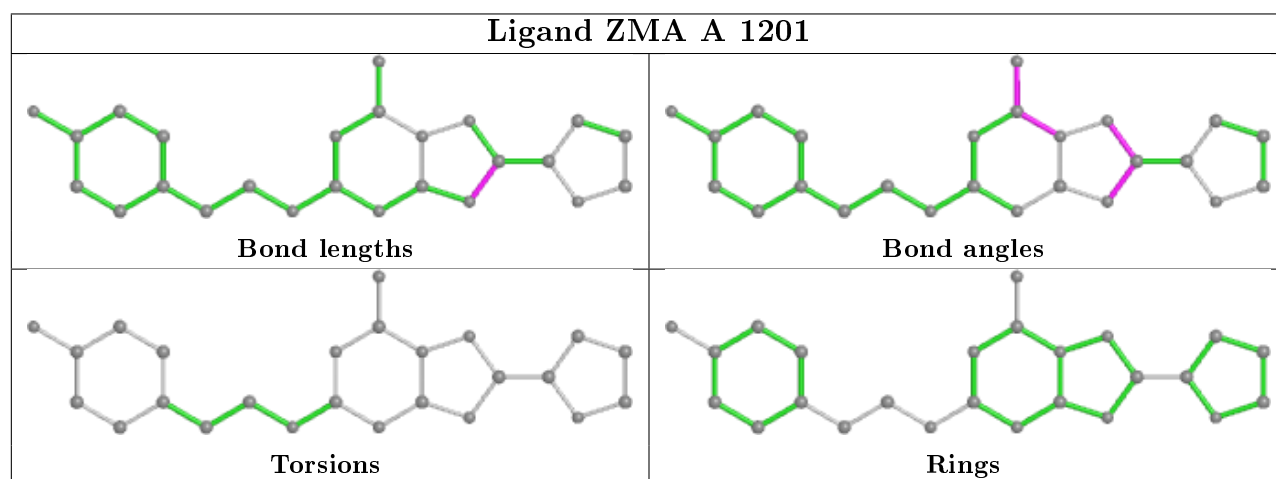
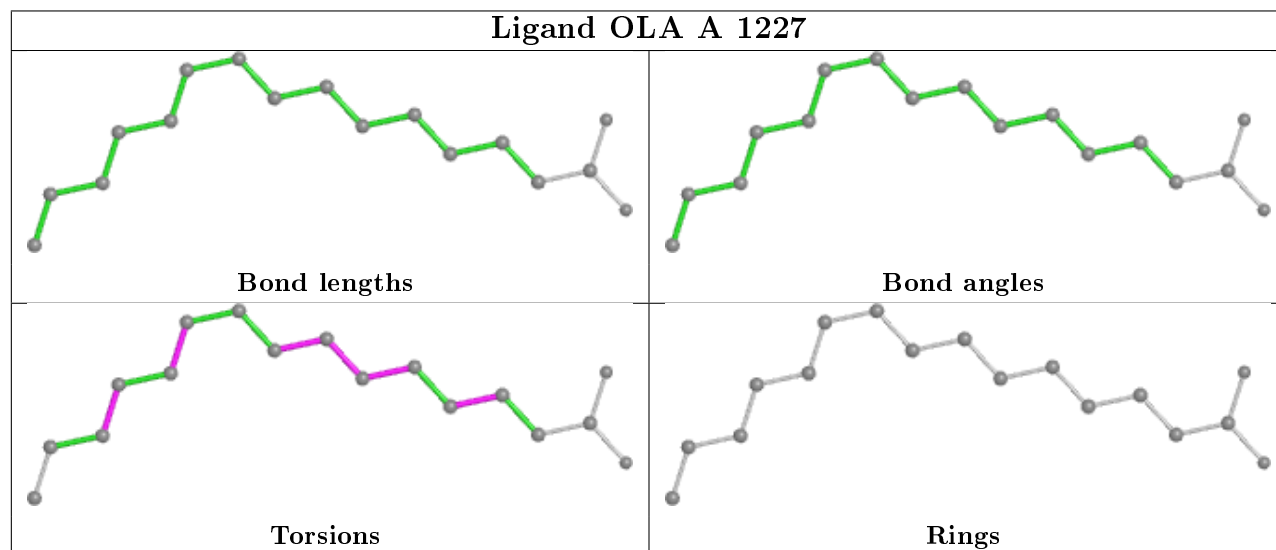
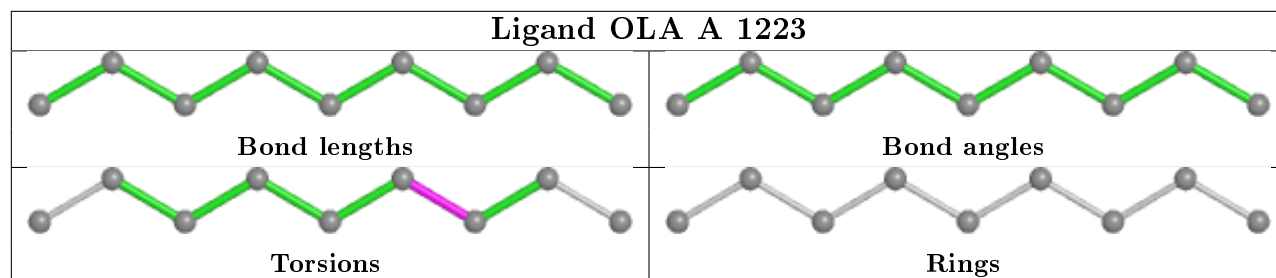




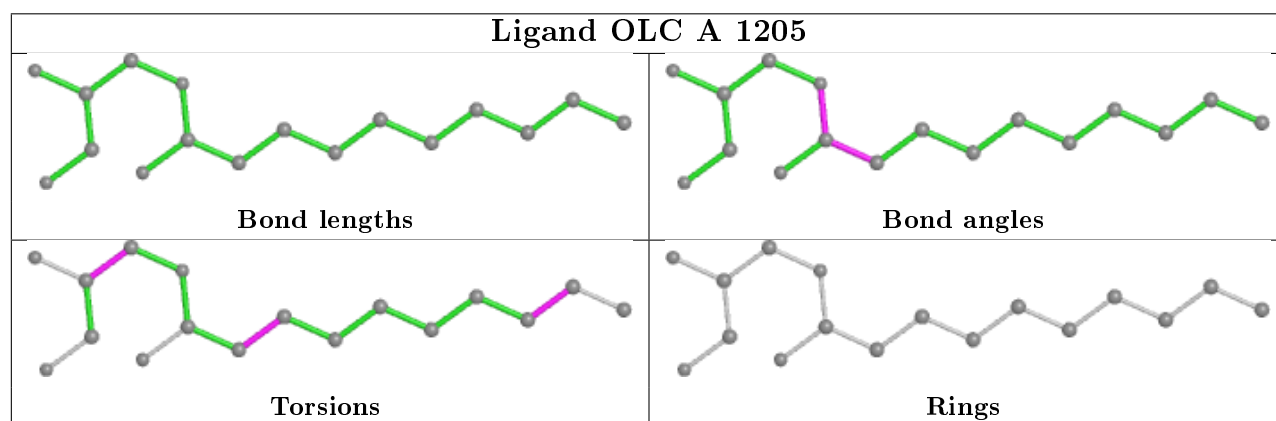
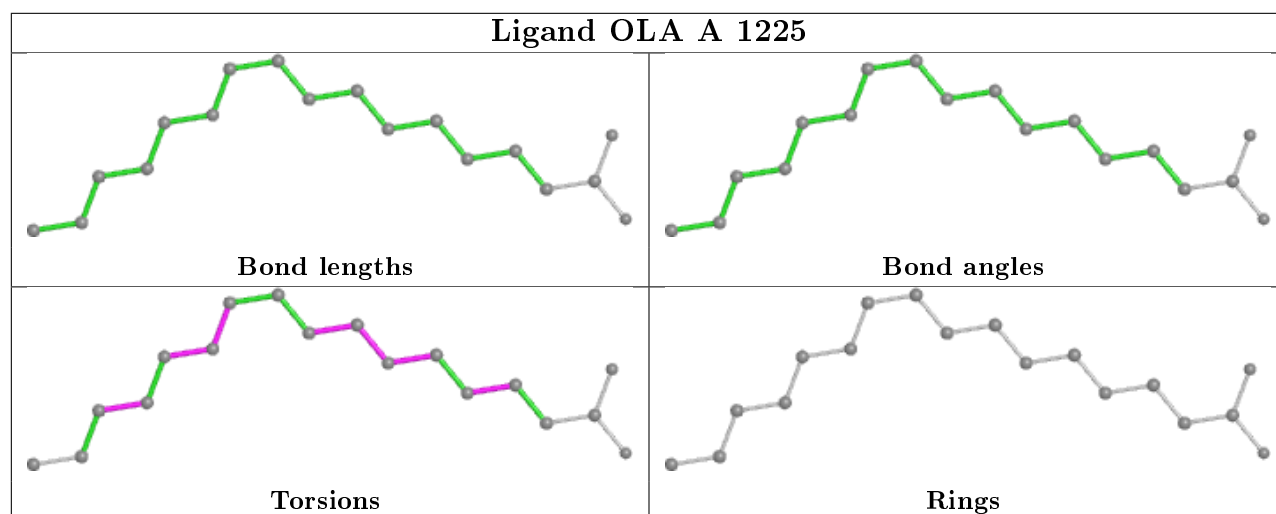
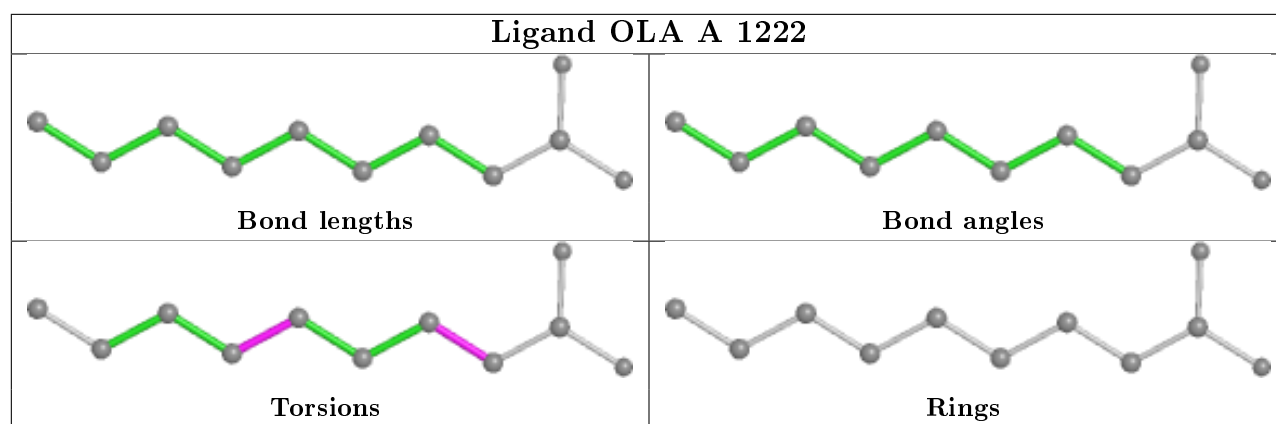


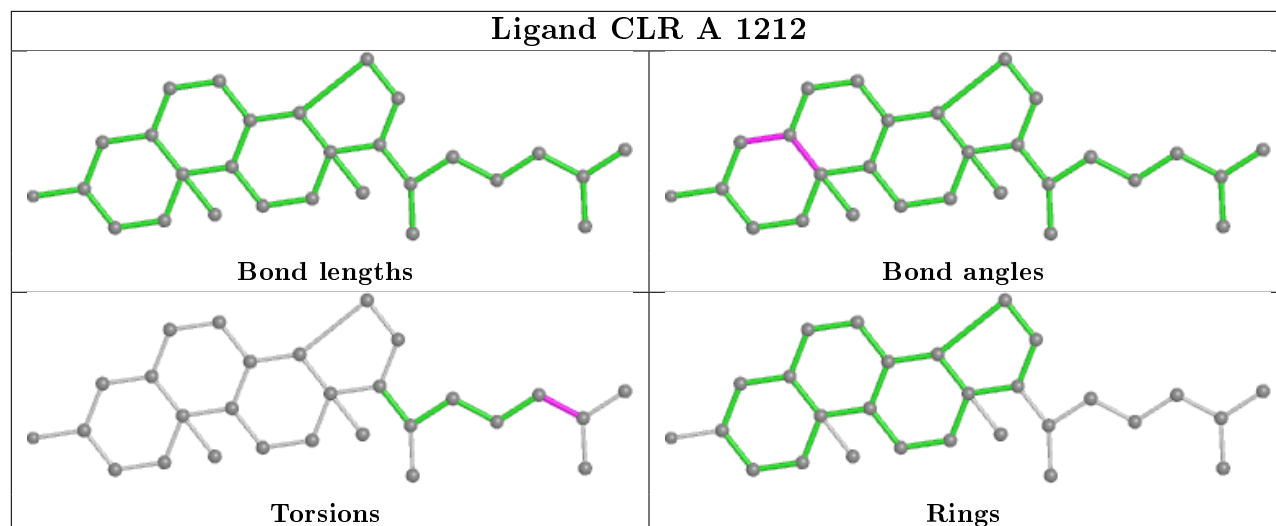












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	392/442 (88%)	1.55	116 (29%) 0 0	23, 37, 99, 128	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1024	ALA	10.4
1	A	1061	PHE	8.6
1	A	1038	LEU	6.9
1	A	307	VAL	6.7
1	A	1060	ASP	6.5
1	A	1059	LYS	6.3
1	A	1062	ARG	6.1
1	A	306	HIS	5.8
1	A	1020	ALA	5.6
1	A	1023	ALA	5.4
1	A	1040	ALA	5.4
1	A	1080	ASN	5.4
1	A	1041	GLN	5.2
1	A	1021	ASP	5.1
1	A	1028	ASP	5.1
1	A	1029	ALA	5.0
1	A	1063	HIS	4.8
1	A	111	ARG	4.8
1	A	1079	ALA	4.7
1	A	1105[A]	TYR	4.6
1	A	1091	ALA	4.5
1	A	1016	VAL	4.5
1	A	1018	GLU	4.5
1	A	1101	TYR	4.5
1	A	1037	ALA	4.4
1	A	1031	THR	4.4
1	A	304	ARG	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1022	ASN	4.3
1	A	1084	VAL	4.3
1	A	1026	VAL	4.2
1	A	1013	ASN	4.1
1	A	303	ILE	4.0
1	A	1089	ALA	3.8
1	A	1077	LYS	3.8
1	A	1039[A]	ASP	3.7
1	A	1035	ALA	3.7
1	A	305	SER	3.7
1	A	172	VAL	3.7
1	A	153	LYS	3.7
1	A	1092	GLU	3.6
1	A	1083	LYS	3.6
1	A	1099	ASN	3.5
1	A	48	LEU	3.5
1	A	1014	LEU	3.5
1	A	1019	LYS	3.4
1	A	1015	LYS	3.4
1	A	1078	LEU	3.4
1	A	84	VAL	3.4
1	A	168	PHE	3.3
1	A	1097	THR	3.3
1	A	1033	MET	3.3
1	A	1025	GLN	3.3
1	A	115	LEU	3.3
1	A	81	ALA	3.3
1	A	1011	ASN	3.2
1	A	55	VAL	3.2
1	A	110	LEU	3.2
1	A	85	LEU	3.1
1	A	1030	LEU	3.1
1	A	1067	ILE	3.1
1	A	87	LEU	3.1
1	A	1017	ILE	3.0
1	A	308	LEU	2.9
1	A	302	ILE	2.9
1	A	114	GLY	2.9
1	A	-1	GLY	2.9
1	A	161	GLU	2.9
1	A	-2	ASP	2.9
1	A	1106[A]	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1081	GLU	2.9
1	A	95	LEU	2.9
1	A	1042	LYS	2.9
1	A	1007	TRP	2.8
1	A	1087	ALA	2.8
1	A	274	ILE	2.8
1	A	1009	THR	2.8
1	A	1032	LYS	2.8
1	A	1100	ALA	2.8
1	A	1095	LYS	2.7
1	A	82	CYS	2.7
1	A	154[A]	ASN	2.7
1	A	1004	GLU	2.7
1	A	1068	LEU	2.7
1	A	92	ILE	2.6
1	A	1096	THR	2.6
1	A	66[A]	ILE	2.6
1	A	1103	GLN	2.6
1	A	88[A]	THR	2.5
1	A	1086	GLU	2.5
1	A	1076	LEU	2.5
1	A	249[A]	LEU	2.5
1	A	1012	ASP	2.5
1	A	108	ILE	2.4
1	A	219	GLU	2.4
1	A	1064	GLY	2.4
1	A	300[A]	ARG	2.4
1	A	290	TYR	2.4
1	A	293	ARG	2.3
1	A	1006	ASN	2.3
1	A	1036	ALA	2.3
1	A	167	LEU	2.3
1	A	1093	GLN	2.2
1	A	242	PHE	2.2
1	A	51	ALA	2.2
1	A	109	PRO	2.2
1	A	119	THR	2.1
1	A	1094	LEU	2.1
1	A	73	ALA	2.1
1	A	63	ALA	2.1
1	A	246	TRP	2.1
1	A	1010	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	157	GLN	2.1
1	A	59	ALA	2.0
1	A	1090	ALA	2.0
1	A	135	ILE	2.0
1	A	301	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 monosaccharides 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.

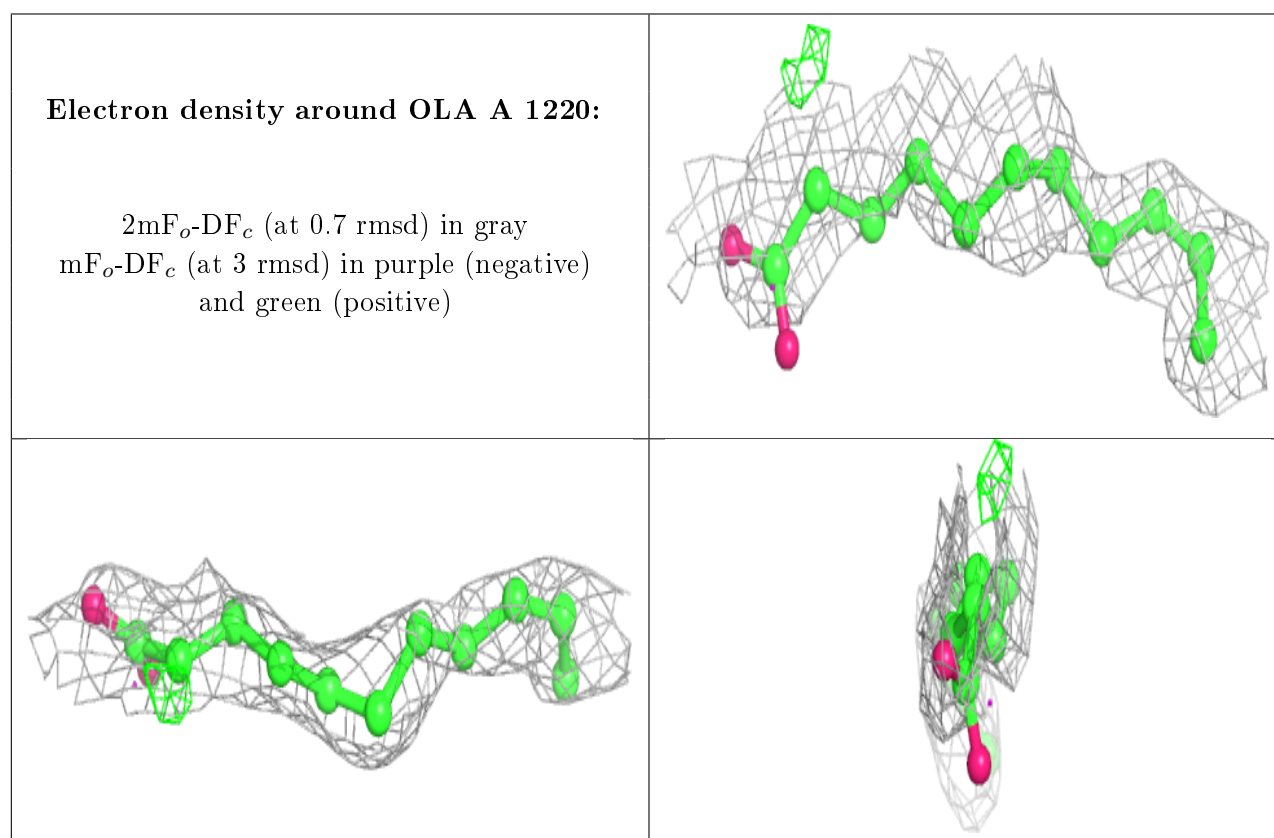
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	OLA	A	1220	13/20	0.43	0.32	72,77,103,104	0
6	OLA	A	1221	12/20	0.45	0.26	64,74,102,110	0
3	OLC	A	1207	11/25	0.50	0.22	81,87,93,93	0
5	OLB	A	1214	17/25	0.50	0.25	69,81,99,100	0
6	OLA	A	1225	18/20	0.57	0.25	74,77,83,83	0
3	OLC	A	1209	11/25	0.58	0.22	69,84,95,105	0
6	OLA	A	1223	9/20	0.61	0.25	73,76,80,81	0
3	OLC	A	1210	17/25	0.69	0.20	77,117,146,149	0
6	OLA	A	1217	9/20	0.70	0.16	67,70,92,93	0
6	OLA	A	1222	11/20	0.70	0.22	85,88,95,99	0
6	OLA	A	1215	16/20	0.73	0.21	57,75,108,111	0
3	OLC	A	1202	17/25	0.73	0.26	58,75,88,92	0
6	OLA	A	1216	9/20	0.74	0.22	56,64,71,76	0
6	OLA	A	1219	11/20	0.76	0.20	46,62,92,94	0
3	OLC	A	1208	11/25	0.77	0.41	78,80,85,85	0
6	OLA	A	1218	12/20	0.78	0.20	70,77,84,84	0
3	OLC	A	1203	16/25	0.78	0.21	58,70,85,88	0
6	OLA	A	1224	8/20	0.79	0.20	72,74,77,81	0

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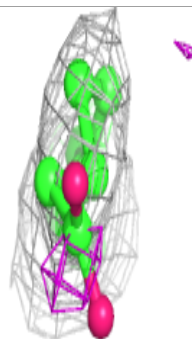
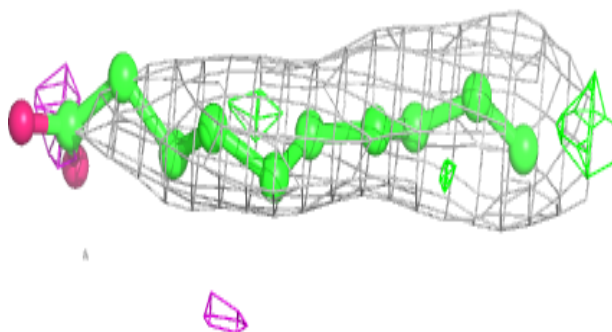
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	OLA	A	1226	12/20	0.80	0.20	56,63,74,78	0
3	OLC	A	1206	17/25	0.82	0.18	50,60,82,86	0
3	OLC	A	1205	17/25	0.83	0.16	61,71,78,84	0
3	OLC	A	1204	18/25	0.84	0.19	64,75,88,93	0
6	OLA	A	1227	17/20	0.85	0.27	55,63,151,152	0
4	CLR	A	1213	28/28	0.86	0.14	38,47,78,82	0
4	CLR	A	1212	28/28	0.87	0.13	41,46,64,69	0
4	CLR	A	1211	28/28	0.90	0.11	37,40,74,77	0
2	ZMA	A	1201	25/25	0.94	0.21	22,25,44,54	0
7	NA	A	1228	1/1	0.98	0.21	33,33,33,33	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.

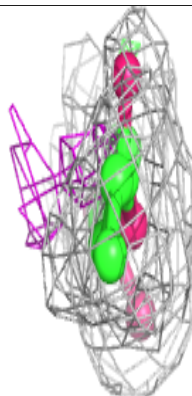
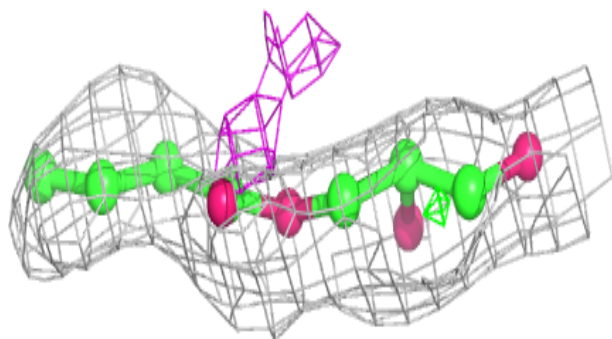
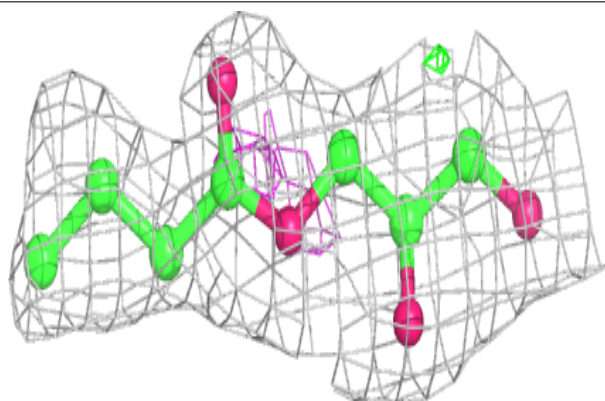


**Electron density around OLA A 1221:**

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

**Electron density around OLC A 1207:**

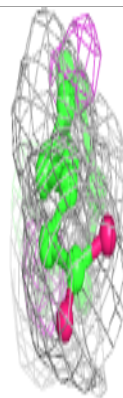
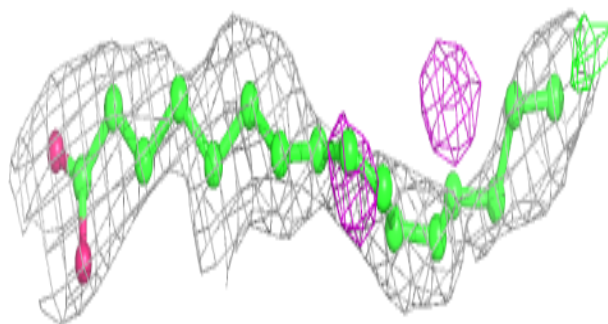
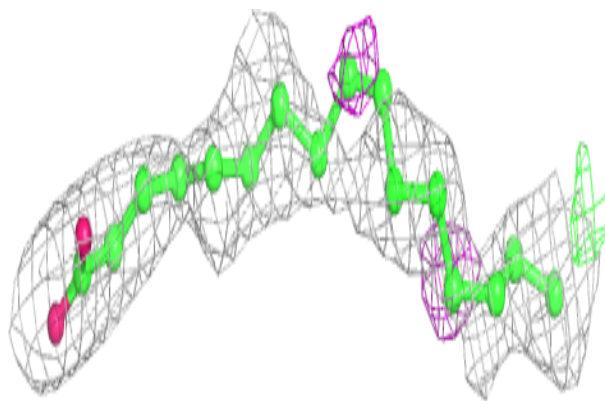
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



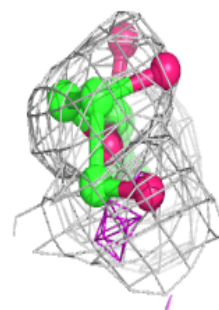
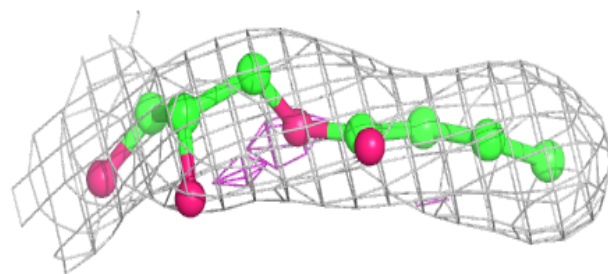
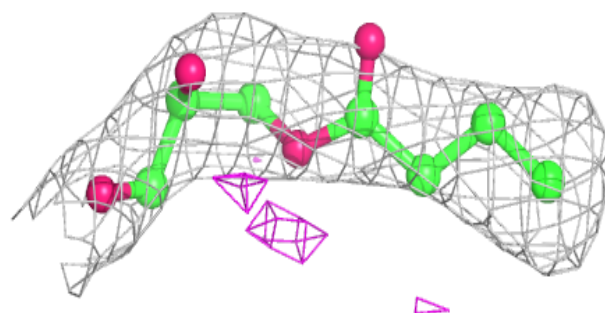


**Electron density around OLA A 1225:**

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

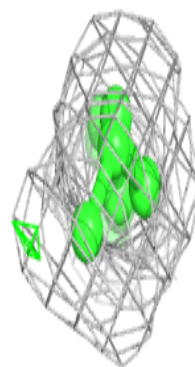
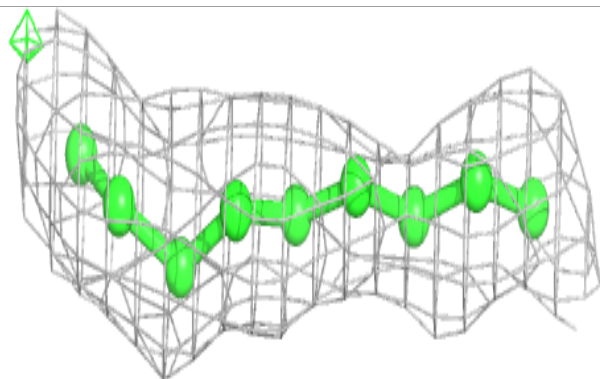
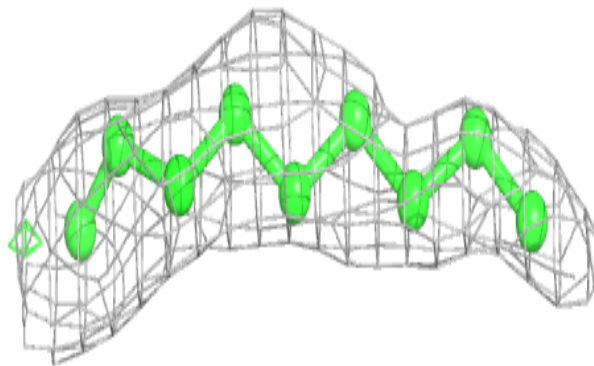
**Electron density around OLC A 1209:**

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

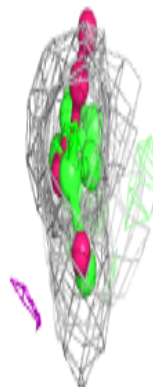
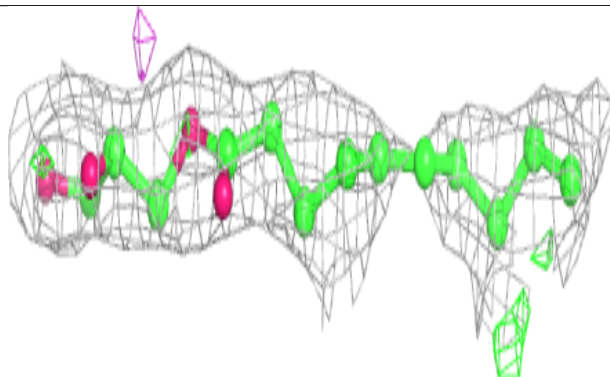
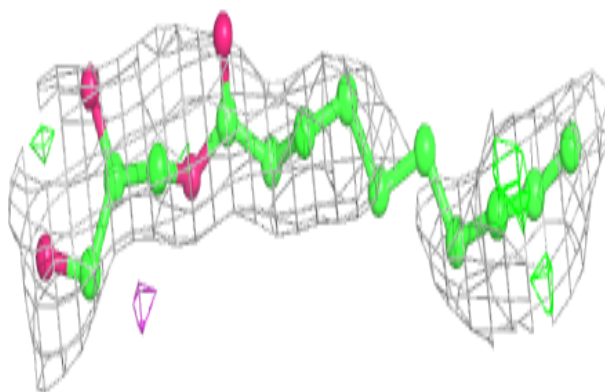


**Electron density around OLA A 1223:**

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

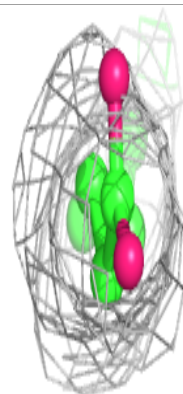
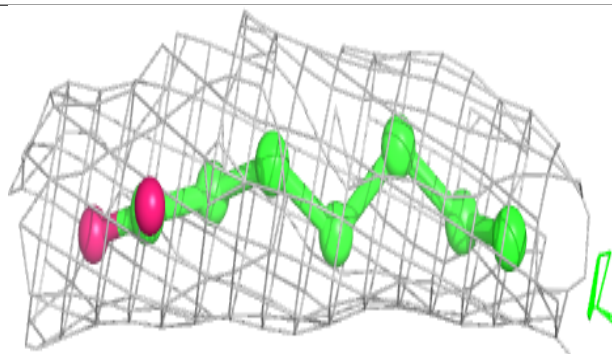
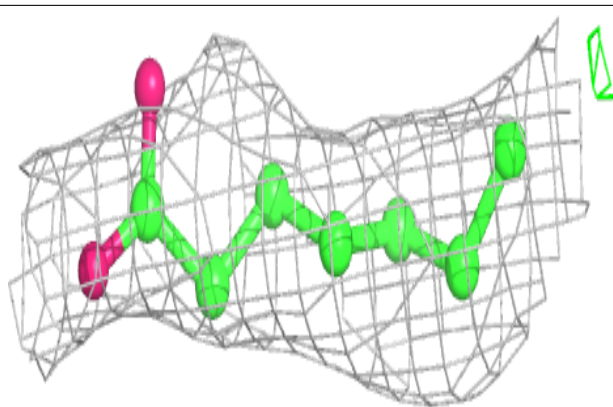
**Electron density around OLC A 1210:**

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

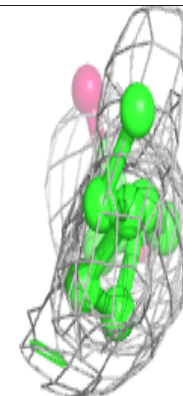
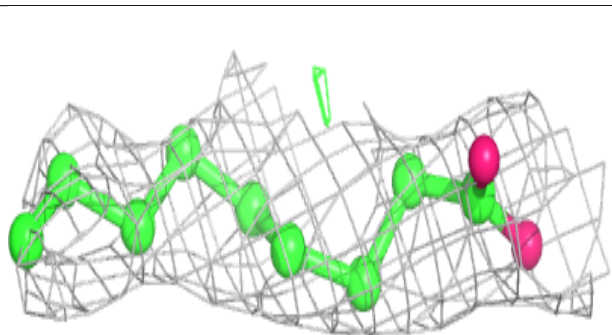
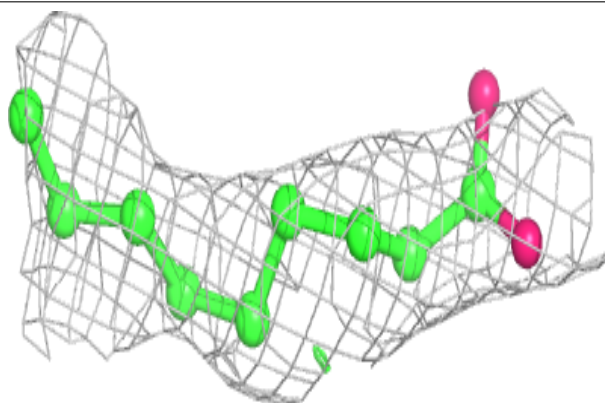


**Electron density around OLA A 1217:**

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

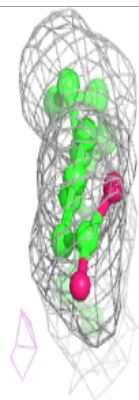
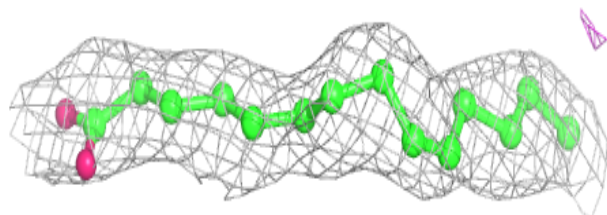
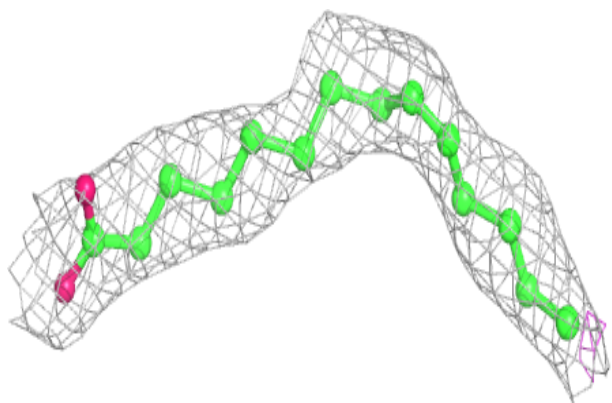
**Electron density around OLA A 1222:**

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

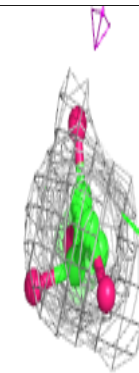
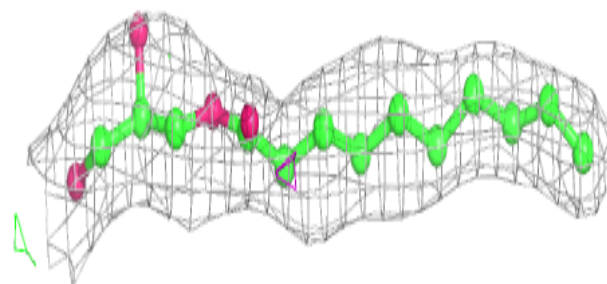
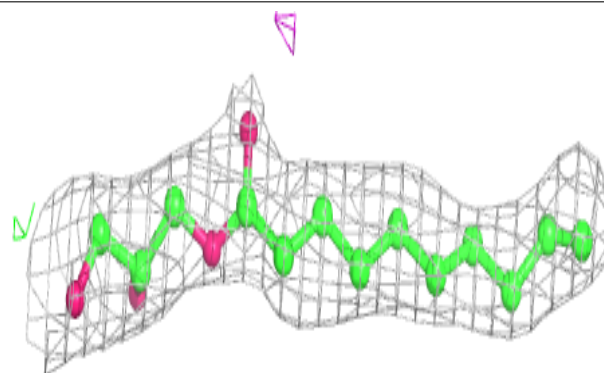


**Electron density around OLA A 1215:**

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

**Electron density around OLC A 1202:**

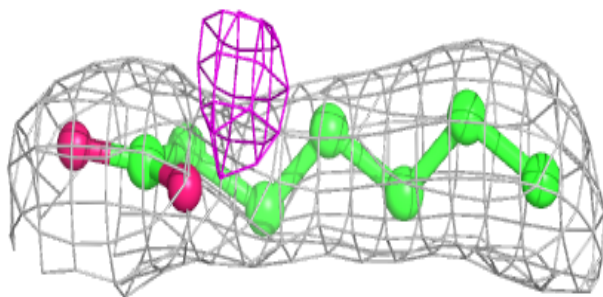
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



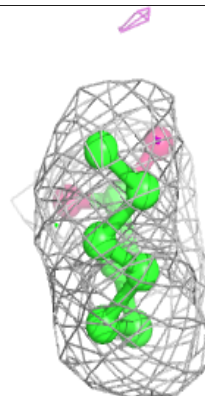
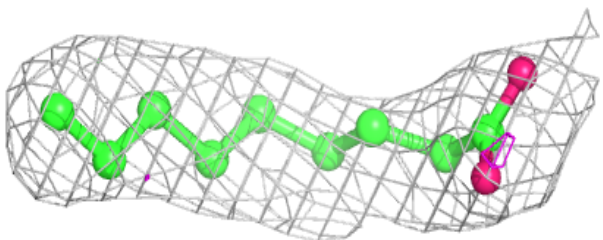
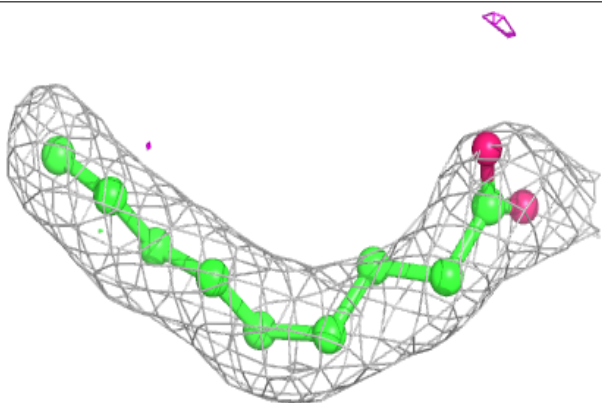


**Electron density around OLA A 1216:**

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

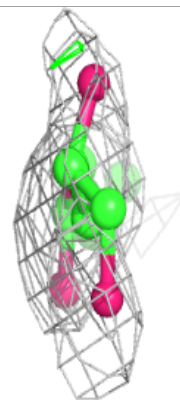
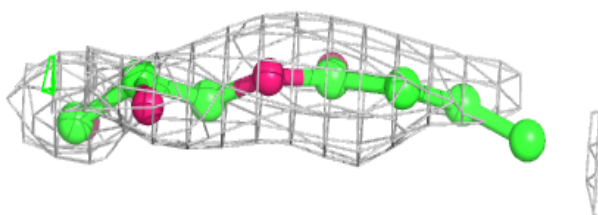
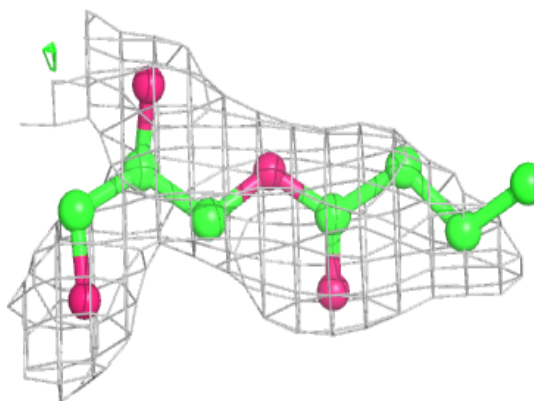
**Electron density around OLA A 1219:**

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

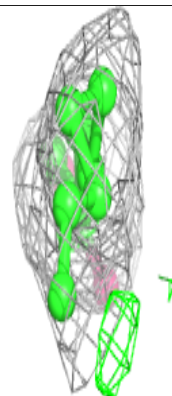
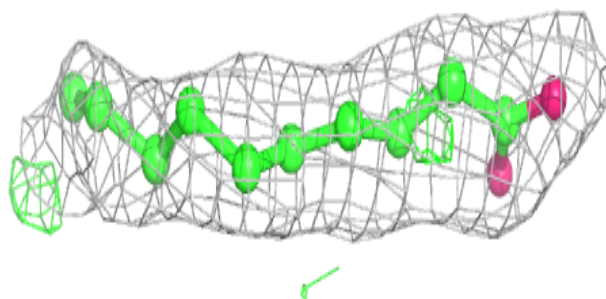
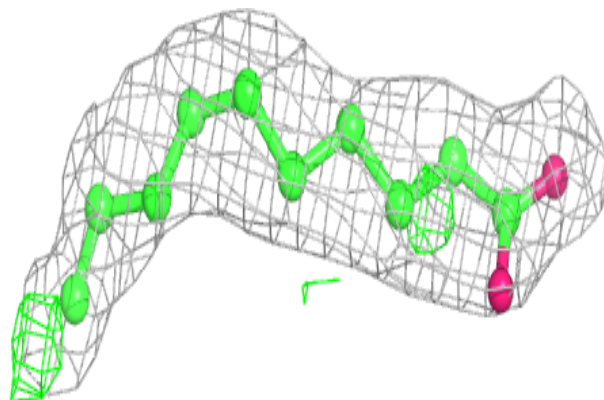


**Electron density around OLC A 1208:**

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

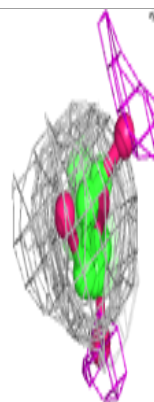
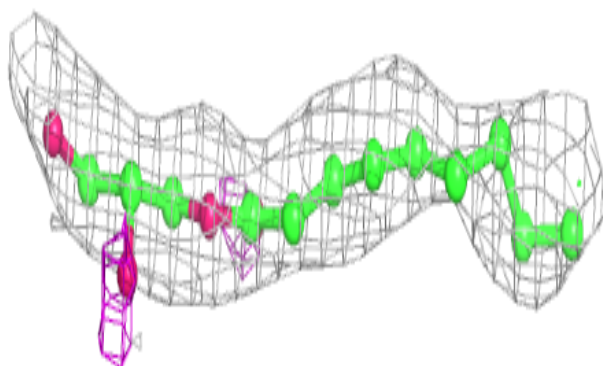
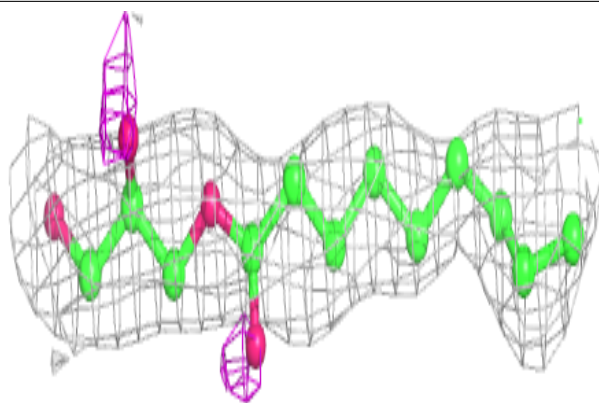
**Electron density around OLA A 1218:**

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

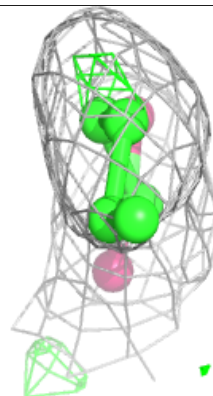
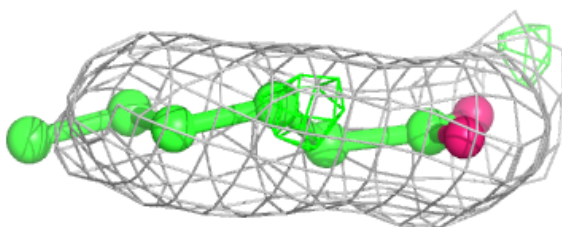
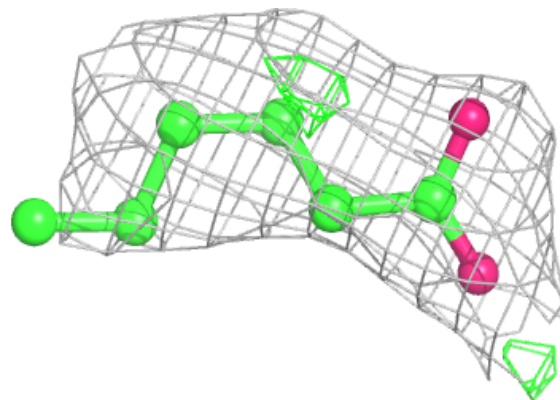


**Electron density around OLC A 1203:**

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

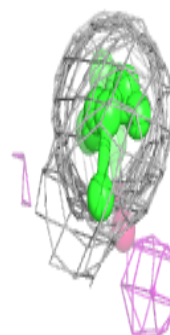
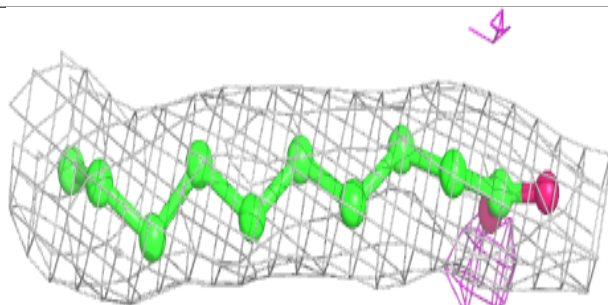
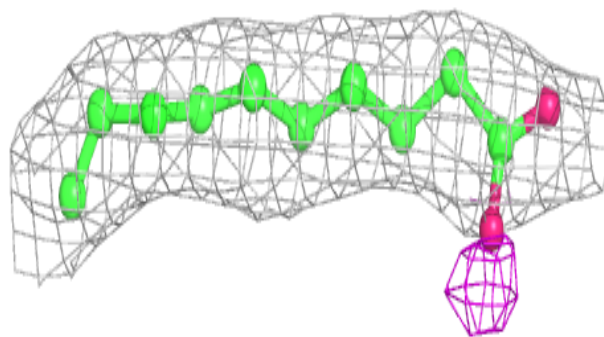
**Electron density around OLA A 1224:**

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

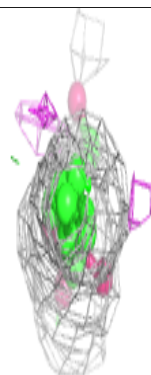
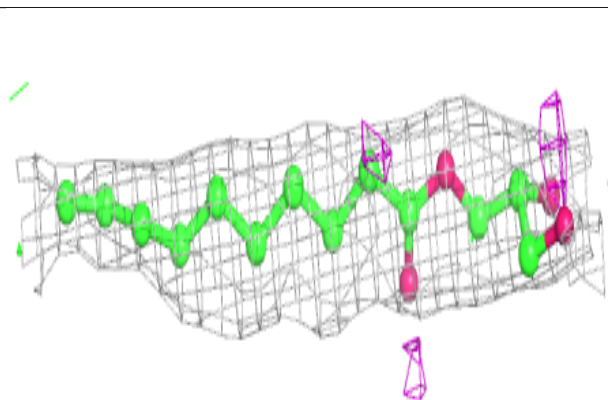
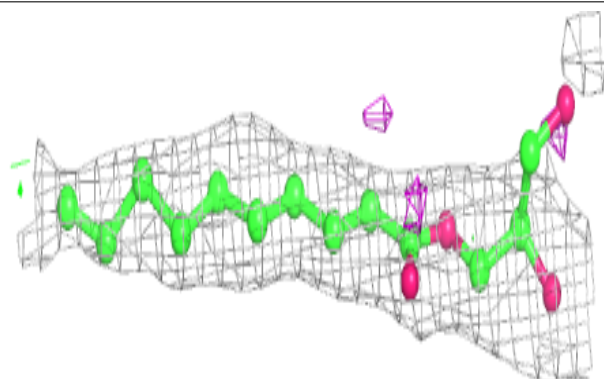


**Electron density around OLA A 1226:**

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

**Electron density around OLC A 1206:**

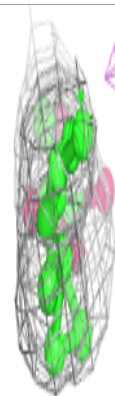
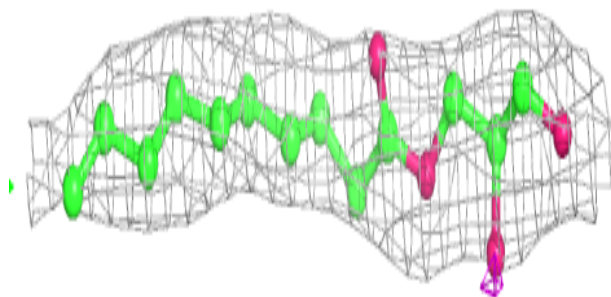
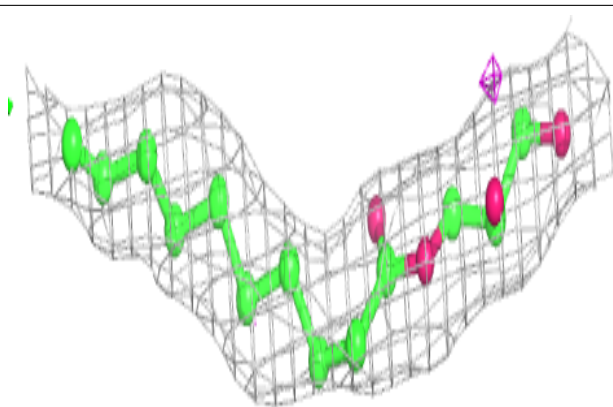
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



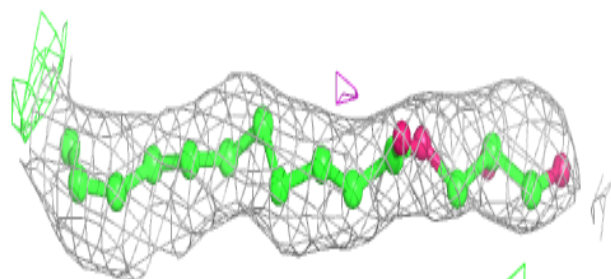
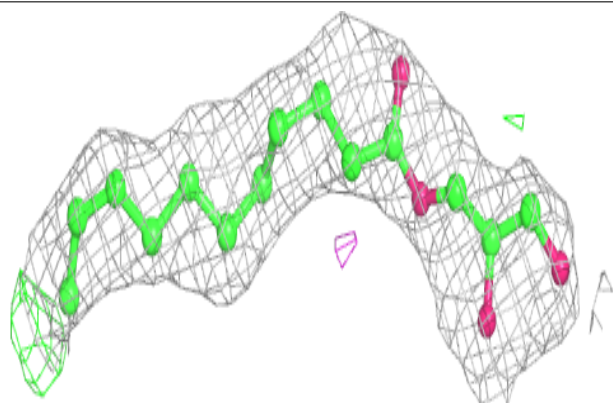


**Electron density around OLC A 1205:**

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

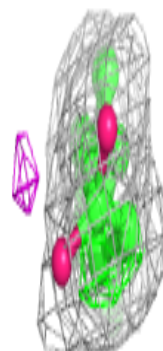
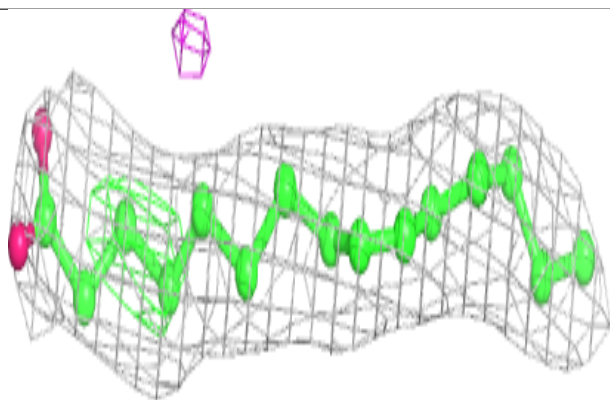
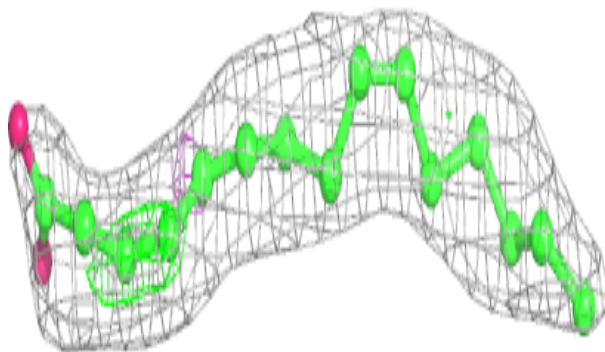
**Electron density around OLC A 1204:**

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

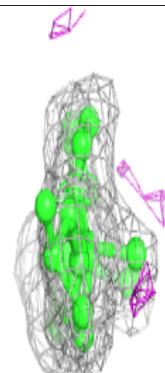
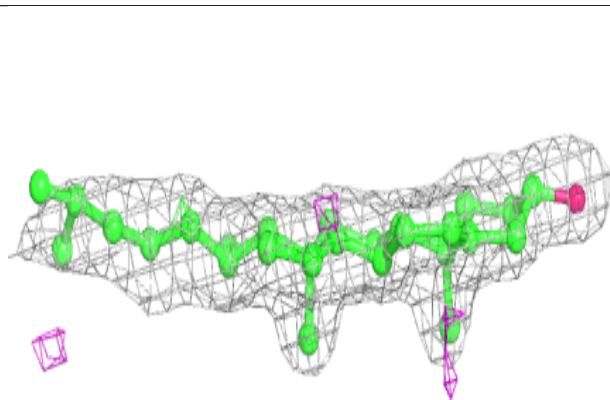
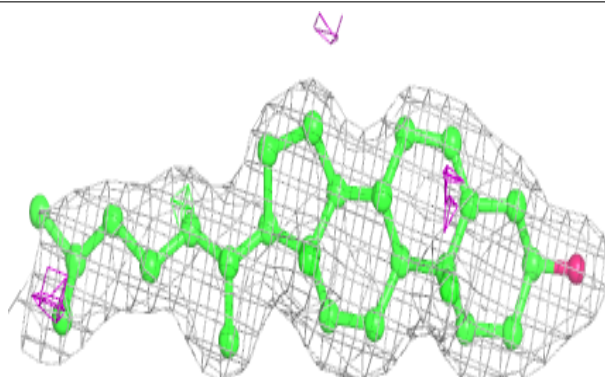


**Electron density around OLA A 1227:**

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

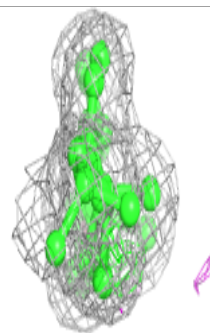
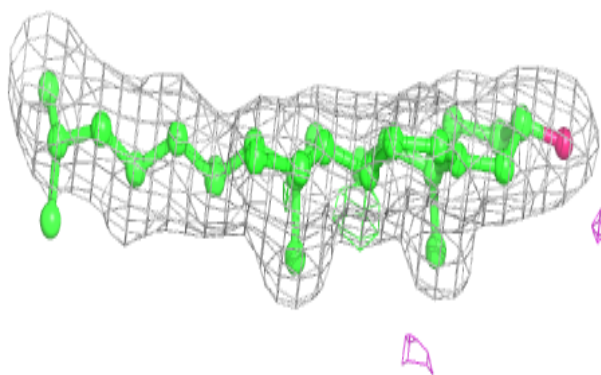
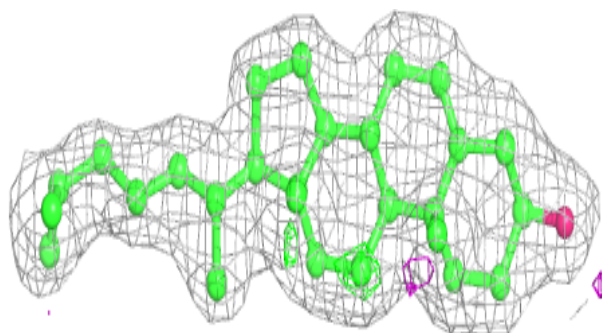
**Electron density around CLR A 1213:**

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

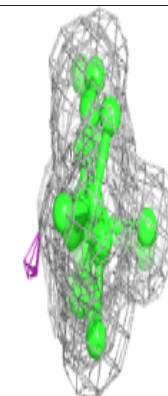
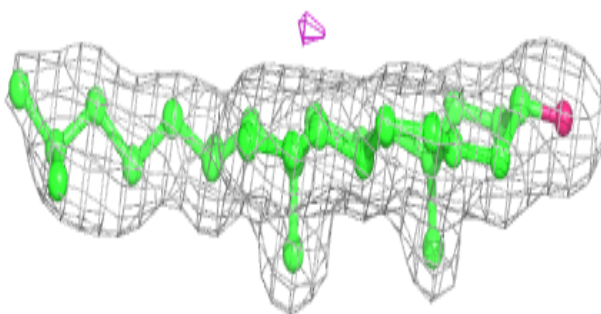
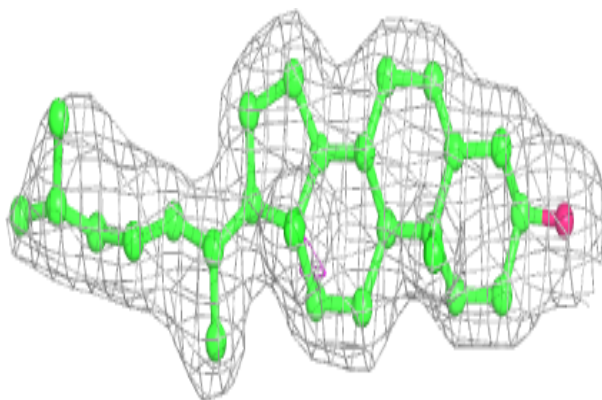


**Electron density around CLR A 1212:**

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

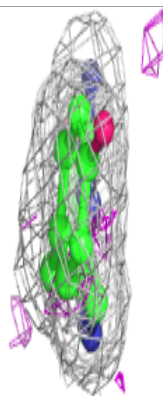
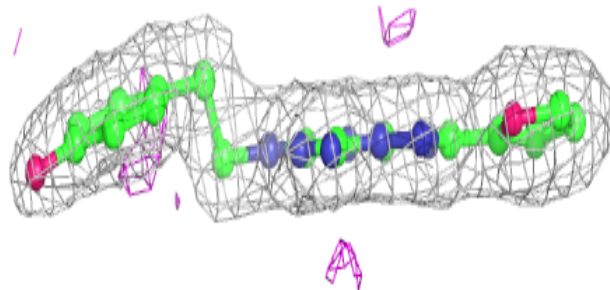
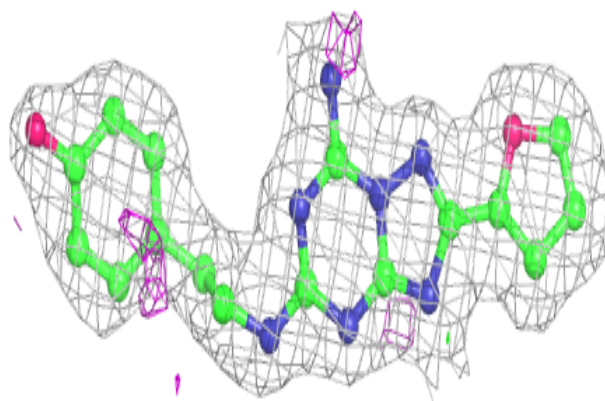
**Electron density around CLR A 1211:**

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



**Electron density around ZMA 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.