



## Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 02:48 AM EDT

PDB ID : 6ZDV  
Title : Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with Chromone 5d  
Authors : Verdon, G.; Jespers, W.; Azuaje, J.; Majellaro, M.; Keranen, H.; Garcia-mera, X.; Congreve, M.; Deflorian, F.; de Graaf, C.; Zhukov, A.; Dore, A.; Mason, J.; Aqvist, J.; Cooke, R.; Sotelo, E.; Gutierrez-de-Teran, H.  
Deposited on : 2020-06-15  
Resolution : 2.13 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

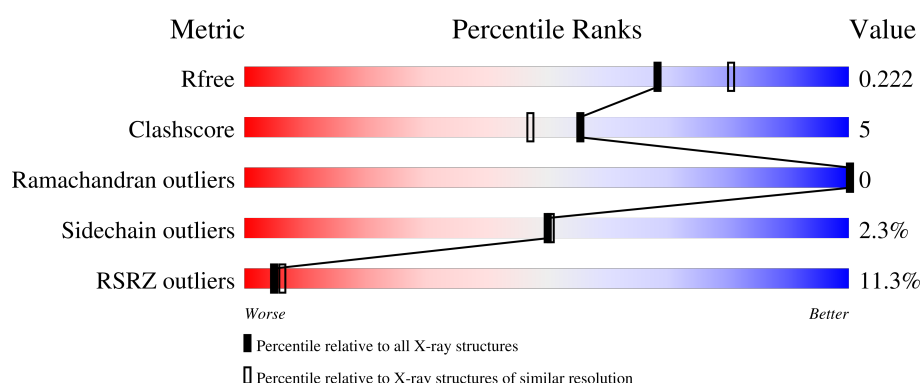
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	433	<div> <div>10%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>12%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3331 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	382	Total	C	N	O	S	0	5	0
			2965	1939	494	511	21			

There are 33 discrepancies between the modelled and reference sequences:

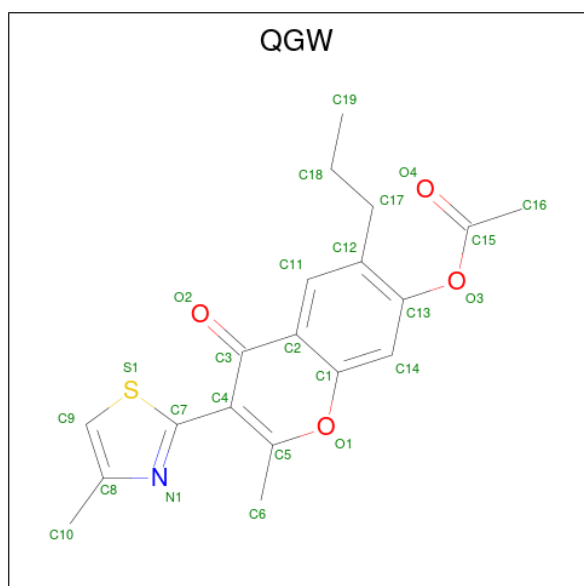
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
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	conflict	UNP P29274
A	88	ALA	THR	conflict	UNP P29274
A	107	ALA	ARG	conflict	UNP P29274
A	122	ALA	LYS	conflict	UNP P29274
A	154	ALA	ASN	conflict	UNP P29274
A	202	ALA	LEU	conflict	UNP P29274
A	1007	TRP	MET	conflict	UNP P0ABE7
A	1102	ILE	HIS	conflict	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	235	ALA	LEU	conflict	UNP P29274
A	239	ALA	VAL	conflict	UNP P29274
A	277	ALA	SER	conflict	UNP P29274
A	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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 [2-methyl-3-(4-methyl-1,3-thiazol-2-yl)-4-oxidanylidene-6-propyl-chromen-7-yl] ethanoate (three-letter code: QGW) (formula: C<sub>19</sub>H<sub>19</sub>NO<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).

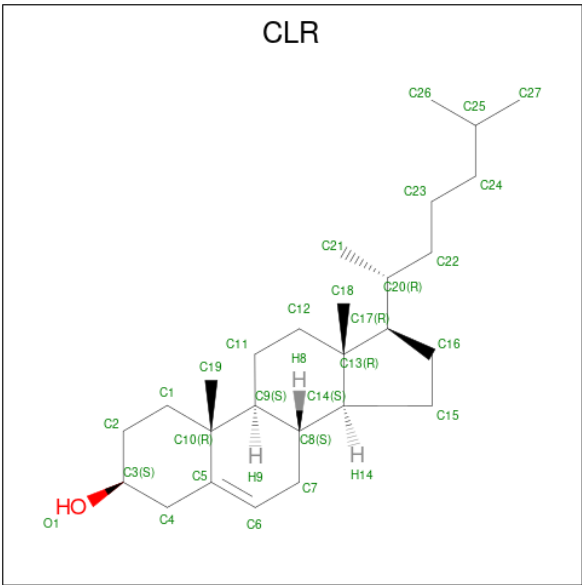


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	19	1	4	1		

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

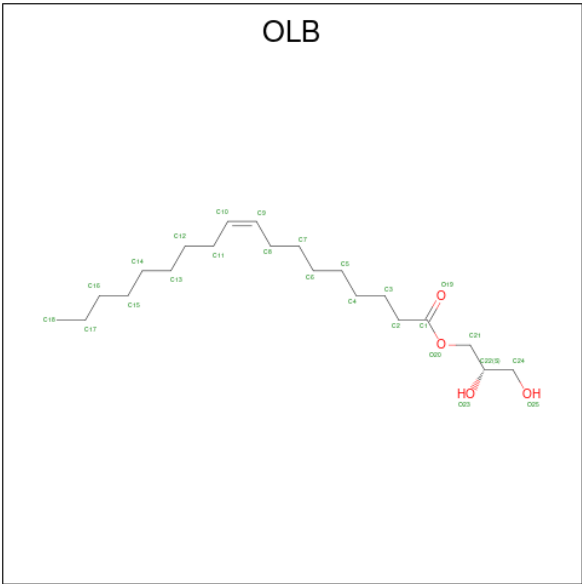
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

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



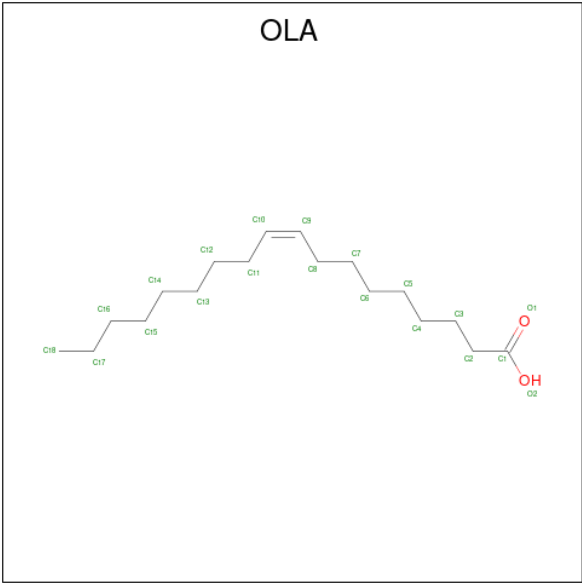
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		
4	A	1	Total	C	O	0	0
			28	27	1		

- 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
			15	11	4		

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



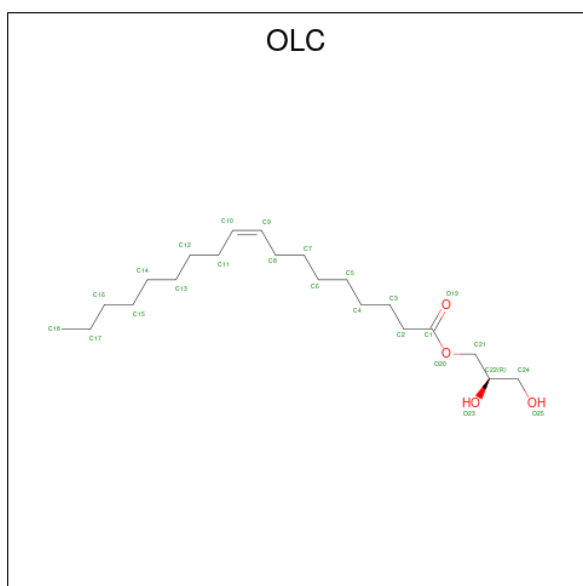
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	9	2		
6	A	1	Total	C	O	0	0
			12	10	2		
6	A	1	Total	C		0	0
			7	7			
6	A	1	Total	C	O	0	0
			15	13	2		
6	A	1	Total	C		0	0
			6	6			
6	A	1	Total	C	O	0	0
			7	5	2		
6	A	1	Total	C		0	0
			5	5			
6	A	1	Total	C		0	0
			7	7			
6	A	1	Total	C	O	0	0
			15	13	2		
6	A	1	Total	C	O	0	0
			11	9	2		
6	A	1	Total	C	O	0	0
			17	15	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 8 2	0	0
6	A	1	Total C 7 7	0	0
6	A	1	Total C 5 5	0	0

- Molecule 7 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
7	A	1	Total C O 17 13 4	0	0

- Molecule 8 is water.

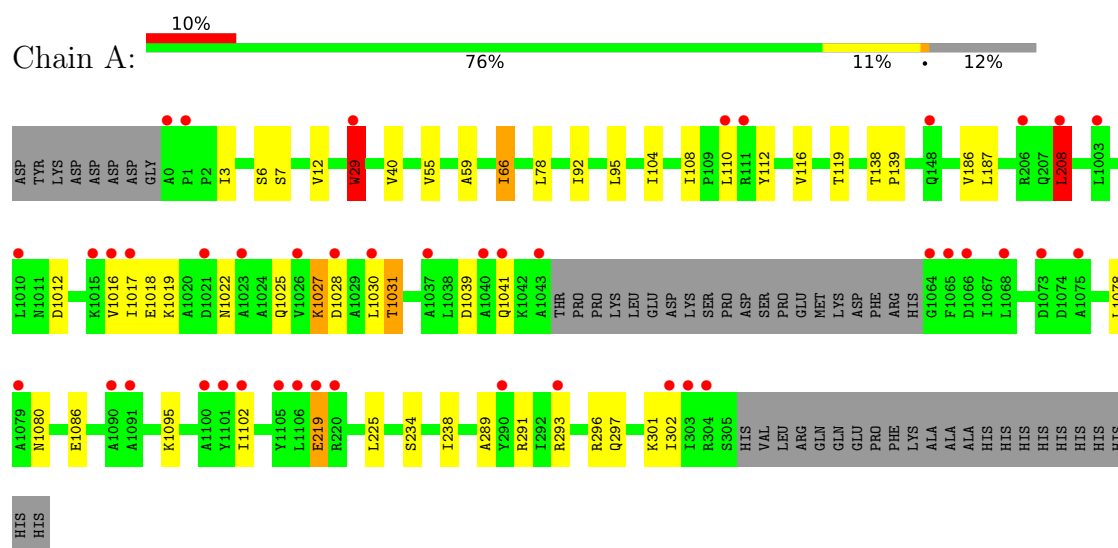
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	89	Total O 89 89	0	0



### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	39.41Å 179.83Å 140.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.80 – 2.13 42.81 – 2.09	Depositor EDS
% Data completeness (in resolution range)	84.0 (42.80-2.13) 84.0 (42.81-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.08Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.215 , 0.224 0.220 , 0.222	Depositor DCC
$R_{free}$ test set	1288 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 69.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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: OLC, CLR, OLA, QGW, OLB, 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	1.18	2/3044 (0.1%)	0.92	13/4146 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLU	C-N	10.34	1.57	1.34
1	A	208	LEU	C-N	8.43	1.53	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	LEU	O-C-N	-21.15	88.86	122.70
1	A	208	LEU	C-N-CA	11.93	151.54	121.70
1	A	6[A]	SER	CA-C-O	6.04	132.79	120.10
1	A	6[B]	SER	CA-C-O	6.04	132.79	120.10
1	A	78[A]	LEU	CA-C-O	5.98	132.66	120.10
1	A	78[B]	LEU	CA-C-O	5.98	132.66	120.10
1	A	7[A]	SER	CA-C-O	5.82	132.31	120.10
1	A	7[B]	SER	CA-C-O	5.82	132.31	120.10
1	A	66[A]	ILE	CA-C-O	5.28	131.18	120.10
1	A	66[B]	ILE	CA-C-O	5.28	131.18	120.10
1	A	208	LEU	CA-C-N	5.17	128.57	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29[A]	TRP	CA-C-O	5.10	130.82	120.10
1	A	29[B]	TRP	CA-C-O	5.10	130.82	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	LEU	Mainchain
1	A	219	GLU	Mainchain
1	A	29[A]	TRP	Mainchain
1	A	29[B]	TRP	Mainchain

## 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	2965	0	3046	31	0
2	A	25	0	0	1	0
3	A	1	0	0	0	0
4	A	84	0	138	2	0
5	A	15	0	19	0	0
6	A	135	0	187	3	0
7	A	17	0	22	0	0
8	A	89	0	0	0	0
All	All	3331	0	3412	34	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 5.

All (34) 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:1018:GLU:OE2	1:A:1095:LYS:NZ	1.90	1.04
1:A:1027:LYS:HE3	1:A:1080:ASN:OD1	1.68	0.93
1:A:1019:LYS:O	1:A:1019:LYS:HG3	1.81	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:LEU:HD13	1:A:1086:GLU:HB3	1.71	0.72
1:A:1017:ILE:HD11	1:A:1030:LEU:HG	1.77	0.66
1:A:289:ALA:O	1:A:296:ARG:HD3	1.97	0.64
1:A:1022:ASN:N	1:A:1022:ASN:OD1	2.30	0.62
2:A:1201:QGW:S1	2:A:1201:QGW:O2	2.57	0.61
1:A:1019:LYS:O	1:A:1019:LYS:CG	2.48	0.59
1:A:234:SER:OG	1:A:291:ARG:HD3	2.06	0.55
1:A:12:VAL:HG21	6:A:1216:OLA:H62	1.87	0.55
1:A:1027:LYS:O	1:A:1031:THR:OG1	2.23	0.52
1:A:1012:ASP:O	1:A:1016:VAL:HG23	2.11	0.51
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.93	0.50
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.43	0.49
1:A:92:ILE:CD1	1:A:186:VAL:HG22	2.43	0.48
1:A:1017:ILE:CD1	1:A:1030:LEU:HG	2.44	0.48
1:A:92:ILE:HD11	1:A:186:VAL:HG22	1.94	0.48
1:A:104:ILE:HG22	1:A:112:TYR:HD2	1.81	0.46
1:A:40:VAL:HG11	1:A:116:VAL:HG12	2.00	0.43
4:A:1205:CLR:H6	6:A:1215:OLA:H62	2.00	0.43
4:A:1205:CLR:H41	6:A:1215:OLA:H41	2.01	0.42
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.88	0.42
1:A:3:ILE:O	1:A:3:ILE:HG12	2.19	0.42
1:A:138:THR:N	1:A:139:PRO:CD	2.83	0.42
1:A:208:LEU:HG	1:A:225:LEU:HD13	2.02	0.42
1:A:293:ARG:HG2	1:A:296:ARG:NH1	2.33	0.41
1:A:297:GLN:O	1:A:301:LYS:HG3	2.20	0.41
1:A:1041:GLN:HE21	1:A:1041:GLN:HB3	1.73	0.41
1:A:108:ILE:HG13	1:A:108:ILE:O	2.21	0.41
1:A:29[B]:TRP:HD1	1:A:302:ILE:HD13	1.86	0.41
1:A:95:LEU:HD21	1:A:238:ILE:HG22	2.03	0.41
1:A:1102:ILE:H	1:A:1102:ILE:HG12	1.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	383/433 (88%)	378 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	310/353 (88%)	303 (98%)	7 (2%)	50	51

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	119	THR
1	A	1025	GLN
1	A	1027	LYS
1	A	1028	ASP
1	A	1031	THR
1	A	1039	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	1041	GLN

### 5.3.3 RNA ⓘ

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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	1216	-	10,10,19	0.61	0	10,10,19	0.75	0
2	QGW	A	1201	-	24,27,27	2.09	6 (25%)	31,39,39	2.46	11 (35%)
6	OLA	A	1211	-	5,5,19	0.28	0	4,4,19	0.43	0
6	OLA	A	1214	-	6,6,19	0.26	0	5,5,19	0.36	0
6	OLA	A	1215	-	14,14,19	0.54	0	14,14,19	0.90	0
4	CLR	A	1203	-	31,31,31	0.60	0	48,48,48	1.07	5 (10%)
6	OLA	A	1212	-	6,6,19	0.80	0	6,6,19	1.18	0
6	OLA	A	1219	-	6,6,19	0.30	0	5,5,19	0.40	0
6	OLA	A	1208	-	11,11,19	0.68	0	11,11,19	0.93	0
7	OLC	A	1221	-	16,16,24	1.19	1 (6%)	17,17,25	0.89	1 (5%)
6	OLA	A	1220	-	4,4,19	0.34	0	3,3,19	0.33	0
6	OLA	A	1218	-	9,9,19	0.73	0	9,9,19	0.91	0
6	OLA	A	1210	-	14,14,19	0.56	0	14,14,19	0.74	0
4	CLR	A	1204	-	31,31,31	0.56	0	48,48,48	1.08	4 (8%)
6	OLA	A	1207	-	10,10,19	0.60	0	10,10,19	1.00	0
5	OLB	A	1206	-	14,14,24	0.28	0	15,15,25	0.31	0
6	OLA	A	1213	-	4,4,19	0.30	0	3,3,19	0.40	0
6	OLA	A	1217	-	16,16,19	0.58	0	16,16,19	0.75	0
4	CLR	A	1205	-	31,31,31	0.68	0	48,48,48	1.08	2 (4%)
6	OLA	A	1209	-	6,6,19	0.26	0	5,5,19	0.43	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
6	OLA	A	1216	-	-	2/8/8/17	-
2	QGW	A	1201	-	-	3/7/11/11	0/3/3/3
6	OLA	A	1211	-	-	0/3/3/17	-
6	OLA	A	1214	-	-	4/4/4/17	-
6	OLA	A	1215	-	-	4/12/12/17	-
4	CLR	A	1203	-	-	2/10/68/68	0/4/4/4
6	OLA	A	1212	-	-	2/4/4/17	-
6	OLA	A	1219	-	-	1/4/4/17	-
6	OLA	A	1208	-	-	5/9/9/17	-
7	OLC	A	1221	-	-	5/16/16/24	-
6	OLA	A	1220	-	-	0/2/2/17	-
6	OLA	A	1218	-	-	3/7/7/17	-
6	OLA	A	1210	-	-	3/12/12/17	-
4	CLR	A	1204	-	-	0/10/68/68	0/4/4/4
6	OLA	A	1207	-	-	7/8/8/17	-
5	OLB	A	1206	-	-	2/14/14/24	-
6	OLA	A	1213	-	-	0/2/2/17	-
6	OLA	A	1217	-	-	6/14/14/17	-
4	CLR	A	1205	-	-	4/10/68/68	0/4/4/4
6	OLA	A	1209	-	-	0/4/4/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	QGW	O1-C5	-7.00	1.30	1.37
7	A	1221	OLC	O20-C1	4.50	1.46	1.33
2	A	1201	QGW	C9-S1	-3.27	1.65	1.70
2	A	1201	QGW	O1-C1	-3.09	1.33	1.38
2	A	1201	QGW	O3-C13	-2.89	1.35	1.41
2	A	1201	QGW	C2-C3	-2.02	1.44	1.48
2	A	1201	QGW	C4-C5	-2.01	1.34	1.39

All (23) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	QGW	O1-C5-C6	-7.52	103.16	109.06
2	A	1201	QGW	C1-O1-C5	-4.62	116.18	119.55
2	A	1201	QGW	C11-C12-C13	4.49	122.98	118.26
2	A	1201	QGW	O1-C5-C4	3.58	128.47	121.26
2	A	1201	QGW	O2-C3-C4	3.56	126.72	121.72
2	A	1201	QGW	O3-C13-C14	3.05	125.78	119.00
2	A	1201	QGW	C10-C8-C9	-2.99	121.14	129.06
2	A	1201	QGW	C13-O3-C15	2.64	123.28	117.65
4	A	1204	CLR	C4-C5-C10	2.58	119.85	116.42
4	A	1203	CLR	C19-C10-C5	-2.51	104.28	108.34
2	A	1201	QGW	C17-C12-C13	-2.47	117.32	121.14
4	A	1204	CLR	C4-C5-C6	-2.41	117.13	120.61
4	A	1204	CLR	C12-C11-C9	-2.38	108.99	113.11
4	A	1203	CLR	C21-C20-C22	-2.28	106.79	110.36
2	A	1201	QGW	C2-C3-C4	-2.24	112.28	116.97
4	A	1205	CLR	C13-C14-C8	-2.23	111.08	114.38
4	A	1205	CLR	C11-C9-C8	2.12	114.81	111.75
7	A	1221	OLC	O20-C1-C2	2.12	118.55	111.91
4	A	1203	CLR	C13-C14-C8	-2.10	111.27	114.38
2	A	1201	QGW	C11-C2-C1	2.09	121.22	118.29
4	A	1203	CLR	C11-C9-C8	2.07	114.73	111.75
4	A	1203	CLR	C4-C5-C10	2.01	119.09	116.42
4	A	1204	CLR	C16-C15-C14	-2.01	101.15	105.13

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1221	OLC	O20-C21-C22-C24
7	A	1221	OLC	O20-C21-C22-O23
4	A	1203	CLR	C23-C24-C25-C26
6	A	1214	OLA	C14-C15-C16-C17
6	A	1210	OLA	C2-C3-C4-C5
7	A	1221	OLC	C2-C3-C4-C5
6	A	1207	OLA	C4-C5-C6-C7
4	A	1205	CLR	C22-C23-C24-C25
6	A	1207	OLA	C3-C4-C5-C6
6	A	1215	OLA	C4-C5-C6-C7
6	A	1207	OLA	C1-C2-C3-C4
6	A	1208	OLA	C5-C6-C7-C8
4	A	1205	CLR	C23-C24-C25-C26
6	A	1208	OLA	C4-C5-C6-C7
6	A	1207	OLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

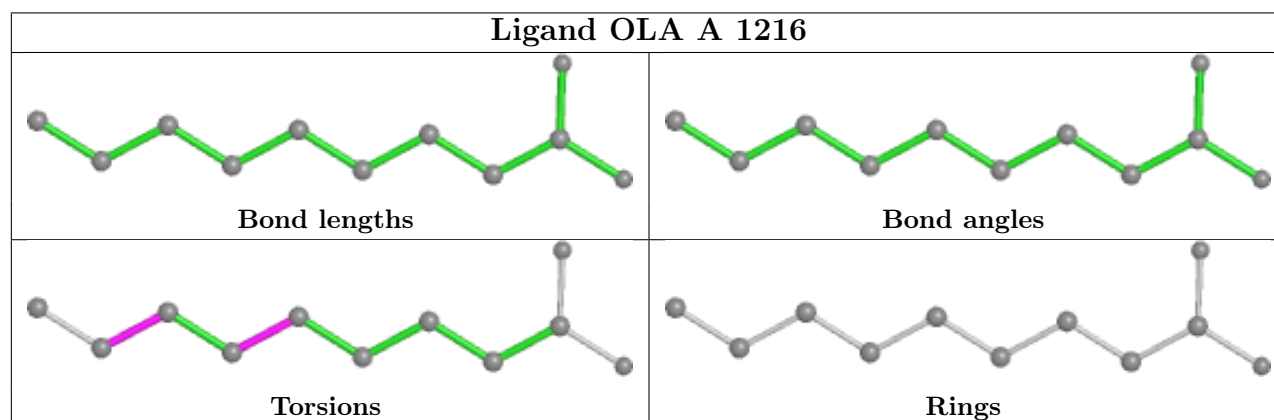
Mol	Chain	Res	Type	Atoms
4	A	1203	CLR	C23-C24-C25-C27
2	A	1201	QGW	C16-C15-O3-C13
6	A	1217	OLA	C2-C3-C4-C5
6	A	1214	OLA	C15-C16-C17-C18
6	A	1214	OLA	C12-C13-C14-C15
6	A	1217	OLA	C10-C11-C12-C13
6	A	1219	OLA	C12-C13-C14-C15
6	A	1218	OLA	C3-C4-C5-C6
6	A	1216	OLA	C4-C5-C6-C7
4	A	1205	CLR	C23-C24-C25-C27
6	A	1215	OLA	C3-C4-C5-C6
7	A	1221	OLC	C1-C2-C3-C4
2	A	1201	QGW	O4-C15-O3-C13
4	A	1205	CLR	C20-C22-C23-C24
6	A	1218	OLA	C4-C5-C6-C7
6	A	1214	OLA	C13-C14-C15-C16
5	A	1206	OLB	C2-C1-O20-C21
6	A	1215	OLA	C7-C8-C9-C10
6	A	1210	OLA	C10-C11-C12-C13
2	A	1201	QGW	C12-C17-C18-C19
6	A	1217	OLA	C6-C7-C8-C9
6	A	1210	OLA	C7-C8-C9-C10
6	A	1217	OLA	O2-C1-C2-C3
6	A	1217	OLA	O1-C1-C2-C3
6	A	1207	OLA	C6-C7-C8-C9
6	A	1215	OLA	C9-C10-C11-C12
6	A	1207	OLA	O2-C1-C2-C3
5	A	1206	OLB	O19-C1-O20-C21
6	A	1212	OLA	O2-C1-C2-C3
6	A	1207	OLA	O1-C1-C2-C3
6	A	1218	OLA	C5-C6-C7-C8
6	A	1217	OLA	C9-C10-C11-C12
7	A	1221	OLC	C7-C8-C9-C10
6	A	1212	OLA	O1-C1-C2-C3
6	A	1208	OLA	C7-C8-C9-C10
6	A	1216	OLA	C6-C7-C8-C9
6	A	1208	OLA	O2-C1-C2-C3
6	A	1208	OLA	O1-C1-C2-C3

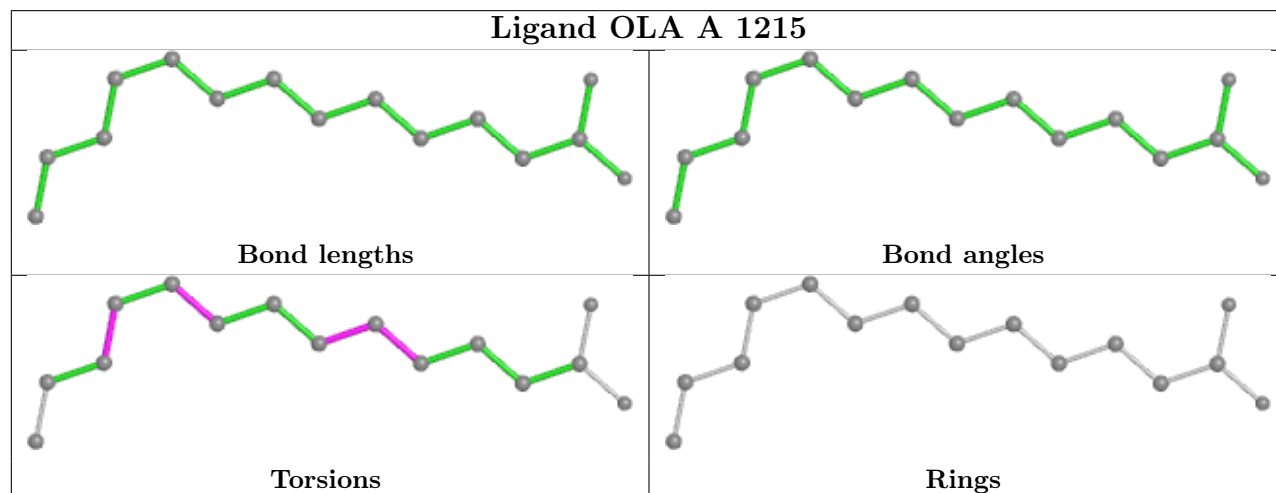
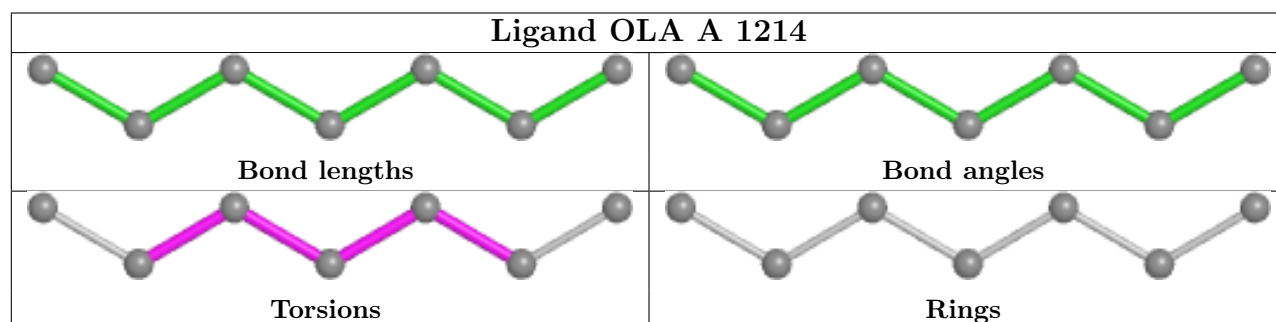
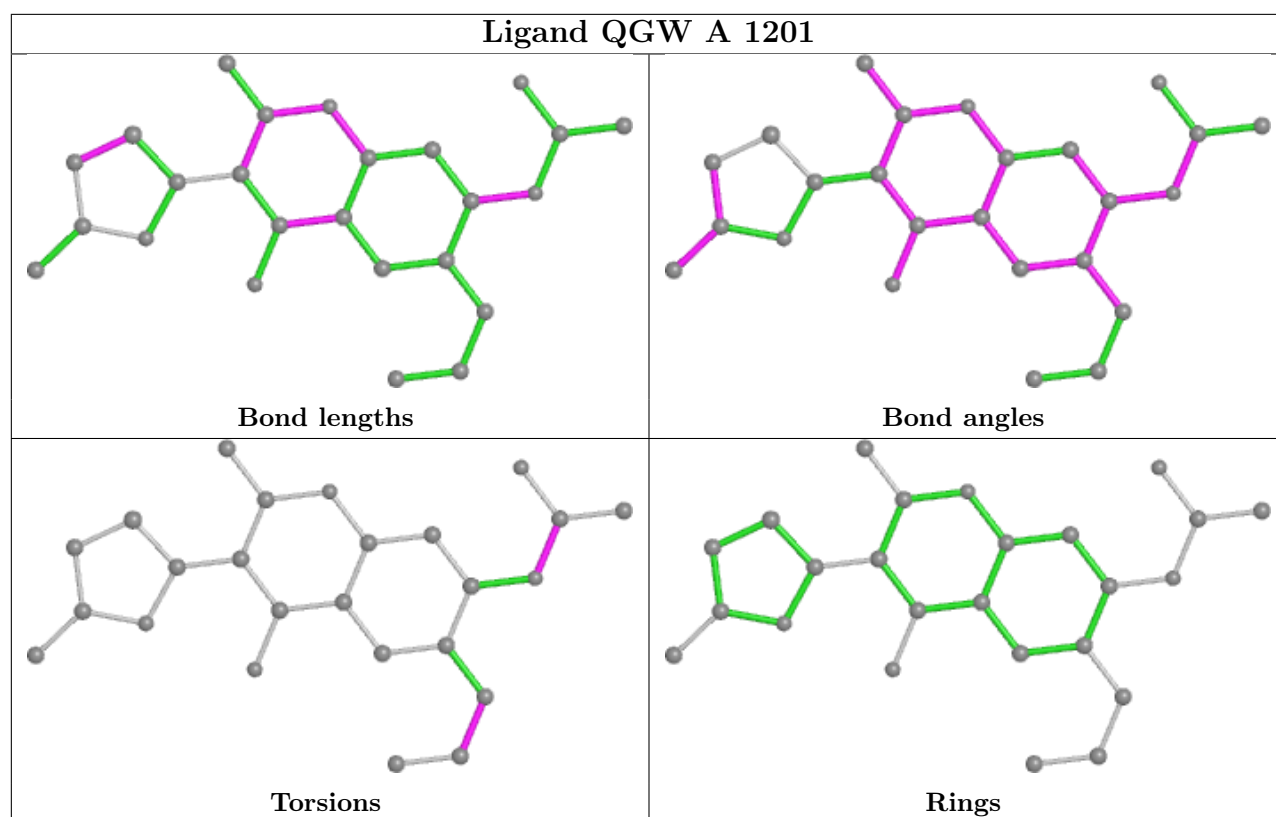
There are no ring outliers.

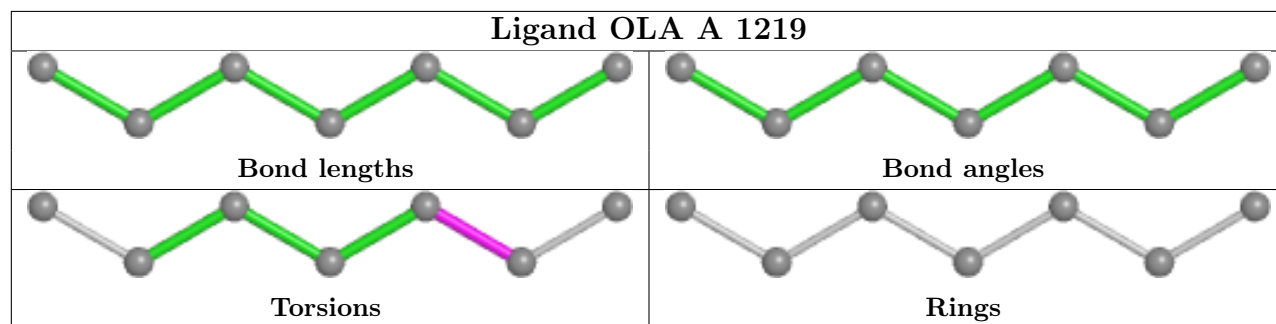
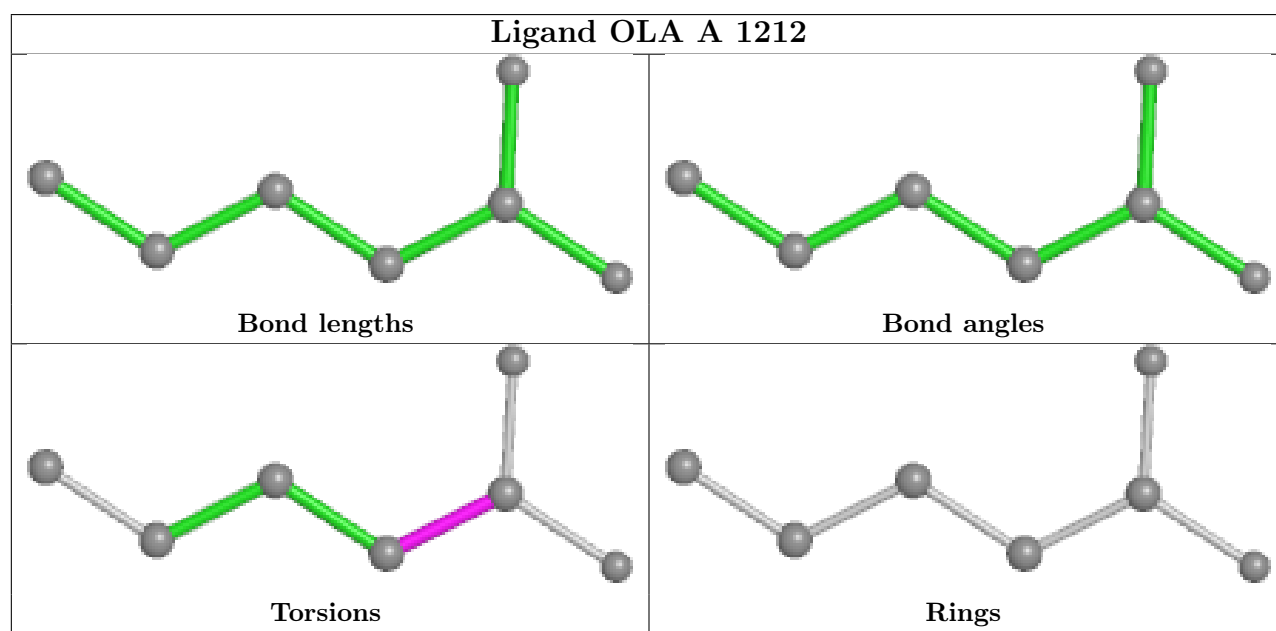
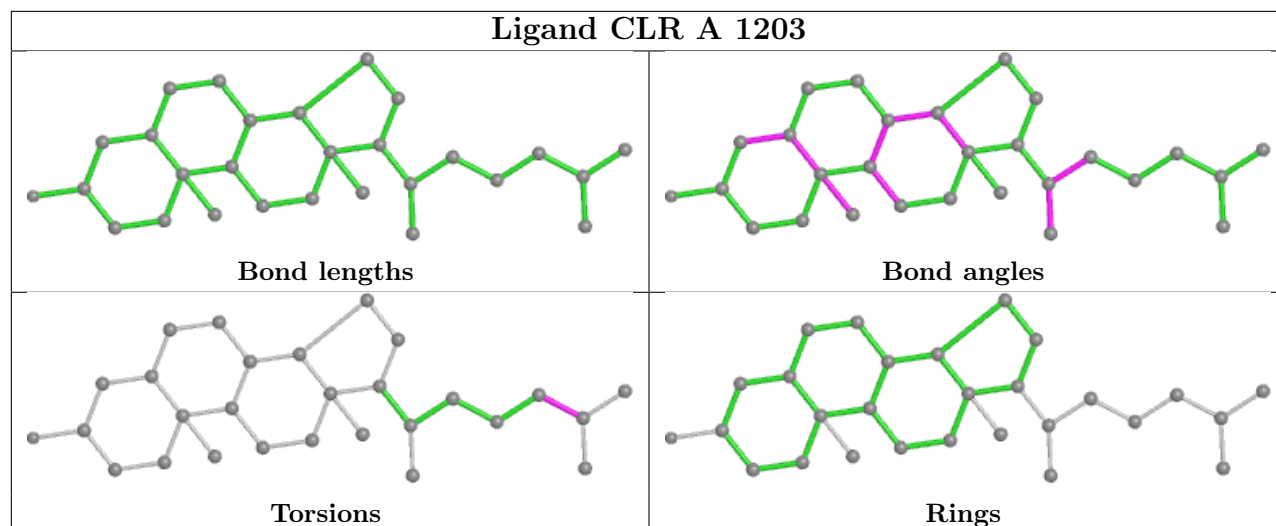
4 monomers are involved in 4 short contacts:

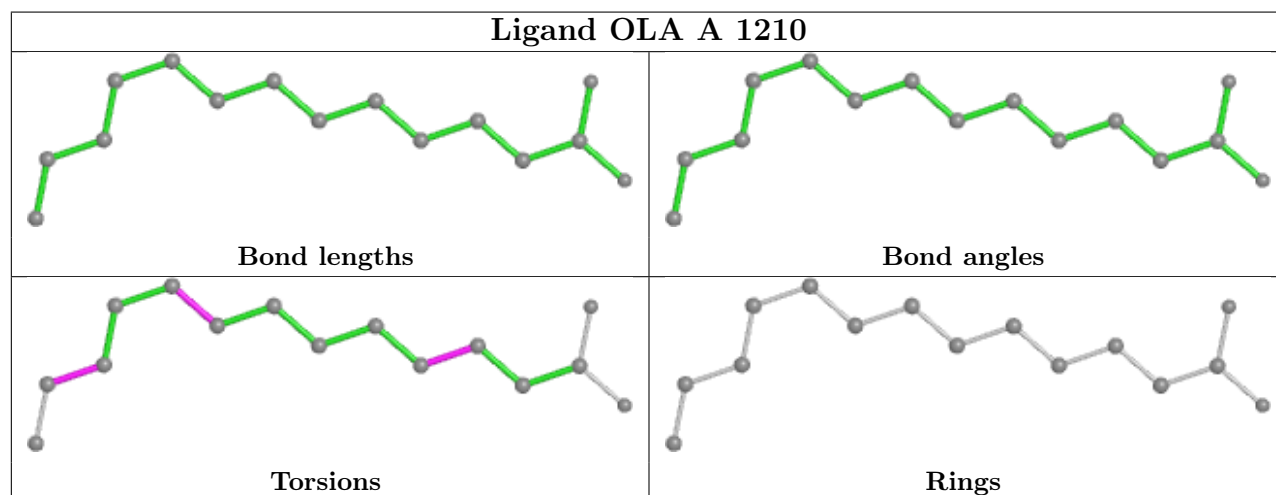
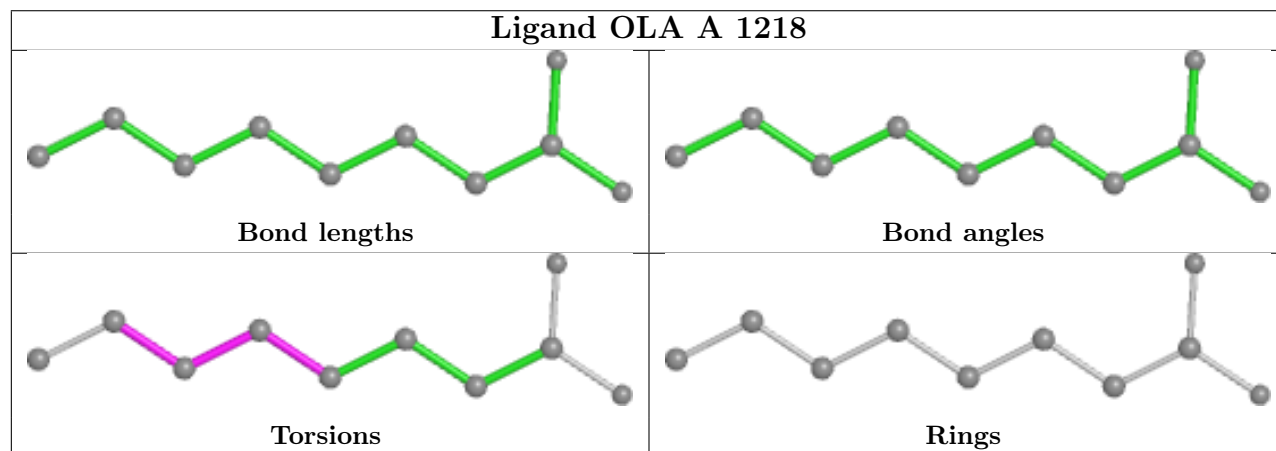
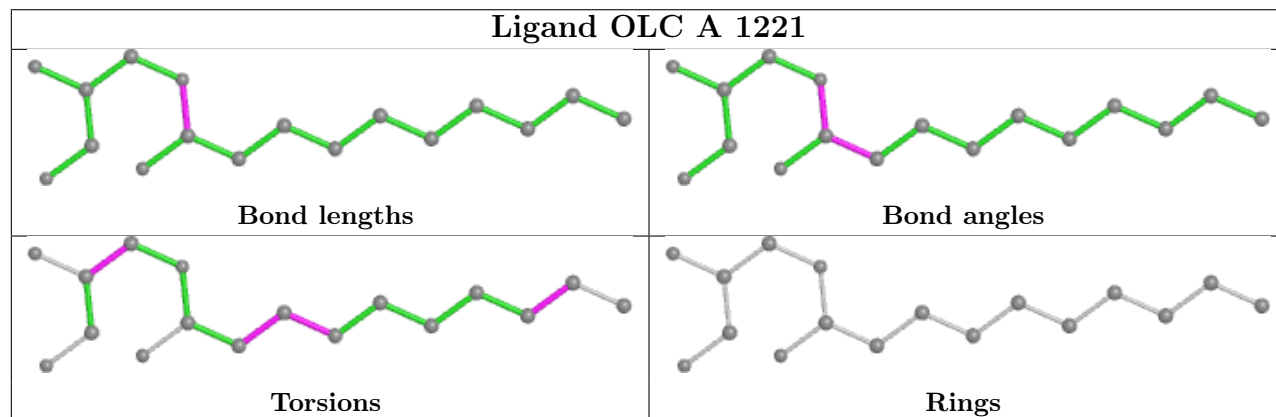
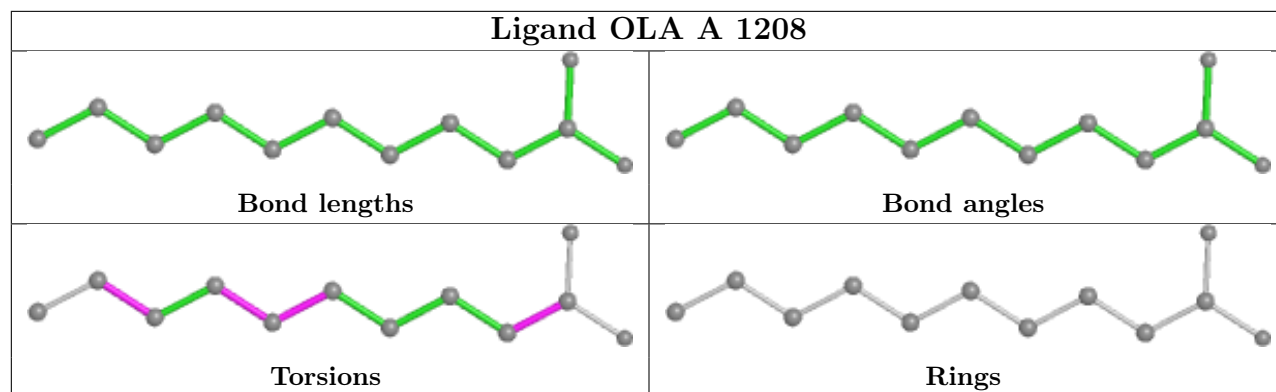
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1216	OLA	1	0
2	A	1201	QGW	1	0
6	A	1215	OLA	2	0
4	A	1205	CLR	2	0

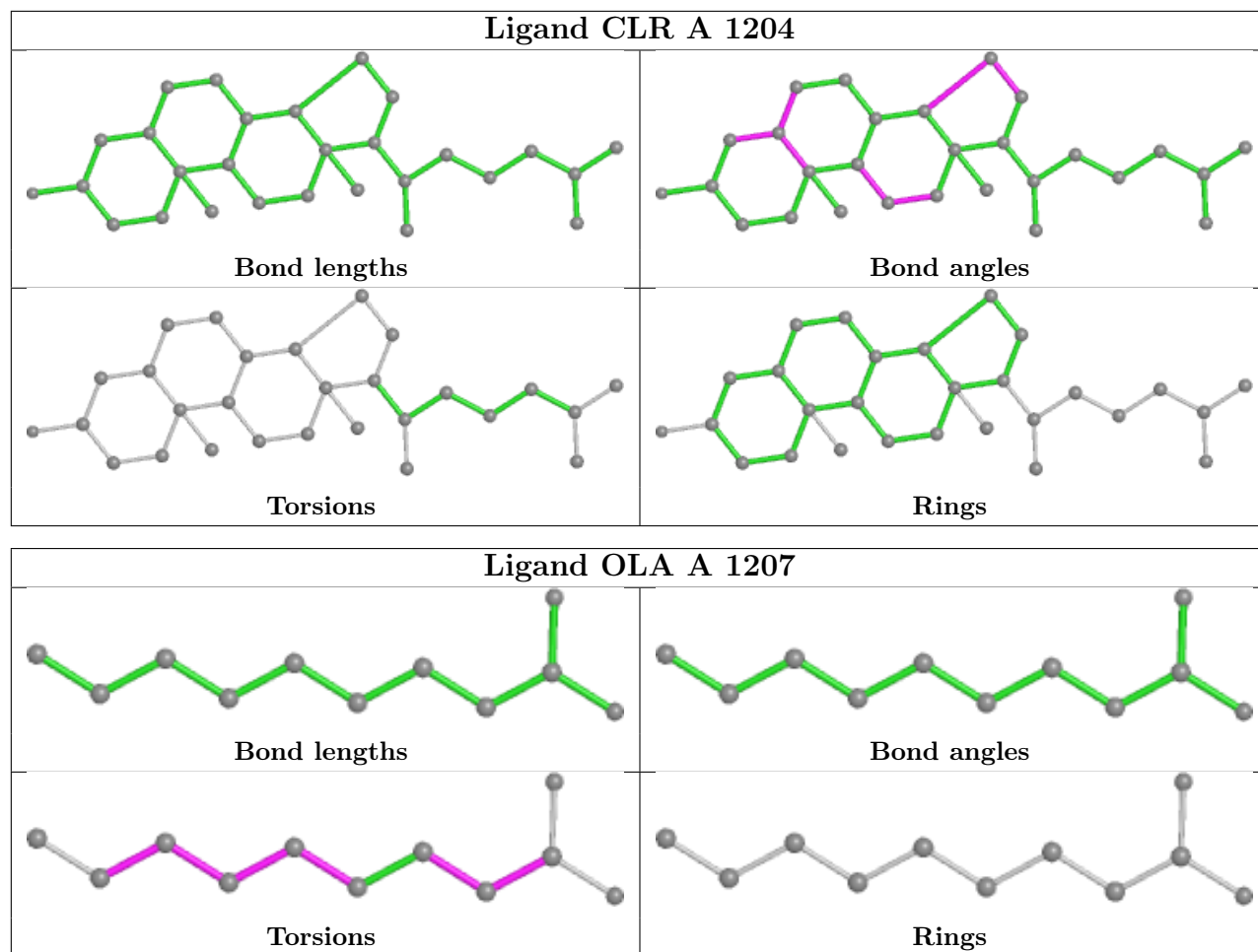
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

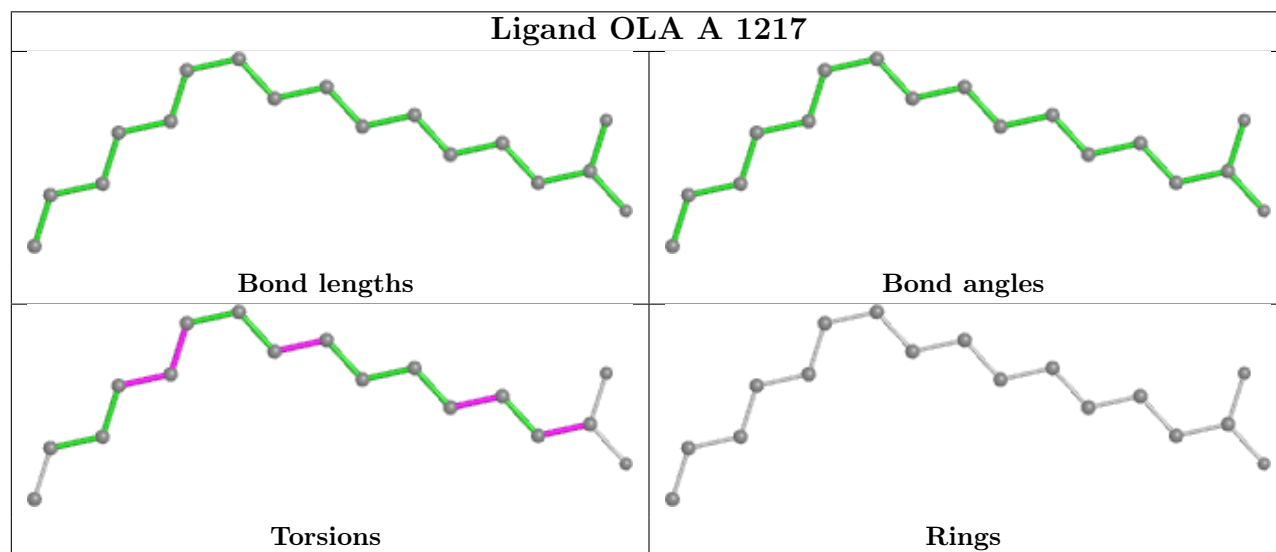
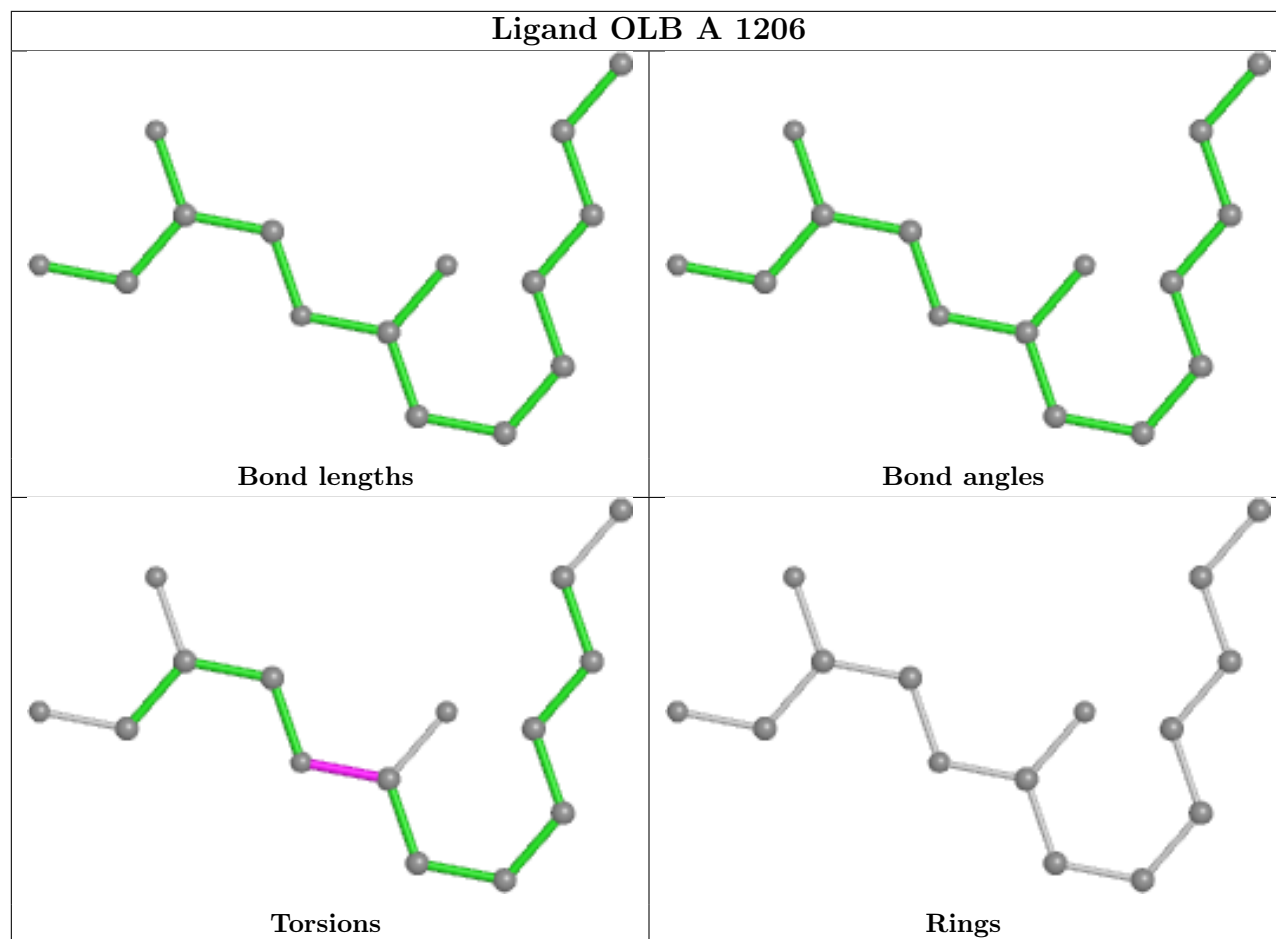




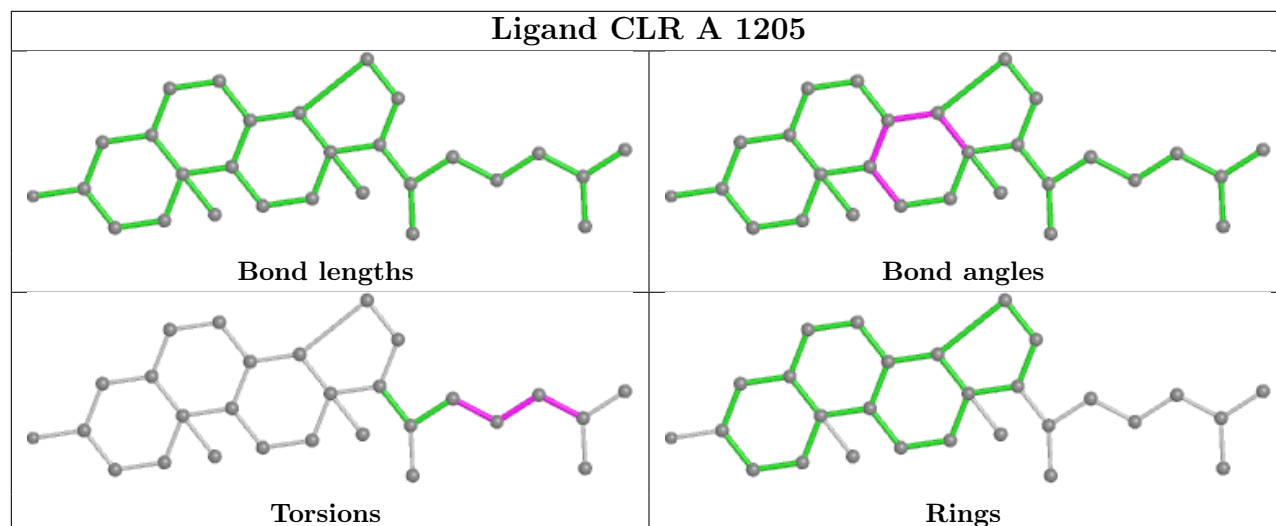












## 5.7 Other polymers [i](#)

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	382/433 (88%)	0.58	43 (11%) <b>5</b> <b>6</b>	20, 44, 89, 122	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1105	TYR	6.3
1	A	290	TYR	4.4
1	A	29[A]	TRP	4.4
1	A	1102	ILE	4.4
1	A	208	LEU	4.3
1	A	1106	LEU	4.2
1	A	302	ILE	4.1
1	A	1021	ASP	4.1
1	A	1101	TYR	4.0
1	A	1026	VAL	3.9
1	A	220	ARG	3.6
1	A	304	ARG	3.3
1	A	111	ARG	3.2
1	A	293	ARG	3.0
1	A	1	PRO	3.0
1	A	148	GLN	3.0
1	A	206	ARG	3.0
1	A	219	GLU	2.9
1	A	1090	ALA	2.9
1	A	1041	GLN	2.8
1	A	1010	LEU	2.8
1	A	1017	ILE	2.7
1	A	1065	PHE	2.7
1	A	1040	ALA	2.7
1	A	1015	LYS	2.7
1	A	1066	ASP	2.6
1	A	1003	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1064	GLY	2.5
1	A	110	LEU	2.5
1	A	1075	ALA	2.5
1	A	303	ILE	2.5
1	A	1030	LEU	2.4
1	A	0	ALA	2.3
1	A	1100	ALA	2.3
1	A	1079	ALA	2.3
1	A	1091	ALA	2.3
1	A	1023	ALA	2.2
1	A	1016	VAL	2.2
1	A	1043	ALA	2.2
1	A	1068	LEU	2.2
1	A	1037	ALA	2.2
1	A	1073	ASP	2.1
1	A	1028	ASP	2.1

## 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.

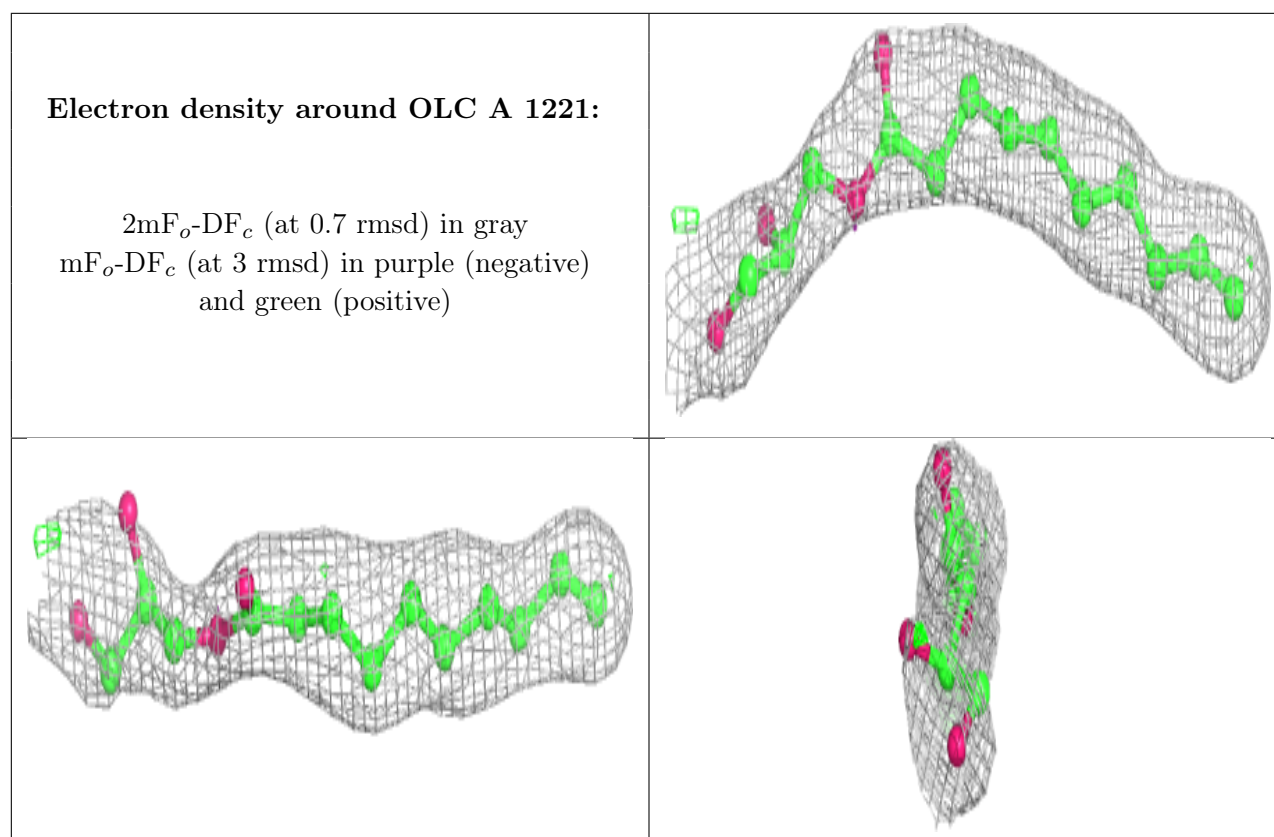
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	OLA	A	1220	5/20	0.47	0.29	60,60,60,60	0
7	OLC	A	1221	17/25	0.63	0.29	55,59,65,66	0
6	OLA	A	1210	15/20	0.65	0.22	69,69,71,71	0
6	OLA	A	1207	11/20	0.68	0.22	52,53,57,57	0
6	OLA	A	1212	7/20	0.69	0.23	77,78,78,78	0
6	OLA	A	1213	5/20	0.72	0.24	54,55,55,55	0
6	OLA	A	1217	17/20	0.74	0.20	54,56,61,61	0

*Continued on next page...*

Continued from previous page...

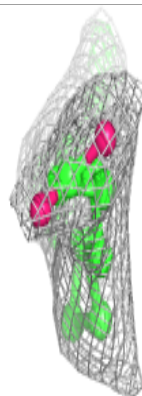
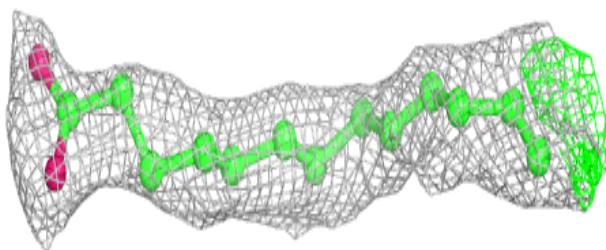
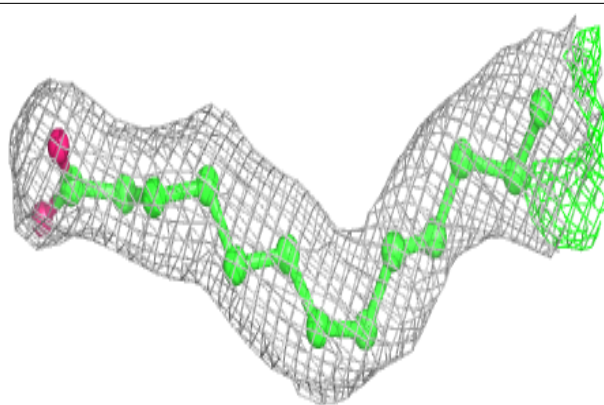
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	OLA	A	1211	6/20	0.76	0.19	45,45,46,46	0
6	OLA	A	1208	12/20	0.76	0.21	59,60,62,62	0
6	OLA	A	1216	11/20	0.78	0.19	62,62,65,65	0
6	OLA	A	1219	7/20	0.79	0.27	43,43,43,43	0
6	OLA	A	1218	10/20	0.80	0.26	49,50,52,52	0
5	OLB	A	1206	15/25	0.81	0.25	53,53,56,56	0
6	OLA	A	1209	7/20	0.82	0.26	51,51,51,51	0
6	OLA	A	1214	7/20	0.87	0.18	46,47,47,47	0
2	QGW	A	1201	25/25	0.89	0.17	28,32,37,37	0
6	OLA	A	1215	15/20	0.89	0.19	43,46,52,52	0
4	CLR	A	1203	28/28	0.91	0.14	42,43,45,46	0
4	CLR	A	1205	28/28	0.91	0.13	34,37,44,45	0
4	CLR	A	1204	28/28	0.92	0.15	37,38,44,44	0
3	NA	A	1202	1/1	0.92	0.17	47,47,47,47	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.

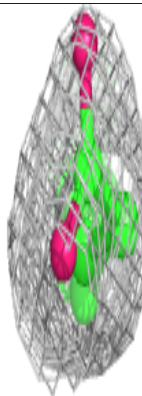
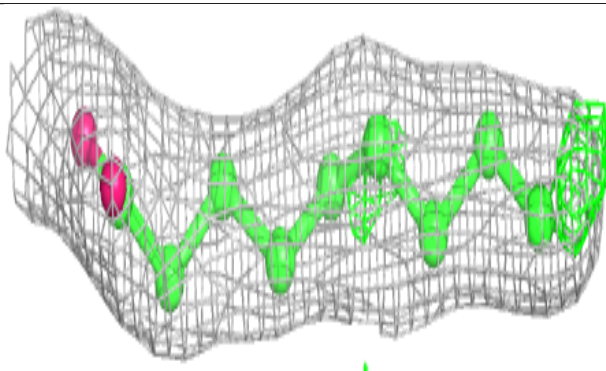
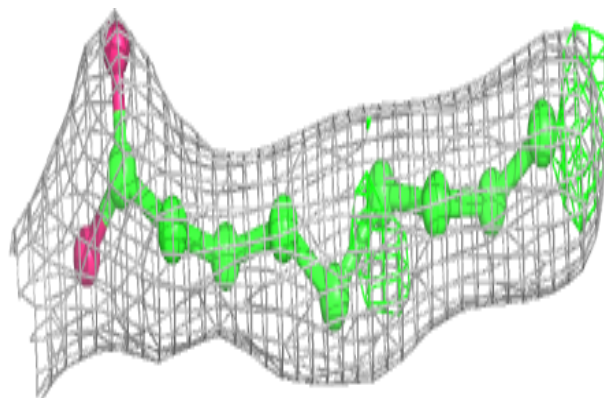


**Electron density around OLA A 1210:**

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

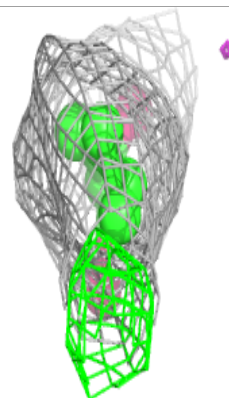
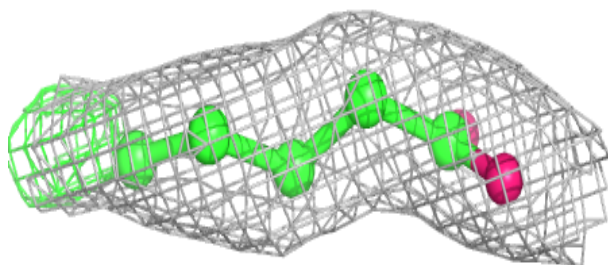
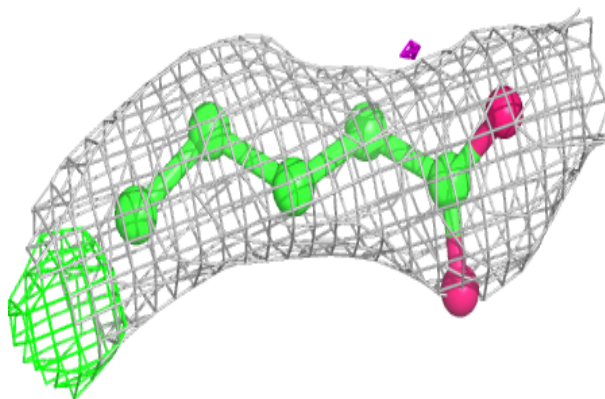
**Electron density around OLA A 1207:**

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

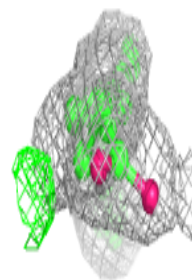
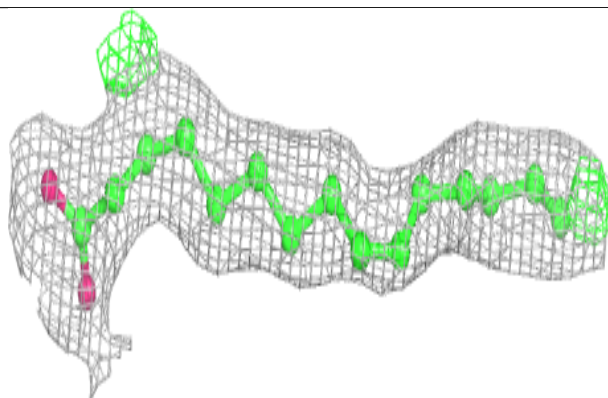
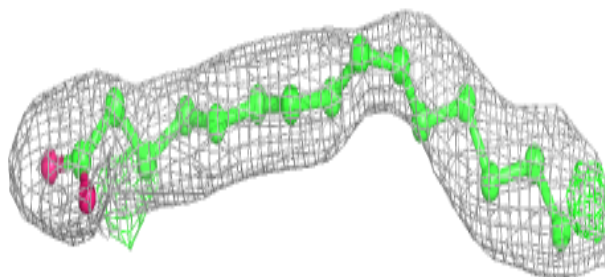


**Electron density around OLA A 1212:**

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

**Electron density around OLA A 1217:**

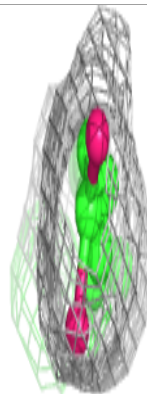
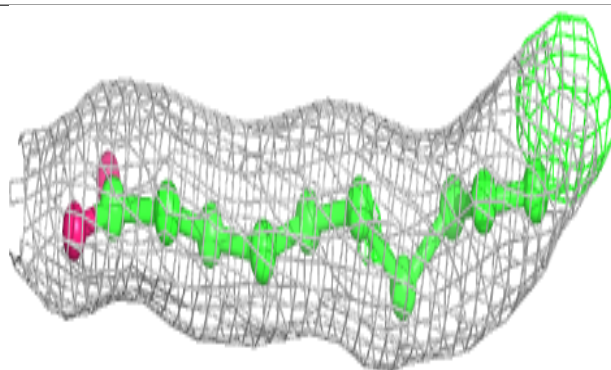
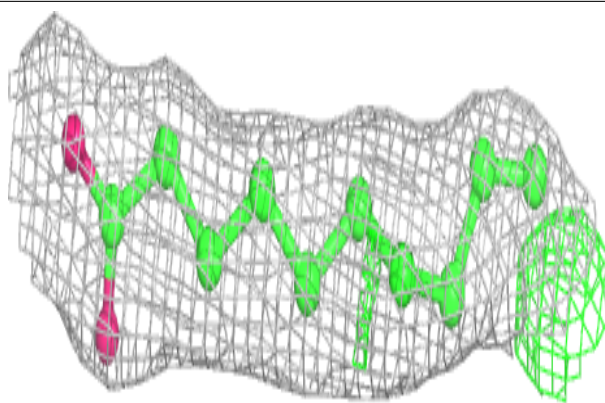
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



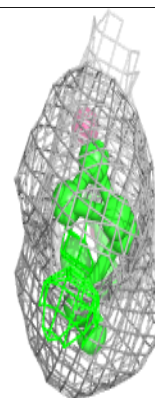
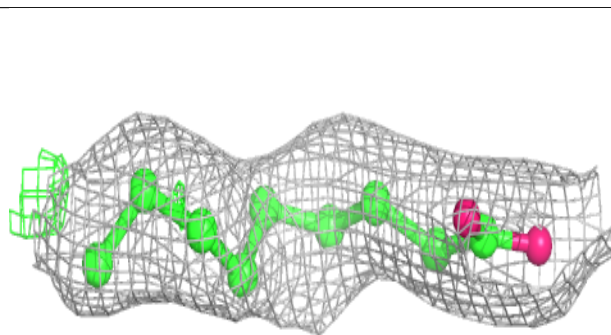
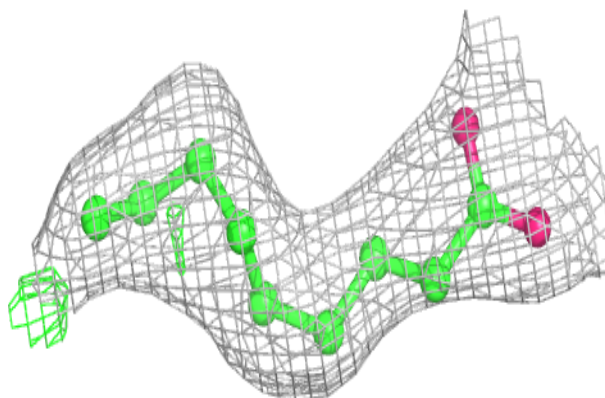


**Electron density around OLA A 1208:**

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

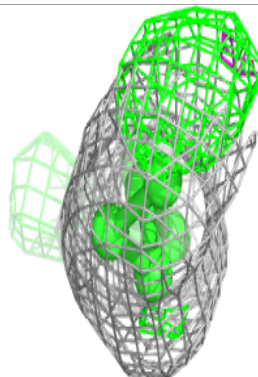
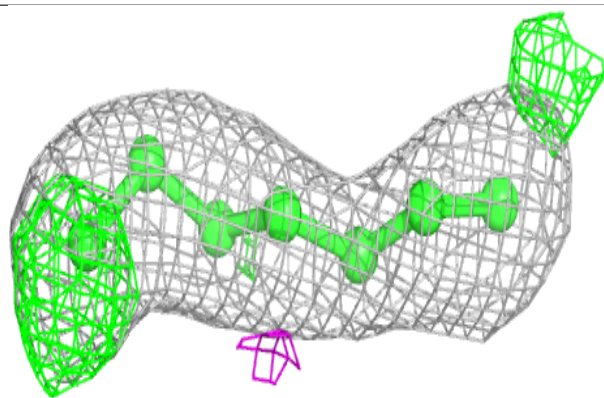
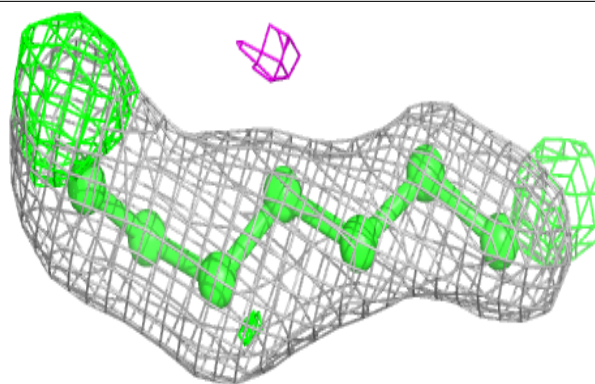
**Electron density around OLA A 1216:**

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

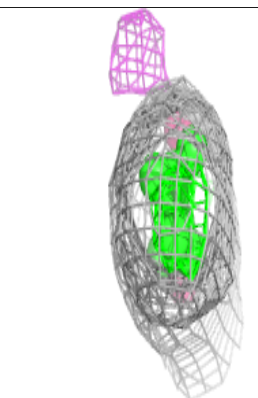
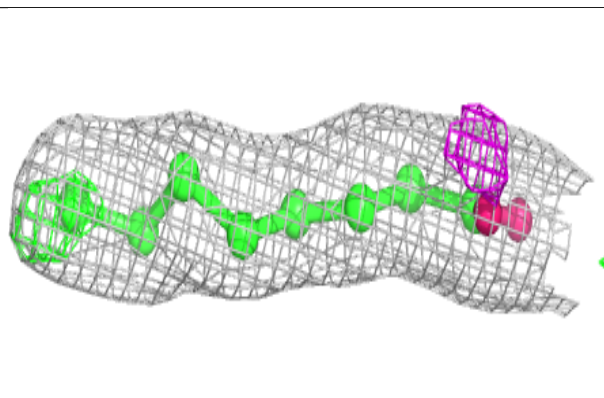
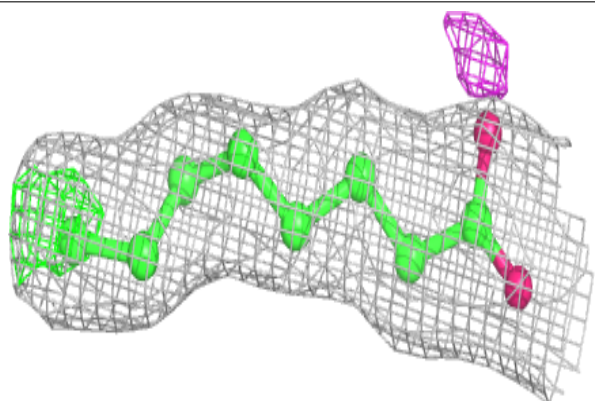


**Electron density around OLA A 1219:**

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

**Electron density around OLA A 1218:**

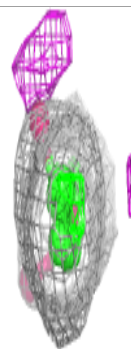
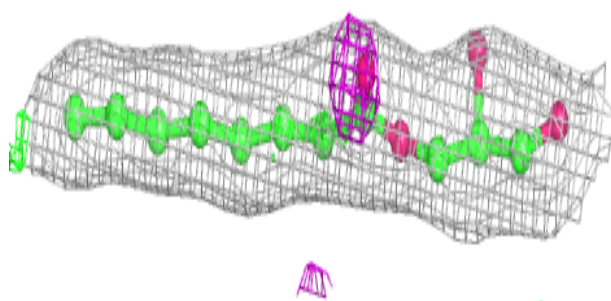
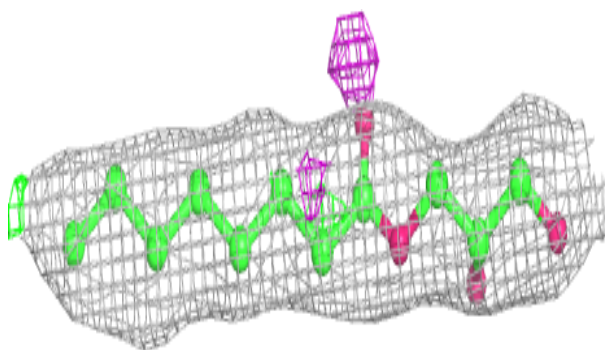
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



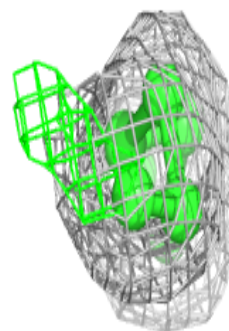
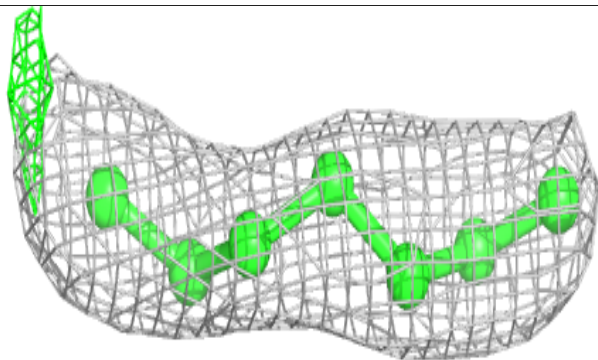
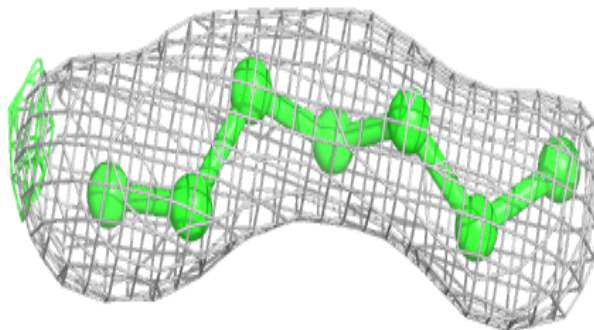


**Electron density around OLB A 1206:**

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

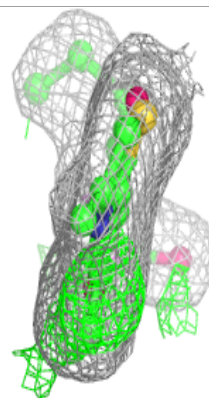
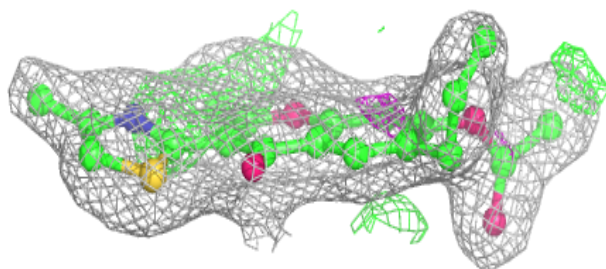
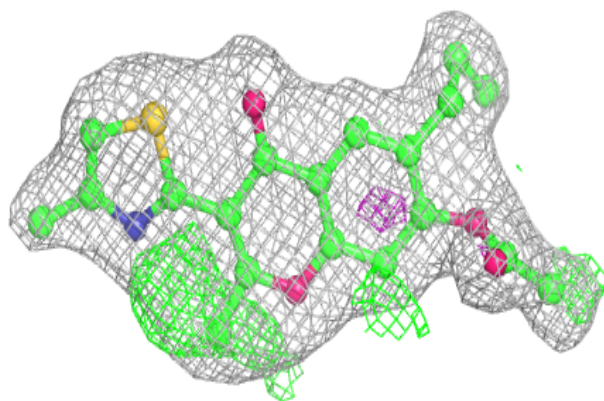
**Electron density around OLA A 1214:**

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

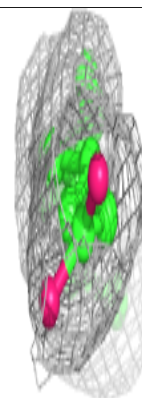
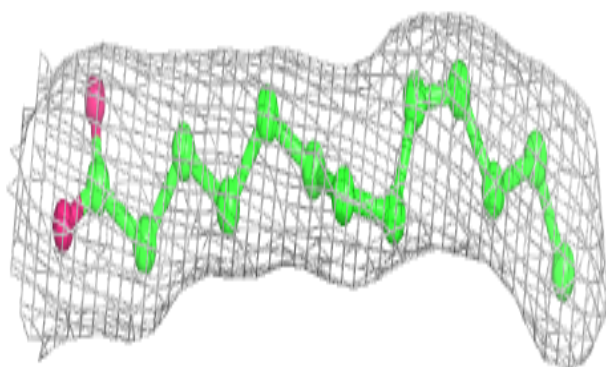
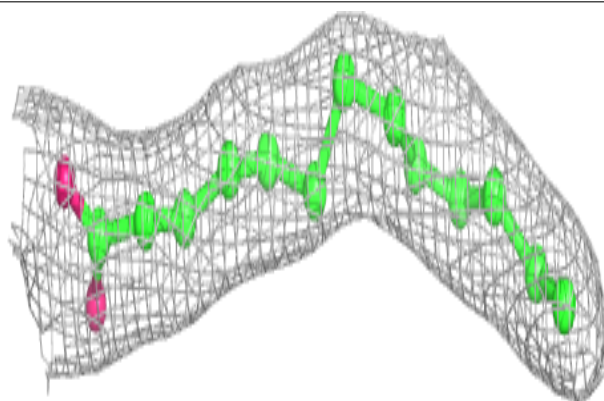


**Electron density around QGW A 1201:**

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

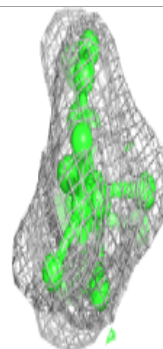
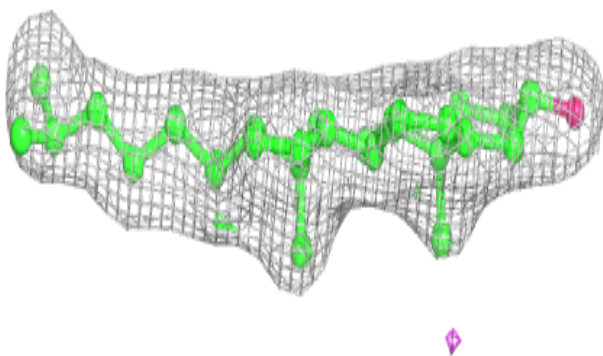
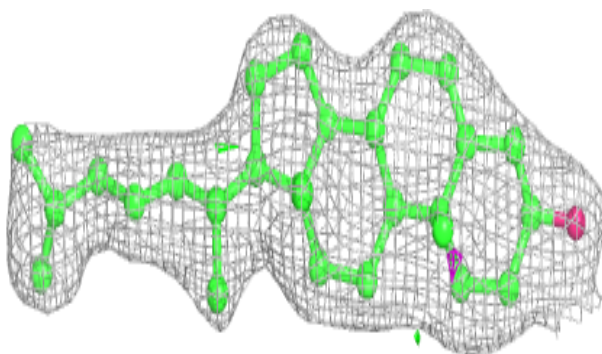
**Electron density around OLA A 1215:**

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

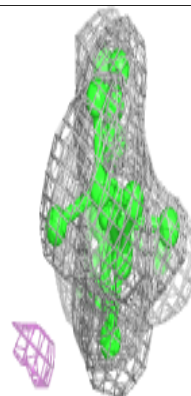
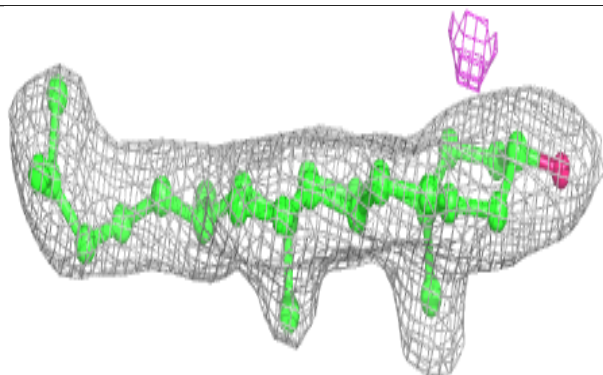
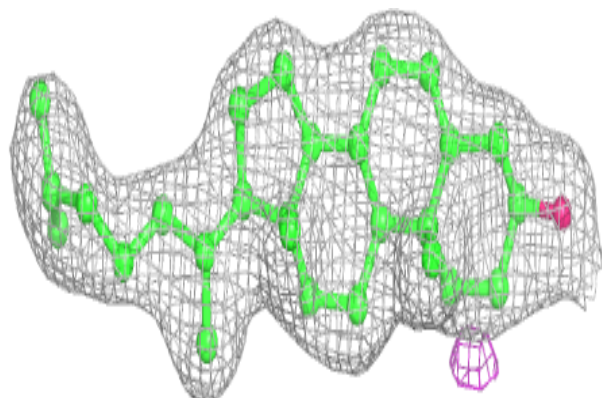


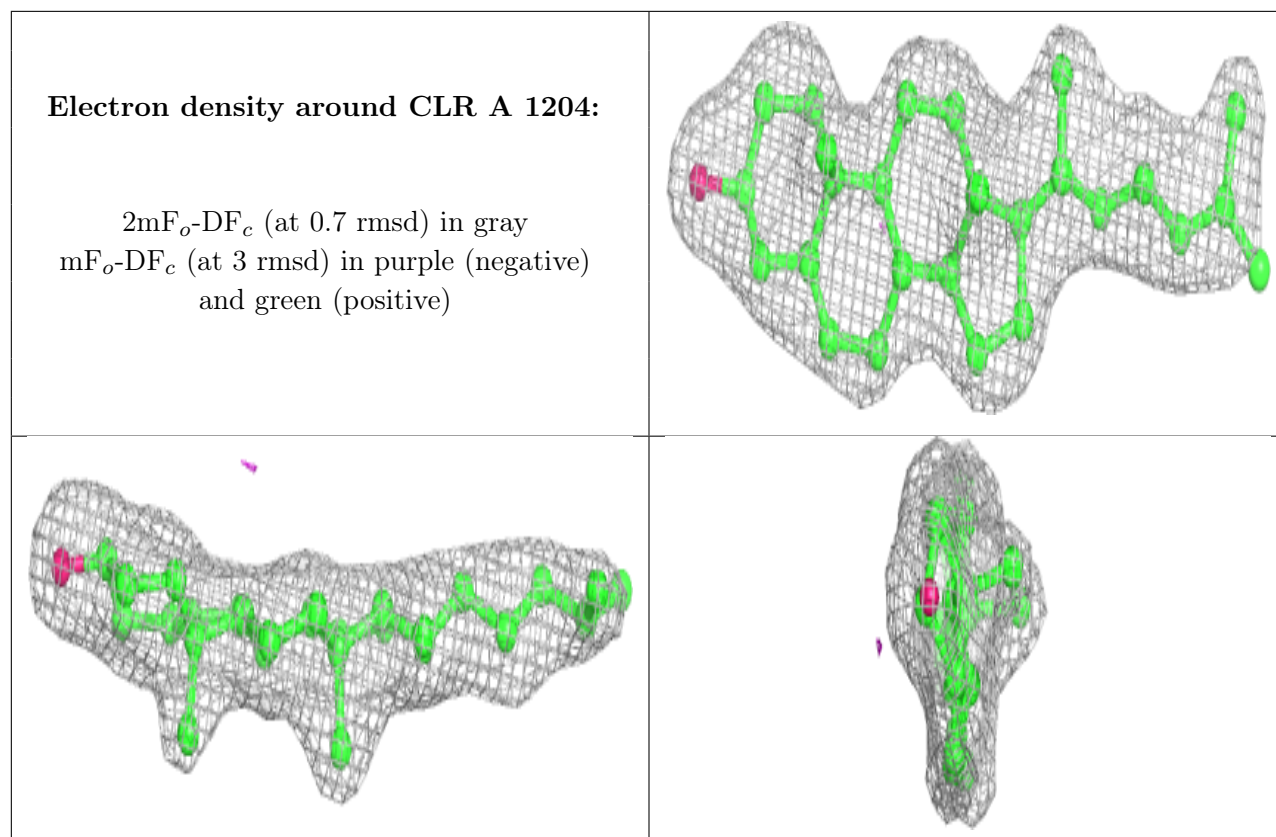
**Electron density around CLR A 1203:**

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

**Electron density around 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.