Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 06:43 PM EDT

PDB ID	:	6AQF
Title	:	Crystal structure of A2AAR-BRIL in complex with the antagonist ZM241385 produced from Pichia pastoris
Authors	:	Eddy, M.T.; Lee, M.Y.; Gao, Z.; White, K.; Didenko, T.; Horst, R.; Audet, M.; Stanczak, P.; McClary, K.M.; Han, G.W.; Jacobson, K.A.; Stevens, R.C.; Wuthrich, K.
Deposited on	:	2017-08-19
Resolution	:	2.51 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

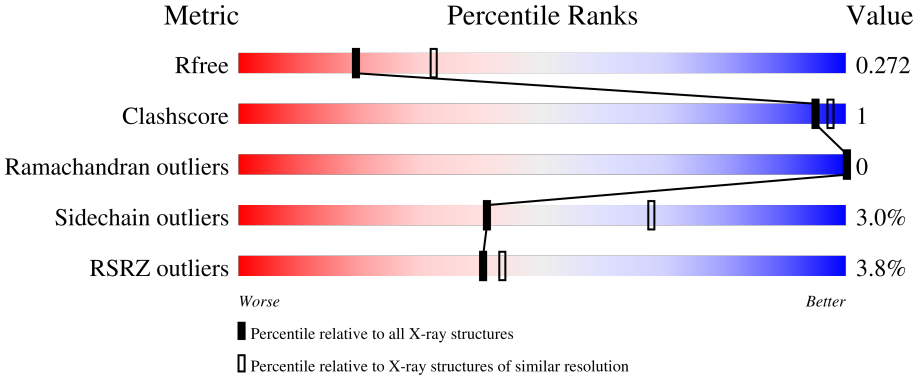
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

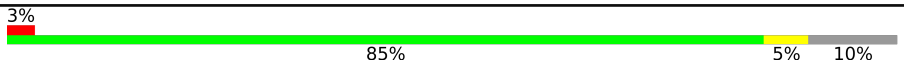
The reported resolution of this entry is 2.51 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	432	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3263 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.

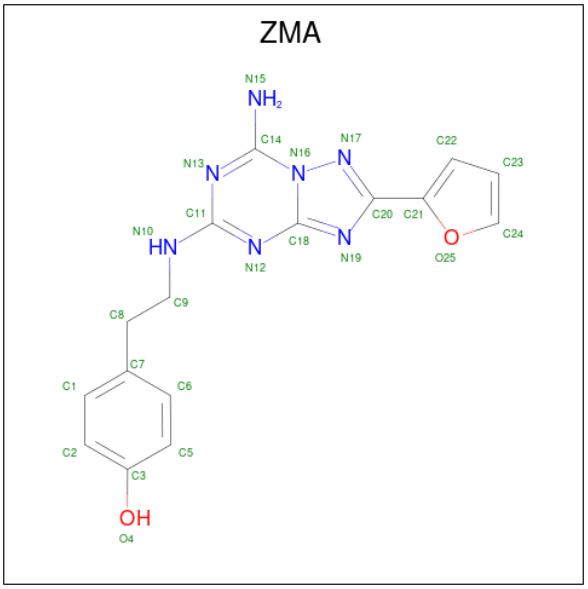
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	2956	1934	483	517	22	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	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
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

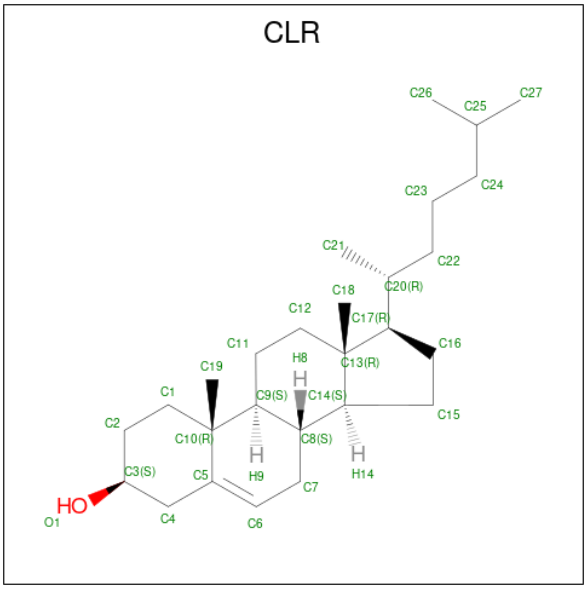
- Molecule 2 is 4-{2-[(7-amino-2-furan-2-yl[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl}

phenol (three-letter code: ZMA) (formula: $C_{16}H_{15}N_7O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

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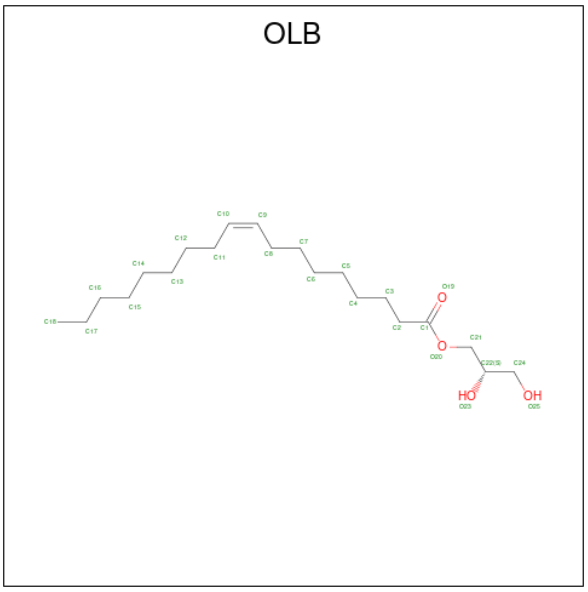
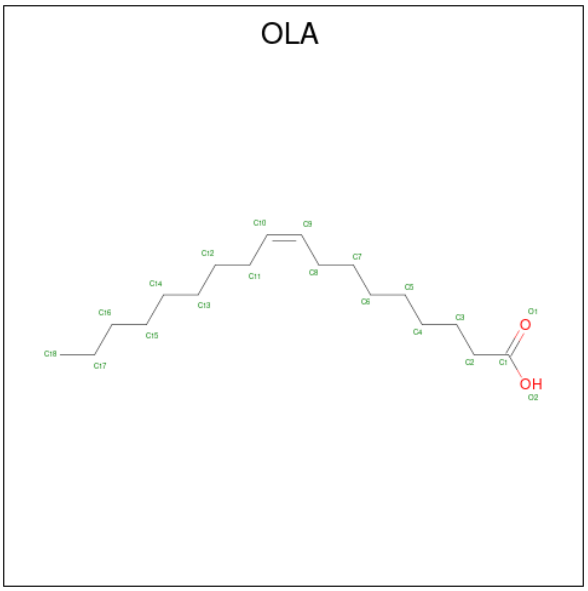
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	28	27	1	0	0
			Total	C	O		
3	A	1	28	27	1	0	0

- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	15	11	4	0	0

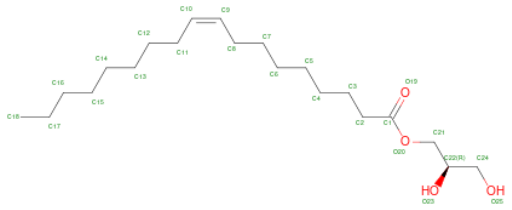
- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	16	14	2	0	0
			Total	C	O		
5	A	1	16	14	2	0	0
			Total	C	O		
5	A	1	14	12	2	0	0
			Total	C	O		
5	A	1	18	16	2	0	0
			Total	C	O		
5	A	1	11	9	2	0	0
			Total	C	O		
5	A	1	9	7	2	0	0
			Total	C	O		
5	A	1	14	12	2	0	0

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).

OLC



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	19	15	4	0	0
			Total	C	O		
6	A	1	16	12	4	0	0
			Total	C	O		
6	A	1	17	13	4	0	0
			Total	C	O		
6	A	1	14	10	4	0	0

- Molecule 7 is water.

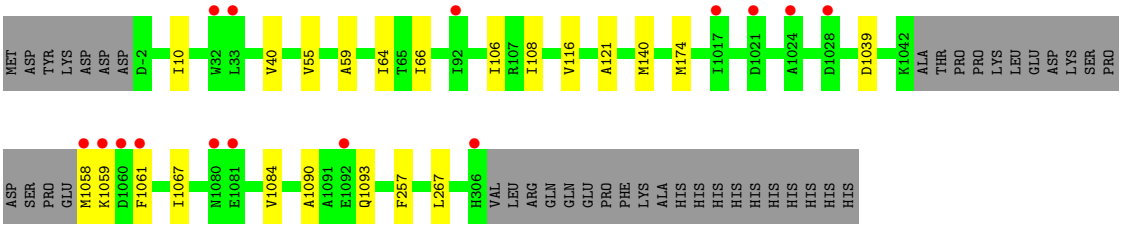
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	19	19	19	0	0

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.84Å 180.97Å 140.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.16 – 2.51 30.05 – 2.51	Depositor EDS
% Data completeness (in resolution range)	89.4 (30.16-2.51) 89.8 (30.05-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.220 , 0.256 0.232 , 0.272	Depositor DCC
R_{free} test set	797 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3263	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: OLB, CLR, OLC, ZMA, OLA

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	0.47	0/3020	0.55	0/4121

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	2956	0	2948	7	0
2	A	25	0	15	0	0
3	A	84	0	138	0	0
4	A	15	0	19	1	0
5	A	98	0	130	0	0
6	A	66	0	85	1	0
7	A	19	0	0	0	0
All	All	3263	0	3335	8	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 1.

All (8) 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:40:VAL:HG11	1:A:116:VAL:HG12	1.80	0.62
1:A:174:MET:HG3	1:A:257:PHE:HB2	1.96	0.48
1:A:40:VAL:HG13	1:A:121:ALA:HB2	2.01	0.43
1:A:1090:ALA:O	1:A:1093:GLN:HG2	2.19	0.43
1:A:10:ILE:HG12	1:A:64:ILE:HG23	1.99	0.43
1:A:55:VAL:HA	1:A:59:ALA:HB3	2.01	0.43
4:A:1205:OLB:H4A	6:A:1214:OLC:H6A	2.02	0.42
1:A:1058:MET:HG3	1:A:1059:LYS:H	1.86	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	387/432 (90%)	383 (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	301/361 (83%)	292 (97%)	9 (3%)	41 68

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ILE
1	A	106	ILE
1	A	108	ILE
1	A	140	MET
1	A	1039	ASP
1	A	1061	PHE
1	A	1067	ILE
1	A	1084	VAL
1	A	267	LEU

Sometimes 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)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	OLB	A	1205	-	14,14,24	0.41	0	15,15,25	1.01	1 (6%)
2	ZMA	A	1201	-	21,28,28	0.73	0	20,39,39	2.17	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	OLA	A	1209	-	17,17,19	0.54	0	17,17,19	0.85	0
5	OLA	A	1208	-	13,13,19	0.61	0	12,13,19	1.07	1 (8%)
5	OLA	A	1212	-	13,13,19	0.59	0	12,13,19	1.07	1 (8%)
3	CLR	A	1204	-	31,31,31	0.60	0	48,48,48	1.17	4 (8%)
3	CLR	A	1202	-	31,31,31	0.59	0	48,48,48	1.17	5 (10%)
5	OLA	A	1206	-	15,15,19	0.56	0	15,15,19	0.99	2 (13%)
5	OLA	A	1210	-	10,10,19	0.67	0	10,10,19	0.97	1 (10%)
6	OLC	A	1216	-	13,13,24	0.42	0	14,14,25	1.04	1 (7%)
5	OLA	A	1211	-	8,8,19	0.68	0	8,8,19	1.28	1 (12%)
6	OLC	A	1215	-	16,16,24	0.45	0	17,17,25	0.96	1 (5%)
6	OLC	A	1213	-	18,18,24	0.42	0	18,19,25	0.89	1 (5%)
6	OLC	A	1214	-	15,15,24	0.39	0	16,16,25	1.03	1 (6%)
5	OLA	A	1207	-	15,15,19	0.54	0	15,15,19	1.00	1 (6%)
3	CLR	A	1203	-	31,31,31	0.60	0	48,48,48	1.22	5 (10%)

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
4	OLB	A	1205	-	-	11/14/14/24	-
2	ZMA	A	1201	-	-	0/6/10/10	0/4/4/4
5	OLA	A	1209	-	-	9/15/15/17	-
5	OLA	A	1208	-	-	8/11/11/17	-
5	OLA	A	1212	-	-	9/11/11/17	-
3	CLR	A	1204	-	-	4/10/68/68	0/4/4/4
3	CLR	A	1202	-	-	8/10/68/68	0/4/4/4
5	OLA	A	1206	-	-	7/13/13/17	-
5	OLA	A	1210	-	-	3/8/8/17	-
6	OLC	A	1216	-	-	8/13/13/24	-
5	OLA	A	1211	-	-	4/6/6/17	-
6	OLC	A	1215	-	-	5/16/16/24	-
6	OLC	A	1213	-	-	6/18/18/24	-
6	OLC	A	1214	-	-	10/15/15/24	-
5	OLA	A	1207	-	-	7/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	A	1203	-	-	5/10/68/68	0/4/4/4

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	ZMA	N15-C14-N16	6.35	122.24	117.97
2	A	1201	ZMA	C23-C22-C21	-4.41	102.62	108.39
2	A	1201	ZMA	N12-C11-N13	-3.80	120.22	126.23
3	A	1204	CLR	C4-C5-C10	3.75	121.40	116.42
3	A	1203	CLR	C21-C20-C22	-3.30	105.20	110.36
3	A	1204	CLR	C4-C5-C6	-3.25	115.92	120.61
3	A	1202	CLR	C4-C5-C10	3.14	120.59	116.42
3	A	1203	CLR	C4-C5-C10	2.99	120.40	116.42
3	A	1204	CLR	C21-C20-C22	-2.82	105.94	110.36
6	A	1214	OLC	O20-C1-C2	2.72	120.44	111.91
6	A	1216	OLC	O20-C1-C2	2.70	120.39	111.91
4	A	1205	OLB	O20-C1-C2	2.64	120.19	111.91
3	A	1202	CLR	C4-C5-C6	-2.59	116.87	120.61
3	A	1203	CLR	C21-C20-C17	2.57	116.85	112.92
3	A	1203	CLR	C7-C8-C14	2.42	114.41	110.91
3	A	1203	CLR	C4-C5-C6	-2.37	117.19	120.61
2	A	1201	ZMA	N10-C11-N13	2.34	121.24	117.19
5	A	1207	OLA	O2-C1-C2	2.30	121.42	114.03
5	A	1206	OLA	O2-C1-C2	2.30	121.41	114.03
3	A	1202	CLR	C16-C17-C20	2.29	115.69	112.15
6	A	1215	OLC	O20-C1-C2	2.28	119.06	111.91
5	A	1212	OLA	O2-C1-C2	2.21	121.13	114.03
6	A	1213	OLC	O20-C1-C2	2.19	118.79	111.91
5	A	1211	OLA	O2-C1-C2	2.13	120.86	114.03
3	A	1202	CLR	C22-C20-C17	2.06	114.54	110.28
3	A	1204	CLR	C21-C20-C17	2.06	116.08	112.92
3	A	1202	CLR	C1-C2-C3	2.05	113.10	110.47
5	A	1208	OLA	O2-C1-C2	2.03	120.56	114.03
5	A	1206	OLA	O2-C1-O1	-2.02	118.26	123.30
5	A	1210	OLA	O2-C1-O1	-2.01	118.29	123.30

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1212	OLA	C9-C10-C11-C12
6	A	1213	OLC	C9-C10-C11-C12
6	A	1214	OLC	C2-C1-O20-C21
6	A	1216	OLC	O19-C1-O20-C21
6	A	1216	OLC	C2-C1-O20-C21
6	A	1214	OLC	O19-C1-O20-C21
3	A	1203	CLR	C17-C20-C22-C23
6	A	1214	OLC	O20-C21-C22-O23
3	A	1204	CLR	C17-C20-C22-C23
3	A	1203	CLR	C21-C20-C22-C23
3	A	1202	CLR	C17-C20-C22-C23
3	A	1202	CLR	C21-C20-C22-C23
4	A	1205	OLB	C2-C1-O20-C21
3	A	1204	CLR	C21-C20-C22-C23
5	A	1208	OLA	C1-C2-C3-C4
3	A	1202	CLR	C22-C23-C24-C25
4	A	1205	OLB	O19-C1-O20-C21
5	A	1212	OLA	C1-C2-C3-C4
6	A	1214	OLC	C1-C2-C3-C4
3	A	1203	CLR	C22-C23-C24-C25
3	A	1204	CLR	C20-C22-C23-C24
4	A	1205	OLB	O20-C21-C22-O23
5	A	1208	OLA	C4-C5-C6-C7
3	A	1202	CLR	C23-C24-C25-C27
4	A	1205	OLB	O20-C21-C22-C24
6	A	1214	OLC	C5-C6-C7-C8
4	A	1205	OLB	C4-C5-C6-C7
5	A	1210	OLA	C4-C5-C6-C7
5	A	1212	OLA	C2-C3-C4-C5
5	A	1208	OLA	C5-C6-C7-C8
5	A	1207	OLA	C4-C5-C6-C7
6	A	1216	OLC	C3-C4-C5-C6
5	A	1211	OLA	C3-C4-C5-C6
5	A	1212	OLA	C3-C4-C5-C6
3	A	1202	CLR	C23-C24-C25-C26
5	A	1210	OLA	C1-C2-C3-C4
6	A	1215	OLC	C2-C1-O20-C21
4	A	1205	OLB	C3-C4-C5-C6
6	A	1215	OLC	O19-C1-O20-C21
6	A	1213	OLC	C4-C5-C6-C7
5	A	1209	OLA	C5-C6-C7-C8
5	A	1207	OLA	C3-C4-C5-C6
6	A	1213	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	A	1212	OLA	C5-C6-C7-C8
5	A	1207	OLA	C10-C11-C12-C13
5	A	1209	OLA	C12-C13-C14-C15
5	A	1206	OLA	C6-C7-C8-C9
5	A	1208	OLA	C6-C7-C8-C9
5	A	1206	OLA	C11-C12-C13-C14
6	A	1214	OLC	C2-C3-C4-C5
6	A	1214	OLC	C6-C7-C8-C9
5	A	1212	OLA	C6-C7-C8-C9
3	A	1203	CLR	C23-C24-C25-C27
6	A	1215	OLC	C1-C2-C3-C4
5	A	1207	OLA	C2-C3-C4-C5
5	A	1206	OLA	C3-C4-C5-C6
5	A	1210	OLA	C3-C4-C5-C6
6	A	1215	OLC	O20-C21-C22-C24
3	A	1202	CLR	C16-C17-C20-C22
5	A	1206	OLA	C10-C11-C12-C13
3	A	1204	CLR	C22-C23-C24-C25
5	A	1211	OLA	C2-C3-C4-C5
4	A	1205	OLB	C2-C3-C4-C5
5	A	1208	OLA	C9-C10-C11-C12
5	A	1209	OLA	C3-C4-C5-C6
6	A	1214	OLC	O20-C21-C22-C24
5	A	1209	OLA	C6-C7-C8-C9
5	A	1209	OLA	C10-C11-C12-C13
3	A	1203	CLR	C23-C24-C25-C26
6	A	1213	OLC	O20-C21-C22-O23
6	A	1216	OLC	O20-C21-C22-O23
6	A	1216	OLC	O20-C21-C22-C24
5	A	1208	OLA	C3-C4-C5-C6
3	A	1202	CLR	C13-C17-C20-C22
5	A	1209	OLA	C13-C14-C15-C16
6	A	1216	OLC	C2-C3-C4-C5
4	A	1205	OLB	C5-C6-C7-C8
5	A	1212	OLA	O2-C1-C2-C3
5	A	1207	OLA	C7-C8-C9-C10
5	A	1206	OLA	O1-C1-C2-C3
5	A	1212	OLA	O1-C1-C2-C3
5	A	1208	OLA	O2-C1-C2-C3
5	A	1206	OLA	O2-C1-C2-C3
5	A	1208	OLA	O1-C1-C2-C3
6	A	1213	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
4	A	1205	OLB	C1-C2-C3-C4
5	A	1211	OLA	O2-C1-C2-C3
5	A	1211	OLA	O1-C1-C2-C3
5	A	1207	OLA	O1-C1-C2-C3
5	A	1209	OLA	O2-C1-C2-C3
5	A	1206	OLA	C7-C8-C9-C10
6	A	1213	OLC	C2-C1-O20-C21
6	A	1215	OLC	O20-C21-C22-O23
4	A	1205	OLB	O20-C1-C2-C3
5	A	1209	OLA	O1-C1-C2-C3
5	A	1207	OLA	O2-C1-C2-C3
6	A	1216	OLC	O20-C1-C2-C3
3	A	1202	CLR	C16-C17-C20-C21
4	A	1205	OLB	O19-C1-C2-C3
6	A	1216	OLC	O19-C1-C2-C3
5	A	1212	OLA	C7-C8-C9-C10
5	A	1209	OLA	C9-C10-C11-C12
6	A	1214	OLC	O20-C1-C2-C3
6	A	1214	OLC	O19-C1-C2-C3

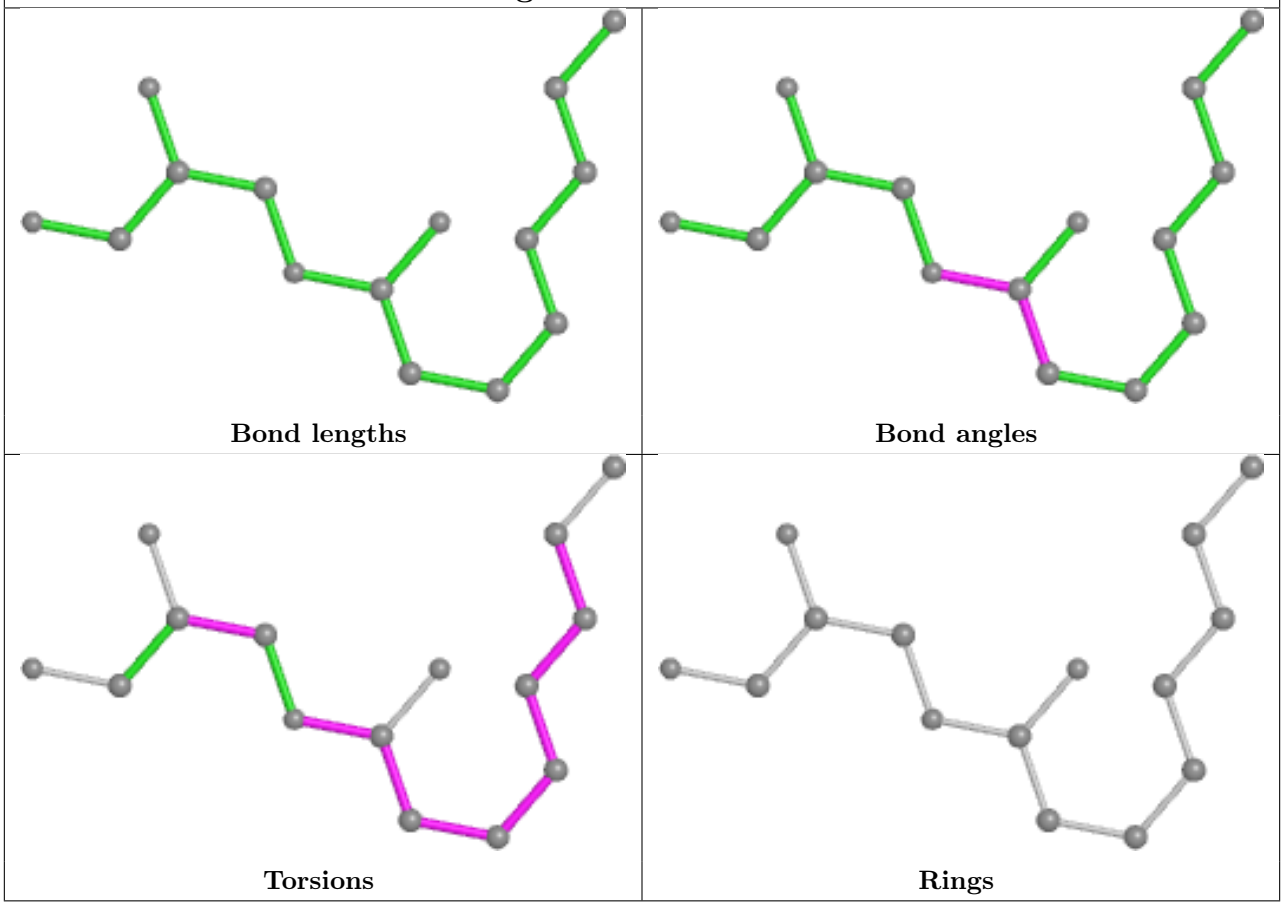
There are no ring outliers.

2 monomers are involved in 1 short contact:

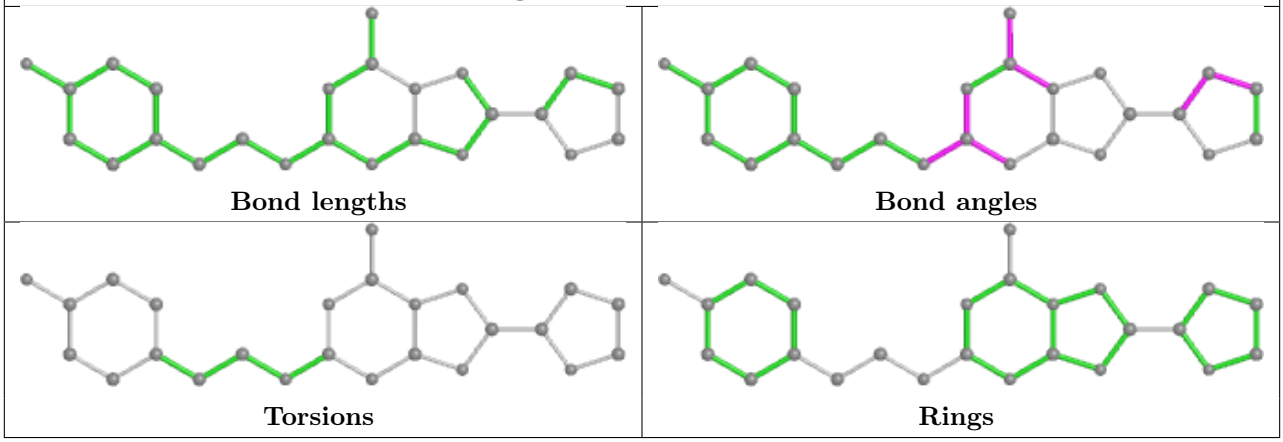
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1205	OLB	1	0
6	A	1214	OLC	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

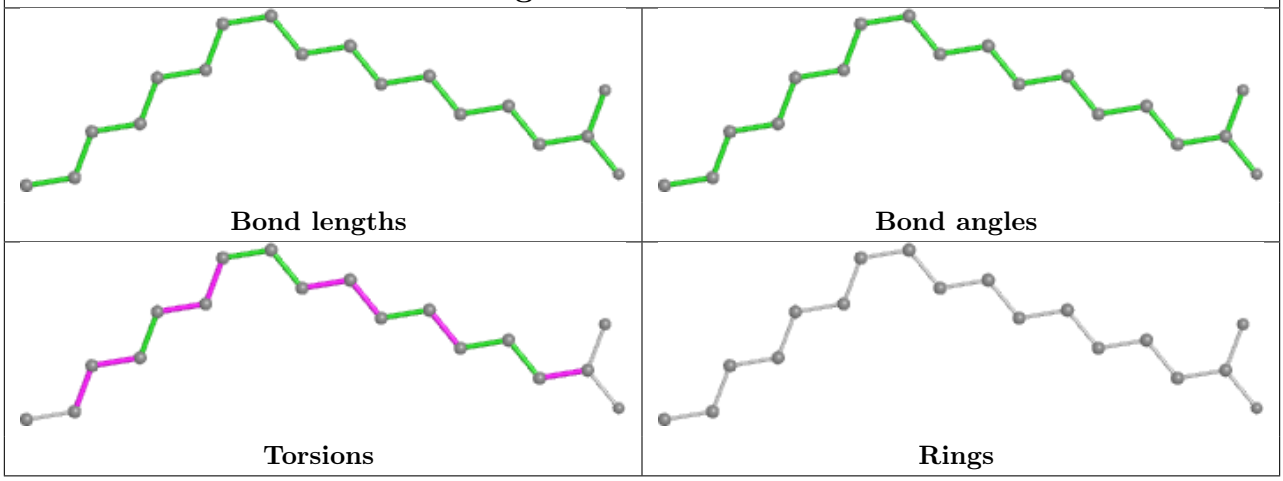
Ligand OLB A 1205



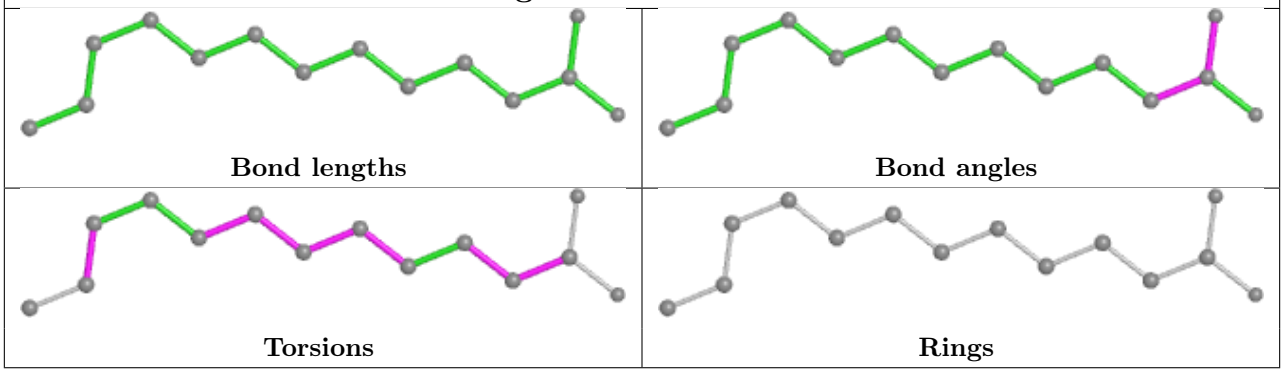
Ligand ZMA A 1201



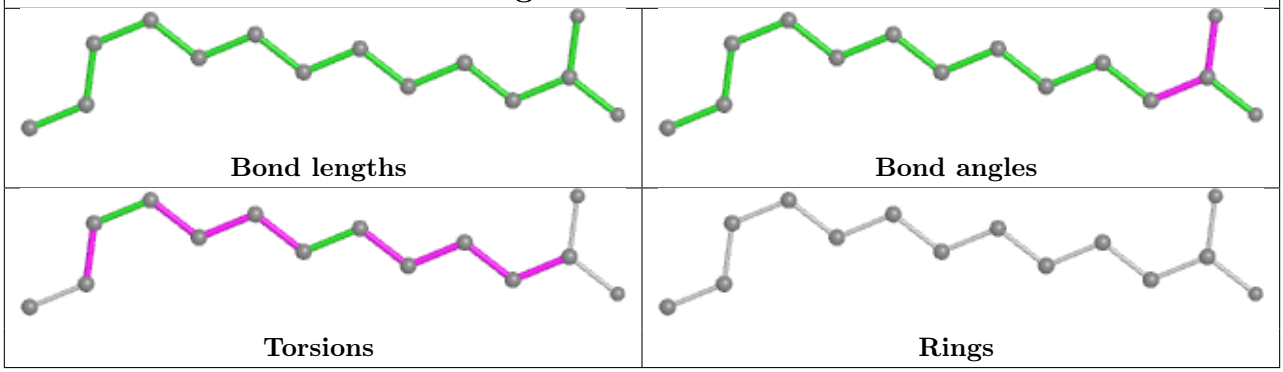
Ligand OLA A 1209



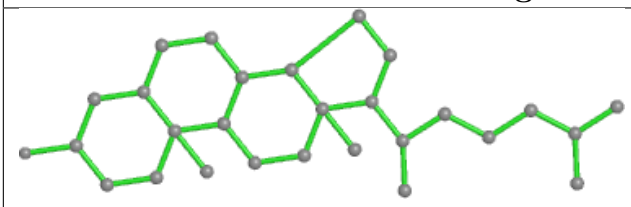
Ligand OLA A 1208



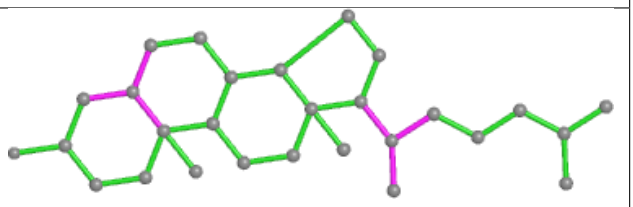
Ligand OLA A 1212



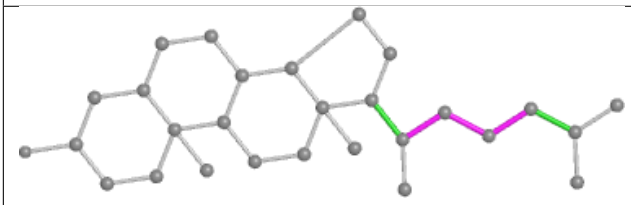
Ligand CLR A 1204



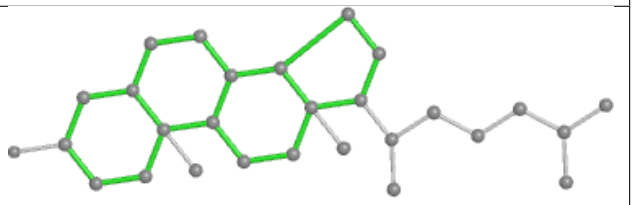
Bond lengths



Bond angles

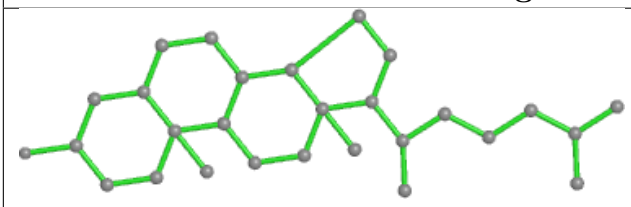


Torsions

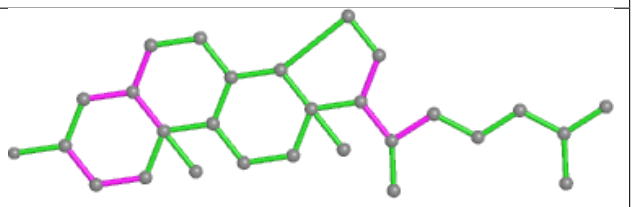


Rings

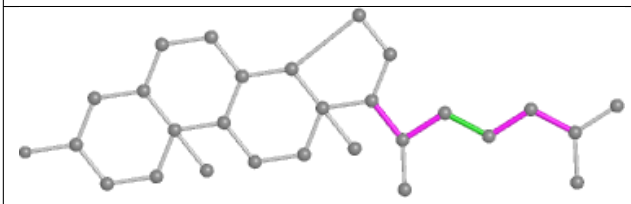
Ligand CLR A 1202



Bond lengths



Bond angles



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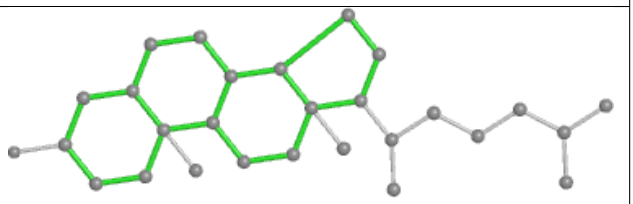
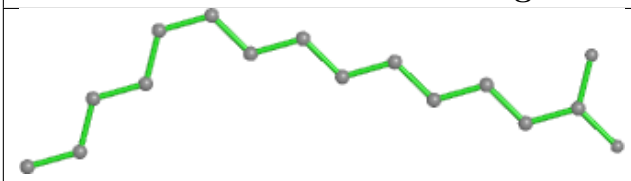
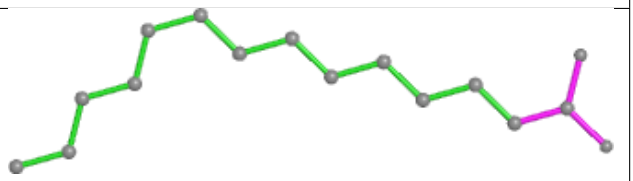


Rings

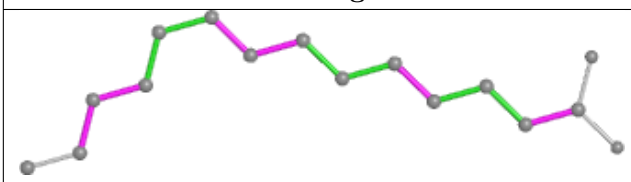
Ligand OLA A 1206



Bond lengths



Bond angles



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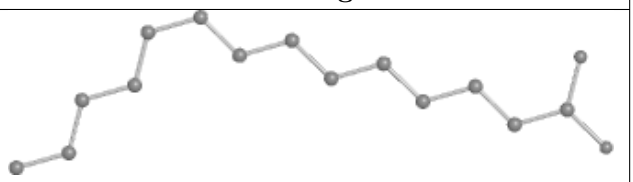
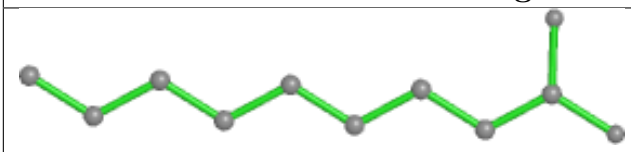


Rings

Ligand OLA A 1210



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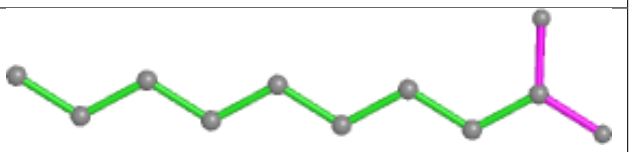

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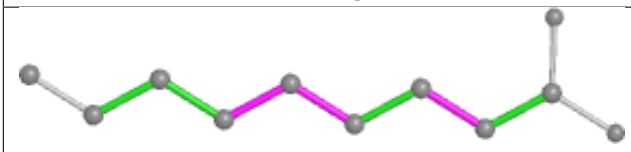

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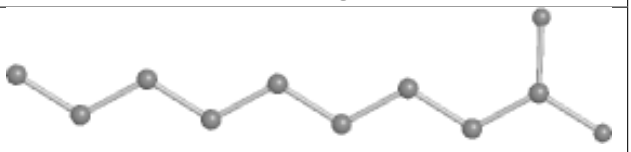
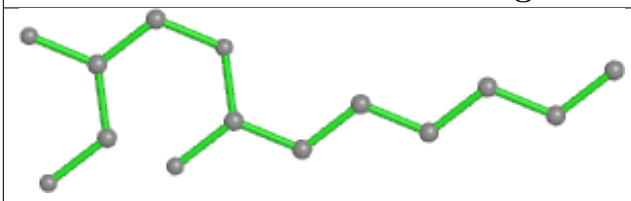


Rings

Ligand OLC A 1216



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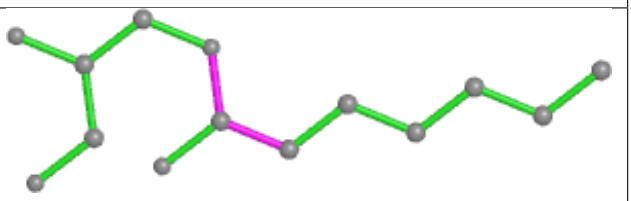
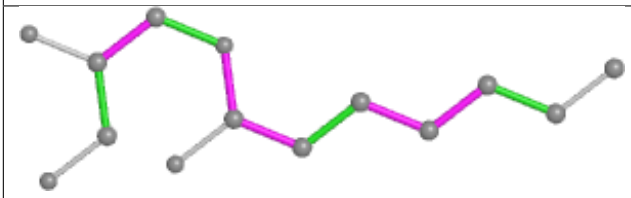


Bond angles



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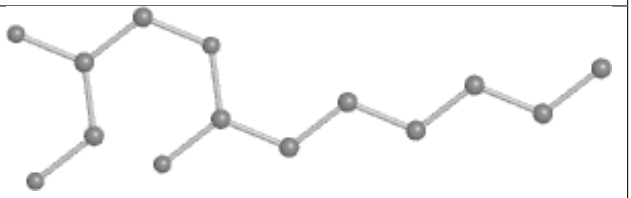
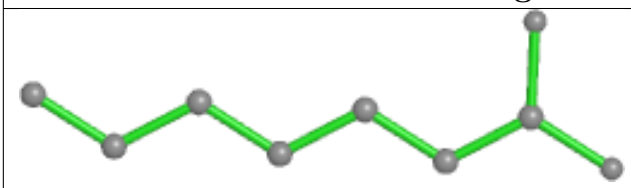


Rings

Ligand OLA A 1211



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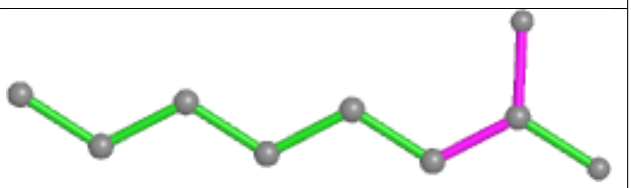
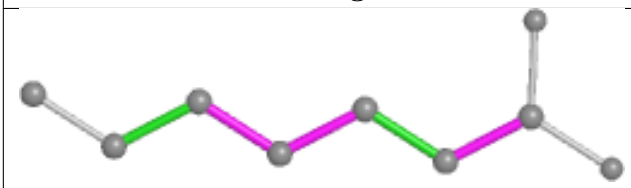
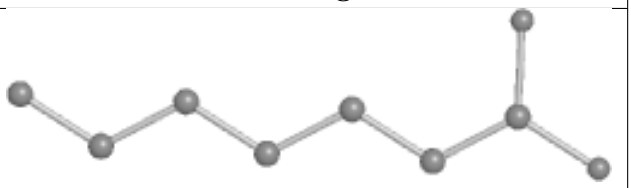


Bond angles

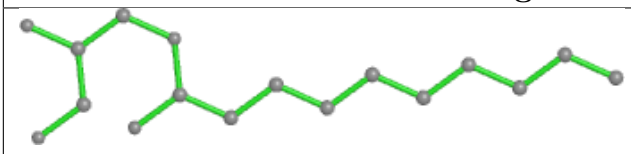


Torsions

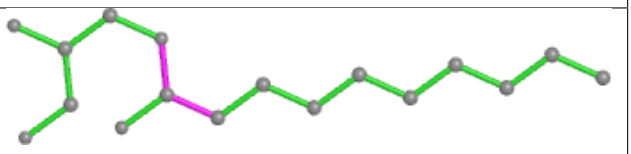


Rings

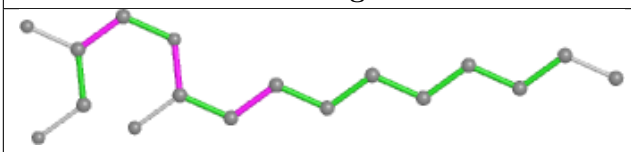
Ligand OLC A 1215



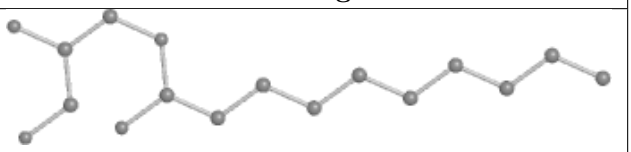
Bond lengths



Bond angles

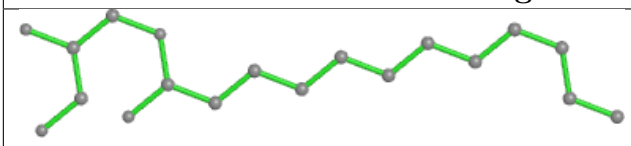


Torsions

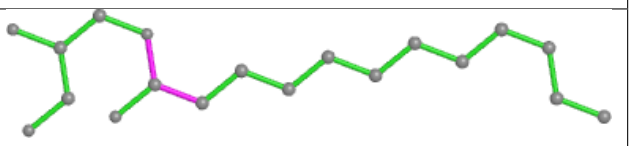


Rings

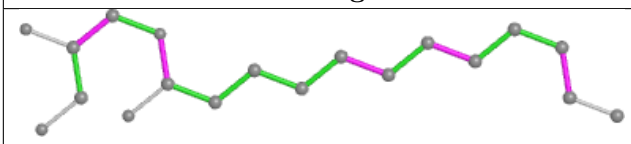
Ligand OLC A 1213



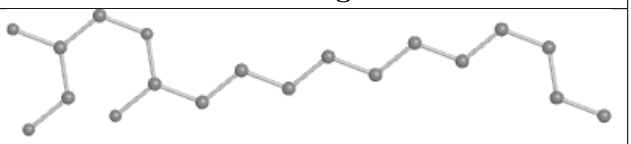
Bond lengths



Bond angles

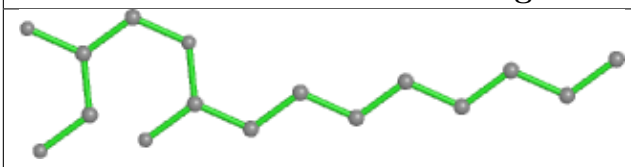


Torsions

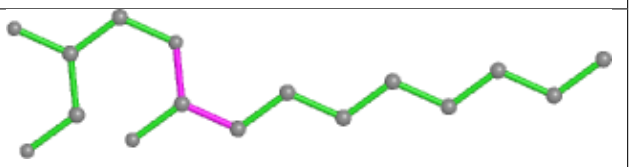


Rings

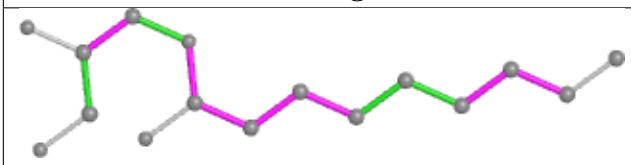
Ligand OLC A 1214



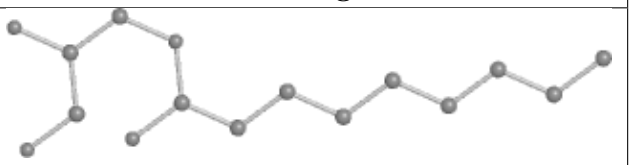
Bond lengths



Bond angles

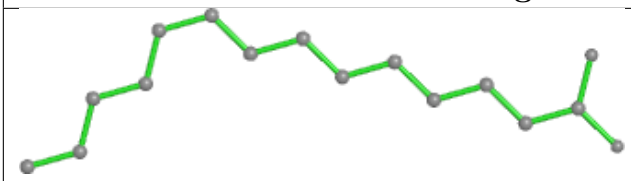


Torsions

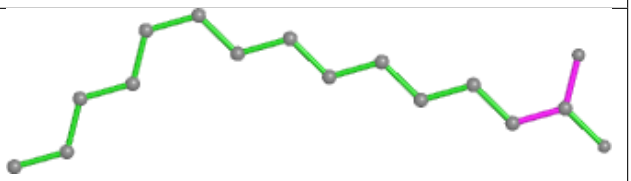


Rings

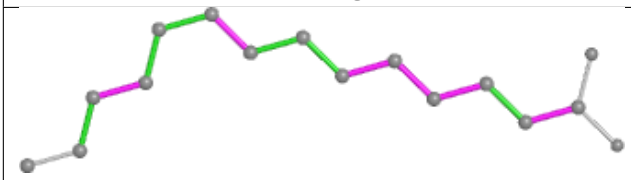
Ligand OLA A 1207



Bond lengths

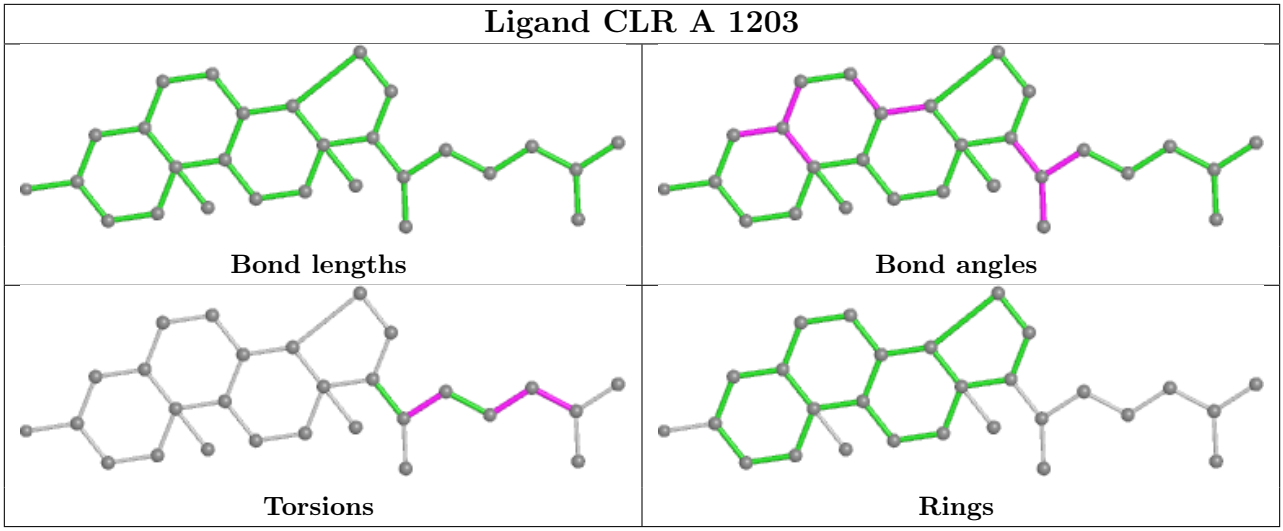


Bond angles



Torsions

Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	390/432 (90%)	0.09	15 (3%) 40 43	35, 51, 98, 148	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	ASP	5.2
1	A	1061	PHE	5.0
1	A	33	LEU	3.1
1	A	1059	LYS	3.0
1	A	1058	MET	2.9
1	A	1024	ALA	2.9
1	A	1060	ASP	2.8
1	A	92	ILE	2.4
1	A	32	TRP	2.4
1	A	1081	GLU	2.3
1	A	1080	ASN	2.3
1	A	306	HIS	2.3
1	A	1017	ILE	2.2
1	A	1092	GLU	2.1
1	A	1028	ASP	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)

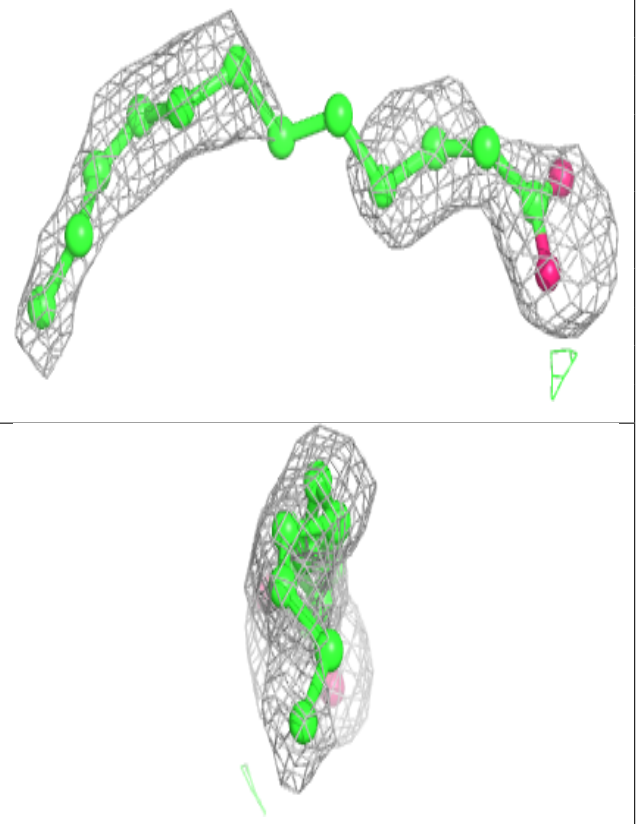
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	OLA	A	1212	14/20	0.69	0.35	69,75,79,80	0
5	OLA	A	1208	14/20	0.70	0.30	88,90,95,96	0
6	OLC	A	1214	16/25	0.76	0.26	124,126,127,127	0
5	OLA	A	1210	11/20	0.77	0.27	81,84,90,90	0
6	OLC	A	1213	19/25	0.78	0.23	63,71,82,83	0
6	OLC	A	1216	14/25	0.80	0.17	92,94,95,95	0
4	OLB	A	1205	15/25	0.82	0.29	80,84,88,89	0
5	OLA	A	1207	16/20	0.86	0.16	66,68,72,73	0
5	OLA	A	1211	9/20	0.86	0.21	65,66,73,73	0
5	OLA	A	1209	18/20	0.86	0.20	70,75,79,80	0
5	OLA	A	1206	16/20	0.87	0.17	67,70,77,77	0
6	OLC	A	1215	17/25	0.89	0.17	73,75,80,81	0
3	CLR	A	1202	28/28	0.91	0.15	58,60,71,74	0
3	CLR	A	1203	28/28	0.92	0.17	51,54,66,67	0
3	CLR	A	1204	28/28	0.93	0.15	56,58,68,69	0
2	ZMA	A	1201	25/25	0.95	0.16	29,37,54,57	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.

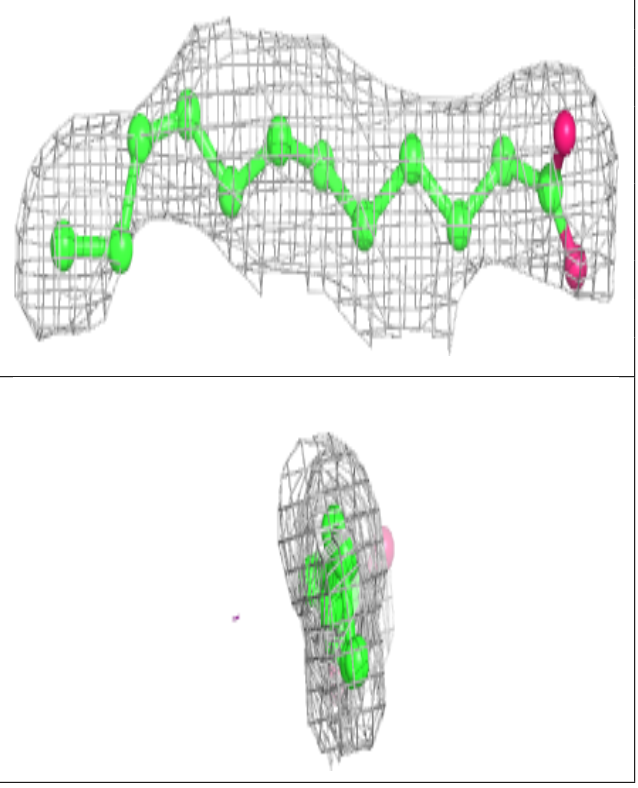
Electron density around OLA A 1212:

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



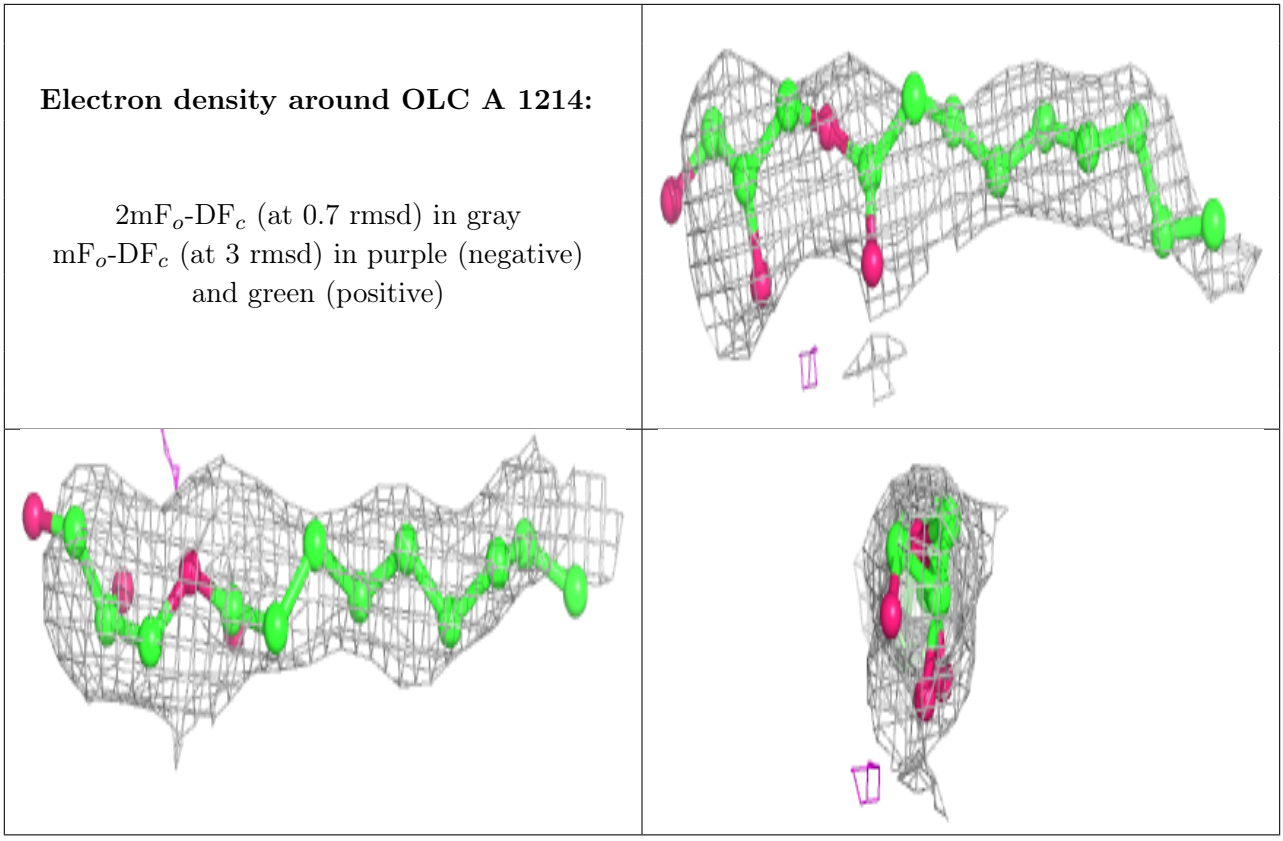
Electron density around OLA A 1208:

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



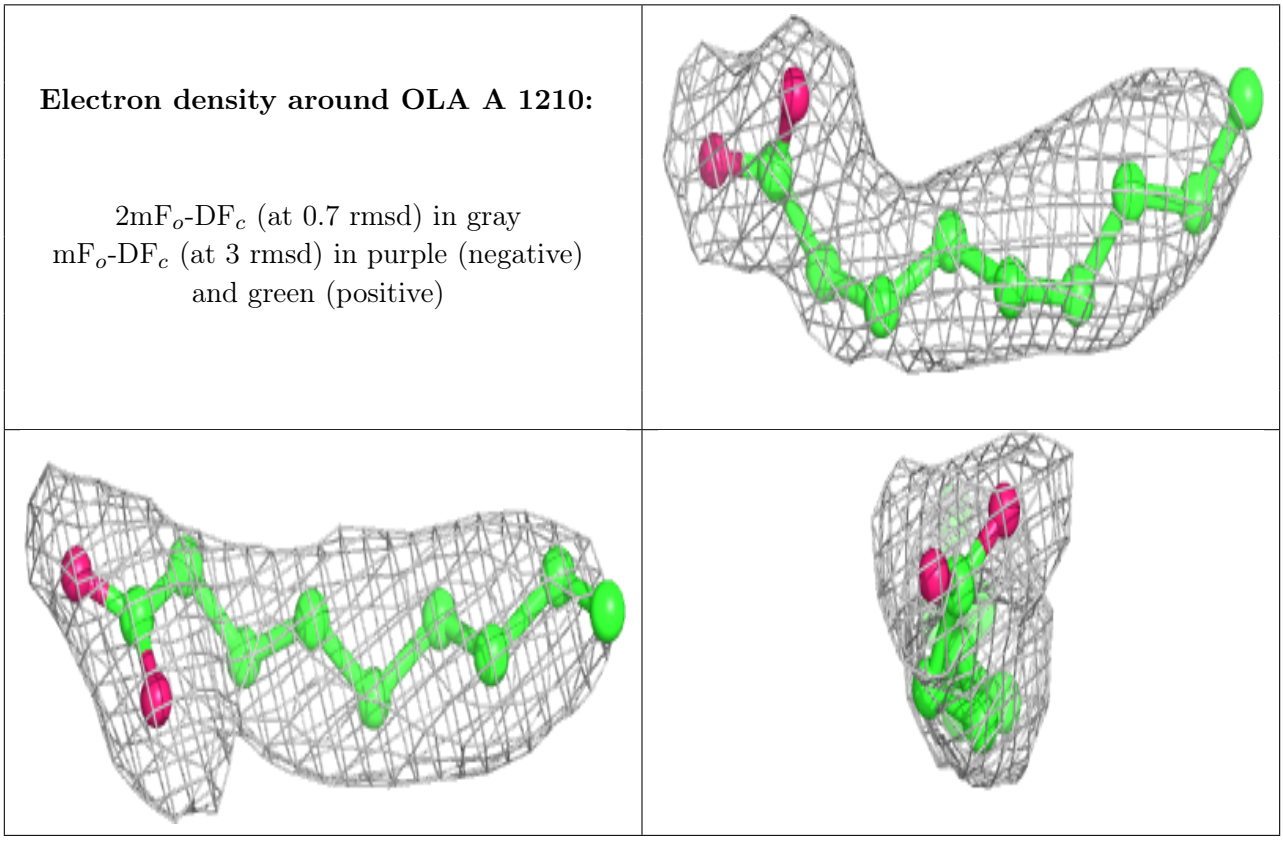
Electron density around OLC A 1214:

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



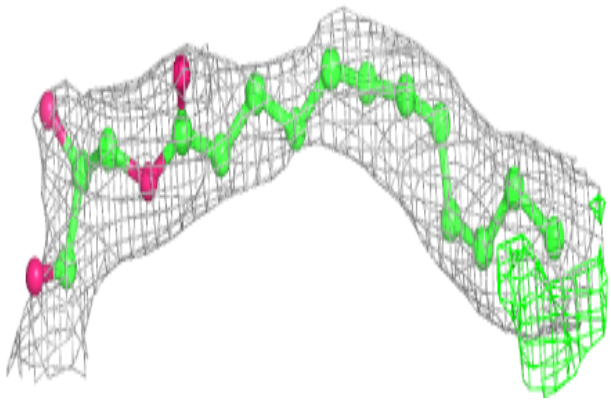
Electron density around OLA A 1210:

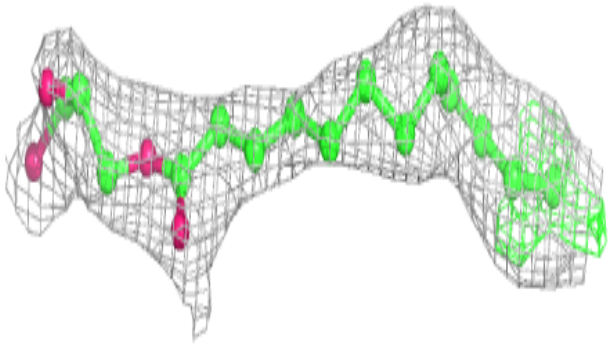
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

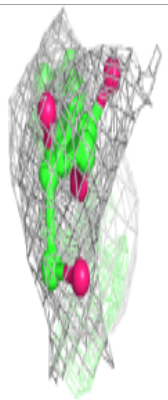


Electron density around OLC A 1213:

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

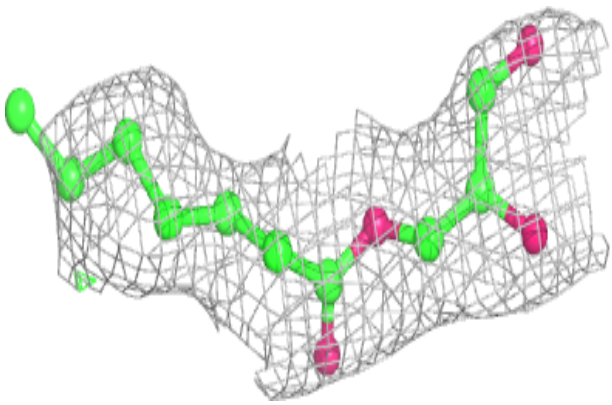


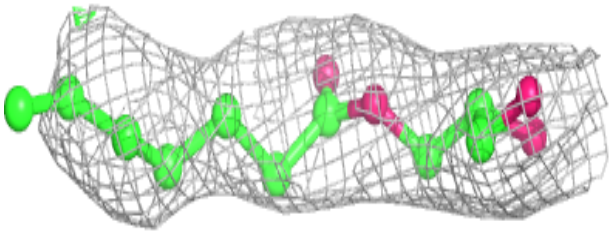


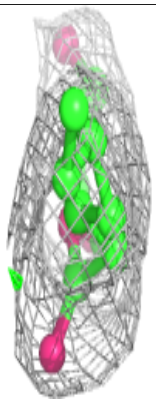


Electron density around OLC A 1216:

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

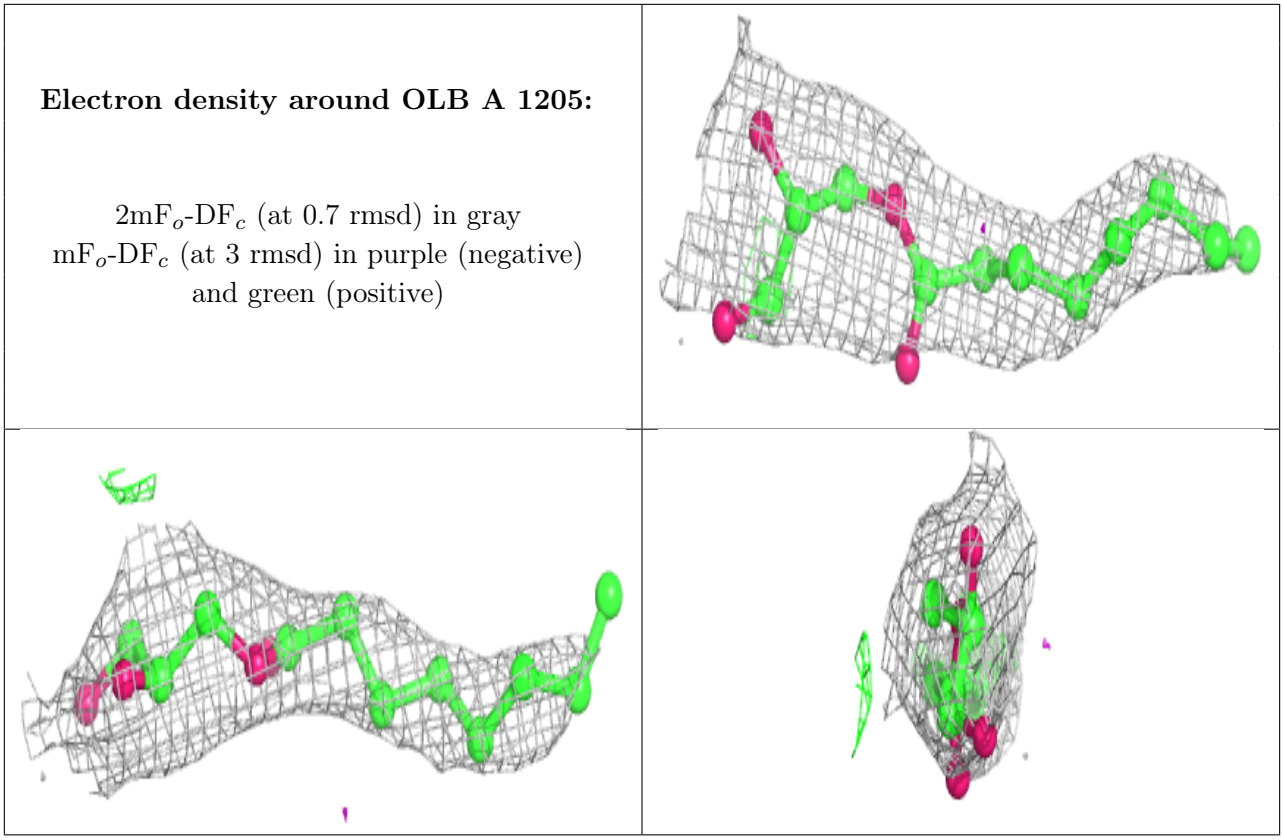






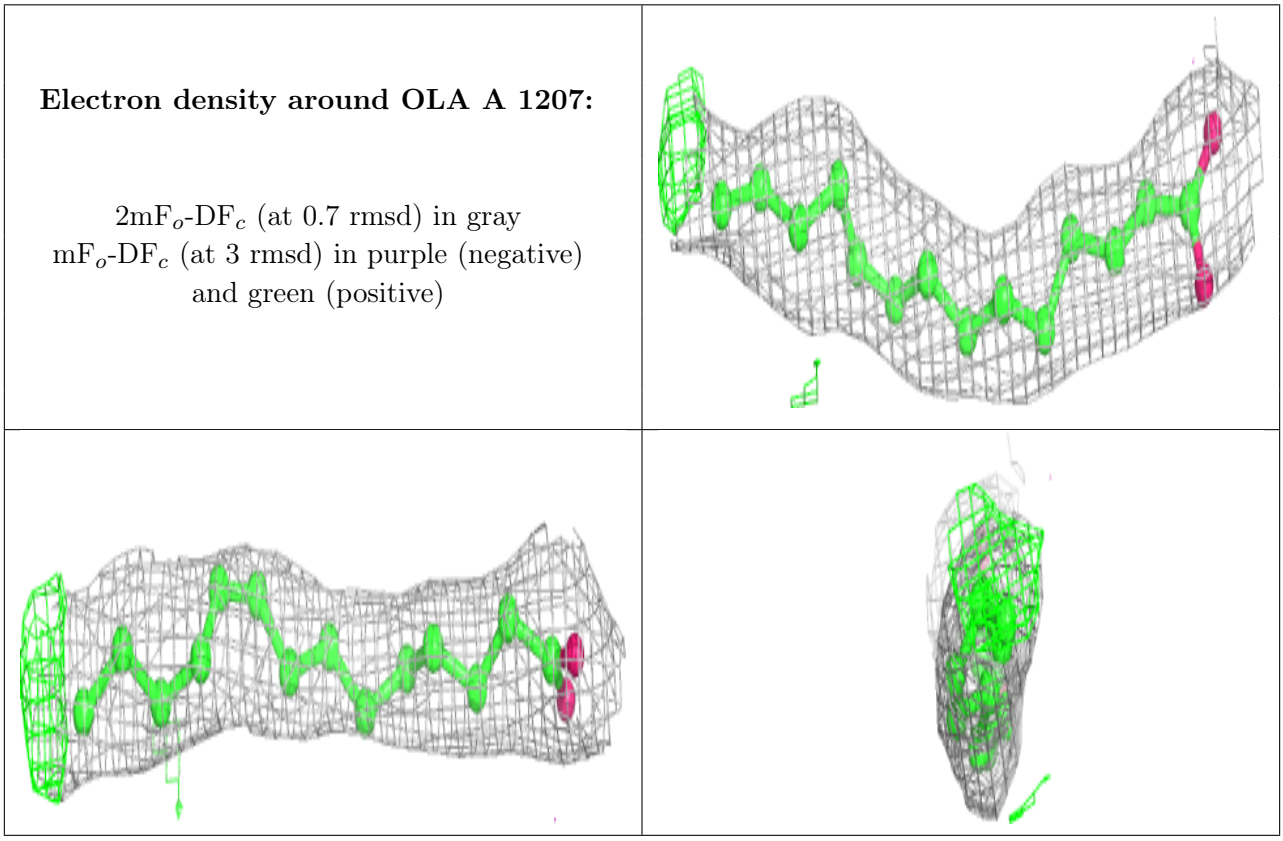
Electron density around OLB A 1205:

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



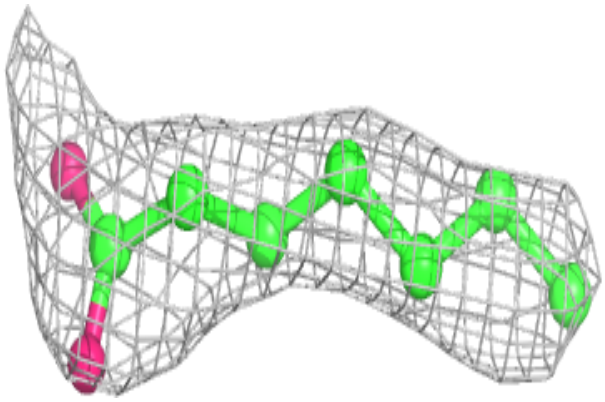
Electron density around OLA A 1207:

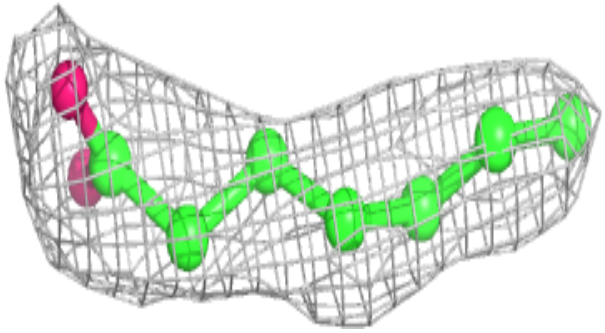
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

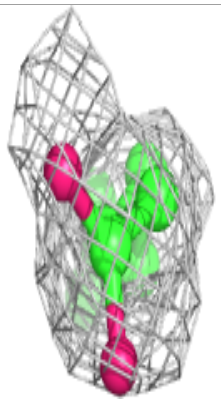


Electron density around OLA A 1211:

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

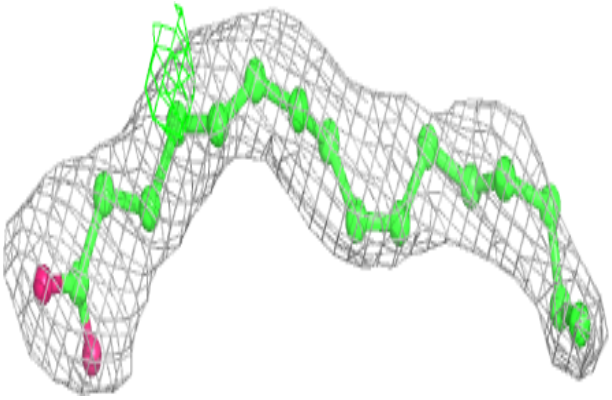


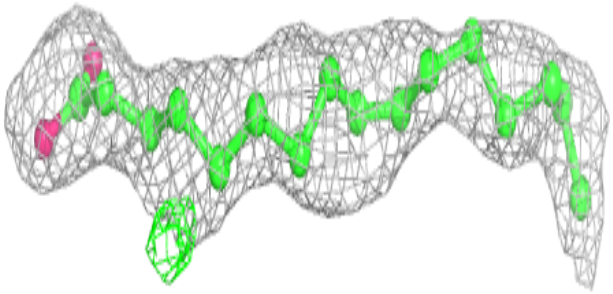


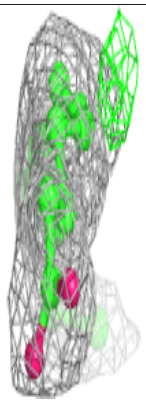


Electron density around OLA A 1209:

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

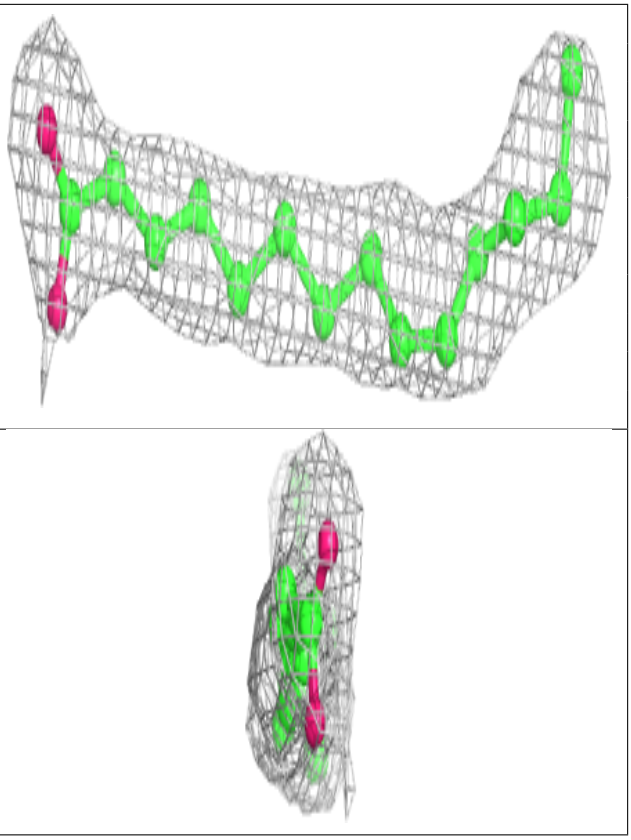


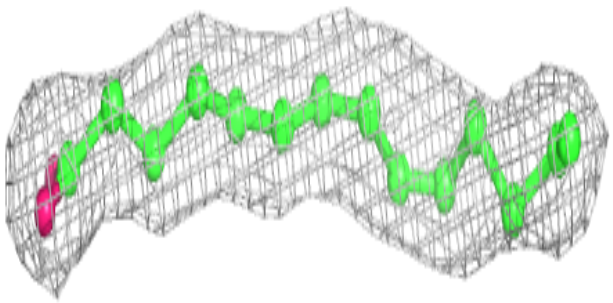




Electron density around OLA A 1206:

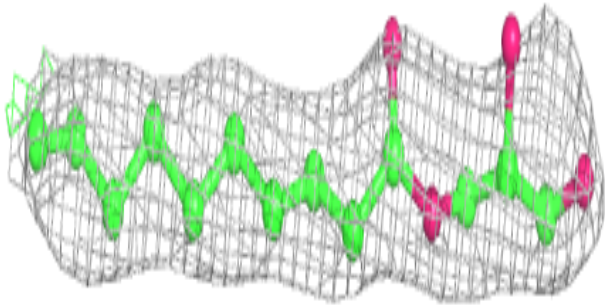
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

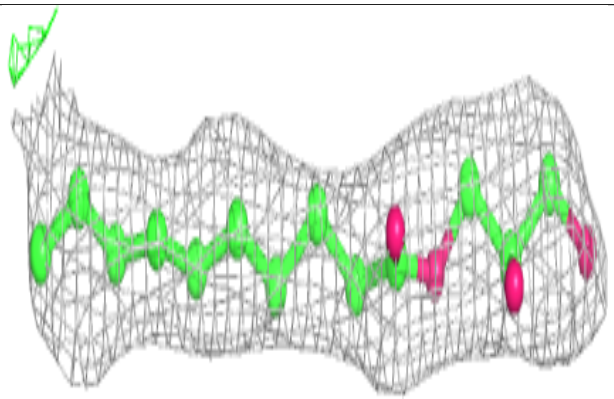


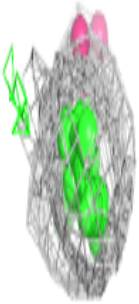


Electron density around OLC A 1215:

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

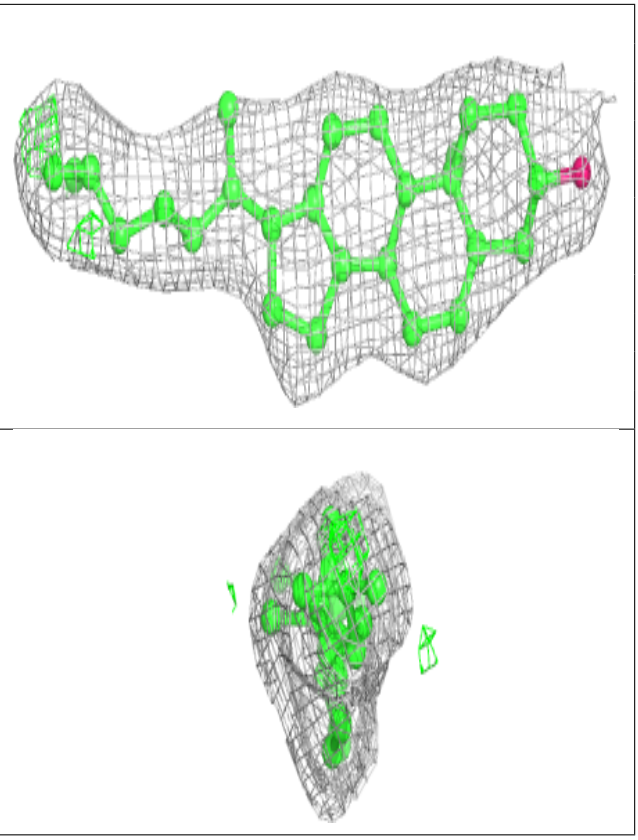






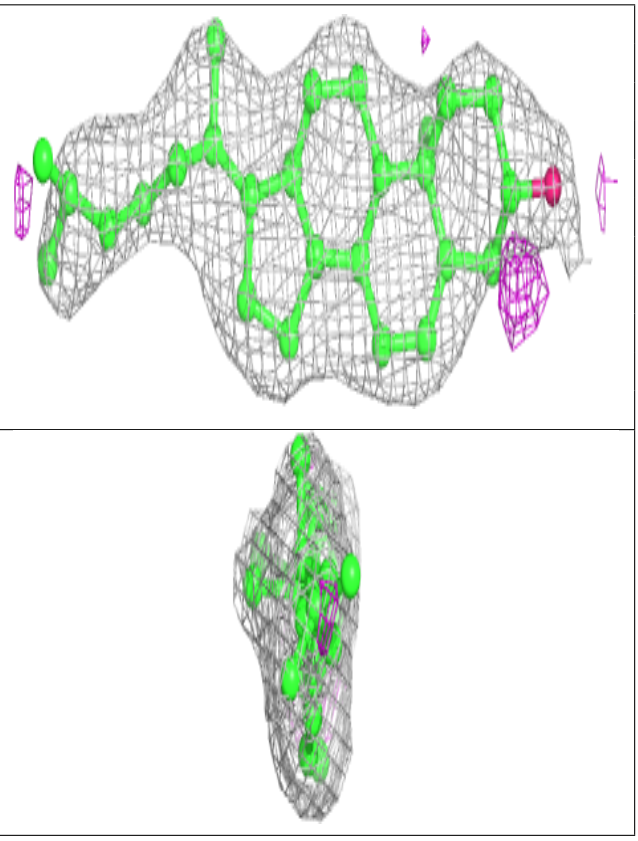
Electron density around CLR A 1202:

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



Electron density around 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 1204:

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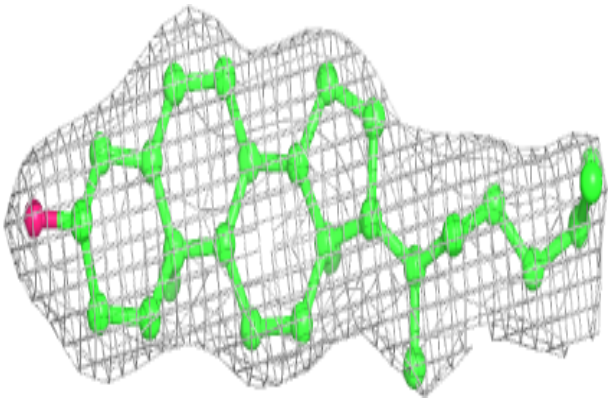
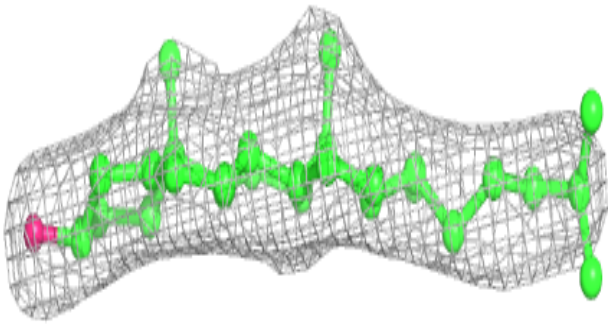
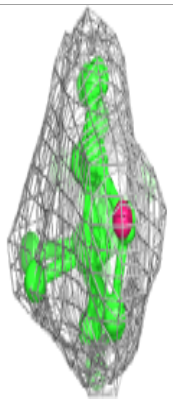
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

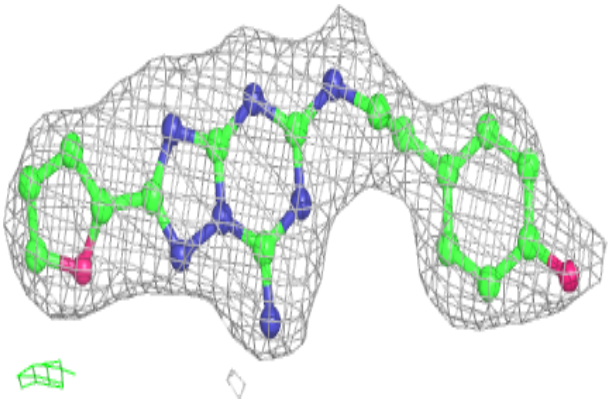


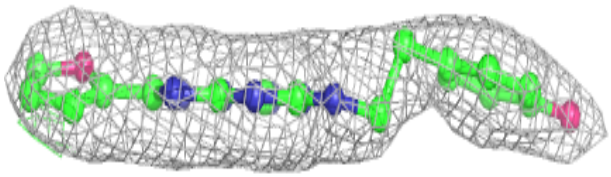


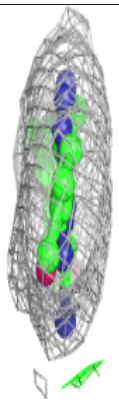


Electron density around ZMA A 1201:

$2mF_o$-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.