wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2020 – 05:31 PM BST

PDB ID	:	6ZDR
Title	:	Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with Chromone 4d
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	:	1.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (i)) were used in the production of this report:

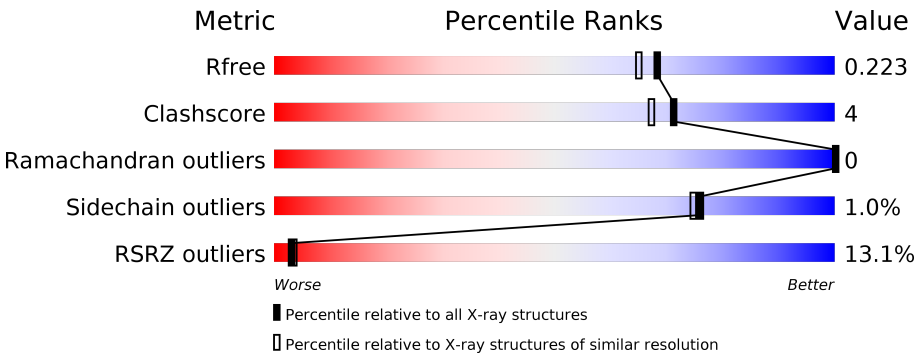
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

1 Overall quality at a glance (i)

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

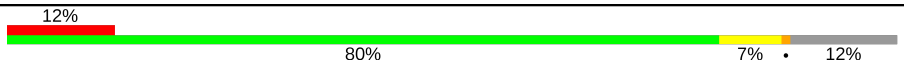
The reported resolution of this entry is 1.92 Å.

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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	433	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3426 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	383	2995	1956	506	512	21	0	6	0

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	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274

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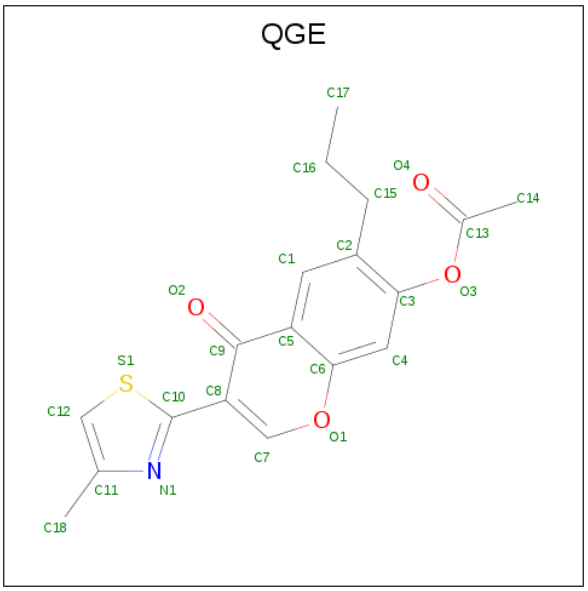
Chain	Residue	Modelled	Actual	Comment	Reference
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is [3-(4-methyl-1,3-thiazol-2-yl)-4-oxidanylidene-6-propyl-chromen-7-yl] ethanoate (three-letter code: QGE) (formula: $C_{18}H_{17}NO_4S$) (labeled as "Ligand of Interest" by author).

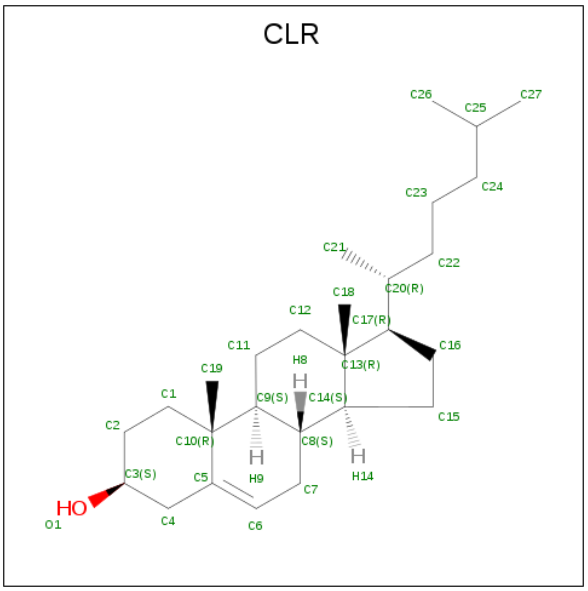


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	24	18	1	4	1	0	0

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

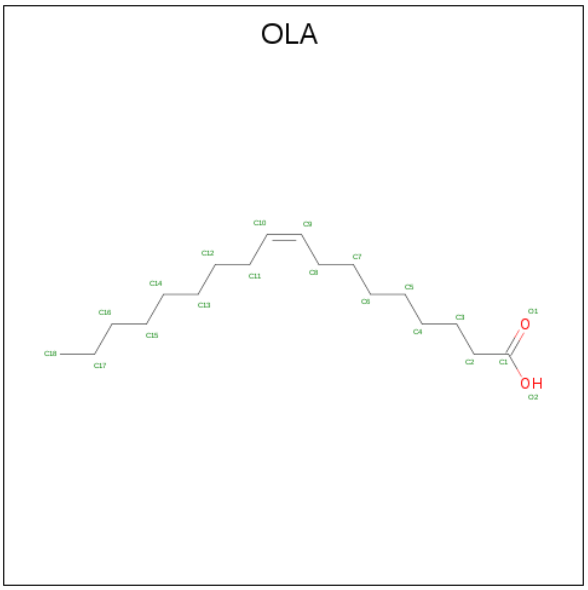
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	15	13	2	0	0

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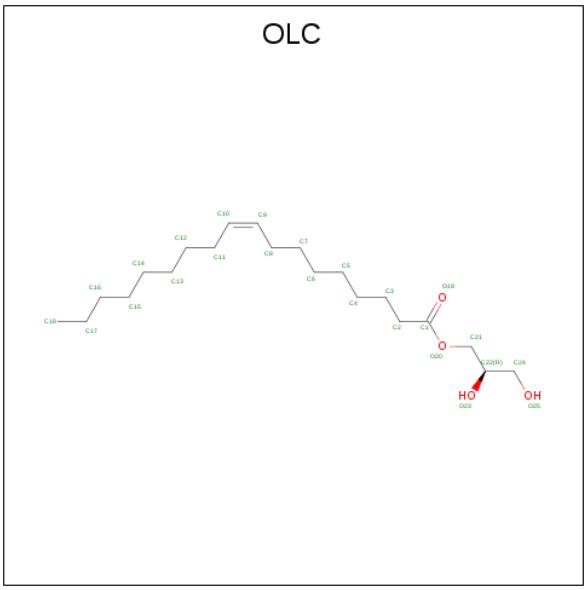
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 5 5	0	0
5	A	1	Total C O 14 12 2	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 16 16	0	0
5	A	1	Total C O 12 10 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C 9 9	0	0

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 19 15 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	20	16	4	0	0
			Total	C	O		
6	A	1	18	14	4	0	0
			Total	C	O		
6	A	1	25	21	4	0	0

- Molecule 7 is water.

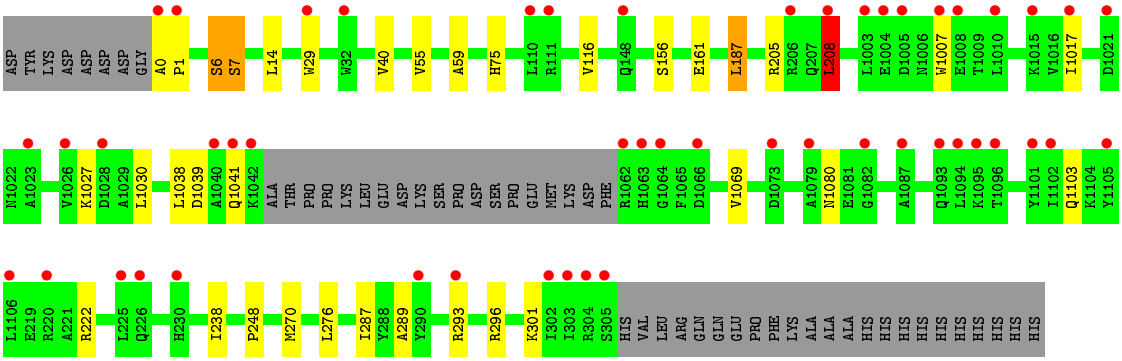
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	104	104	104	0	0

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	39.26Å 180.23Å 140.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.06 – 1.92 45.06 – 1.92	Depositor EDS
% Data completeness (in resolution range)	84.4 (45.06-1.92) 84.3 (45.06-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.92Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.208 , 0.218 0.214 , 0.223	Depositor DCC
R_{free} test set	1636 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3426	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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: OLA, QGE, OLC, CLR, 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	1.12	0/3079	0.85	21/4190 (0.5%)

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

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	LEU	O-C-N	-8.73	108.74	122.70
1	A	29[A]	TRP	CA-C-O	6.52	133.79	120.10
1	A	29[B]	TRP	CA-C-O	6.52	133.79	120.10
1	A	75[A]	HIS	CA-C-O	6.34	133.42	120.10
1	A	75[B]	HIS	CA-C-O	6.34	133.42	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	6[A]	SER	Mainchain
1	A	6[B]	SER	Mainchain
1	A	7[B]	SER	Mainchain

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	2995	0	3080	22	0
2	A	24	0	0	1	0
3	A	1	0	0	0	0
4	A	84	0	138	1	0
5	A	136	0	193	2	0
6	A	82	0	111	1	0
7	A	104	0	0	0	0
All	All	3426	0	3522	24	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 4.

The worst 5 of 24 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:301:LYS:HB3	1:A:301:LYS:NZ	1.97	0.80
1:A:270:MET:HG3	2:A:1201:QGE:C14	2.13	0.77
1:A:1027:LYS:HE3	1:A:1080:ASN:OD1	1.87	0.74
1:A:1041:GLN:HG2	1:A:1041:GLN:O	1.94	0.66
1:A:1038:LEU:HD21	1:A:1069:VAL:HG21	1.84	0.59

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	385/433 (89%)	383 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/353 (89%)	311 (99%)	3 (1%)	76	75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	SER
1	A	161	GLU
1	A	1039	ASP

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

Mol	Chain	Res	Type
1	A	1025	GLN
1	A	1041	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	OLC	A	1211	-	18,18,24	0.99	1 (5%)	18,19,25	1.28	2 (11%)
5	OLA	A	1215	-	16,19,19	0.28	0	15,19,19	0.57	0
5	OLA	A	1219	-	7,10,19	0.26	0	6,10,19	0.60	0
5	OLA	A	1206	-	11,14,19	0.25	0	10,14,19	0.51	0
5	OLA	A	1218	-	11,14,19	0.27	0	10,14,19	0.52	0
2	QGE	A	1201	-	19,26,26	1.11	1 (5%)	21,37,37	1.91	5 (23%)
5	OLA	A	1210	-	14,14,19	0.27	0	12,12,19	0.45	0
5	OLA	A	1214	-	8,11,19	0.27	0	7,11,19	0.96	0
6	OLC	A	1212	-	18,18,24	1.11	1 (5%)	18,18,25	1.15	2 (11%)
4	CLR	A	1205	-	31,31,31	0.62	0	48,48,48	1.26	6 (12%)
5	OLA	A	1207	-	4,4,19	0.26	0	3,3,19	0.43	0
5	OLA	A	1220	-	8,8,19	0.20	0	7,7,19	0.57	0
5	OLA	A	1208	-	10,13,19	0.33	0	8,13,19	0.50	0
6	OLC	A	1213	-	17,17,24	1.14	1 (5%)	18,18,25	1.14	2 (11%)
5	OLA	A	1217	-	7,10,19	0.24	0	6,10,19	0.59	0
6	OLC	A	1216	-	24,24,24	0.97	1 (4%)	25,25,25	0.87	2 (8%)
4	CLR	A	1204	-	31,31,31	0.67	0	48,48,48	1.04	1 (2%)
4	CLR	A	1203	-	31,31,31	0.61	0	48,48,48	1.10	4 (8%)
5	OLA	A	1209	-	7,7,19	0.24	0	6,6,19	0.48	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	OLC	A	1211	-	-	5/18/18/24	-
5	OLA	A	1215	-	-	3/15/17/17	-
5	OLA	A	1219	-	-	1/6/8/17	-
5	OLA	A	1206	-	-	6/10/12/17	-
5	OLA	A	1218	-	-	2/10/12/17	-
2	QGE	A	1201	-	-	5/7/11/11	0/3/3/3
5	OLA	A	1210	-	-	3/10/10/17	-
5	OLA	A	1214	-	-	1/7/9/17	-
6	OLC	A	1212	-	-	6/17/17/24	-
4	CLR	A	1205	-	-	0/10/68/68	0/4/4/4
5	OLA	A	1207	-	-	0/2/2/17	-
5	OLA	A	1220	-	-	1/6/6/17	-
5	OLA	A	1208	-	-	2/9/11/17	-
6	OLC	A	1213	-	-	6/17/17/24	-
5	OLA	A	1217	-	-	1/6/8/17	-
6	OLC	A	1216	-	-	6/24/24/24	-
4	CLR	A	1204	-	-	0/10/68/68	0/4/4/4
4	CLR	A	1203	-	-	0/10/68/68	0/4/4/4
5	OLA	A	1209	-	-	3/5/5/17	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1216	OLC	O20-C1	4.52	1.46	1.33
6	A	1212	OLC	O20-C1	4.45	1.46	1.33
6	A	1213	OLC	O20-C1	4.39	1.46	1.33
6	A	1211	OLC	O20-C1	3.84	1.44	1.33
2	A	1201	QGE	C5-C6	-3.14	1.37	1.41

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	QGE	C1-C5-C6	4.12	121.03	116.39
2	A	1201	QGE	C4-C6-C5	-4.00	118.62	123.05
2	A	1201	QGE	O1-C6-C5	3.74	124.82	121.20
4	A	1205	CLR	C4-C5-C6	-3.72	115.24	120.61
6	A	1211	OLC	O20-C1-C2	3.41	122.61	111.91

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1219	OLA	C1-C2-C3-C4
5	A	1206	OLA	C1-C2-C3-C4
6	A	1212	OLC	C21-C22-C24-O25
5	A	1208	OLA	C9-C10-C11-C12
6	A	1213	OLC	O20-C21-C22-C24

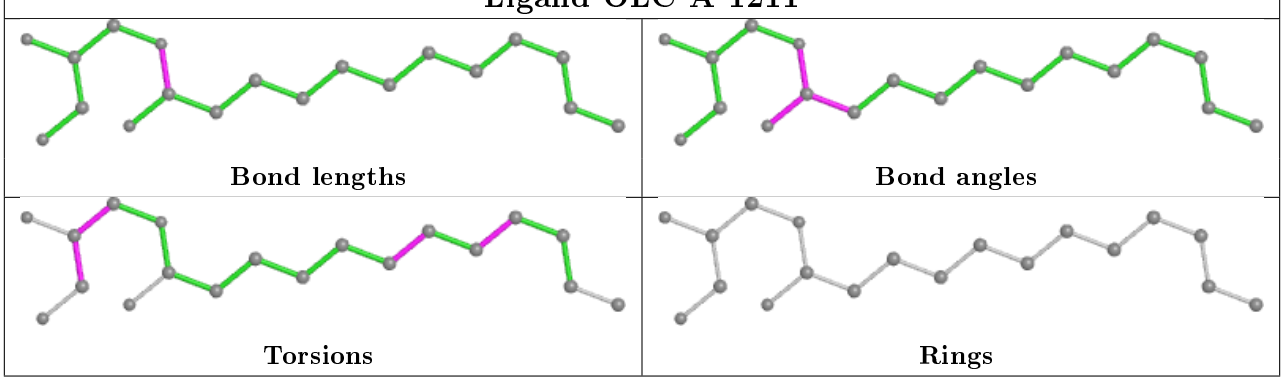
There are no ring outliers.

6 monomers are involved in 4 short contacts:

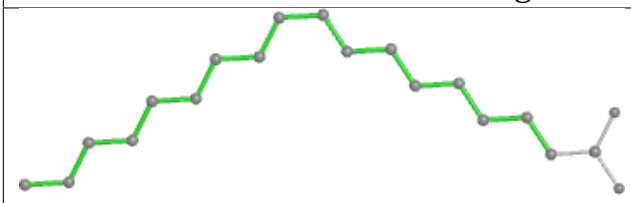
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1211	OLC	1	0
5	A	1215	OLA	1	0
2	A	1201	QGE	1	0
5	A	1214	OLA	1	0
4	A	1205	CLR	1	0
5	A	1220	OLA	1	0

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

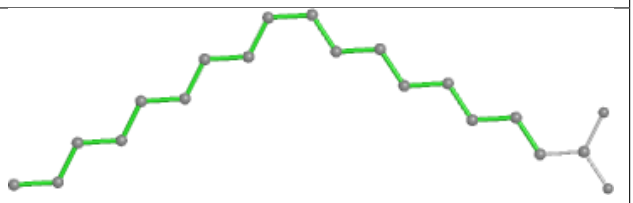
Ligand OLC A 1211



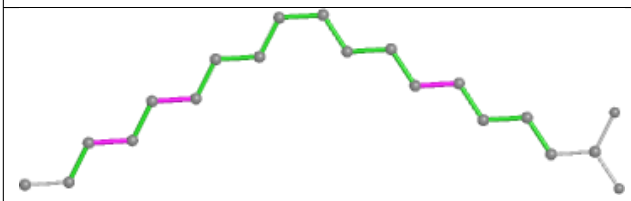
Ligand OLA A 1215



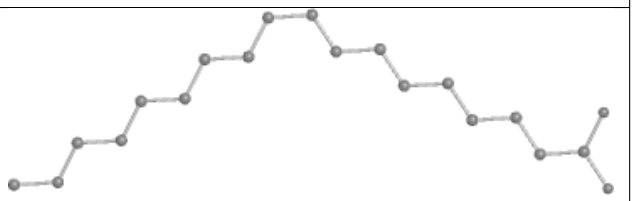
Bond lengths



Bond angles

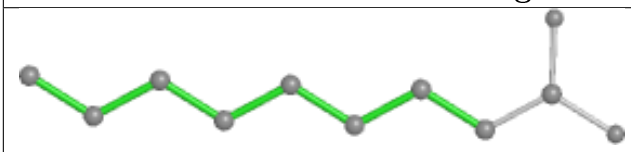


Torsions

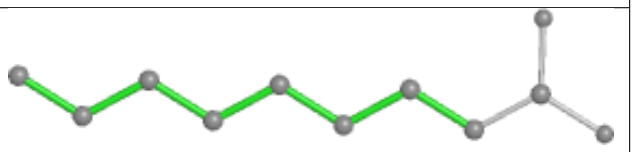


Rings

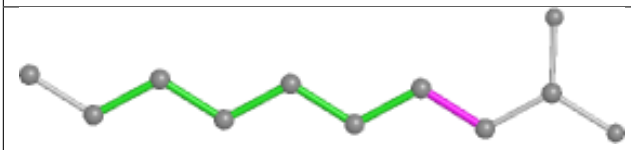
Ligand OLA A 1219



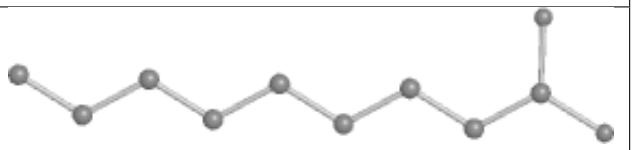
Bond lengths



Bond angles

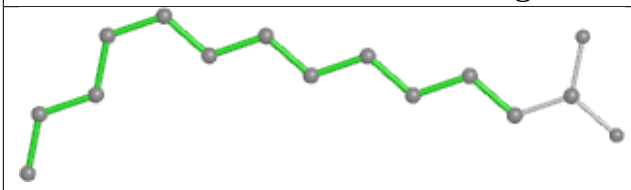


Torsions

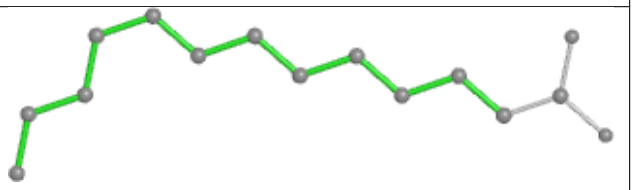


Rings

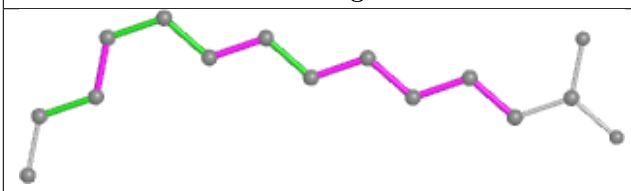
Ligand OLA A 1206



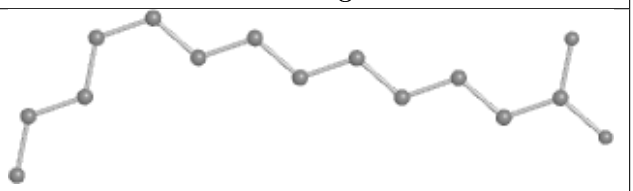
Bond lengths



Bond angles

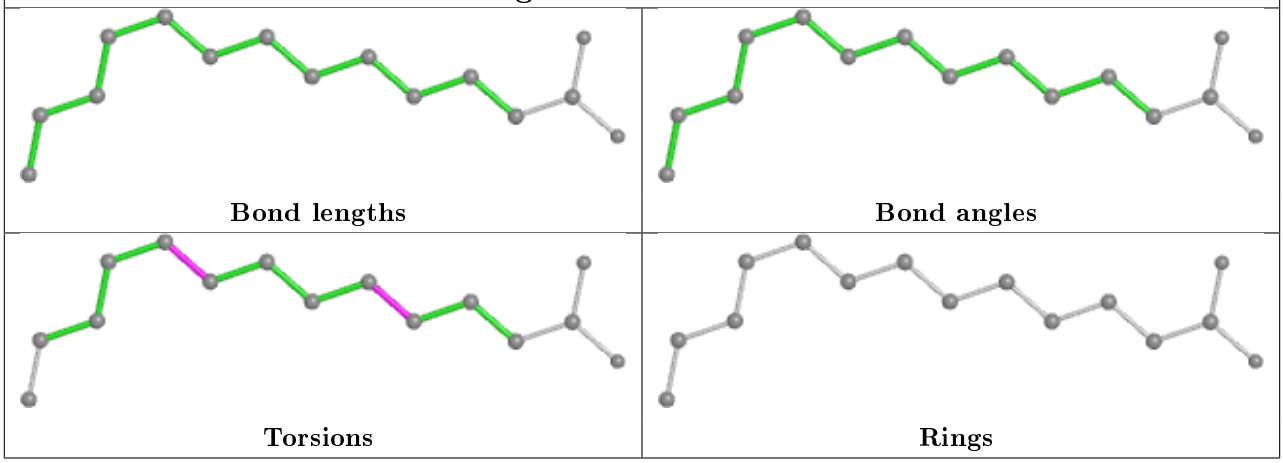


Torsions

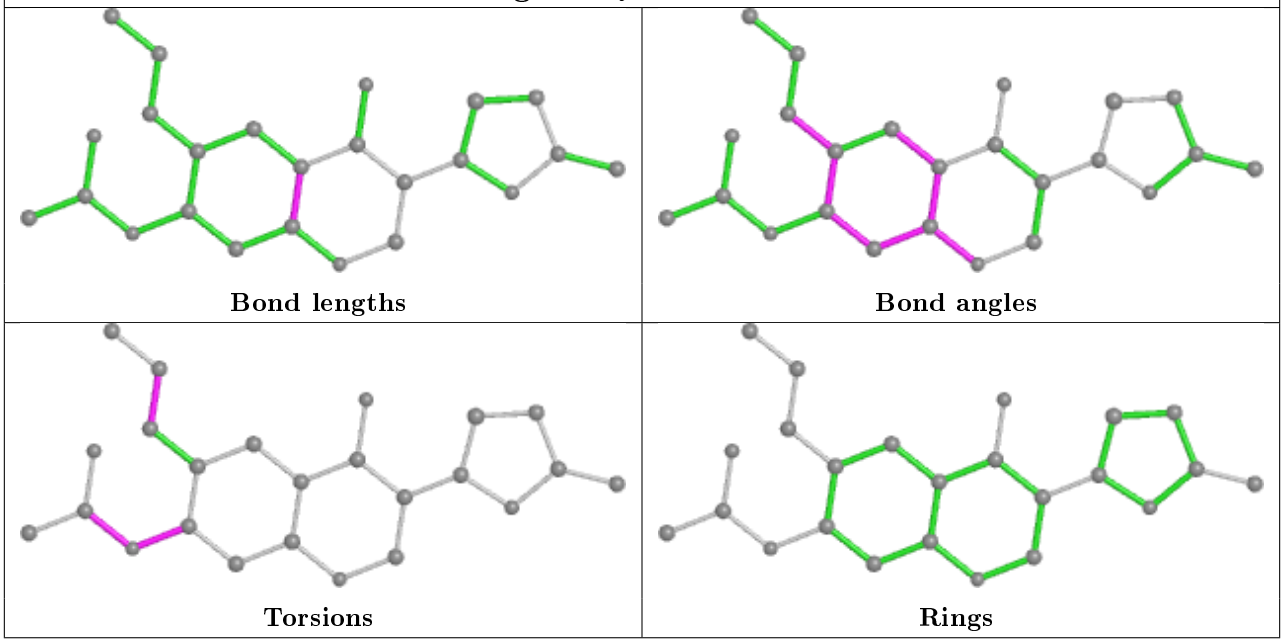


Rings

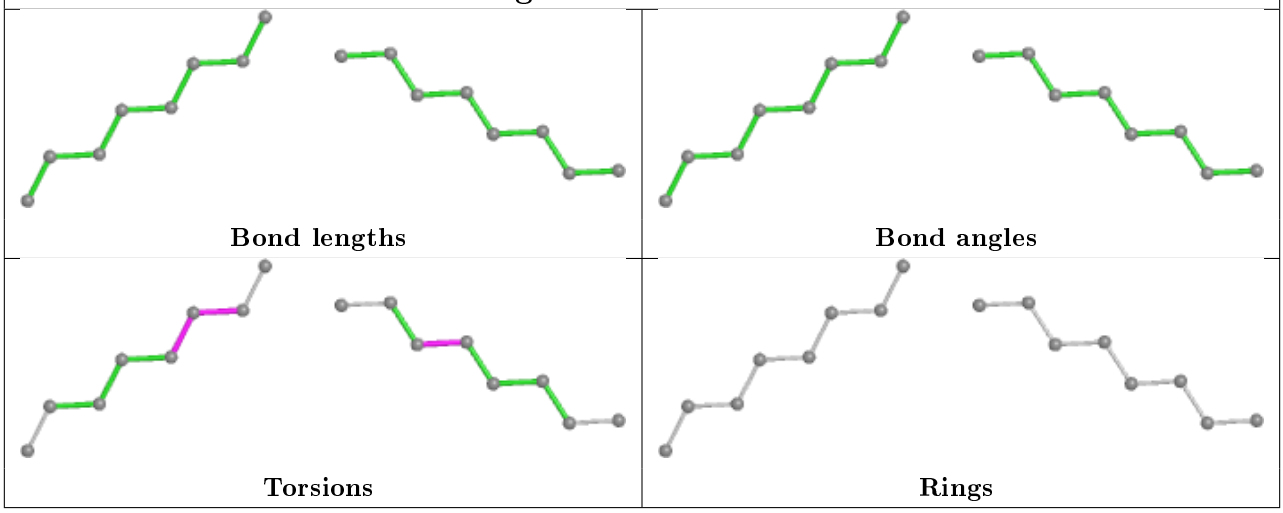
Ligand OLA A 1218



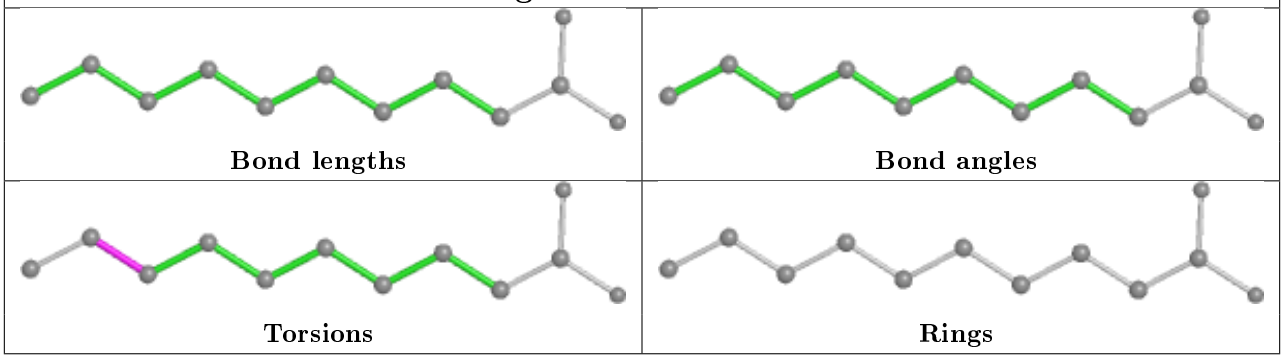
Ligand QGE A 1201



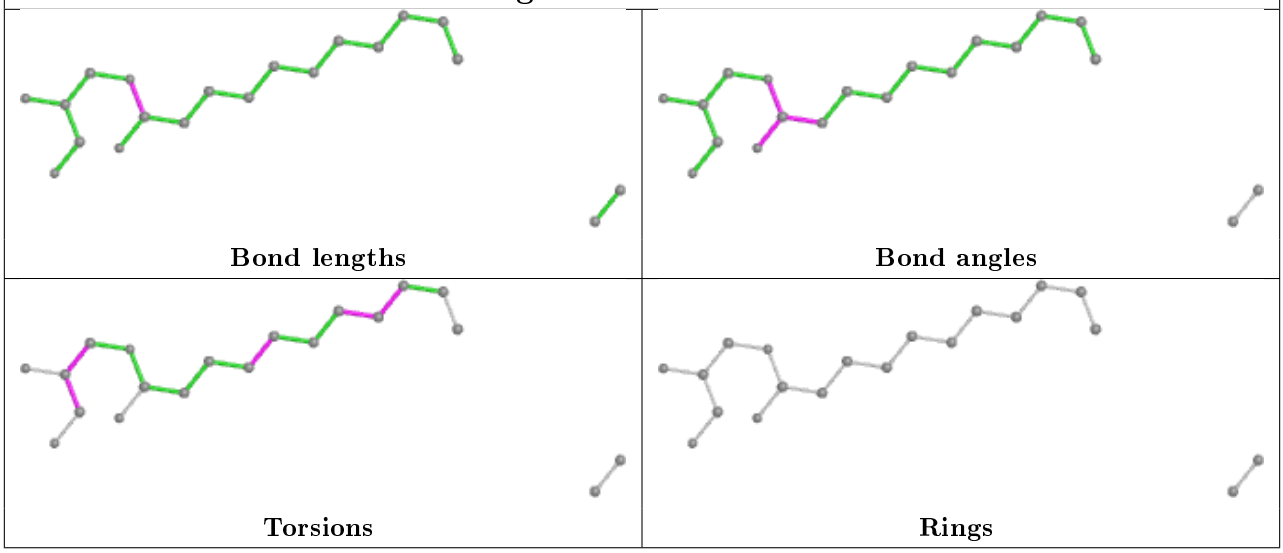
Ligand OLA A 1210



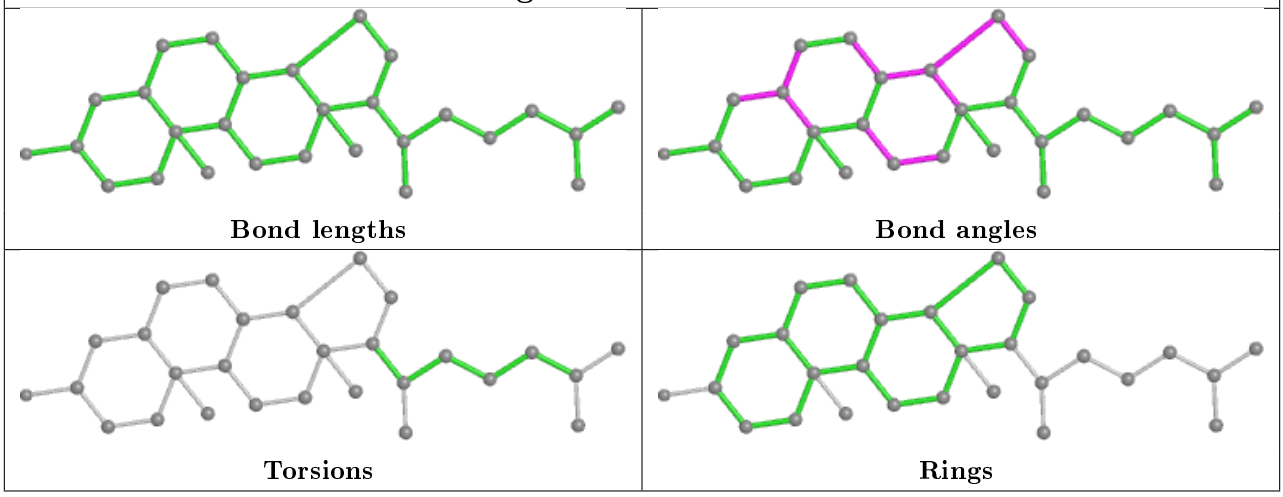
Ligand OLA A 1214



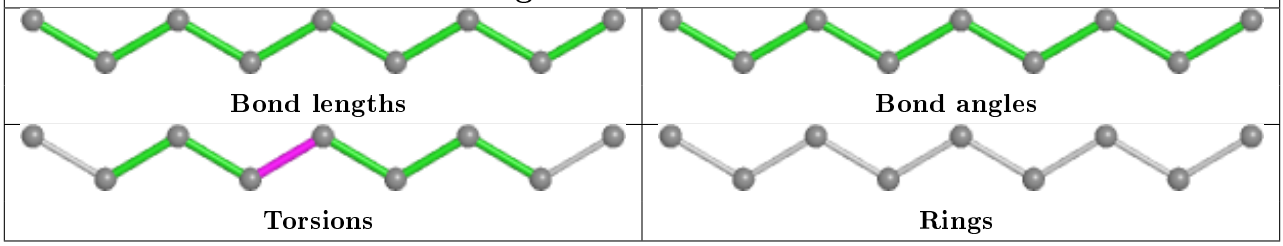
Ligand OLC A 1212



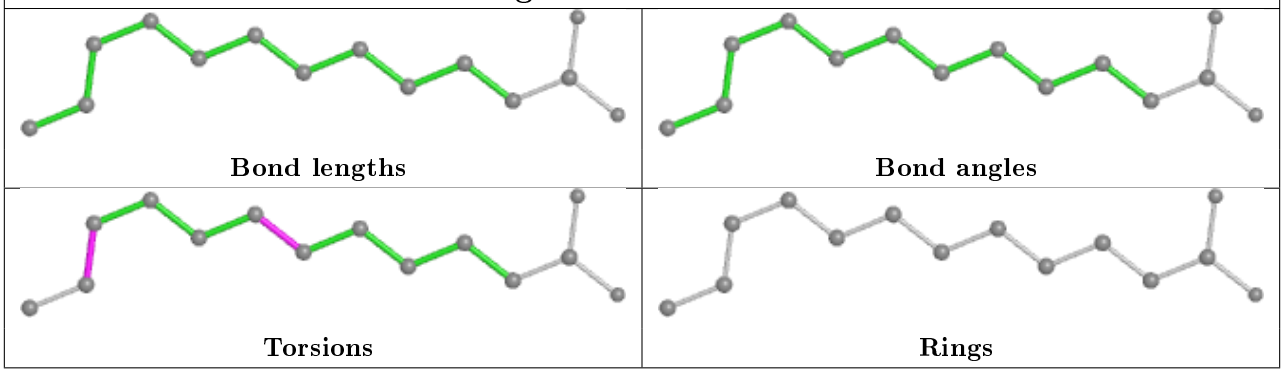
Ligand CLR A 1205



Ligand OLA A 1220

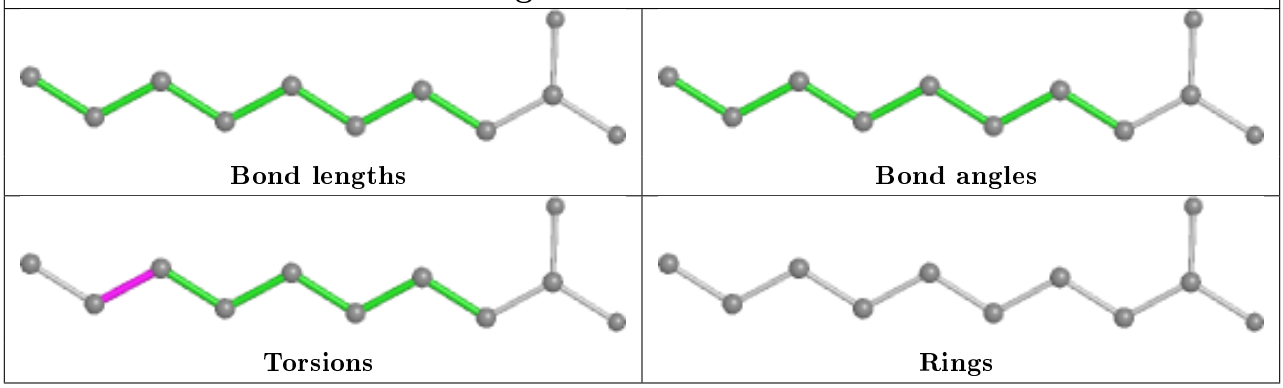


Ligand OLA A 1208

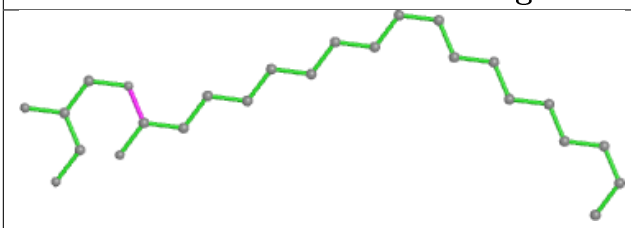


Ligand OLC A 1213

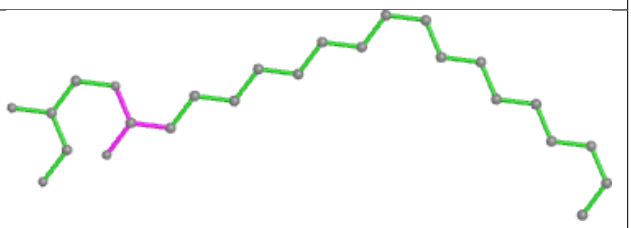
Ligand OLA A 1217



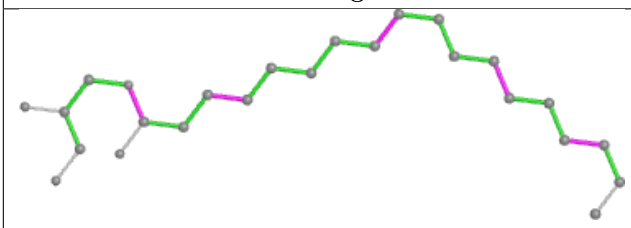
Ligand OLC A 1216



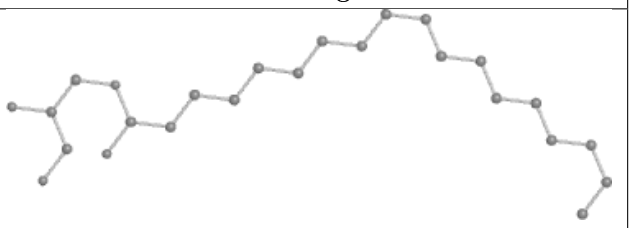
Bond lengths



Bond angles

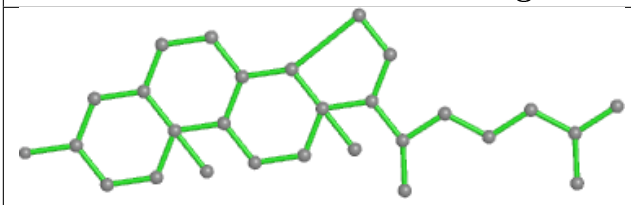


Torsions

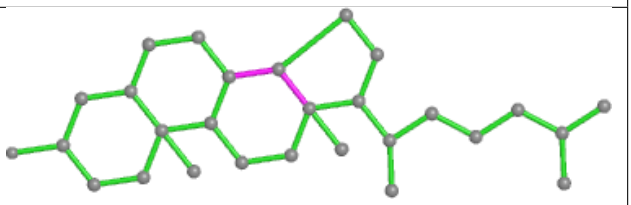


Rings

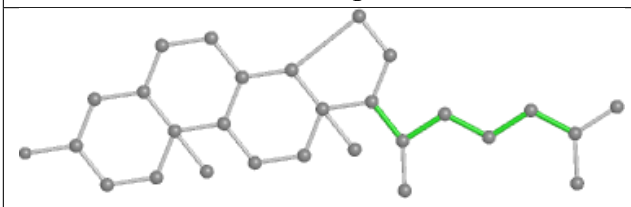
Ligand CLR A 1204



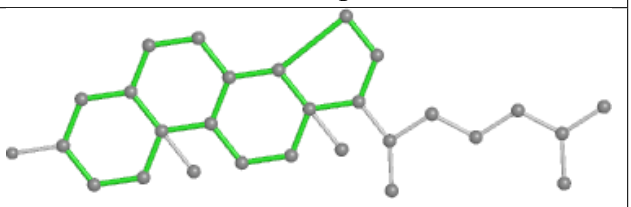
Bond lengths



Bond angles

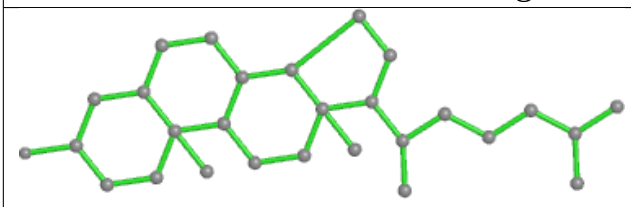


Torsions

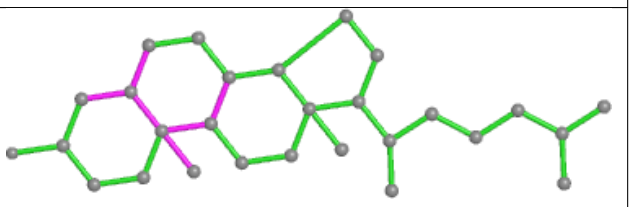


Rings

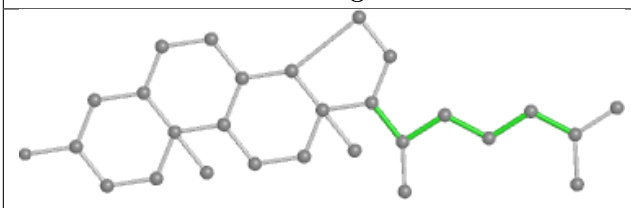
Ligand CLR A 1203



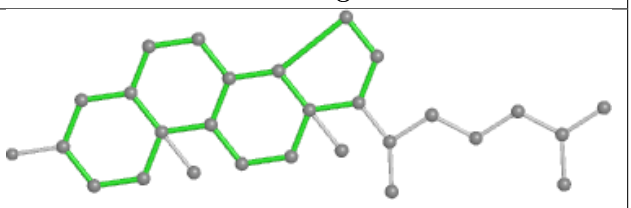
Bond lengths



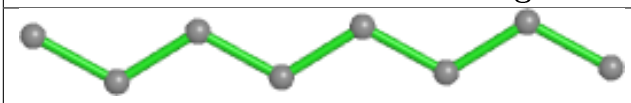
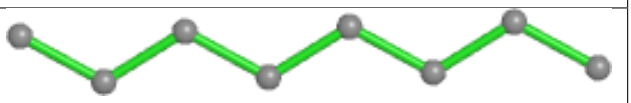
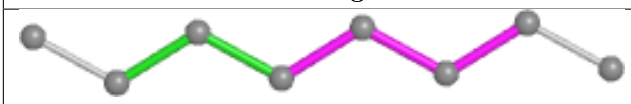
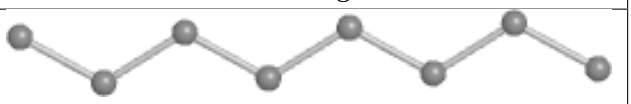
Bond angles



Torsions



Rings

Ligand OLA A 1209	
 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	383/433 (88%)	0.65	50 (13%) 3 3	16, 40, 94, 143	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1063	HIS	8.1
1	A	290	TYR	5.0
1	A	1062	ARG	4.4
1	A	208	LEU	4.4
1	A	1105	TYR	4.0

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	1217	11/20	0.57	0.29	55,56,60,60	0
5	OLA	A	1219	11/20	0.63	0.19	52,54,57,57	0

Continued on next page...

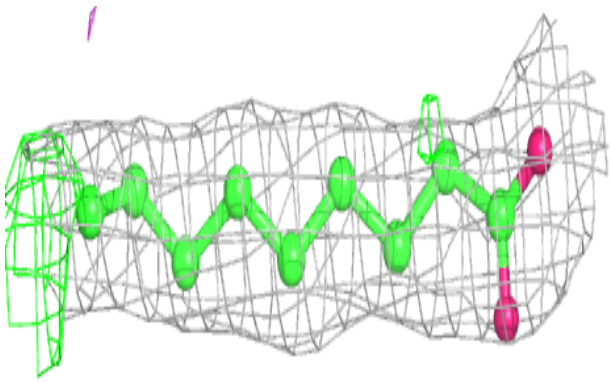
Continued from previous page...

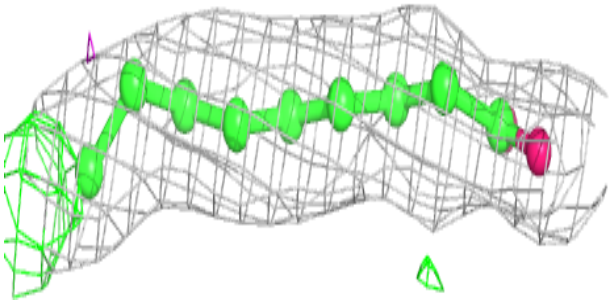
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OLC	A	1216	25/25	0.63	0.27	60,62,67,68	0
5	OLA	A	1208	14/20	0.64	0.21	68,70,72,72	0
6	OLC	A	1212	20/25	0.66	0.24	43,57,62,62	0
5	OLA	A	1218	15/20	0.66	0.22	60,60,65,65	0
5	OLA	A	1215	20/20	0.68	0.26	56,57,60,60	0
6	OLC	A	1211	19/25	0.74	0.24	52,54,56,56	0
5	OLA	A	1206	15/20	0.77	0.18	61,62,64,65	0
6	OLC	A	1213	18/25	0.80	0.20	47,50,56,56	0
5	OLA	A	1209	8/20	0.83	0.17	46,48,49,49	0
5	OLA	A	1210	16/20	0.86	0.18	50,50,58,59	0
5	OLA	A	1214	12/20	0.88	0.23	48,50,53,53	0
5	OLA	A	1207	5/20	0.89	0.19	45,45,46,46	0
2	QGE	A	1201	24/24	0.89	0.20	27,32,45,47	0
5	OLA	A	1220	9/20	0.91	0.20	51,51,52,52	0
4	CLR	A	1205	28/28	0.92	0.15	31,32,39,40	0
4	CLR	A	1203	28/28	0.93	0.12	36,37,42,43	0
4	CLR	A	1204	28/28	0.94	0.11	28,30,41,42	0
3	NA	A	1202	1/1	0.98	0.13	41,41,41,41	0

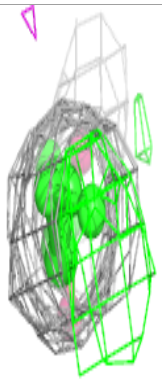
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1217:

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

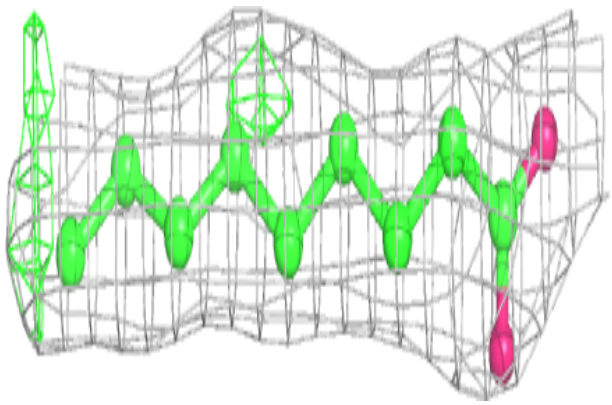


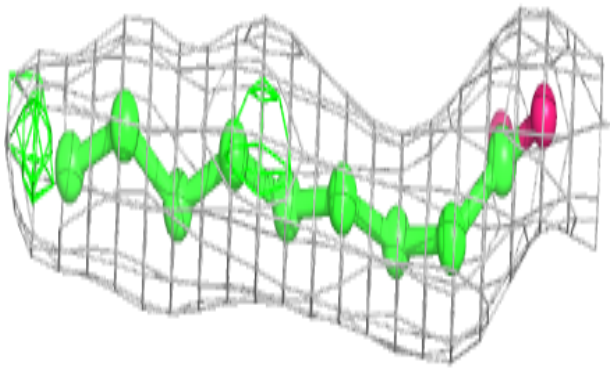


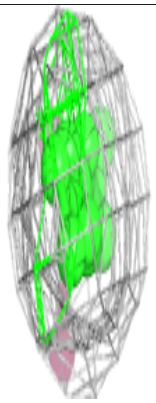


Electron density around OLA A 1219:

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

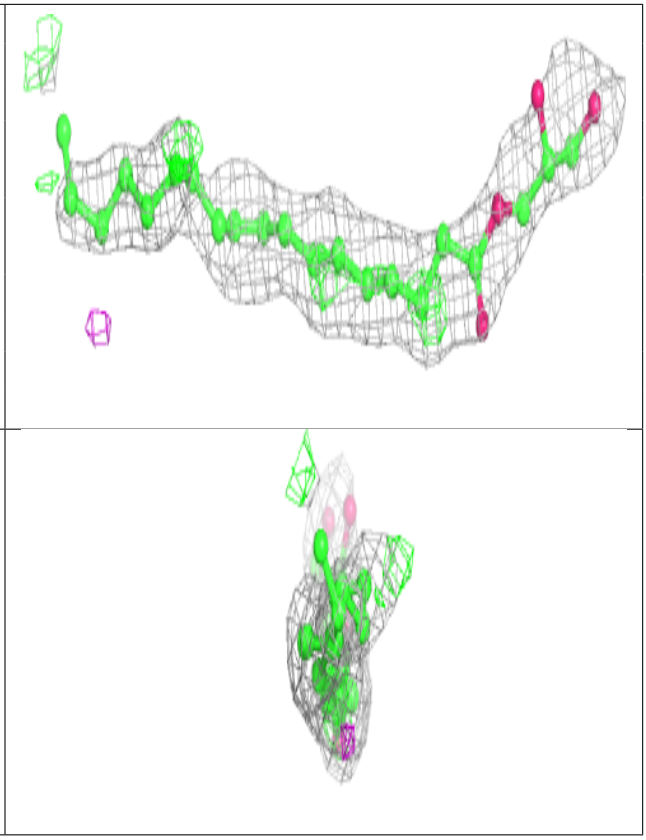






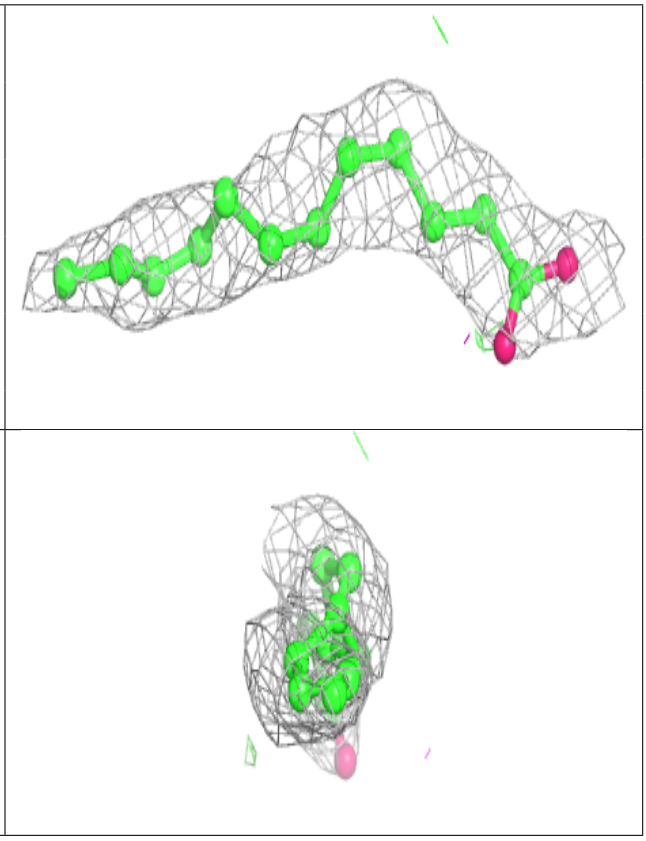
Electron density around OLC A 1216:

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



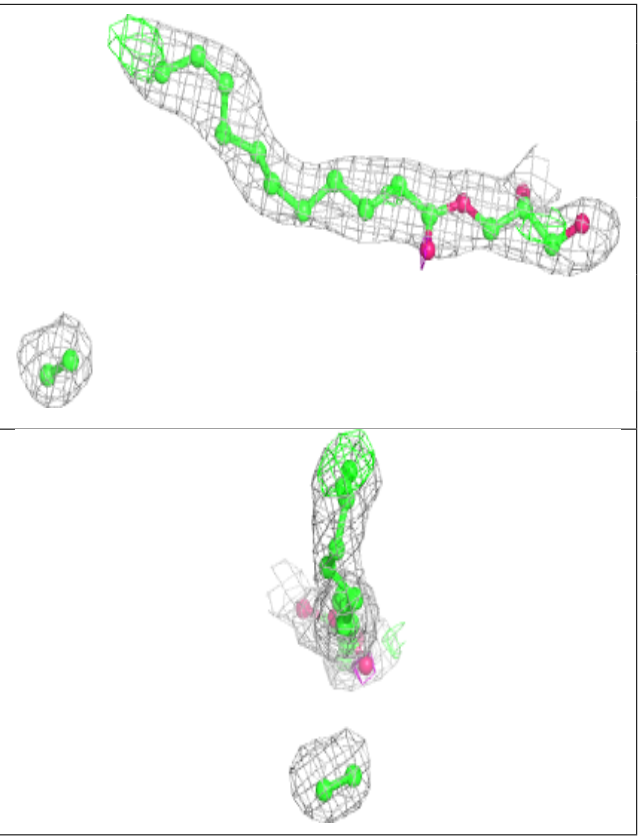
Electron density around OLA A 1208:

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



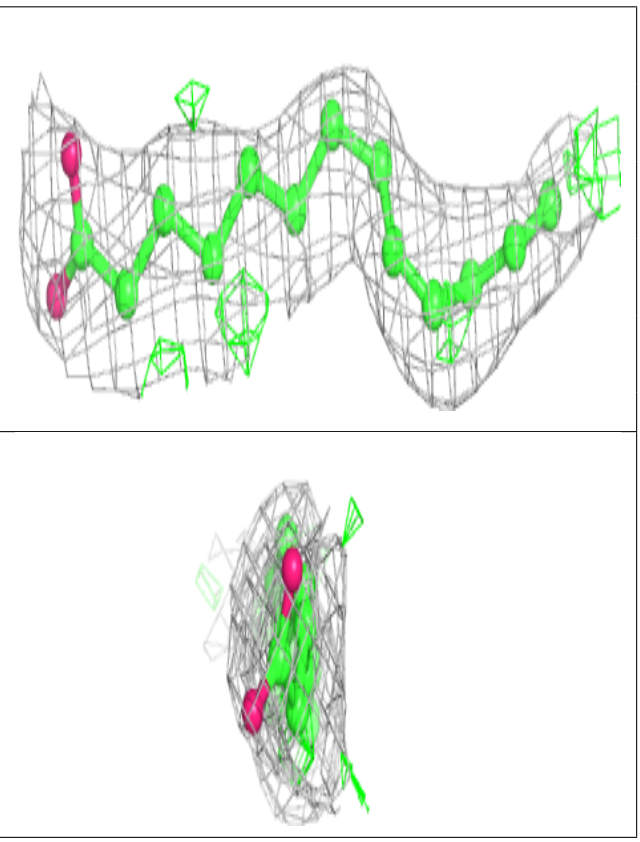
Electron density around OLC A 1212:

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



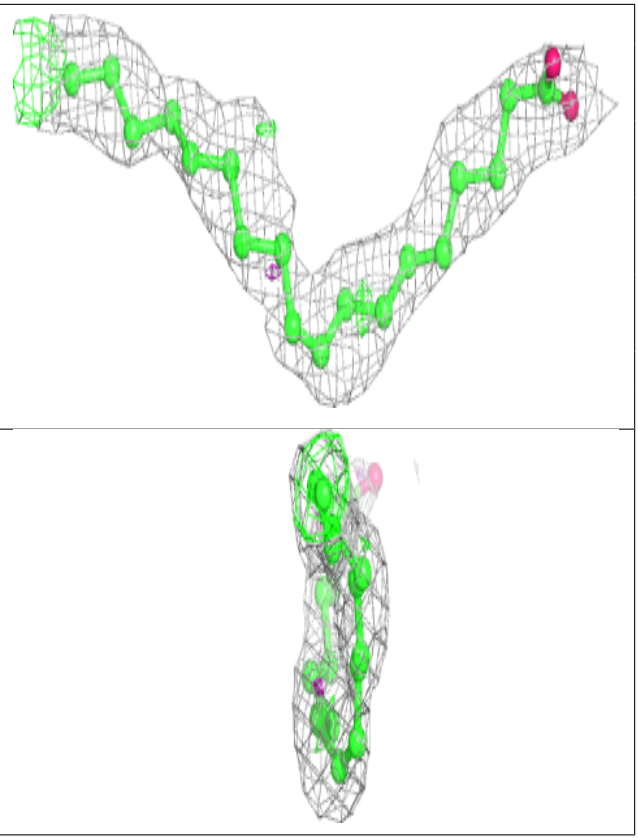
Electron density around OLA A 1218:

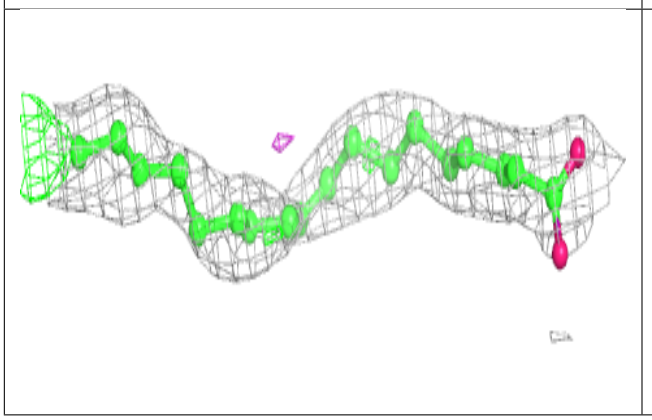
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLA A 1215:

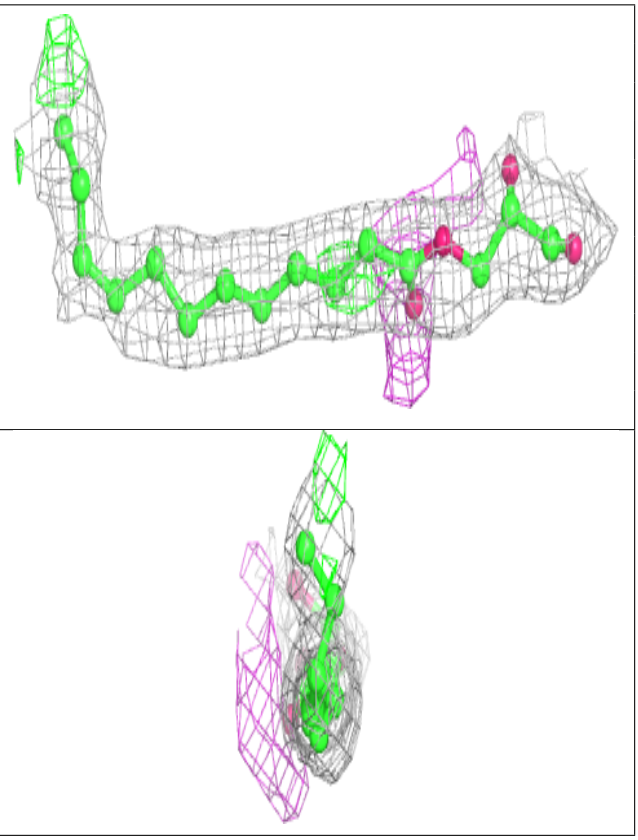
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

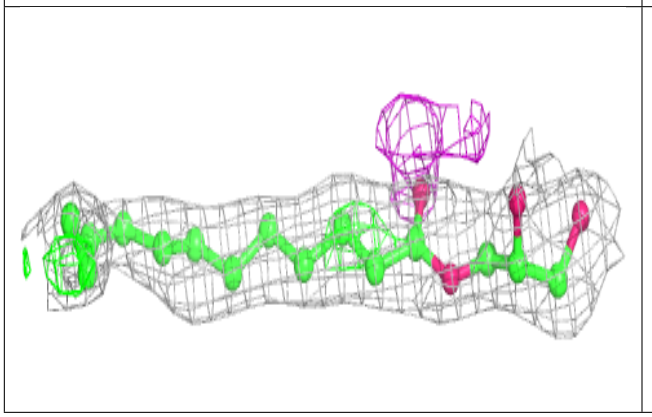




Electron density around OLC A 1211:

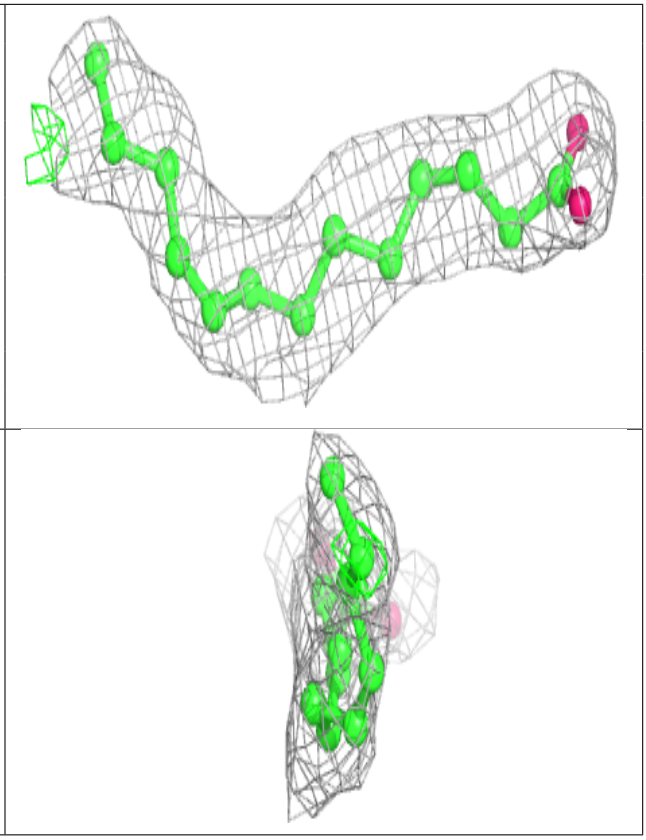
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





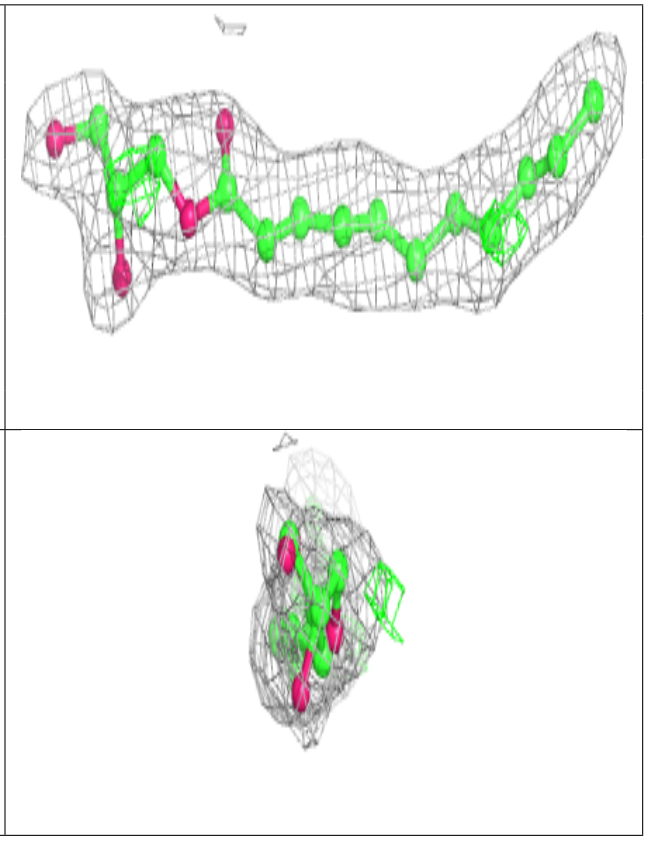
Electron density around OLA A 1206:

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



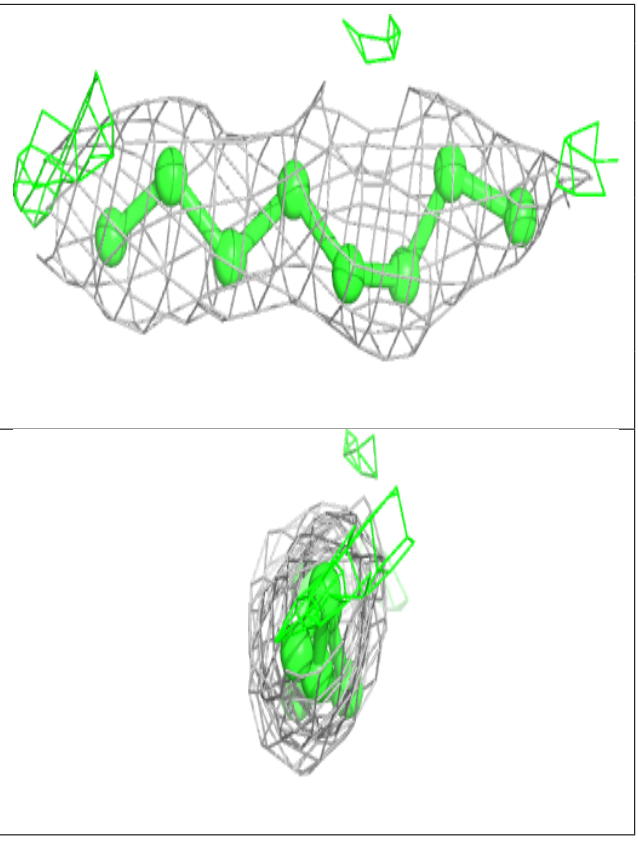
Electron density around OLC A 1213:

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



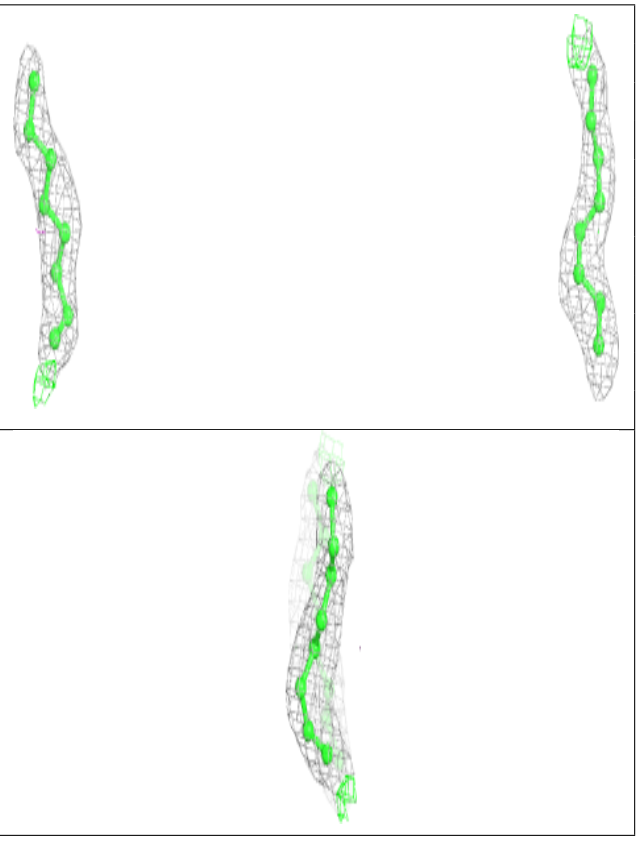
Electron density around OLA A 1209:

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



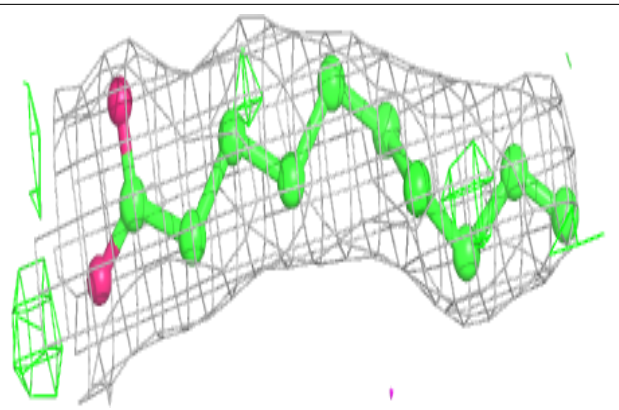
Electron density around OLA A 1210:

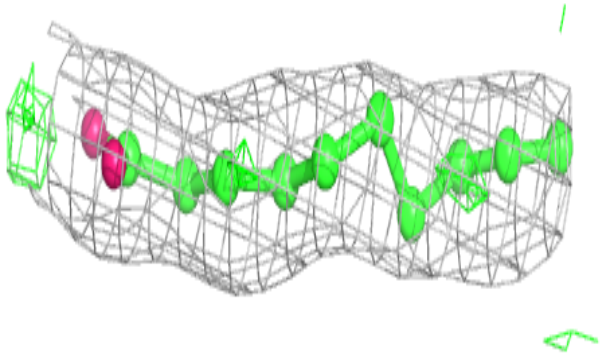
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

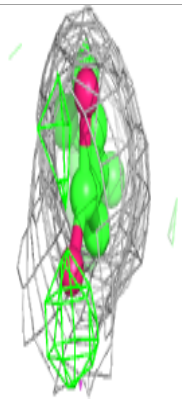


Electron density around OLA A 1214:

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

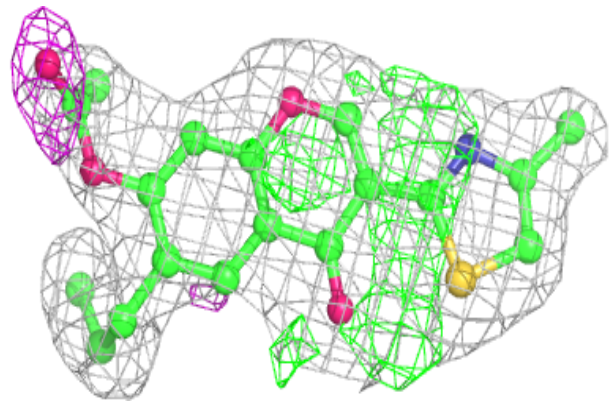


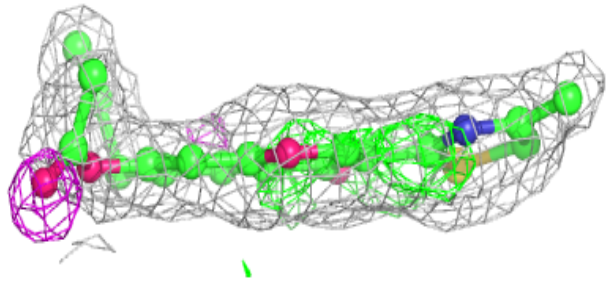


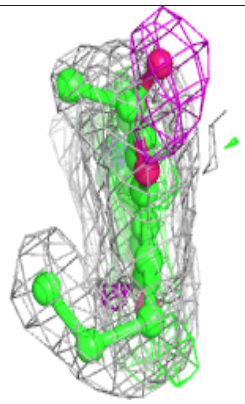


Electron density around QGE A 1201:

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

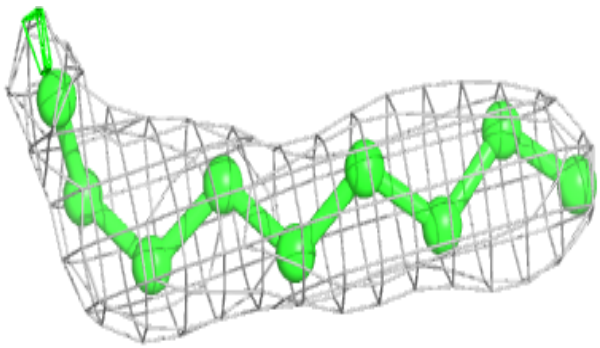


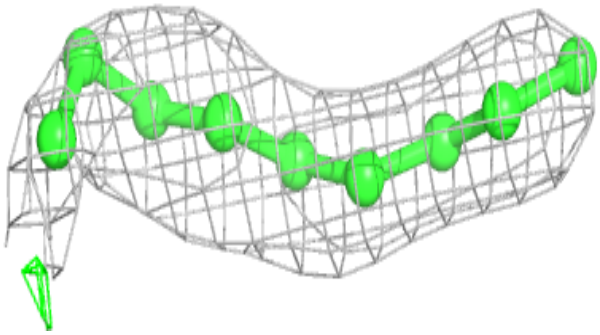


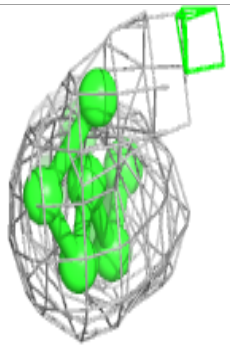


Electron density around OLA A 1220:

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

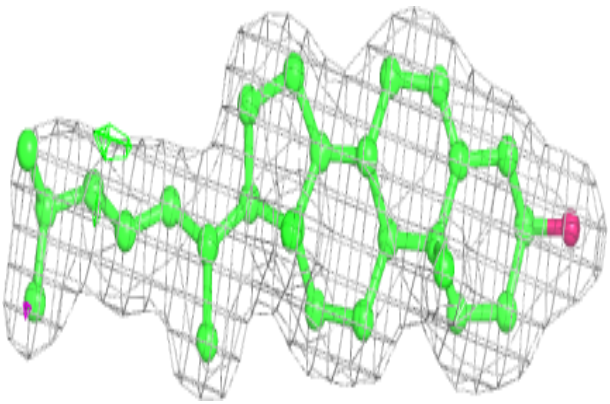


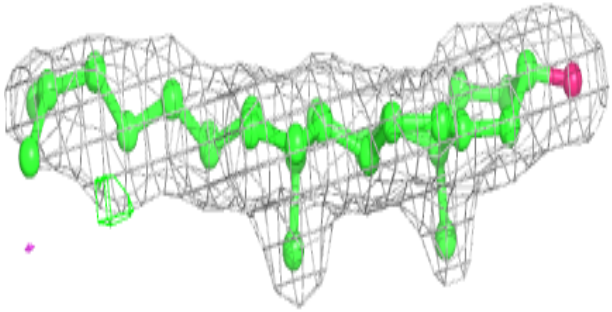


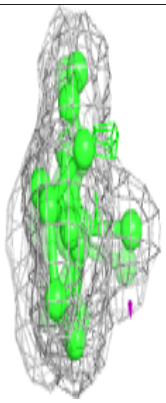


Electron density around CLR A 1205:

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

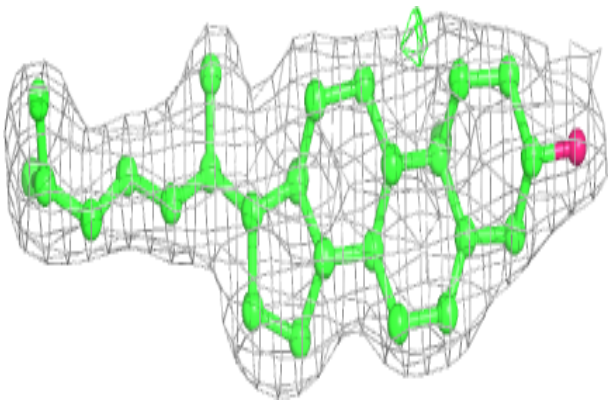


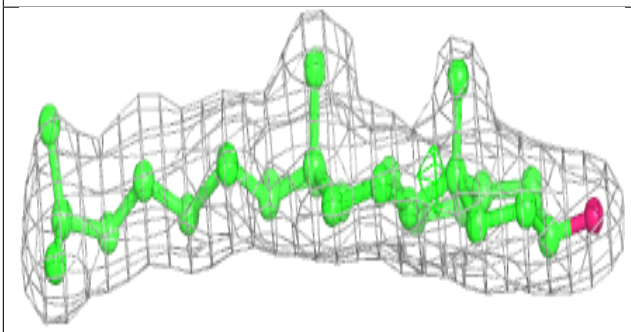


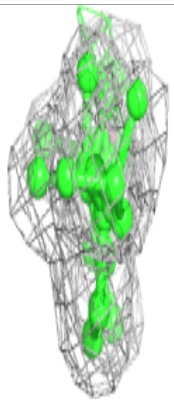


Electron density around CLR A 1203:

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

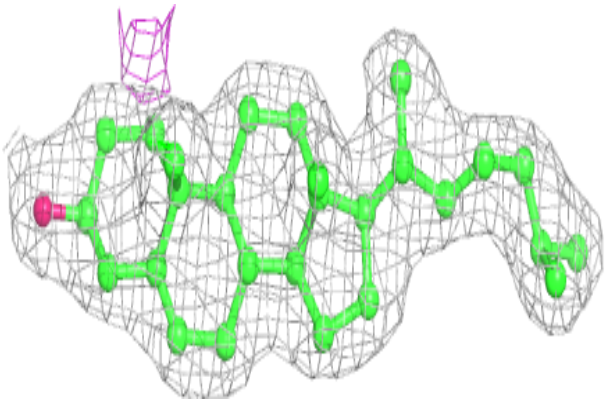


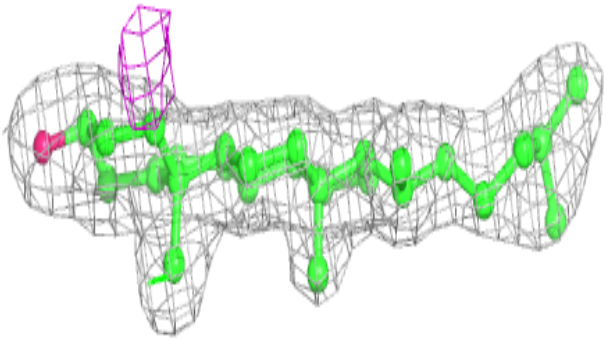


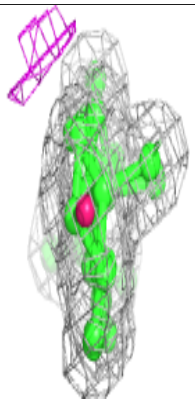


Electron density around CLR A 1204:

$2mF_o$-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.