Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 08:53 PM EDT

PDB ID	:	5JTB
Title	:	Crystal structure of the chimeric protein of A2aAR-BRIL with bound iodide ions
Authors	:	Melnikov, I.; Polovinkin, V.; Shevtsov, M.; Borshchevskiy, V.; Cherezov, V.; Popov, A.; Gordeliy, V.
Deposited on	:	2016-05-09
Resolution	:	2.80 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:

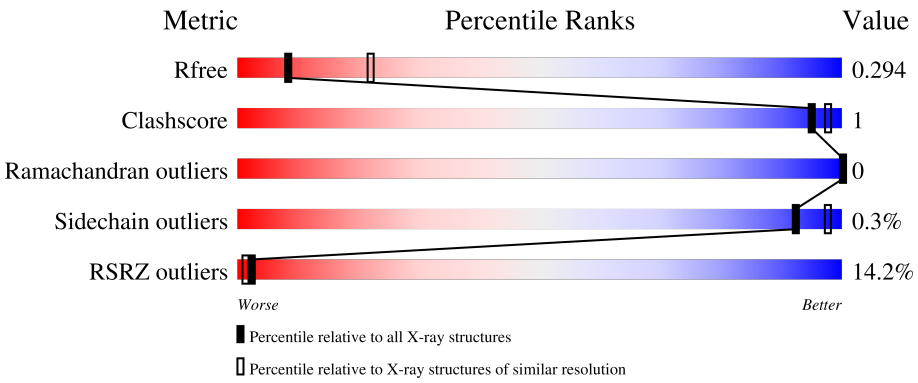
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

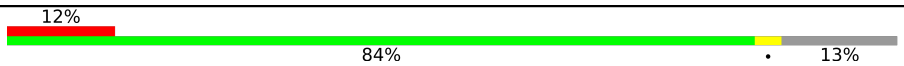
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	447	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OLA	A	1213	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3436 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	388	3043	1984	517	521	21	0	3	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274

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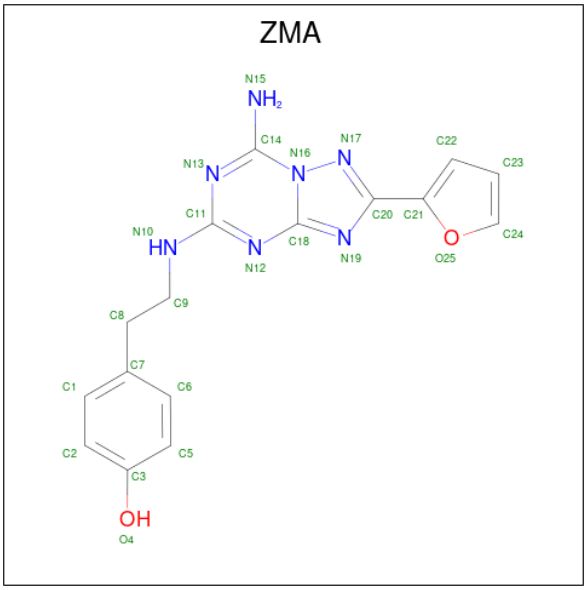
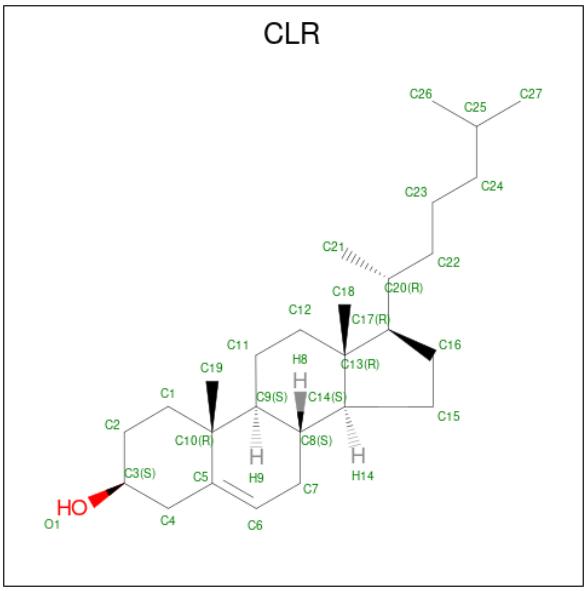
Chain	Residue	Modelled	Actual	Comment	Reference
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	Arg	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	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: $C_{16}H_{15}N_7O_2$).



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: $C_{27}H_{46}O$).

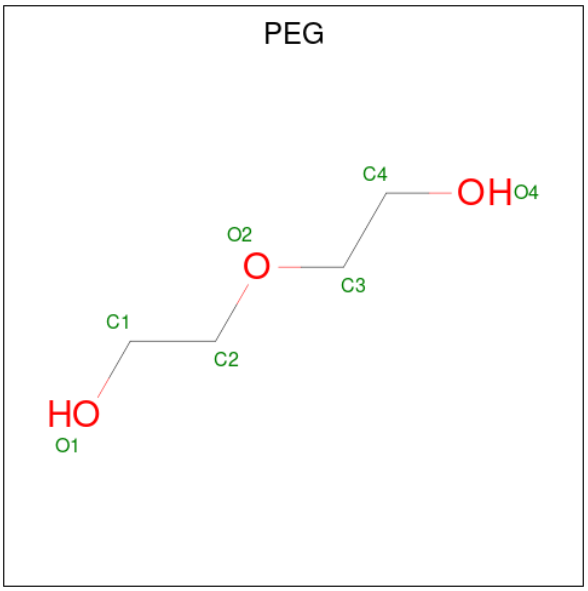


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

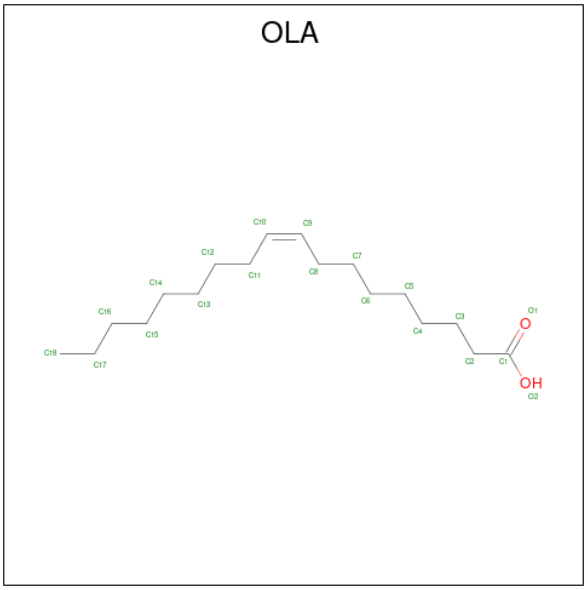
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total I 6 6	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 20 18 2	0	0
6	A	1	Total C O 20 18 2	0	0

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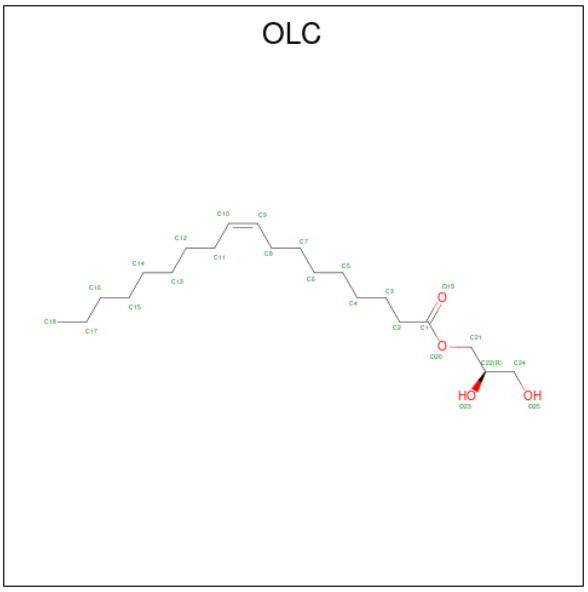
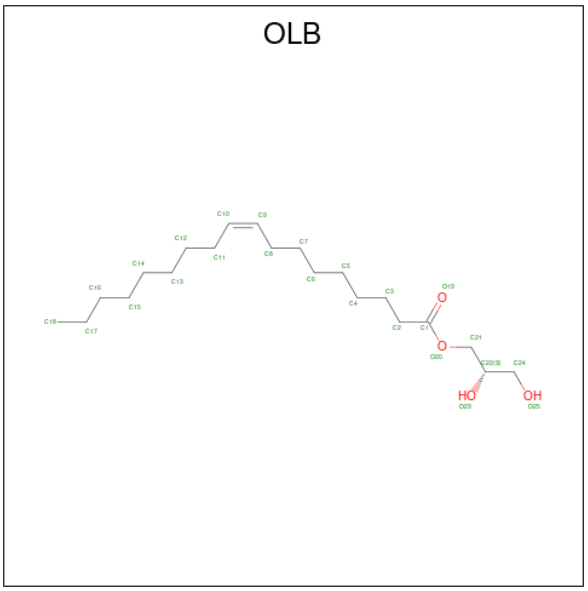
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	20	18	2	0	0
			Total	C	O		
6	A	1	20	18	2	0	0

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

- Molecule 8 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	18	14	4	0	0

- Molecule 9 is water.

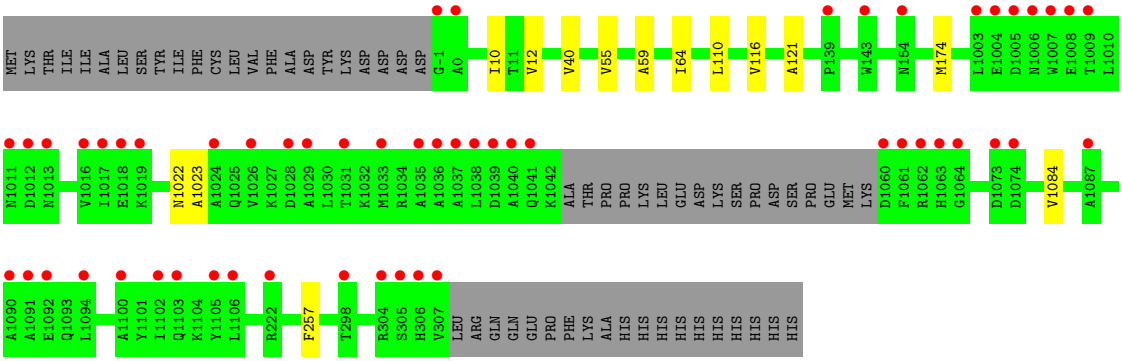
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	64	64	64	0	0

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	39.65Å 179.79Å 139.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.90 – 2.80 55.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.90-2.80) 99.7 (55.18-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.234 , 0.294 0.234 , 0.294	Depositor DCC
R_{free} test set	661 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3436	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% 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, PEG, IOD, ZMA, OLA, OLC

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	0.43	0/3119	0.57	0/4242

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	3043	0	3120	8	0
2	A	25	0	15	0	0
3	A	84	0	138	0	0
4	A	6	0	0	1	0
5	A	14	0	20	0	0
6	A	80	0	132	1	0
7	A	102	0	132	0	0
8	A	18	0	23	0	0
9	A	64	0	0	0	0
All	All	3436	0	3580	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	1.76	0.68
1:A:110:LEU:HB2	4:A:1209:IOD:I	2.80	0.51
1:A:1023:ALA:HB2	1:A:1084:VAL:HG22	1.95	0.48
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.95	0.48
1:A:40:VAL:HG13	1:A:121:ALA:HB2	1.98	0.46
1:A:12:VAL:HG21	6:A:1215:OLA:H112	1.99	0.45
1:A:174:MET:HG3	1:A:257:PHE:HB2	2.01	0.42
1:A:10:ILE:HG12	1:A:64:ILE:HG23	2.01	0.41

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	387/447 (87%)	379 (98%)	8 (2%)	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	322/374 (86%)	321 (100%)	1 (0%)	92 98

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

Mol	Chain	Res	Type
1	A	1022	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	145	ASN
1	A	1013	ASN

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 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
7	OLC	A	1220	-	16,16,24	1.17	1 (6%)	17,17,25	0.80	0
3	CLR	A	1203	-	31,31,31	1.91	7 (22%)	48,48,48	1.30	5 (10%)
7	OLC	A	1221	-	16,16,24	1.11	1 (6%)	17,17,25	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	OLC	A	1219	-	16,16,24	1.15	1 (6%)	17,17,25	0.94	0
3	CLR	A	1204	-	31,31,31	1.91	6 (19%)	48,48,48	1.29	5 (10%)
5	PEG	A	1211	-	6,6,6	0.61	0	5,5,5	0.52	0
6	OLA	A	1214	-	19,19,19	1.19	1 (5%)	19,19,19	0.96	0
7	OLC	A	1218	-	16,16,24	1.13	1 (6%)	17,17,25	0.86	0
3	CLR	A	1202	-	31,31,31	1.91	8 (25%)	48,48,48	1.25	5 (10%)
8	OLB	A	1223	-	17,17,24	1.09	1 (5%)	18,18,25	0.83	0
7	OLC	A	1217	-	16,16,24	1.12	1 (6%)	17,17,25	0.88	0
6	OLA	A	1215	-	19,19,19	1.18	1 (5%)	19,19,19	0.90	1 (5%)
6	OLA	A	1216	-	19,19,19	1.15	1 (5%)	19,19,19	0.98	1 (5%)
6	OLA	A	1213	-	19,19,19	1.12	1 (5%)	19,19,19	1.03	0
5	PEG	A	1212	-	6,6,6	0.49	0	5,5,5	0.49	0
2	ZMA	A	1201	-	21,28,28	1.27	3 (14%)	20,39,39	1.80	4 (20%)
7	OLC	A	1222	-	16,16,24	1.13	1 (6%)	17,17,25	0.83	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
7	OLC	A	1220	-	-	7/16/16/24	-
3	CLR	A	1203	-	-	6/10/68/68	0/4/4/4
7	OLC	A	1221	-	-	5/16/16/24	-
7	OLC	A	1219	-	-	8/16/16/24	-
3	CLR	A	1204	-	-	6/10/68/68	0/4/4/4
5	PEG	A	1211	-	-	3/4/4/4	-
6	OLA	A	1214	-	-	12/17/17/17	-
7	OLC	A	1218	-	-	9/16/16/24	-
3	CLR	A	1202	-	-	4/10/68/68	0/4/4/4
8	OLB	A	1223	-	-	4/17/17/24	-
7	OLC	A	1217	-	-	8/16/16/24	-
6	OLA	A	1215	-	-	11/17/17/17	-
6	OLA	A	1216	-	-	10/17/17/17	-
6	OLA	A	1213	-	-	11/17/17/17	-
5	PEG	A	1212	-	-	1/4/4/4	-
2	ZMA	A	1201	-	-	0/6/10/10	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	1222	-	-	11/16/16/24	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1203	CLR	C4-C5	-4.49	1.41	1.51
3	A	1202	CLR	C4-C5	-4.40	1.42	1.51
3	A	1203	CLR	C7-C6	-4.27	1.41	1.50
3	A	1204	CLR	C4-C5	-4.26	1.42	1.51
3	A	1202	CLR	C7-C6	-4.25	1.41	1.50
3	A	1204	CLR	C7-C6	-4.11	1.41	1.50
6	A	1214	OLA	C10-C9	4.06	1.55	1.31
6	A	1216	OLA	C10-C9	4.03	1.55	1.31
6	A	1213	OLA	C10-C9	4.01	1.55	1.31
6	A	1215	OLA	C10-C9	4.01	1.55	1.31
2	A	1201	ZMA	C8-C7	-3.83	1.40	1.51
3	A	1204	CLR	C10-C5	-3.76	1.45	1.52
7	A	1217	OLC	C10-C9	3.72	1.53	1.28
7	A	1220	OLC	C10-C9	3.72	1.53	1.28
7	A	1219	OLC	C10-C9	3.72	1.53	1.28
7	A	1218	OLC	C10-C9	3.71	1.53	1.28
3	A	1204	CLR	C6-C5	3.69	1.41	1.33
7	A	1221	OLC	C10-C9	3.69	1.53	1.28
7	A	1222	OLC	C10-C9	3.68	1.53	1.28
3	A	1203	CLR	C10-C5	-3.68	1.45	1.52
3	A	1202	CLR	C6-C5	3.67	1.41	1.33
3	A	1203	CLR	C6-C5	3.65	1.41	1.33
3	A	1202	CLR	C10-C5	-3.63	1.45	1.52
3	A	1204	CLR	C11-C9	3.56	1.59	1.53
8	A	1223	OLB	C9-C10	3.42	1.55	1.29
3	A	1203	CLR	C11-C9	3.02	1.58	1.53
3	A	1202	CLR	C11-C9	2.89	1.58	1.53
3	A	1203	CLR	C8-C9	2.51	1.58	1.53
3	A	1204	CLR	C8-C9	2.51	1.58	1.53
3	A	1202	CLR	C8-C9	2.28	1.58	1.53
3	A	1203	CLR	C13-C17	2.26	1.59	1.55
2	A	1201	ZMA	C22-C21	-2.16	1.33	1.42
3	A	1202	CLR	C8-C14	2.15	1.57	1.53
3	A	1202	CLR	C16-C17	2.06	1.58	1.54
2	A	1201	ZMA	C18-N19	-2.05	1.32	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	ZMA	N15-C14-N16	5.38	121.59	117.97
2	A	1201	ZMA	N12-C11-N13	-4.12	119.71	126.23
3	A	1203	CLR	C4-C5-C6	-4.07	114.74	120.61
3	A	1202	CLR	C4-C5-C6	-4.07	114.75	120.61
3	A	1203	CLR	C4-C5-C10	4.07	121.82	116.42
3	A	1202	CLR	C4-C5-C10	4.04	121.79	116.42
3	A	1204	CLR	C4-C5-C10	3.83	121.50	116.42
3	A	1203	CLR	C17-C13-C14	-3.79	95.58	100.07
3	A	1204	CLR	C4-C5-C6	-3.53	115.52	120.61
3	A	1204	CLR	C21-C20-C22	-2.90	105.81	110.36
3	A	1202	CLR	C17-C13-C14	-2.84	96.71	100.07
3	A	1204	CLR	C12-C13-C17	-2.78	112.41	116.57
2	A	1201	ZMA	N10-C11-N13	2.66	121.79	117.19
3	A	1204	CLR	C17-C13-C14	-2.33	97.32	100.07
2	A	1201	ZMA	N15-C14-N13	2.32	120.08	117.03
3	A	1203	CLR	C12-C13-C17	-2.21	113.26	116.57
3	A	1203	CLR	C21-C20-C22	-2.18	106.94	110.36
6	A	1215	OLA	O1-C1-C2	-2.18	116.08	123.08
3	A	1202	CLR	C12-C13-C17	-2.15	113.36	116.57
3	A	1202	CLR	C16-C15-C14	-2.03	101.11	105.13
6	A	1216	OLA	O1-C1-C2	-2.02	116.60	123.08

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1219	OLC	O20-C21-C22-O23
7	A	1217	OLC	C2-C1-O20-C21
7	A	1219	OLC	O19-C1-O20-C21
7	A	1217	OLC	O19-C1-O20-C21
3	A	1204	CLR	C17-C20-C22-C23
7	A	1219	OLC	C2-C1-O20-C21
3	A	1204	CLR	C21-C20-C22-C23
7	A	1222	OLC	C2-C1-O20-C21
8	A	1223	OLB	C2-C1-O20-C21
7	A	1222	OLC	O20-C21-C22-C24
6	A	1213	OLA	C1-C2-C3-C4
6	A	1216	OLA	C1-C2-C3-C4
7	A	1217	OLC	C1-C2-C3-C4
5	A	1211	PEG	O2-C3-C4-O4
8	A	1223	OLB	O19-C1-O20-C21
3	A	1203	CLR	C20-C22-C23-C24
7	A	1222	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
7	A	1222	OLC	O20-C21-C22-O23
5	A	1212	PEG	O2-C3-C4-O4
3	A	1204	CLR	C23-C24-C25-C26
7	A	1219	OLC	O20-C21-C22-C24
6	A	1214	OLA	C12-C13-C14-C15
6	A	1213	OLA	C4-C5-C6-C7
6	A	1214	OLA	C14-C15-C16-C17
7	A	1222	OLC	C1-C2-C3-C4
3	A	1202	CLR	C23-C24-C25-C26
3	A	1202	CLR	C23-C24-C25-C27
6	A	1213	OLA	C14-C15-C16-C17
6	A	1216	OLA	C3-C4-C5-C6
7	A	1218	OLC	O20-C21-C22-O23
7	A	1219	OLC	C2-C3-C4-C5
3	A	1204	CLR	C23-C24-C25-C27
6	A	1215	OLA	C11-C12-C13-C14
7	A	1217	OLC	C3-C4-C5-C6
7	A	1219	OLC	C5-C6-C7-C8
6	A	1215	OLA	C2-C3-C4-C5
6	A	1213	OLA	C13-C14-C15-C16
6	A	1215	OLA	C1-C2-C3-C4
7	A	1222	OLC	C6-C7-C8-C9
7	A	1220	OLC	C4-C5-C6-C7
7	A	1221	OLC	C3-C4-C5-C6
6	A	1213	OLA	C3-C4-C5-C6
7	A	1221	OLC	C1-C2-C3-C4
3	A	1202	CLR	C20-C22-C23-C24
6	A	1216	OLA	C13-C14-C15-C16
6	A	1213	OLA	C10-C11-C12-C13
6	A	1216	OLA	C10-C11-C12-C13
7	A	1217	OLC	C6-C7-C8-C9
7	A	1220	OLC	C6-C7-C8-C9
7	A	1221	OLC	C6-C7-C8-C9
3	A	1204	CLR	C20-C22-C23-C24
6	A	1214	OLA	C2-C3-C4-C5
6	A	1215	OLA	C14-C15-C16-C17
6	A	1216	OLA	C11-C12-C13-C14
3	A	1203	CLR	C16-C17-C20-C22
6	A	1215	OLA	C10-C11-C12-C13
7	A	1222	OLC	C3-C4-C5-C6
3	A	1203	CLR	C17-C20-C22-C23
7	A	1218	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	1211	PEG	O1-C1-C2-O2
6	A	1214	OLA	C15-C16-C17-C18
6	A	1215	OLA	C15-C16-C17-C18
6	A	1213	OLA	C2-C3-C4-C5
6	A	1216	OLA	C15-C16-C17-C18
6	A	1214	OLA	C6-C7-C8-C9
8	A	1223	OLB	C6-C7-C8-C9
7	A	1222	OLC	C2-C3-C4-C5
6	A	1213	OLA	C12-C13-C14-C15
7	A	1218	OLC	C1-C2-C3-C4
7	A	1218	OLC	O20-C21-C22-C24
7	A	1221	OLC	C5-C6-C7-C8
6	A	1214	OLA	C4-C5-C6-C7
6	A	1215	OLA	C12-C13-C14-C15
3	A	1203	CLR	C21-C20-C22-C23
7	A	1217	OLC	C5-C6-C7-C8
7	A	1220	OLC	C2-C1-O20-C21
3	A	1204	CLR	C22-C23-C24-C25
6	A	1216	OLA	C4-C5-C6-C7
6	A	1214	OLA	C10-C11-C12-C13
7	A	1218	OLC	C4-C5-C6-C7
7	A	1220	OLC	O20-C21-C22-O23
8	A	1223	OLB	O20-C21-C22-O23
7	A	1220	OLC	O19-C1-O20-C21
5	A	1211	PEG	C4-C3-O2-C2
6	A	1216	OLA	C2-C3-C4-C5
7	A	1220	OLC	C3-C4-C5-C6
3	A	1202	CLR	C22-C23-C24-C25
6	A	1215	OLA	C4-C5-C6-C7
7	A	1222	OLC	C7-C8-C9-C10
7	A	1220	OLC	O20-C21-C22-C24
7	A	1222	OLC	C4-C5-C6-C7
7	A	1218	OLC	C2-C1-O20-C21
7	A	1218	OLC	O19-C1-O20-C21
3	A	1203	CLR	C23-C24-C25-C26
3	A	1203	CLR	C23-C24-C25-C27
6	A	1213	OLA	C7-C8-C9-C10
6	A	1214	OLA	C3-C4-C5-C6
6	A	1214	OLA	O1-C1-C2-C3
6	A	1216	OLA	O1-C1-C2-C3
7	A	1222	OLC	O23-C22-C24-O25
7	A	1217	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
7	A	1219	OLC	C4-C5-C6-C7
6	A	1214	OLA	O2-C1-C2-C3
6	A	1213	OLA	O2-C1-C2-C3
7	A	1219	OLC	C7-C8-C9-C10
6	A	1213	OLA	O1-C1-C2-C3
6	A	1214	OLA	C9-C10-C11-C12
6	A	1216	OLA	O2-C1-C2-C3
7	A	1221	OLC	C7-C8-C9-C10
6	A	1215	OLA	C7-C8-C9-C10
7	A	1217	OLC	O20-C21-C22-C24
7	A	1218	OLC	C2-C3-C4-C5
7	A	1218	OLC	C7-C8-C9-C10
6	A	1215	OLA	C6-C7-C8-C9
6	A	1214	OLA	C13-C14-C15-C16
6	A	1215	OLA	C3-C4-C5-C6

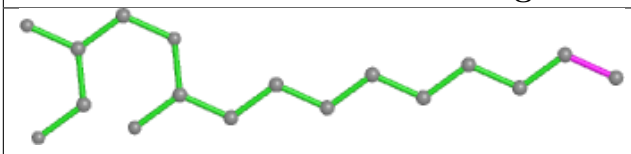
There are no ring outliers.

1 monomer is involved in 1 short contact:

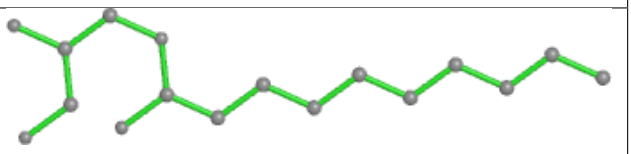
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1215	OLA	1	0

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.

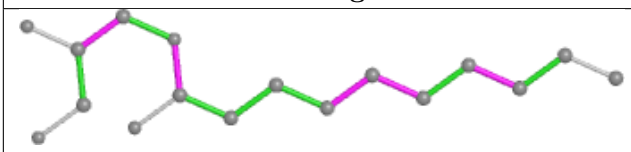
Ligand OLC A 1220



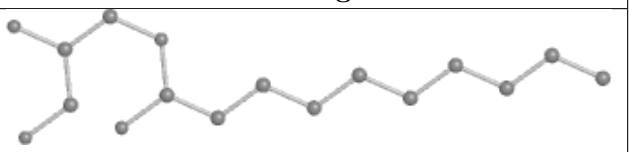
Bond lengths



Bond angles

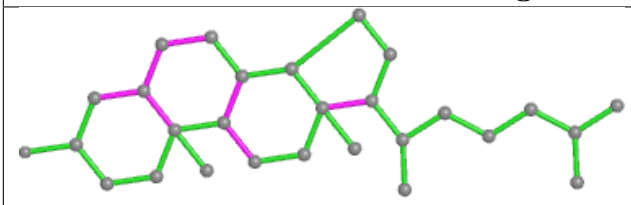


Torsions

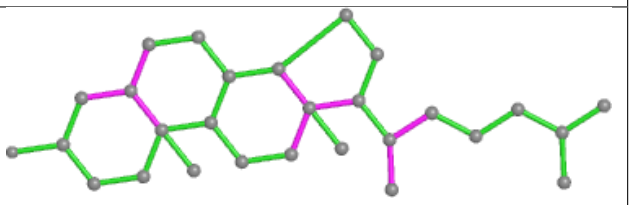


Rings

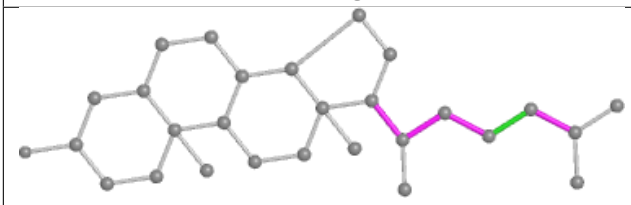
Ligand CLR A 1203



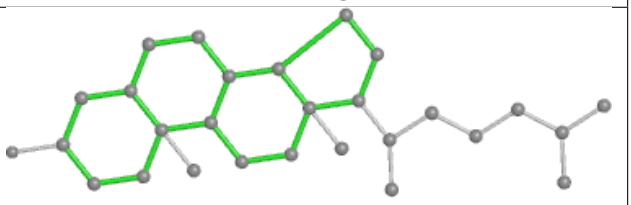
Bond lengths



Bond angles

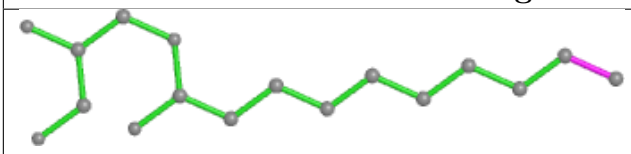


Torsions

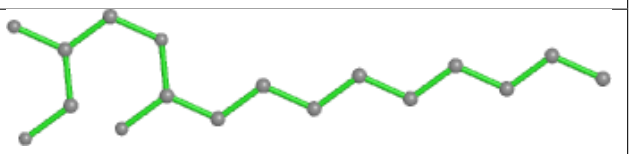


Rings

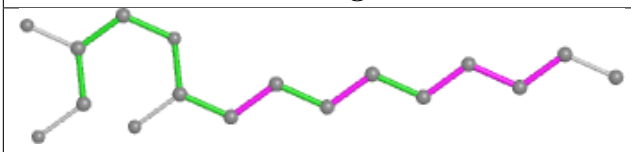
Ligand OLC A 1221



Bond lengths



Bond angles



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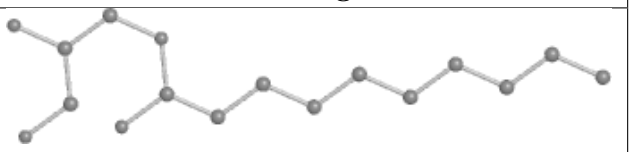
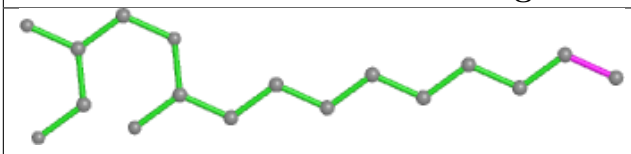


Rings

Ligand OLC A 1219



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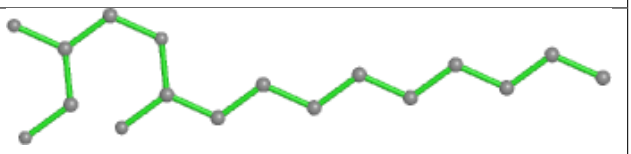
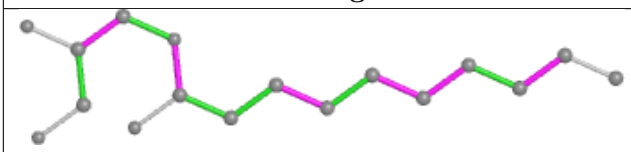
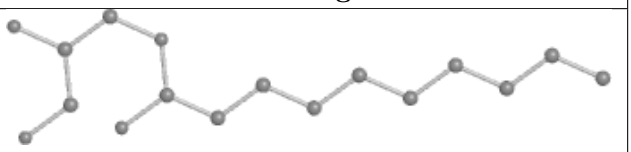


Bond angles

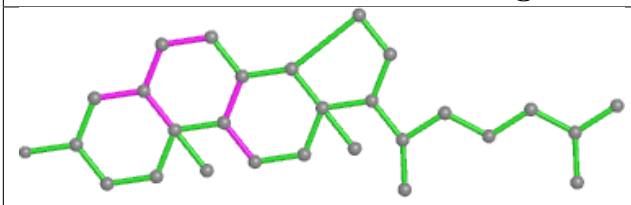


Torsions



Rings

Ligand CLR A 1204



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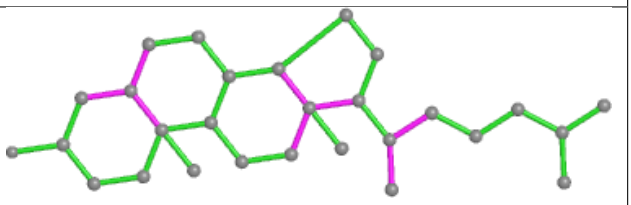
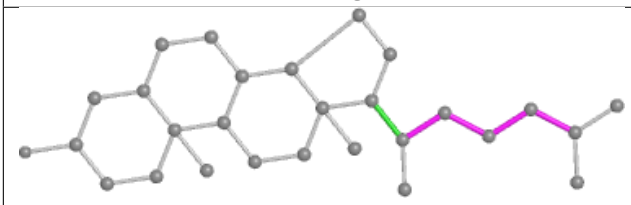


Bond angles



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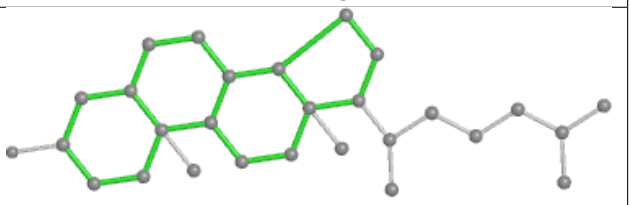
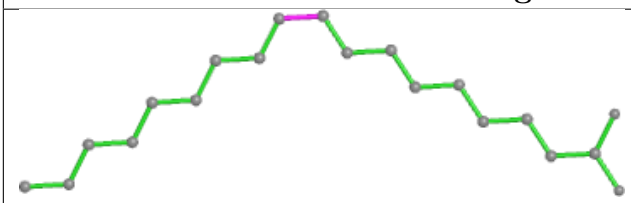


Rings

Ligand OLA A 1214



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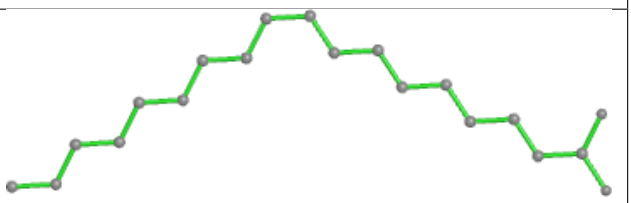
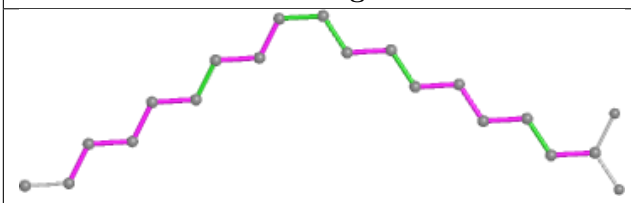
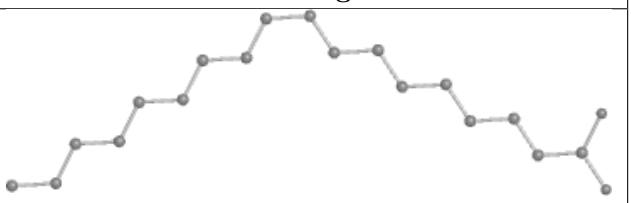


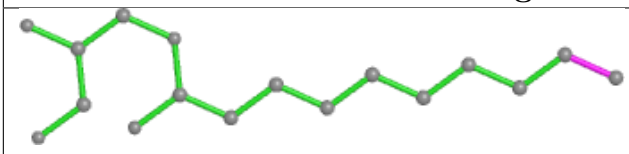
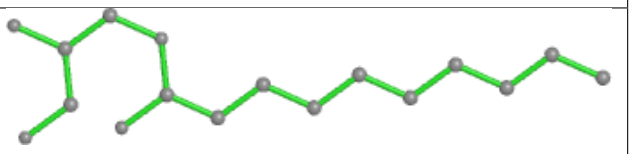
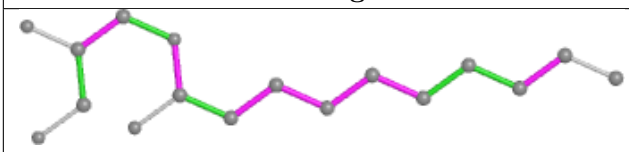
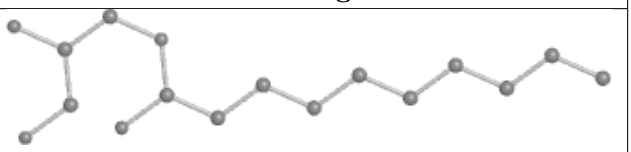
Bond angles

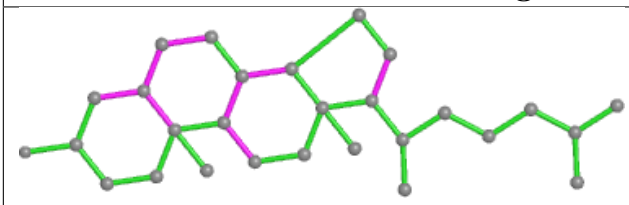
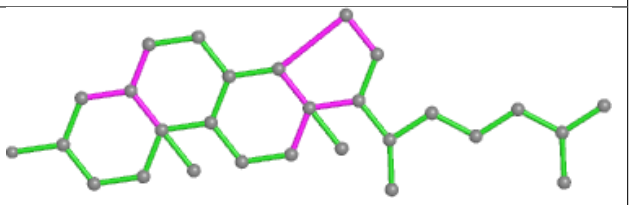
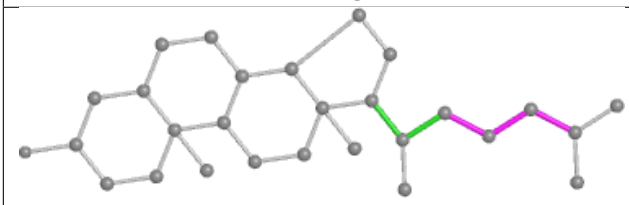
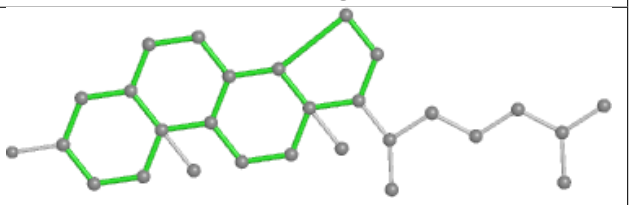


Torsions

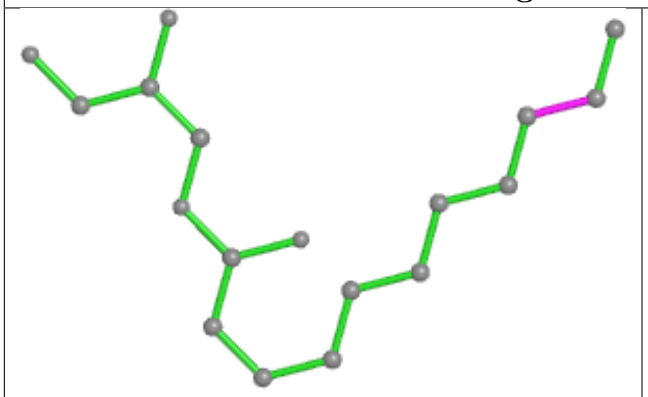


Rings

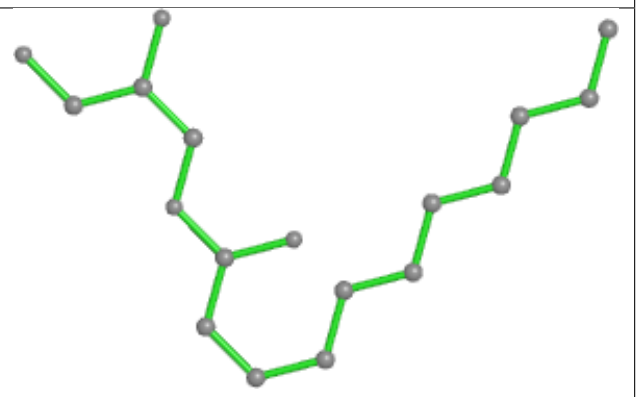
Ligand OLC A 1218	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLR A 1202	
 Bond lengths	 Bond angles
 Torsions	 Rings

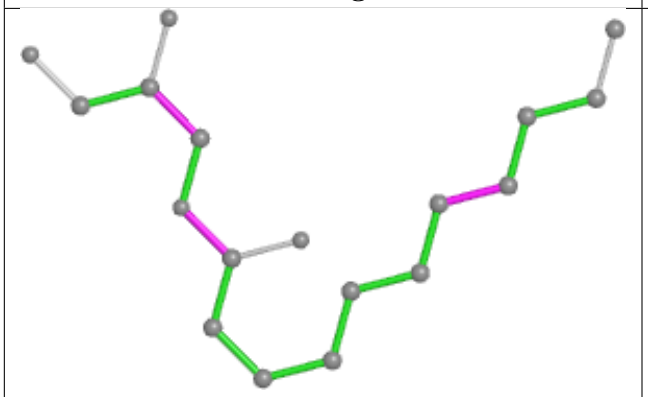
Ligand OLB A 1223



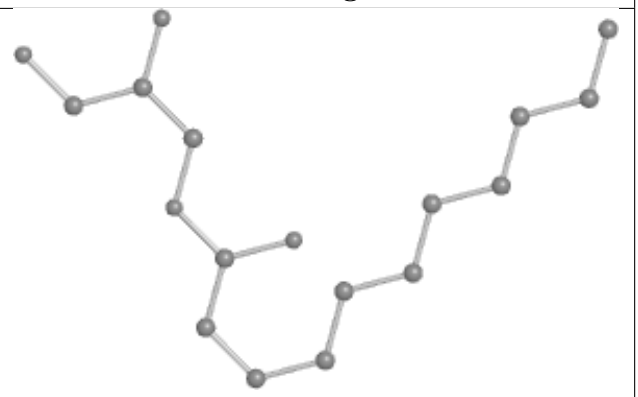
Bond lengths



Bond angles

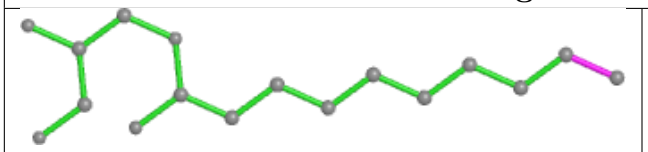


Torsions

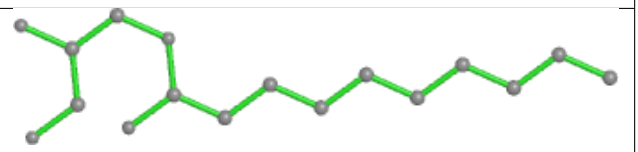


Rings

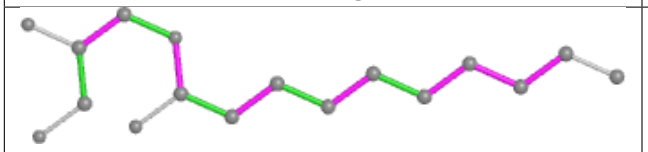
Ligand OLC A 1217



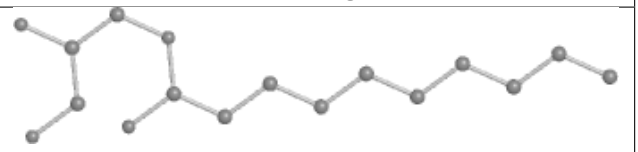
Bond lengths



Bond angles

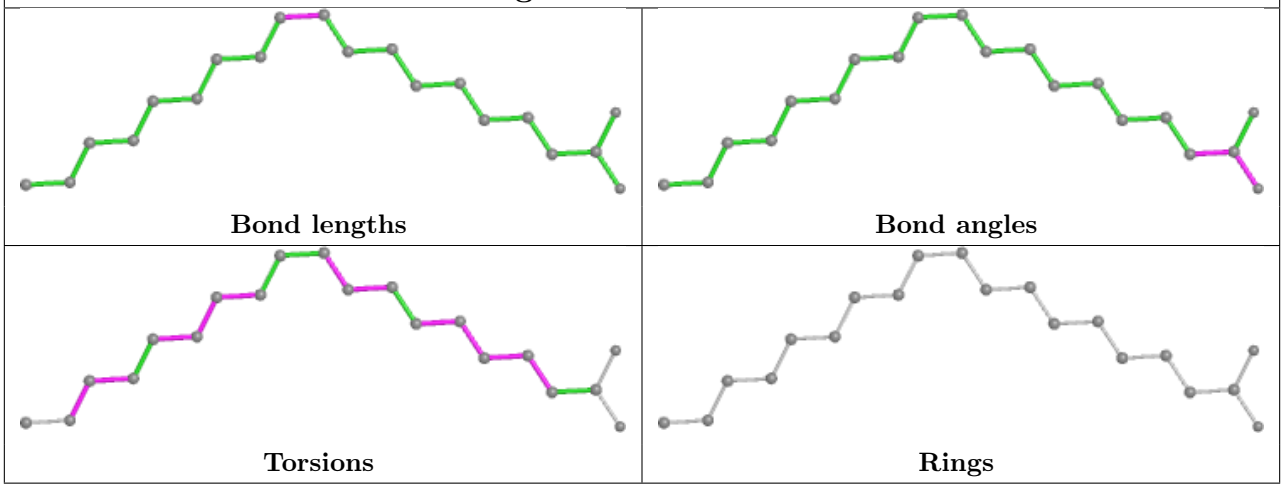


Torsions

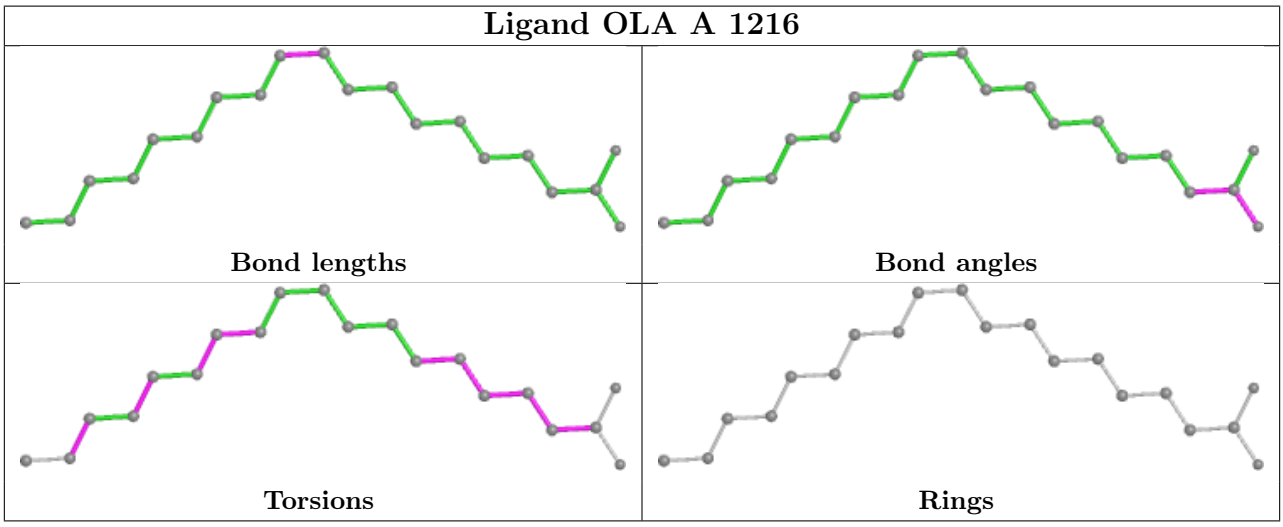


Rings

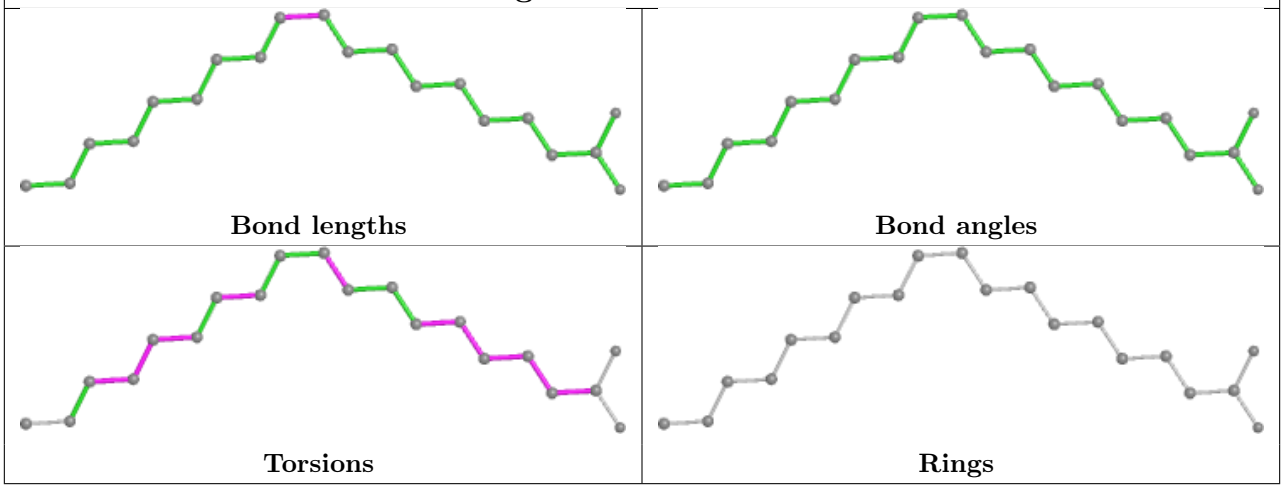
Ligand OLA A 1215

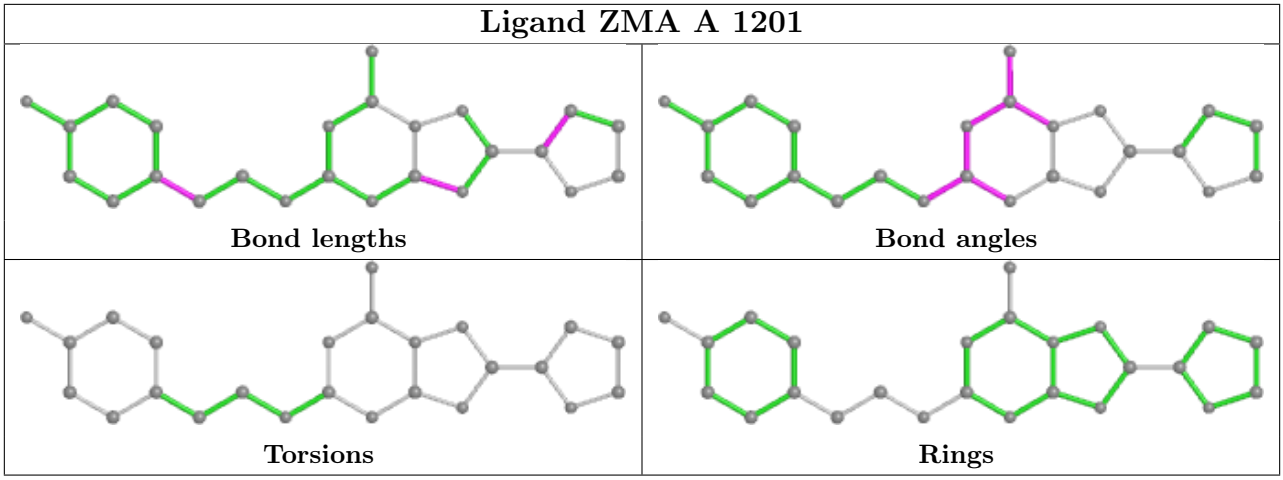


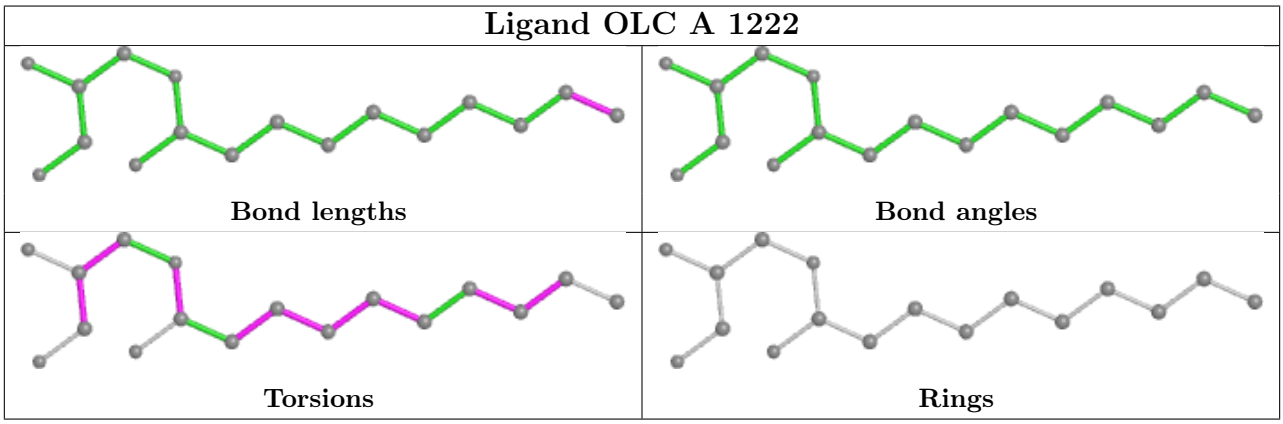
Ligand OLA A 1216



Ligand OLA A 1213







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	388/447 (86%)	0.50	55 (14%) 2 1	16, 32, 77, 96	26 (6%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1039	ASP	5.1
1	A	1028	ASP	5.0
1	A	306	HIS	4.7
1	A	1041	GLN	4.5
1	A	1033	MET	4.4
1	A	1037	ALA	4.1
1	A	1091	ALA	4.0
1	A	1061	PHE	3.9
1	A	1012	ASP	3.8
1	A	1060	ASP	3.8
1	A	1040	ALA	3.6
1	A	1013	ASN	3.6
1	A	1063	HIS	3.5
1	A	1016	VAL	3.5
1	A	1029	ALA	3.4
1	A	1006	ASN	3.3
1	A	1036	ALA	3.3
1	A	1106	LEU	3.3
1	A	1038	LEU	3.2
1	A	1003	LEU	3.1
1	A	1031	THR	3.1
1	A	1018	GLU	3.0
1	A	1062	ARG	3.0
1	A	1011	ASN	3.0
1	A	1026	VAL	2.9
1	A	-1	GLY	2.9
1	A	1102	ILE	2.9

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
1	A	1009	THR	2.8
1	A	305	SER	2.8
1	A	1017	ILE	2.8
1	A	1092	GLU	2.8
1	A	222	ARG	2.8
1	A	1094	LEU	2.7
1	A	1005	ASP	2.7
1	A	304	ARG	2.7
1	A	154[A]	ASN	2.7
1	A	1105	TYR	2.6
1	A	1024	ALA	2.6
1	A	1004	GLU	2.6
1	A	1035	ALA	2.6
1	A	1087	ALA	2.5
1	A	1064	GLY	2.5
1	A	307	VAL	2.5
1	A	0	ALA	2.4
1	A	1007	TRP	2.4
1	A	298	THR	2.4
1	A	1074	ASP	2.3
1	A	1019	LYS	2.3
1	A	1090	ALA	2.3
1	A	1073	ASP	2.2
1	A	143	TRP	2.1
1	A	1008	GLU	2.1
1	A	139	PRO	2.1
1	A	1100	ALA	2.1
1	A	1103	GLN	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,

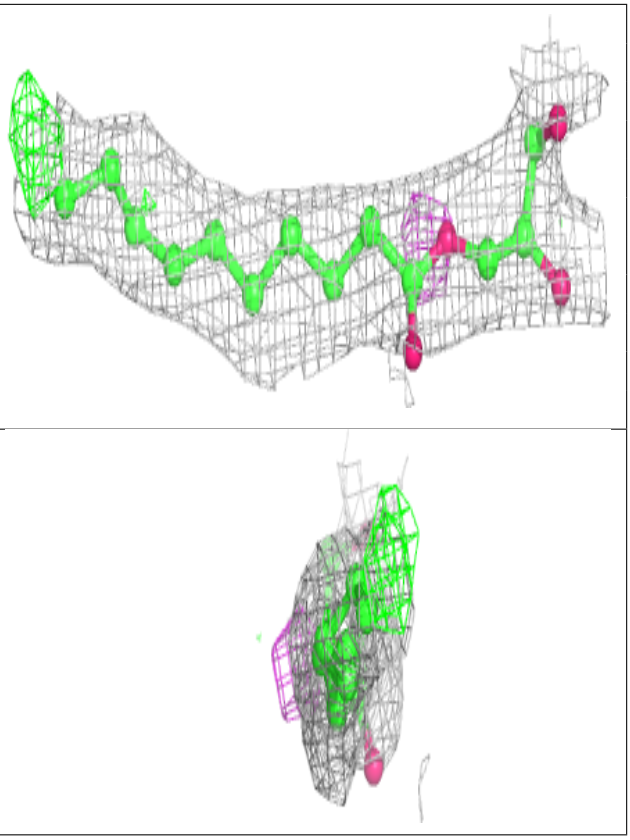
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

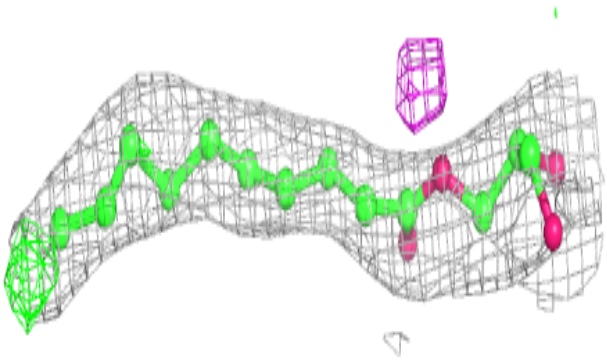
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	OLC	A	1220	17/25	0.70	0.32	45,52,61,62	0
6	OLA	A	1213	20/20	0.74	0.47	59,61,65,66	9
7	OLC	A	1222	17/25	0.75	0.35	66,68,71,72	0
5	PEG	A	1211	7/7	0.76	0.29	79,79,79,79	0
6	OLA	A	1214	20/20	0.77	0.33	53,57,60,60	0
7	OLC	A	1219	17/25	0.78	0.38	62,63,66,66	0
7	OLC	A	1217	17/25	0.80	0.32	59,60,63,64	0
7	OLC	A	1221	17/25	0.81	0.32	79,80,81,81	2
6	OLA	A	1215	20/20	0.82	0.28	60,61,65,65	0
7	OLC	A	1218	17/25	0.85	0.29	49,50,56,56	0
5	PEG	A	1212	7/7	0.86	0.23	58,59,61,61	0
8	OLB	A	1223	18/25	0.86	0.31	58,61,65,65	0
6	OLA	A	1216	20/20	0.87	0.29	51,52,54,54	0
3	CLR	A	1202	28/28	0.90	0.24	31,32,35,35	0
4	IOD	A	1206	1/1	0.93	0.09	40,40,40,40	1
4	IOD	A	1210	1/1	0.93	0.16	61,61,61,61	1
3	CLR	A	1203	28/28	0.93	0.20	32,33,35,35	0
3	CLR	A	1204	28/28	0.94	0.17	27,28,32,32	0
2	ZMA	A	1201	25/25	0.94	0.18	15,15,20,21	0
4	IOD	A	1209	1/1	0.96	0.12	39,39,39,39	1
4	IOD	A	1207	1/1	0.97	0.07	36,36,36,36	1
4	IOD	A	1205	1/1	0.97	0.13	44,44,44,44	1
4	IOD	A	1208	1/1	0.98	0.09	44,44,44,44	1

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

Electron density around OLC A 1220:

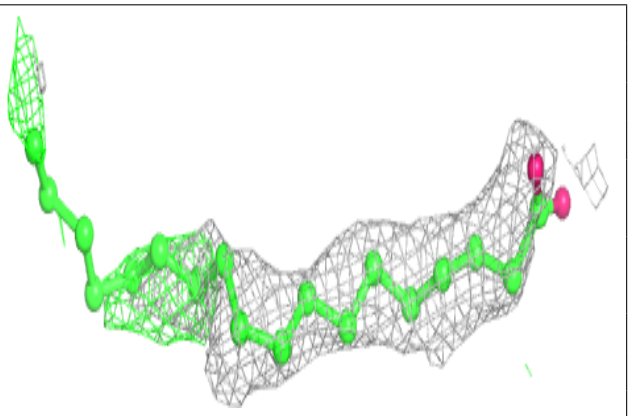
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

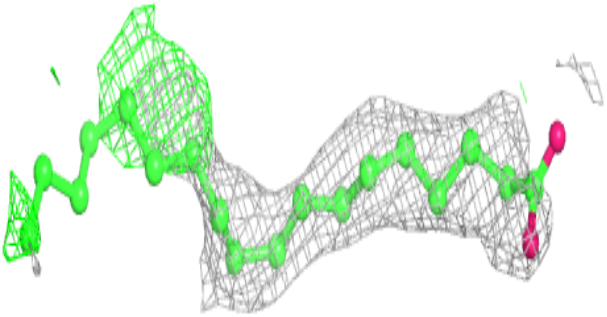


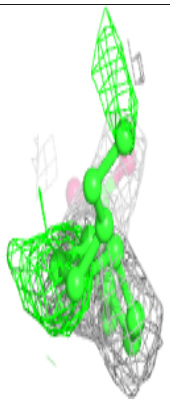


Electron density around OLA A 1213:

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







Electron density around OLC A 1222:

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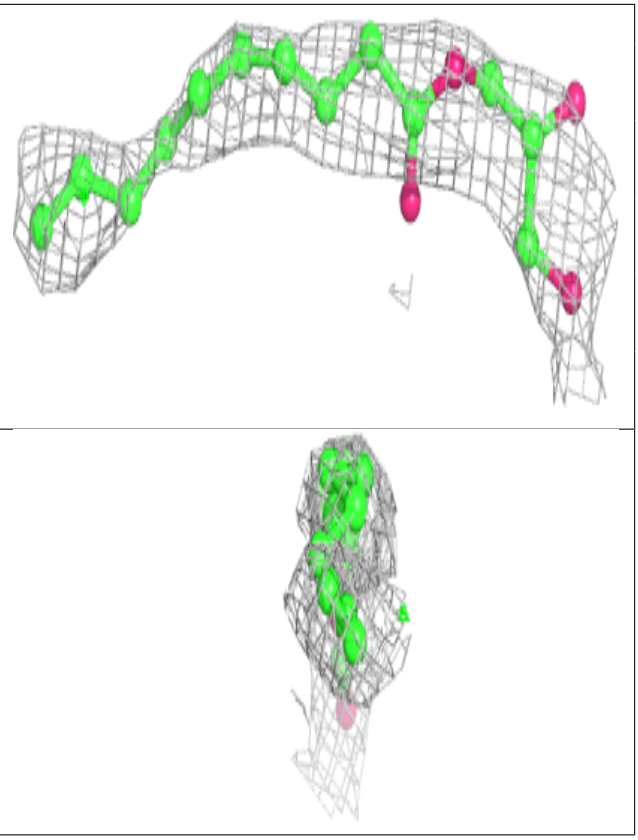
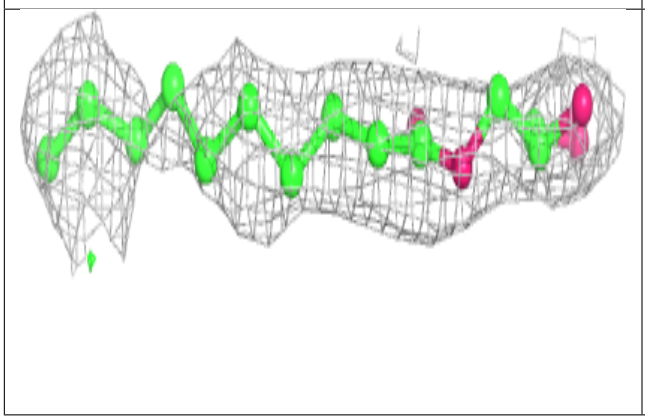
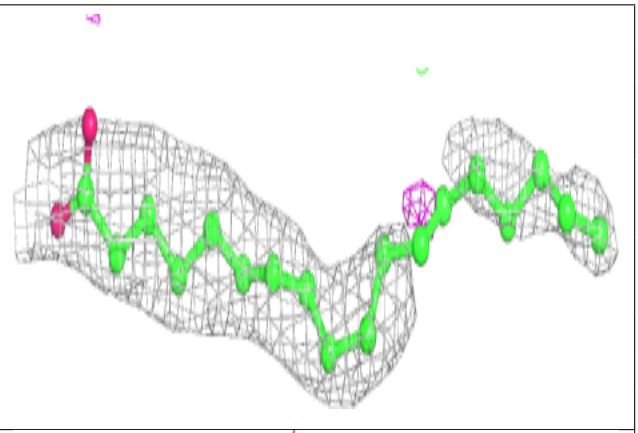
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

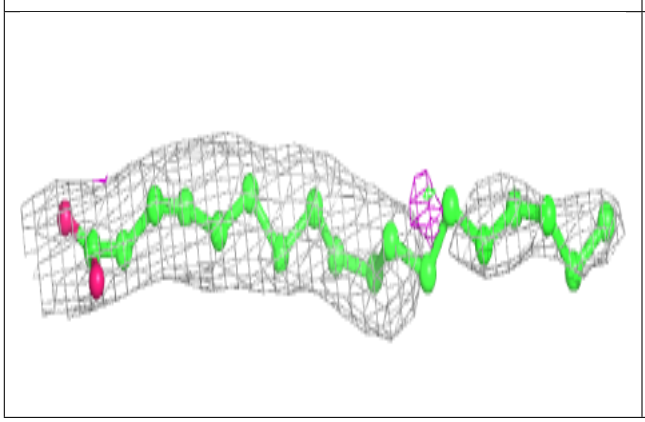


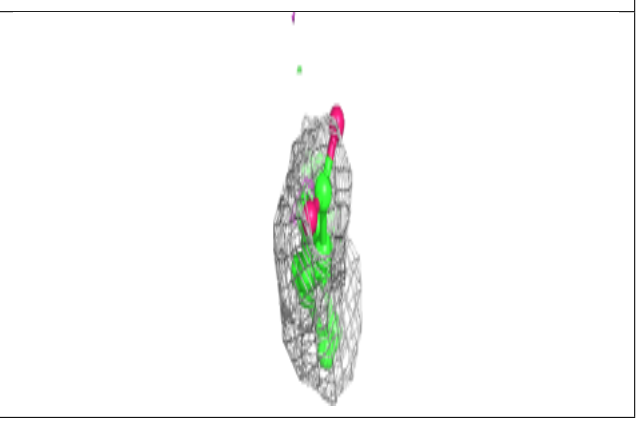


Electron density around OLA A 1214:

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

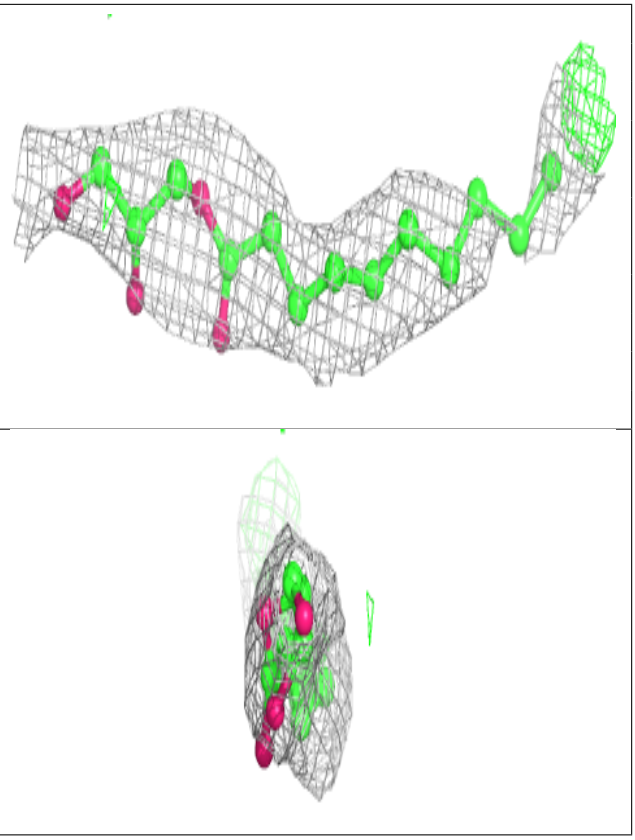






Electron density around OLC A 1219:

$2mF_o$-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 1217:

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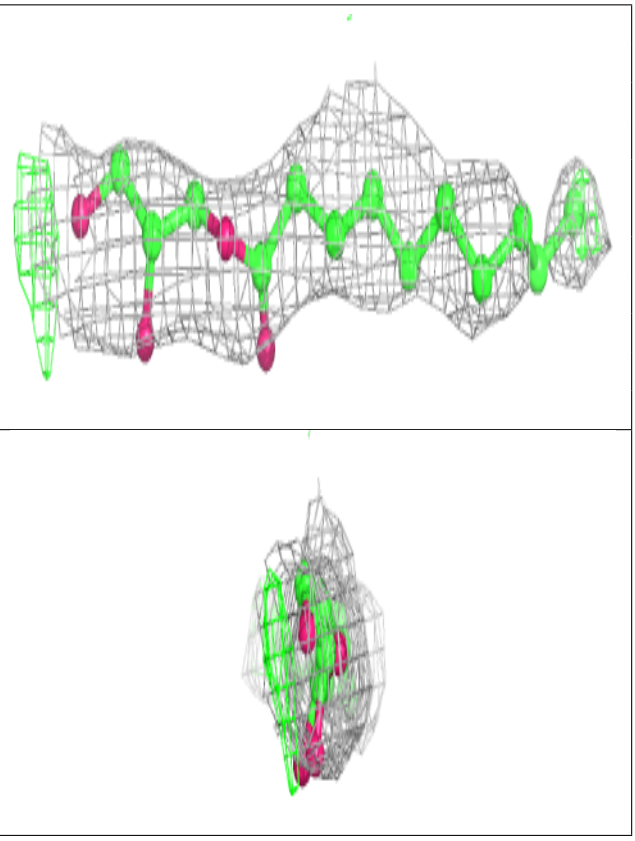
and green (positive)



Electron density around OLC A 1221:

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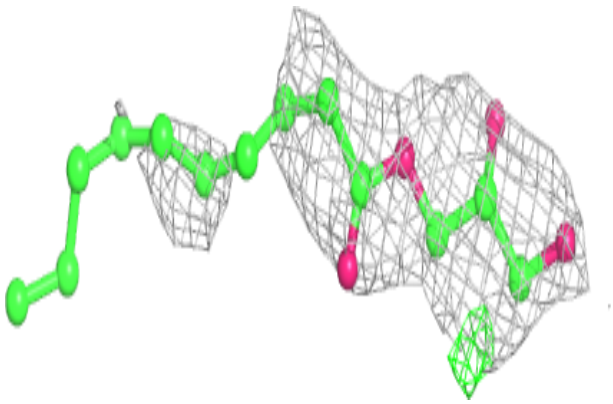
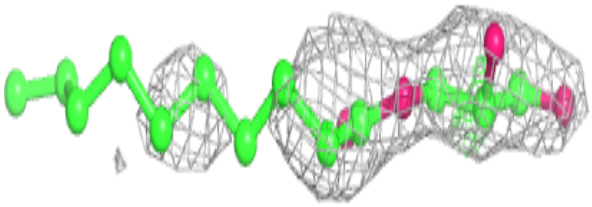
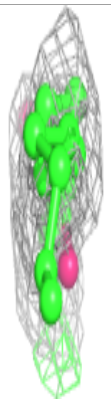
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

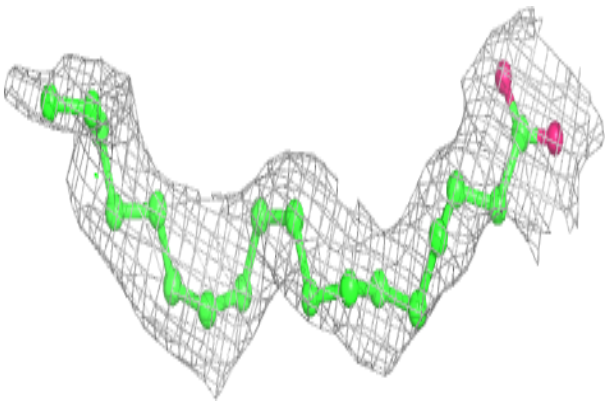


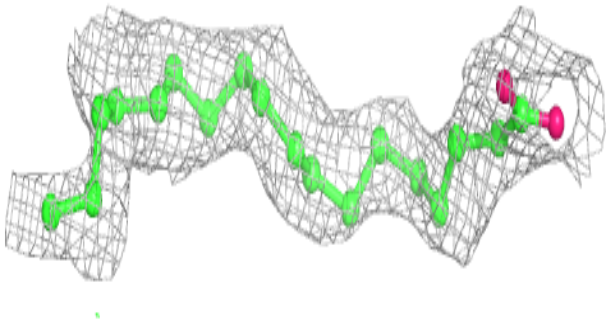


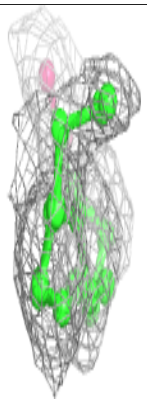


Electron density around OLA A 1215:

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

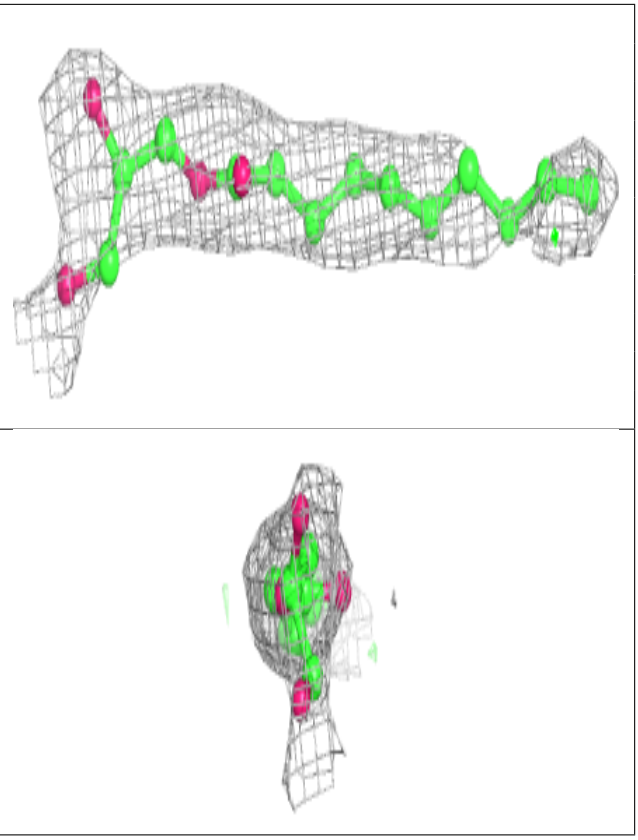






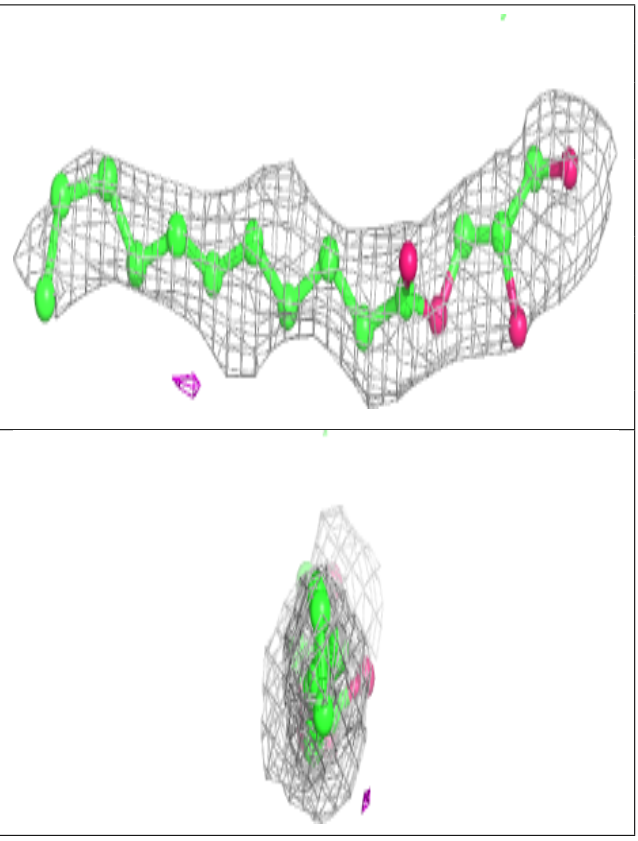
Electron density around OLC A 1218:

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



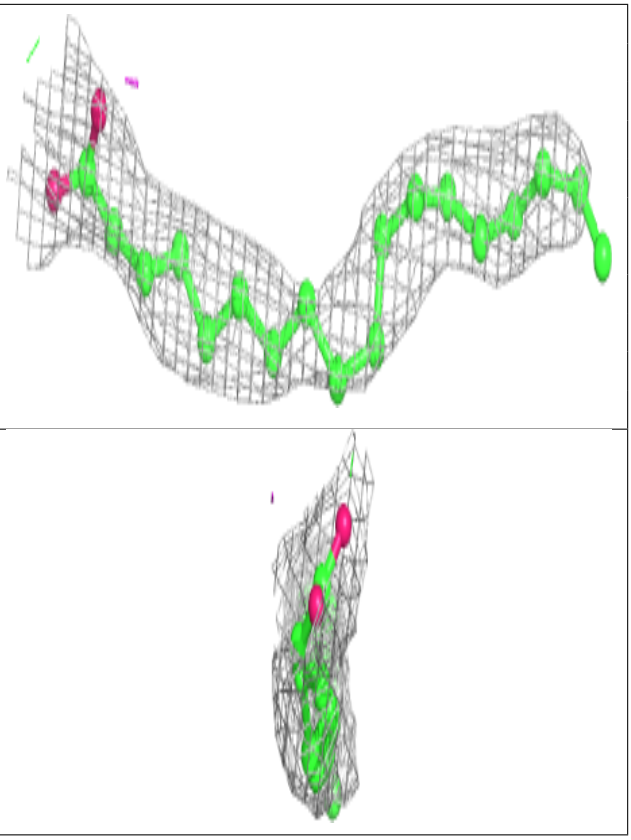
Electron density around OLB A 1223:

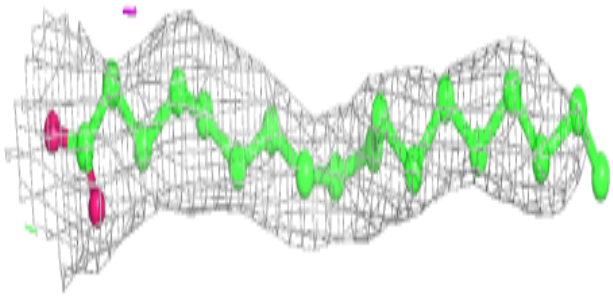
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLA A 1216:

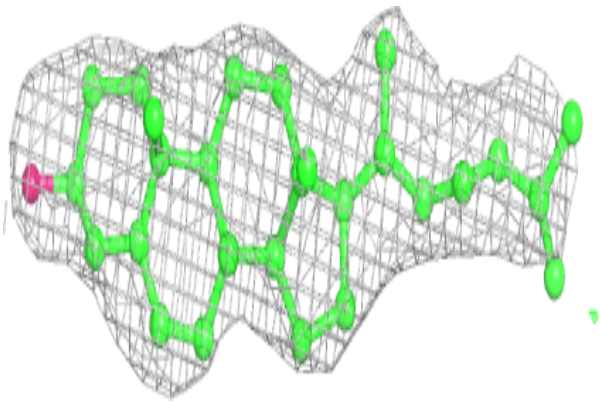
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

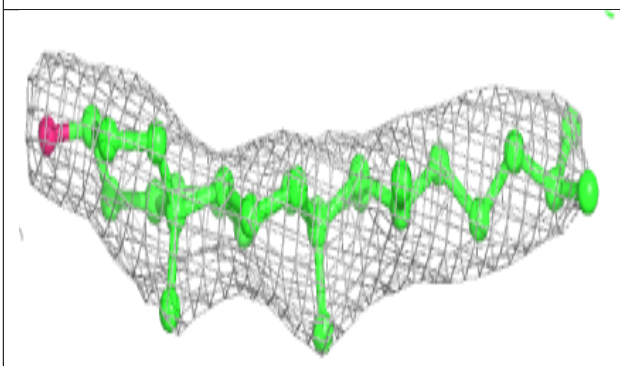


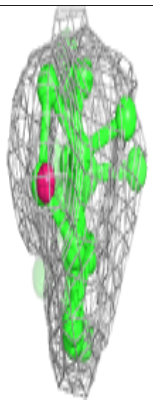


Electron density around CLR A 1202:

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

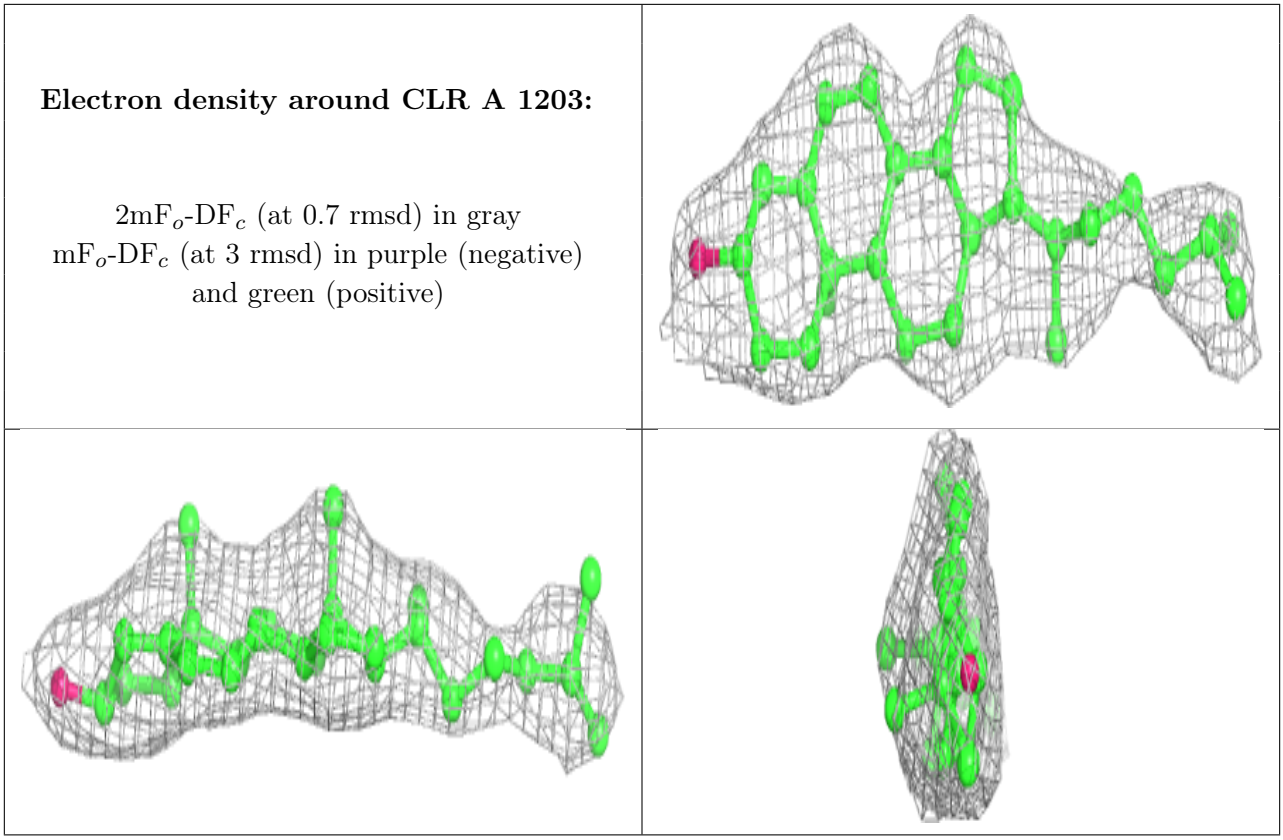






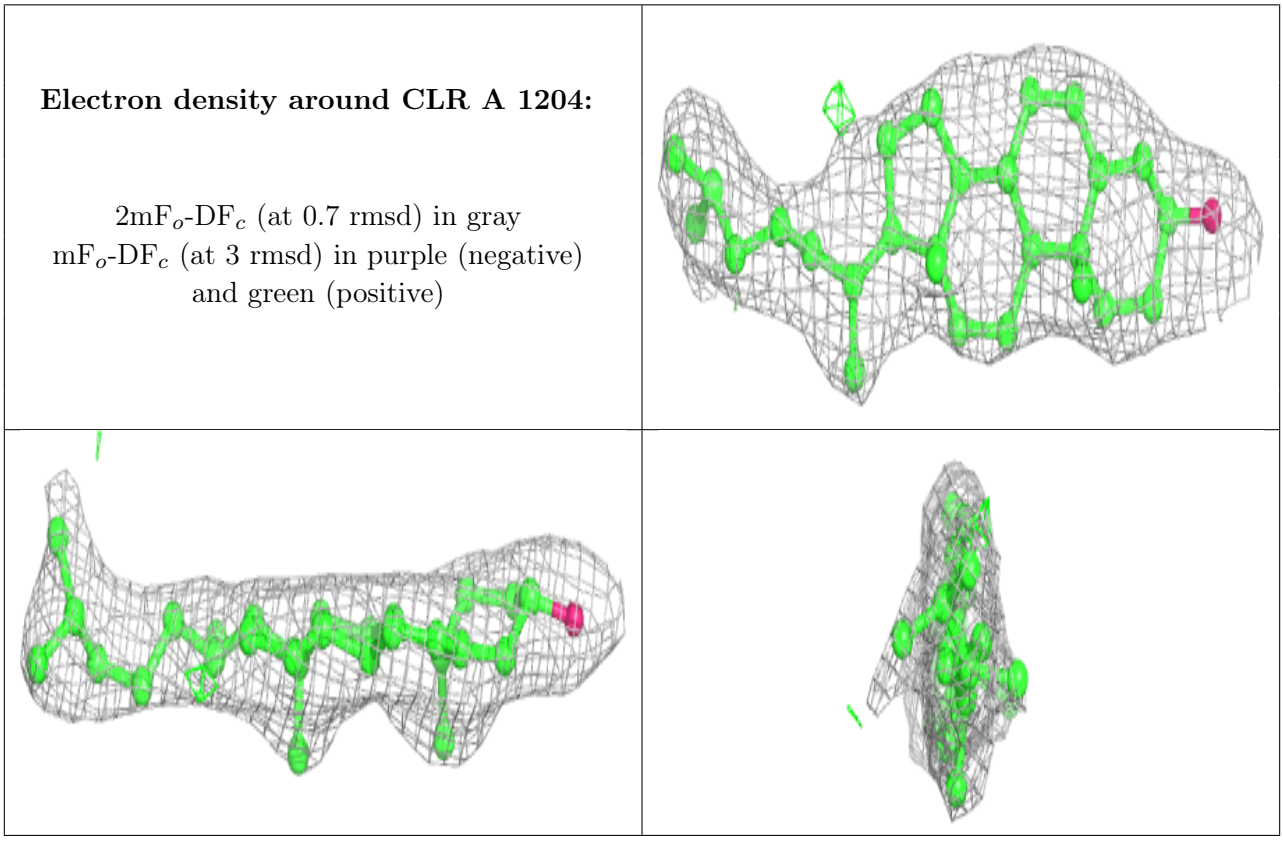
Electron density around CLR A 1203:

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



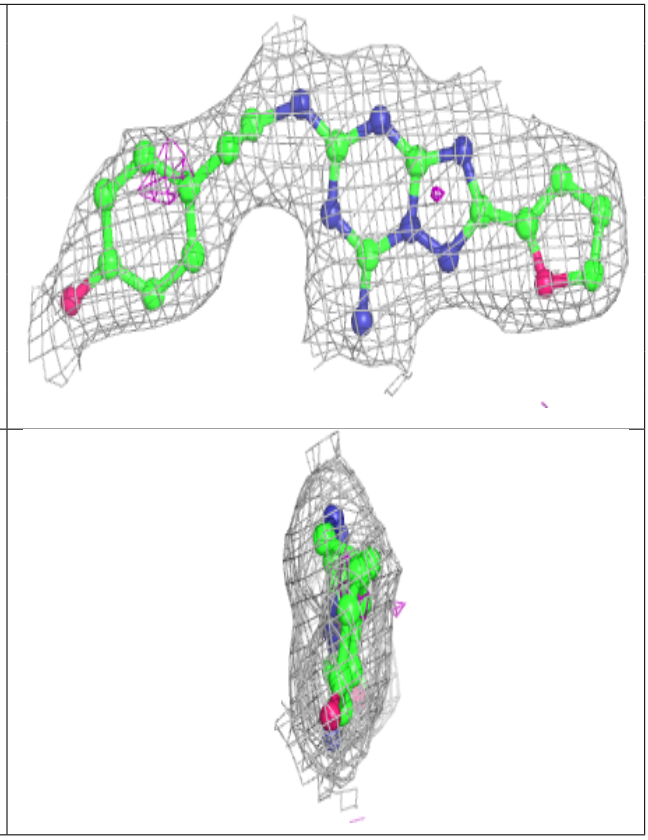
Electron density around CLR A 1204:

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



Electron density around ZMA A 1201:

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



6.5 Other polymers (i)

There are no such residues in this entry.