Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:05 AM EDT

PDB ID	:	5OQT
Title	:	Crystal structure of a bacterial cationic amino acid transporter (CAT) homologue
Authors	:	Jungnickel, K.E.J.; Newstead, S.
Deposited on	:	2017-08-14
Resolution	:	2.86 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:

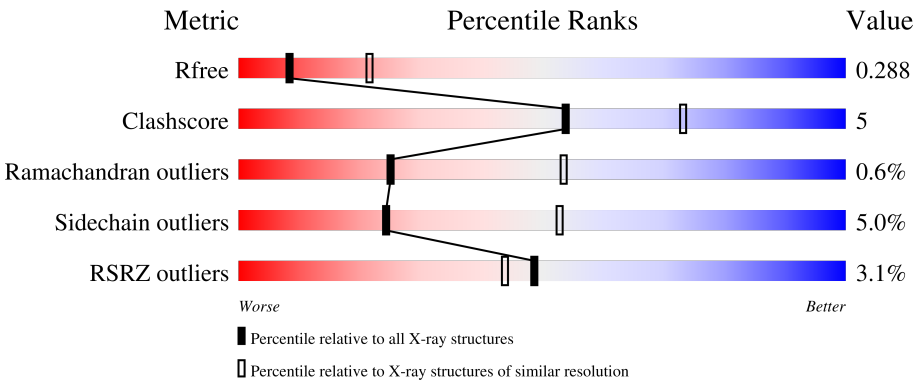
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	471	3% 82% 13% • •
2	C	31	71% 16% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLC	A	501	-	-	-	X
3	OLC	A	502	-	-	-	X
3	OLC	A	508	-	-	-	X
3	OLC	A	512	-	-	-	X
3	OLC	C	102	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4127 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.

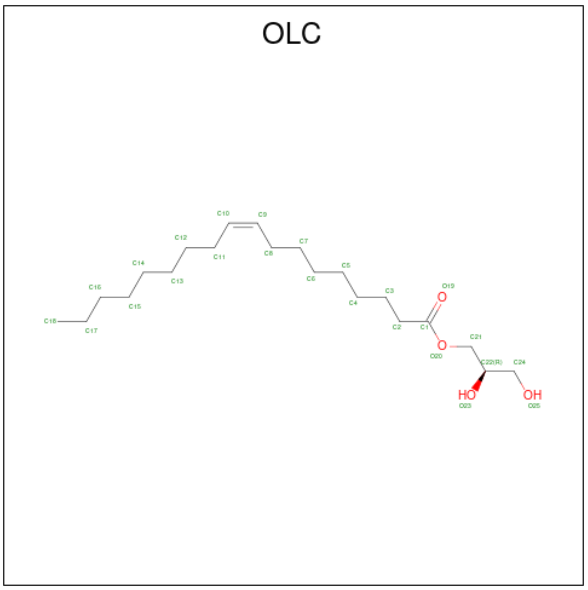
- Molecule 1 is a protein called Amino acid transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	3478	2331	547	589	11	0	0	0

- Molecule 2 is a protein called Uncharacterized protein YneM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	27	207	141	31	32	3	0	0	0

- Molecule 3 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		
3	A	1	25	21	4	0	0
3	A	1	Total 25	C 21	O 4	0	0

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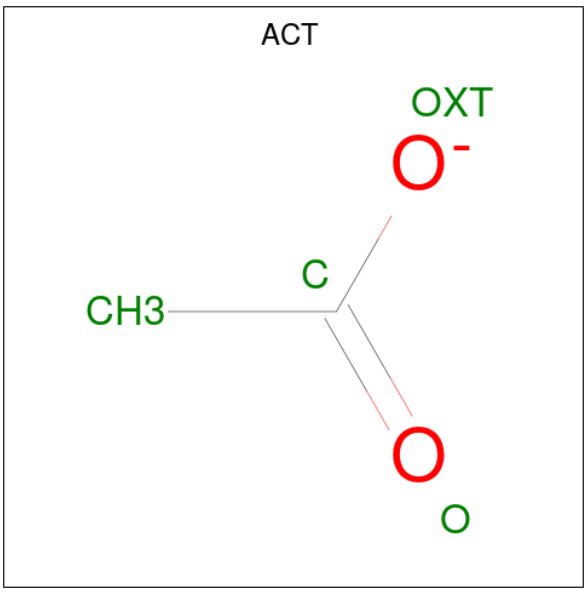
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	C	1	Total C O 25 21 4	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

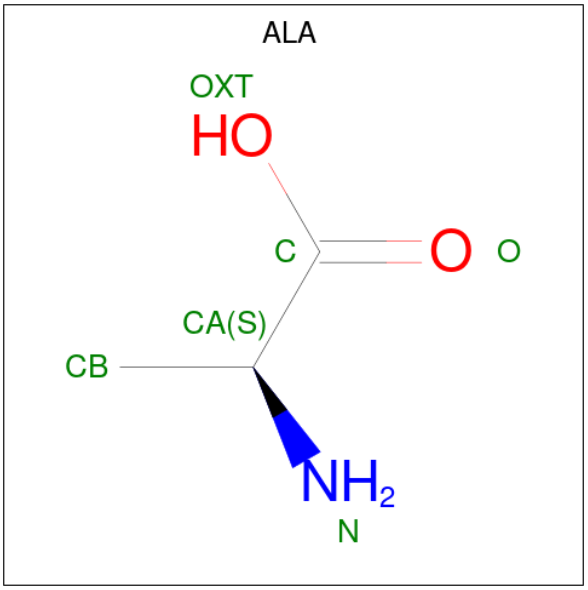


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	4	2	2		0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

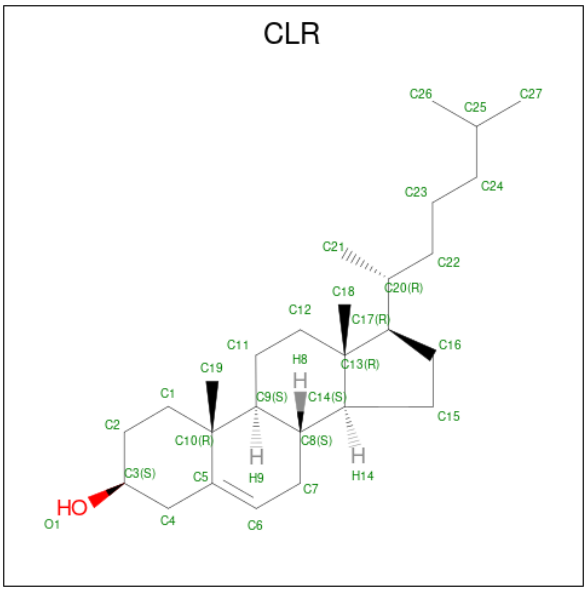
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	5	3	1	1	0	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 8 is water.

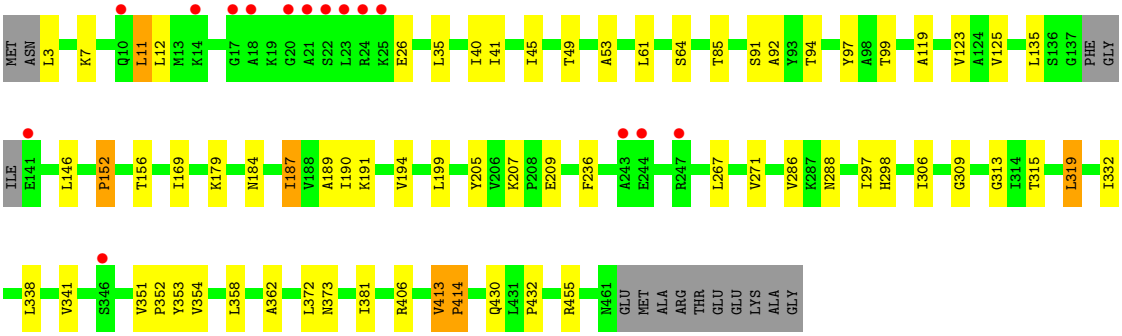
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	106	Total O 106 106	0	0
8	C	2	Total O 2 2	0	0

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.

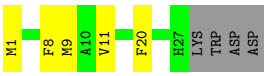
• Molecule 1: Amino acid transporter

Chain A:



• Molecule 2: Uncharacterized protein YneM

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.92Å 83.15Å 119.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.72 – 2.86 64.72 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.2 (64.72-2.86) 99.2 (64.72-2.86)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.215 , 0.271 0.229 , 0.288	Depositor DCC
R_{free} test set	901 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 75.8	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	0.92	EDS
Total number of atoms	4127	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: ACT, OLC, CLR, CL

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	0.49	0/3568	0.65	0/4875
2	C	0.44	0/212	0.67	0/284
All	All	0.49	0/3780	0.65	0/5159

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	3478	0	3631	38	0
2	C	207	0	211	6	0
3	A	271	0	434	13	0
3	C	25	0	40	1	0
4	A	4	0	3	0	0
5	A	1	0	0	0	0
6	A	5	0	4	0	0
7	C	28	0	46	1	0
8	A	106	0	0	0	0
8	C	2	0	0	0	0
All	All	4127	0	4369	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (44) 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:413:VAL:HG13	1:A:414:PRO:HD3	1.60	0.82
1:A:207:LYS:HG3	3:A:501:OLC:H24	1.74	0.67
1:A:85:THR:CG2	1:A:406:ARG:HG2	2.29	0.62
3:A:503:OLC:H11	3:A:512:OLC:H2A	1.82	0.61
1:A:53:ALA:HB2	1:A:61:LEU:HD22	1.83	0.61
1:A:205:TYR:HB3	1:A:297:ILE:HG12	1.83	0.59
1:A:191:LYS:HG3	1:A:313:GLY:HA3	1.86	0.58
1:A:169:ILE:HD11	1:A:315:THR:HG23	1.87	0.56
1:A:184:ASN:HB2	3:A:509:OLC:H22	1.88	0.55
1:A:199:LEU:HB3	3:A:501:OLC:H14	1.90	0.54
1:A:85:THR:HG22	1:A:406:ARG:HG2	1.90	0.53
1:A:179:LYS:HB2	3:A:509:OLC:H24A	1.90	0.53
1:A:12:LEU:HD22	1:A:94:THR:HG23	1.90	0.53
1:A:286:VAL:HG12	1:A:288:ASN:H	1.74	0.53
1:A:267:LEU:O	1:A:271:VAL:HG23	2.11	0.51
1:A:189:ALA:CB	2:C:11:VAL:HG23	2.40	0.51
1:A:152:PRO:HD3	1:A:156:THR:O	2.12	0.50
1:A:189:ALA:HB1	2:C:11:VAL:HG23	1.94	0.48
3:A:501:OLC:H17A	3:A:512:OLC:H10	1.96	0.47
2:C:9:MET:HB3	3:C:102:OLC:H4	1.97	0.46
1:A:351:VAL:HB	1:A:352:PRO:HD2	1.97	0.46
2:C:20:PHE:CD1	7:C:101:CLR:H211	2.50	0.46
1:A:362:ALA:HB2	3:A:506:OLC:H6	1.98	0.45
1:A:7:LYS:HE3	1:A:11:LEU:HD12	1.98	0.45
1:A:205:TYR:CB	1:A:297:ILE:HG12	2.46	0.45
1:A:45:ILE:O	1:A:49:THR:CG2	2.65	0.45
1:A:194:VAL:HG11	1:A:309:GLY:HA3	1.99	0.44
3:A:503:OLC:H13	3:A:512:OLC:H4A	1.99	0.44
1:A:40:ILE:HD11	1:A:236:PHE:HB3	1.99	0.44
1:A:125:VAL:HG11	1:A:372:LEU:HB2	1.99	0.44
1:A:358:LEU:HB3	3:A:506:OLC:H4	1.99	0.44
1:A:319:LEU:HD13	3:A:509:OLC:H3	1.99	0.43
1:A:119:ALA:O	1:A:123:VAL:HG23	2.18	0.43
1:A:3:LEU:HG	1:A:455:ARG:HH22	1.83	0.43
1:A:189:ALA:HB3	2:C:11:VAL:CG2	2.49	0.42
1:A:41:ILE:HB	1:A:191:LYS:HD2	2.02	0.42
1:A:338:LEU:HD23	1:A:338:LEU:HA	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HA	1:A:190:ILE:HD12	2.02	0.42
1:A:354:VAL:HG22	3:A:506:OLC:H24	2.01	0.42
1:A:332:ILE:HG22	1:A:338:LEU:HB2	2.02	0.41
3:A:504:OLC:H7A	3:A:509:OLC:H4A	2.02	0.41
1:A:189:ALA:HB2	2:C:8:PHE:CD1	2.55	0.41
1:A:432:PRO:HA	3:A:507:OLC:H4A	2.03	0.41
1:A:341:VAL:HG12	1:A:353:TYR:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	452/471 (96%)	424 (94%)	25 (6%)	3 (1%)	22	50
2	C	25/31 (81%)	24 (96%)	1 (4%)	0	100	100
All	All	477/502 (95%)	448 (94%)	26 (6%)	3 (1%)	25	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	PRO
1	A	92	ALA
1	A	414	PRO

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	362/373 (97%)	344 (95%)	18 (5%)	24	53
2	C	21/25 (84%)	20 (95%)	1 (5%)	25	55
All	All	383/398 (96%)	364 (95%)	19 (5%)	24	53

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	26	GLU
1	A	35	LEU
1	A	64	SER
1	A	91	SER
1	A	97	TYR
1	A	99	THR
1	A	135	LEU
1	A	146	LEU
1	A	187	ILE
1	A	209	GLU
1	A	298	HIS
1	A	306	ILE
1	A	319	LEU
1	A	373	ASN
1	A	381	ILE
1	A	413	VAL
1	A	430	GLN
2	C	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	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 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	OLC	A	508	-	9,9,24	0.50	0	8,8,25	0.62	0
3	OLC	A	507	-	24,24,24	0.85	1 (4%)	25,25,25	0.91	1 (4%)
7	CLR	C	101	-	31,31,31	1.69	10 (32%)	48,48,48	1.56	7 (14%)
6	ALA	A	515	-	3,4,5	0.83	0	2,4,6	1.51	1 (50%)
4	ACT	A	513	-	3,3,3	1.11	0	3,3,3	0.85	0
3	OLC	A	509	-	24,24,24	0.78	0	25,25,25	0.72	0
3	OLC	A	511	-	24,24,24	0.75	0	25,25,25	0.67	0
3	OLC	C	102	-	24,24,24	0.86	1 (4%)	25,25,25	0.88	2 (8%)
3	OLC	A	505	-	10,10,24	0.44	0	8,9,25	0.72	0
3	OLC	A	501	-	24,24,24	0.92	2 (8%)	25,25,25	0.72	0
3	OLC	A	502	-	24,24,24	0.91	1 (4%)	25,25,25	0.97	2 (8%)
3	OLC	A	504	-	24,24,24	0.87	1 (4%)	25,25,25	0.97	2 (8%)
3	OLC	A	503	-	24,24,24	0.93	1 (4%)	25,25,25	0.94	2 (8%)
3	OLC	A	512	-	24,24,24	0.80	1 (4%)	25,25,25	0.73	0
3	OLC	A	506	-	24,24,24	0.79	0	25,25,25	0.74	0
3	OLC	A	510	-	24,24,24	0.80	1 (4%)	25,25,25	0.65	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
3	OLC	A	508	-	-	2/7/7/24	-
3	OLC	A	507	-	-	8/24/24/24	-
7	CLR	C	101	-	-	9/10/68/68	0/4/4/4
6	ALA	A	515	-	-	0/0/2/4	-
3	OLC	A	509	-	-	4/24/24/24	-
3	OLC	A	511	-	-	8/24/24/24	-
3	OLC	C	102	-	-	7/24/24/24	-
3	OLC	A	505	-	-	2/8/8/24	-
3	OLC	A	501	-	-	9/24/24/24	-
3	OLC	A	502	-	-	9/24/24/24	-
3	OLC	A	504	-	-	8/24/24/24	-
3	OLC	A	503	-	-	10/24/24/24	-
3	OLC	A	512	-	-	6/24/24/24	-
3	OLC	A	506	-	-	4/24/24/24	-
3	OLC	A	510	-	-	9/24/24/24	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	101	CLR	C10-C9	3.31	1.61	1.56
7	C	101	CLR	C13-C17	3.30	1.61	1.55
7	C	101	CLR	C8-C9	2.97	1.59	1.53
3	A	503	OLC	O20-C1	2.96	1.42	1.33
7	C	101	CLR	C13-C14	2.60	1.59	1.55
3	A	502	OLC	O20-C1	2.57	1.40	1.33
7	C	101	CLR	C18-C13	2.52	1.58	1.54
3	A	504	OLC	O20-C1	2.51	1.40	1.33
3	A	501	OLC	O20-C1	2.46	1.40	1.33
3	C	102	OLC	O20-C1	2.39	1.40	1.33
7	C	101	CLR	C12-C13	2.39	1.58	1.54
7	C	101	CLR	C2-C3	2.35	1.57	1.51
3	A	507	OLC	O20-C1	2.33	1.40	1.33
7	C	101	CLR	C4-C3	2.33	1.56	1.52
3	A	512	OLC	O20-C1	2.29	1.40	1.33
7	C	101	CLR	C11-C9	2.29	1.57	1.53
3	A	510	OLC	O20-C1	2.20	1.39	1.33
7	C	101	CLR	C1-C10	2.20	1.58	1.54
3	A	501	OLC	C21-C22	2.04	1.58	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	101	CLR	C17-C13-C14	-5.64	93.39	100.07
7	C	101	CLR	C21-C20-C22	-4.31	103.60	110.36
7	C	101	CLR	C13-C17-C20	2.95	124.10	119.49
3	A	502	OLC	O20-C1-O19	-2.92	116.23	123.59
3	A	504	OLC	O20-C1-O19	-2.85	116.40	123.59
3	A	507	OLC	O20-C1-O19	-2.57	117.12	123.59
7	C	101	CLR	C18-C13-C14	2.47	116.33	111.71
3	C	102	OLC	O20-C1-O19	-2.43	117.45	123.59
3	A	503	OLC	O20-C1-O19	-2.38	117.59	123.59
3	A	504	OLC	C21-O20-C1	2.32	125.72	117.12
3	A	503	OLC	C21-O20-C1	2.31	125.66	117.12
3	A	502	OLC	C21-O20-C1	2.31	125.66	117.12
3	C	102	OLC	C21-O20-C1	2.30	125.64	117.12
6	A	515	ALA	O-C-CA	-2.14	117.50	124.28
7	C	101	CLR	C1-C2-C3	2.12	113.19	110.47
7	C	101	CLR	C2-C3-C4	2.08	113.15	110.31
7	C	101	CLR	C16-C17-C13	-2.01	101.42	103.84

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	OLC	O23-C22-C24-O25
3	A	502	OLC	O20-C21-C22-O23
3	A	502	OLC	C2-C1-O20-C21
3	A	502	OLC	O19-C1-O20-C21
3	A	503	OLC	C2-C1-O20-C21
3	A	503	OLC	O19-C1-O20-C21
3	A	504	OLC	C2-C1-O20-C21
3	A	504	OLC	O19-C1-O20-C21
3	A	505	OLC	C9-C10-C11-C12
3	A	507	OLC	C2-C1-O20-C21
3	A	507	OLC	O19-C1-O20-C21
3	C	102	OLC	C2-C1-O20-C21
3	C	102	OLC	O19-C1-O20-C21
7	C	101	CLR	C13-C17-C20-C21
7	C	101	CLR	C16-C17-C20-C22
7	C	101	CLR	C13-C17-C20-C22
3	A	501	OLC	O20-C21-C22-O23
7	C	101	CLR	C16-C17-C20-C21
3	A	501	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
7	C	101	CLR	C17-C20-C22-C23
7	C	101	CLR	C21-C20-C22-C23
3	A	504	OLC	C13-C14-C15-C16
3	A	510	OLC	C2-C3-C4-C5
3	A	509	OLC	C11-C12-C13-C14
3	A	501	OLC	C4-C5-C6-C7
3	A	512	OLC	C3-C4-C5-C6
3	A	512	OLC	C4-C5-C6-C7
3	A	501	OLC	C21-C22-C24-O25
3	A	503	OLC	C21-C22-C24-O25
3	A	510	OLC	C21-C22-C24-O25
3	A	511	OLC	C21-C22-C24-O25
3	A	503	OLC	C4-C5-C6-C7
3	A	501	OLC	C11-C12-C13-C14
3	A	510	OLC	C14-C15-C16-C17
3	A	503	OLC	C14-C15-C16-C17
3	A	512	OLC	C14-C15-C16-C17
3	A	511	OLC	C6-C7-C8-C9
3	A	512	OLC	C10-C11-C12-C13
3	C	102	OLC	C10-C11-C12-C13
3	A	507	OLC	C1-C2-C3-C4
3	A	511	OLC	C3-C4-C5-C6
3	A	501	OLC	C12-C13-C14-C15
3	A	504	OLC	C4-C5-C6-C7
3	A	511	OLC	C11-C12-C13-C14
3	A	510	OLC	C11-C12-C13-C14
3	A	504	OLC	C6-C7-C8-C9
3	A	508	OLC	C15-C16-C17-C18
3	A	502	OLC	C2-C3-C4-C5
3	C	102	OLC	C11-C12-C13-C14
3	A	509	OLC	C5-C6-C7-C8
3	A	502	OLC	C14-C15-C16-C17
3	A	506	OLC	C15-C16-C17-C18
3	A	504	OLC	C11-C12-C13-C14
3	A	503	OLC	C15-C16-C17-C18
3	A	502	OLC	O20-C21-C22-C24
3	A	503	OLC	C3-C4-C5-C6
3	A	503	OLC	C2-C3-C4-C5
3	A	510	OLC	C13-C14-C15-C16
3	A	512	OLC	C15-C16-C17-C18
3	A	511	OLC	C15-C16-C17-C18
7	C	101	CLR	C23-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
3	A	503	OLC	C6-C7-C8-C9
3	A	511	OLC	O20-C21-C22-O23
3	A	511	OLC	C4-C5-C6-C7
7	C	101	CLR	C23-C24-C25-C26
3	C	102	OLC	C15-C16-C17-C18
3	A	508	OLC	C9-C10-C11-C12
3	A	504	OLC	C10-C11-C12-C13
3	A	506	OLC	C6-C7-C8-C9
3	A	504	OLC	C9-C10-C11-C12
3	A	506	OLC	C7-C8-C9-C10
3	A	510	OLC	C3-C4-C5-C6
3	A	512	OLC	C7-C8-C9-C10
3	A	509	OLC	C13-C14-C15-C16
3	A	502	OLC	C9-C10-C11-C12
3	A	505	OLC	C7-C8-C9-C10
3	A	502	OLC	O23-C22-C24-O25
3	A	511	OLC	O23-C22-C24-O25
3	A	503	OLC	C13-C14-C15-C16
3	A	501	OLC	C1-C2-C3-C4
3	A	506	OLC	C2-C3-C4-C5
3	A	507	OLC	C14-C15-C16-C17
3	A	510	OLC	C9-C10-C11-C12
3	A	507	OLC	O20-C1-C2-C3
3	A	509	OLC	C14-C15-C16-C17
3	A	510	OLC	O20-C1-C2-C3
3	C	102	OLC	C13-C14-C15-C16
3	A	507	OLC	C7-C8-C9-C10
3	A	510	OLC	O19-C1-C2-C3
3	A	502	OLC	C21-C22-C24-O25
3	A	507	OLC	O20-C21-C22-O23
3	A	501	OLC	C9-C10-C11-C12
3	A	507	OLC	O19-C1-C2-C3
3	C	102	OLC	C14-C15-C16-C17
7	C	101	CLR	C22-C23-C24-C25

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	OLC	1	0
7	C	101	CLR	1	0
3	A	509	OLC	4	0

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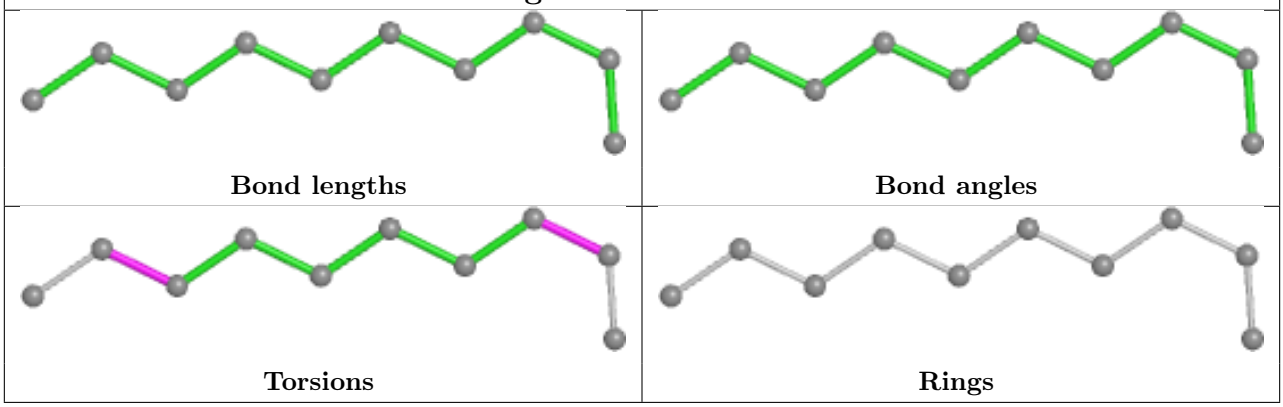
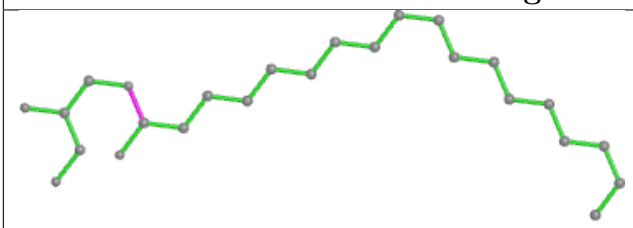
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	102	OLC	1	0
3	A	501	OLC	3	0
3	A	504	OLC	1	0
3	A	503	OLC	2	0
3	A	512	OLC	3	0
3	A	506	OLC	3	0

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.

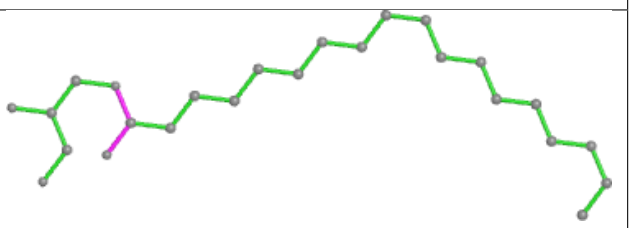
Ligand OLC A 508



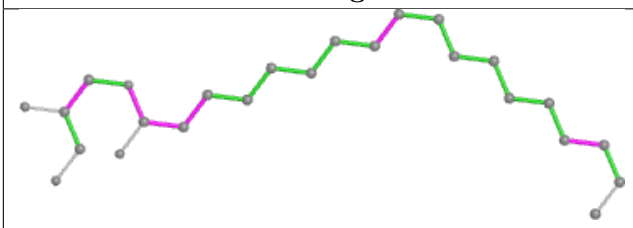
Ligand OLC A 507



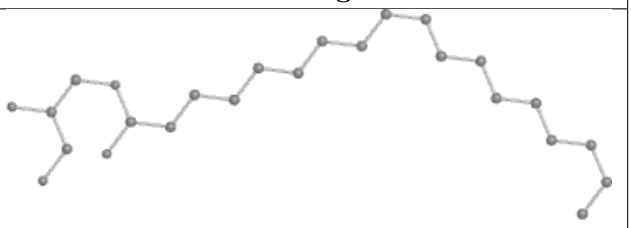
Bond lengths



Bond angles

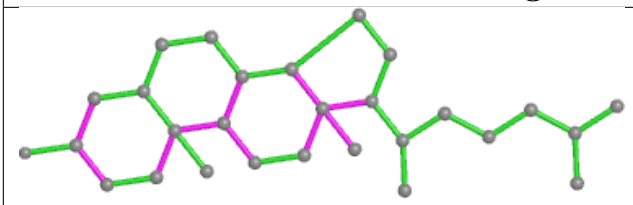


Torsions

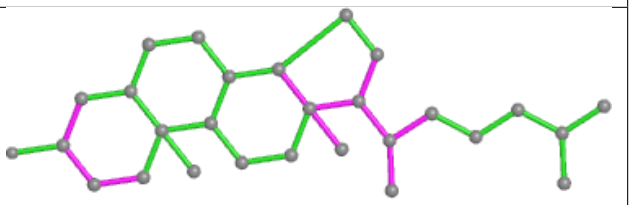


Rings

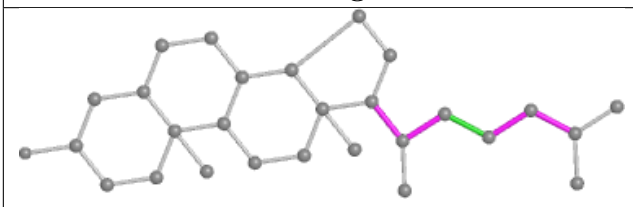
Ligand CLR C 101



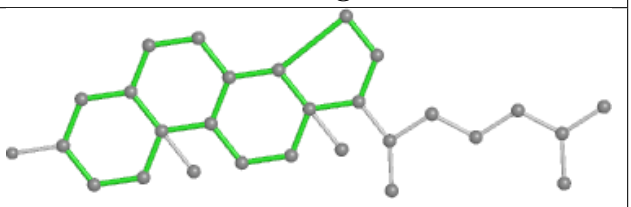
Bond lengths



Bond angles

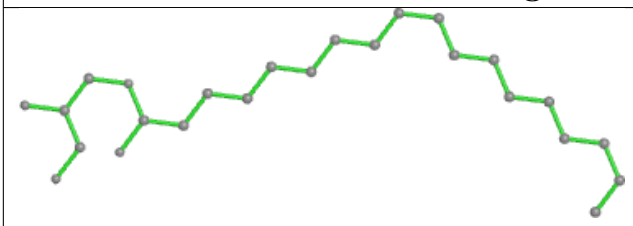


Torsions

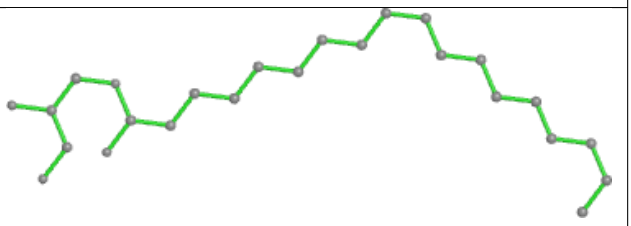


Rings

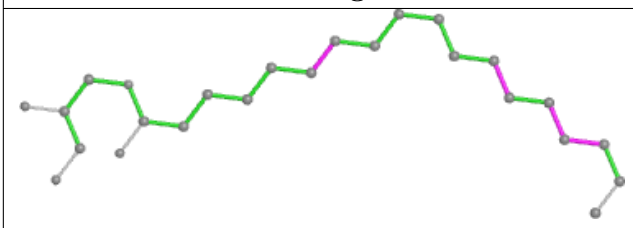
Ligand OLC A 509



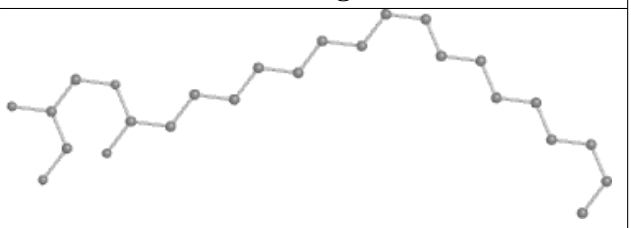
Bond lengths



Bond angles

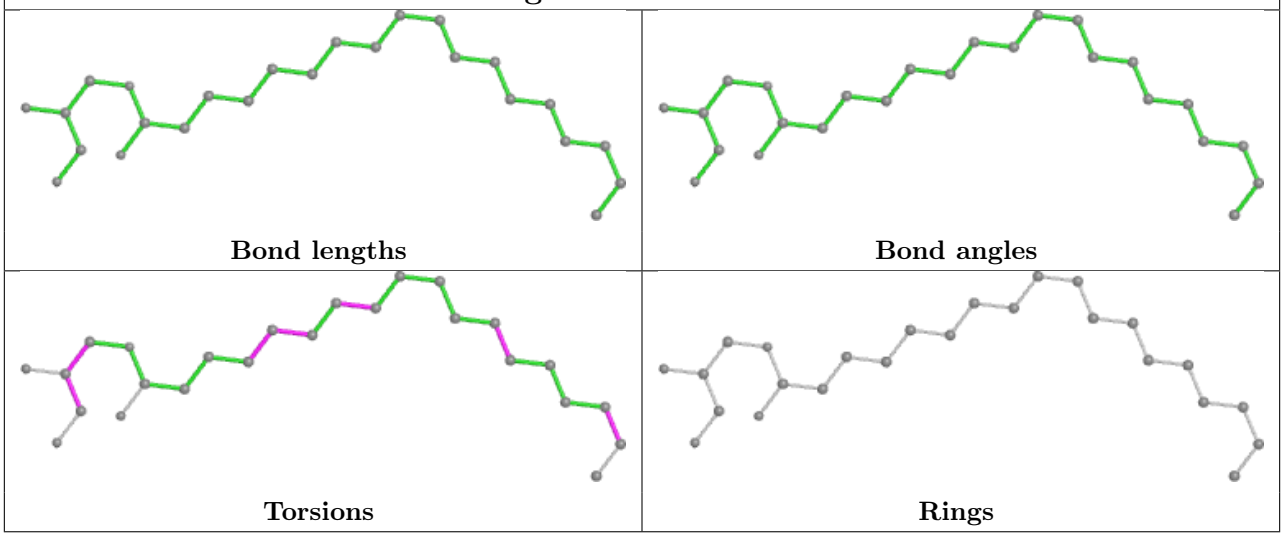


Torsions

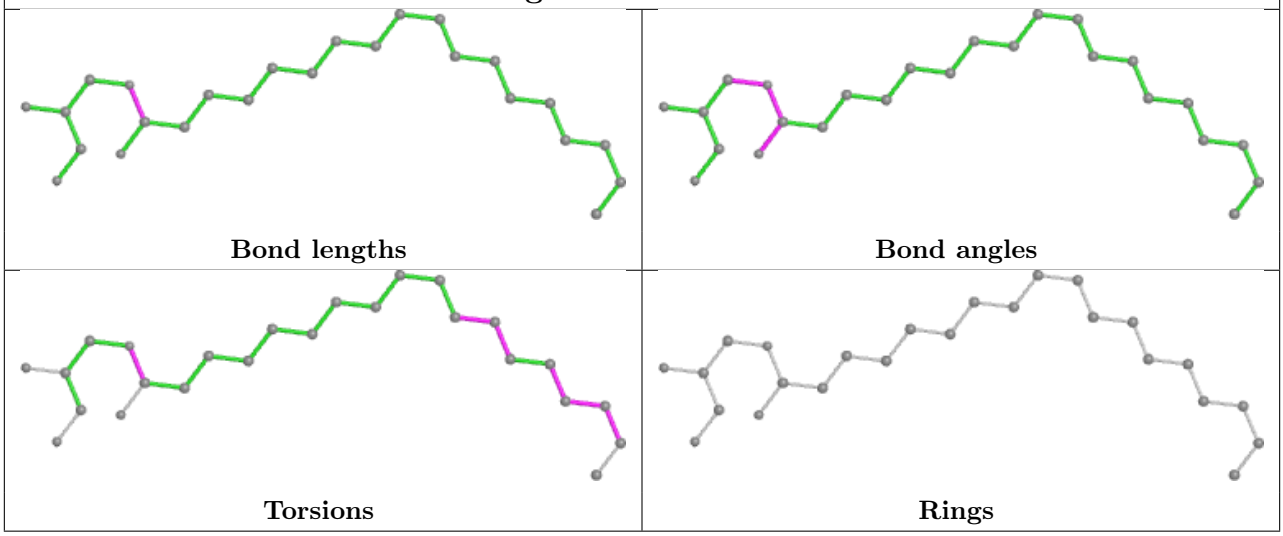


Rings

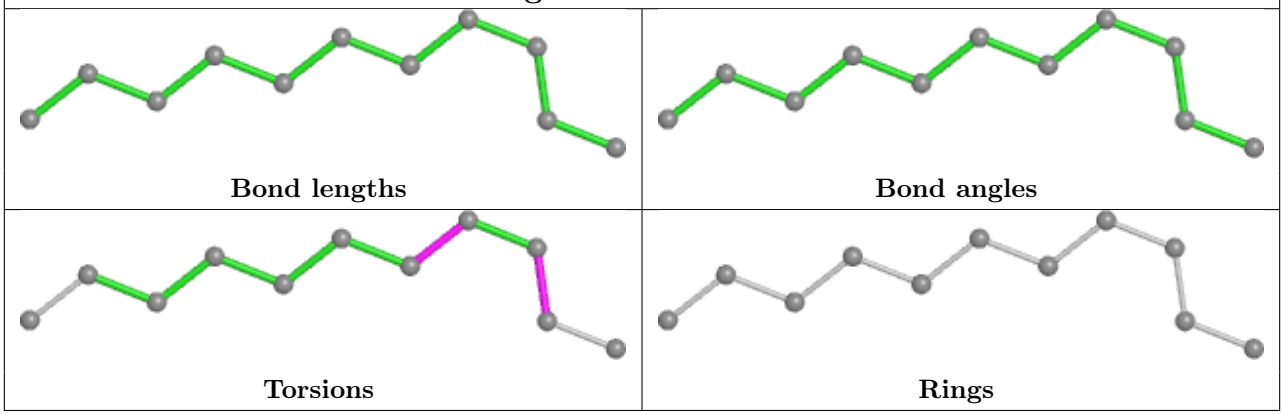
Ligand OLC A 511



Ligand OLC C 102



Ligand OLC A 505



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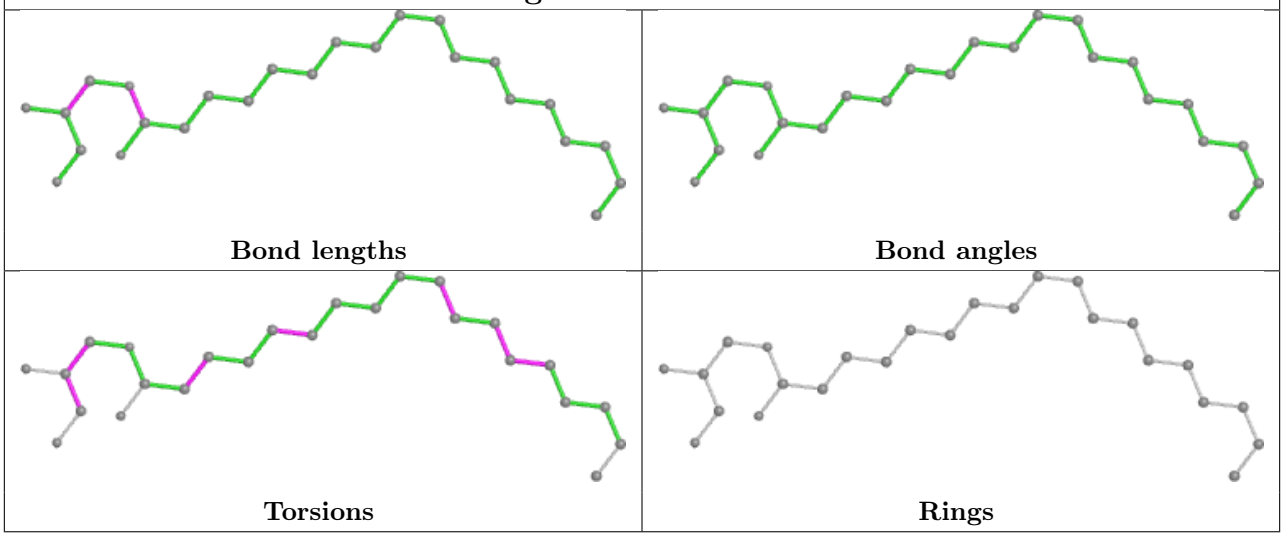

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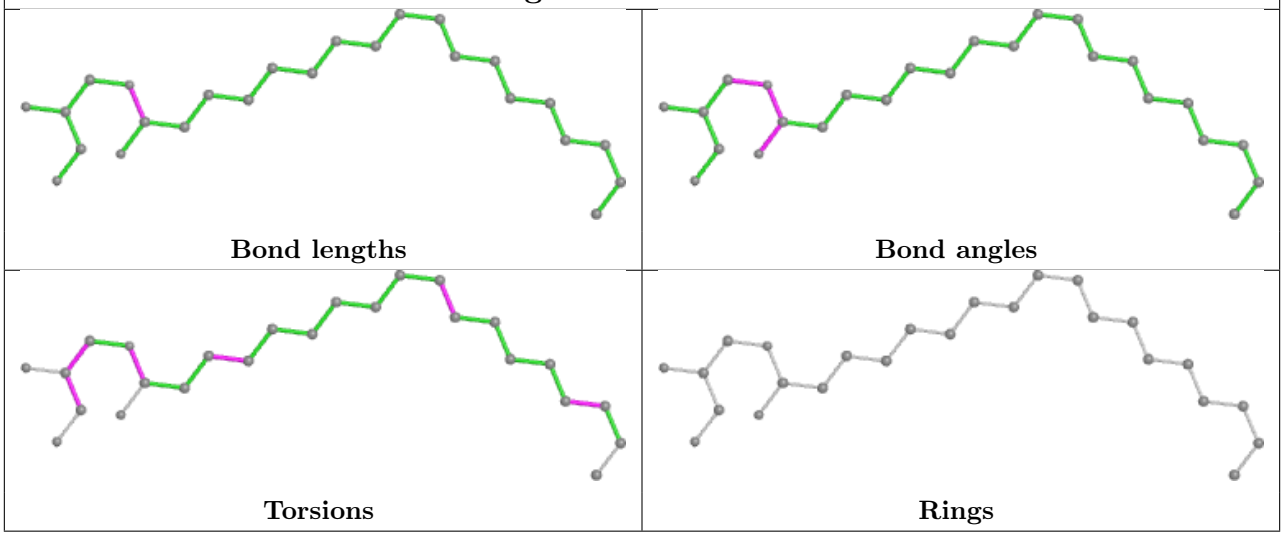

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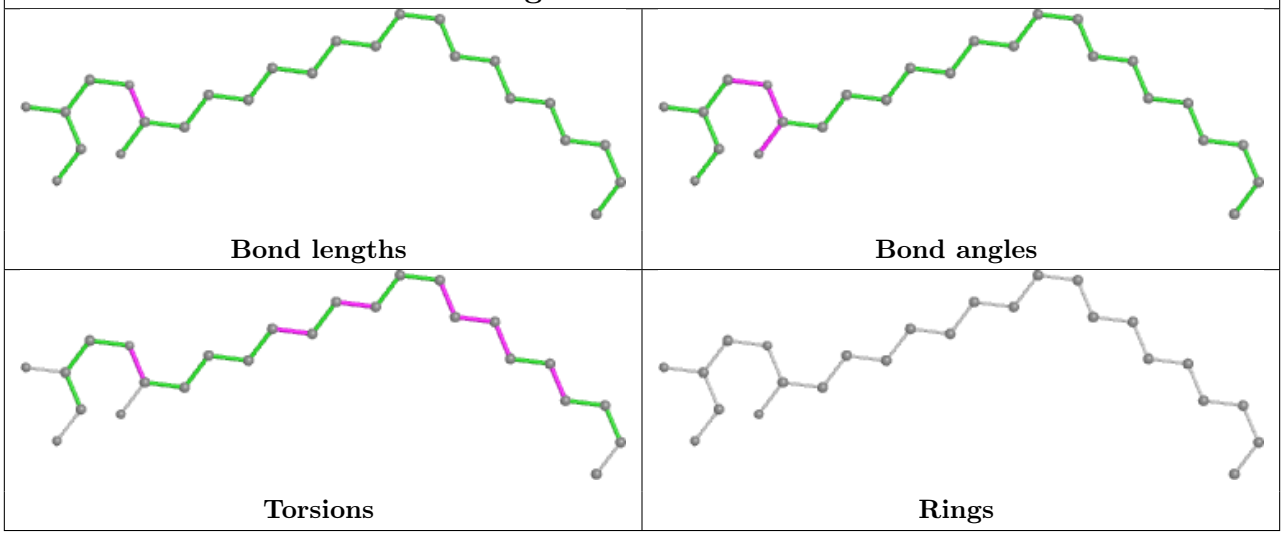

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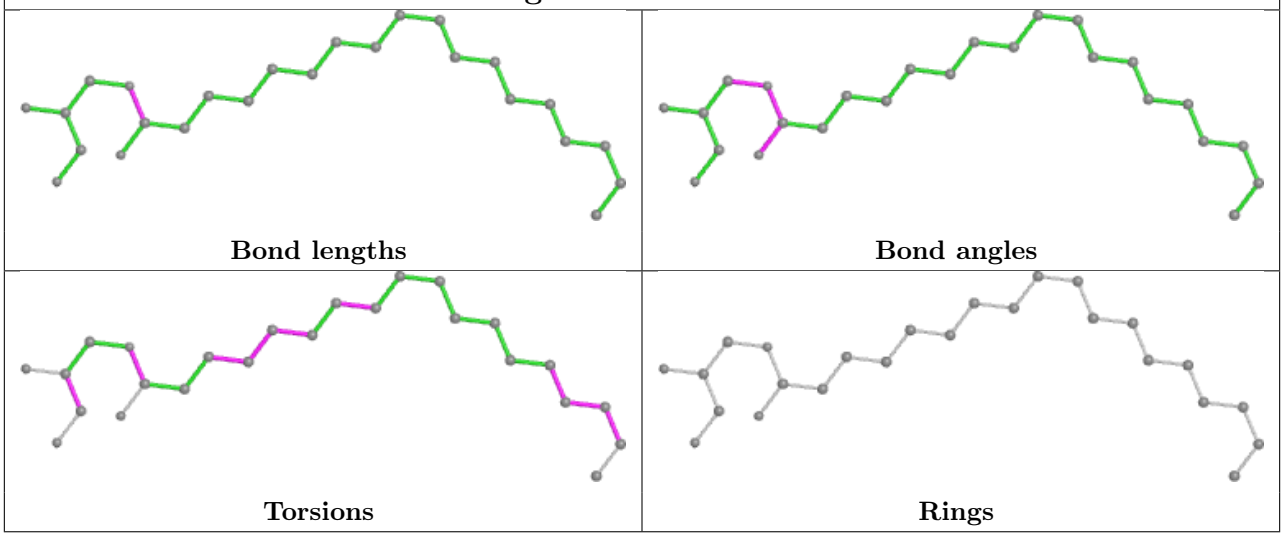
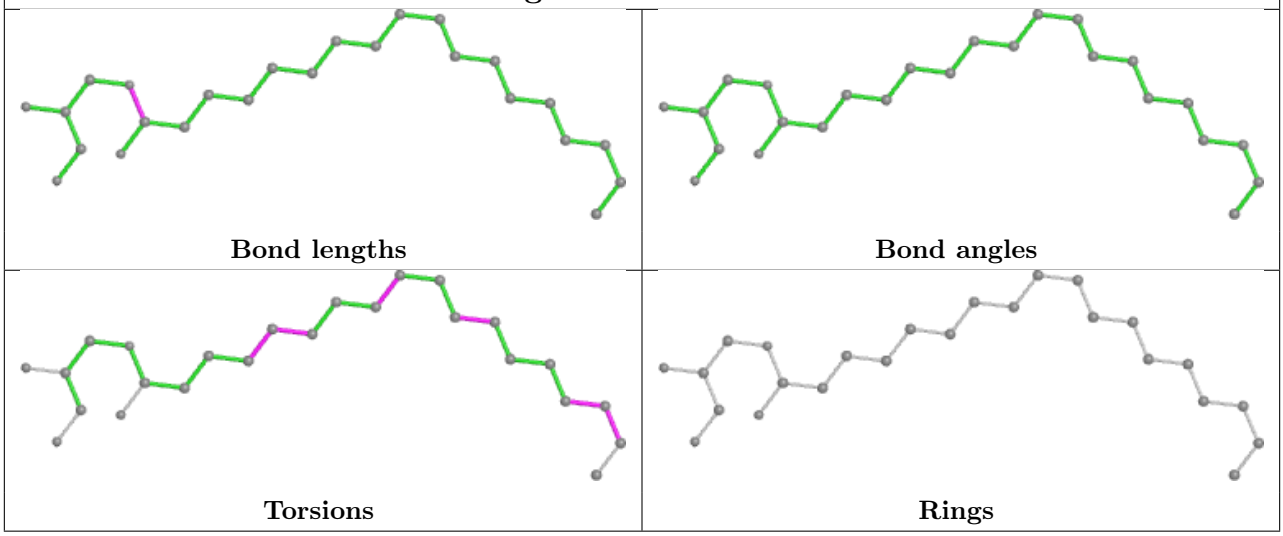


Ligand OLC A 512



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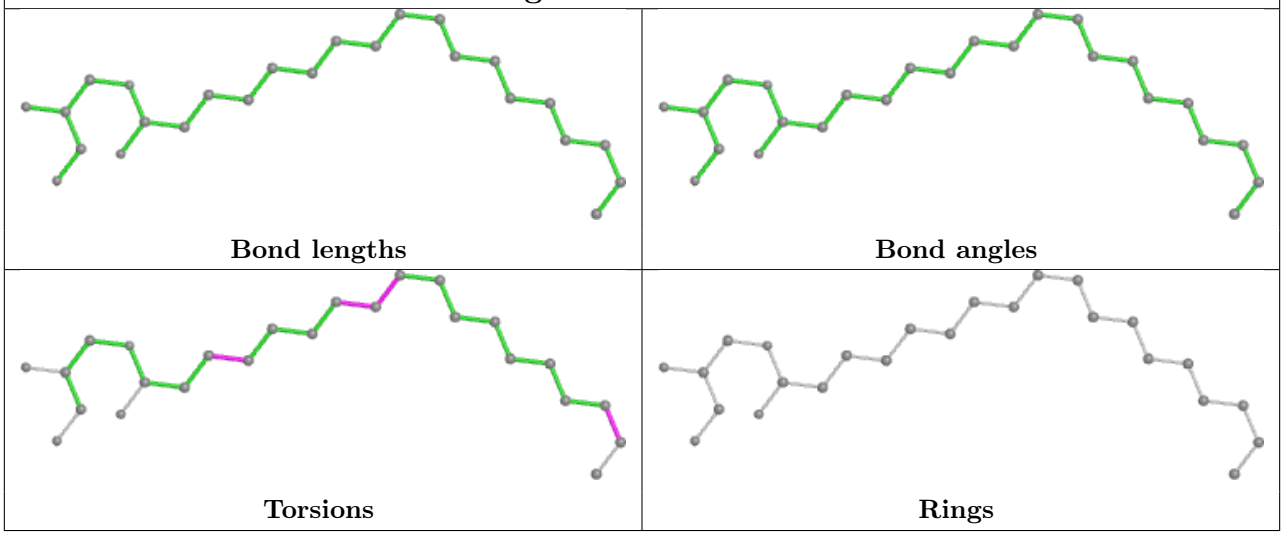
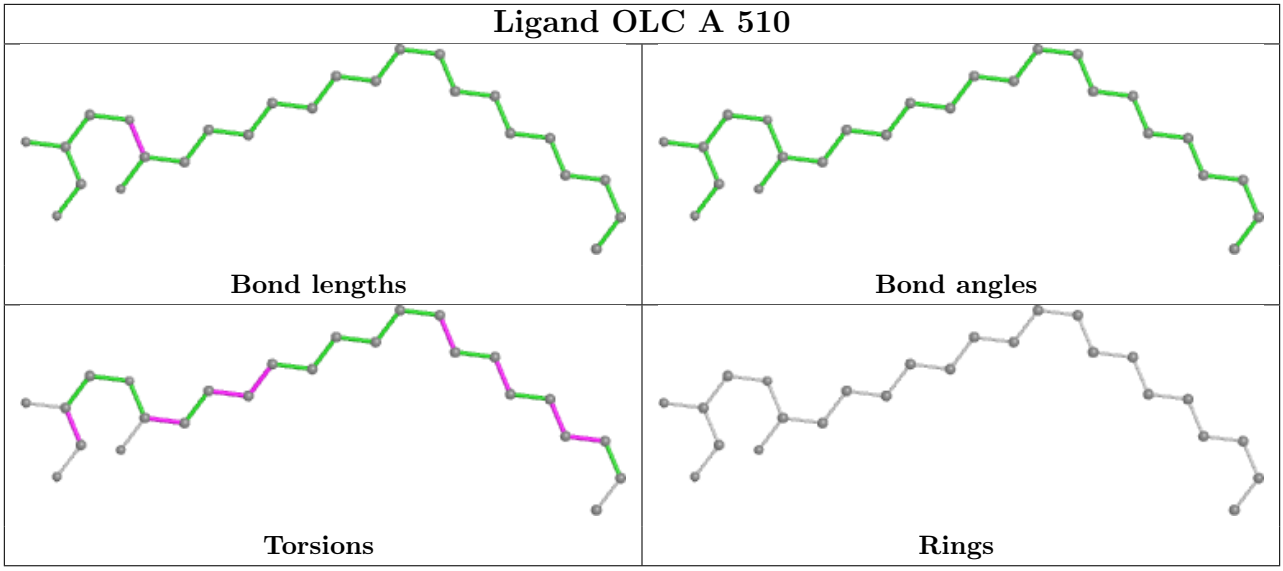




5.7 Other polymers (i)

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	456/471 (96%)	0.01	15 (3%) 46 41	49, 72, 117, 135	0
2	C	27/31 (87%)	0.01	0 100 100	59, 69, 106, 134	0
All	All	483/502 (96%)	0.01	15 (3%) 49 44	49, 72, 117, 135	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	SER	6.8
1	A	10	GLN	5.2
1	A	23	LEU	4.7
1	A	21	ALA	4.5
1	A	20	GLY	4.1
1	A	244	GLU	3.9
1	A	141	GLU	3.8
1	A	247	ARG	3.6
1	A	17	GLY	3.4
1	A	14	LYS	3.3
1	A	25	LYS	3.0
1	A	243	ALA	2.6
1	A	346	SER	2.3
1	A	24	ARG	2.3
1	A	18	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

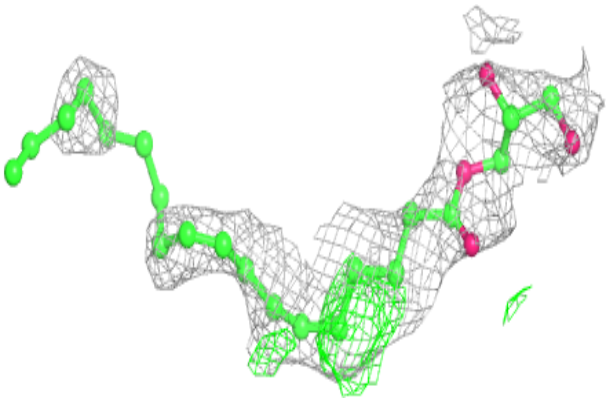
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

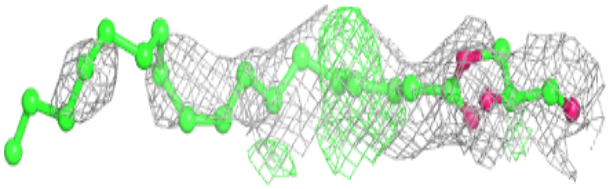
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLC	A	509	25/25	0.53	0.31	130,132,145,146	0
3	OLC	A	510	25/25	0.62	0.37	119,123,140,141	0
3	OLC	A	511	25/25	0.67	0.36	143,148,151,151	0
3	OLC	A	507	25/25	0.69	0.35	111,124,131,131	0
3	OLC	A	502	25/25	0.71	0.54	91,97,102,103	0
3	OLC	A	512	25/25	0.71	0.56	99,103,116,116	0
3	OLC	A	508	10/25	0.72	0.41	80,81,83,84	0
3	OLC	C	102	25/25	0.72	0.46	71,84,119,122	0
4	ACT	A	513	4/4	0.77	0.18	139,139,139,140	0
3	OLC	A	501	25/25	0.78	0.45	73,86,105,106	0
3	OLC	A	503	25/25	0.78	0.35	66,86,113,114	0
3	OLC	A	504	25/25	0.83	0.16	106,121,135,135	0
3	OLC	A	505	11/25	0.84	0.22	71,72,75,75	0
5	CL	A	514	1/1	0.84	0.37	79,79,79,79	0
3	OLC	A	506	25/25	0.85	0.41	93,95,99,99	0
7	CLR	C	101	28/28	0.89	0.29	71,83,90,91	0
6	ALA	A	515	5/6	0.94	0.20	32,35,49,57	0

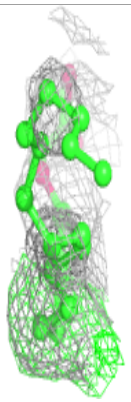
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 509:

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

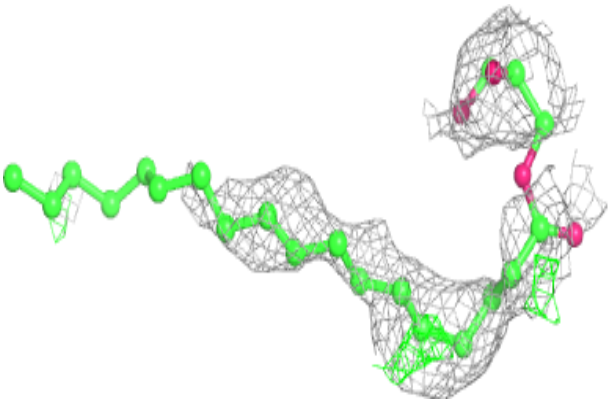


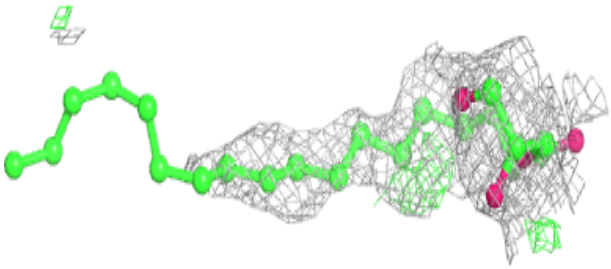


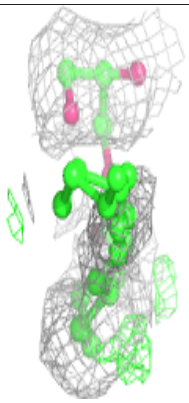


Electron density around OLC A 510:

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

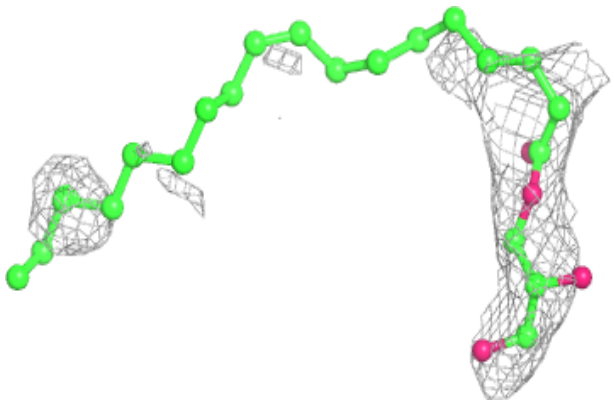


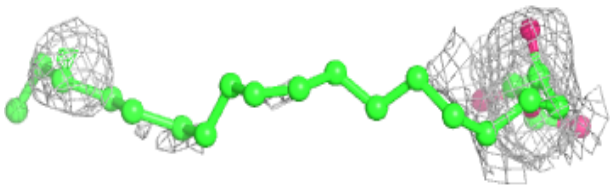


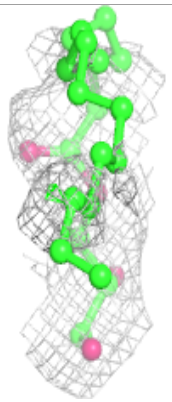


Electron density around OLC A 511:

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

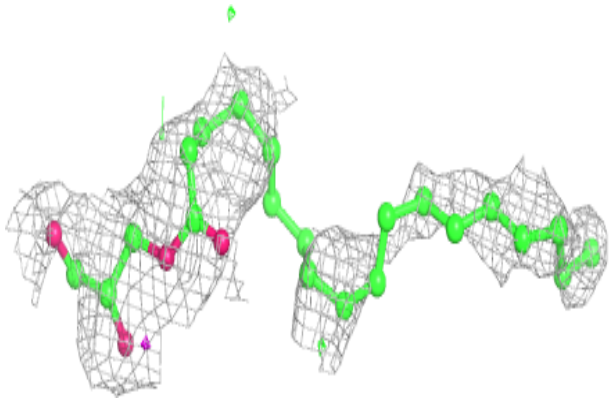


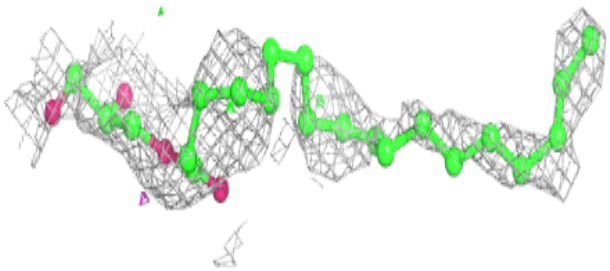


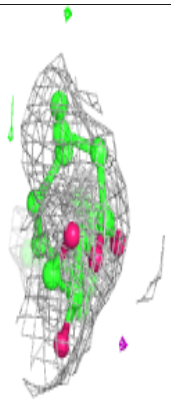


Electron density around OLC A 507:

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

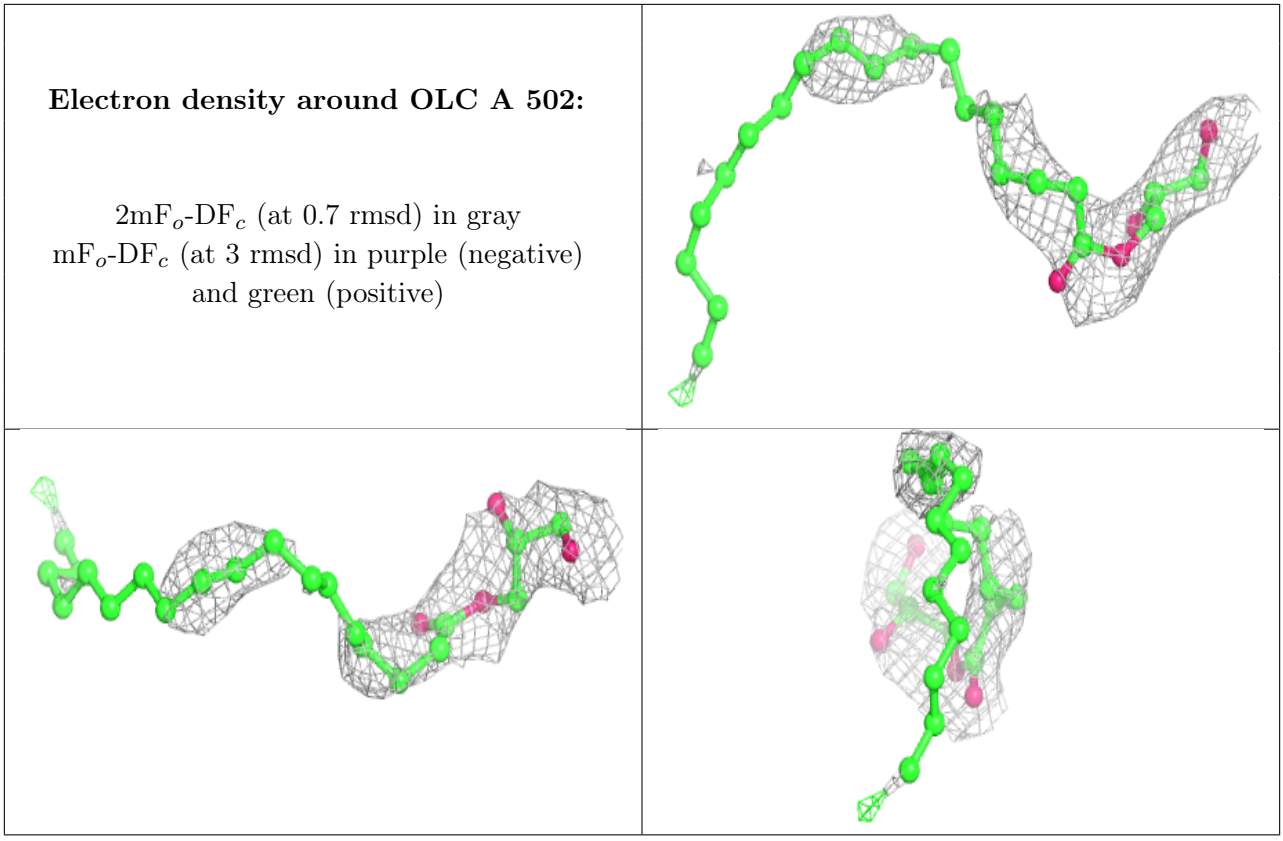






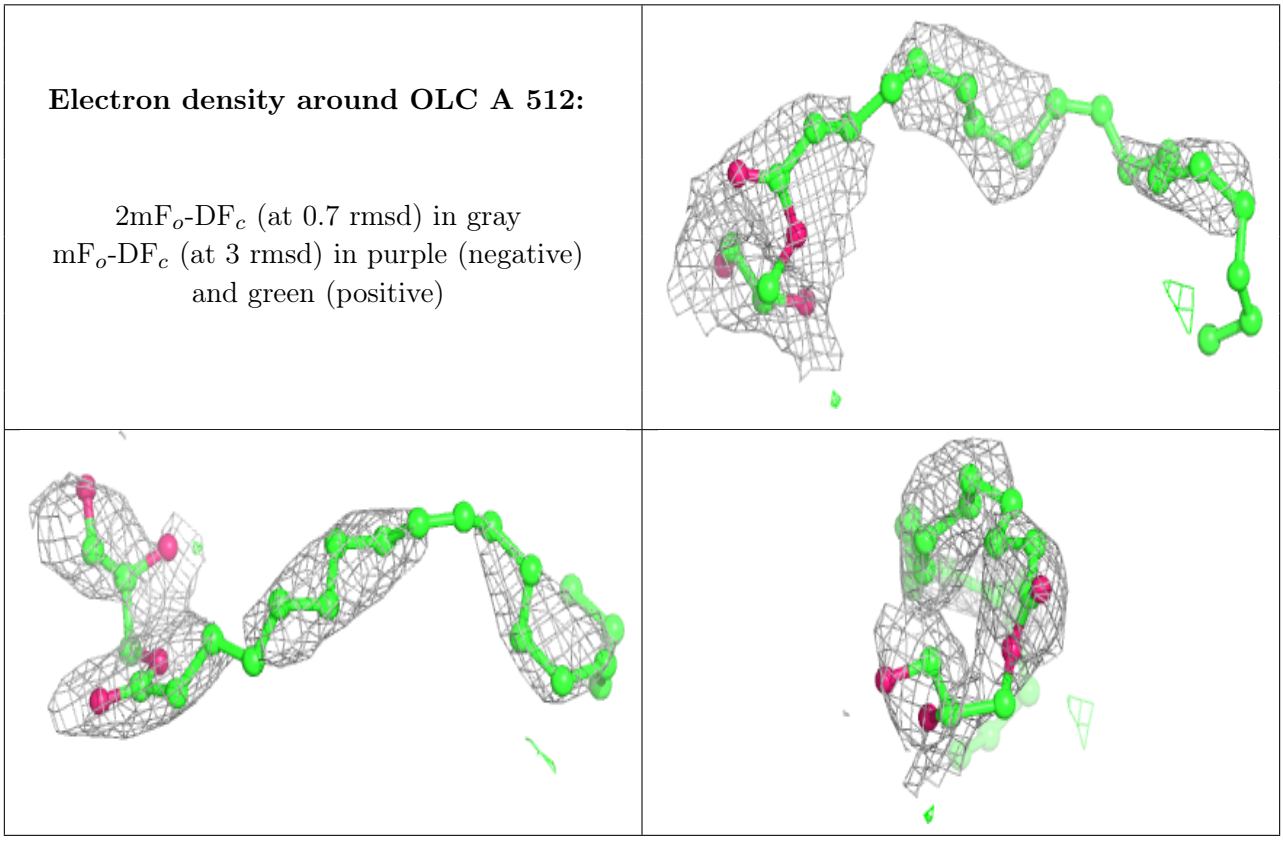
Electron density around OLC A 502:

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



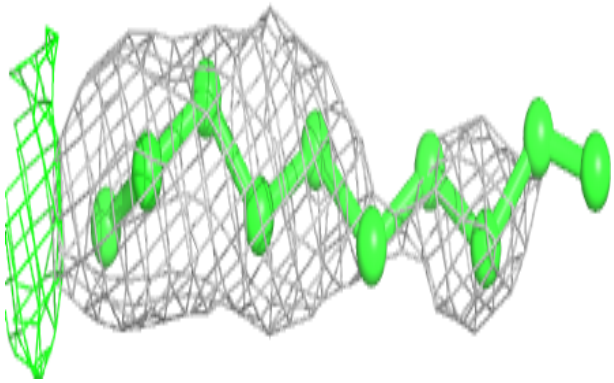
Electron density around OLC A 512:

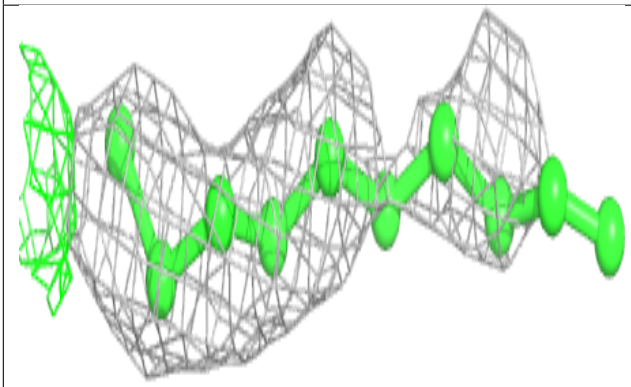
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

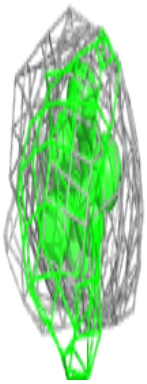


Electron density around OLC A 508:

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

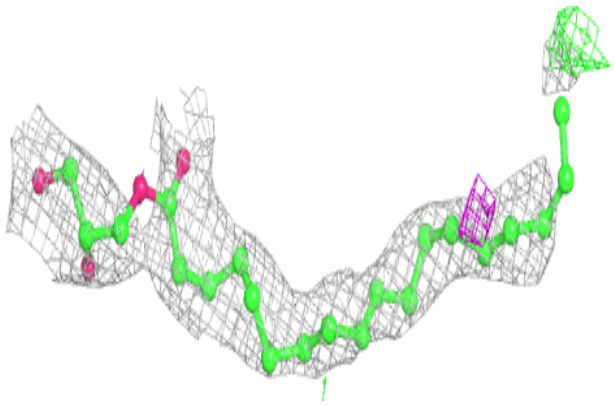


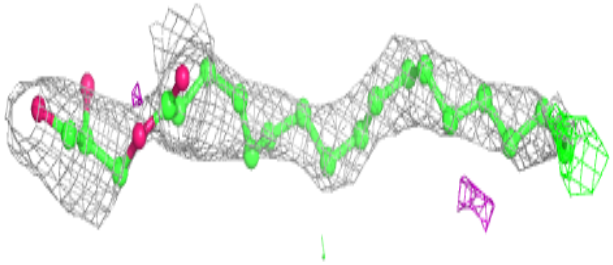


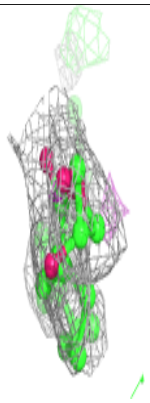


Electron density around OLC C 102:

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

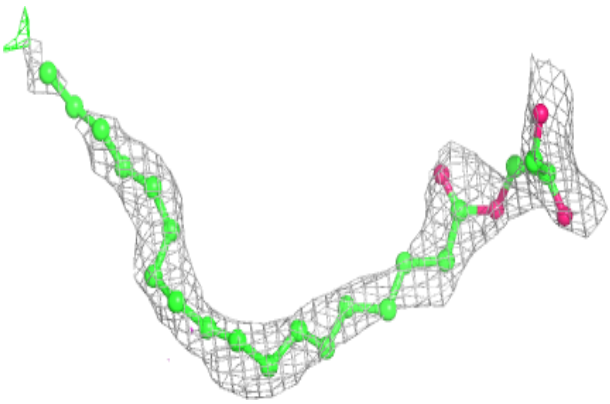


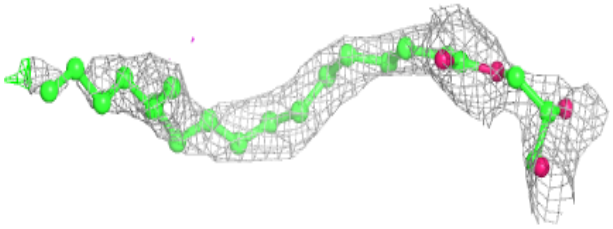


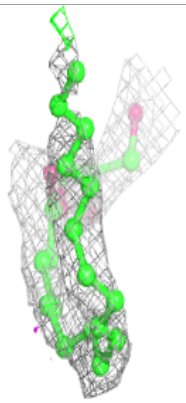


Electron density around OLC A 501:

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

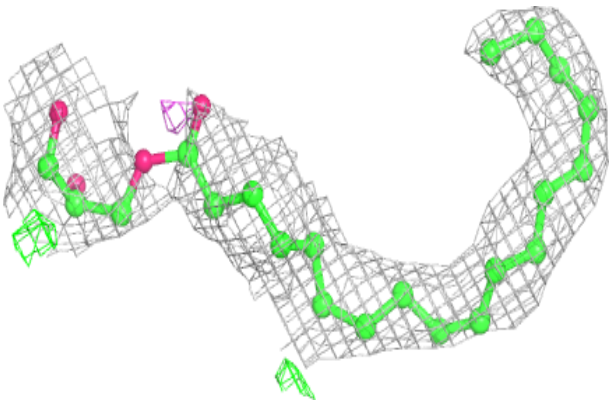


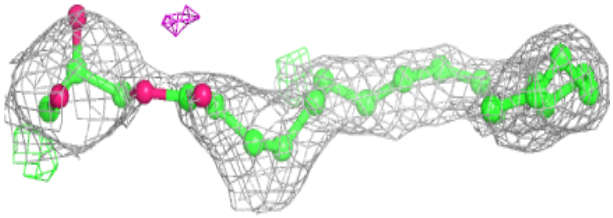


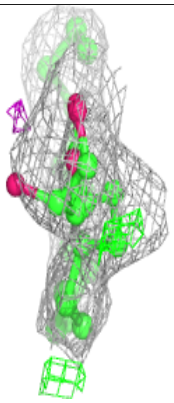


Electron density around OLC A 503:

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

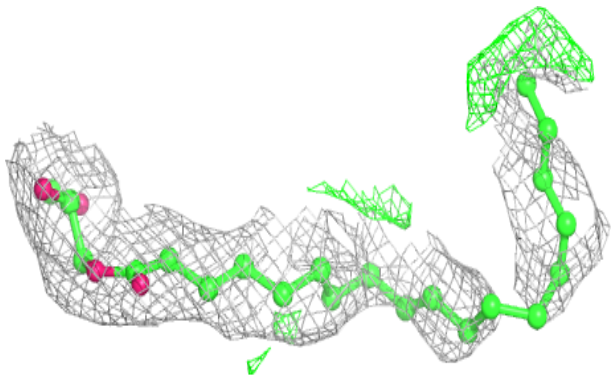


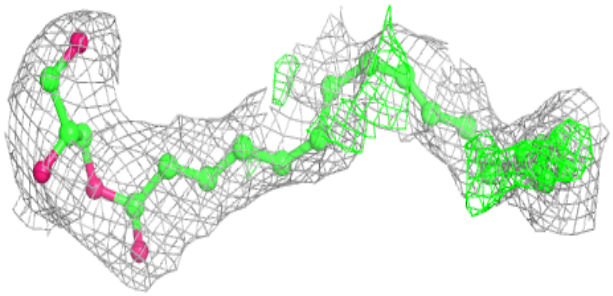


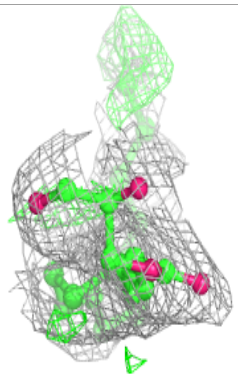


Electron density around OLC A 504:

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

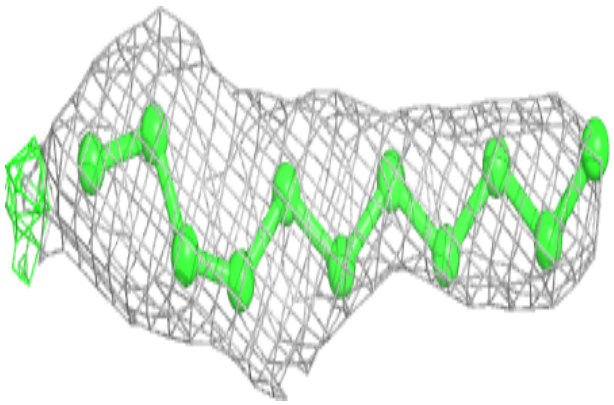


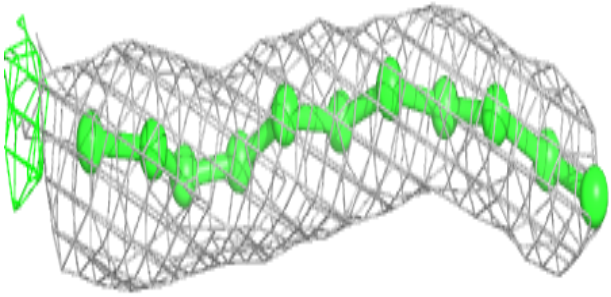


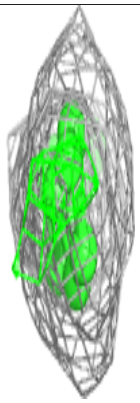


Electron density around OLC A 505:

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

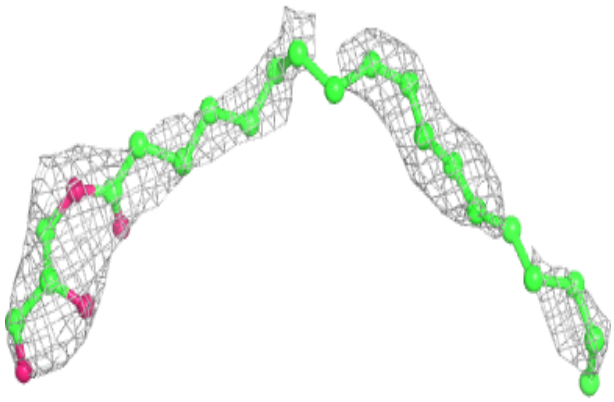


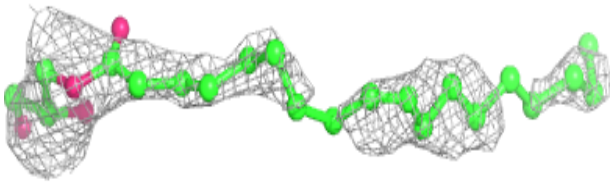


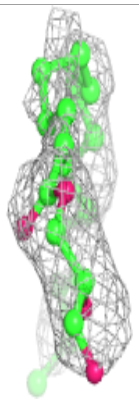


Electron density around OLC A 506:

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

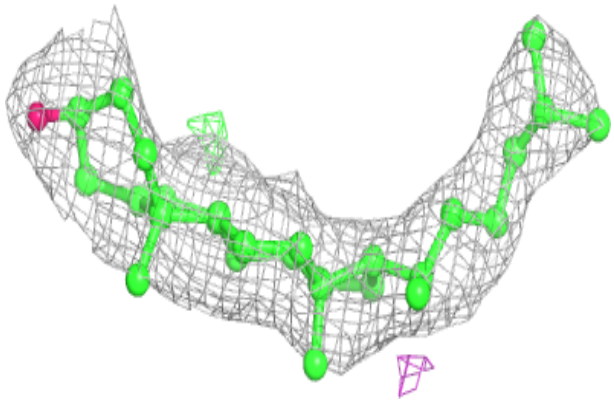


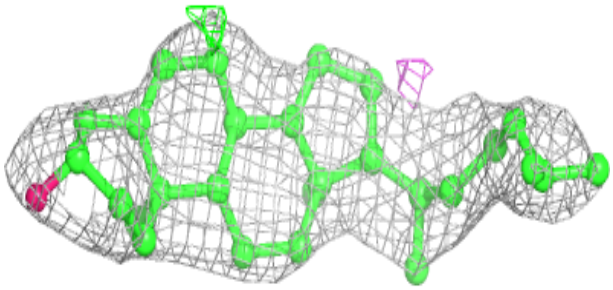


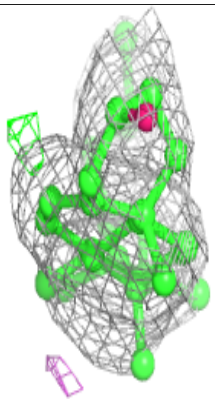


Electron density around CLR C 101:

$2mF_o$-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.