wwPDB X-ray Structure Validation Summary Report (i)

May 31, 2022 – 06:21 pm BST

PDB ID	:	7Z0C
Title	:	Crystal structure of the K state of bacteriorhodopsin at 1.53 Angstrom resolution
Authors	:	Borshchevskiy, V.; Kovalev, K.; Round, E.; Efremov, R.; Bourenkov, G.; Gordeliy, V.
Deposited on	:	2022-02-22
Resolution	:	1.53 Å(reported)

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

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

The following versions of software and data (see references (i)) were used in the production of this report:

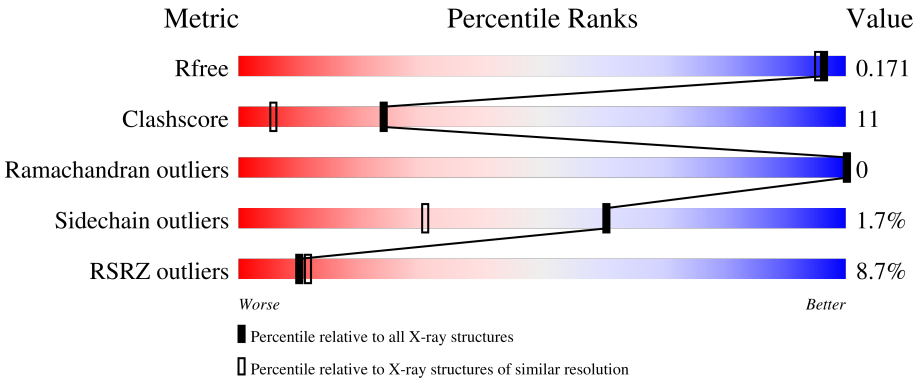
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 1.53 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	248	8% 80% 11% · 7%

2 Entry composition (i)

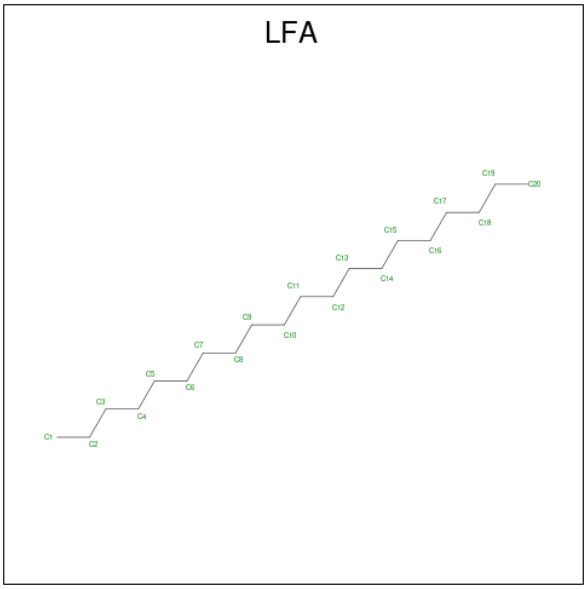
There are 5 unique types of molecules in this entry. The entry contains 4825 atoms, of which 2470 are hydrogens and 0 are deuteriums.

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 Bacteriorhodopsin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	44	0
			4102	1362	2093	297	338	12			

- Molecule 2 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C		0	0
			7	7			
2	A	1	Total	C	H	0	0
			19	6	13		
2	A	1	Total	C	H	0	0
			25	8	17		
2	A	1	Total	C	H	0	0
			19	6	13		
2	A	1	Total	C	H	0	0
			28	10	18		

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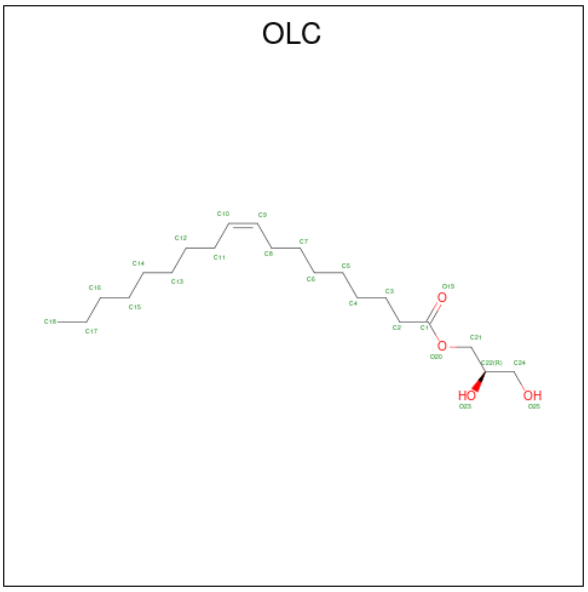
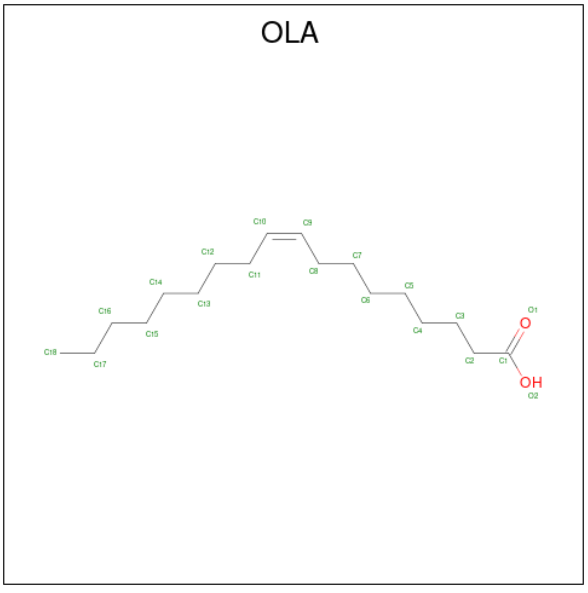
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H 31 10 21	0	0
2	A	1	Total C H 13 4 9	0	0
2	A	1	Total C H 31 10 21	0	0
2	A	1	Total C H 34 11 23	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C H 25 8 17	0	0
2	A	1	Total C H 13 4 9	0	0
2	A	1	Total C H 31 10 21	0	0
2	A	1	Total C H 25 8 17	0	0
2	A	1	Total C H 43 14 29	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C H 49 16 33	0	0
2	A	1	Total C H 19 6 13	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 2 2	0	0
2	A	1	Total C H 13 4 9	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
3	A	1	Total C H O 65 21 40 4	0	0
3	A	1	Total C H O 46 16 26 4	0	0
3	A	1	Total C H O 17 9 4 4	0	0

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 40 14 24 2	0	0

- Molecule 5 is water.

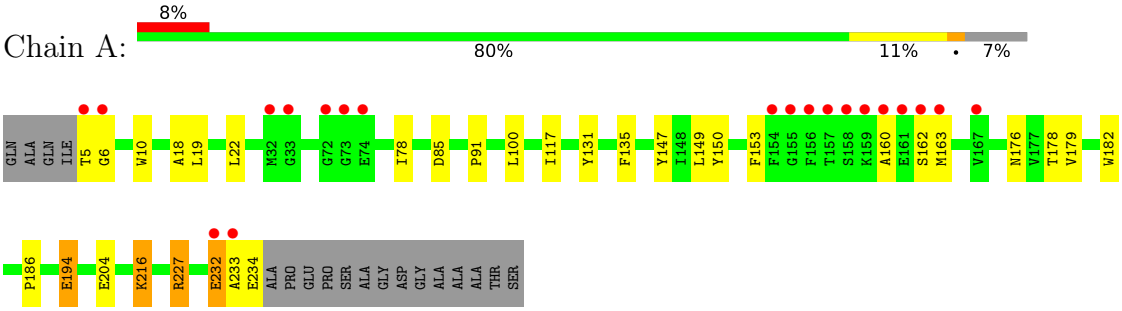
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	81	Total O 89 89	0	7

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: Bacteriorhodopsin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	60.99Å 60.99Å 110.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.11 – 1.53 38.11 – 1.53	Depositor EDS
% Data completeness (in resolution range)	85.1 (38.11-1.53) 85.1 (38.11-1.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 1.53Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.149 , 0.171 0.150 , 0.171	Depositor DCC
R_{free} test set	1010 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	4825	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLC, LYR, LFA

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	0.51	0/2139	0.61	1/2923 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	ASP	CB-CG-OD1	5.18	122.96	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194[A]	GLU	Mainchain
1	A	6	GLY	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2009	2093	1939	38	0
2	A	183	283	333	17	0
3	A	58	70	82	9	0
4	A	16	24	22	3	0
5	A	89	0	0	6	0
All	All	2355	2470	2376	53	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 11.

The worst 5 of 53 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)
3:A:811:OLC:H5A	3:A:811:OLC:H9	1.50	0.93
2:A:814:LFA:H11	2:A:828:LFA:H22	1.48	0.93
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.38	0.88
1:A:216[D]:LYR:H192	1:A:216[D]:LYR:H9	1.54	0.87
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.11	0.84

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	271/248 (109%)	269 (99%)	2 (1%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	215/193 (111%)	211 (98%)	4 (2%)	57 26

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22[A]	LEU
1	A	22[B]	LEU
1	A	227	ARG
1	A	232	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LYR	A	216[D]	1	27,29,30	1.26	2 (7%)	30,37,39	1.38	4 (13%)
1	LYR	A	216[A]	1	27,29,30	0.67	0	30,37,39	1.13	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYR	A	216[D]	1	-	3/22/40/42	0/1/1/1
1	LYR	A	216[A]	1	-	3/22/40/42	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216[D]	LYR	C7-C80	3.83	1.40	1.35
1	A	216[D]	LYR	C9-C80	-2.72	1.40	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216[D]	LYR	C8-C80-C7	-4.33	116.85	122.92
1	A	216[D]	LYR	C1-NZ-CE	3.21	118.42	113.33
1	A	216[D]	LYR	C9-C80-C7	3.03	123.59	118.94
1	A	216[A]	LYR	C19-C17-C11	2.67	114.64	110.30
1	A	216[D]	LYR	C7-C6-C5	2.51	131.06	123.22

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	216[A]	LYR	C1-C2-C3-C4
1	A	216[A]	LYR	C1-C2-C3-C5
1	A	216[D]	LYR	C1-C2-C3-C5
1	A	216[D]	LYR	CG-CD-CE-NZ
1	A	216[A]	LYR	CD-CE-NZ-C1

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	216[D]	LYR	6	0
1	A	216[A]	LYR	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LFA	A	804	-	7,7,19	0.15	0	6,6,18	0.17	0
2	LFA	A	821	-	6,6,19	0.13	0	5,5,18	0.12	0
2	LFA	A	813	-	7,7,19	0.12	0	6,6,18	0.07	0
2	LFA	A	814	-	3,3,19	0.19	0	2,2,18	0.46	0
2	LFA	A	817	-	13,13,19	0.30	0	12,12,18	0.85	0
2	LFA	A	802	-	5,5,19	0.13	0	4,4,18	0.10	0
2	LFA	A	807	-	9,9,19	0.28	0	8,8,18	0.78	0
2	LFA	A	805	-	5,5,19	0.15	0	4,4,18	0.13	0
2	LFA	A	810	-	10,10,19	0.23	0	9,9,18	0.10	0
2	LFA	A	827	-	1,1,19	0.05	0	-		
4	OLA	A	826	-	12,15,19	0.35	0	11,15,19	0.15	0
2	LFA	A	819	-	5,5,19	0.14	0	4,4,18	0.08	0
3	OLC	A	803	-	24,24,24	0.82	1 (4%)	25,25,25	1.04	2 (8%)
2	LFA	A	809	-	9,9,19	0.19	0	8,8,18	0.20	0
2	LFA	A	822	-	15,15,19	0.30	0	14,14,18	0.82	0
2	LFA	A	828	-	3,3,19	0.40	0	2,2,18	0.73	0
2	LFA	A	820	-	2,2,19	0.17	0	0,1,18	-	-
3	OLC	A	811	-	19,19,24	1.04	1 (5%)	20,20,25	0.92	1 (5%)
2	LFA	A	818	-	7,7,19	0.16	0	6,6,18	0.12	0
2	LFA	A	825	-	4,4,19	0.16	0	3,3,18	0.28	0
2	LFA	A	806	-	9,9,19	0.10	0	8,8,18	0.11	0
2	LFA	A	808	-	3,3,19	0.18	0	2,2,18	0.44	0
2	LFA	A	823	-	5,5,19	0.14	0	4,4,18	0.06	0
2	LFA	A	801	-	6,6,19	0.15	0	5,5,18	0.21	0
2	LFA	A	812	-	9,9,19	0.14	0	8,8,18	0.12	0
2	LFA	A	816	-	7,7,19	0.11	0	6,6,18	0.10	0
2	LFA	A	815	-	9,9,19	0.15	0	8,8,18	0.12	0
3	OLC	A	824	-	12,12,24	1.20	1 (8%)	13,13,25	1.31	2 (15%)

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
2	LFA	A	804	-	-	2/5/5/17	-
2	LFA	A	821	-	-	2/4/4/17	-
2	LFA	A	813	-	-	4/5/5/17	-
2	LFA	A	814	-	-	1/1/1/17	-
2	LFA	A	817	-	-	6/11/11/17	-
2	LFA	A	802	-	-	1/3/3/17	-
2	LFA	A	807	-	-	4/7/7/17	-
2	LFA	A	805	-	-	0/3/3/17	-
2	LFA	A	810	-	-	4/8/8/17	-
4	OLA	A	826	-	-	7/11/13/17	-
2	LFA	A	819	-	-	2/3/3/17	-
3	OLC	A	803	-	-	6/24/24/24	-
2	LFA	A	809	-	-	5/7/7/17	-
2	LFA	A	822	-	-	4/13/13/17	-
2	LFA	A	828	-	-	1/1/1/17	-
3	OLC	A	811	-	-	7/19/19/24	-
2	LFA	A	818	-	-	3/5/5/17	-
2	LFA	A	825	-	-	2/2/2/17	-
2	LFA	A	806	-	-	6/7/7/17	-
2	LFA	A	808	-	-	1/1/1/17	-
2	LFA	A	823	-	-	1/3/3/17	-
2	LFA	A	801	-	-	0/4/4/17	-
2	LFA	A	812	-	-	5/7/7/17	-
2	LFA	A	816	-	-	3/5/5/17	-
2	LFA	A	815	-	-	4/7/7/17	-
3	OLC	A	824	-	-	9/12/12/24	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	811	OLC	O20-C1	4.19	1.45	1.33
3	A	824	OLC	O20-C1	3.90	1.44	1.33
3	A	803	OLC	O20-C1	3.43	1.43	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	824	OLC	O20-C1-C2	3.32	122.32	111.91
3	A	803	OLC	O20-C1-C2	2.89	120.97	111.91
3	A	811	OLC	O20-C1-C2	2.68	120.31	111.91
3	A	824	OLC	O20-C1-O19	-2.43	117.46	123.59
3	A	803	OLC	O20-C1-O19	-2.11	118.26	123.59

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	808	LFA	C1-C2-C3-C4
2	A	814	LFA	C1-C2-C3-C4
2	A	828	LFA	C1-C2-C3-C4
3	A	811	OLC	C10-C11-C12-C13
3	A	811	OLC	C21-C22-C24-O25

There are no ring outliers.

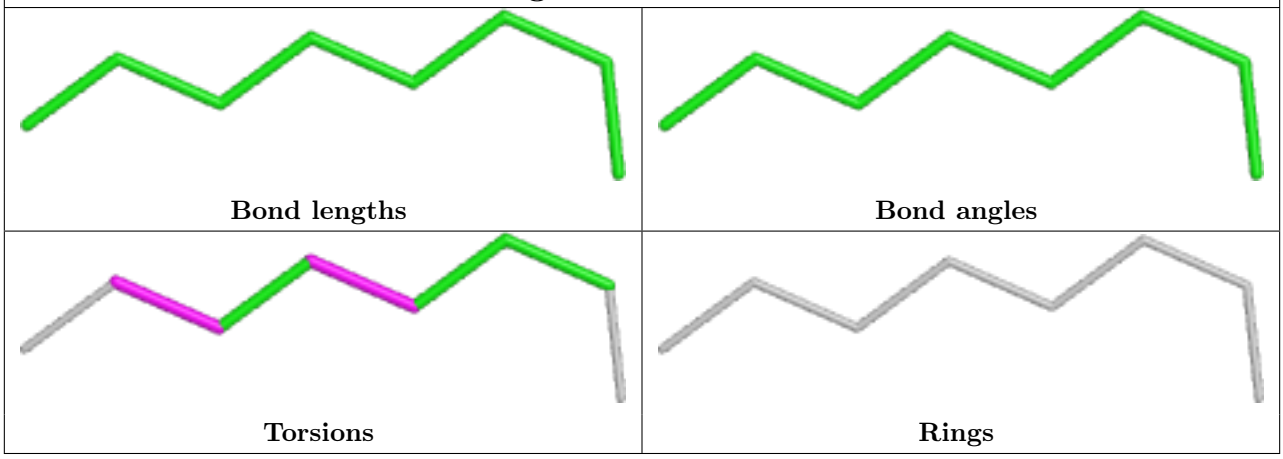
16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	821	LFA	1	0
2	A	813	LFA	1	0
2	A	814	LFA	4	0
2	A	807	LFA	1	0
2	A	810	LFA	1	0
2	A	827	LFA	1	0
4	A	826	OLA	3	0
2	A	819	LFA	4	0
3	A	803	OLC	3	0
2	A	822	LFA	1	0
2	A	828	LFA	3	0
3	A	811	OLC	5	0
2	A	818	LFA	1	0
2	A	806	LFA	4	0
2	A	812	LFA	2	0
3	A	824	OLC	1	0

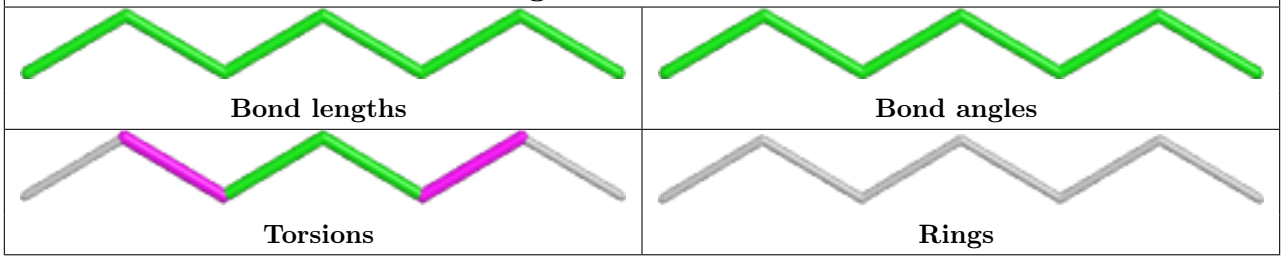
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

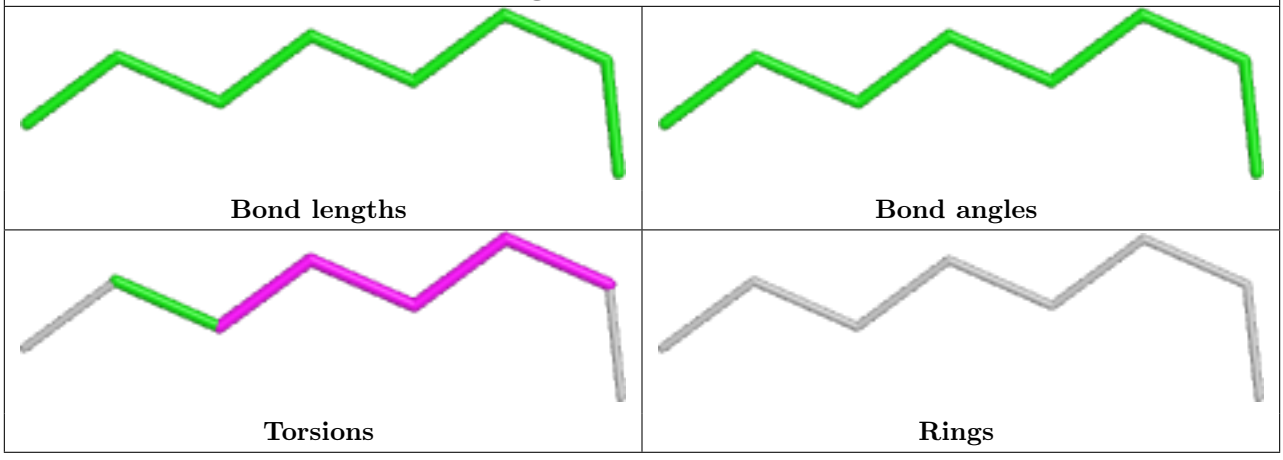
Ligand LFA A 804



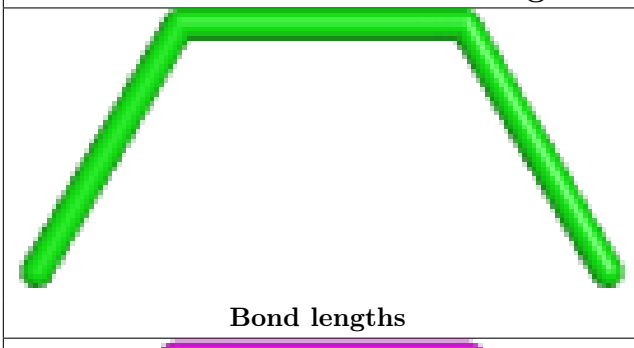
Ligand LFA A 821



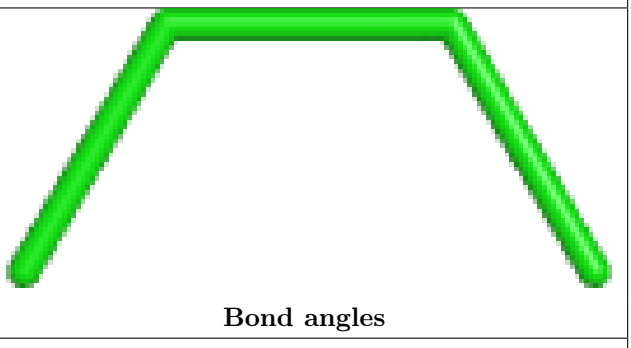
Ligand LFA A 813



Ligand LFA A 814



Bond lengths

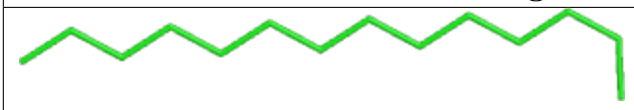


Bond angles

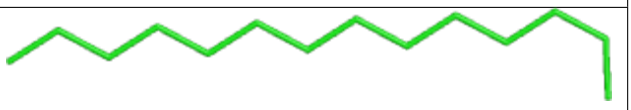
Torsions

Rings

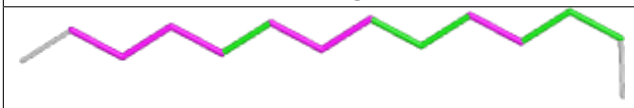
Ligand LFA A 817



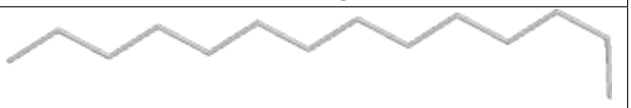
Bond lengths



Bond angles

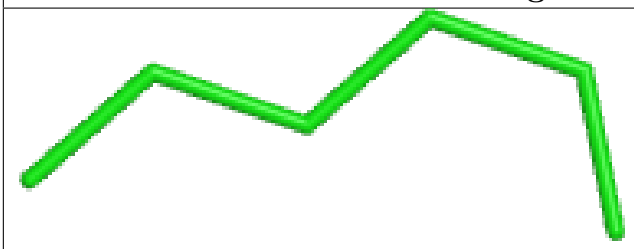


Torsions

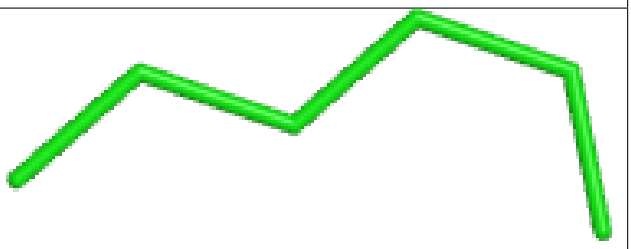


Rings

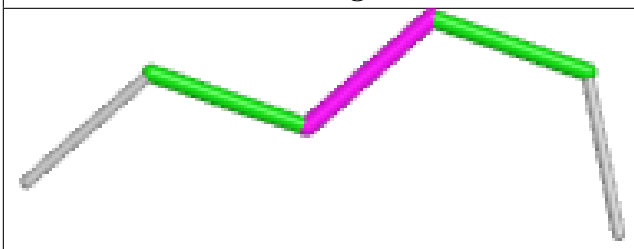
Ligand LFA A 802



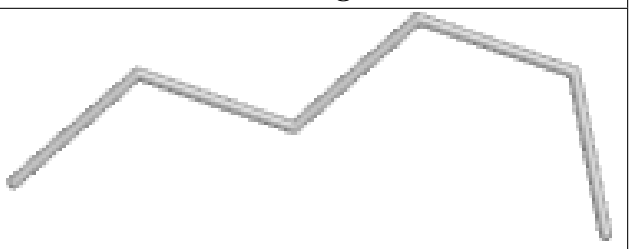
Bond lengths



Bond angles

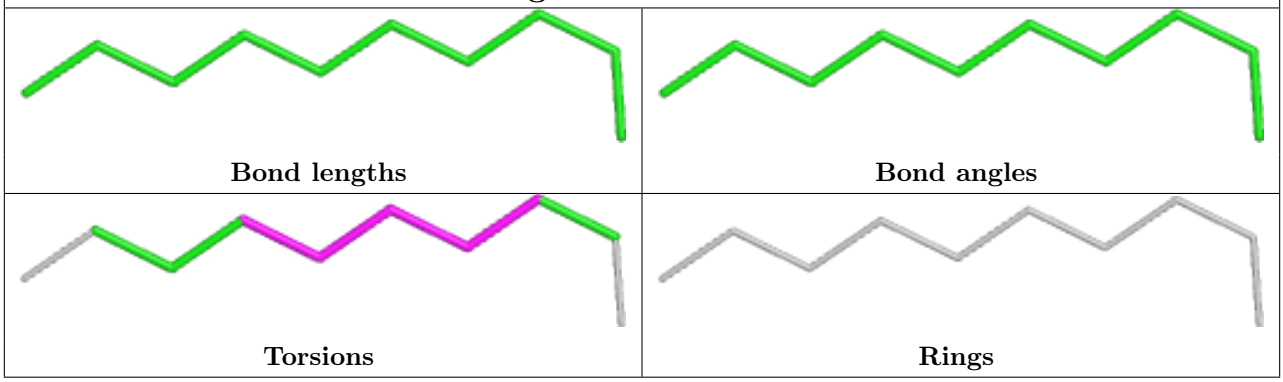


Torsions

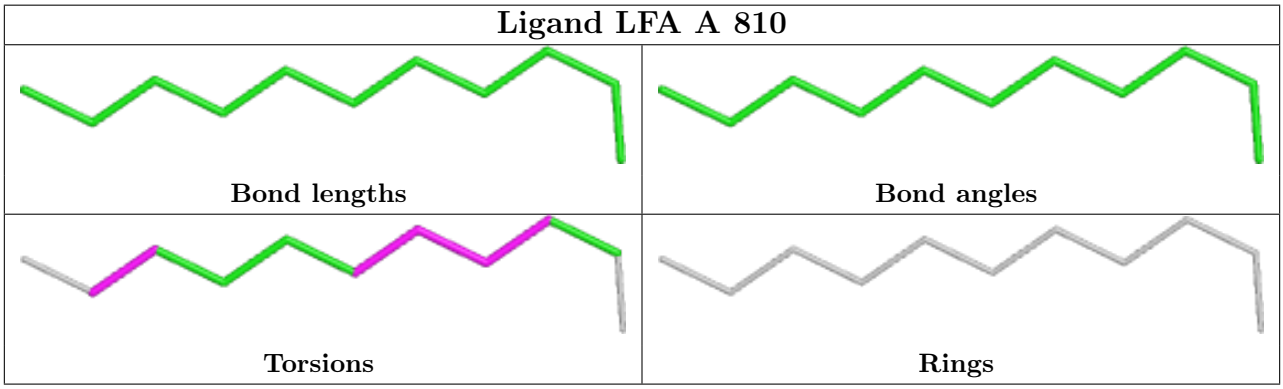


Rings

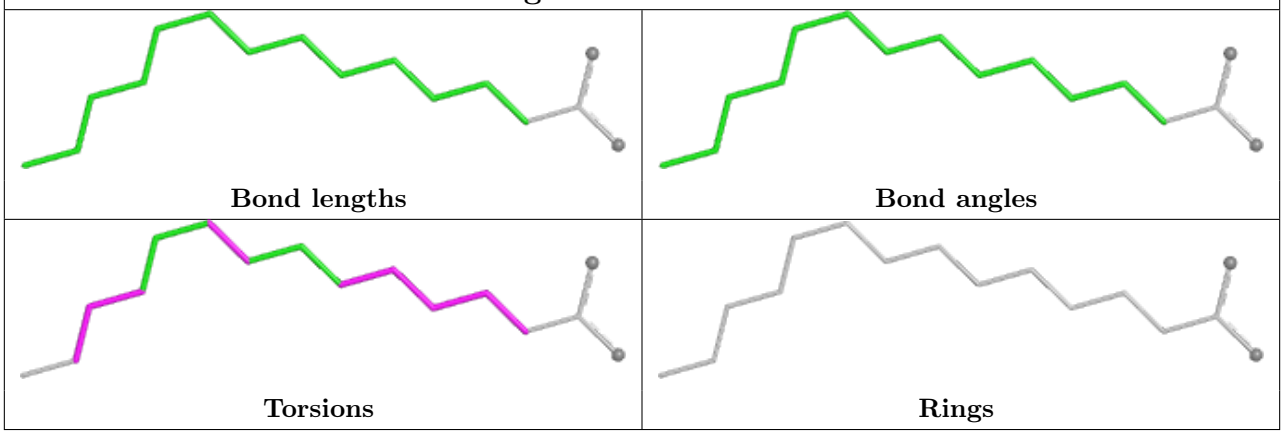
Ligand LFA A 807



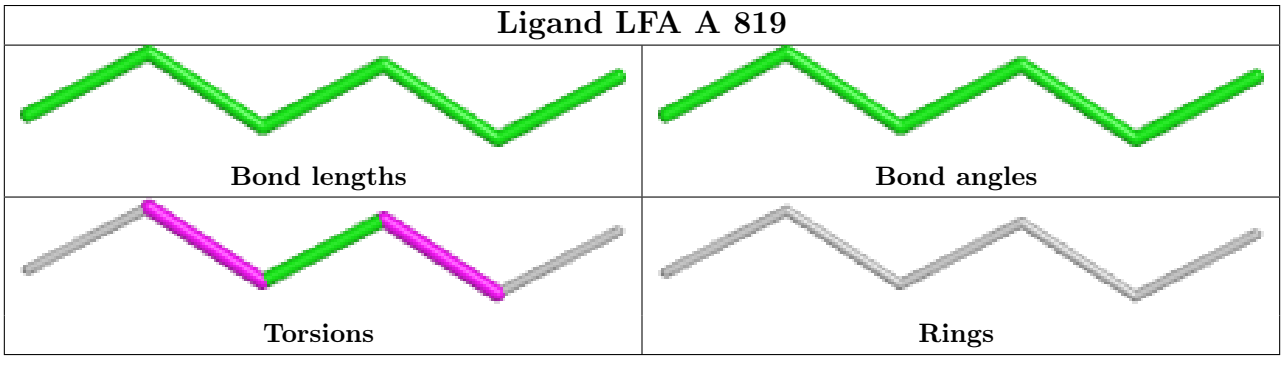
Ligand LFA A 810



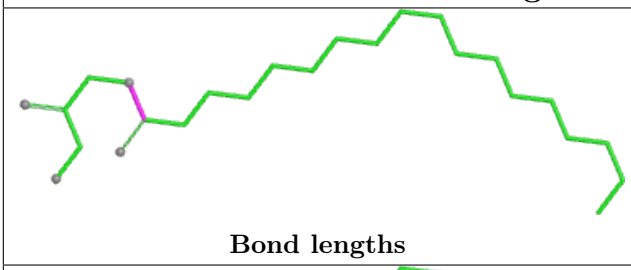
Ligand OLA A 826



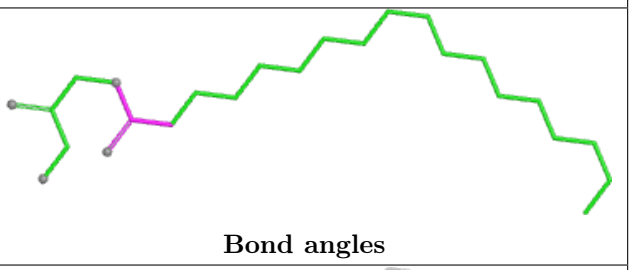
Ligand LFA A 819



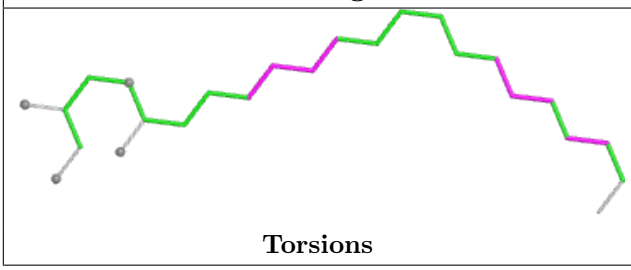
Ligand OLC A 803



Bond lengths



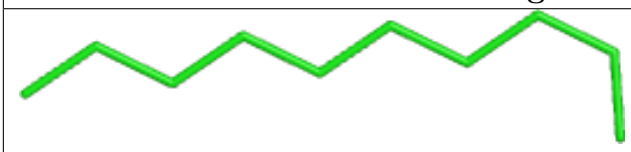
Bond angles



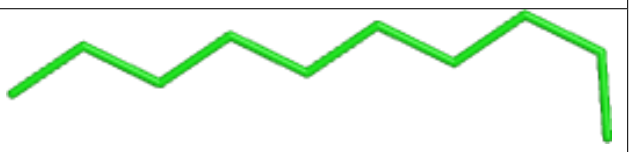
Torsions

Rings

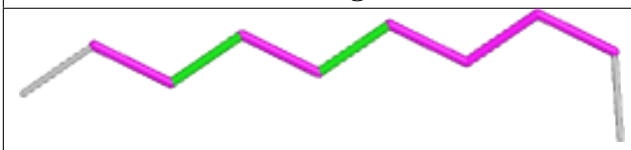
Ligand LFA A 809



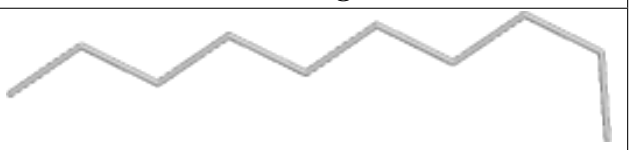
Bond lengths



Bond angles

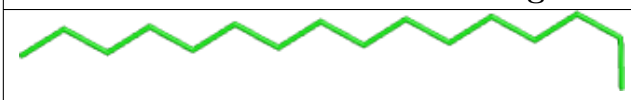


Torsions



Rings

Ligand LFA A 822



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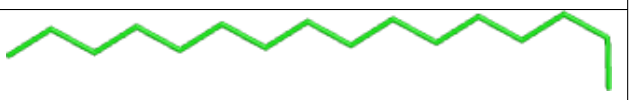
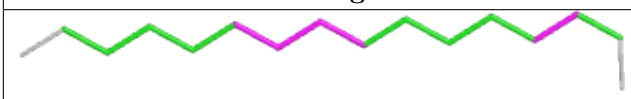


Bond angles



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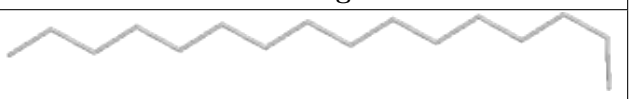
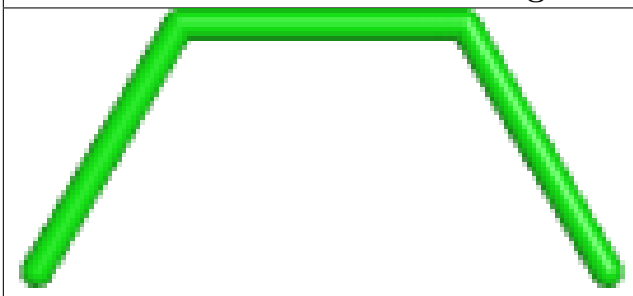


Rings

Ligand LFA A 828



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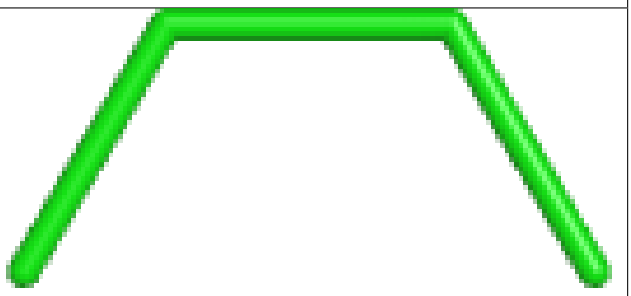
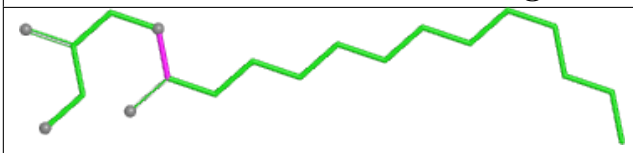


Bond angles

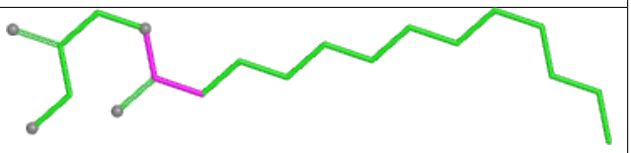
Torsions

Rings

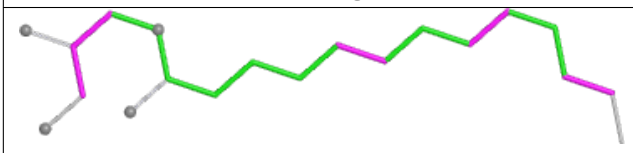
Ligand OLC A 811



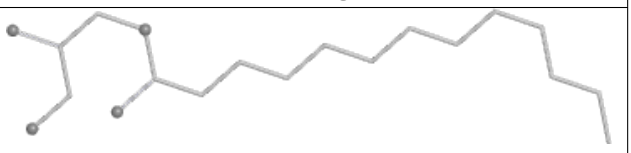
Bond lengths



Bond angles



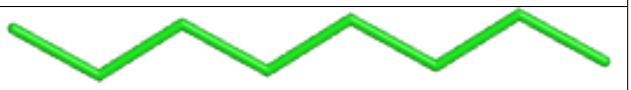
Torsions



Rings

Ligand LFA A 818

Bond lengths

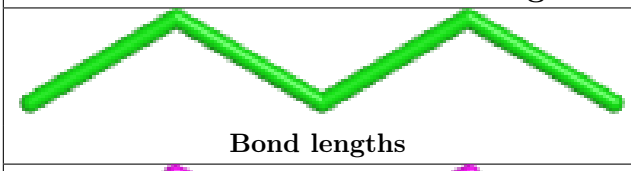


Bond angles

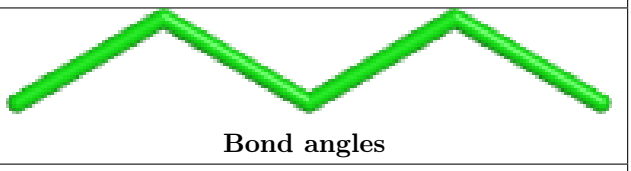
Torsions

Rings

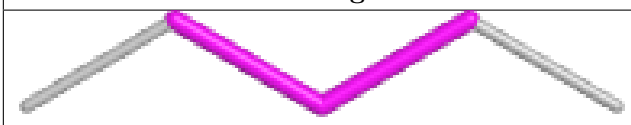
Ligand LFA A 825



Bond lengths



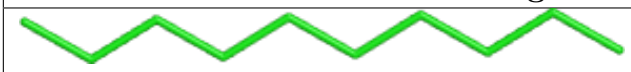
Bond angles



Torsions

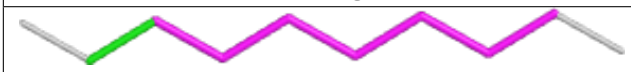
Rings

Ligand LFA A 806



Bond lengths

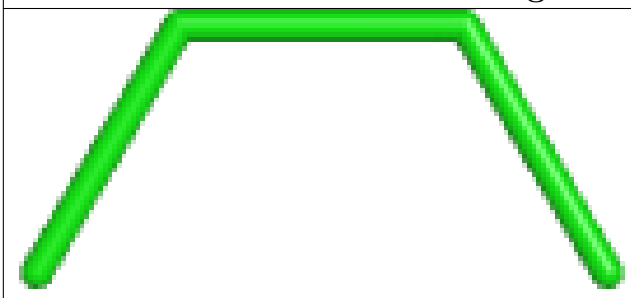
Bond angles



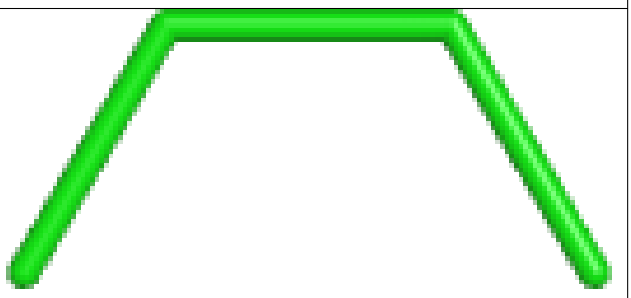
Torsions

Rings

Ligand LFA A 808



Bond lengths

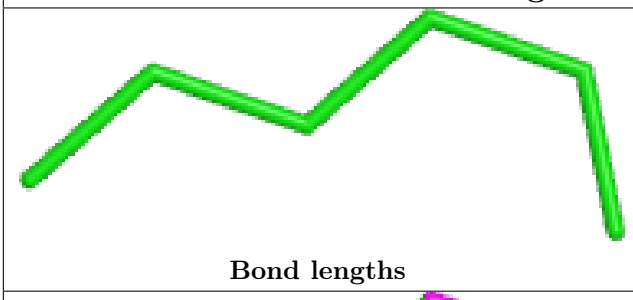


Bond angles

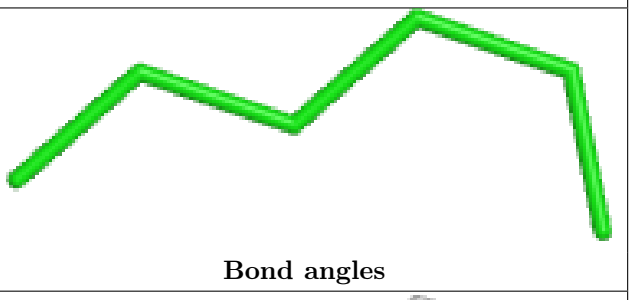
Torsions

Rings

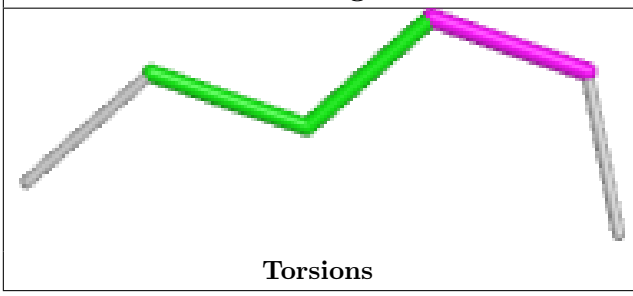
Ligand LFA A 823



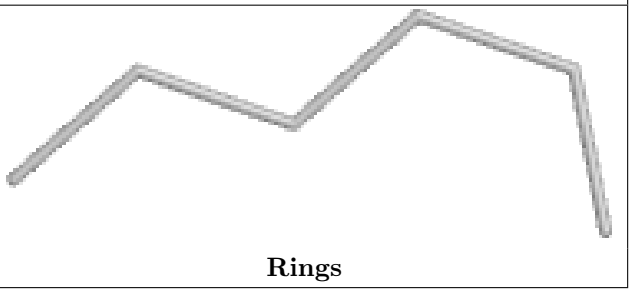
Bond lengths



Bond angles



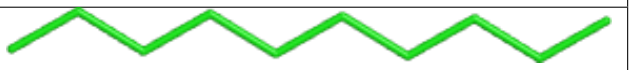
Torsions



Rings

Ligand LFA A 812

Bond lengths

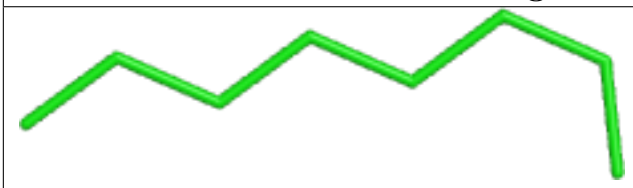


Bond angles

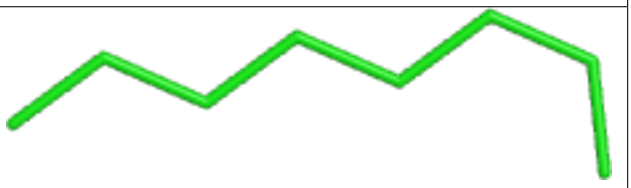
Torsions

Rings

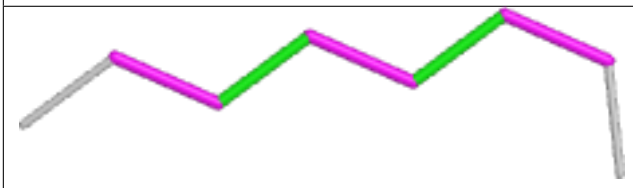
Ligand LFA A 816



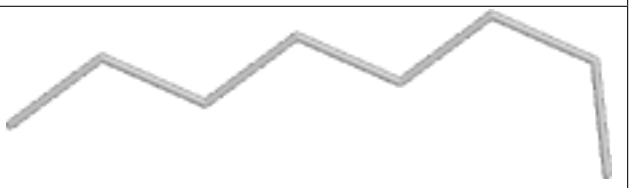
Bond lengths



Bond angles

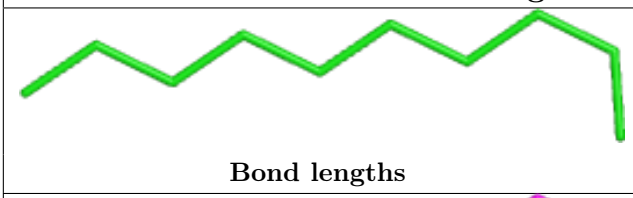


Torsions

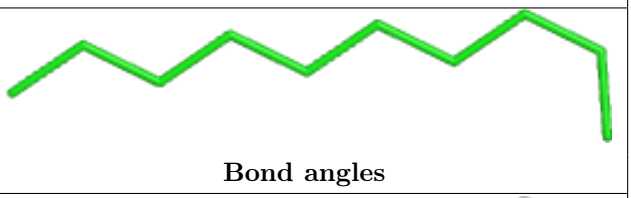


Rings

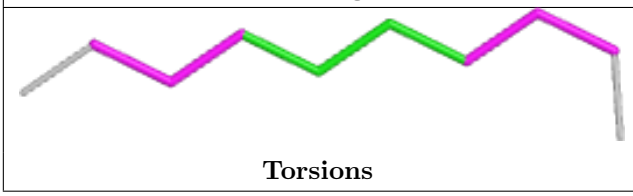
Ligand LFA A 815



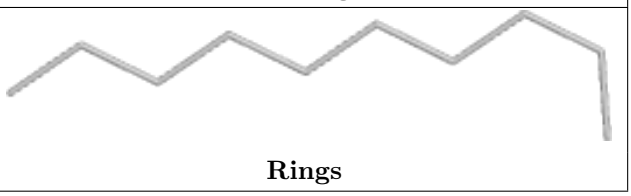
Bond lengths



Bond angles

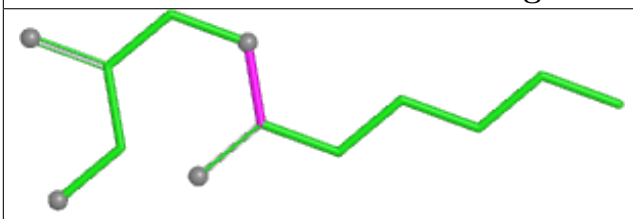


Torsions

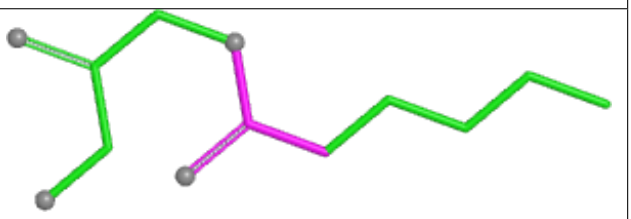


Rings

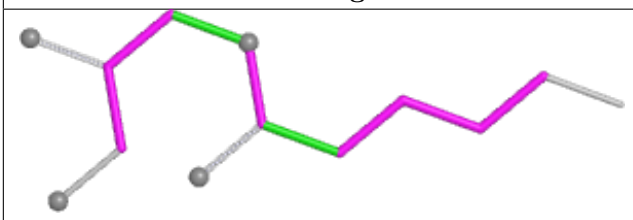
Ligand OLC A 824



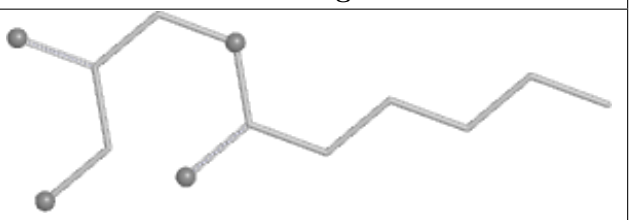
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	229/248 (92%)	0.28	20 (8%)	10	11	18, 26, 55, 83	2 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	THR	9.8
1	A	160	ALA	7.8
1	A	159	LYS	7.1
1	A	162	SER	4.9
1	A	161	GLU	4.3

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
1	LYR	A	216[A]	29/30	0.96	0.10	19,24,29,30	68
1	LYR	A	216[D]	29/30	0.96	0.10	19,24,29,30	68

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

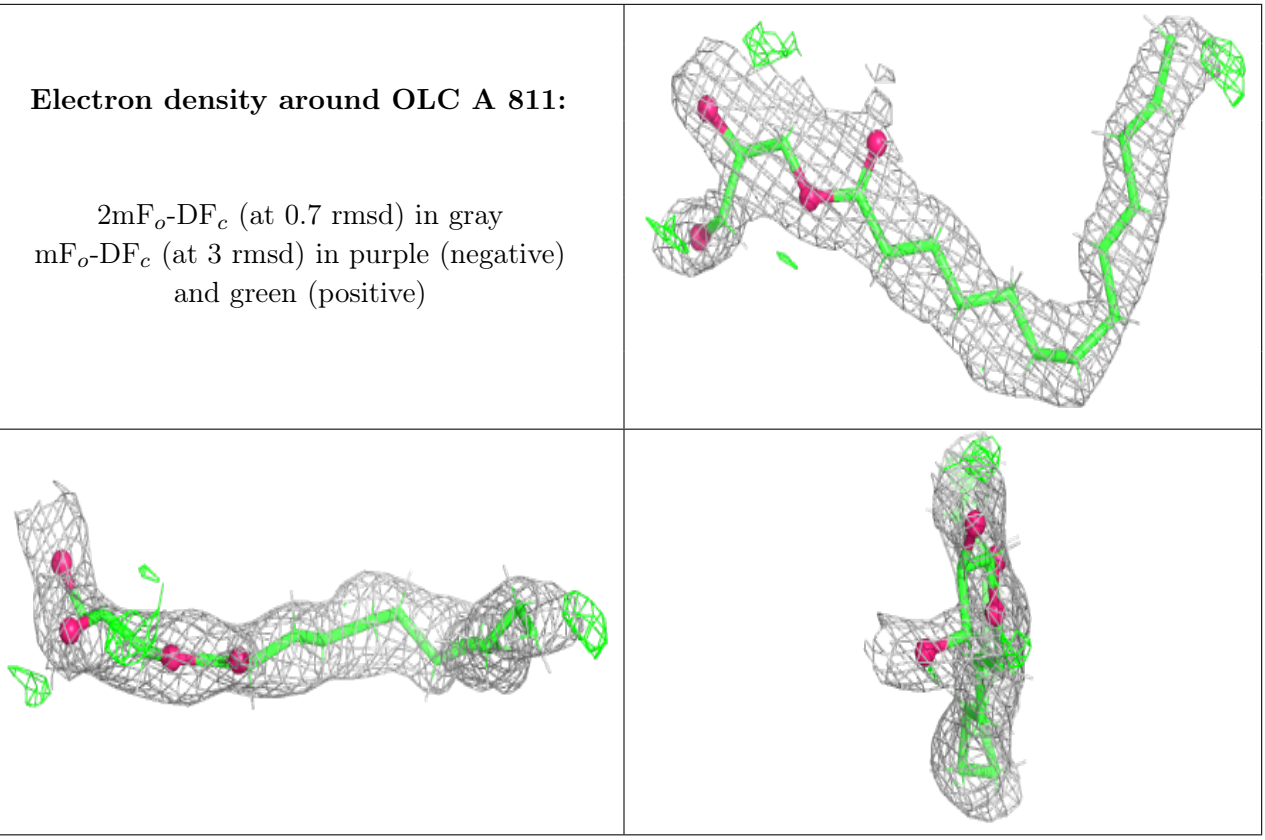
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLC	A	811	20/25	0.62	0.17	54,66,78,79	0
2	LFA	A	816	8/20	0.67	0.23	61,74,81,81	0
4	OLA	A	826	16/20	0.70	0.19	49,61,69,72	0
2	LFA	A	806	10/20	0.73	0.17	53,64,66,66	0
2	LFA	A	805	6/20	0.73	0.15	50,60,62,62	0
3	OLC	A	824	13/25	0.75	0.21	58,59,77,77	0
2	LFA	A	815	10/20	0.76	0.14	65,79,84,84	0
2	LFA	A	817	14/20	0.77	0.16	67,82,83,83	0
2	LFA	A	812	10/20	0.77	0.21	47,48,49,49	0
2	LFA	A	819	6/20	0.78	0.12	48,49,49,49	0
2	LFA	A	804	8/20	0.80	0.12	52,63,70,70	0
2	LFA	A	828	4/20	0.82	0.15	58,70,71,71	0
2	LFA	A	814	4/20	0.83	0.12	54,65,66,66	0
2	LFA	A	822	16/20	0.83	0.15	48,59,65,65	0
2	LFA	A	818	8/20	0.83	0.13	51,52,53,53	0
2	LFA	A	802	6/20	0.84	0.09	46,55,58,58	0
2	LFA	A	813	8/20	0.86	0.23	58,70,72,72	0
2	LFA	A	825	5/20	0.87	0.13	48,48,50,50	0
2	LFA	A	821	7/20	0.88	0.15	47,48,50,50	0
2	LFA	A	827	2/20	0.89	0.30	45,45,45,45	0
2	LFA	A	809	10/20	0.89	0.10	46,56,61,61	0
3	OLC	A	803	25/25	0.89	0.10	40,49,60,62	0
2	LFA	A	808	4/20	0.90	0.14	55,66,66,66	0
2	LFA	A	801	7/20	0.90	0.11	44,44,45,45	0
2	LFA	A	810	11/20	0.90	0.13	45,55,58,58	0
2	LFA	A	807	10/20	0.90	0.10	47,59,70,71	0
2	LFA	A	823	6/20	0.91	0.08	49,60,64,64	0
2	LFA	A	820	3/20	0.91	0.19	44,44,44,44	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.

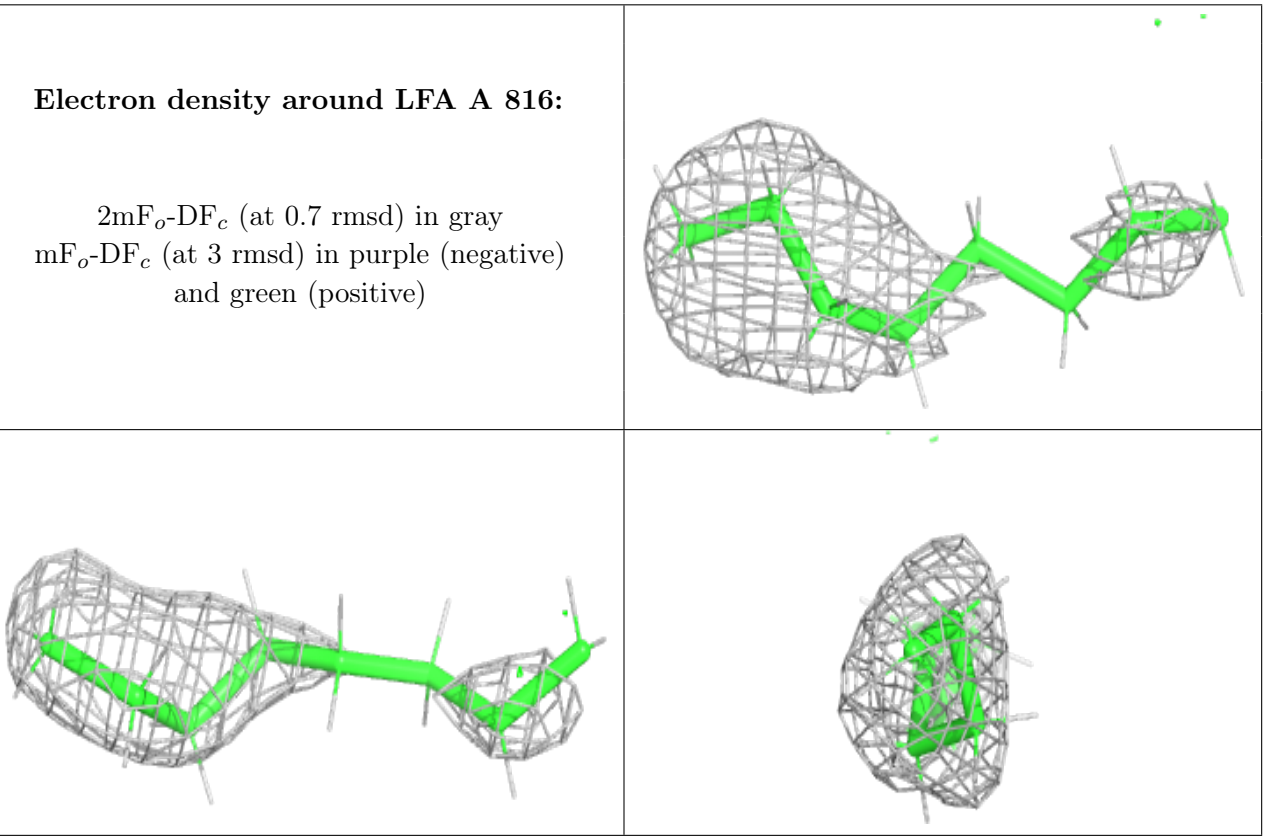
Electron density around OLC A 811:

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



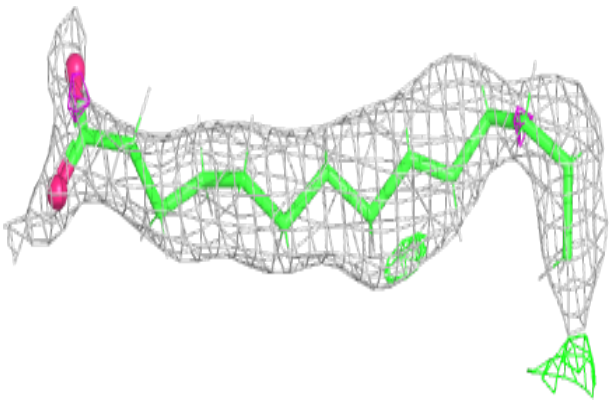
Electron density around LFA A 816:

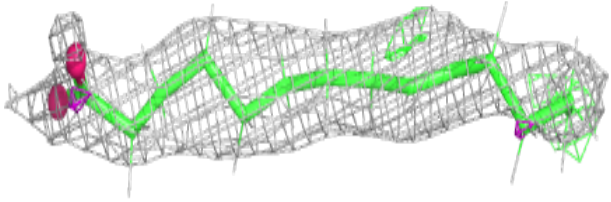
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

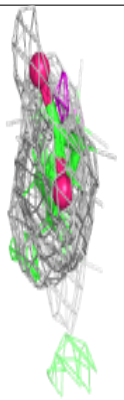


Electron density around OLA A 826:

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

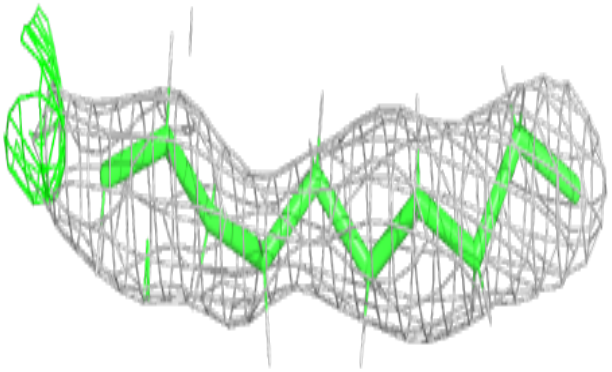


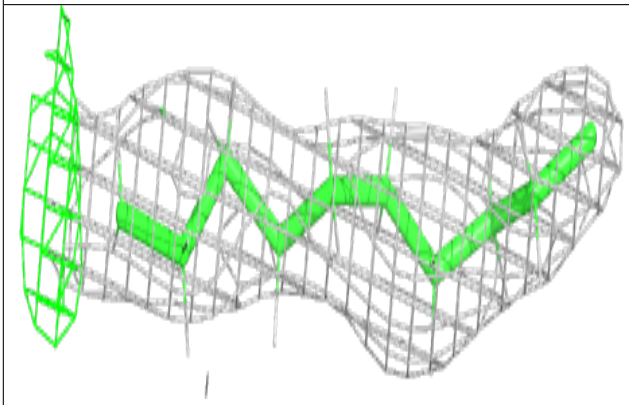


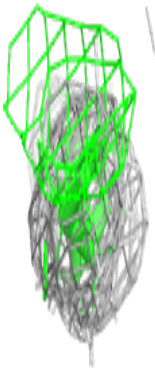


Electron density around LFA A 806:

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

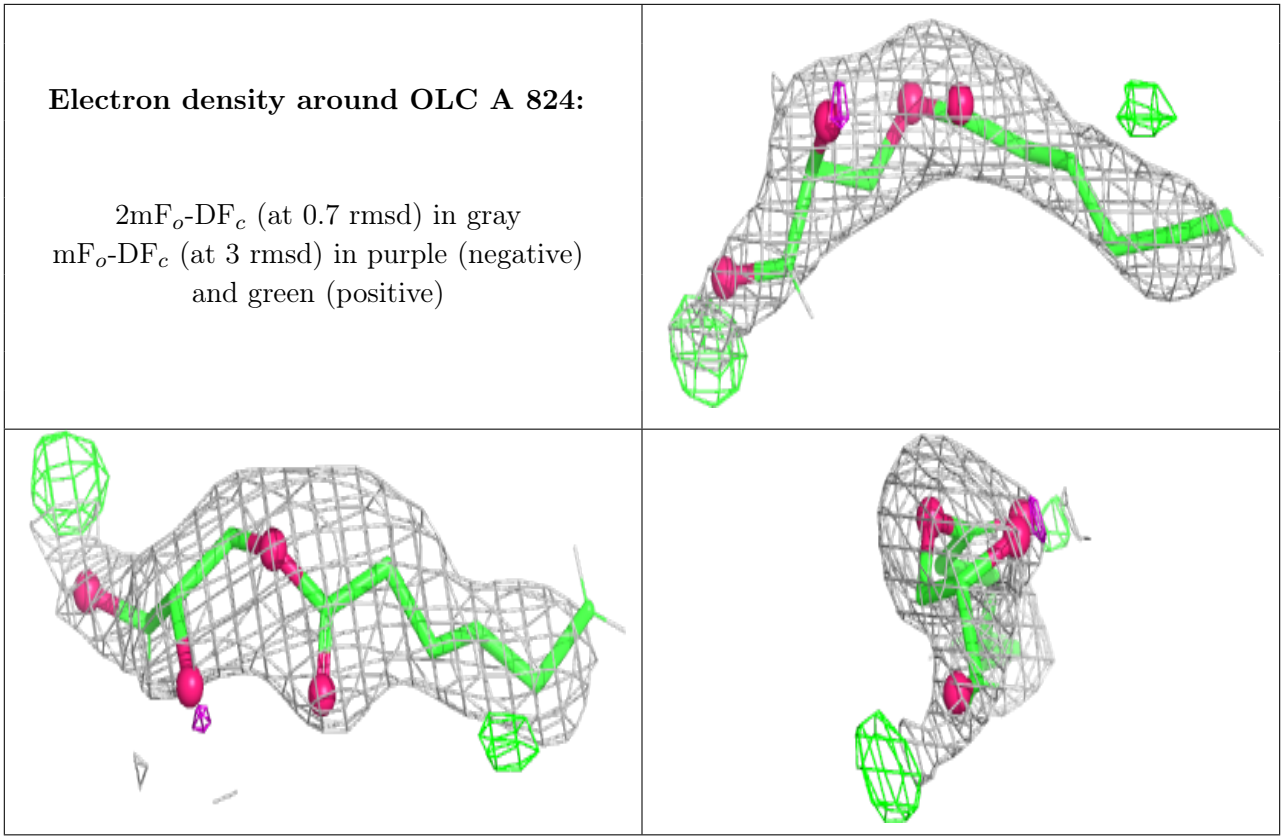






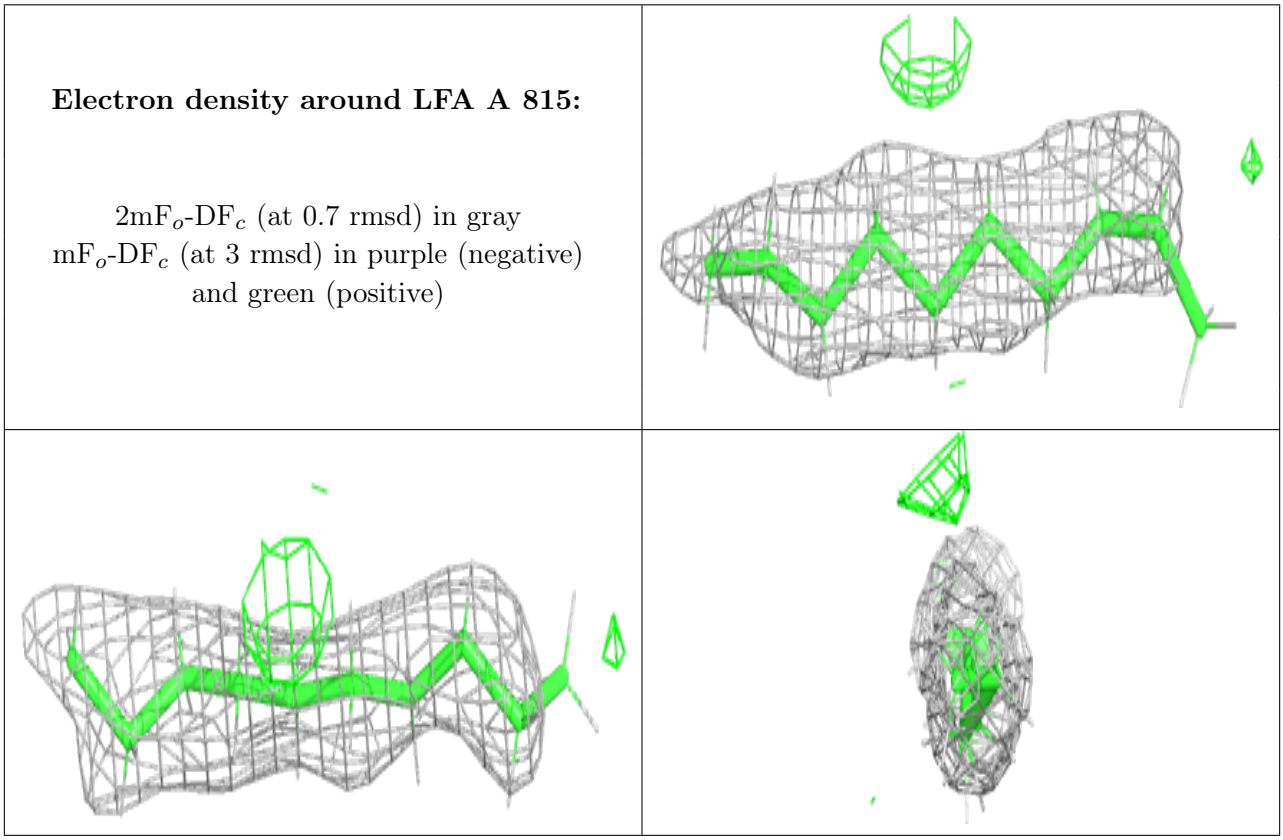
Electron density around OLC A 824:

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



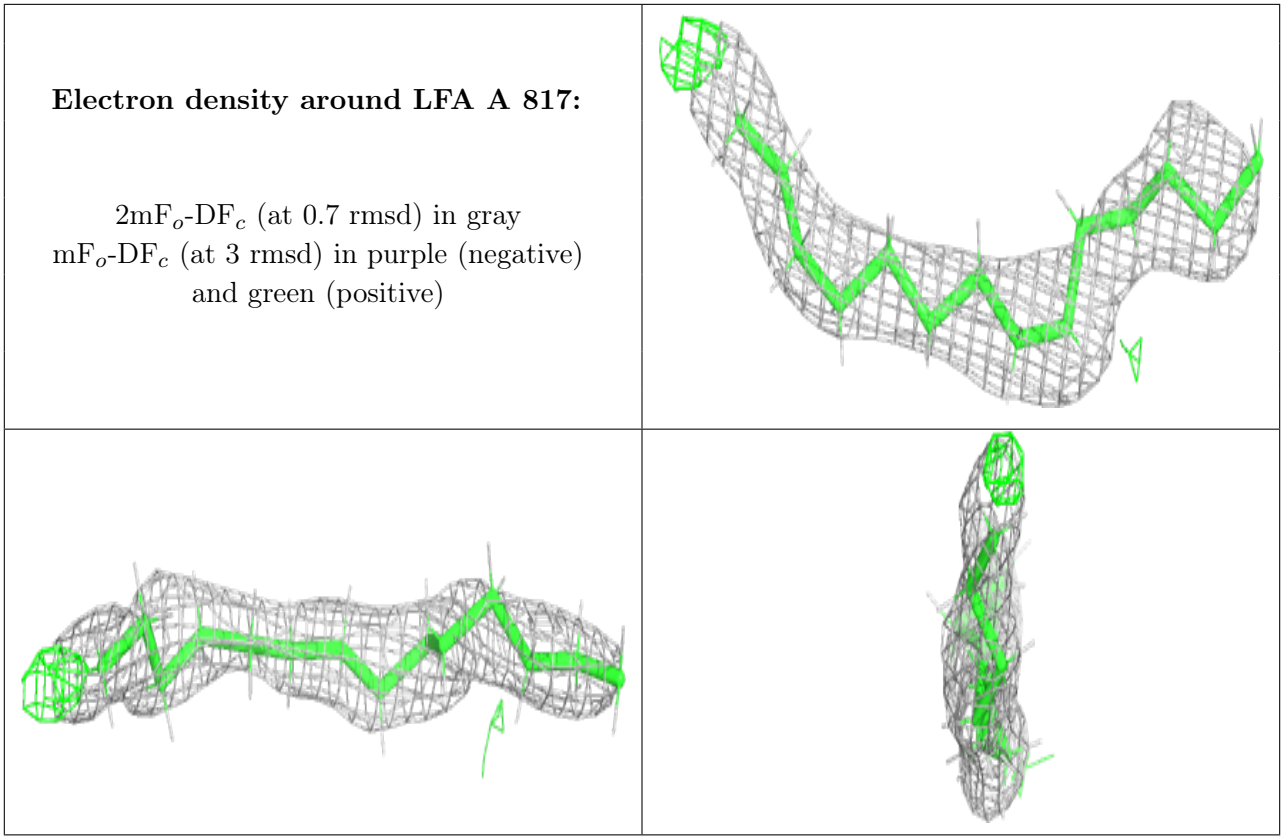
Electron density around LFA A 815:

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



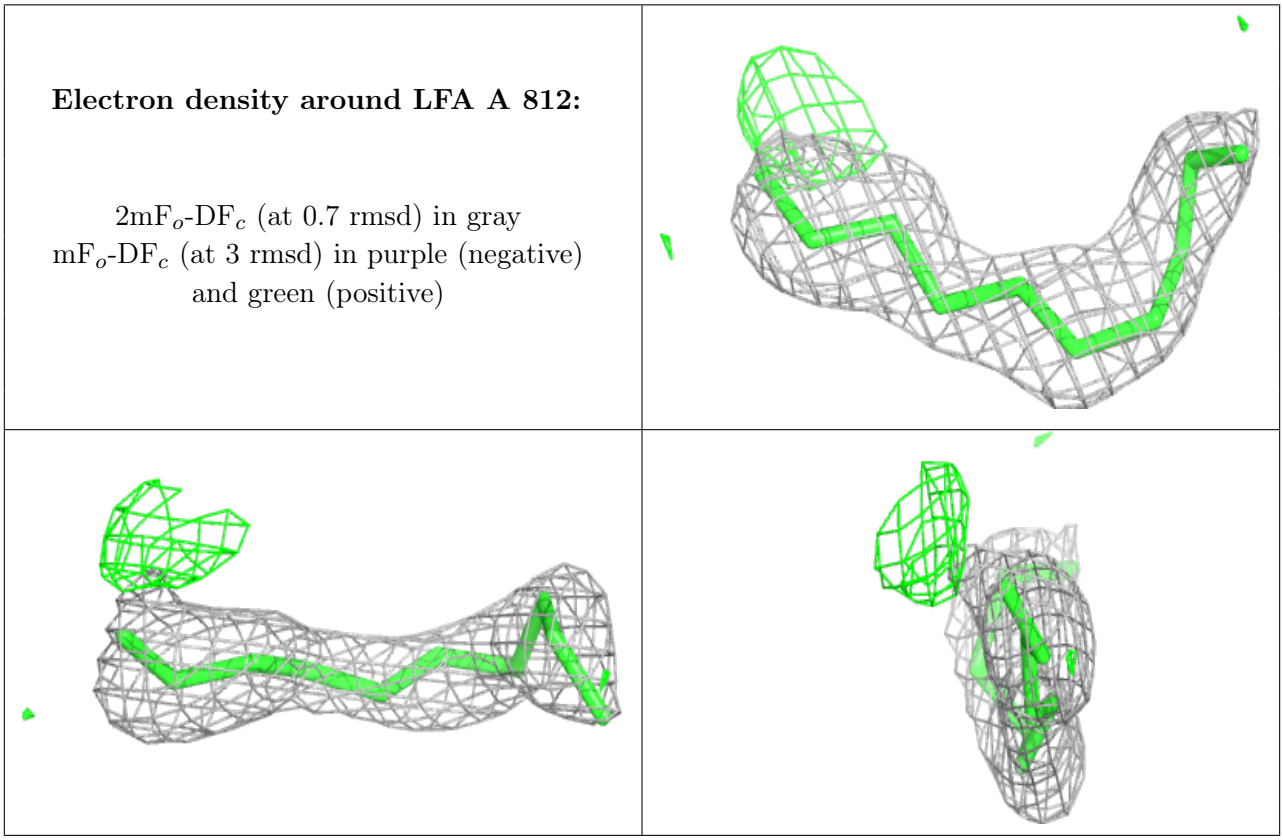
Electron density around LFA A 817:

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



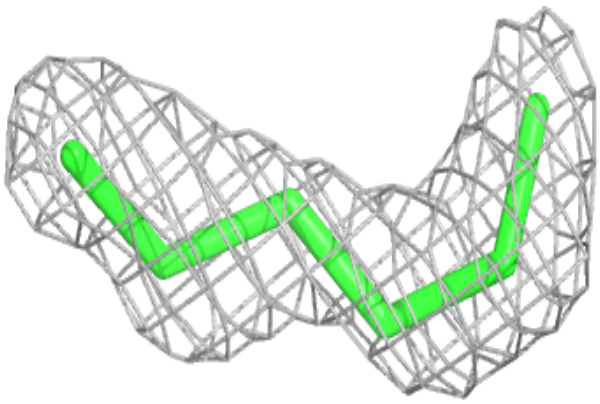
Electron density around LFA A 812:

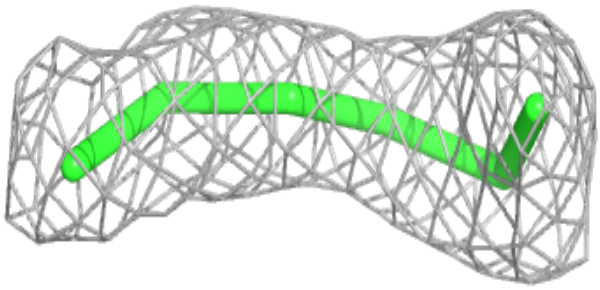
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

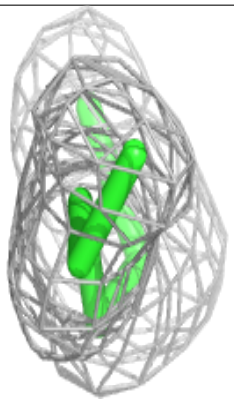


Electron density around LFA A 819:

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

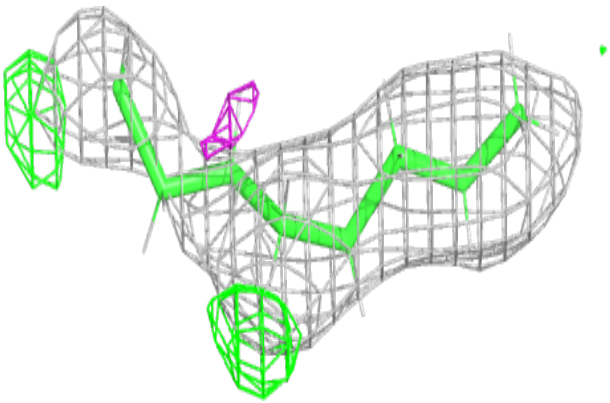


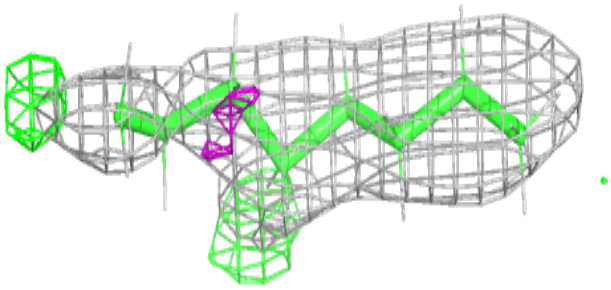


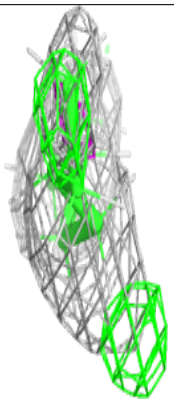


Electron density around LFA A 804:

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

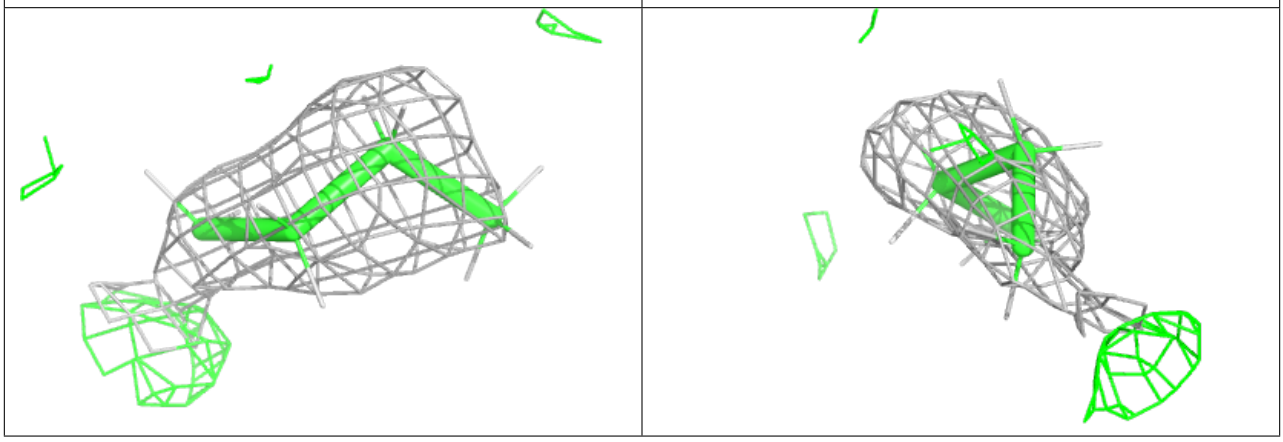






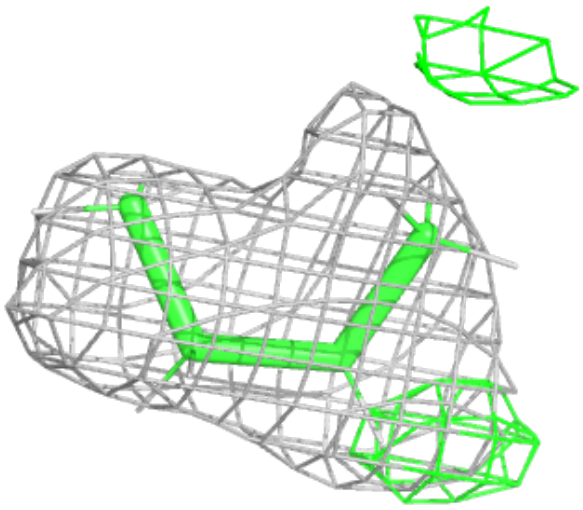
Electron density around LFA A 828:

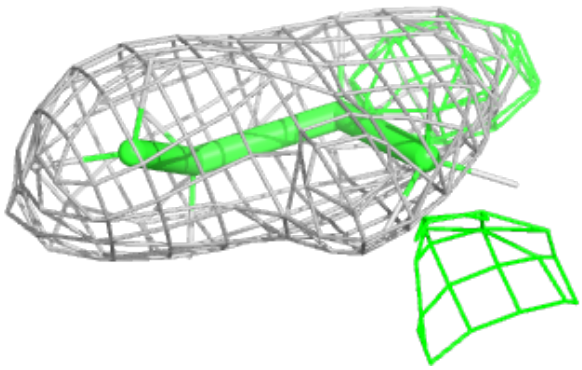
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

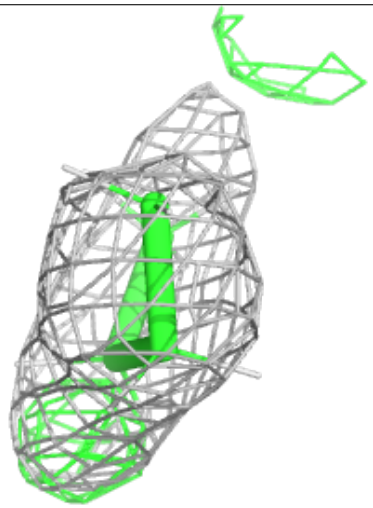


Electron density around LFA A 814:

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

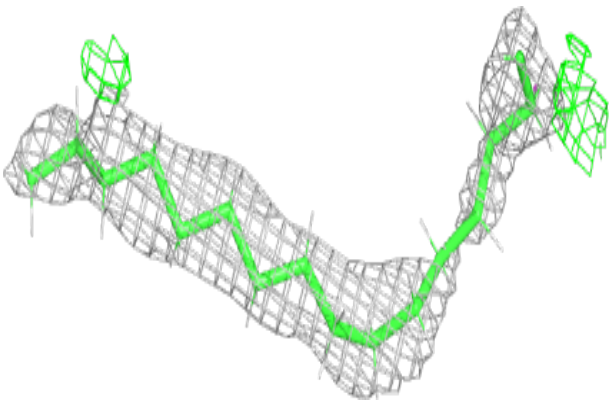


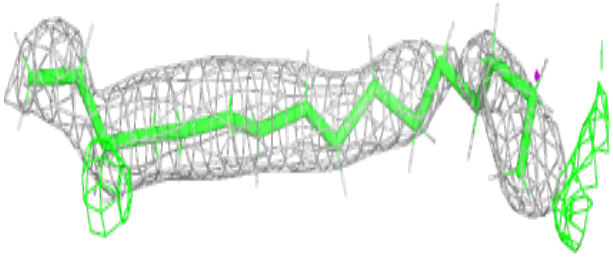


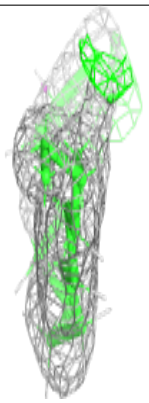


Electron density around LFA A 822:

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

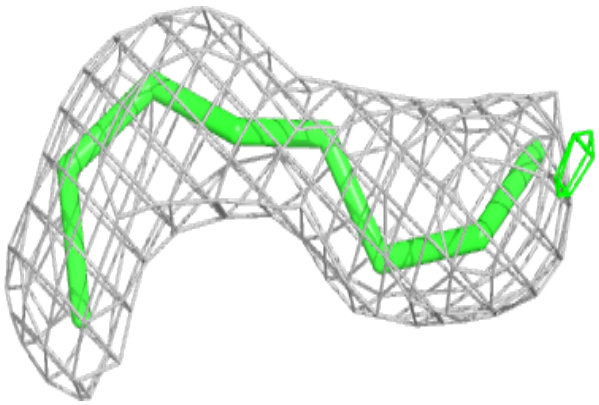


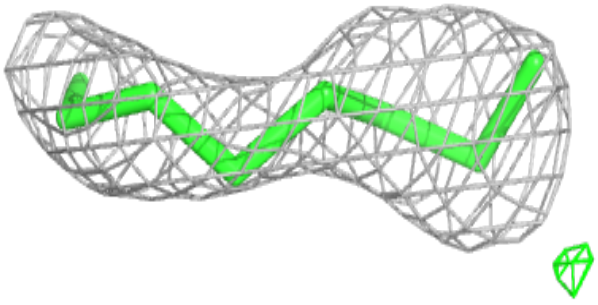


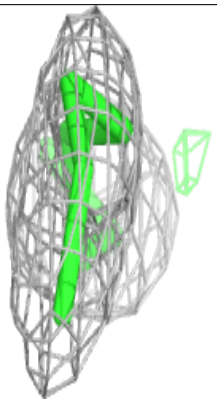


Electron density around LFA A 818:

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

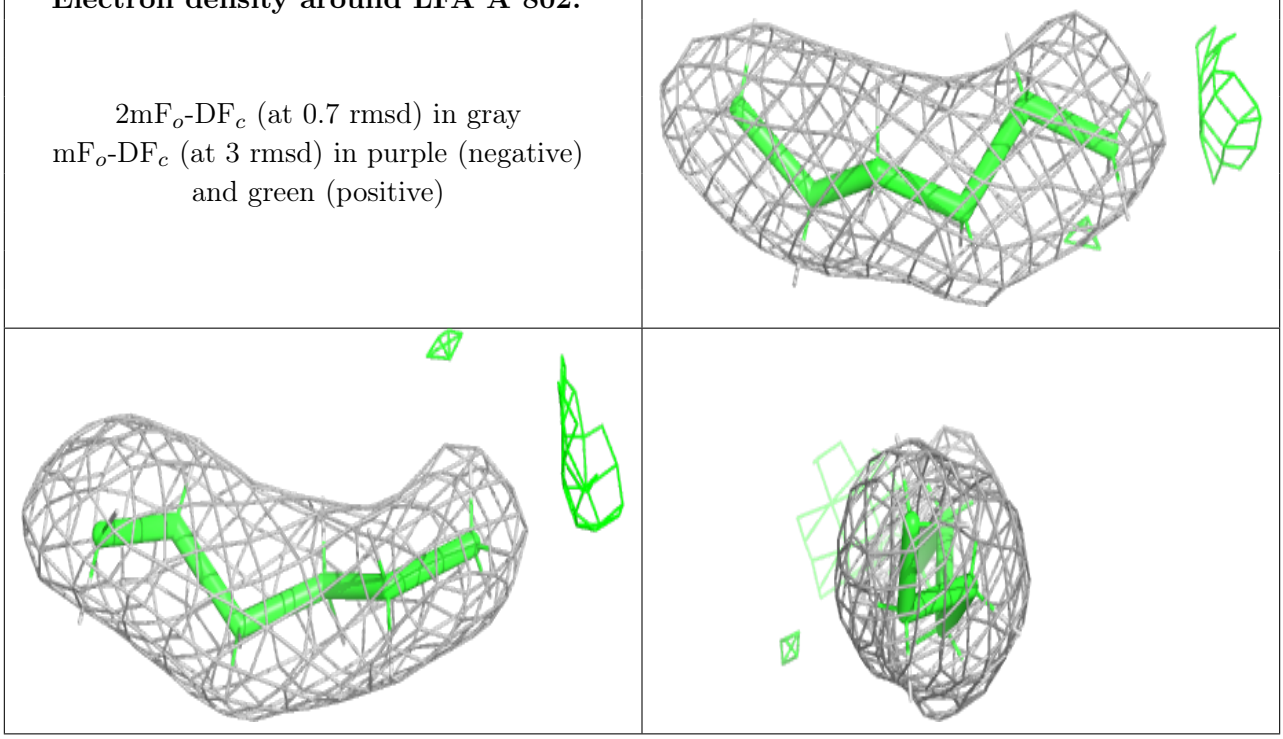






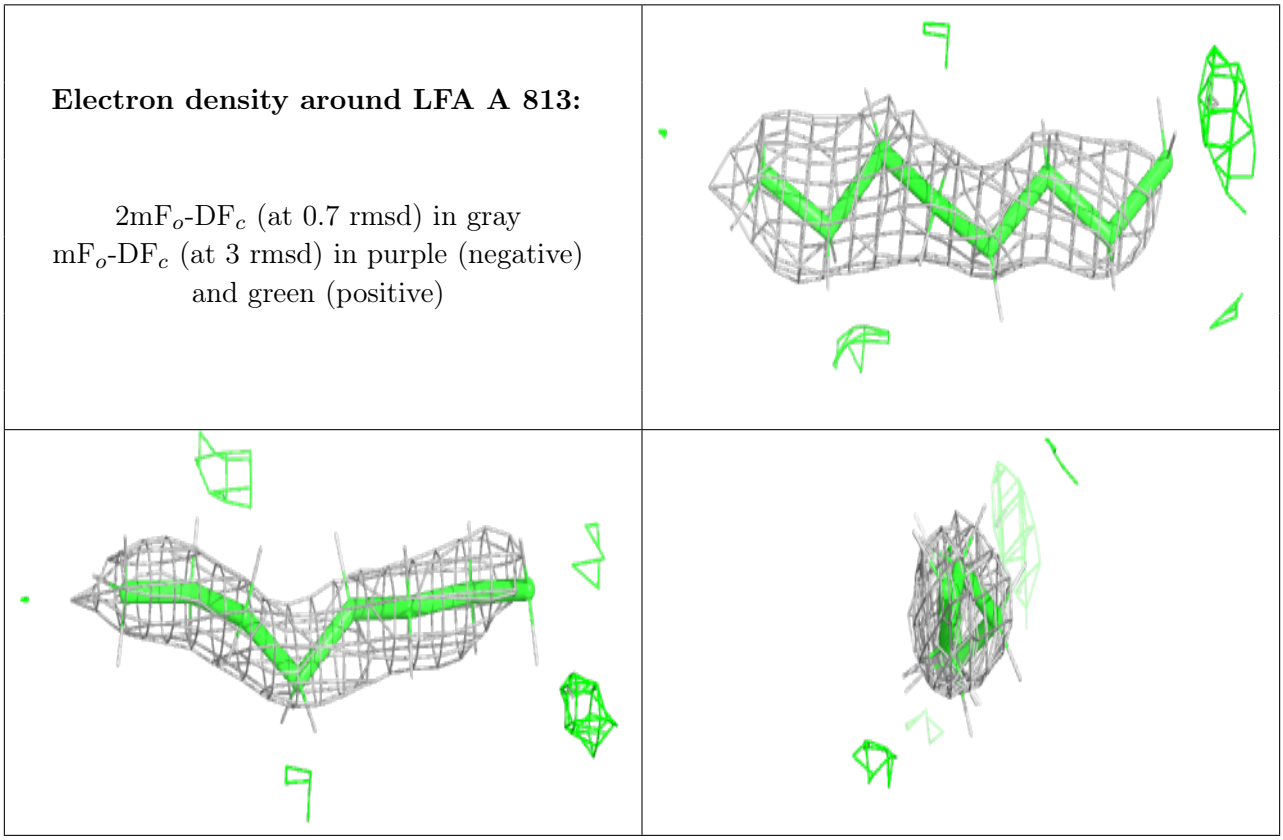
Electron density around LFA A 802:

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



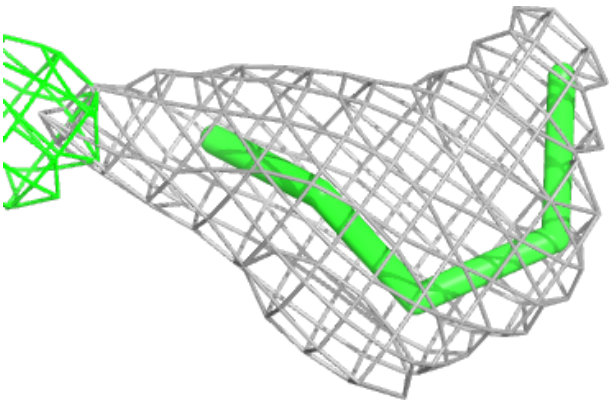
Electron density around LFA A 813:

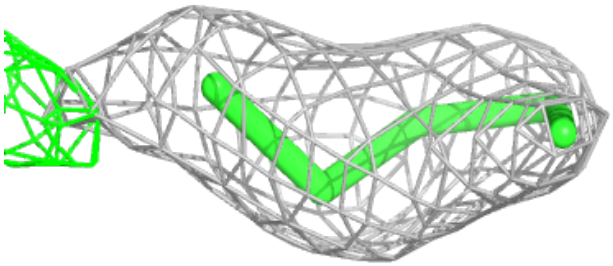
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

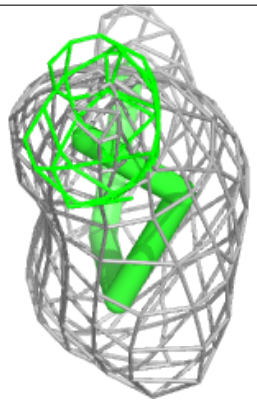


Electron density around LFA A 825:

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

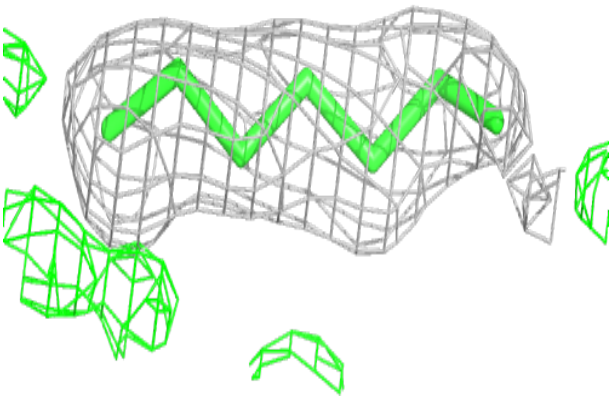


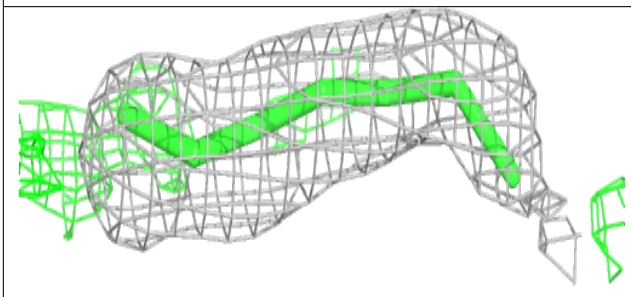


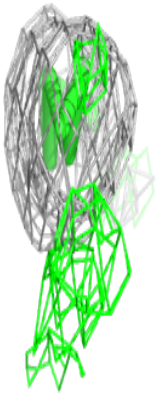


Electron density around LFA A 821:

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

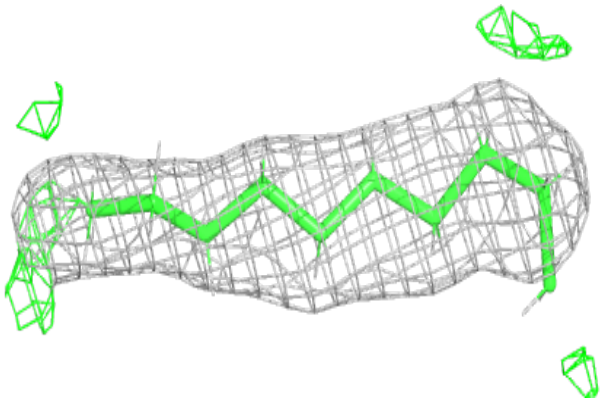


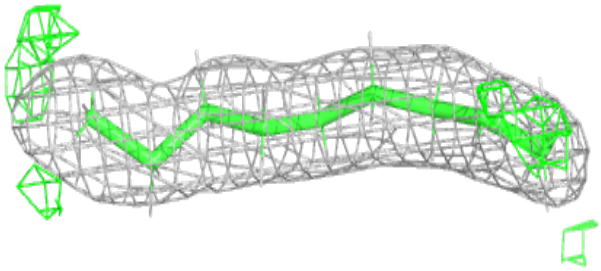


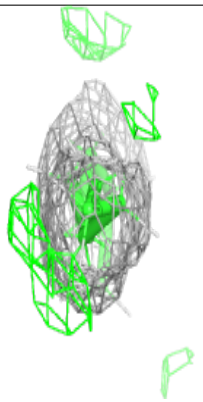


Electron density around LFA A 809:

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

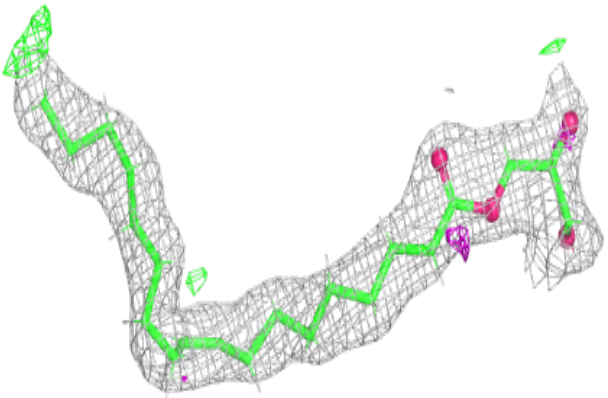


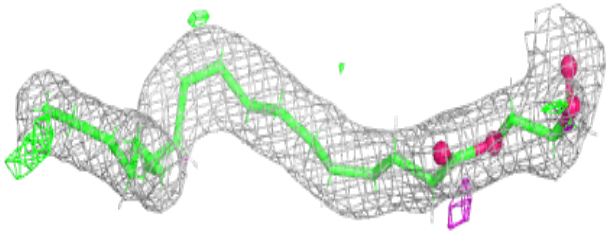


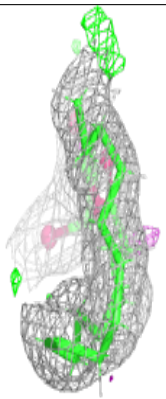


Electron density around OLC A 803:

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

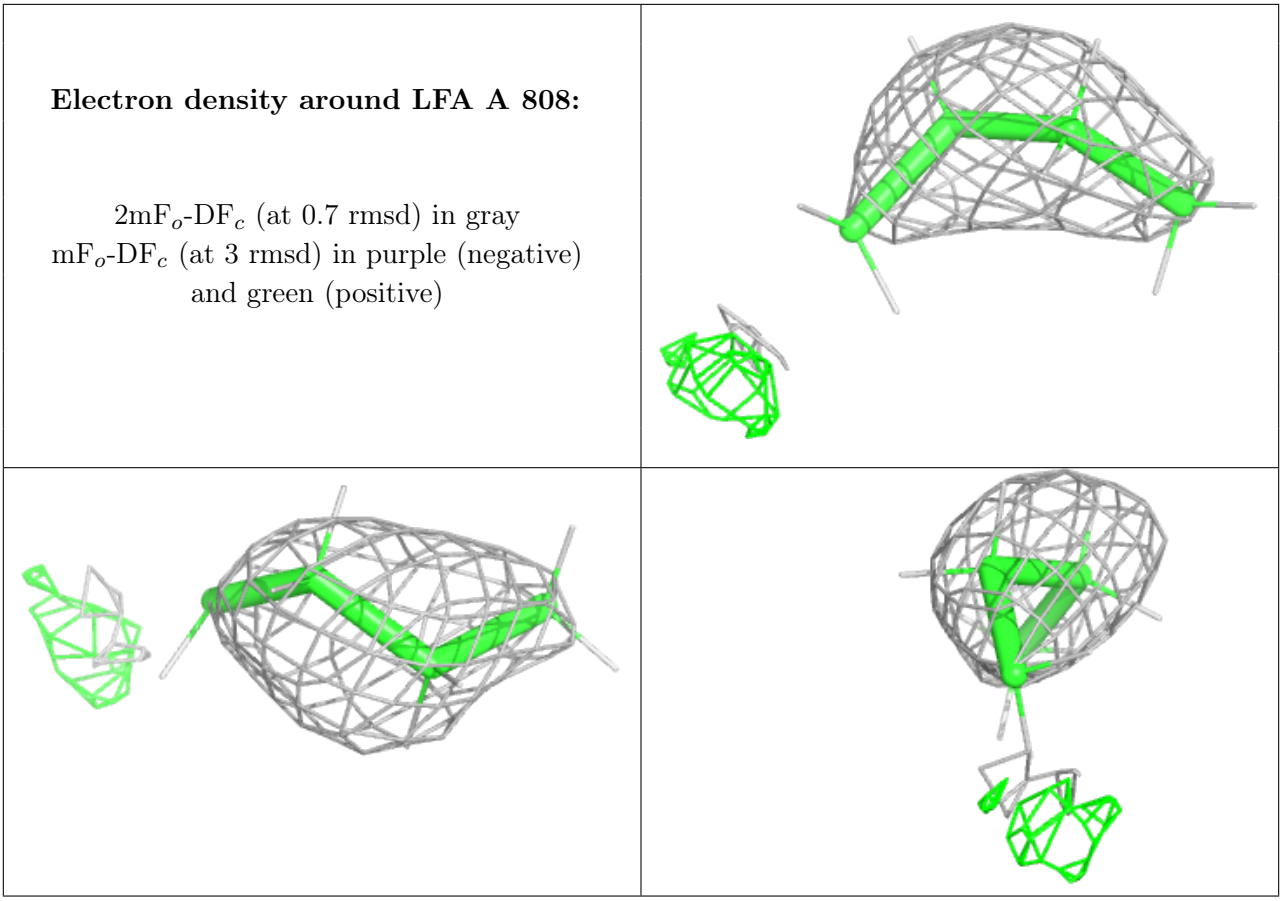






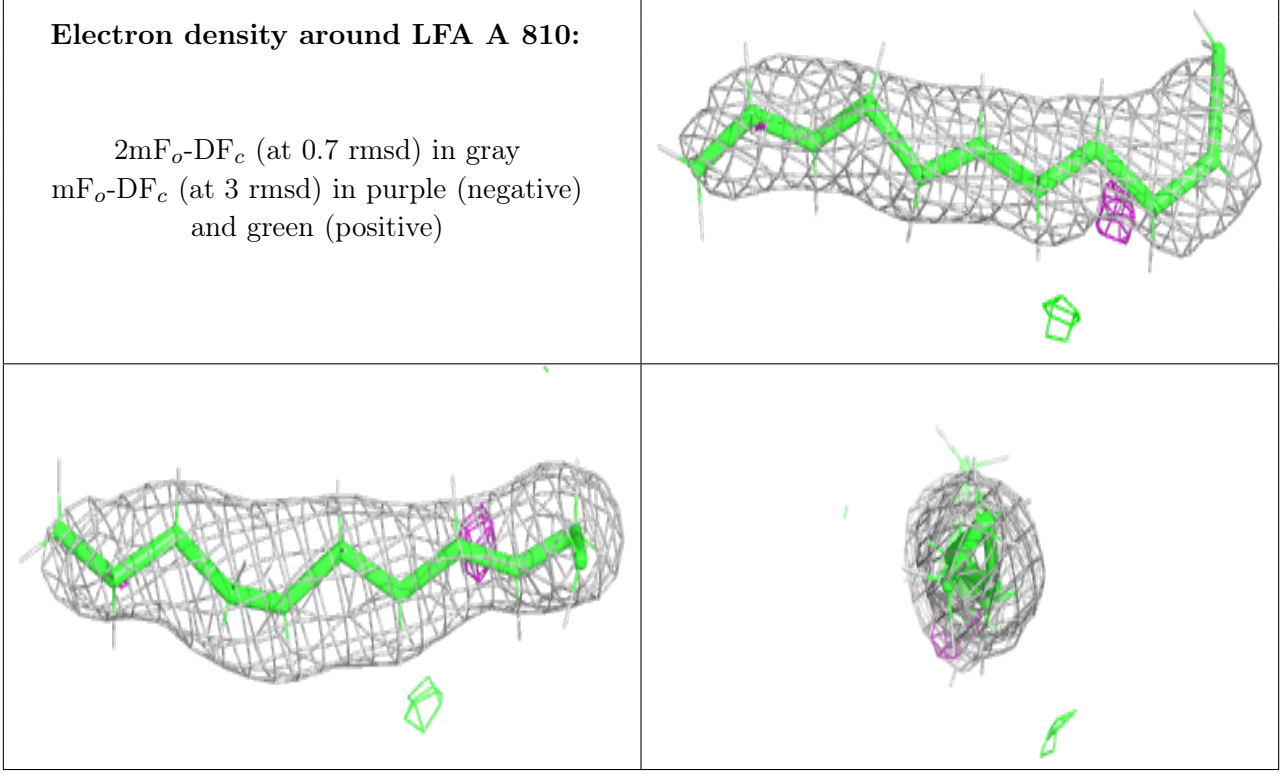
Electron density around LFA A 808:

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



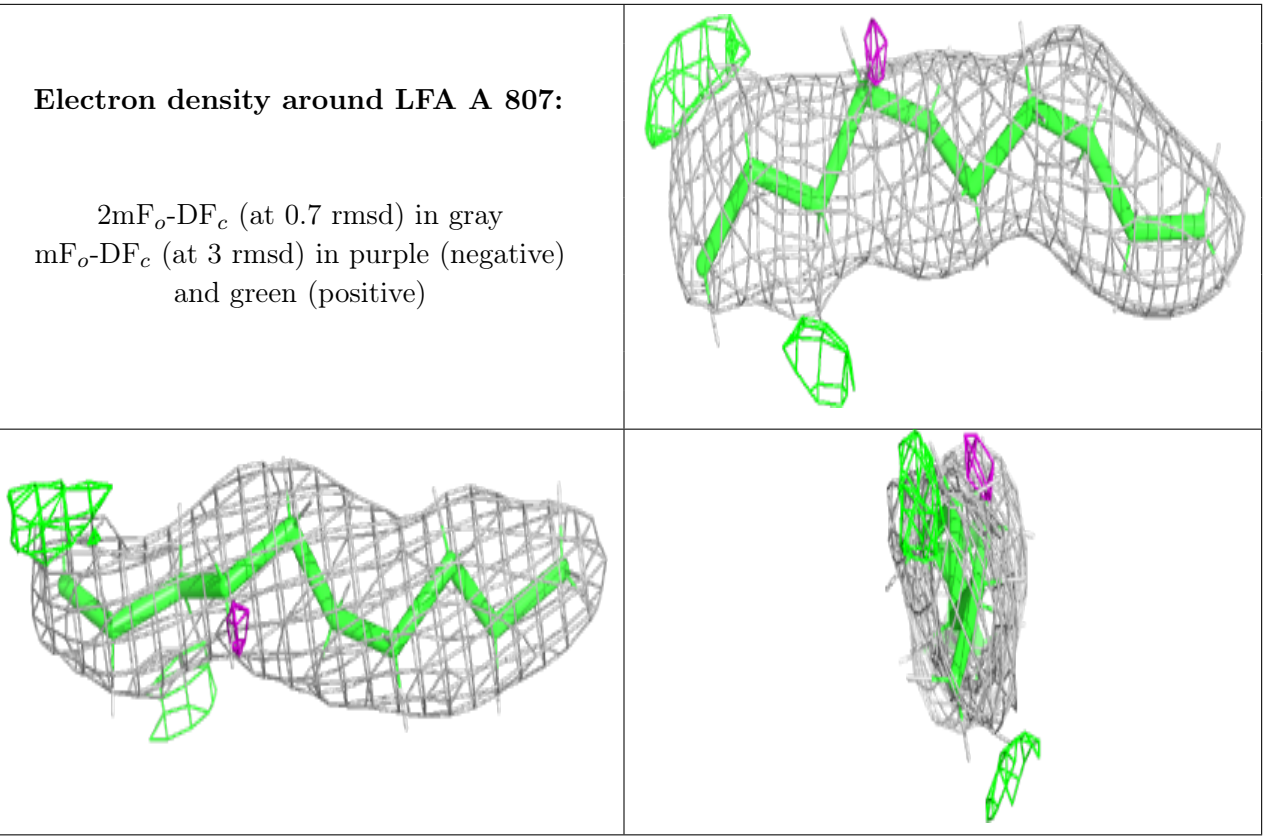
Electron density around LFA A 810:

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



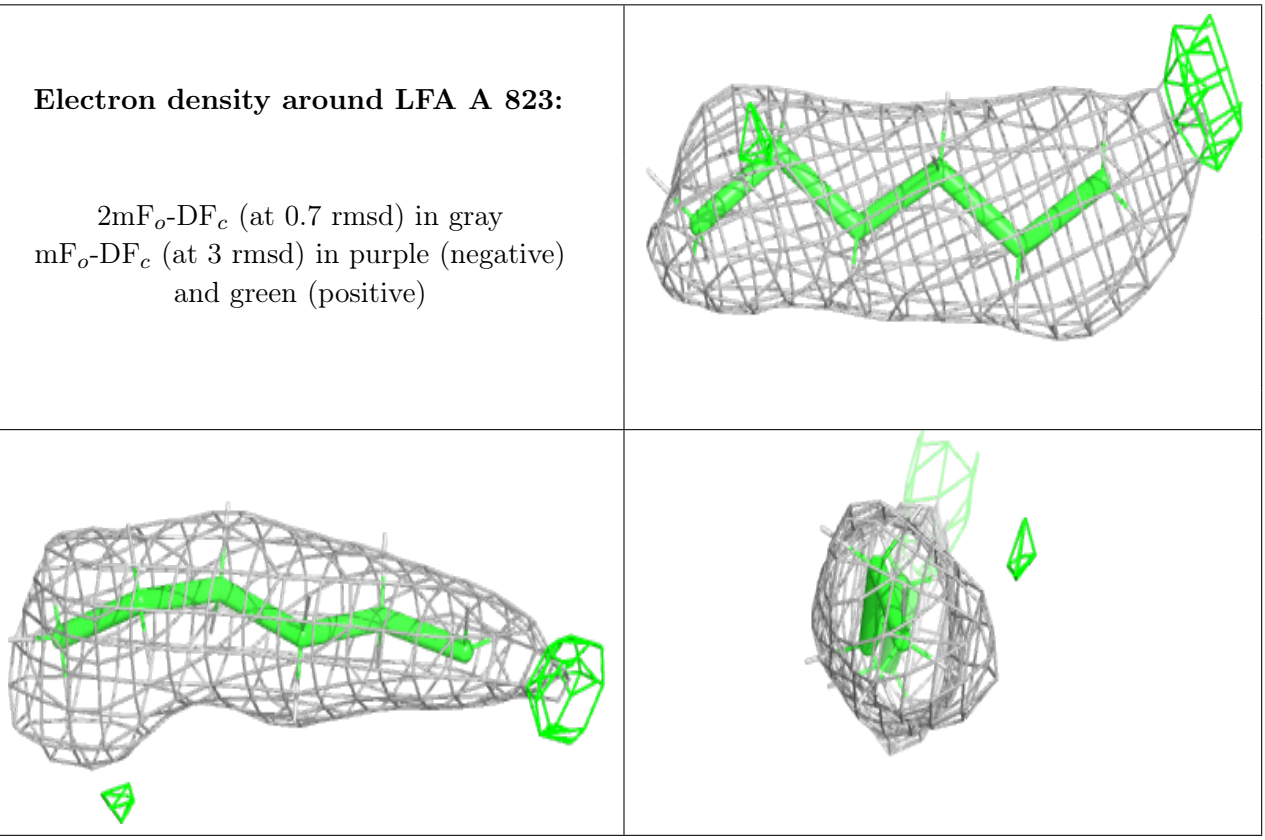
Electron density around LFA A 807:

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



Electron density around LFA A 823:

$2mF_o$-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.