Full wwPDB X-ray Structure Validation Report (i)

Jun 26, 2024 – 05:15 AM EDT

PDB ID	:	7AKY
Title	:	Crystal structure of the viral rhodopsin OLPVR1 in P21212 space group
Authors	:	Kovalev, K.; Zabelskii, D.; Alekseev, A.; Astashkin, R.; Gordeliy, V.
Deposited on	:	2020-10-02
Resolution	:	1.40 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:

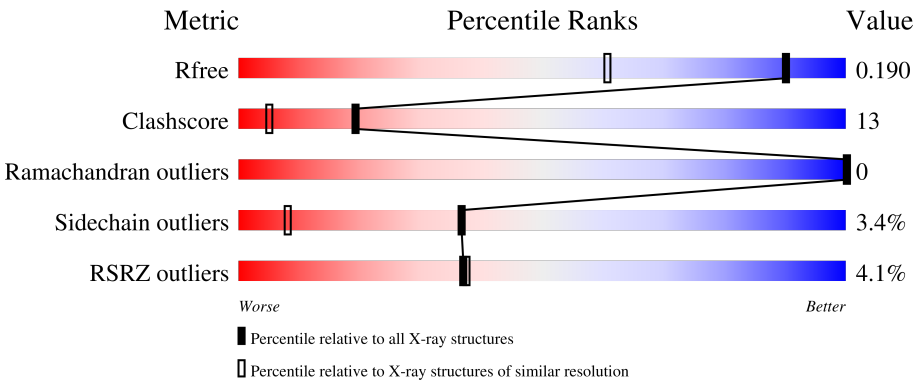
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	231	4% 78% 16% · ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2378 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.

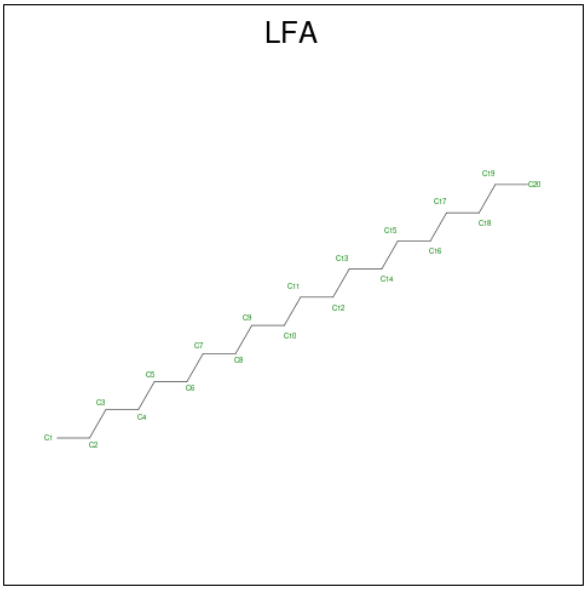
- Molecule 1 is a protein called viral rhodopsin OLPVR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	2052	1434	282	323	13	0	15	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	LEU	-	expression tag	UNP F2Y337
A	225	GLU	-	expression tag	UNP F2Y337
A	226	HIS	-	expression tag	UNP F2Y337
A	227	HIS	-	expression tag	UNP F2Y337
A	228	HIS	-	expression tag	UNP F2Y337
A	229	HIS	-	expression tag	UNP F2Y337
A	230	HIS	-	expression tag	UNP F2Y337
A	231	HIS	-	expression tag	UNP F2Y337

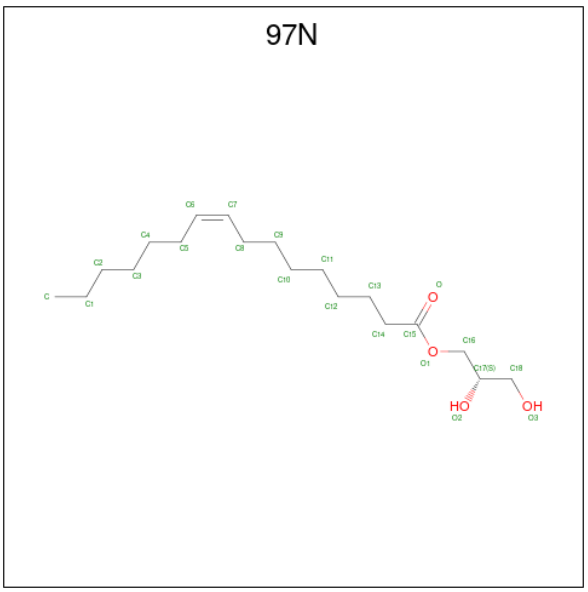
- Molecule 2 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 12	C 12	0	0
2	A	1	Total 15	C 15	0	0
2	A	1	Total 15	C 15	0	0
2	A	1	Total 7	C 7	0	0
2	A	1	Total 10	C 10	0	0
2	A	1	Total 11	C 11	0	0
2	A	1	Total 9	C 9	0	0
2	A	1	Total 3	C 3	0	0
2	A	1	Total 7	C 7	0	0
2	A	1	Total 11	C 11	0	0
2	A	1	Total 5	C 5	0	0
2	A	1	Total 5	C 5	0	0
2	A	1	Total 8	C 8	0	0
2	A	1	Total 16	C 16	0	0
2	A	1	Total 15	C 15	0	0
2	A	1	Total 12	C 12	0	0
2	A	1	Total 8	C 8	0	0
2	A	1	Total 11	C 11	0	0
2	A	1	Total 6	C 6	0	0
2	A	1	Total 18	C 18	0	0
2	A	1	Total 4	C 4	0	0

- Molecule 3 is (2S)-2,3-dihydroxypropyl (9Z)-hexadec-9-enoate (three-letter code: 97N)

(formula: $C_{19}H_{36}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 7 4	0	0

- Molecule 4 is water.

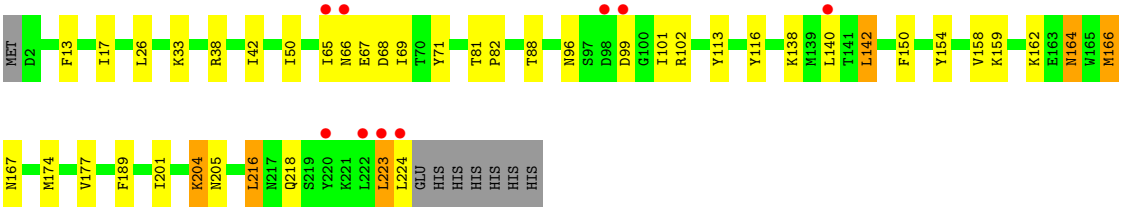
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	106	Total O 107 107	0	1

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: viral rhodopsin OLPVR1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	46.52Å 115.80Å 53.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.40 48.59 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.40) 99.9 (48.59-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.143 , 0.188 0.147 , 0.190	Depositor DCC
R_{free} test set	2897 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2378	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.94% 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: 97N, 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	0.65	1/2066 (0.0%)	0.52	0/2801

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	LEU	C-N	15.53	1.69	1.34

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	2052	0	2125	53	2
2	A	208	0	386	27	1
3	A	11	0	0	0	0
4	A	107	0	0	6	1
All	All	2378	0	2511	62	3

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 13.

All (62) 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:223:LEU:C	1:A:224:LEU:N	1.69	1.45
1:A:67:GLU:CG	2:A:412:LFA:H182	1.70	1.22
1:A:38:ARG:CZ	2:A:410:LFA:H12	1.77	1.12
1:A:67:GLU:CG	2:A:412:LFA:C18	2.42	0.96
1:A:204[B]:LYR:H192	1:A:204[B]:LYR:H9	1.48	0.93
1:A:96:ASN:HD21	1:A:167:ASN:HD21	1.19	0.91
1:A:204[A]:LYR:H9	1:A:204[A]:LYR:H183	1.55	0.88
1:A:26:LEU:O	2:A:410:LFA:H13	1.77	0.84
1:A:67:GLU:CG	2:A:412:LFA:C17	2.57	0.83
1:A:174[B]:MET:HE2	4:A:576:HOH:O	1.79	0.83
1:A:166[A]:MET:HE3	1:A:166[A]:MET:H	1.49	0.77
1:A:177:VAL:HG22	2:A:415:LFA:H11	1.69	0.75
1:A:38:ARG:NH2	2:A:410:LFA:H12	2.02	0.73
1:A:204[B]:LYR:H192	1:A:204[B]:LYR:C9	2.19	0.73
1:A:38:ARG:CZ	2:A:410:LFA:C1	2.64	0.72
1:A:205[B]:ASN:ND2	4:A:502:HOH:O	2.21	0.70
1:A:65:ILE:HD11	1:A:189:PHE:CZ	2.27	0.69
1:A:204[A]:LYR:H183	1:A:204[A]:LYR:C9	2.22	0.67
1:A:67:GLU:CG	2:A:412:LFA:H171	2.26	0.66
2:A:403:LFA:C15	2:A:412:LFA:C20	2.73	0.66
1:A:166[A]:MET:H	1:A:166[A]:MET:CE	2.08	0.66
2:A:403:LFA:C15	2:A:412:LFA:H202	2.29	0.63
1:A:33:LYS:HE3	4:A:511:HOH:O	1.99	0.61
1:A:88:THR:CG2	1:A:174[B]:MET:HE1	2.30	0.61
1:A:150[B]:PHE:CD1	2:A:418:LFA:H181	2.36	0.61
1:A:201:ILE:HA	1:A:205[B]:ASN:HD22	1.66	0.60
2:A:412:LFA:C16	4:A:526:HOH:O	2.50	0.59
1:A:65:ILE:CD1	1:A:189:PHE:CZ	2.87	0.58
1:A:26:LEU:O	2:A:410:LFA:H31	2.04	0.58
1:A:88:THR:HG23	1:A:174[B]:MET:HE1	1.86	0.57
1:A:223:LEU:CA	1:A:224:LEU:N	2.66	0.56
1:A:13:PHE:CE1	1:A:17[A]:ILE:HD11	2.40	0.56
2:A:403:LFA:C15	2:A:412:LFA:H192	2.37	0.55
1:A:33:LYS:NZ	1:A:218:GLN:OE1	2.40	0.54
1:A:13:PHE:CE1	1:A:17[A]:ILE:CD1	2.90	0.54
1:A:71:TYR:OH	2:A:412:LFA:H181	2.07	0.53
1:A:113:TYR:CD1	1:A:159:LYS:HD3	2.44	0.53
1:A:68:ASP:OD2	4:A:501:HOH:O	2.18	0.52
1:A:50[B]:ILE:HD12	2:A:403:LFA:H22	1.91	0.52
1:A:164:ASN:C	1:A:164:ASN:HD22	2.13	0.52
1:A:204[B]:LYR:C9	1:A:204[B]:LYR:C19	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:403:LFA:H41	2:A:403:LFA:H71	1.53	0.49
1:A:204[A]:LYR:C9	1:A:204[A]:LYR:C18	2.93	0.46
1:A:116:TYR:CD2	2:A:407:LFA:H122	2.51	0.46
1:A:204[B]:LYR:H81	1:A:204[B]:LYR:H10	1.68	0.46
1:A:204[A]:LYR:H81	1:A:204[A]:LYR:H10	1.67	0.45
2:A:420:LFA:H121	2:A:420:LFA:H151	1.49	0.45
1:A:67:GLU:CG	2:A:412:LFA:C16	2.93	0.45
1:A:69:ILE:C	1:A:69:ILE:HD12	2.37	0.45
1:A:65:ILE:HD11	1:A:189:PHE:HZ	1.80	0.45
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.84	0.44
1:A:216[A]:LEU:HD23	1:A:216[A]:LEU:HA	1.84	0.44
1:A:162:LYS:H	1:A:167:ASN:ND2	2.15	0.43
1:A:38:ARG:NH1	2:A:410:LFA:C1	2.80	0.43
2:A:403:LFA:C15	2:A:412:LFA:C19	2.96	0.43
1:A:81:THR:N	1:A:82:PRO:HD2	2.33	0.43
1:A:150[B]:PHE:HD1	2:A:418:LFA:H191	1.84	0.43
2:A:416:LFA:H161	2:A:416:LFA:H132	1.85	0.43
1:A:26:LEU:O	2:A:410:LFA:C1	2.58	0.41
2:A:418:LFA:H202	2:A:418:LFA:H171	1.71	0.41
1:A:154:TYR:CZ	1:A:158:VAL:HG11	2.56	0.41
1:A:42:ILE:HD12	4:A:592:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:420:LFA:C14	2:A:420:LFA:C17[2_555]	1.95	0.25
1:A:66:ASN:OD1	1:A:102:ARG:NH1[1_554]	2.09	0.11
1:A:99:ASP:CB	4:A:570:HOH:O[1_556]	2.16	0.04

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	234/231 (101%)	232 (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	221/220 (100%)	211 (96%)	10 (4%)	27	4

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ILE
1	A	138[A]	LYS
1	A	138[B]	LYS
1	A	140	LEU
1	A	142	LEU
1	A	164	ASN
1	A	166[A]	MET
1	A	166[B]	MET
1	A	216[A]	LEU
1	A	216[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	63	GLN
1	A	164	ASN
1	A	167	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)

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	204[A]	1	27,29,30	1.24	3 (11%)	30,37,39	2.05	8 (26%)
1	LYR	A	204[B]	1	27,29,30	1.21	3 (11%)	30,37,39	2.08	8 (26%)

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	204[A]	1	-	3/22/40/42	0/1/1/1
1	LYR	A	204[B]	1	-	2/22/40/42	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204[A]	LYR	C7-C80	3.25	1.40	1.35
1	A	204[B]	LYR	C7-C80	3.06	1.39	1.35
1	A	204[A]	LYR	C2-C3	2.48	1.40	1.33
1	A	204[B]	LYR	C2-C3	2.47	1.40	1.33
1	A	204[A]	LYR	C6-C5	2.25	1.40	1.34
1	A	204[B]	LYR	C6-C5	2.17	1.40	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204[B]	LYR	C10-C9-C80	-5.05	118.60	126.23
1	A	204[A]	LYR	C1-NZ-CE	4.97	121.20	113.33
1	A	204[A]	LYR	C10-C9-C80	-4.93	118.78	126.23
1	A	204[B]	LYR	C13-C12-C11	-4.91	119.01	124.53
1	A	204[B]	LYR	C1-NZ-CE	4.90	121.10	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204[A]	LYR	C13-C12-C11	-4.58	119.39	124.53
1	A	204[B]	LYR	C7-C6-C5	-3.15	113.38	123.22
1	A	204[A]	LYR	C7-C6-C5	-2.95	114.01	123.22
1	A	204[A]	LYR	C4-C3-C2	-2.60	118.50	123.59
1	A	204[A]	LYR	C8-C80-C7	-2.59	119.30	122.92
1	A	204[B]	LYR	C15-C14-C12	-2.50	109.61	114.08
1	A	204[A]	LYR	C15-C14-C12	-2.48	109.65	114.08
1	A	204[B]	LYR	C4-C3-C2	-2.47	118.74	123.59
1	A	204[B]	LYR	C8-C80-C7	-2.32	119.68	122.92
1	A	204[A]	LYR	C6-C7-C80	-2.10	124.31	127.31
1	A	204[B]	LYR	C6-C7-C80	-2.09	124.33	127.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	204[A]	LYR	NZ-C1-C2-C3
1	A	204[B]	LYR	CG-CD-CE-NZ
1	A	204[A]	LYR	CG-CD-CE-NZ
1	A	204[B]	LYR	CD-CE-NZ-C1
1	A	204[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	204[A]	LYR	4	0
1	A	204[B]	LYR	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	411	-	4,4,19	0.14	0	3,3,18	0.22	0
2	LFA	A	401	-	11,11,19	0.09	0	10,10,18	0.08	0
2	LFA	A	404	-	6,6,19	0.11	0	5,5,18	0.11	0
2	LFA	A	416	-	11,11,19	0.09	0	10,10,18	0.09	0
2	LFA	A	420	-	17,17,19	0.22	0	16,16,18	0.18	0
2	LFA	A	409	-	6,6,19	0.12	0	5,5,18	0.14	0
2	LFA	A	405	-	9,9,19	0.12	0	8,8,18	0.16	0
2	LFA	A	414	-	15,15,19	0.13	0	14,14,18	0.12	0
2	LFA	A	402	-	14,14,19	0.10	0	13,13,18	0.10	0
2	LFA	A	406	-	10,10,19	0.12	0	9,9,18	0.11	0
2	LFA	A	407	-	8,8,19	0.09	0	7,7,18	0.10	0
3	97N	A	422	-	10,10,22	0.24	0	11,11,23	0.31	0
2	LFA	A	403	-	14,14,19	0.08	0	13,13,18	0.14	0
2	LFA	A	408	-	2,2,19	0.08	0	0,1,18	-	-
2	LFA	A	421	-	3,3,19	0.21	0	2,2,18	0.45	0
2	LFA	A	412	-	4,4,19	0.14	0	3,3,18	0.24	0
2	LFA	A	410	-	10,10,19	0.13	0	9,9,18	0.14	0
2	LFA	A	419	-	5,5,19	0.12	0	4,4,18	0.14	0
2	LFA	A	413	-	7,7,19	0.11	0	6,6,18	0.12	0
2	LFA	A	417	-	7,7,19	0.11	0	6,6,18	0.13	0
2	LFA	A	415	-	14,14,19	0.17	0	13,13,18	0.14	0
2	LFA	A	418	-	10,10,19	0.10	0	9,9,18	0.12	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
2	LFA	A	411	-	-	1/2/2/17	-
2	LFA	A	401	-	-	3/9/9/17	-
2	LFA	A	404	-	-	0/4/4/17	-
2	LFA	A	416	-	-	6/9/9/17	-
2	LFA	A	420	-	-	12/15/15/17	-
2	LFA	A	409	-	-	2/4/4/17	-
2	LFA	A	405	-	-	2/7/7/17	-
2	LFA	A	414	-	-	6/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	402	-	-	7/12/12/17	-
2	LFA	A	406	-	-	7/8/8/17	-
2	LFA	A	407	-	-	2/6/6/17	-
3	97N	A	422	-	-	3/10/10/22	-
2	LFA	A	403	-	-	10/12/12/17	-
2	LFA	A	421	-	-	0/1/1/17	-
2	LFA	A	412	-	-	0/2/2/17	-
2	LFA	A	410	-	-	3/8/8/17	-
2	LFA	A	419	-	-	1/3/3/17	-
2	LFA	A	413	-	-	3/5/5/17	-
2	LFA	A	417	-	-	2/5/5/17	-
2	LFA	A	415	-	-	8/12/12/17	-
2	LFA	A	418	-	-	6/8/8/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	LFA	C6-C7-C8-C9
2	A	403	LFA	C4-C5-C6-C7
2	A	420	LFA	C12-C13-C14-C15
2	A	401	LFA	C2-C3-C4-C5
2	A	403	LFA	C3-C4-C5-C6
2	A	415	LFA	C7-C8-C9-C10
2	A	416	LFA	C14-C15-C16-C17
2	A	417	LFA	C5-C6-C7-C8
2	A	418	LFA	C12-C13-C14-C15
2	A	420	LFA	C6-C7-C8-C9
2	A	420	LFA	C11-C10-C9-C8
2	A	402	LFA	C11-C12-C13-C14
2	A	420	LFA	C2-C3-C4-C5
2	A	413	LFA	C16-C17-C18-C19
2	A	402	LFA	C6-C7-C8-C9
2	A	414	LFA	C11-C12-C13-C14
2	A	401	LFA	C3-C4-C5-C6
2	A	403	LFA	C5-C6-C7-C8
2	A	406	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	414	LFA	C10-C11-C12-C13
2	A	407	LFA	C14-C15-C16-C17
2	A	418	LFA	C14-C15-C16-C17
3	A	422	97N	C12-C13-C14-C15
2	A	415	LFA	C4-C5-C6-C7
2	A	410	LFA	C7-C8-C9-C10
2	A	410	LFA	C4-C5-C6-C7
2	A	416	LFA	C10-C11-C12-C13
2	A	418	LFA	C17-C18-C19-C20
2	A	402	LFA	C10-C11-C12-C13
2	A	416	LFA	C12-C13-C14-C15
2	A	415	LFA	C5-C6-C7-C8
2	A	417	LFA	C4-C5-C6-C7
2	A	402	LFA	C2-C3-C4-C5
2	A	406	LFA	C3-C4-C5-C6
2	A	415	LFA	C9-C10-C11-C12
2	A	409	LFA	C2-C3-C4-C5
2	A	401	LFA	C11-C10-C9-C8
2	A	413	LFA	C14-C15-C16-C17
2	A	420	LFA	C14-C15-C16-C17
2	A	403	LFA	C11-C12-C13-C14
2	A	411	LFA	C17-C18-C19-C20
2	A	419	LFA	C2-C3-C4-C5
2	A	414	LFA	C13-C14-C15-C16
2	A	418	LFA	C11-C12-C13-C14
2	A	413	LFA	C17-C18-C19-C20
2	A	416	LFA	C15-C16-C17-C18
2	A	403	LFA	C1-C2-C3-C4
2	A	406	LFA	C7-C8-C9-C10
2	A	416	LFA	C9-C10-C11-C12
2	A	420	LFA	C15-C16-C17-C18
2	A	420	LFA	C1-C2-C3-C4
2	A	402	LFA	C1-C2-C3-C4
2	A	406	LFA	C5-C6-C7-C8
2	A	418	LFA	C16-C17-C18-C19
2	A	420	LFA	C11-C12-C13-C14
2	A	415	LFA	C12-C13-C14-C15
2	A	405	LFA	C7-C8-C9-C10
2	A	407	LFA	C12-C13-C14-C15
2	A	403	LFA	C9-C10-C11-C12
2	A	409	LFA	C1-C2-C3-C4
2	A	414	LFA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	415	LFA	C6-C7-C8-C9
2	A	402	LFA	C4-C5-C6-C7
2	A	402	LFA	C3-C4-C5-C6
2	A	415	LFA	C10-C11-C12-C13
2	A	420	LFA	C10-C11-C12-C13
2	A	406	LFA	C1-C2-C3-C4
2	A	414	LFA	C5-C6-C7-C8
3	A	422	97N	O-C15-O1-C16
3	A	422	97N	C14-C15-O1-C16
2	A	416	LFA	C13-C14-C15-C16
2	A	405	LFA	C5-C6-C7-C8
2	A	414	LFA	C12-C13-C14-C15
2	A	403	LFA	C11-C10-C9-C8
2	A	420	LFA	C9-C10-C11-C12
2	A	410	LFA	C2-C3-C4-C5
2	A	403	LFA	C12-C13-C14-C15
2	A	420	LFA	C7-C8-C9-C10
2	A	415	LFA	C2-C3-C4-C5
2	A	406	LFA	C6-C7-C8-C9
2	A	403	LFA	C7-C8-C9-C10
2	A	406	LFA	C2-C3-C4-C5
2	A	418	LFA	C13-C14-C15-C16
2	A	420	LFA	C3-C4-C5-C6

There are no ring outliers.

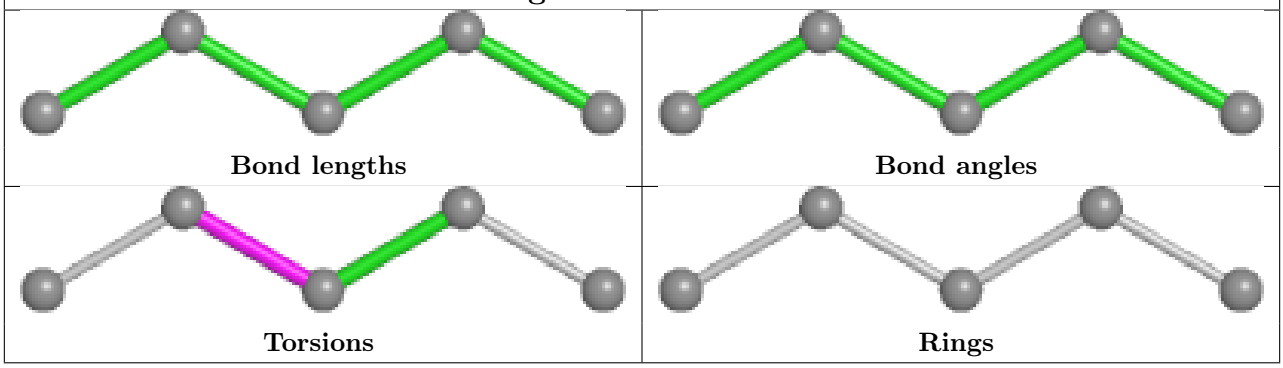
8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	416	LFA	1	0
2	A	420	LFA	1	1
2	A	407	LFA	1	0
2	A	403	LFA	6	0
2	A	412	LFA	11	0
2	A	410	LFA	7	0
2	A	415	LFA	1	0
2	A	418	LFA	3	0

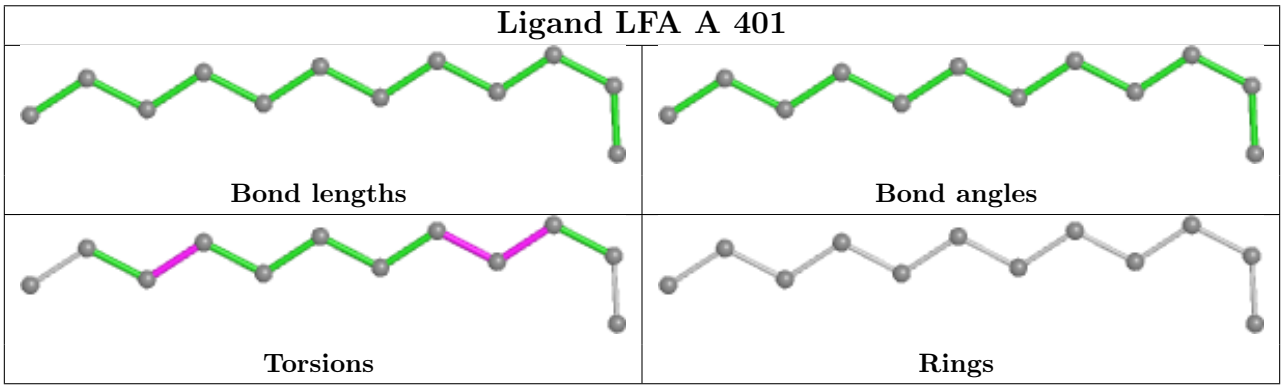
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

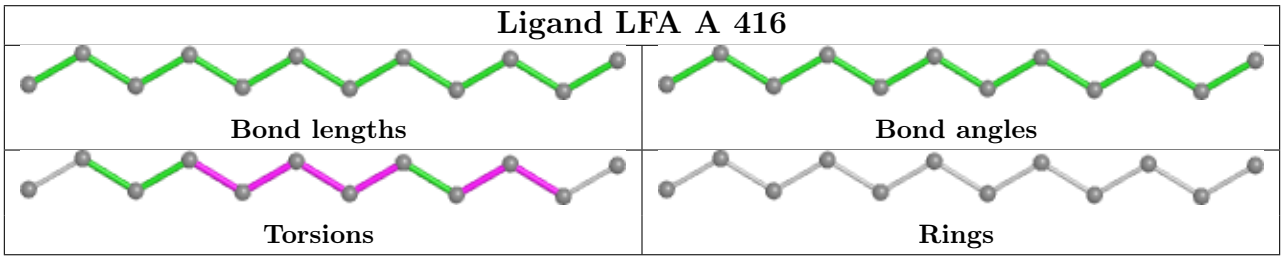
Ligand LFA A 411



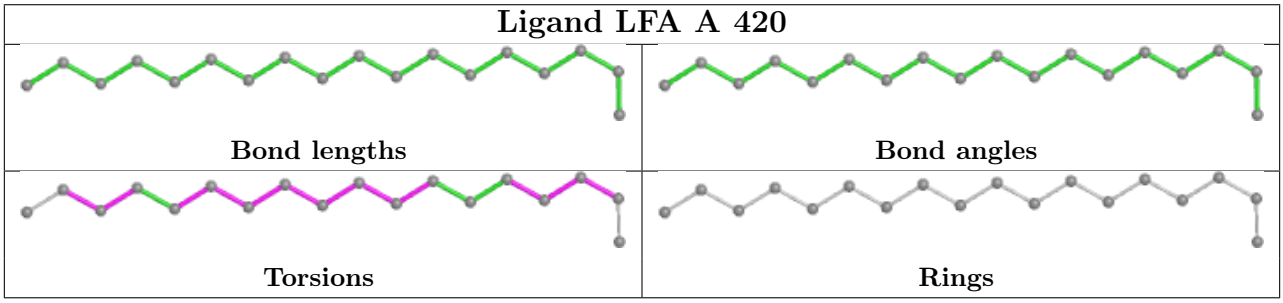
Ligand LFA A 401



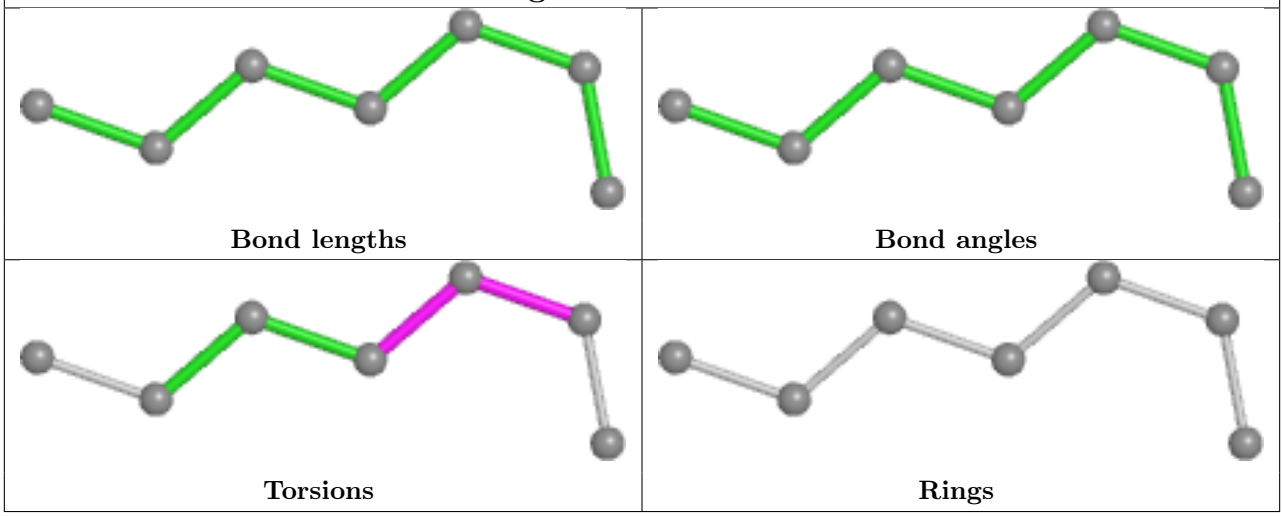
Ligand LFA A 416



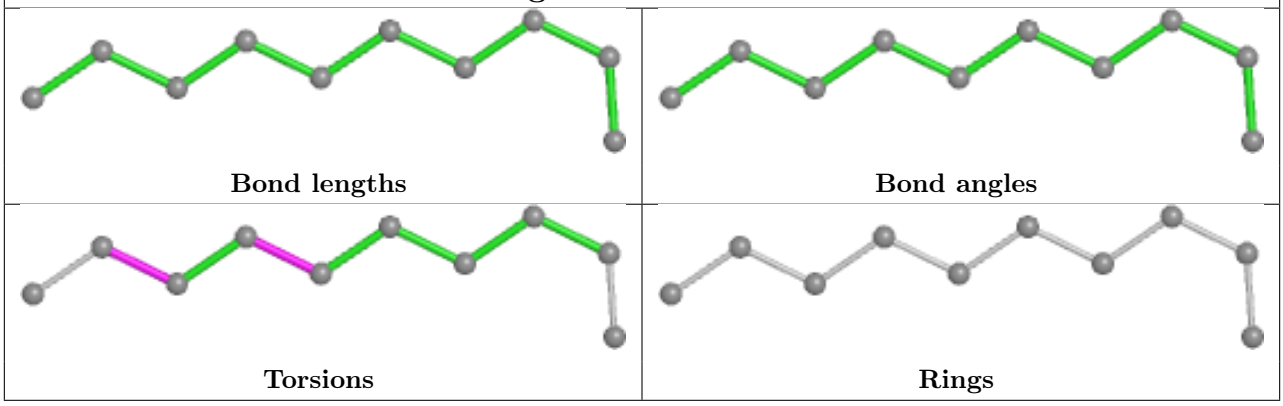
Ligand LFA A 420



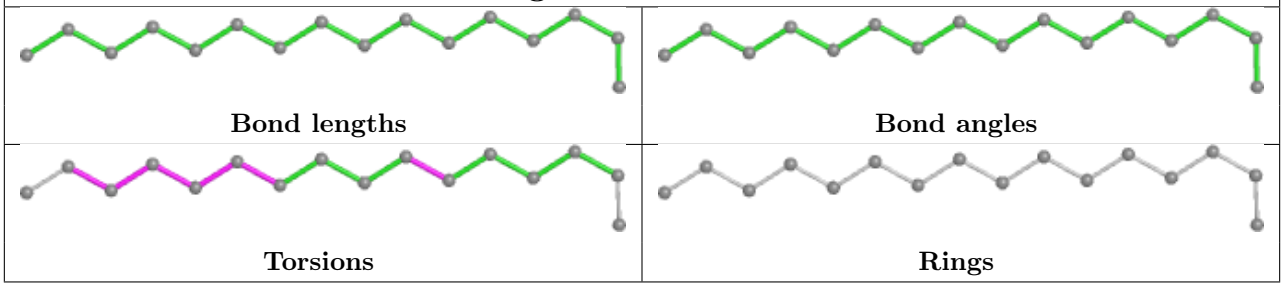
Ligand LFA A 409



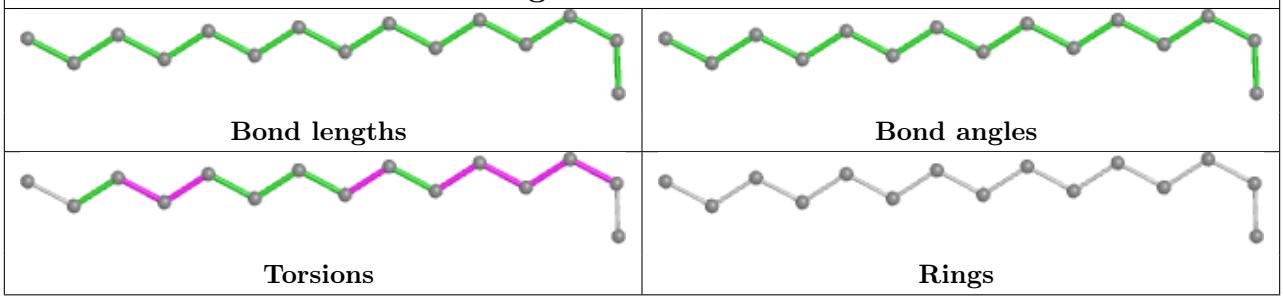
Ligand LFA A 405



Ligand LFA A 414



Ligand LFA A 402



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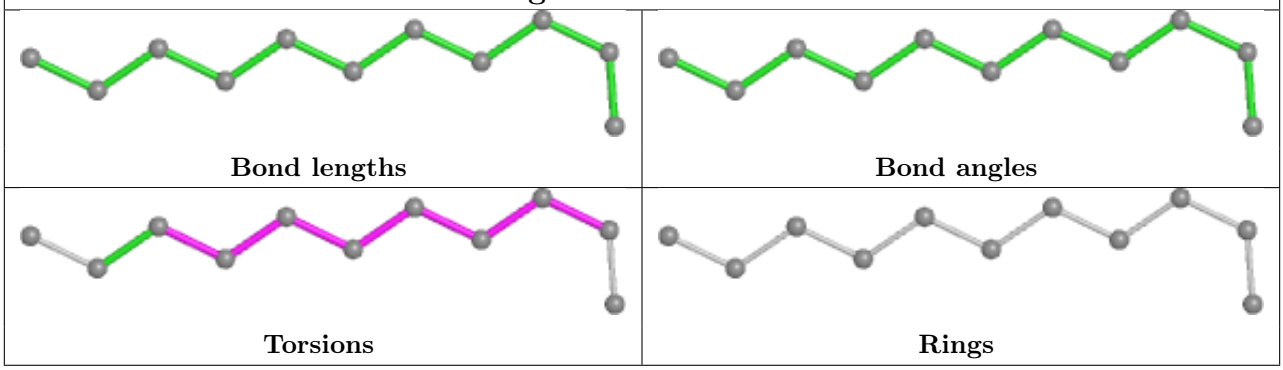
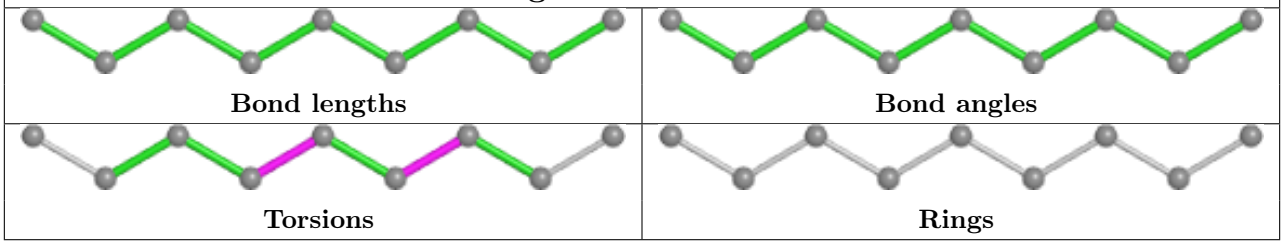
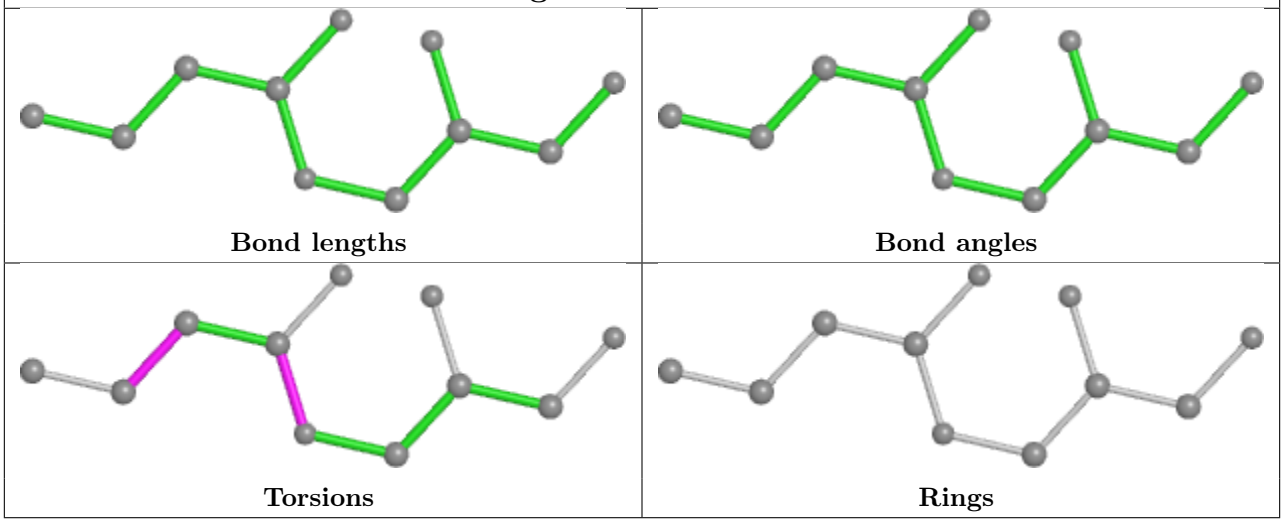


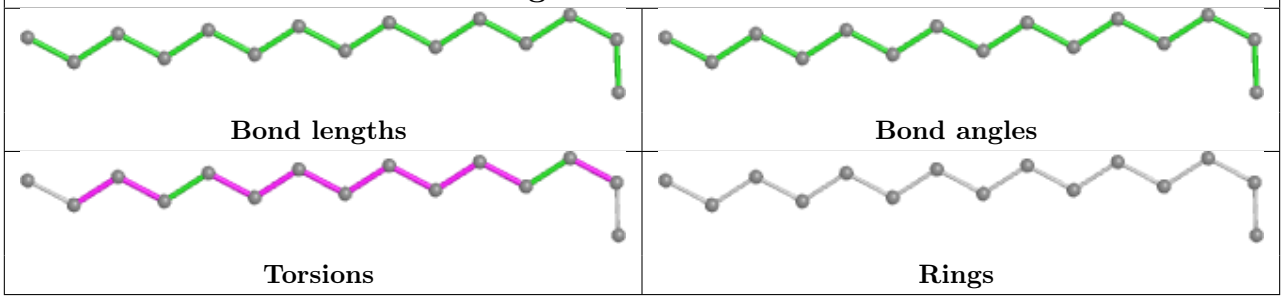
Ligand LFA A 407



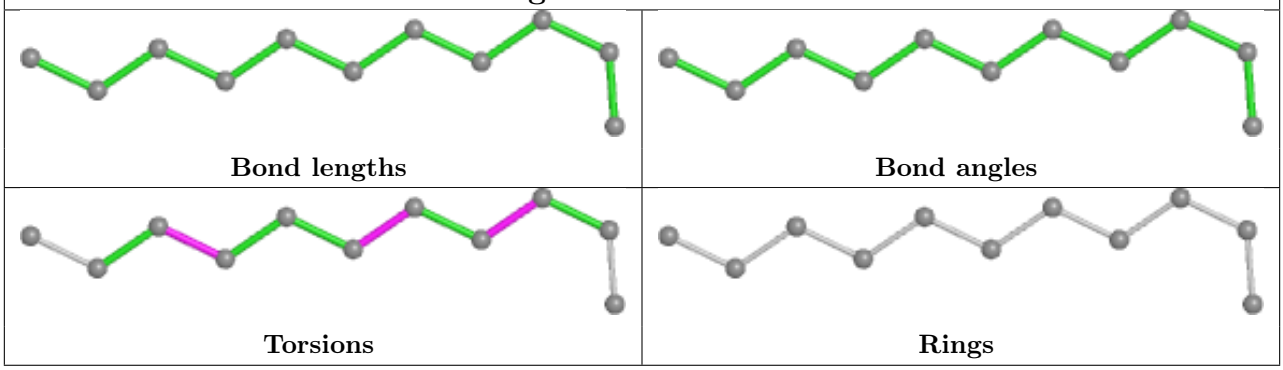
Ligand 97N A 422



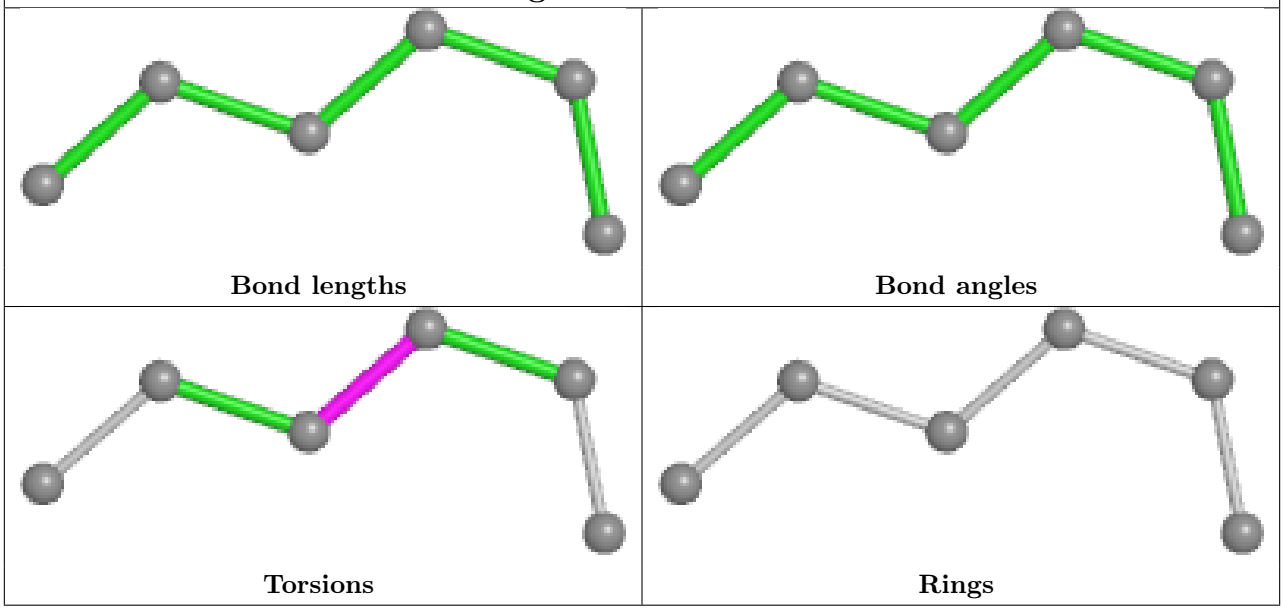
Ligand LFA A 403



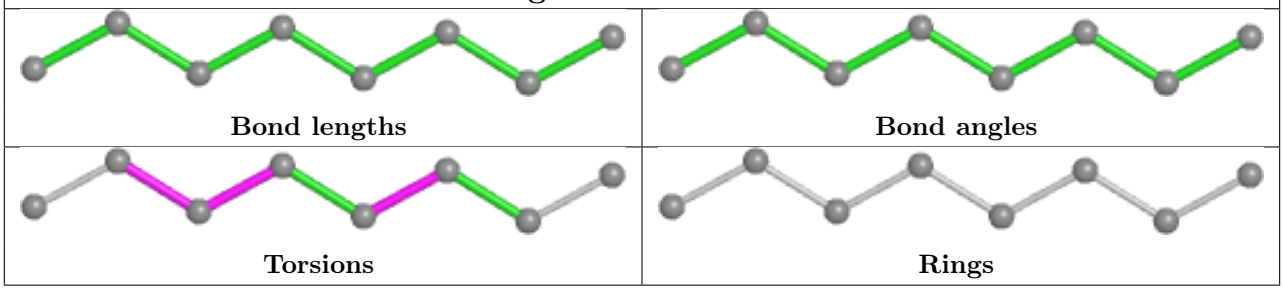
Ligand LFA A 410



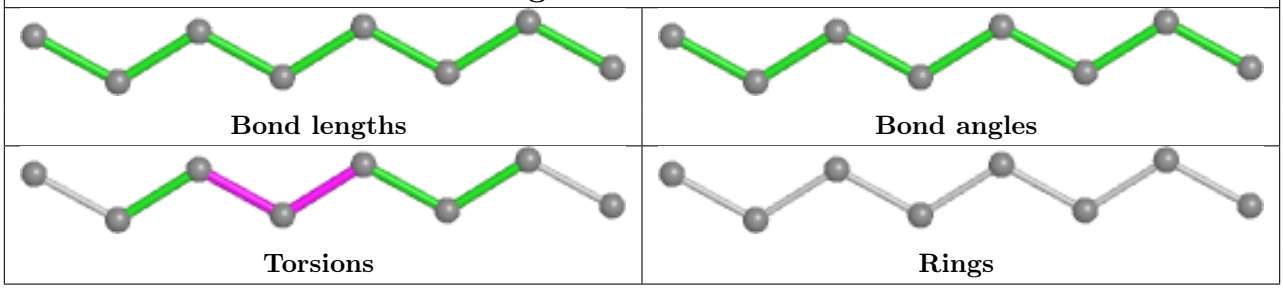
Ligand LFA A 419

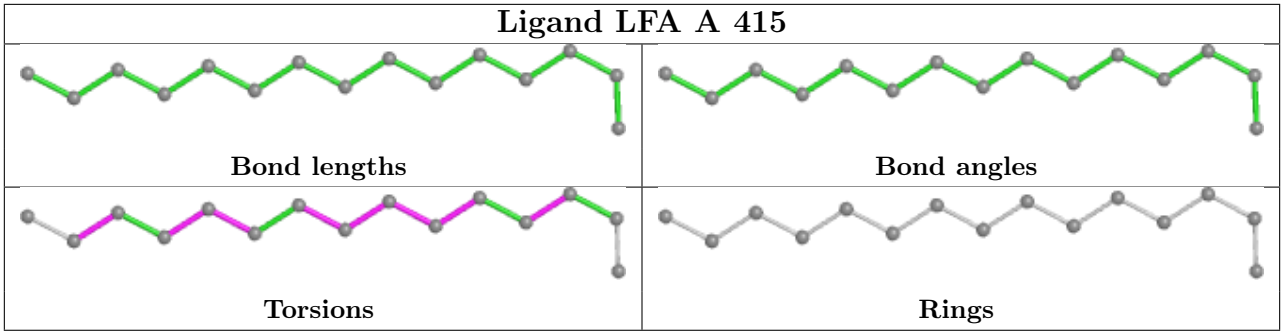


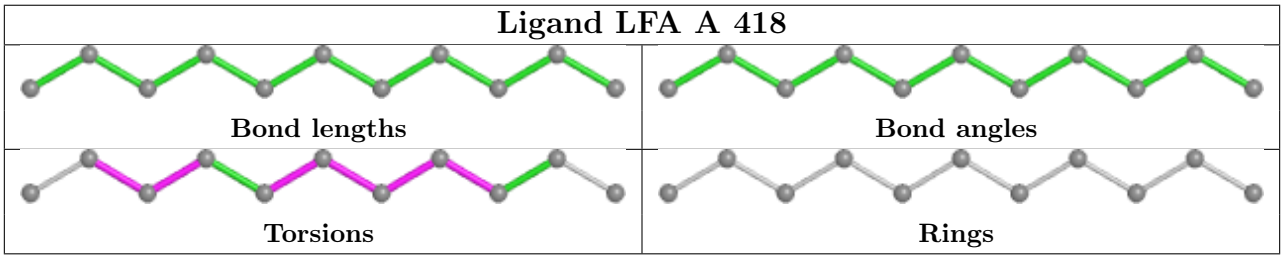
Ligand LFA A 413



Ligand LFA A 417







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	223:LEU	C	224:LEU	N	1.69

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	222/231 (96%)	-0.39	9 (4%) 37 37	15, 20, 44, 60	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	LEU	5.0
1	A	220	TYR	4.3
1	A	65	ILE	3.6
1	A	224	LEU	2.9
1	A	66	ASN	2.8
1	A	98	ASP	2.6
1	A	140	LEU	2.6
1	A	222	LEU	2.4
1	A	99	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	LYR	A	204[A]	29/30	0.96	0.08	14,16,20,21	29
1	LYR	A	204[B]	29/30	0.96	0.08	14,16,20,22	29

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

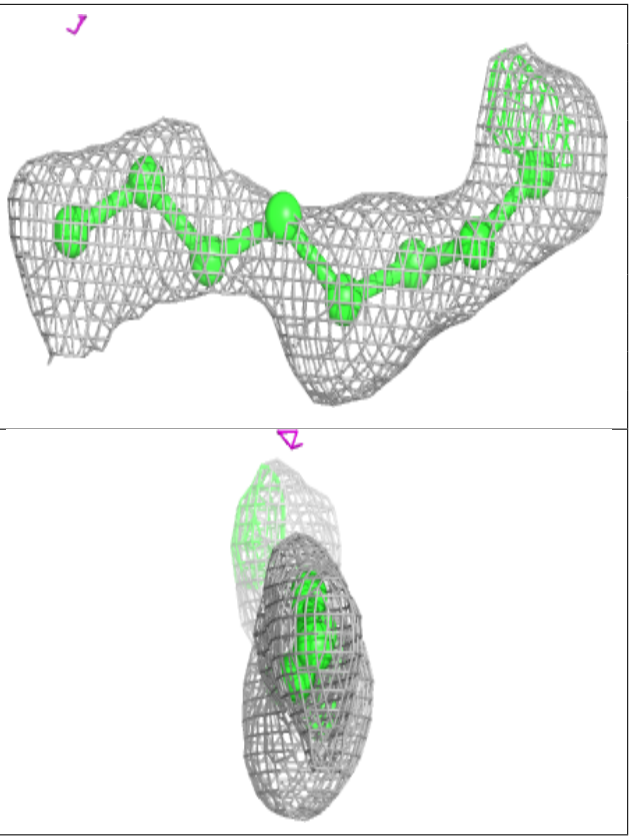
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

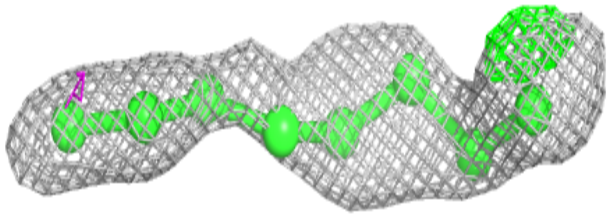
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	A	417	8/20	0.48	0.19	41,45,55,58	0
2	LFA	A	416	12/20	0.76	0.13	41,45,49,50	0
2	LFA	A	410	11/20	0.77	0.14	46,51,55,59	0
3	97N	A	422	11/23	0.77	0.15	32,43,47,54	2
2	LFA	A	420	18/20	0.79	0.24	26,32,36,38	4
2	LFA	A	414	16/20	0.82	0.14	38,50,58,62	0
2	LFA	A	405	10/20	0.85	0.12	46,52,65,85	0
2	LFA	A	419	6/20	0.86	0.09	41,48,50,52	0
2	LFA	A	412	5/20	0.86	0.37	40,45,56,60	0
2	LFA	A	421	4/20	0.86	0.14	31,35,36,36	0
2	LFA	A	411	5/20	0.86	0.09	39,44,50,61	0
2	LFA	A	401	12/20	0.88	0.17	41,45,56,72	0
2	LFA	A	406	11/20	0.89	0.15	39,47,56,57	0
2	LFA	A	409	7/20	0.89	0.11	37,42,55,61	0
2	LFA	A	413	8/20	0.90	0.08	36,41,47,51	0
2	LFA	A	418	11/20	0.91	0.09	35,42,53,57	0
2	LFA	A	404	7/20	0.91	0.08	35,42,55,59	0
2	LFA	A	402	15/20	0.91	0.10	31,44,62,66	0
2	LFA	A	403	15/20	0.91	0.09	34,46,59,61	0
2	LFA	A	407	9/20	0.91	0.11	35,48,56,58	0
2	LFA	A	415	15/20	0.93	0.11	33,37,47,65	0
2	LFA	A	408	3/20	0.95	0.09	35,35,36,38	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 LFA A 417:

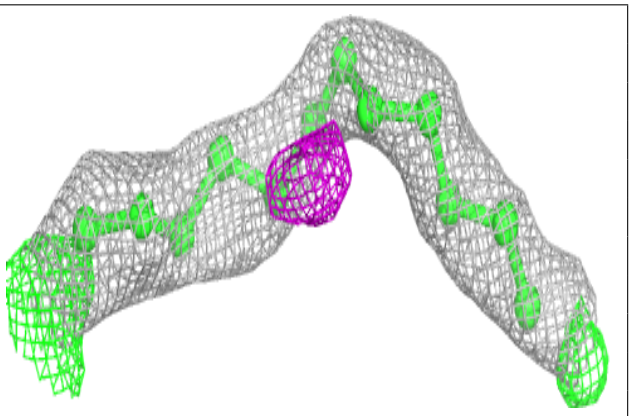
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

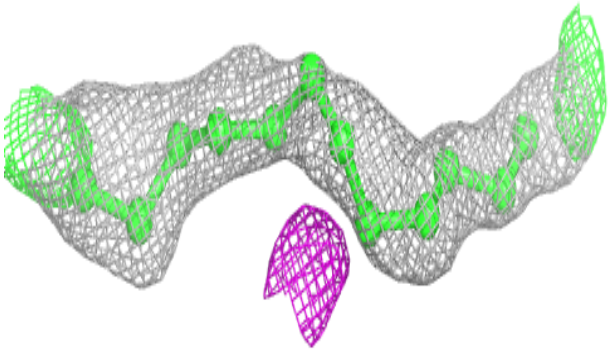


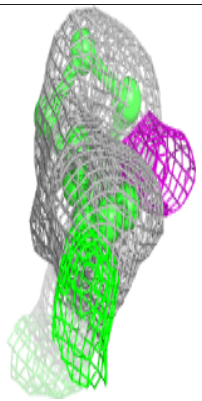


Electron density around LFA A 416:

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

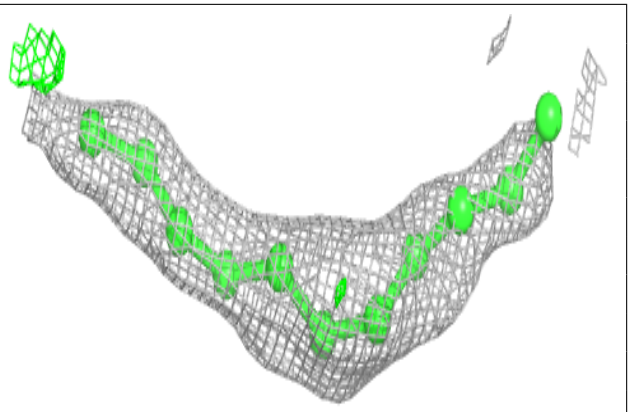


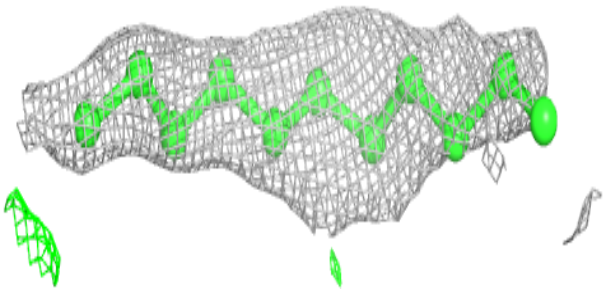


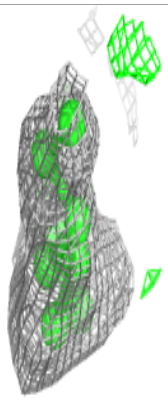


Electron density around LFA A 410:

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

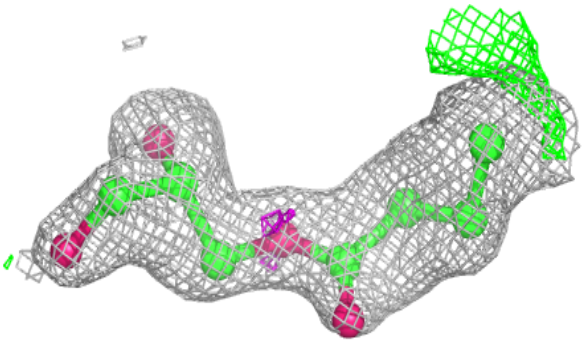


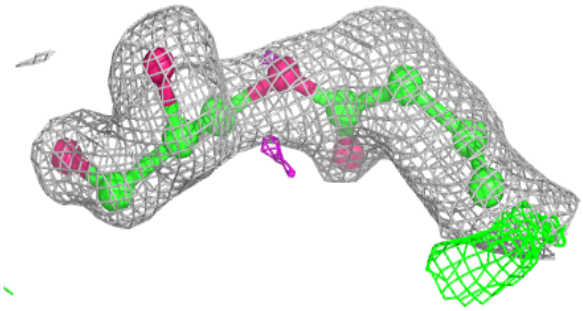


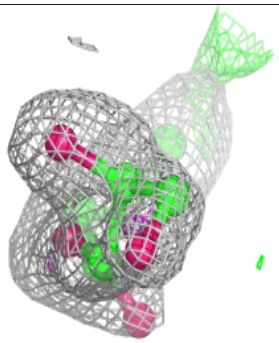


Electron density around 97N A 422:

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

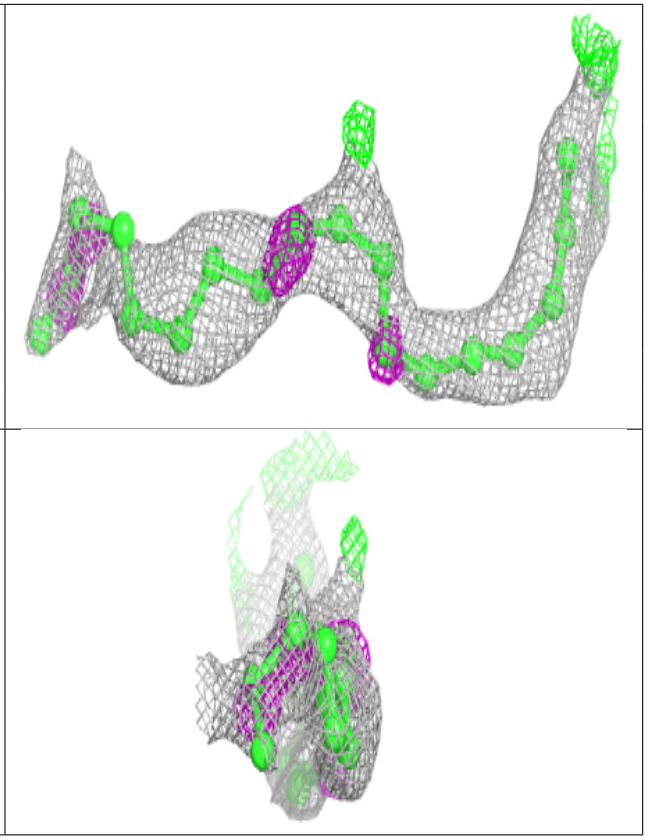






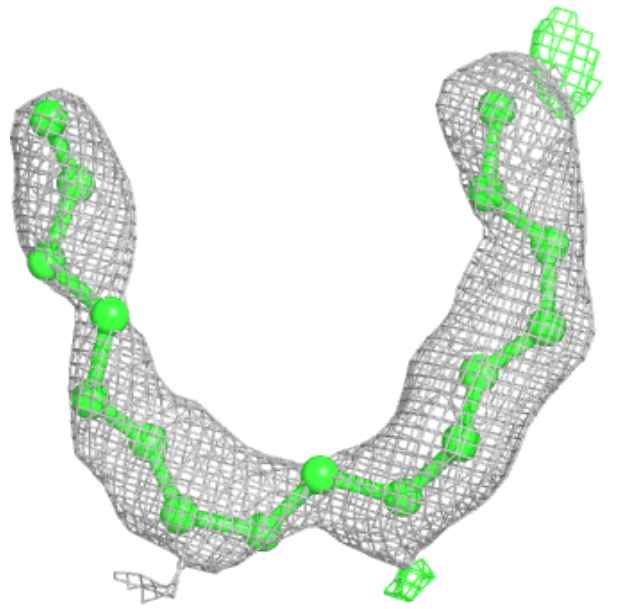
Electron density around LFA A 420:

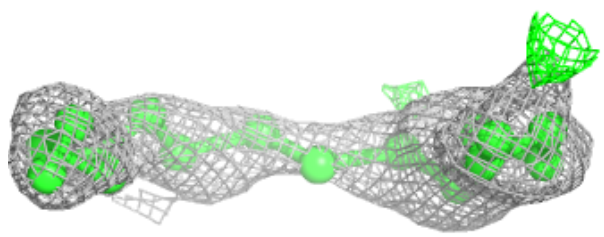
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

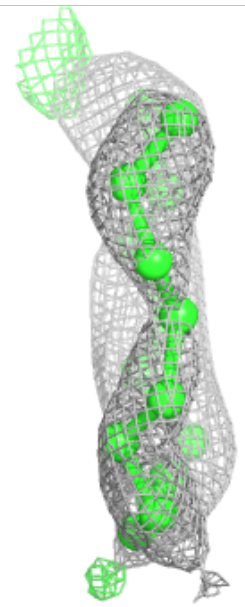


Electron density around LFA A 414:

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

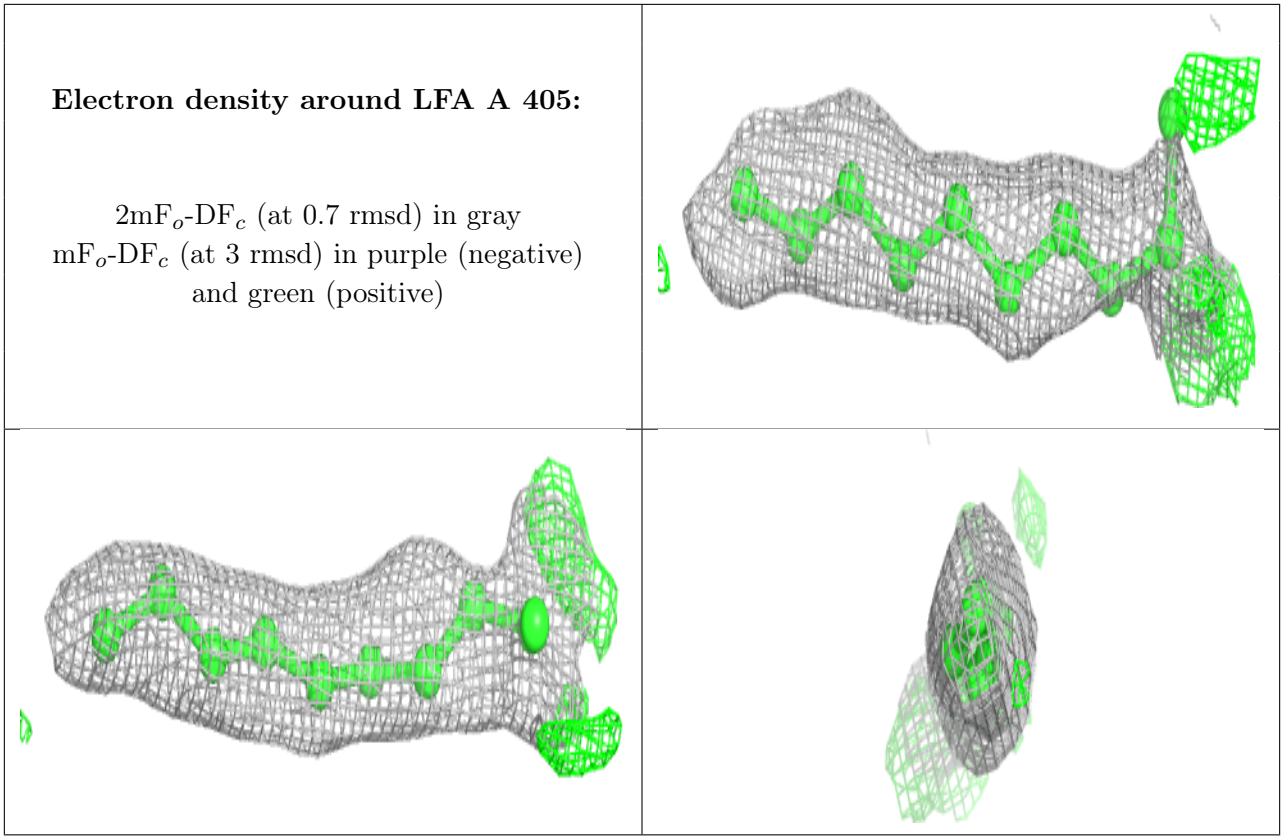






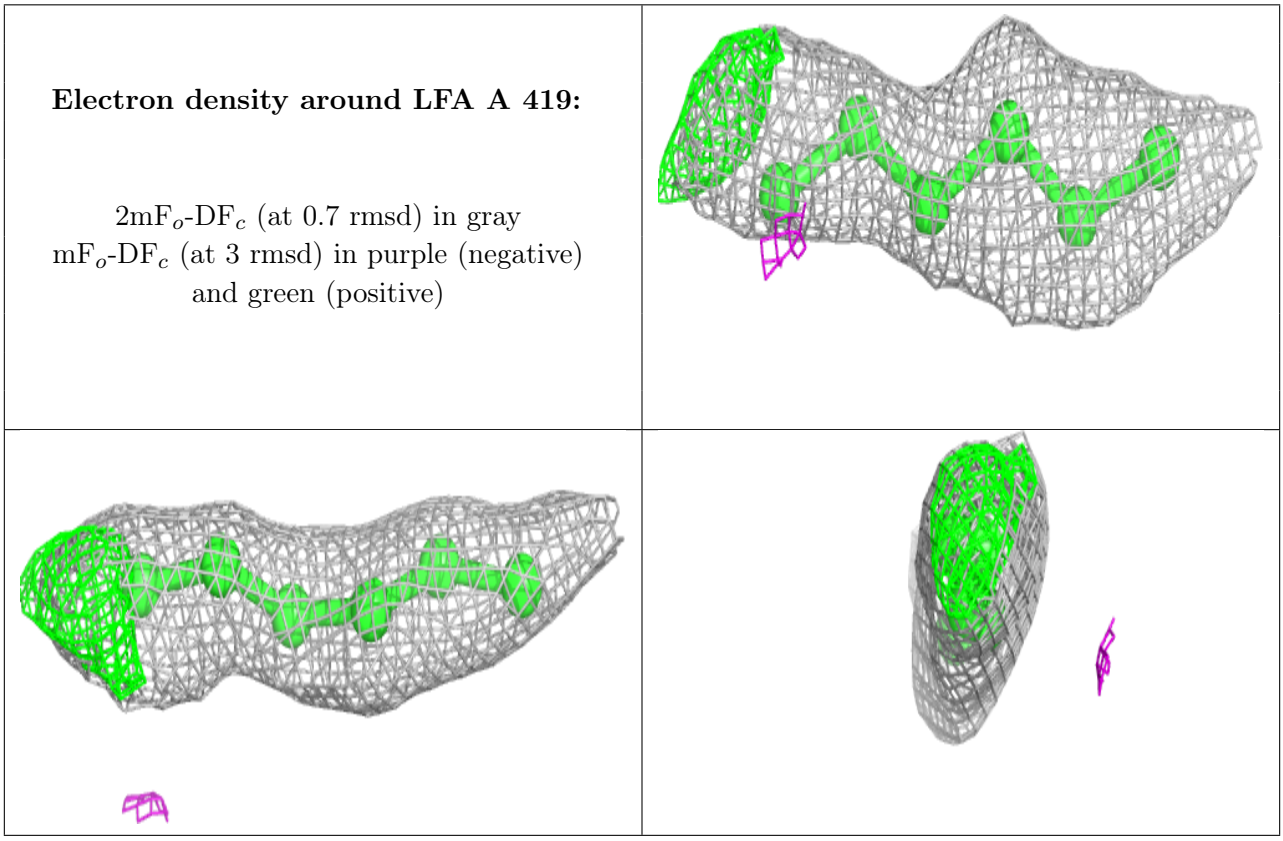
Electron density around LFA A 405:

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



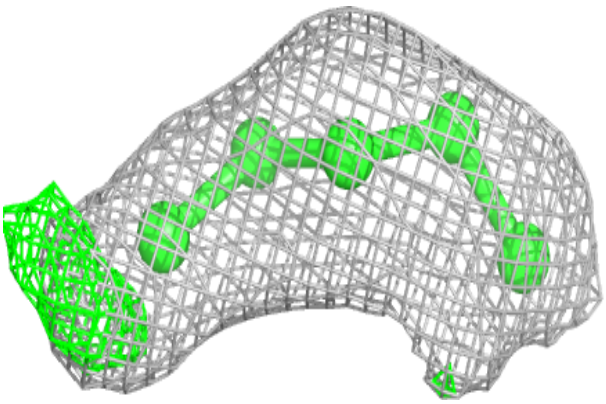
Electron density around LFA A 419:

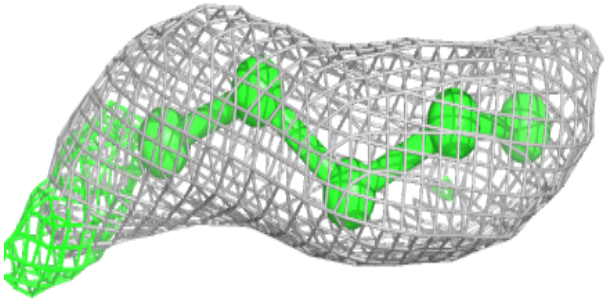
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

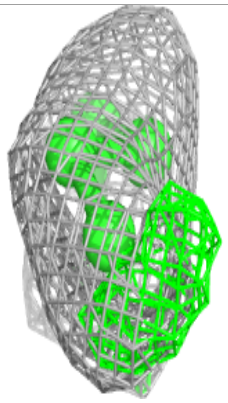


Electron density around LFA A 411:

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

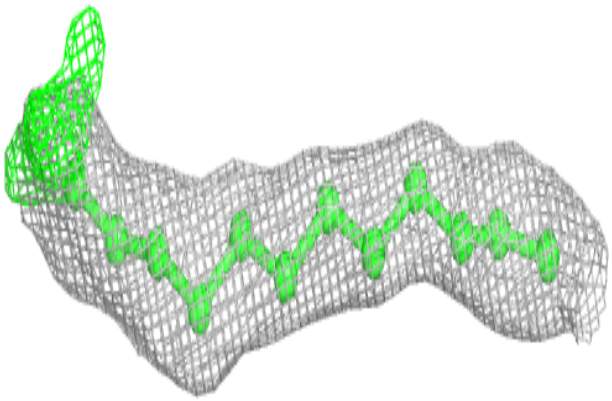


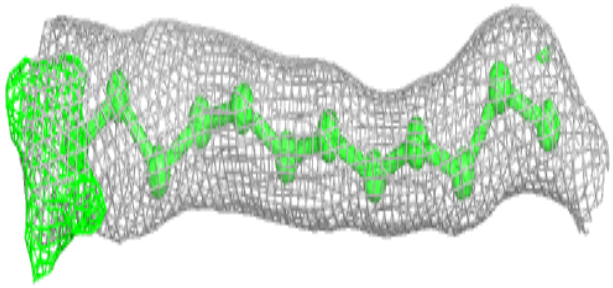


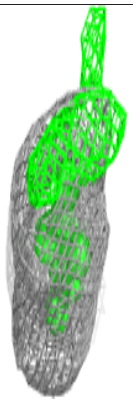


Electron density around LFA A 401:

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

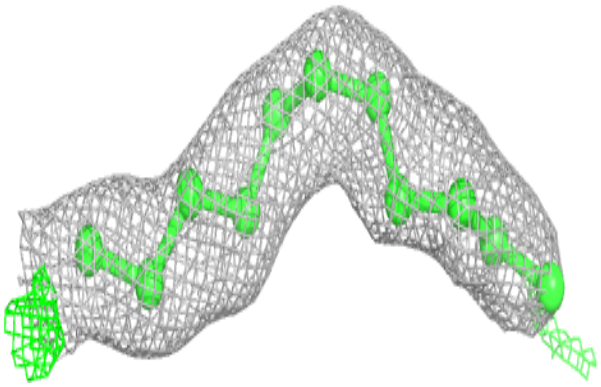


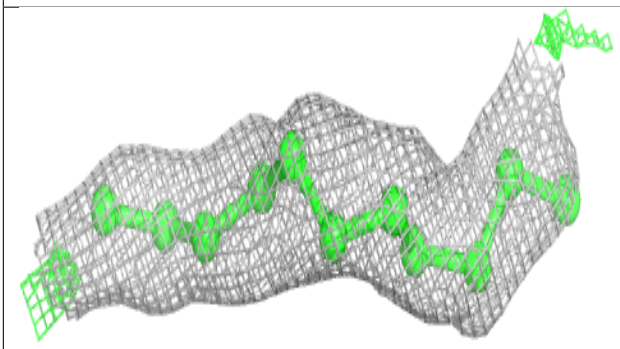


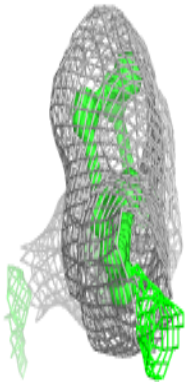


Electron density around LFA A 406:

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

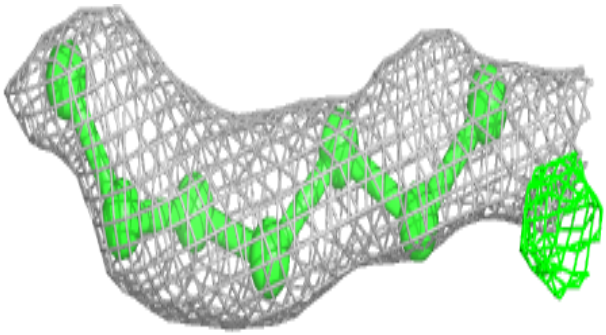


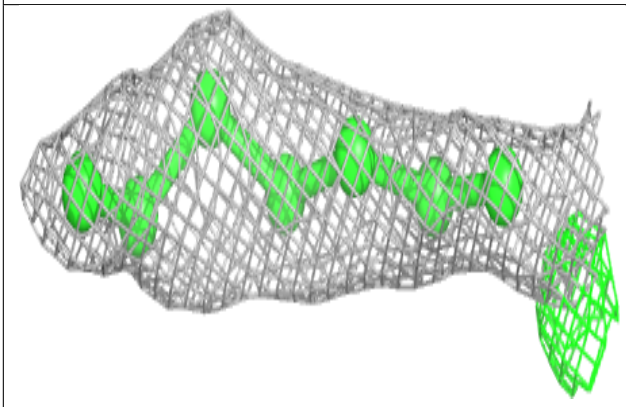


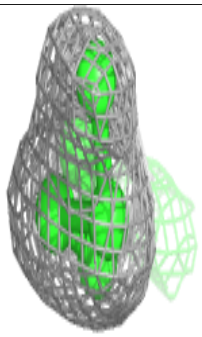


Electron density around LFA A 409:

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

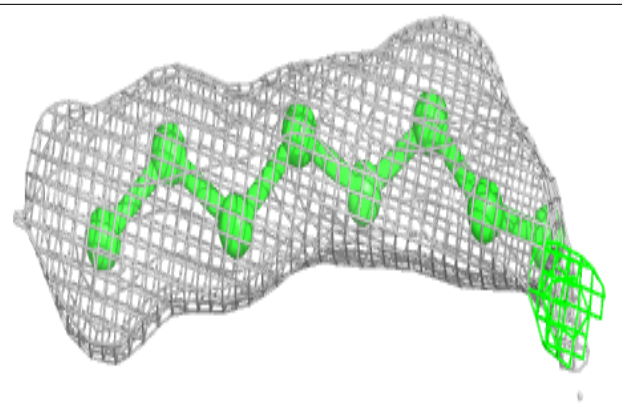


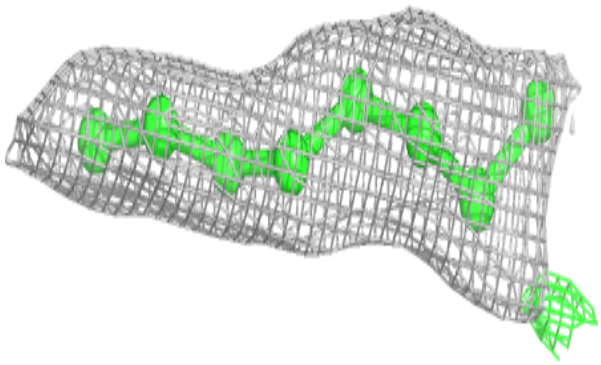


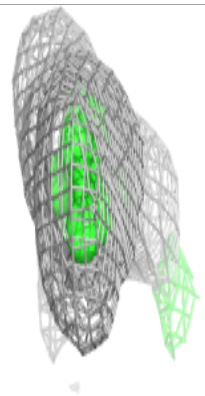


Electron density around LFA A 413:

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

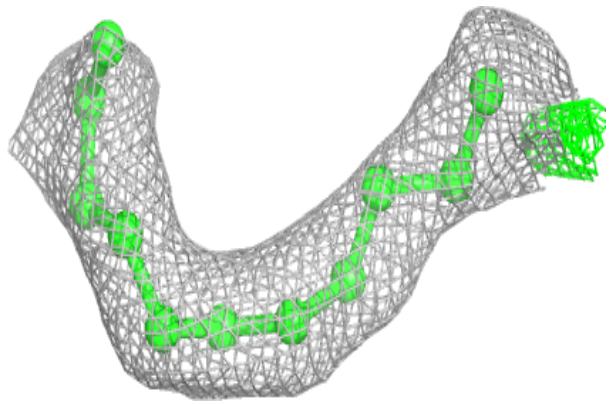


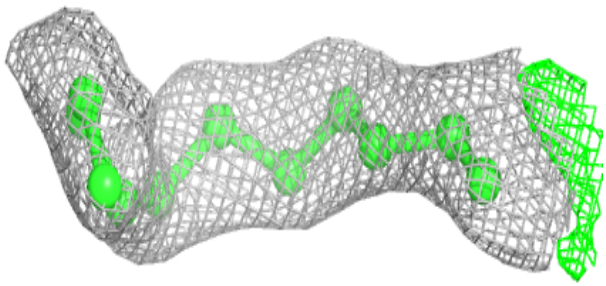


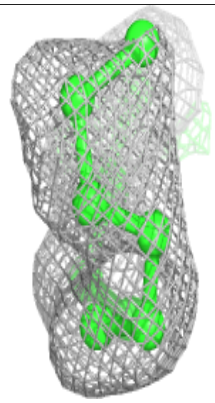


Electron density around LFA A 418:

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

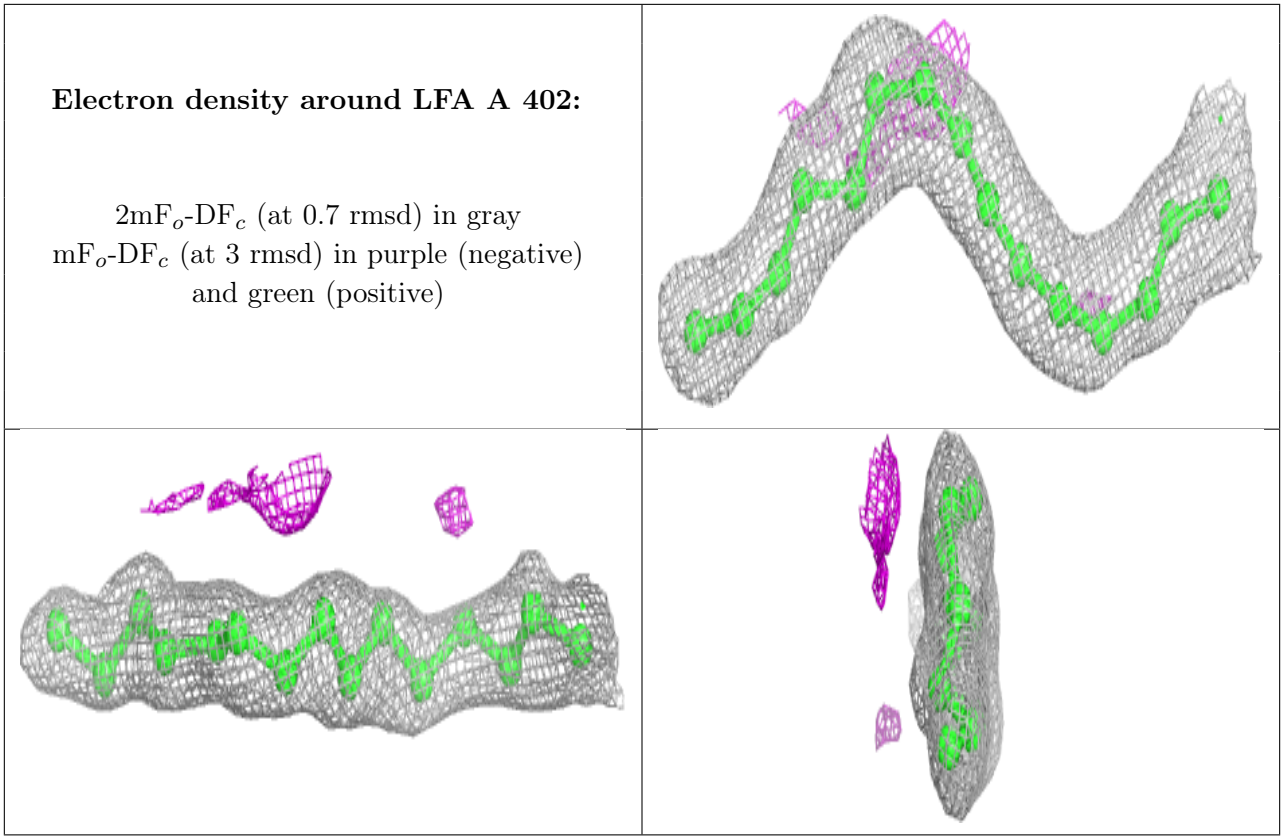






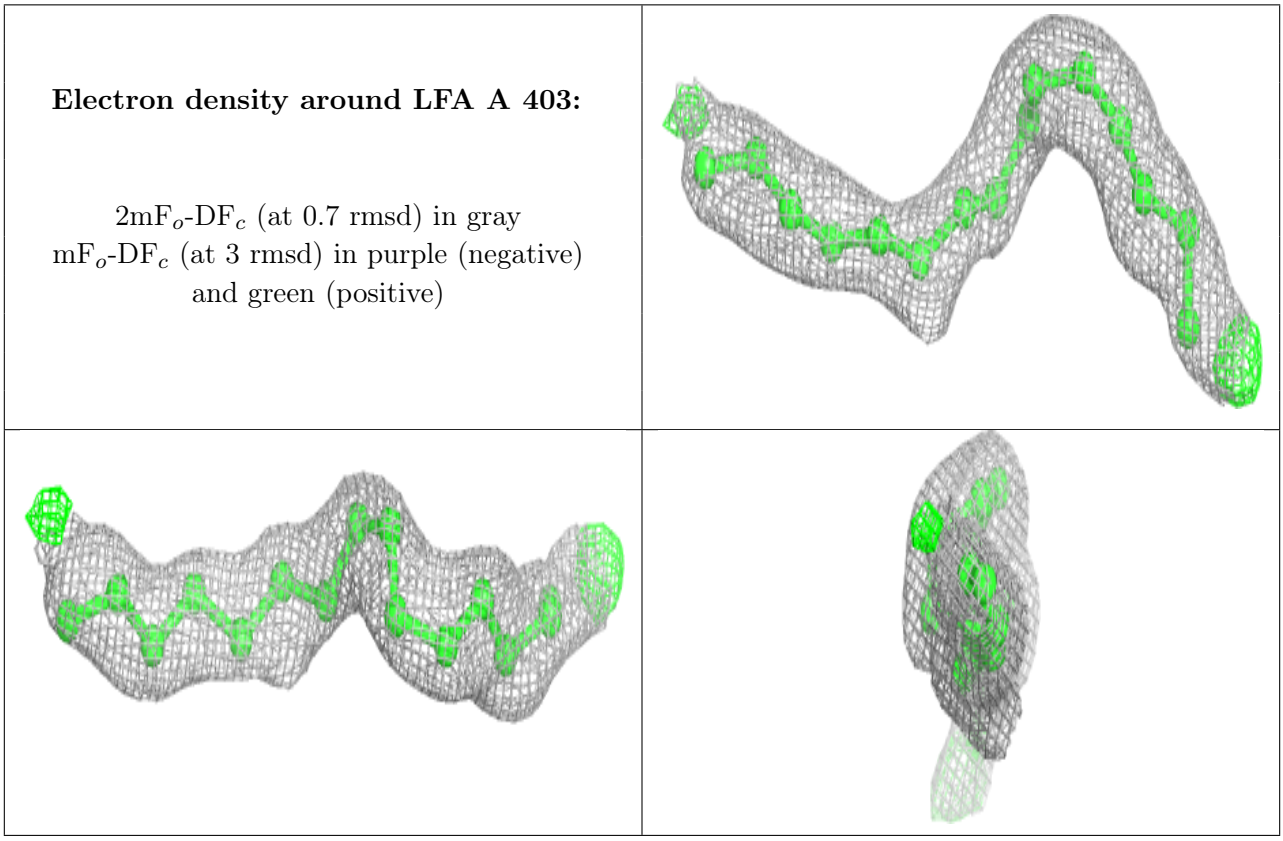
Electron density around LFA A 402:

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



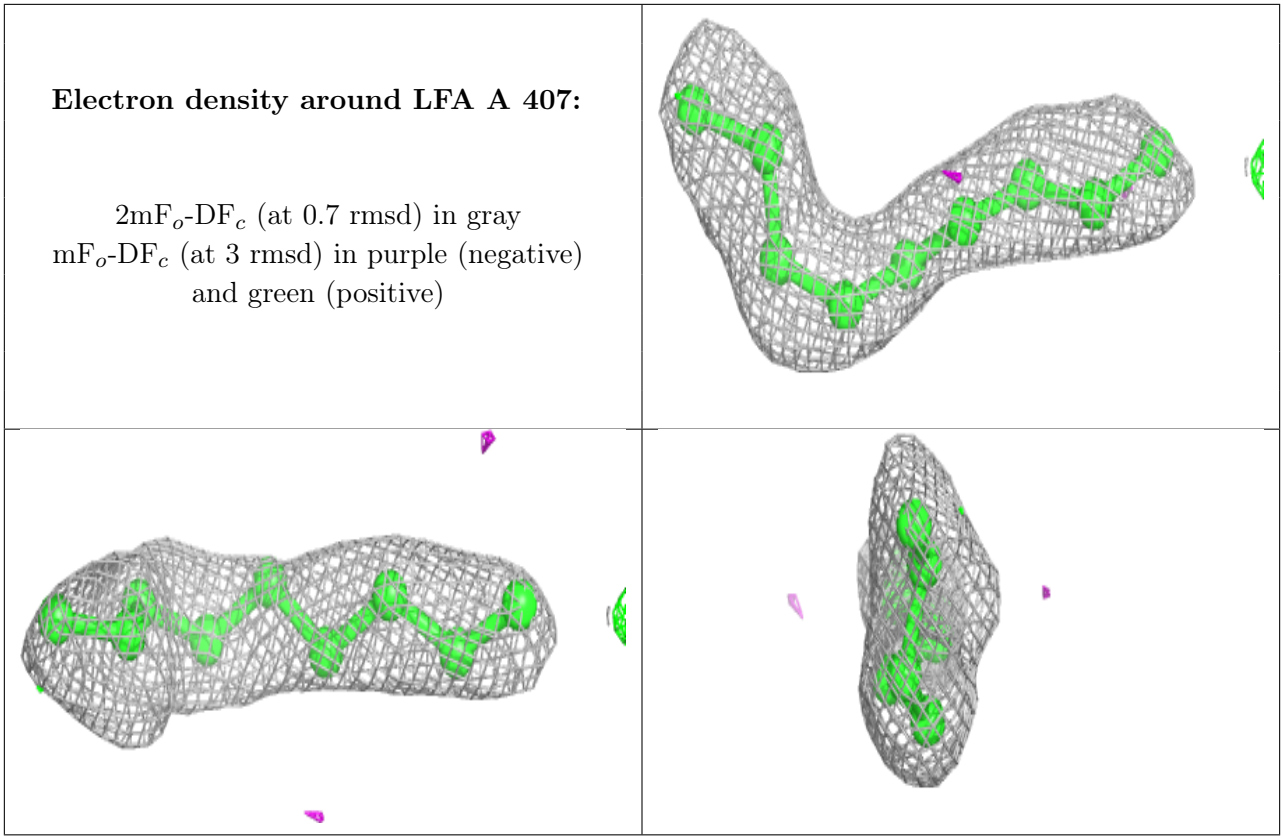
Electron density around LFA A 403:

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



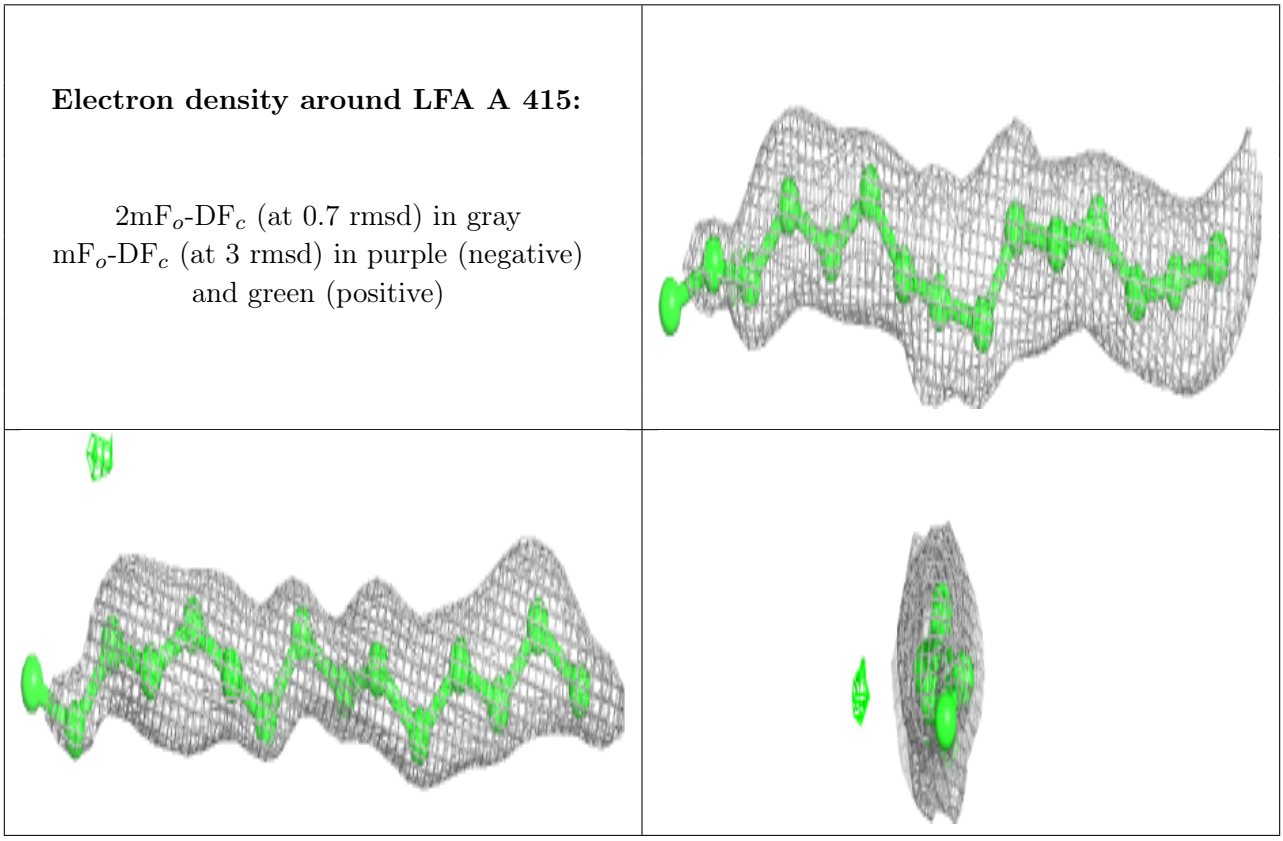
Electron density around LFA A 407:

$2mF_o$-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 415:

$2mF_o$-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.