W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 23, 2020 – 04:18 pm GMT

PDB ID	:	6SU3
Title	:	Crystal structure of the 48C12 heliorhodopsin in the violet form at pH 8.8
Authors	:	Kovalev, K.; Volkov, D.; Astashkin, R.; Alekseev, A.; Gushchin, I.; Gordeliy, V.
Deposited on	:	2019-09-12
Resolution	:	1.50 Å(reported)

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

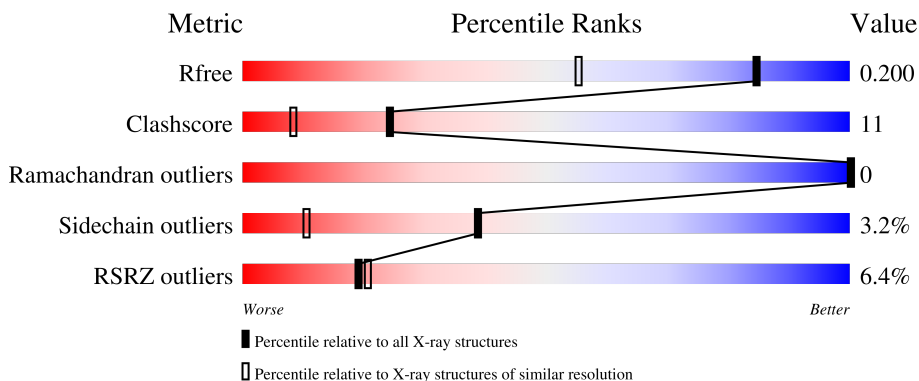|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.50 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	Percentile Ranks	Value
Rfree		0.200
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		3.2%
RSRZ outliers		6.4%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	6% / 86% 10%
1	X	264	6% / 82% 14%

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

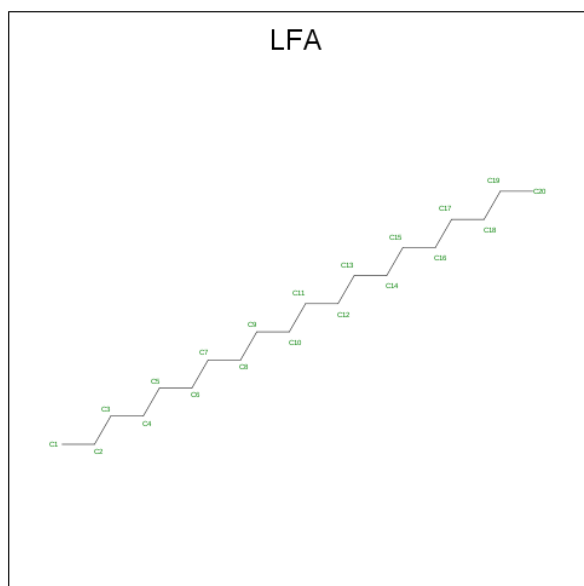| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	801	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4753 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 48C12 heliorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	256	Total	C	N	O	S	0	12	0
			2061	1378	323	353	7			
1	A	256	Total	C	N	O	S	0	6	0
			2005	1346	310	342	7			

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

LFA

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	C	0	0
			12	12		
2	X	1	Total	C	0	0
			16	16		
2	X	1	Total	C	0	0
			14	14		
2	X	1	Total	C	0	0
			14	14		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total 14	C 14	0	0
2	X	1	Total 17	C 17	0	0
2	X	1	Total 8	C 8	0	0
2	X	1	Total 9	C 9	0	0
2	X	1	Total 10	C 10	0	0
2	X	1	Total 10	C 10	0	0
2	X	1	Total 7	C 7	0	0
2	X	1	Total 17	C 17	0	0
2	X	1	Total 9	C 9	0	0
2	A	1	Total 15	C 15	0	0
2	A	1	Total 15	C 15	0	0
2	A	1	Total 10	C 10	0	0
2	A	1	Total 18	C 18	0	0
2	A	1	Total 13	C 13	0	0
2	A	1	Total 7	C 7	0	0
2	A	1	Total 11	C 11	0	0
2	A	1	Total 13	C 13	0	0
2	A	1	Total 15	C 15	0	0
2	A	1	Total 11	C 11	0	0
2	A	1	Total 7	C 7	0	0
2	A	1	Total 8	C 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 7	C 7	0	0

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).
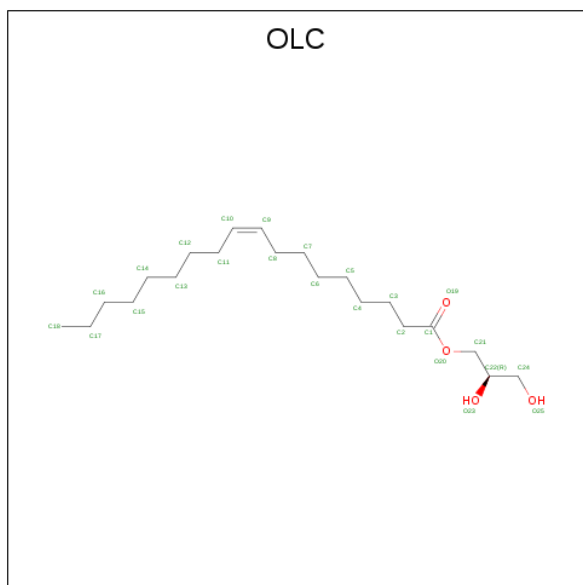
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total 22	C 18	O 4	0	0
3	X	1	Total 23	C 19	O 4	0	0
3	A	1	Total 16	C 12	O 4	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
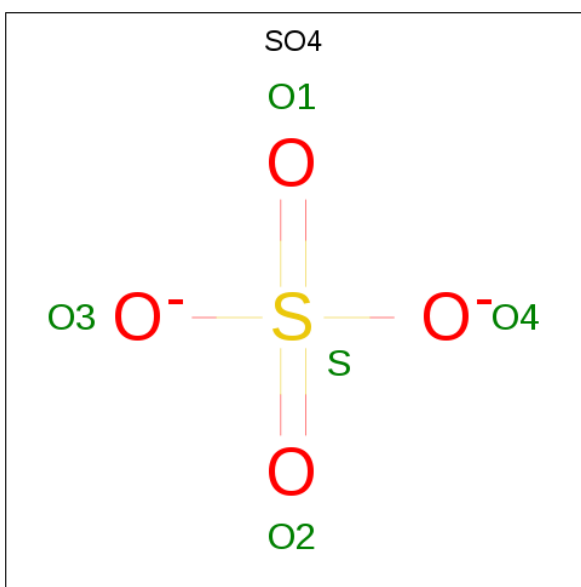
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total 5	O 4	S 1	0	0

- Molecule 5 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).
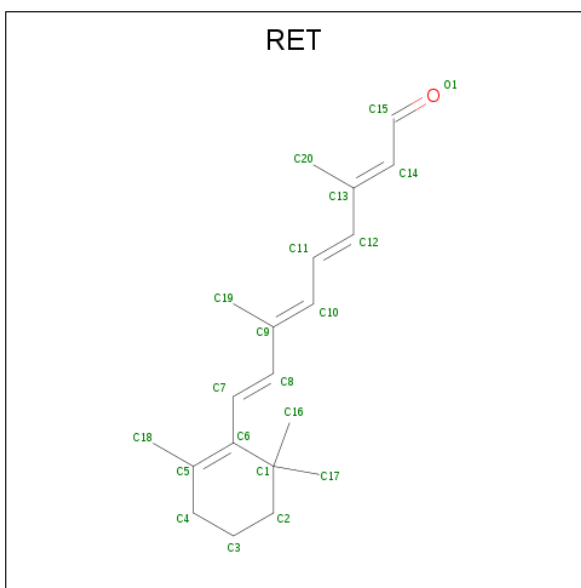
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	1	Total 20	C 20	0	0
5	A	1	Total 20	C 20	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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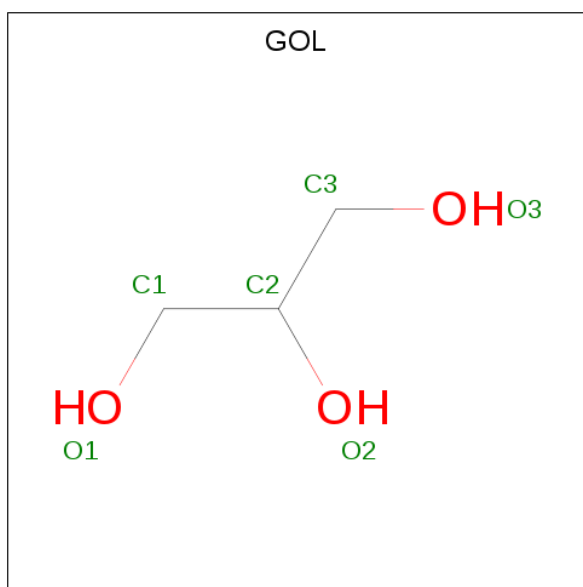
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	C 3	O 3	0	0

- Molecule 7 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).

OLA
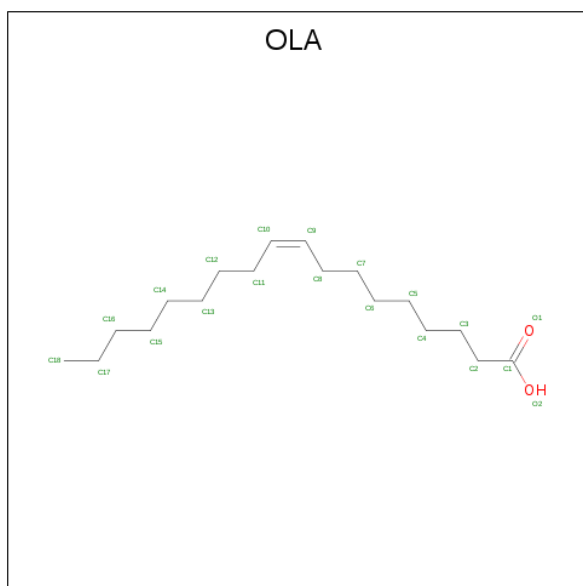
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 16	C 14	O 2	0	0
7	A	1	Total 19	C 17	O 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	X	109	Total O 112 112	0	2
8	A	121	Total O 121 121	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 48C12 heliorhodopsin
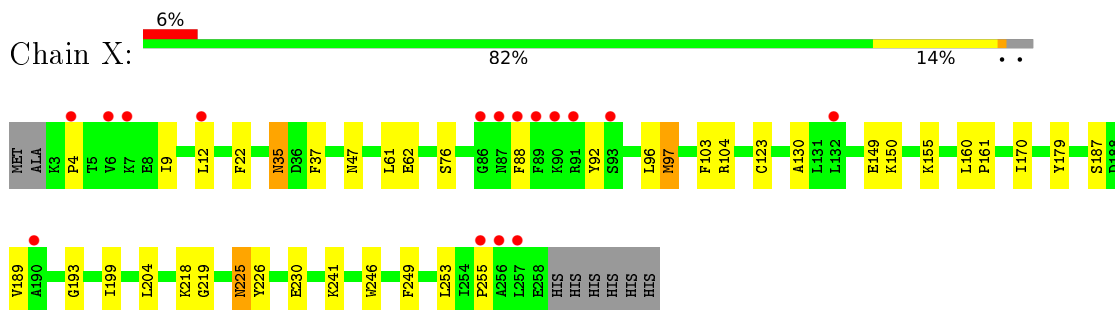
- Molecule 1: 48C12 heliorhodopsin
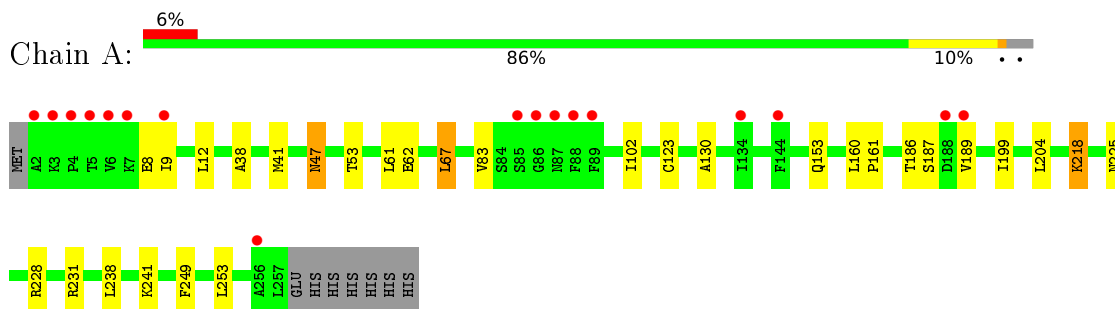
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.12Å 59.75Å 94.32Å 90.00° 92.30° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 49.06 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-1.50) 98.5 (49.06-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.153 , 0.199 0.155 , 0.200	Depositor DCC
R_{free} test set	4924 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å²)	18.9	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.39 , 73.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4753	wwPDB-VP
Average B, all atoms (Å²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, OLC, LFA, OLA, RET, SO4

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	0.66	1/2060 (0.0%)	0.64	0/2814
1	X	0.64	1/2117 (0.0%)	0.63	0/2888
All	All	0.65	2/4177 (0.0%)	0.63	0/5702

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	LYS	C-N	9.73	1.56	1.34
1	X	255	PRO	C-N	5.26	1.46	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	2005	0	2025	26	0
1	X	2061	0	2082	43	0
2	A	150	0	281	15	0
2	X	157	0	301	14	0
3	A	16	0	21	1	0
3	X	45	0	64	4	0
4	X	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	20	0	27	3	0
5	X	20	0	27	4	0
6	A	6	0	8	4	0
7	A	35	0	50	3	0
8	A	121	0	0	6	0
8	X	112	0	0	4	0
All	All	4753	0	4886	104	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 104 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)
2:A:811:LFA:C1	2:A:812:LFA:H41	1.73	1.18
6:A:801:GOL:H32	8:A:910:HOH:O	1.48	1.09
1:X:187[A]:SER:OG	1:X:189:VAL:HG12	1.55	1.06
2:A:811:LFA:C1	2:A:812:LFA:C4	2.33	1.06
2:X:313:LFA:H13	2:X:315:LFA:C2	1.87	1.04

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	260/264 (98%)	256 (98%)	4 (2%)	0	100	100
1	X	266/264 (101%)	263 (99%)	3 (1%)	0	100	100
All	All	526/528 (100%)	519 (99%)	7 (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	207/218 (95%)	198 (96%)	9 (4%)	29	5
1	X	216/218 (99%)	211 (98%)	5 (2%)	50	20
All	All	423/436 (97%)	409 (97%)	14 (3%)	39	10

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	83	VAL
1	A	228	ARG
1	A	47	ASN
1	A	225	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	225	ASN
1	A	153	GLN
1	X	213	GLN
1	A	47	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

35 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	X	314	-	6,6,19	0.14	0	5,5,18	0.14	0
5	RET	A	818	1	20,20,21	1.60	4 (20%)	27,27,28	1.19	2 (7%)
3	OLC	X	303	-	22,22,24	0.96	1 (4%)	23,23,25	0.89	0
2	LFA	X	313	-	9,9,19	0.11	0	8,8,18	0.10	0
2	LFA	A	809	-	12,12,19	0.11	0	11,11,18	0.13	0
2	LFA	A	807	-	9,9,19	0.11	0	8,8,18	0.13	0
7	OLA	A	802	-	12,15,19	0.40	0	11,15,19	0.14	0
2	LFA	X	312	-	9,9,19	0.12	0	8,8,18	0.25	0
6	GOL	A	801	-	5,5,5	0.18	0	5,5,5	0.29	0
3	OLC	A	804	-	15,15,24	1.01	1 (6%)	16,16,25	1.18	2 (12%)
2	LFA	X	309	-	16,16,19	0.11	0	15,15,18	0.11	0
5	RET	X	317	1	20,20,21	1.47	4 (20%)	27,27,28	1.13	2 (7%)
2	LFA	A	805	-	14,14,19	0.09	0	13,13,18	0.15	0
2	LFA	X	306	-	13,13,19	0.10	0	12,12,18	0.08	0
2	LFA	A	812	-	12,12,19	0.11	0	11,11,18	0.08	0
7	OLA	A	803	-	15,18,19	0.43	0	14,18,19	0.16	0
2	LFA	A	806	-	14,14,19	0.10	0	13,13,18	0.11	0
2	LFA	X	305	-	15,15,19	0.13	0	14,14,18	0.11	0
2	LFA	X	308	-	13,13,19	0.13	0	12,12,18	0.06	0
2	LFA	A	808	-	17,17,19	0.12	0	16,16,18	0.11	0
2	LFA	X	307	-	13,13,19	0.13	0	12,12,18	0.16	0
2	LFA	A	817	-	6,6,19	0.17	0	5,5,18	0.05	0
2	LFA	X	310	-	7,7,19	0.17	0	6,6,18	0.09	0
2	LFA	A	814	-	10,10,19	0.17	0	9,9,18	0.09	0
2	LFA	X	301	-	11,11,19	0.18	0	10,10,18	0.18	0
2	LFA	A	813	-	14,14,19	0.22	0	13,13,18	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	LFA	A	816	-	7,7,19	0.14	0	6,6,18	0.16	0
2	LFA	X	315	-	16,16,19	0.20	0	15,15,18	0.11	0
3	OLC	X	302	-	21,21,24	1.06	1 (4%)	22,22,25	1.08	1 (4%)
2	LFA	A	815	-	6,6,19	0.12	0	5,5,18	0.08	0
2	LFA	A	811	-	10,10,19	0.10	0	9,9,18	0.09	0
2	LFA	X	316	-	8,8,19	0.09	0	7,7,18	0.09	0
2	LFA	A	810	-	6,6,19	0.15	0	5,5,18	0.13	0
4	SO4	X	304	-	4,4,4	0.34	0	6,6,6	0.06	0
2	LFA	X	311	-	8,8,19	0.18	0	7,7,18	0.09	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	X	314	-	-	3/4/4/17	-
5	RET	A	818	1	-	0/13/30/31	0/1/1/1
3	OLC	X	303	-	-	6/22/22/24	-
2	LFA	X	313	-	-	4/7/7/17	-
2	LFA	A	809	-	-	5/10/10/17	-
2	LFA	A	807	-	-	3/7/7/17	-
7	OLA	A	802	-	-	6/11/13/17	-
2	LFA	X	312	-	-	1/7/7/17	-
6	GOL	A	801	-	-	2/4/4/4	-
3	OLC	A	804	-	-	5/15/15/24	-
2	LFA	X	309	-	-	9/14/14/17	-
5	RET	X	317	1	-	0/13/30/31	0/1/1/1
2	LFA	A	805	-	-	3/12/12/17	-
2	LFA	X	306	-	-	7/11/11/17	-
2	LFA	A	812	-	-	7/10/10/17	-
7	OLA	A	803	-	-	9/14/16/17	-
2	LFA	A	806	-	-	5/12/12/17	-
2	LFA	X	305	-	-	3/13/13/17	-
2	LFA	X	308	-	-	7/11/11/17	-
2	LFA	A	808	-	-	6/15/15/17	-
2	LFA	X	307	-	-	4/11/11/17	-
2	LFA	A	817	-	-	3/4/4/17	-

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wwPDB X-ray Structure Validation Summary Report 6SU3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	X	310	-	-	5/5/5/17	-
2	LFA	A	814	-	-	2/8/8/17	-
2	LFA	X	301	-	-	1/9/9/17	-
2	LFA	A	813	-	-	9/12/12/17	-
2	LFA	A	816	-	-	1/5/5/17	-
2	LFA	X	315	-	-	11/14/14/17	-
2	LFA	A	815	-	-	1/4/4/17	-
2	LFA	A	811	-	-	5/8/8/17	-
2	LFA	X	316	-	-	5/6/6/17	-
2	LFA	A	810	-	-	2/4/4/17	-
3	OLC	X	302	-	-	11/21/21/24	-
2	LFA	X	311	-	-	4/6/6/17	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	302	OLC	O20-C1	4.66	1.46	1.33
3	X	303	OLC	O20-C1	4.04	1.45	1.33
3	A	804	OLC	O20-C1	3.68	1.44	1.33
5	A	818	RET	C14-C13	3.63	1.36	1.33
5	X	317	RET	C14-C13	3.37	1.36	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	317	RET	C19-C9-C10	-4.07	117.22	122.92
5	A	818	RET	C19-C9-C10	-3.95	117.39	122.92
3	X	302	OLC	O20-C1-C2	3.22	122.02	111.91
3	A	804	OLC	O20-C1-C2	3.10	121.63	111.91
3	A	804	OLC	O20-C1-O19	-2.36	117.63	123.59

There are no chirality outliers.

5 of 155 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	802	OLA	C1-C2-C3-C4
7	A	803	OLA	C11-C10-C9-C8
3	X	302	OLC	O20-C21-C22-C24
3	X	302	OLC	O20-C21-C22-O23
7	A	802	OLA	C11-C10-C9-C8

There are no ring outliers.

19 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	314	LFA	1	0
5	A	818	RET	3	0
2	X	313	LFA	9	0
2	A	807	LFA	2	0
7	A	802	OLA	2	0
6	A	801	GOL	4	0
3	A	804	OLC	1	0
2	X	309	LFA	1	0
5	X	317	RET	4	0
2	X	306	LFA	2	0
2	A	812	LFA	12	0
7	A	803	OLA	1	0
2	A	806	LFA	1	0
2	X	305	LFA	1	0
2	A	813	LFA	1	0
2	X	315	LFA	8	0
3	X	302	OLC	4	0
2	A	811	LFA	11	0
2	X	316	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 X 314

Bond lengths

Bond angles

Torsions

Rings

Ligand RET A 818

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC X 303

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 313

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 809

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 807

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 802

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 312

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 804

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 309

Bond lengths

Bond angles

Torsions

Rings

Ligand RET X 317

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 805

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 306

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 812

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 803

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 806

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 305

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 308

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 808

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 307

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 817

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 310

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 814

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 301

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 813

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 816

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 315

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC X 302

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 815

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 811

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA X 316

Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 810

Ligand LFA X 311

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	256/264 (96%)	0.08	17 (6%)	18	19	15, 22, 45, 59	0
1	X	256/264 (96%)	0.06	16 (6%)	20	21	15, 22, 44, 58	0
All	All	512/528 (96%)	0.07	33 (6%)	19	20	15, 22, 44, 59	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	PRO	7.4
1	A	9	ILE	6.9
1	X	89	PHE	5.9
1	A	6	VAL	5.9
1	A	87	ASN	5.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	X	309	17/20	0.74	0.21	27,35,43,44	0
2	LFA	X	310	8/20	0.75	0.15	31,37,38,39	0
2	LFA	X	316	9/20	0.75	0.18	34,37,41,42	0
7	OLA	A	802	16/20	0.76	0.23	30,35,39,41	0
2	LFA	A	808	18/20	0.77	0.14	32,35,39,43	0
2	LFA	A	809	13/20	0.78	0.16	34,35,40,43	0
3	OLC	X	303	23/25	0.79	0.13	25,29,35,48	0
2	LFA	A	817	7/20	0.79	0.14	33,35,40,42	0
3	OLC	X	302	22/25	0.79	0.30	29,35,43,44	0
2	LFA	X	308	14/20	0.81	0.18	32,37,40,42	0
2	LFA	A	813	15/20	0.81	0.17	34,37,43,46	0
2	LFA	X	315	17/20	0.83	0.21	33,35,39,41	0
2	LFA	X	306	14/20	0.84	0.15	44,51,64,72	0
6	GOL	A	801	6/6	0.85	0.25	28,37,41,42	0
2	LFA	A	815	7/20	0.85	0.16	35,36,39,43	0
2	LFA	A	812	13/20	0.86	0.22	33,35,39,46	0
2	LFA	X	312	10/20	0.86	0.15	30,36,38,40	0
2	LFA	X	314	7/20	0.88	0.23	37,38,41,43	0
7	OLA	A	803	19/20	0.89	0.10	25,32,39,41	0
2	LFA	X	307	14/20	0.90	0.10	30,34,39,42	0
2	LFA	A	816	8/20	0.90	0.11	28,35,37,40	0
2	LFA	X	311	9/20	0.90	0.17	33,35,41,41	0
2	LFA	A	811	11/20	0.92	0.14	35,37,40,41	0
2	LFA	A	807	10/20	0.92	0.15	32,33,37,38	0
2	LFA	A	810	7/20	0.92	0.15	31,35,38,43	0
2	LFA	A	806	15/20	0.92	0.11	33,37,61,66	0
2	LFA	X	305	16/20	0.92	0.10	22,29,46,59	0
2	LFA	A	805	15/20	0.93	0.10	22,25,37,41	0
3	OLC	A	804	16/25	0.94	0.20	26,32,38,41	0
2	LFA	A	814	11/20	0.94	0.12	30,35,40,45	0
2	LFA	X	301	12/20	0.94	0.07	29,34,44,45	0
2	LFA	X	313	10/20	0.94	0.14	32,35,41,43	0
5	RET	A	818	20/21	0.96	0.09	16,17,22,26	0
5	RET	X	317	20/21	0.96	0.11	14,17,21,24	0
4	SO4	X	304	5/5	0.96	0.10	55,58,65,69	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 X 309:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
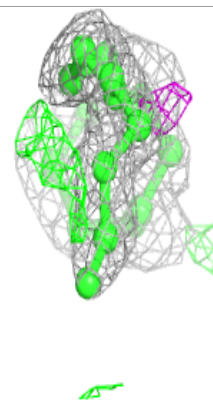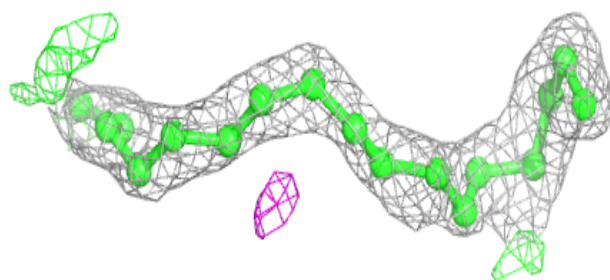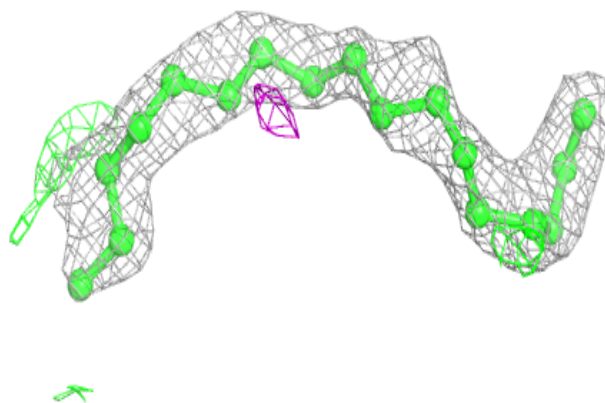
Electron density around LFA X 310:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
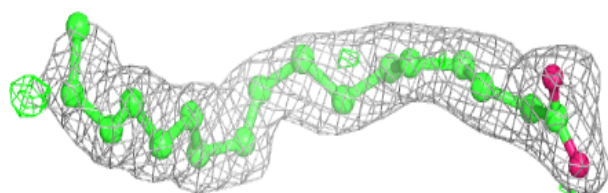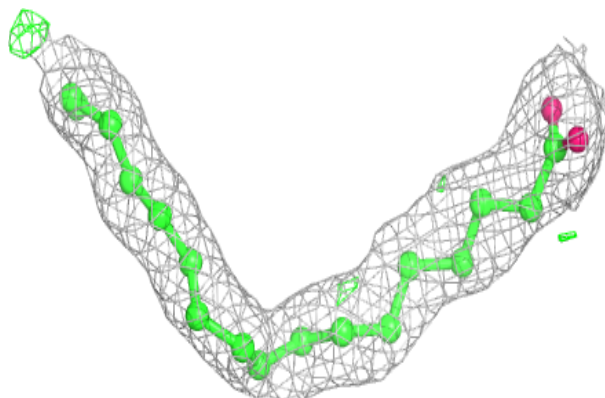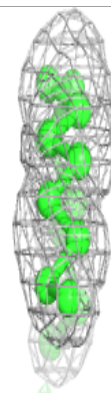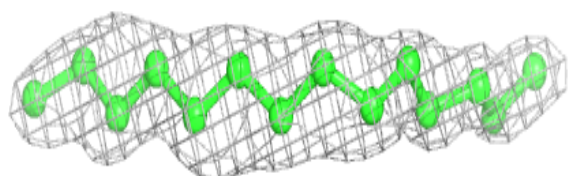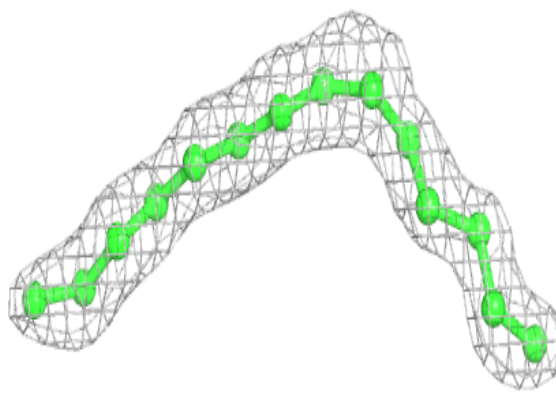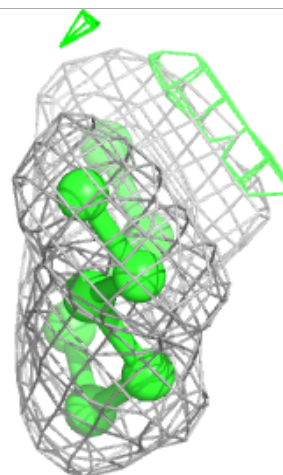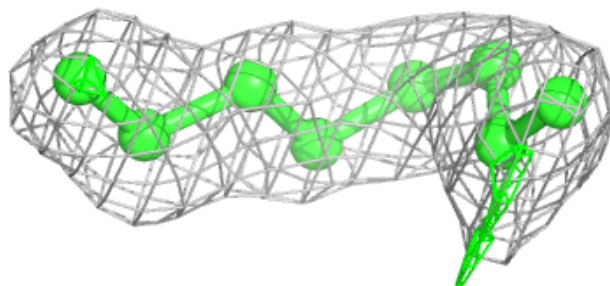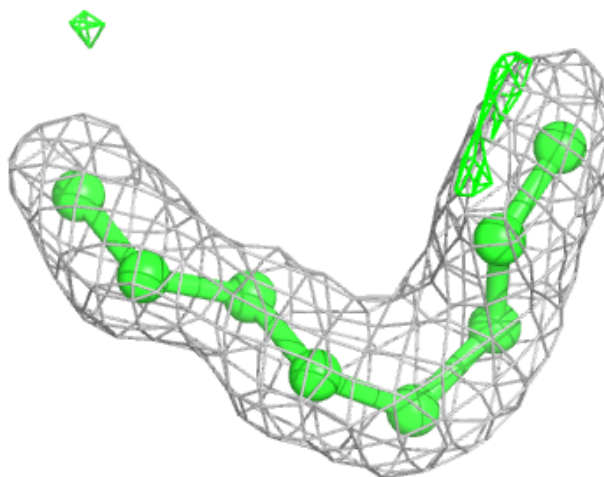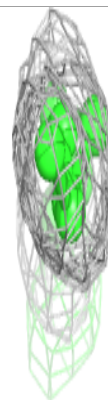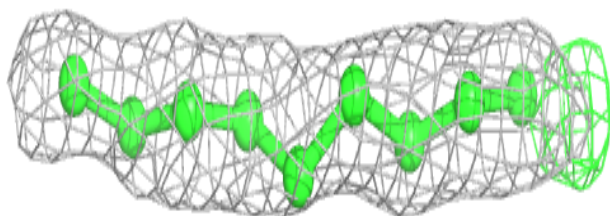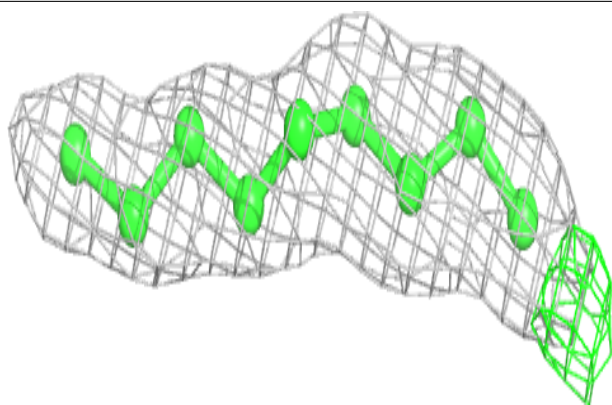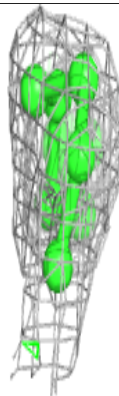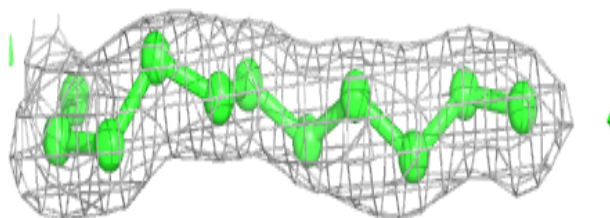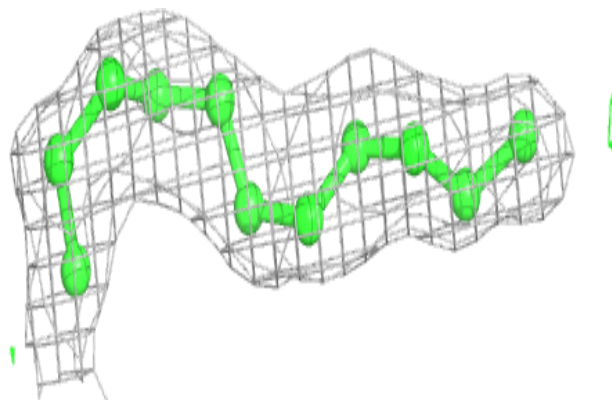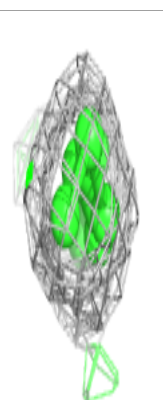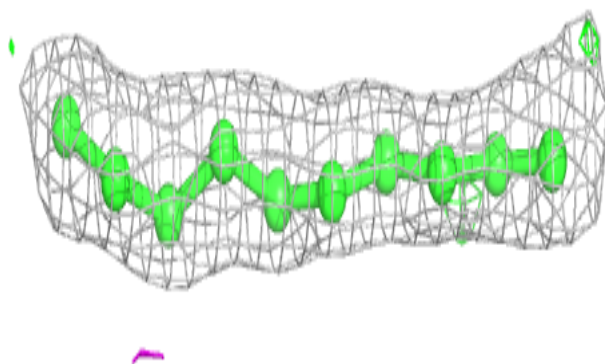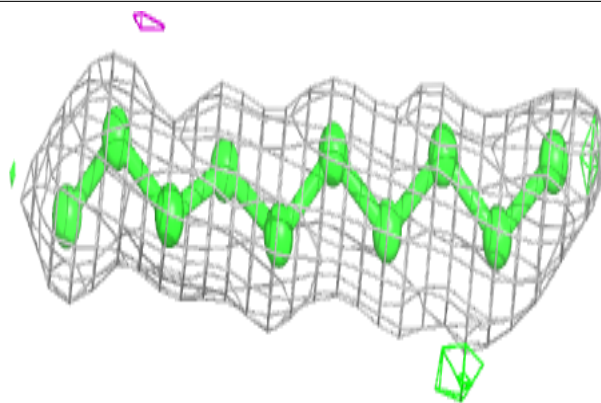$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
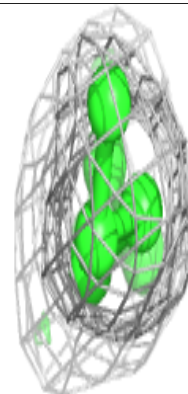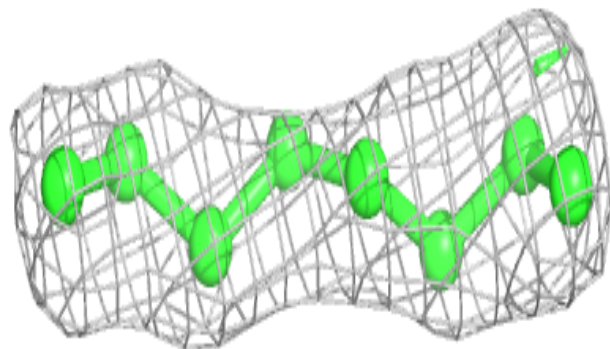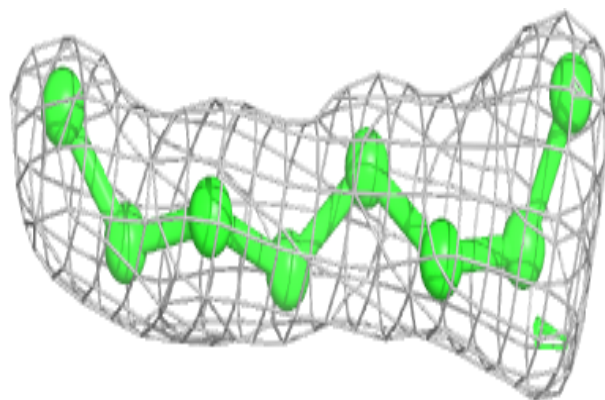
Electron density around LFA X 316:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
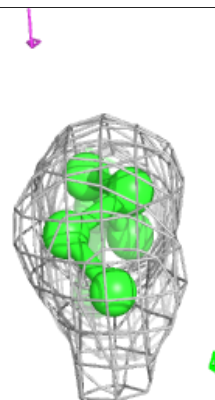mF_o-DF_c (at 3 rmsd) in purple (negative)
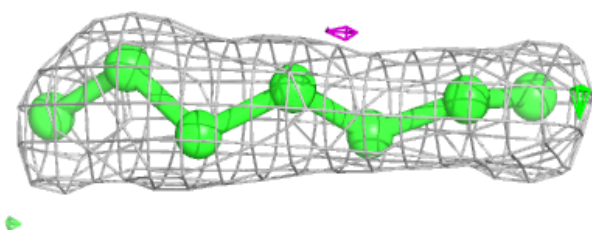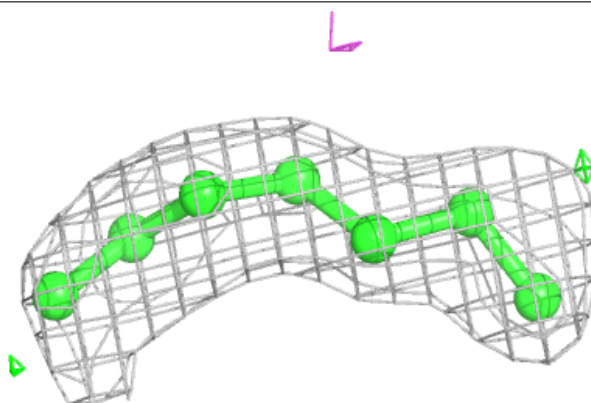and green (positive)
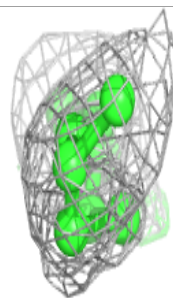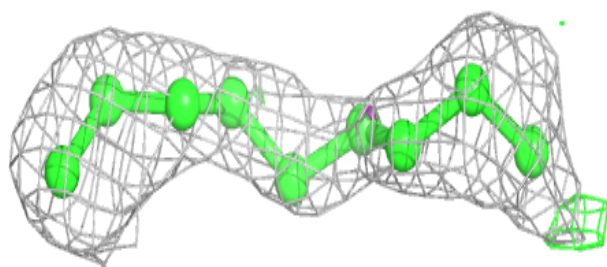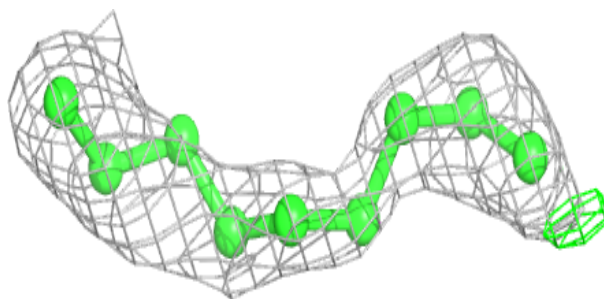
Electron density around OLA A 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
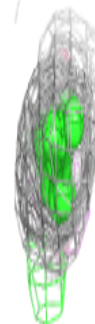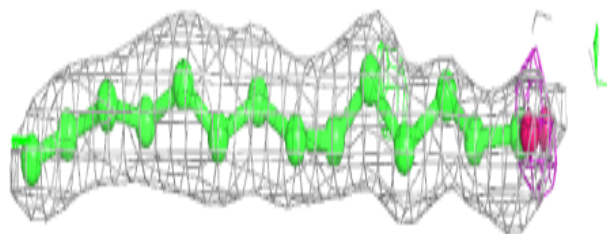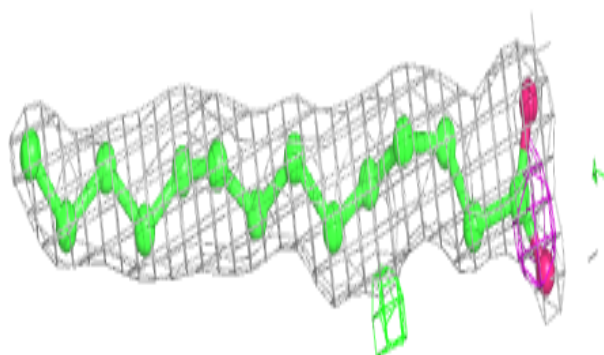
Electron density around LFA A 808:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
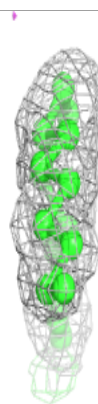and green (positive)
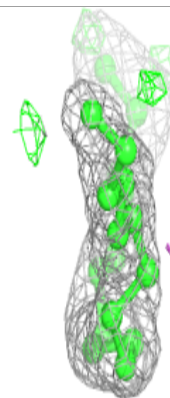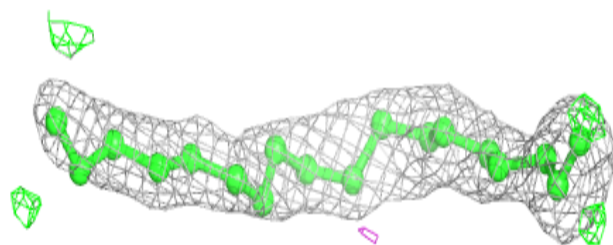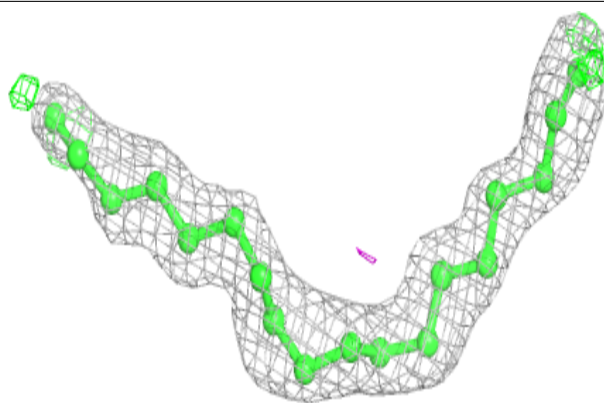
Electron density around LFA A 809:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
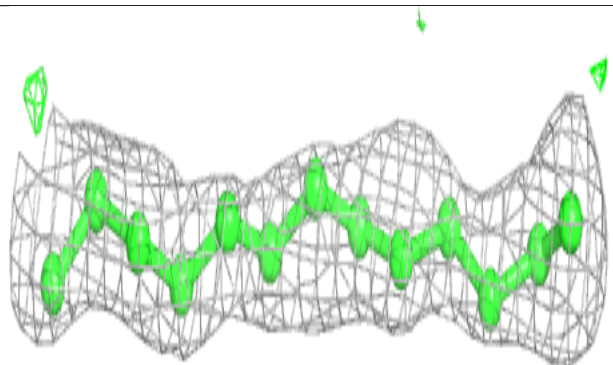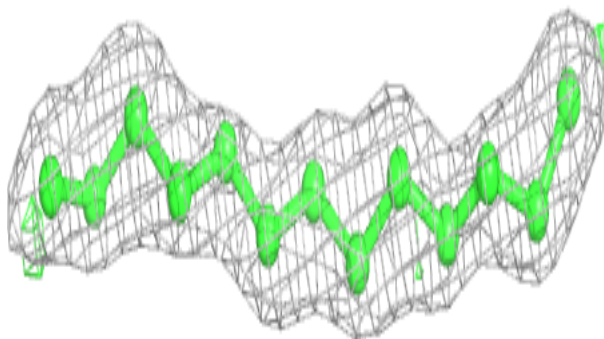
Electron density around OLC X 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
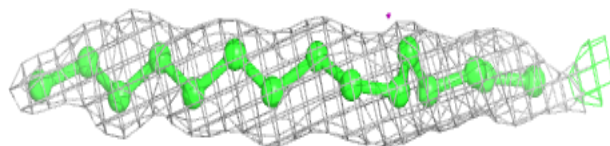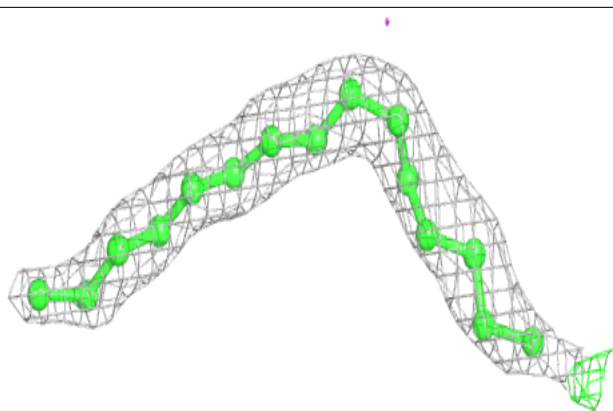and green (positive)
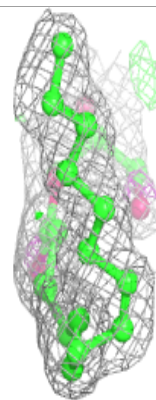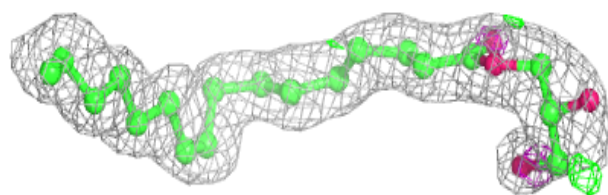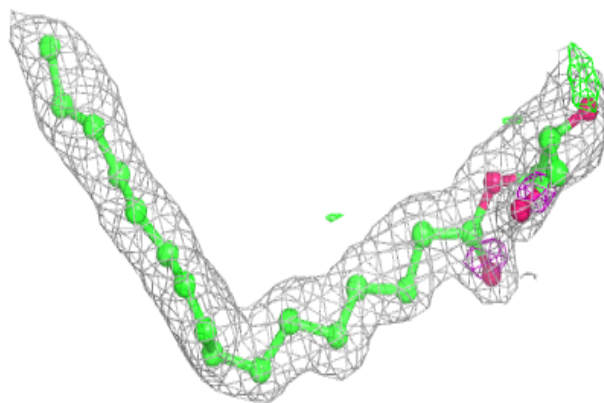
Electron density around LFA A 817:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
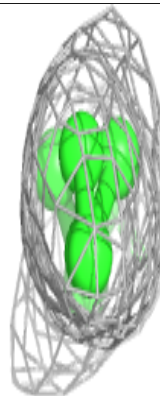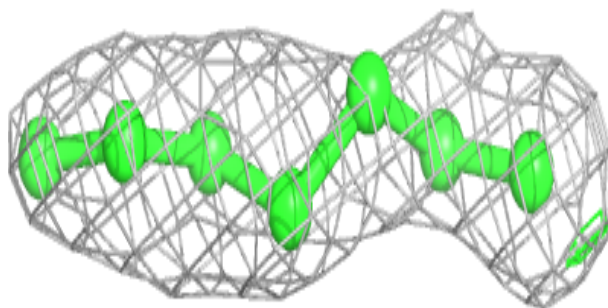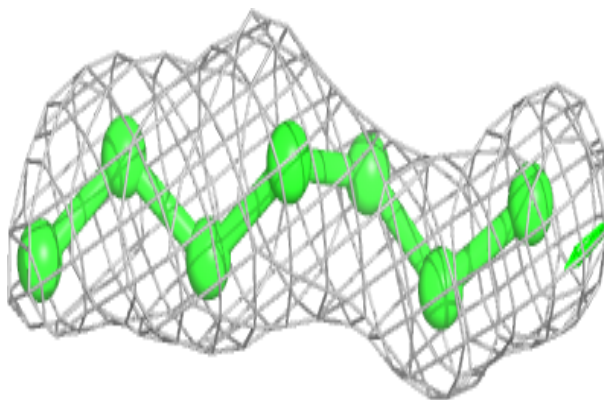
Electron density around OLC X 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
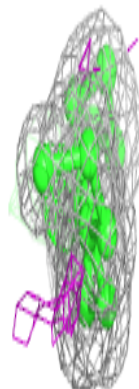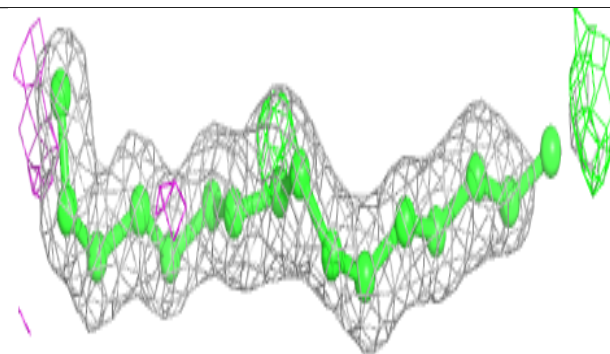and green (positive)
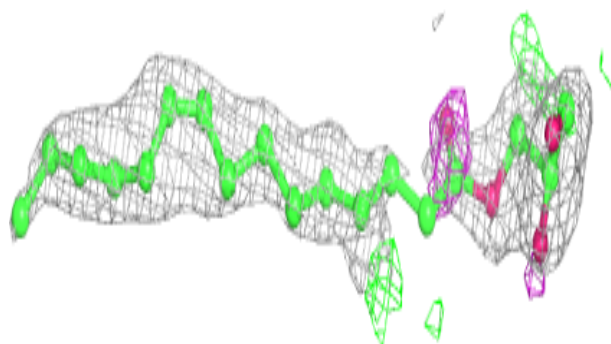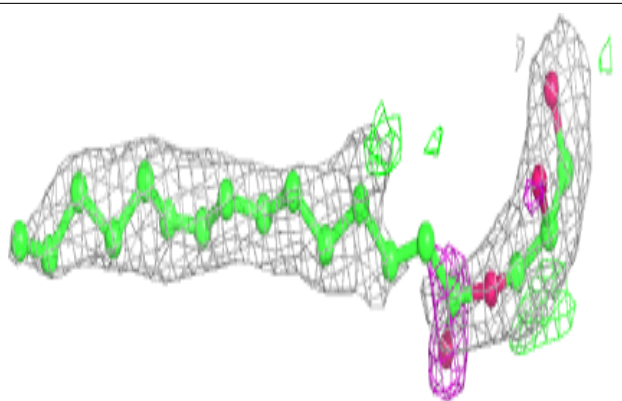
Electron density around LFA X 308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
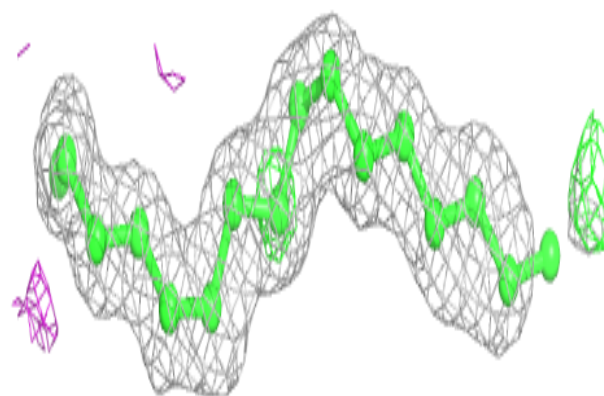mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
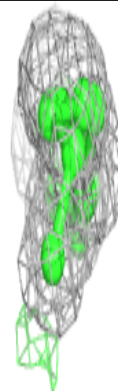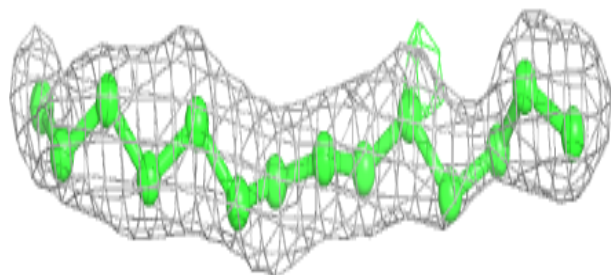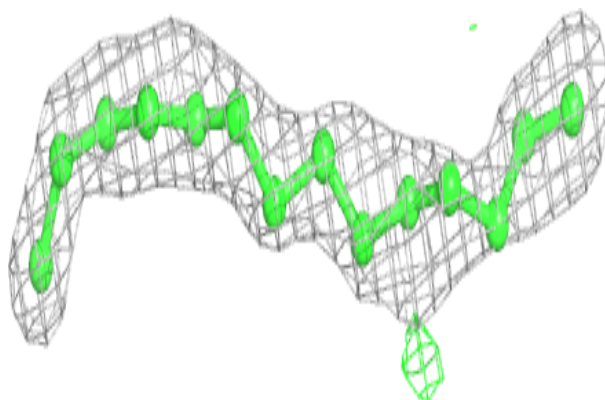
Electron density around LFA A 813:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
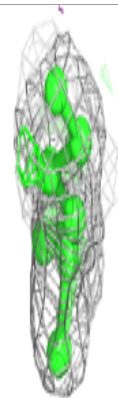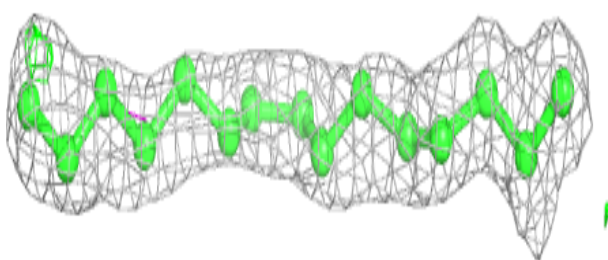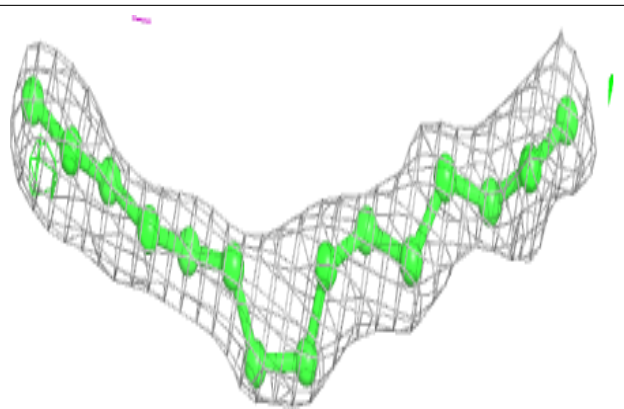
Electron density around LFA X 315:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
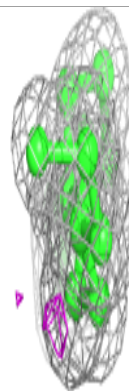$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
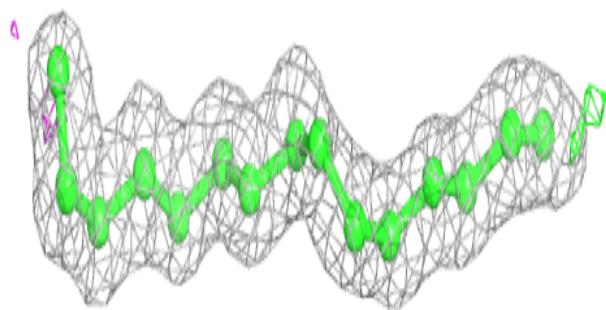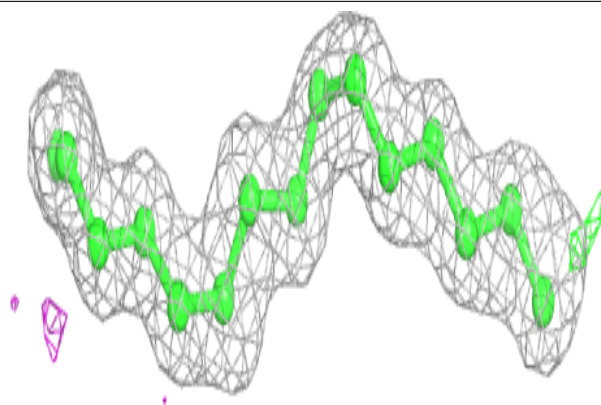and green (positive)
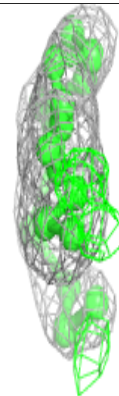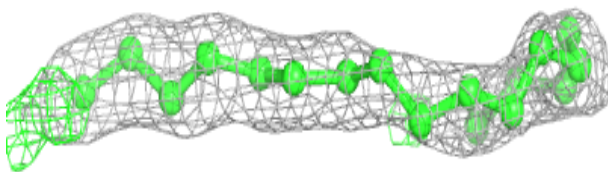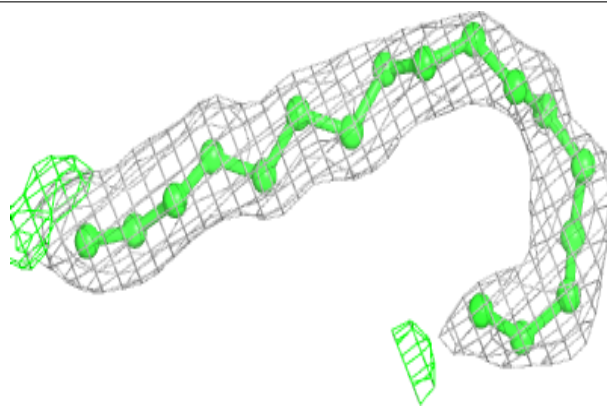
Electron density around LFA X 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
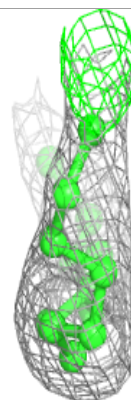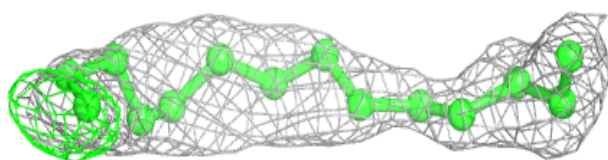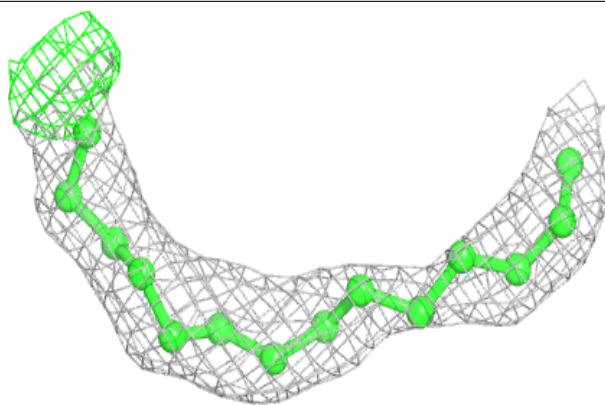
Electron density around LFA A 815:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
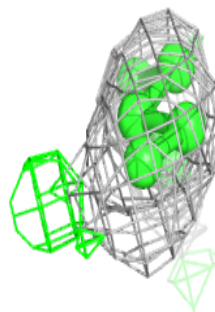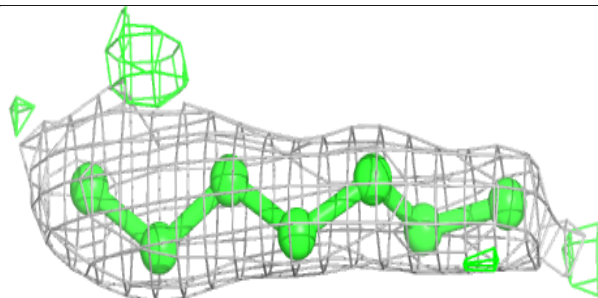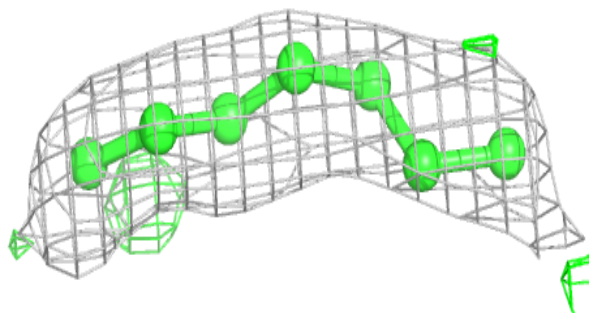
Electron density around LFA A 812:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
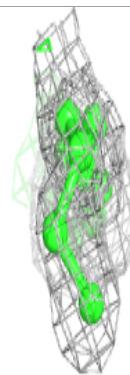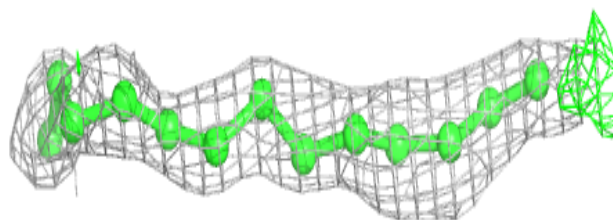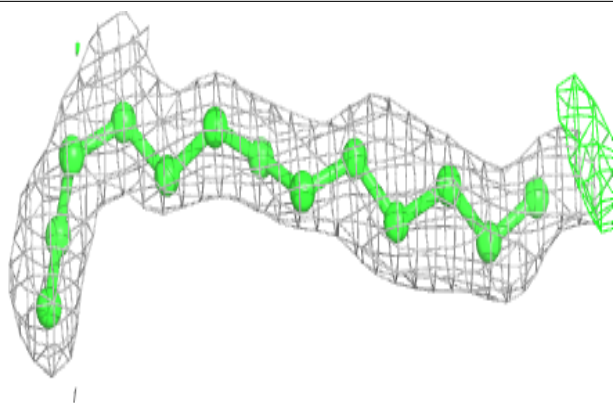
Electron density around LFA X 312:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
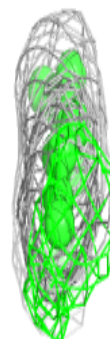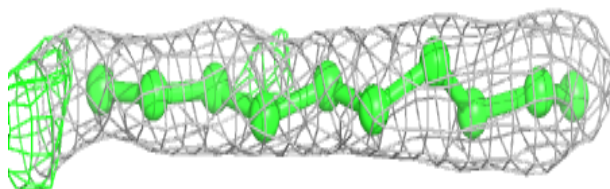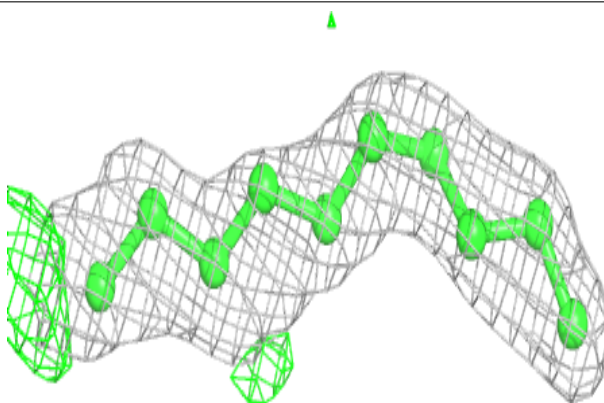
Electron density around LFA X 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
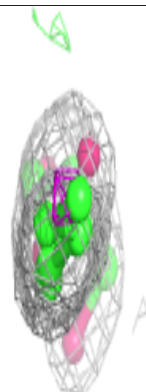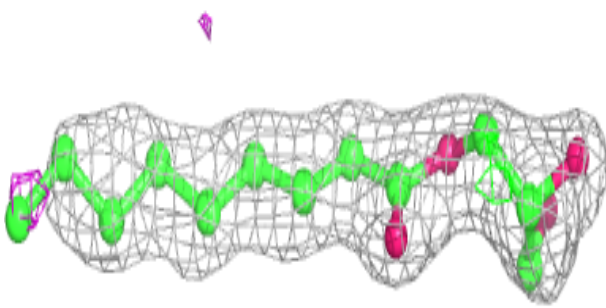mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
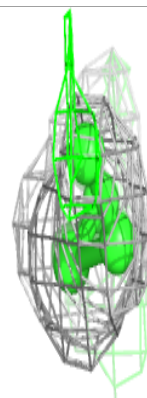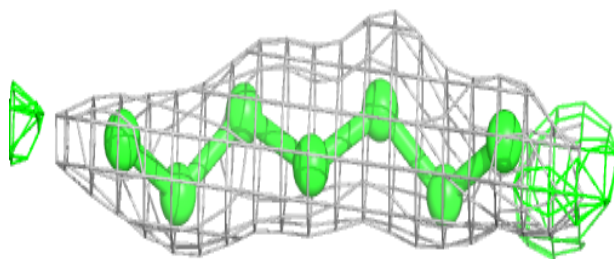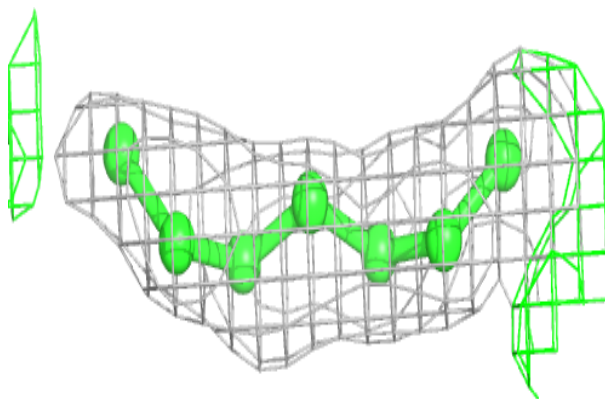
Electron density around OLA A 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
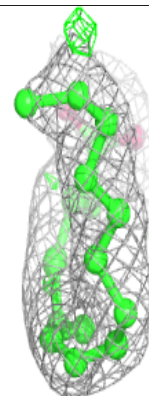
Electron density around LFA X 307:

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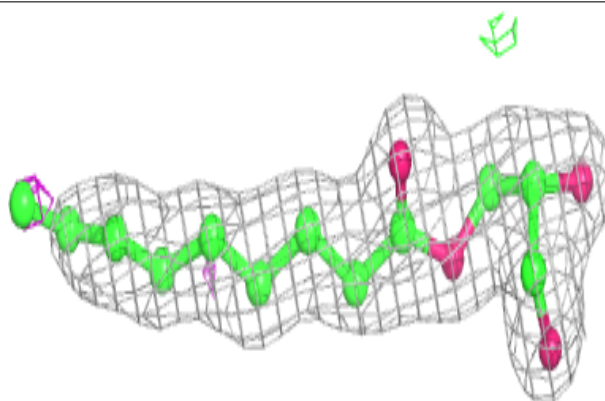mF_o-DF_c (at 3 rmsd) in purple (negative)
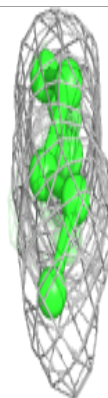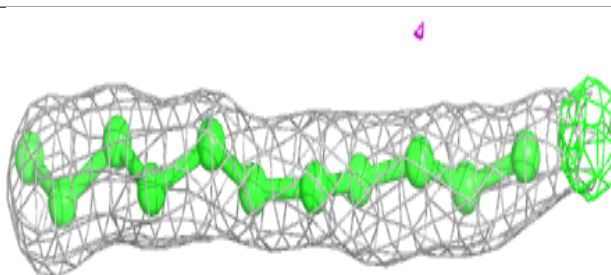and green (positive)

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 LFA X 311:

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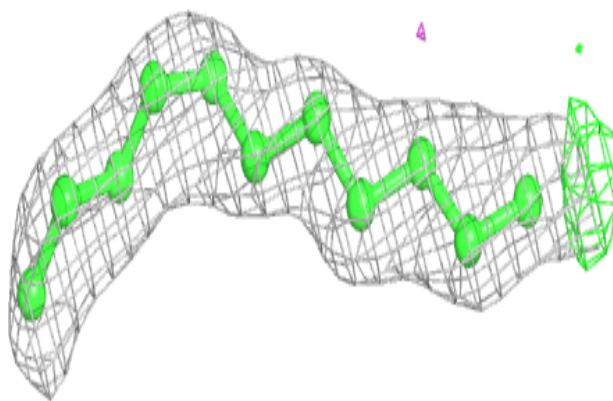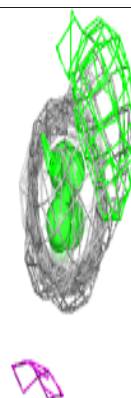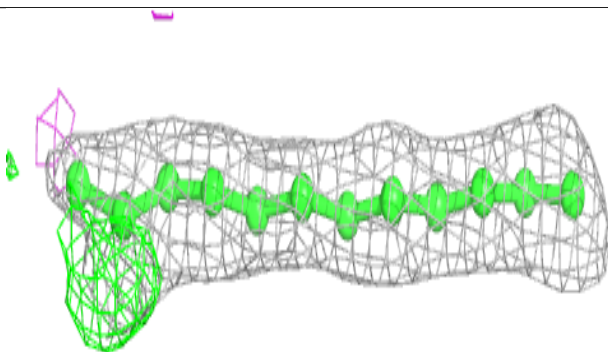and green (positive)

Electron density around LFA A 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 807:

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

Electron density around LFA A 810:

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

Electron density around LFA A 806:

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

Electron density around LFA X 305:

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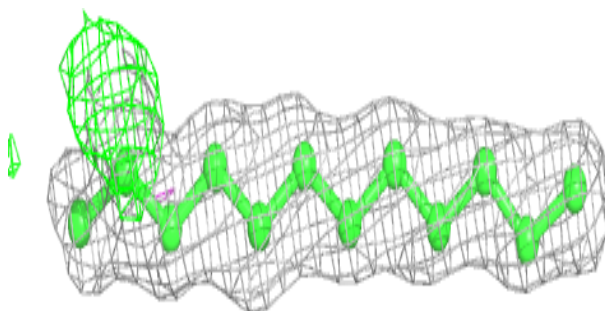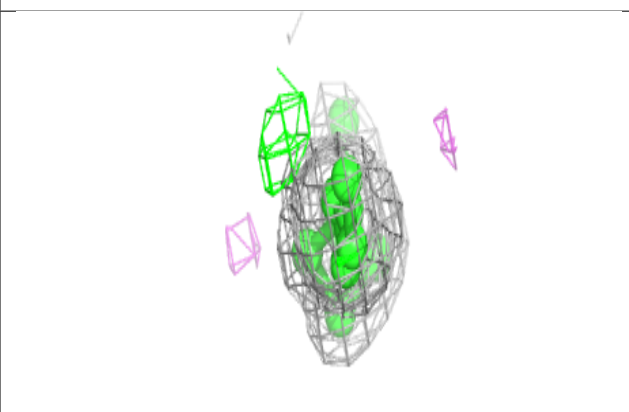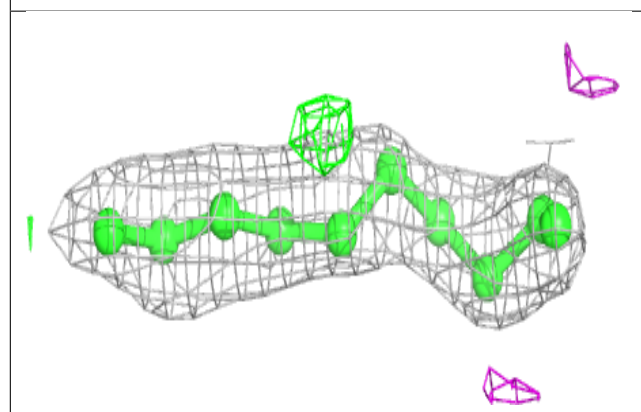$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around LFA A 805:

$2mF_o$-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 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 814:

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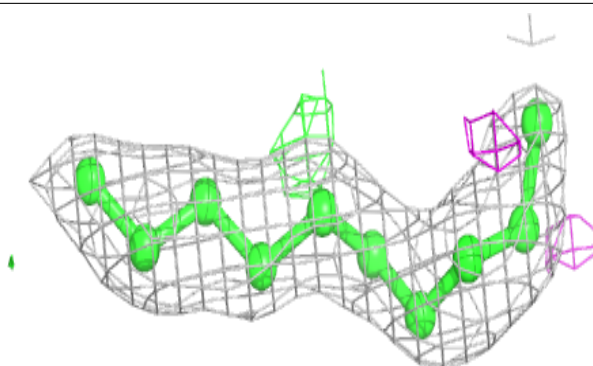mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around LFA X 301:

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

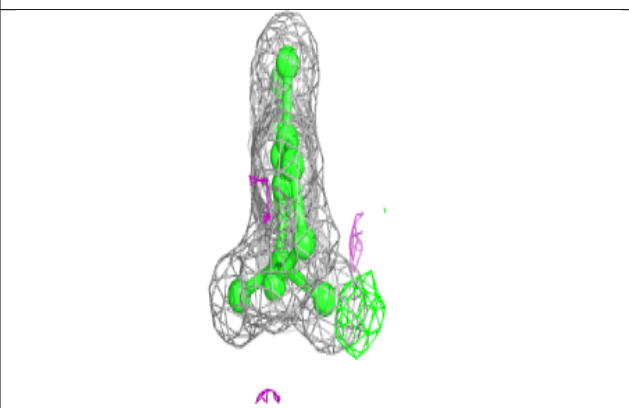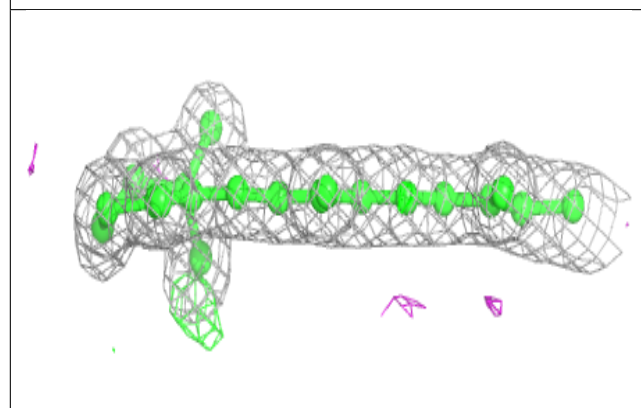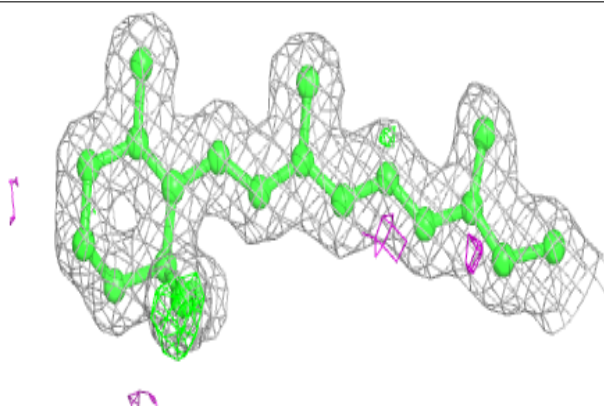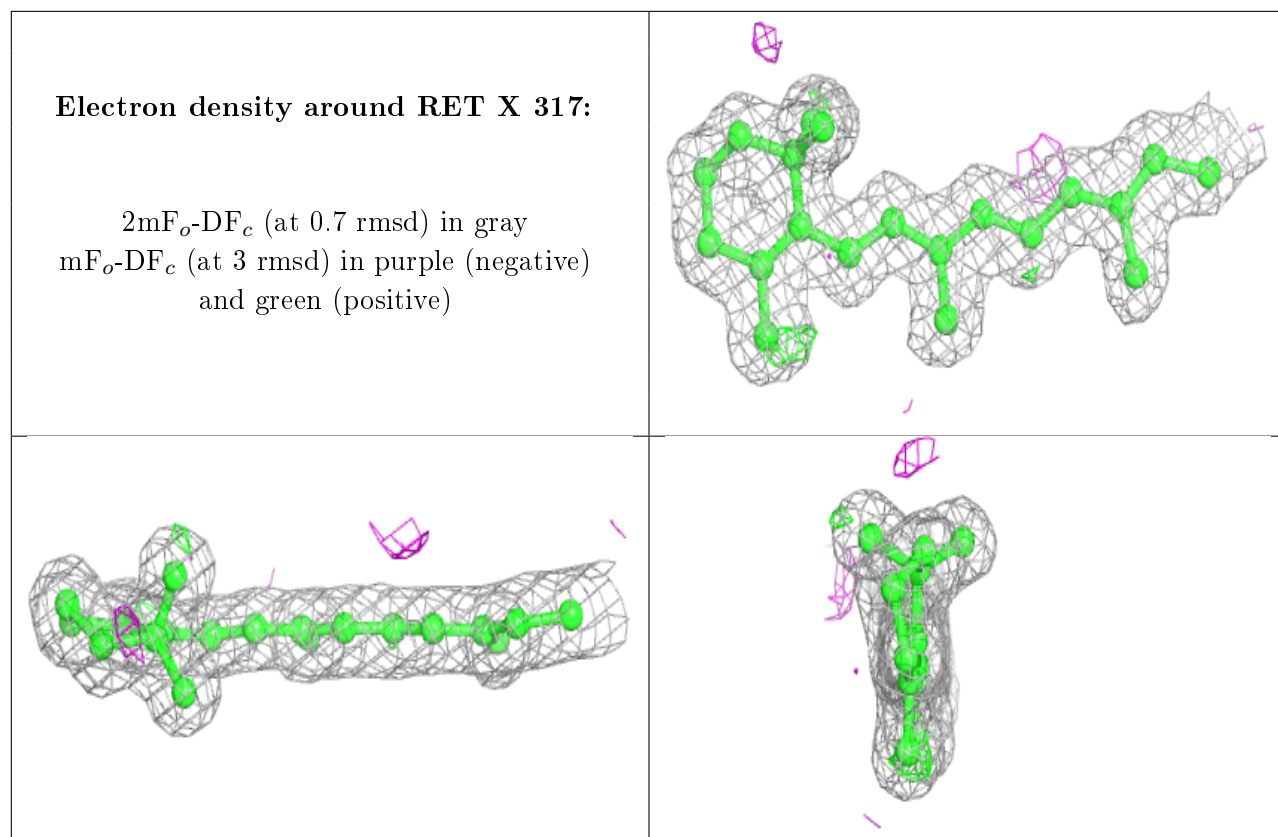**Electron density around LFA X 313:**

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

Electron density around RET A 818:

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

Electron density around RET X 317:

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

6.5 Other polymers (i)

There are no such residues in this entry.