Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 12:24 PM EST

PDB ID	:	3QAP
Title	:	Crystal structure of Natronomonas pharaonis sensory rhodopsin II in the ground state
Authors	:	Gushchin, I.; Reshetnyak, A.; Borshchevskiy, V.; Ishchenko, A.; Round, E.; Grudinin, S.; Engelhard, M.; Buldt, G.; Gordeliy, V.
Deposited on	:	2011-01-11
Resolution	:	1.90 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:

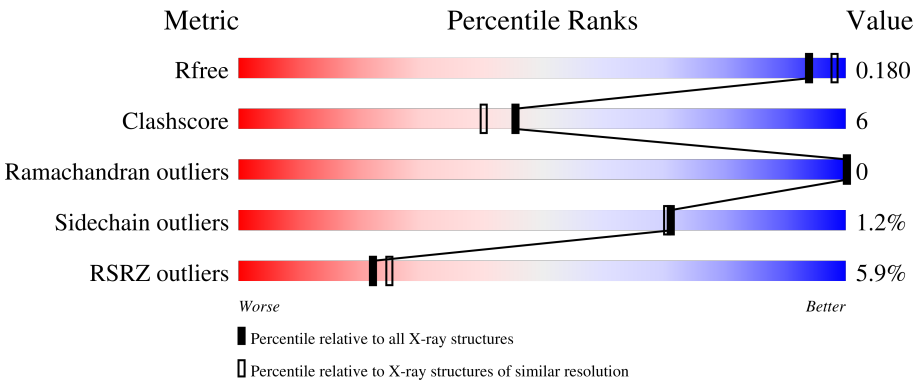
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

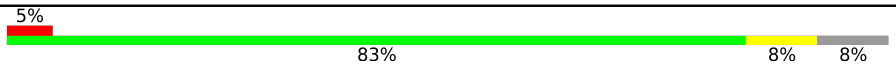
The reported resolution of this entry is 1.90 Å.

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	239	

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
4	LFA	A	253	-	-	-	X

2 Entry composition (i)

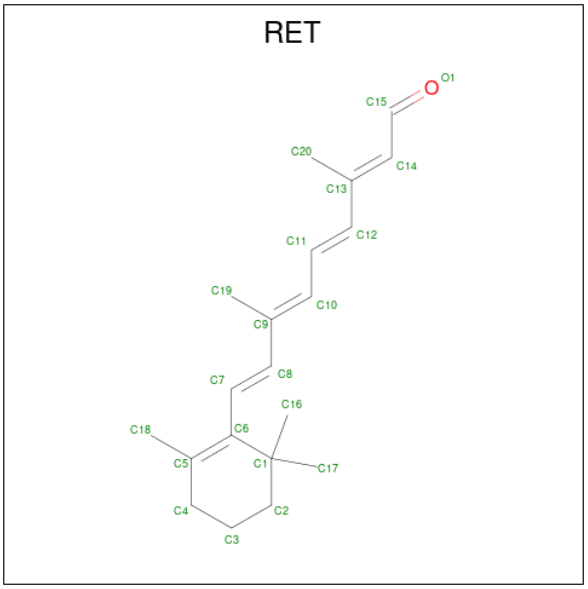
There are 6 unique types of molecules in this entry. The entry contains 2142 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sensory rhodopsin-2.

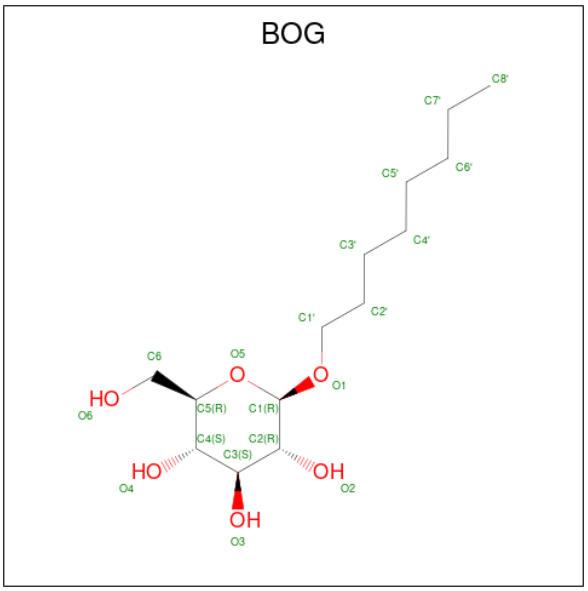
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	219	1694	1153	261	274	6	2	11	0

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



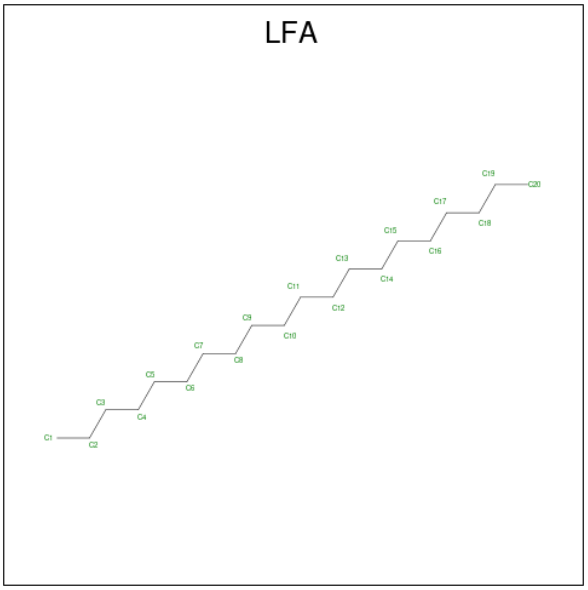
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
2	A	1	20	20	0	0

- Molecule 3 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	20	14	6	0	0

- Molecule 4 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
4	A	1	10	10	0	0
			Total	C		
4	A	1	6	6	0	0
			Total	C		
4	A	1	10	10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 6 6	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 14 14	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 4 4	0	0
4	A	1	Total C 14 14	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 20 20	0	0

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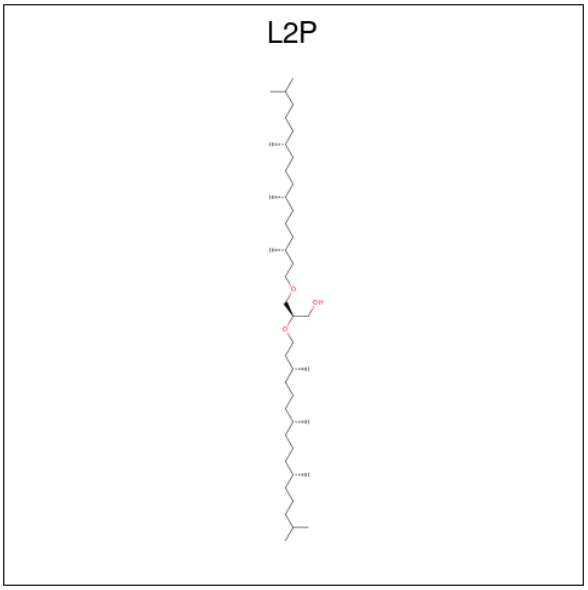
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 7 7	0	0
4	A	1	Total C 4 4	0	0
4	A	1	Total C 4 4	0	0
4	A	1	Total C 20 20	0	0
4	A	1	Total C 12 12	0	0

- Molecule 5 is 2,3-DI-PHYTANYL-GLYCEROL (three-letter code: L2P) (formula: $C_{43}H_{88}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 46 43 3	0	0
5	A	1	Total C 20 20	0	0

- Molecule 6 is water.

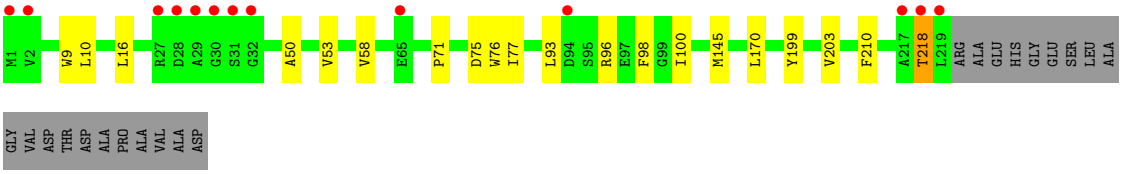
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	73	Total O 73 73	0	0

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: Sensory rhodopsin-2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	86.99Å 128.09Å 50.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.00 – 1.90 22.11 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (22.00-1.90) 95.9 (22.11-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.152 , 0.173 0.169 , 0.180	Depositor DCC
R_{free} test set	1107 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 91.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2142	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.64% 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: RET, BOG, LFA, L2P

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	0.76	2/1767 (0.1%)	0.67	2/2422 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	THR	CB-OG1	-13.62	1.16	1.43
1	A	218	THR	CB-CG2	-5.78	1.33	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	218	THR	OG1-CB-CG2	14.06	142.34	110.00
1	A	75	ASP	CB-CG-OD1	5.53	123.28	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	218	THR	CB

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	1694	0	1806	20	0
2	A	20	0	27	3	0
3	A	20	0	28	0	0
4	A	269	0	515	12	0
5	A	66	0	127	7	0
6	A	73	0	0	0	0
All	All	2142	0	2503	29	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 6.

All (29) 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:210[B]:PHE:HD2	4:A:255:LFA:H92	1.51	0.76
4:A:252:LFA:H11	4:A:261:LFA:H61	1.67	0.75
4:A:259:LFA:H21	4:A:261:LFA:H111	1.73	0.70
1:A:16[B]:LEU:HD23	4:A:261:LFA:H12	1.78	0.65
1:A:96[B]:ARG:HH11	1:A:100:ILE:HD11	1.62	0.65
1:A:210[B]:PHE:CD2	4:A:255:LFA:H92	2.33	0.63
1:A:50:ALA:HB2	5:A:257:L2P:H491	1.80	0.62
1:A:9:TRP:HZ3	4:A:252:LFA:H13	1.70	0.56
1:A:170:LEU:HD13	1:A:203[B]:VAL:HG13	1.86	0.55
2:A:240:RET:H8	2:A:240:RET:H171	1.91	0.52
1:A:10:LEU:HB3	4:A:267:LFA:H121	1.91	0.52
1:A:77:ILE:HG21	5:A:257:L2P:H241	1.92	0.52
1:A:53:VAL:HG13	1:A:58:VAL:HB	1.92	0.51
1:A:96[B]:ARG:NH1	1:A:100:ILE:HD11	2.25	0.50
1:A:93[B]:LEU:HD21	1:A:145:MET:HG2	1.94	0.49
1:A:76:TRP:CD1	2:A:240:RET:H14	2.51	0.46
1:A:199:TYR:HB2	4:A:267:LFA:H161	1.98	0.46
4:A:245:LFA:H21	5:A:257:L2P:H243	1.98	0.45
1:A:16[A]:LEU:HD23	1:A:16[A]:LEU:HA	1.83	0.45
4:A:255:LFA:H12	4:A:267:LFA:H152	2.00	0.44
5:A:257:L2P:H492	5:A:257:L2P:H462	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ALA:CB	5:A:257:L2P:H491	2.47	0.43
4:A:252:LFA:C1	4:A:261:LFA:H61	2.42	0.43
2:A:240:RET:H8	2:A:240:RET:H161	2.01	0.43
1:A:71:PRO:HG3	5:A:257:L2P:H421	2.00	0.42
1:A:16[B]:LEU:CD2	4:A:261:LFA:H12	2.48	0.42
1:A:93[B]:LEU:HD11	1:A:145:MET:HG2	2.02	0.42
5:A:257:L2P:H542	5:A:257:L2P:H512	1.89	0.42
1:A:170:LEU:HD13	1:A:203[B]:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	228/239 (95%)	226 (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	172/180 (96%)	170 (99%)	2 (1%)	71 70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	PHE
1	A	218	THR

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

Mol	Chain	Res	Type
1	A	151	GLN

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)

33 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	$\#\|Z\| > 2$
4	LFA	A	255	-	13,13,19	0.36	0	12,12,18	0.55	0
4	LFA	A	253	-	5,5,19	0.41	0	4,4,18	0.33	0
4	LFA	A	269	-	3,3,19	0.48	0	2,2,18	0.62	0
4	LFA	A	246	-	7,7,19	0.36	0	6,6,18	0.54	0
4	LFA	A	266	-	9,9,19	0.41	0	8,8,18	0.47	0
4	LFA	A	272	-	11,11,19	0.40	0	10,10,18	0.45	0
4	LFA	A	270	-	3,3,19	0.44	0	2,2,18	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	LFA	A	261	-	13,13,19	0.35	0	12,12,18	0.61	0
4	LFA	A	249	-	4,4,19	0.36	0	3,3,18	0.45	0
4	LFA	A	264	-	8,8,19	0.34	0	7,7,18	0.51	0
4	LFA	A	248	-	6,6,19	0.34	0	5,5,18	0.48	0
4	LFA	A	263	-	9,9,19	0.39	0	8,8,18	0.48	0
5	L2P	A	257	-	45,45,45	0.50	0	51,53,53	0.75	1 (1%)
4	LFA	A	258	-	5,5,19	0.39	0	4,4,18	0.36	0
4	LFA	A	242	-	9,9,19	0.42	0	8,8,18	0.52	0
3	BOG	A	241	-	20,20,20	0.61	0	25,25,25	1.03	1 (4%)
4	LFA	A	247	-	4,4,19	0.39	0	3,3,18	0.43	0
4	LFA	A	259	-	3,3,19	0.45	0	2,2,18	0.60	0
4	LFA	A	243	-	5,5,19	0.40	0	4,4,18	0.33	0
4	LFA	A	245	-	5,5,19	0.39	0	4,4,18	0.33	0
4	LFA	A	265	-	7,7,19	0.41	0	6,6,18	0.47	0
4	LFA	A	267	-	19,19,19	0.39	0	18,18,18	0.53	0
4	LFA	A	268	-	6,6,19	0.38	0	5,5,18	0.46	0
4	LFA	A	254	-	15,15,19	0.37	0	14,14,18	0.57	0
4	LFA	A	271	-	19,19,19	0.38	0	18,18,18	0.56	0
4	LFA	A	252	-	11,11,19	0.34	0	10,10,18	0.61	0
4	LFA	A	262	-	5,5,19	0.40	0	4,4,18	0.34	0
4	LFA	A	256	-	4,4,19	0.39	0	3,3,18	0.35	0
4	LFA	A	251	-	15,15,19	0.40	0	14,14,18	0.51	0
5	L2P	A	260	-	19,19,45	0.33	0	22,22,53	0.61	0
4	LFA	A	244	-	9,9,19	0.42	0	8,8,18	0.51	0
4	LFA	A	250	-	8,8,19	0.39	0	7,7,18	0.43	0
2	RET	A	240	-	20,20,21	2.61	13 (65%)	27,27,28	1.82	9 (33%)

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
4	LFA	A	255	-	-	5/11/11/17	-
4	LFA	A	253	-	-	1/3/3/17	-
4	LFA	A	269	-	-	0/1/1/17	-
4	LFA	A	246	-	-	3/5/5/17	-
4	LFA	A	266	-	-	4/7/7/17	-
4	LFA	A	272	-	-	4/9/9/17	-
4	LFA	A	270	-	-	0/1/1/17	-
4	LFA	A	261	-	-	7/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LFA	A	249	-	-	0/2/2/17	-
4	LFA	A	264	-	-	5/6/6/17	-
4	LFA	A	248	-	-	1/4/4/17	-
4	LFA	A	263	-	-	5/7/7/17	-
5	L2P	A	257	-	-	26/51/51/51	-
4	LFA	A	258	-	-	1/3/3/17	-
4	LFA	A	242	-	-	4/7/7/17	-
3	BOG	A	241	-	-	6/11/31/31	0/1/1/1
4	LFA	A	247	-	-	0/2/2/17	-
4	LFA	A	259	-	-	0/1/1/17	-
4	LFA	A	243	-	-	1/3/3/17	-
4	LFA	A	245	-	-	2/3/3/17	-
4	LFA	A	265	-	-	4/5/5/17	-
4	LFA	A	267	-	-	9/17/17/17	-
4	LFA	A	268	-	-	2/4/4/17	-
4	LFA	A	254	-	-	10/13/13/17	-
4	LFA	A	271	-	-	14/17/17/17	-
4	LFA	A	252	-	-	6/9/9/17	-
4	LFA	A	262	-	-	1/3/3/17	-
4	LFA	A	256	-	-	1/2/2/17	-
4	LFA	A	251	-	-	8/13/13/17	-
5	L2P	A	260	-	-	11/20/20/51	-
4	LFA	A	244	-	-	2/7/7/17	-
4	LFA	A	250	-	-	3/6/6/17	-
2	RET	A	240	-	-	0/13/30/31	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	240	RET	C14-C13	4.90	1.37	1.33
2	A	240	RET	C1-C6	4.39	1.59	1.53
2	A	240	RET	C5-C6	4.18	1.41	1.34
2	A	240	RET	C10-C9	3.89	1.40	1.35
2	A	240	RET	C15-C14	-3.00	1.38	1.49
2	A	240	RET	C18-C5	2.69	1.55	1.50
2	A	240	RET	C8-C7	2.68	1.41	1.33
2	A	240	RET	C12-C13	-2.54	1.40	1.45
2	A	240	RET	C19-C9	2.50	1.56	1.50
2	A	240	RET	C20-C13	2.31	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	240	RET	C8-C9	-2.24	1.41	1.45
2	A	240	RET	C17-C1	2.07	1.57	1.53
2	A	240	RET	C11-C12	2.04	1.39	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	240	RET	C10-C11-C12	-3.61	111.94	123.22
3	A	241	BOG	C1'-O1-C1	-3.30	108.36	113.84
2	A	240	RET	C11-C10-C9	-3.22	122.72	127.31
2	A	240	RET	C3-C4-C5	-2.95	108.82	114.08
2	A	240	RET	C20-C13-C12	2.76	122.42	118.08
2	A	240	RET	C18-C5-C6	-2.42	121.81	124.53
2	A	240	RET	C1-C6-C7	2.39	122.54	115.78
2	A	240	RET	C7-C8-C9	-2.32	122.73	126.23
2	A	240	RET	C19-C9-C10	-2.31	119.69	122.92
5	A	257	L2P	C41-O2-C2	-2.27	110.19	115.40
2	A	240	RET	C2-C3-C4	-2.21	106.43	111.38

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	257	L2P	C1-C2-C3-O3
5	A	257	L2P	O2-C2-C3-O3
5	A	257	L2P	C41-C42-C43-C44
5	A	260	L2P	C41-C42-C43-C45
3	A	241	BOG	O5-C5-C6-O6
3	A	241	BOG	C4-C5-C6-O6
5	A	257	L2P	C16-C17-C18-C19
4	A	271	LFA	C9-C10-C11-C12
5	A	257	L2P	C45-C46-C47-C48
5	A	257	L2P	C43-C45-C46-C47
5	A	260	L2P	C45-C46-C47-C48
5	A	257	L2P	C16-C17-C18-C20
5	A	257	L2P	O2-C41-C42-C43
4	A	264	LFA	C5-C6-C7-C8
4	A	264	LFA	C2-C3-C4-C5
3	A	241	BOG	C2'-C3'-C4'-C5'
4	A	254	LFA	C12-C13-C14-C15
5	A	260	L2P	C48-C50-C51-C52
4	A	242	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	A	251	LFA	C3-C4-C5-C6
4	A	251	LFA	C4-C5-C6-C7
4	A	255	LFA	C4-C5-C6-C7
4	A	261	LFA	C2-C3-C4-C5
4	A	251	LFA	C2-C3-C4-C5
4	A	254	LFA	C11-C10-C9-C8
5	A	257	L2P	C50-C51-C52-C53
4	A	271	LFA	C2-C3-C4-C5
4	A	261	LFA	C3-C4-C5-C6
4	A	264	LFA	C4-C5-C6-C7
4	A	261	LFA	C5-C6-C7-C8
4	A	263	LFA	C3-C4-C5-C6
4	A	264	LFA	C3-C4-C5-C6
4	A	266	LFA	C4-C5-C6-C7
4	A	267	LFA	C3-C4-C5-C6
4	A	267	LFA	C11-C12-C13-C14
4	A	271	LFA	C4-C5-C6-C7
4	A	271	LFA	C15-C16-C17-C18
5	A	257	L2P	C26-C27-C28-C29
5	A	257	L2P	C26-C27-C28-C30
3	A	241	BOG	C3'-C4'-C5'-C6'
4	A	254	LFA	C4-C5-C6-C7
4	A	255	LFA	C7-C8-C9-C10
4	A	267	LFA	C6-C7-C8-C9
4	A	254	LFA	C9-C10-C11-C12
4	A	265	LFA	C3-C4-C5-C6
4	A	271	LFA	C6-C7-C8-C9
4	A	272	LFA	C3-C4-C5-C6
5	A	257	L2P	C23-C25-C26-C27
4	A	265	LFA	C2-C3-C4-C5
4	A	261	LFA	C10-C11-C12-C13
3	A	241	BOG	C1'-C2'-C3'-C4'
4	A	263	LFA	C5-C6-C7-C8
5	A	257	L2P	C42-C43-C45-C46
5	A	257	L2P	C47-C48-C50-C51
4	A	251	LFA	C7-C8-C9-C10
4	A	242	LFA	C5-C6-C7-C8
4	A	271	LFA	C12-C13-C14-C15
4	A	271	LFA	C5-C6-C7-C8
4	A	271	LFA	C7-C8-C9-C10
4	A	242	LFA	C4-C5-C6-C7
5	A	257	L2P	C44-C43-C45-C46

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Mol	Chain	Res	Type	Atoms
5	A	257	L2P	C49-C48-C50-C51
4	A	255	LFA	C6-C7-C8-C9
4	A	267	LFA	C10-C11-C12-C13
4	A	262	LFA	C1-C2-C3-C4
4	A	261	LFA	C1-C2-C3-C4
4	A	271	LFA	C3-C4-C5-C6
4	A	265	LFA	C5-C6-C7-C8
4	A	244	LFA	C7-C8-C9-C10
4	A	250	LFA	C5-C6-C7-C8
4	A	265	LFA	C4-C5-C6-C7
4	A	264	LFA	C6-C7-C8-C9
5	A	257	L2P	C18-C20-C21-C22
4	A	271	LFA	C10-C11-C12-C13
4	A	252	LFA	C7-C8-C9-C10
4	A	255	LFA	C5-C6-C7-C8
4	A	272	LFA	C1-C2-C3-C4
4	A	252	LFA	C11-C10-C9-C8
5	A	260	L2P	C47-C48-C50-C51
5	A	257	L2P	C54-C53-C55-C56
5	A	260	L2P	C49-C48-C50-C51
4	A	245	LFA	C3-C4-C5-C6
3	A	241	BOG	C4'-C5'-C6'-C7'
4	A	263	LFA	C7-C8-C9-C10
4	A	271	LFA	C14-C15-C16-C17
4	A	263	LFA	C4-C5-C6-C7
4	A	252	LFA	C1-C2-C3-C4
4	A	243	LFA	C3-C4-C5-C6
4	A	261	LFA	C11-C12-C13-C14
5	A	257	L2P	O1-C1-C2-C3
4	A	252	LFA	C6-C7-C8-C9
4	A	248	LFA	C2-C3-C4-C5
4	A	251	LFA	C13-C14-C15-C16
4	A	255	LFA	C3-C4-C5-C6
4	A	256	LFA	C2-C3-C4-C5
4	A	252	LFA	C9-C10-C11-C12
4	A	258	LFA	C1-C2-C3-C4
5	A	257	L2P	O1-C1-C2-O2
4	A	254	LFA	C11-C12-C13-C14
4	A	266	LFA	C2-C3-C4-C5
5	A	260	L2P	C41-C42-C43-C44
4	A	244	LFA	C5-C6-C7-C8
4	A	251	LFA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	254	LFA	C10-C11-C12-C13
5	A	257	L2P	C15-C16-C17-C18
5	A	257	L2P	C41-C42-C43-C45
4	A	261	LFA	C4-C5-C6-C7
4	A	250	LFA	C2-C3-C4-C5
4	A	254	LFA	C7-C8-C9-C10
4	A	272	LFA	C11-C10-C9-C8
4	A	267	LFA	C5-C6-C7-C8
4	A	246	LFA	C3-C4-C5-C6
4	A	254	LFA	C13-C14-C15-C16
4	A	253	LFA	C2-C3-C4-C5
4	A	242	LFA	C7-C8-C9-C10
4	A	268	LFA	C1-C2-C3-C4
4	A	250	LFA	C3-C4-C5-C6
4	A	254	LFA	C3-C4-C5-C6
4	A	266	LFA	C6-C7-C8-C9
4	A	245	LFA	C2-C3-C4-C5
4	A	267	LFA	C11-C10-C9-C8
4	A	272	LFA	C6-C7-C8-C9
4	A	246	LFA	C1-C2-C3-C4
4	A	267	LFA	C15-C16-C17-C18
4	A	263	LFA	C2-C3-C4-C5
4	A	267	LFA	C1-C2-C3-C4
4	A	267	LFA	C4-C5-C6-C7
4	A	266	LFA	C5-C6-C7-C8
4	A	268	LFA	C4-C5-C6-C7
4	A	271	LFA	C17-C18-C19-C20
5	A	257	L2P	C52-C53-C55-C56
5	A	260	L2P	C46-C47-C48-C50
4	A	246	LFA	C2-C3-C4-C5
5	A	260	L2P	C53-C55-C56-C57
4	A	251	LFA	C6-C7-C8-C9
4	A	271	LFA	C1-C2-C3-C4
5	A	257	L2P	C12-C11-O1-C1
4	A	271	LFA	C11-C12-C13-C14
4	A	254	LFA	C1-C2-C3-C4
4	A	251	LFA	C9-C10-C11-C12
5	A	260	L2P	C46-C47-C48-C49
5	A	260	L2P	C56-C57-C58-C59
5	A	260	L2P	C54-C53-C55-C56
4	A	252	LFA	C5-C6-C7-C8
5	A	257	L2P	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
5	A	257	L2P	C22-C23-C25-C26

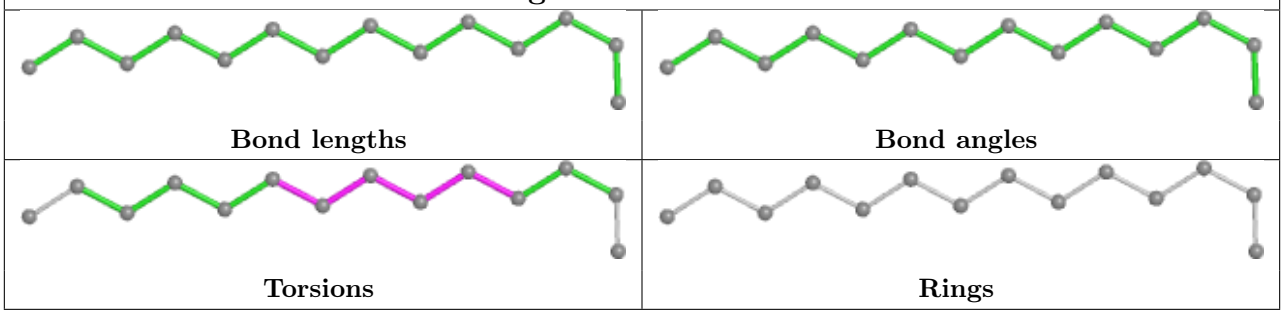
There are no ring outliers.

8 monomers are involved in 21 short contacts:

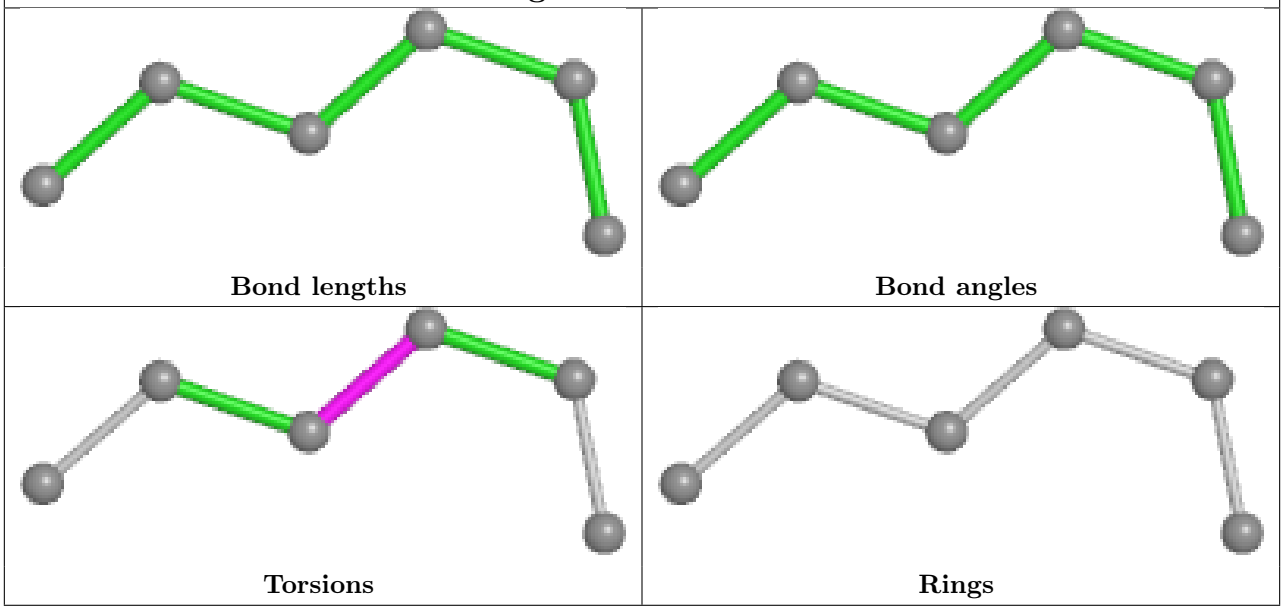
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	255	LFA	3	0
4	A	261	LFA	5	0
5	A	257	L2P	7	0
4	A	259	LFA	1	0
4	A	245	LFA	1	0
4	A	267	LFA	3	0
4	A	252	LFA	3	0
2	A	240	RET	3	0

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.

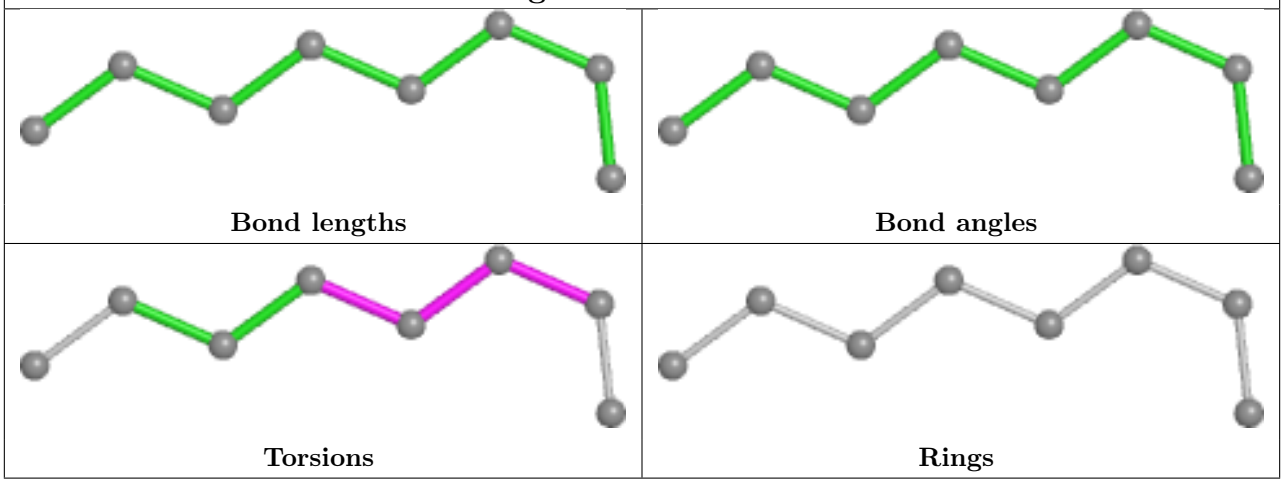
Ligand LFA A 255



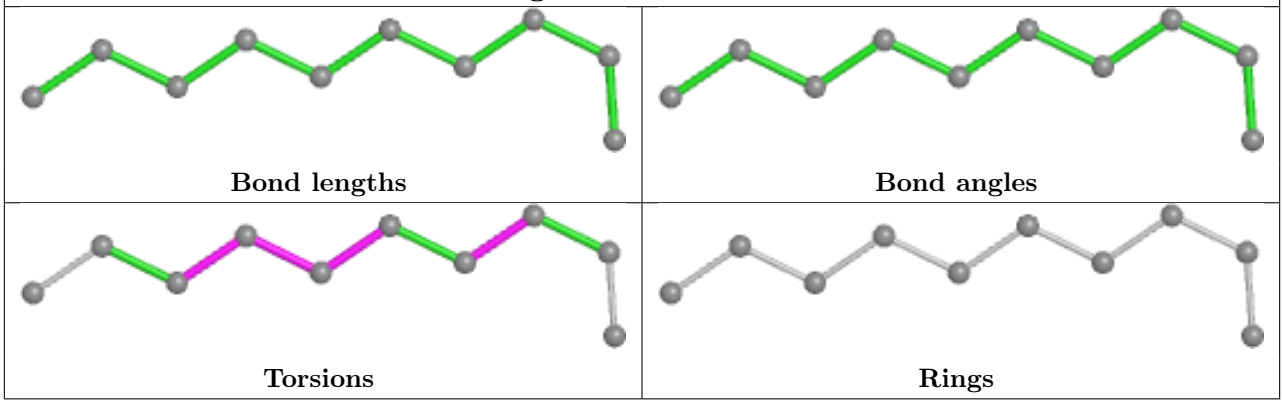
Ligand LFA A 253



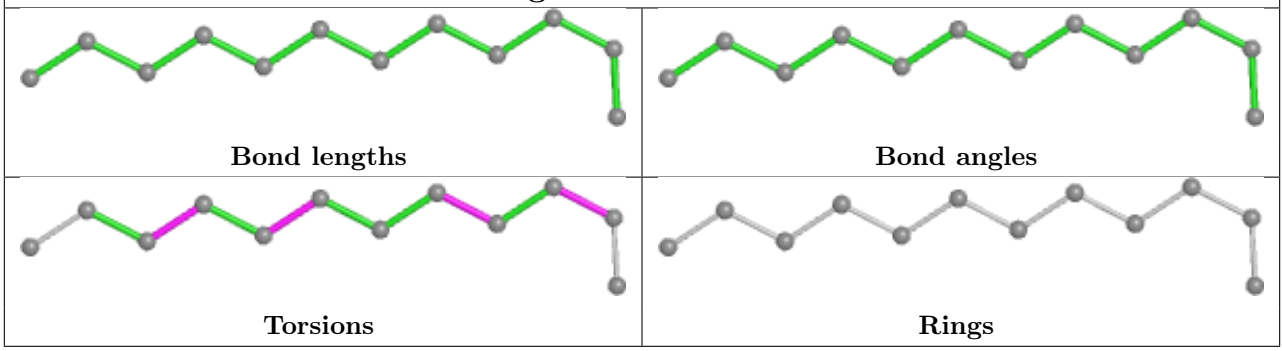
Ligand LFA A 246



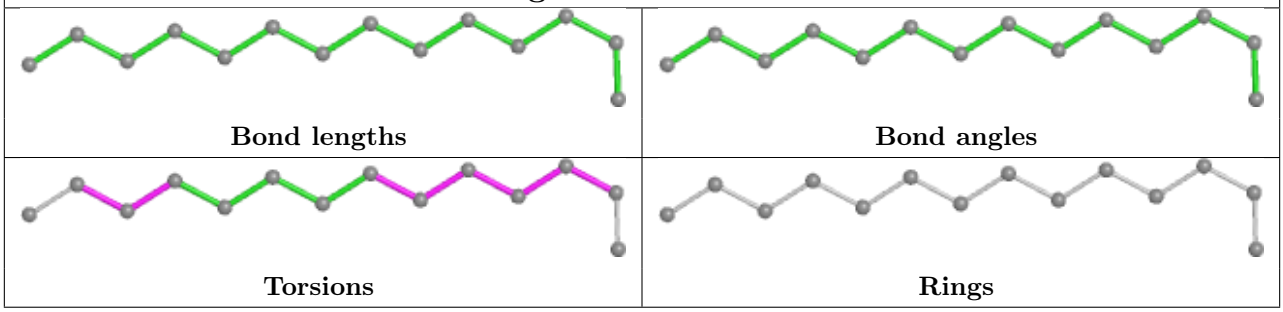
Ligand LFA A 266



Ligand LFA A 272



Ligand LFA A 261



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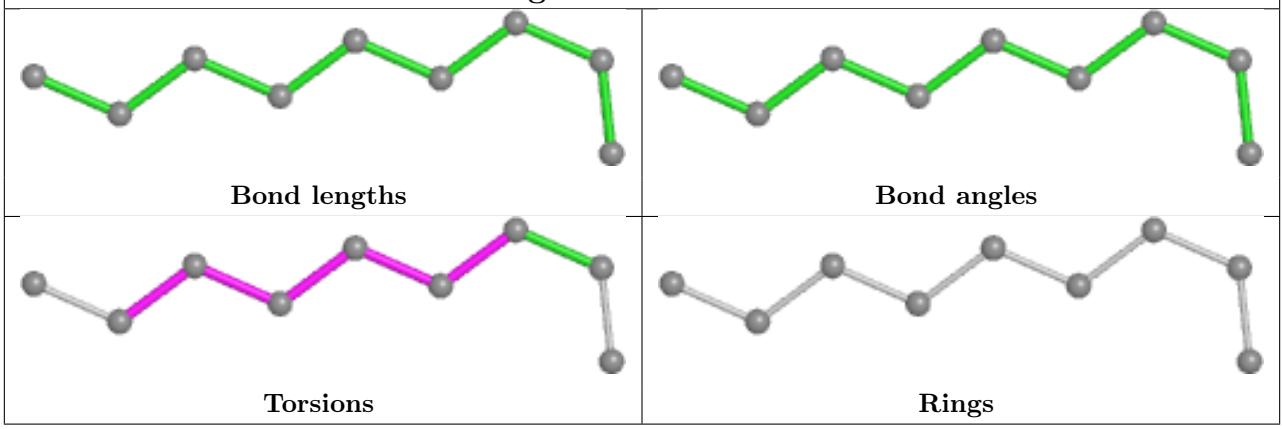

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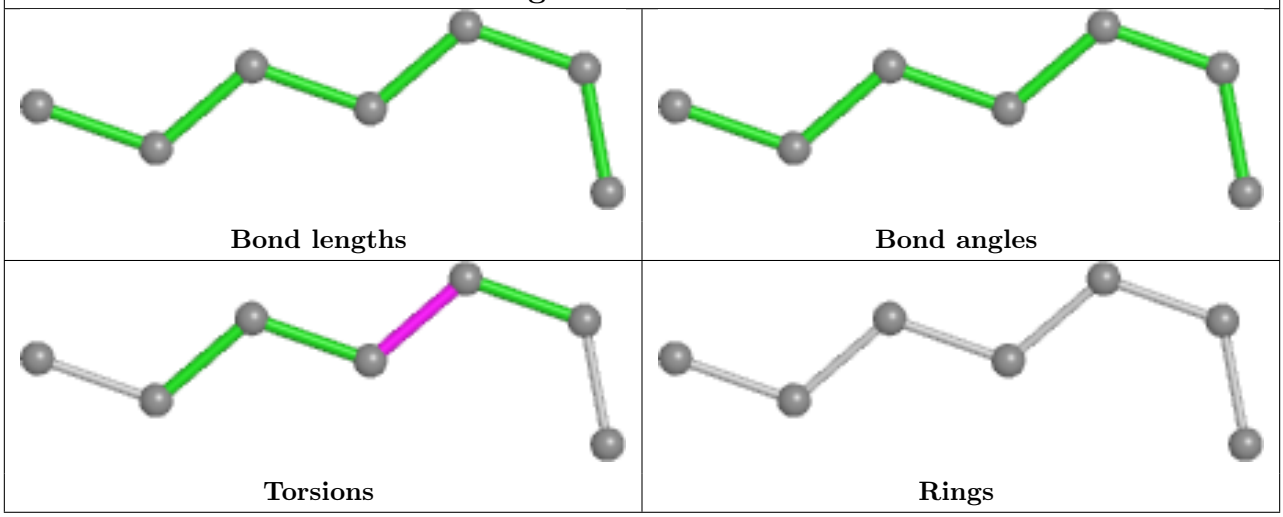
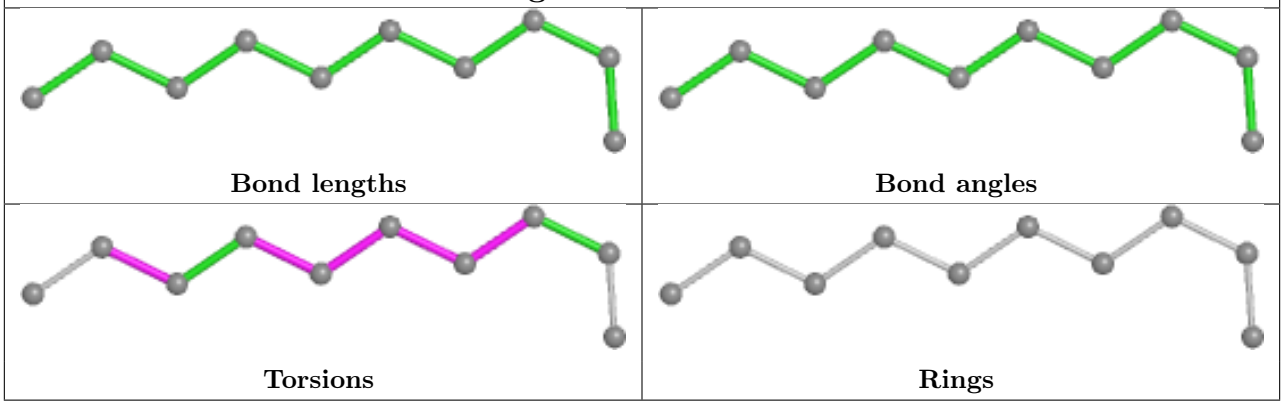
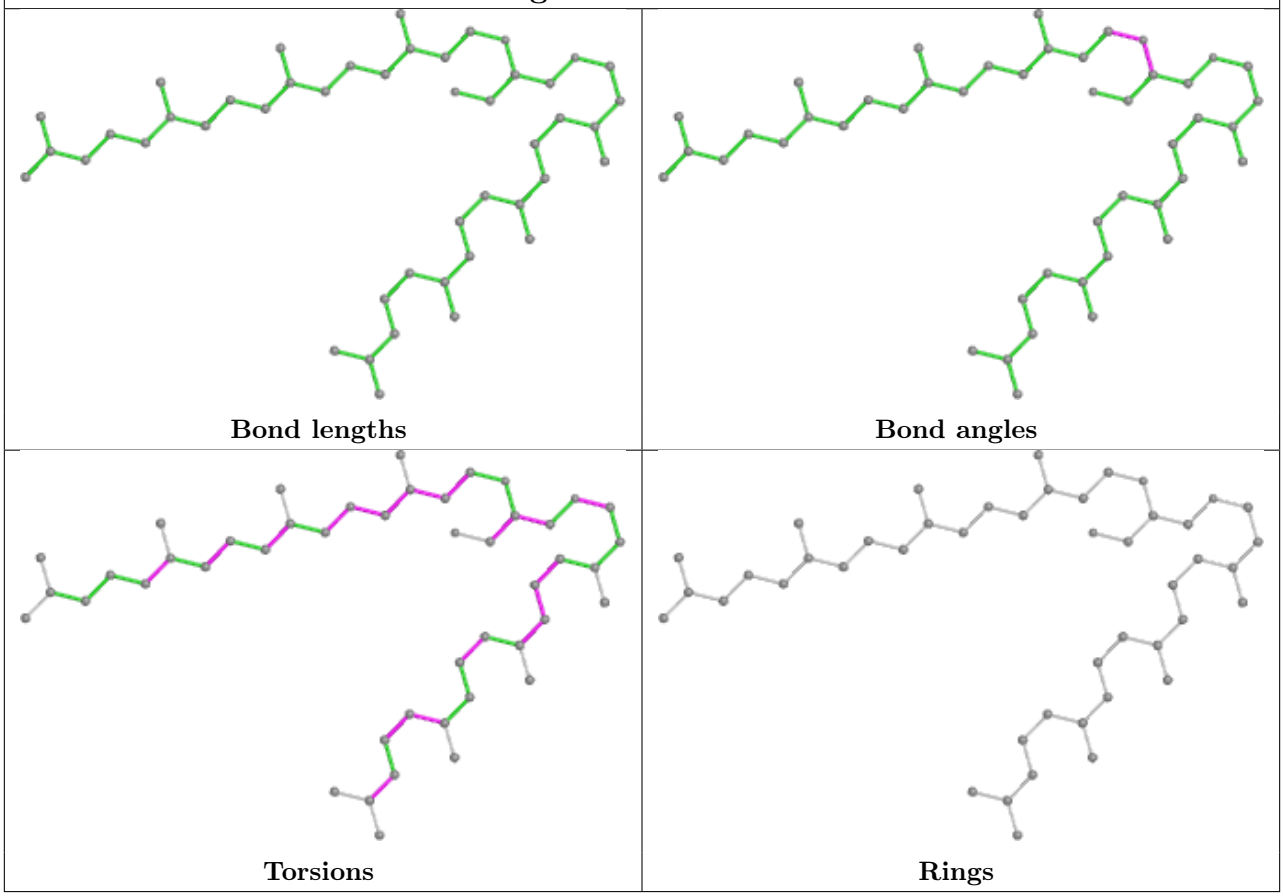


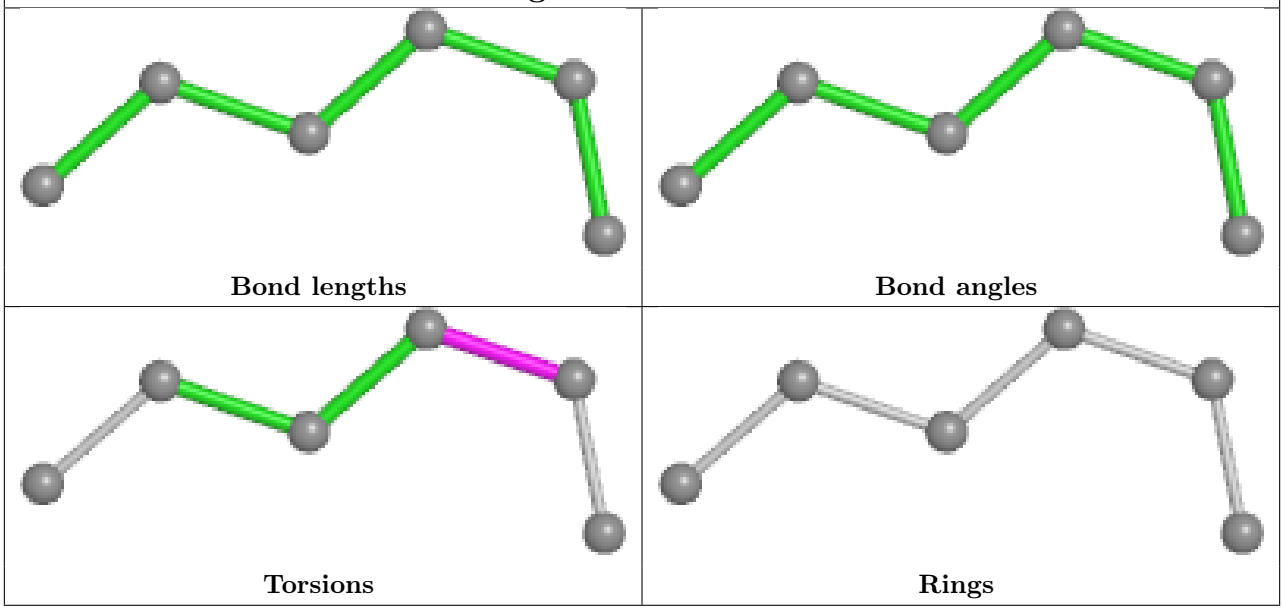
Ligand LFA A 263



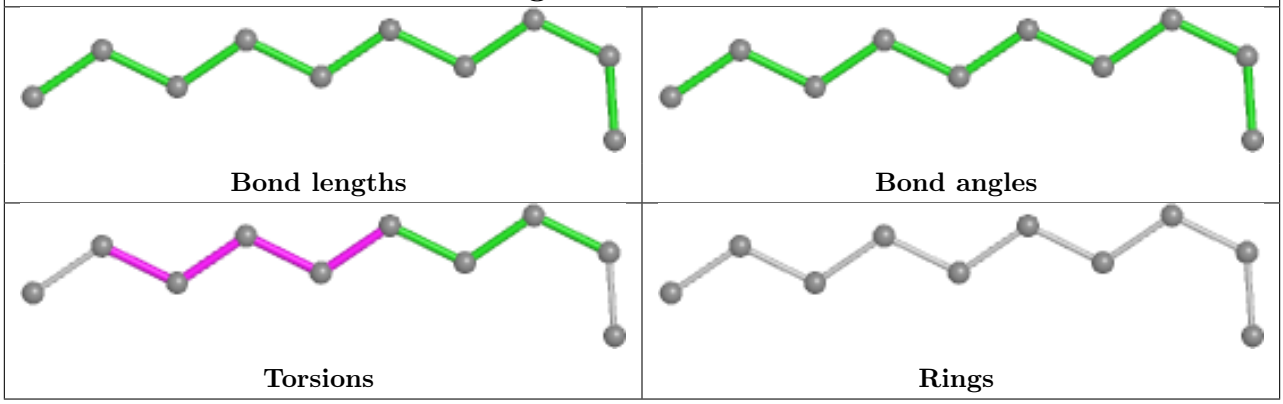
Ligand L2P A 257



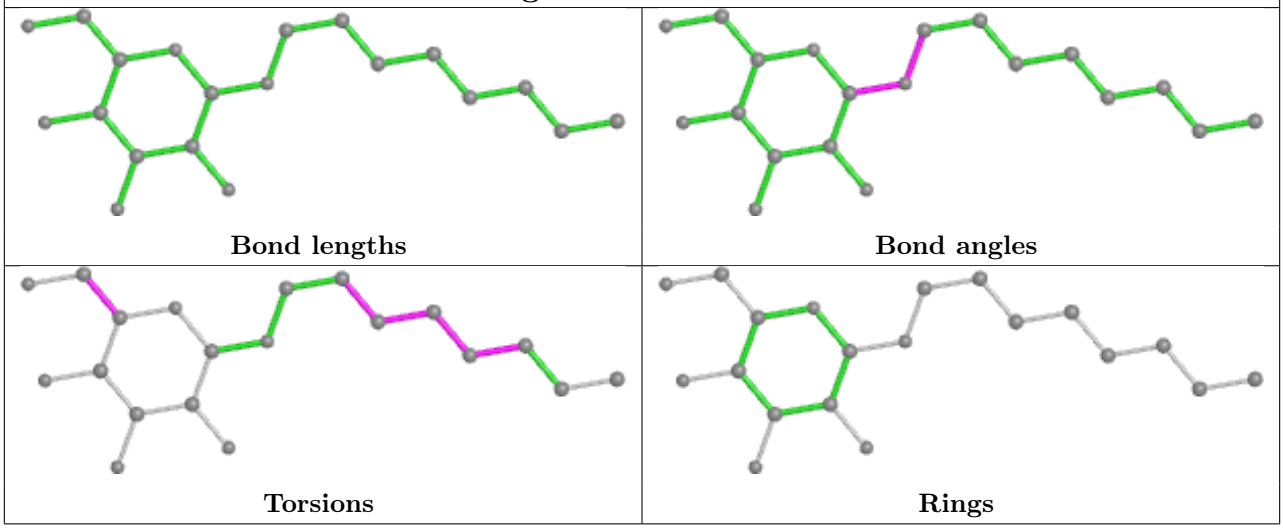
Ligand LFA A 258



Ligand LFA A 242



Ligand BOG A 241



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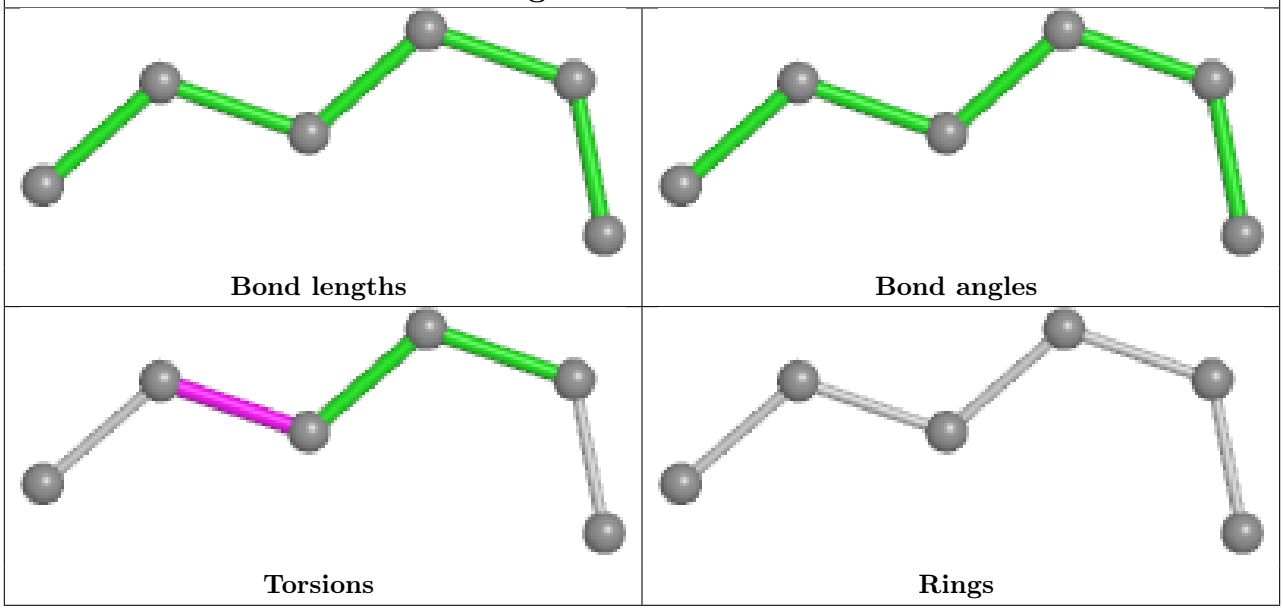

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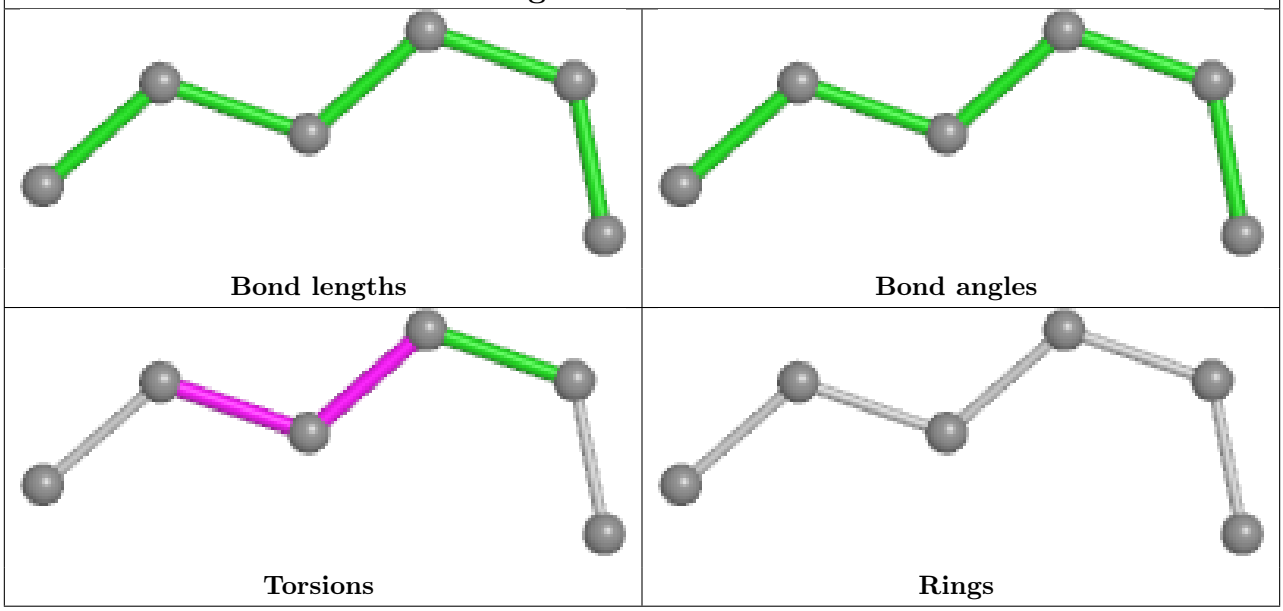
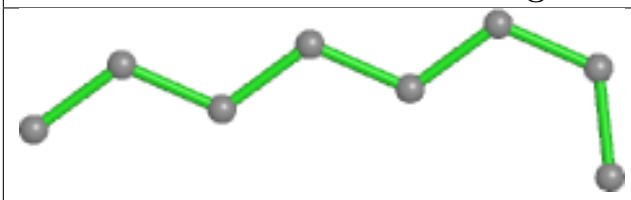
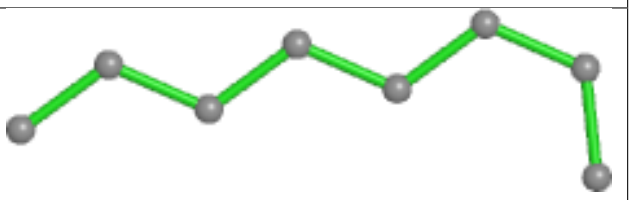


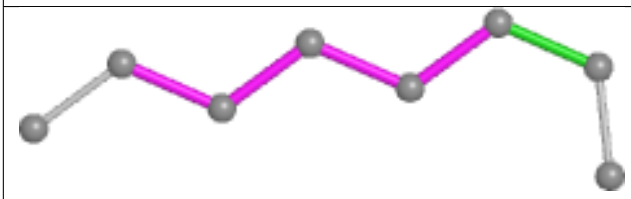
Ligand LFA A 265



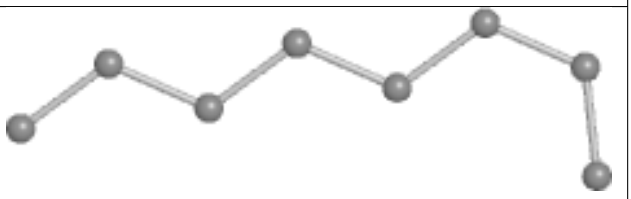
Bond lengths



Bond angles

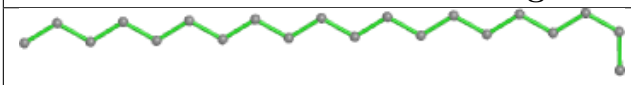


Torsions

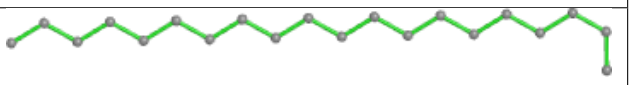


Rings

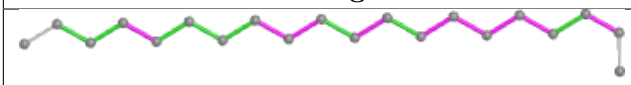
Ligand LFA A 267



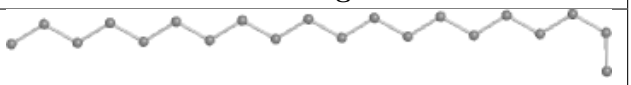
Bond lengths



Bond angles

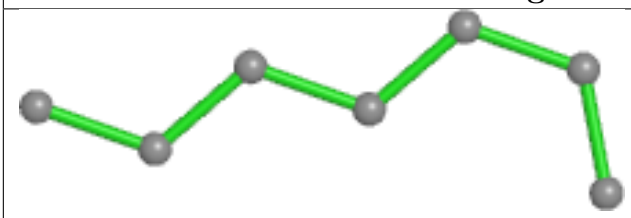


Torsions

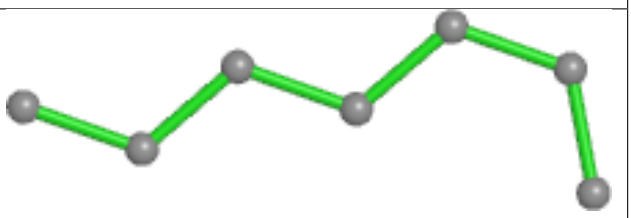


Rings

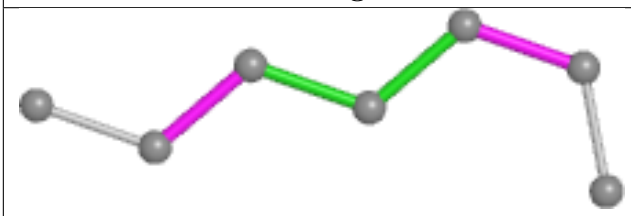
Ligand LFA A 268



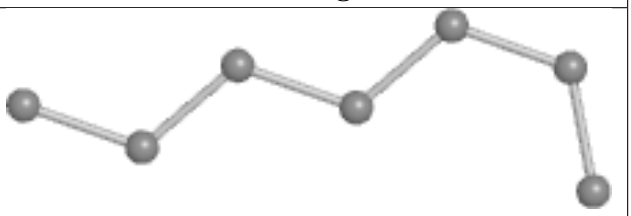
Bond lengths



Bond angles

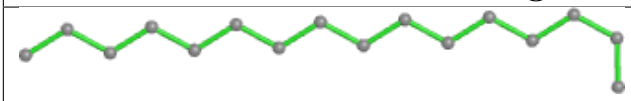


Torsions

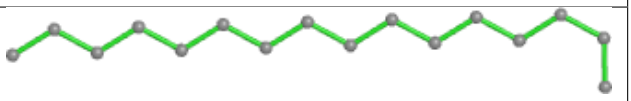


Rings

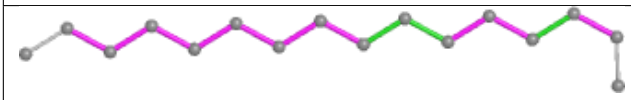
Ligand LFA A 254



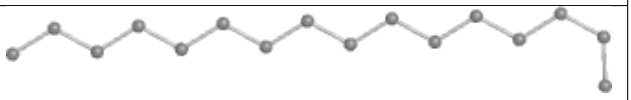
Bond lengths



Bond angles

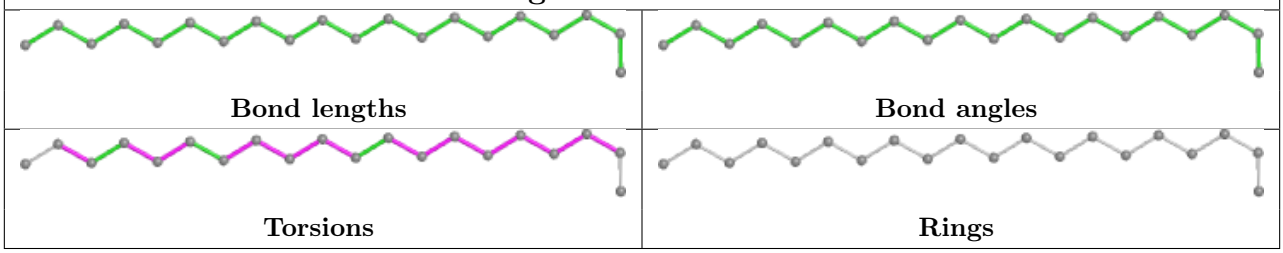


Torsions

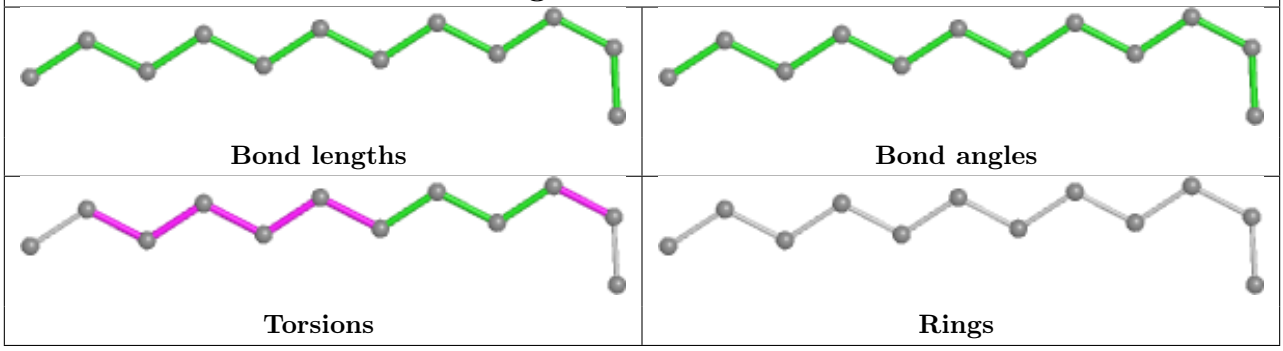


Rings

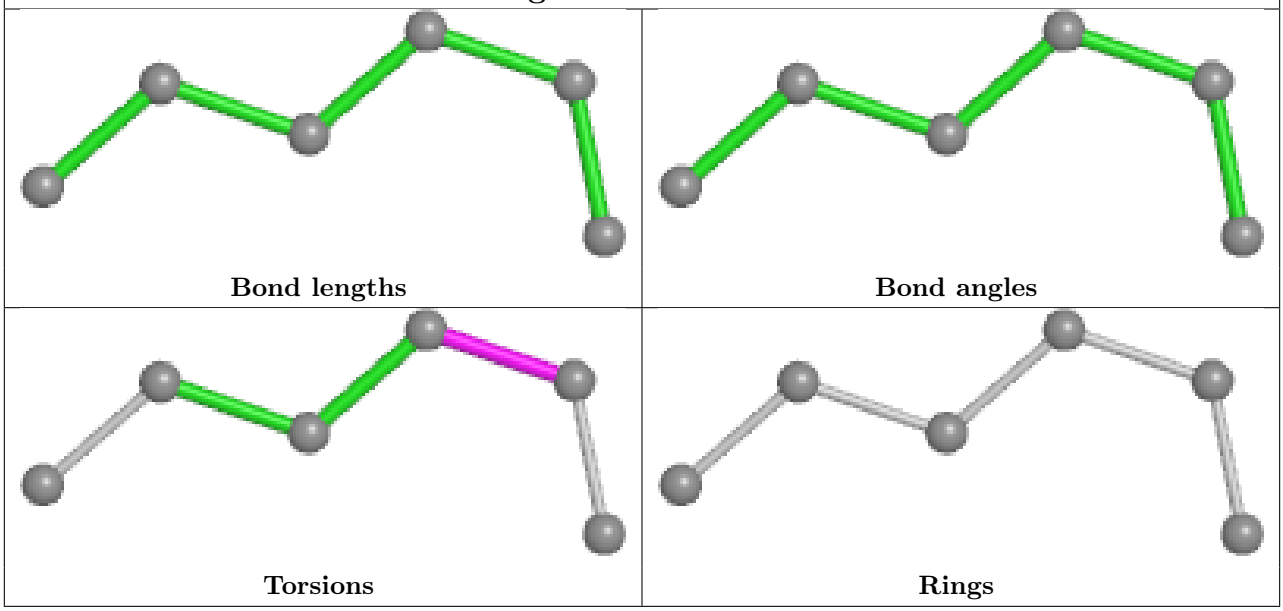
Ligand LFA A 271



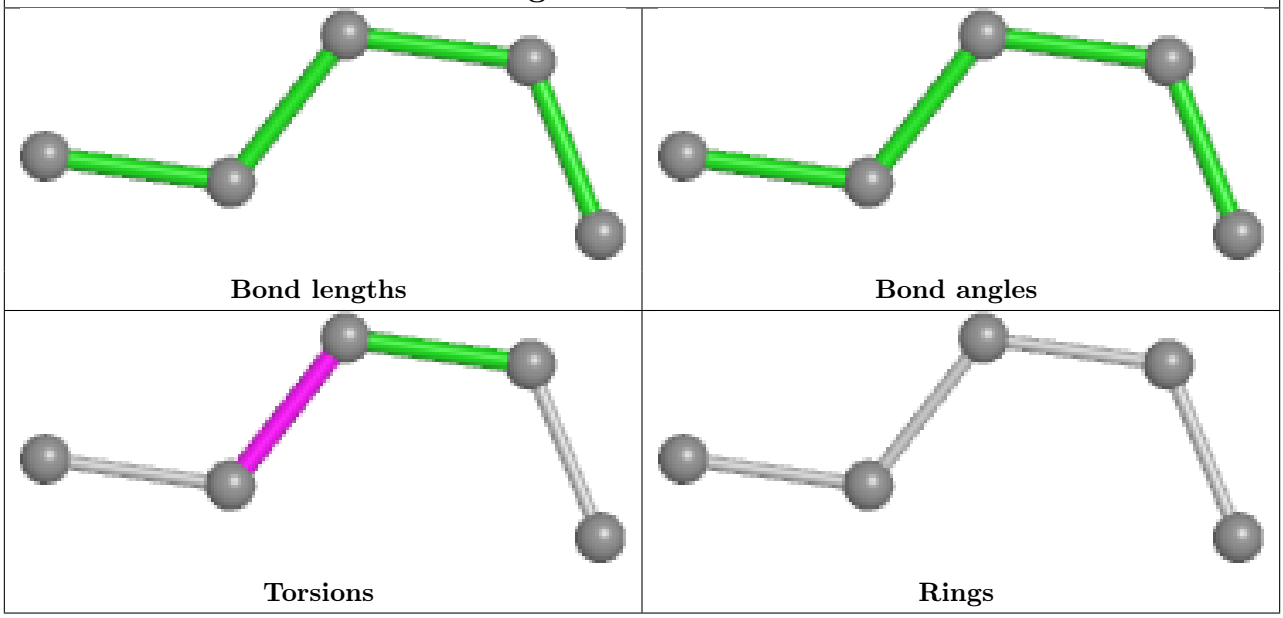
Ligand LFA A 252



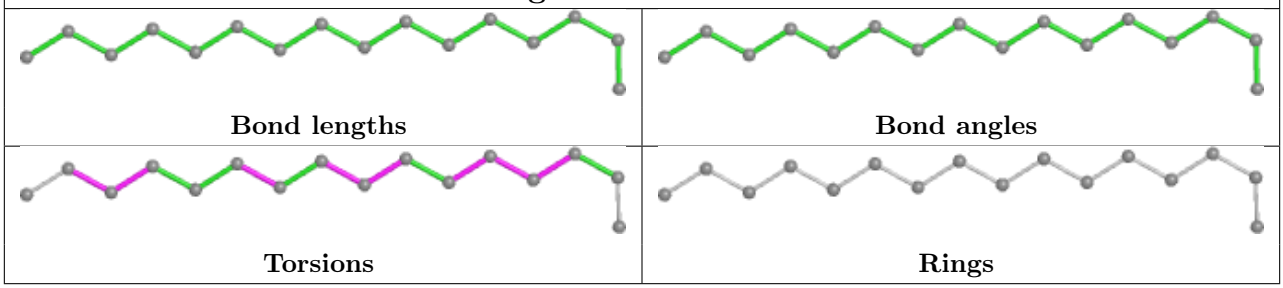
Ligand LFA A 262



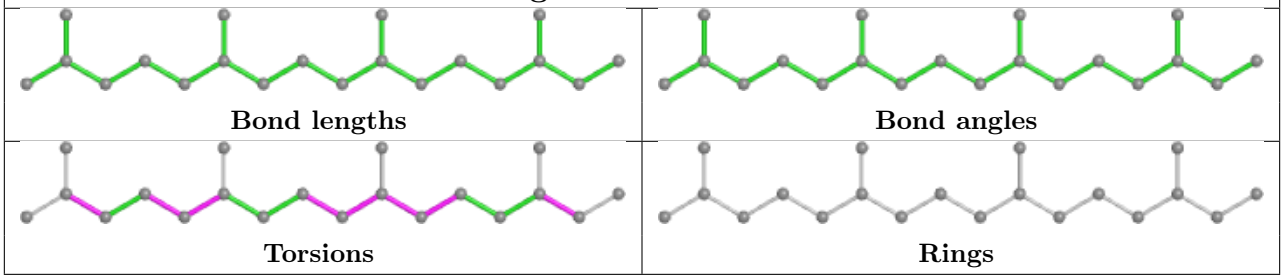
Ligand LFA A 256



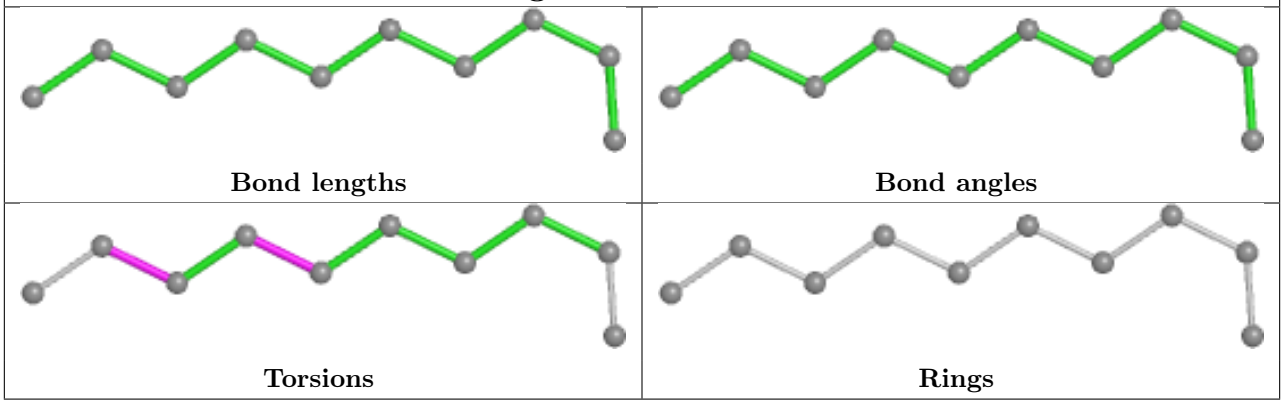
Ligand LFA A 251



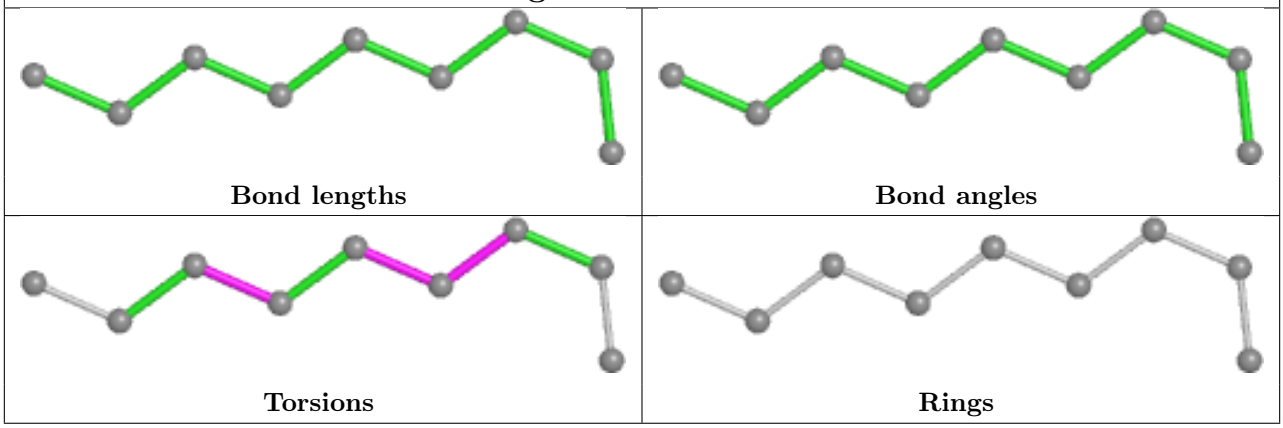
Ligand L2P A 260



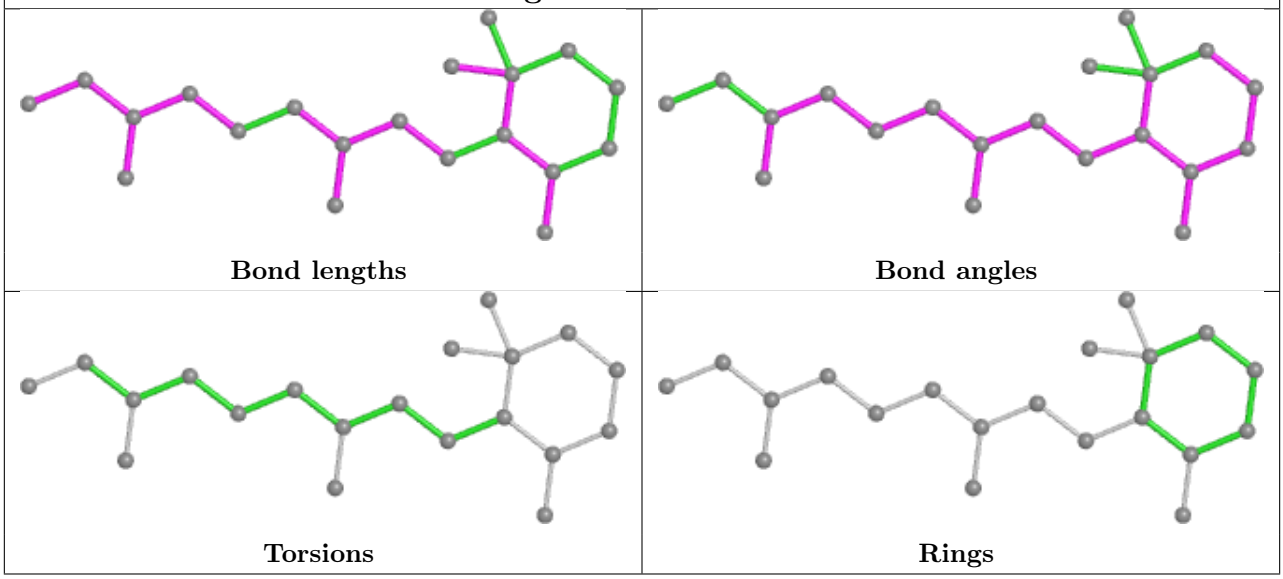
Ligand LFA A 244



Ligand LFA A 250



Ligand RET A 240



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	219/239 (91%)	-0.10	13 (5%)	22	25	13, 21, 45, 66	11 (5%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	ALA	9.4
1	A	31	SER	6.2
1	A	30	GLY	5.3
1	A	2	VAL	4.4
1	A	217	ALA	4.3
1	A	32	GLY	4.3
1	A	27	ARG	3.3
1	A	219	LEU	3.1
1	A	1	MET	3.1
1	A	218	THR	3.0
1	A	28	ASP	2.6
1	A	94	ASP	2.5
1	A	65	GLU	2.5

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.

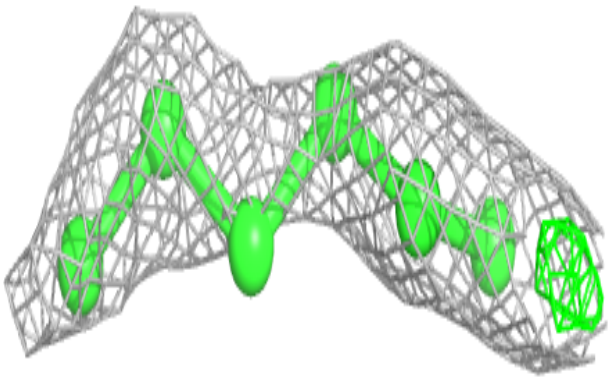
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LFA	A	262	6/20	0.45	0.23	69,69,70,70	0
4	LFA	A	253	6/20	0.49	0.40	67,68,68,68	0
4	LFA	A	263	10/20	0.50	0.22	50,56,58,59	0
4	LFA	A	269	4/20	0.59	0.24	68,68,69,69	0
4	LFA	A	259	4/20	0.60	0.32	64,64,65,65	0
4	LFA	A	266	10/20	0.65	0.25	56,61,61,61	0
4	LFA	A	272	12/20	0.66	0.21	77,78,79,79	0
3	BOG	A	241	20/20	0.68	0.20	37,60,64,65	0
4	LFA	A	271	20/20	0.69	0.20	66,71,75,75	0
5	L2P	A	257	46/46	0.69	0.24	59,69,80,81	0
4	LFA	A	261	14/20	0.72	0.18	58,59,65,66	0
4	LFA	A	255	14/20	0.72	0.22	43,46,50,50	0
4	LFA	A	252	12/20	0.73	0.21	78,79,79,79	0
5	L2P	A	260	20/46	0.74	0.21	59,64,70,70	0
4	LFA	A	268	7/20	0.75	0.16	56,57,57,57	0
4	LFA	A	242	10/20	0.76	0.22	46,50,55,55	0
4	LFA	A	270	4/20	0.76	0.37	59,60,60,60	0
4	LFA	A	265	8/20	0.76	0.22	60,62,63,63	0
4	LFA	A	256	5/20	0.77	0.16	63,63,63,63	0
4	LFA	A	258	6/20	0.78	0.17	70,70,71,71	0
4	LFA	A	251	16/20	0.79	0.14	55,57,58,58	0
4	LFA	A	250	9/20	0.81	0.16	59,59,60,60	0
4	LFA	A	244	10/20	0.81	0.15	54,55,56,56	0
4	LFA	A	245	6/20	0.81	0.16	57,57,58,58	0
4	LFA	A	246	8/20	0.81	0.15	47,49,50,51	0
4	LFA	A	264	9/20	0.82	0.19	69,69,71,71	0
4	LFA	A	267	20/20	0.83	0.19	47,51,57,57	0
4	LFA	A	243	6/20	0.84	0.16	50,52,52,52	0
4	LFA	A	254	16/20	0.84	0.16	45,50,59,60	0
4	LFA	A	249	5/20	0.86	0.21	34,35,37,40	0
4	LFA	A	248	7/20	0.90	0.10	46,46,47,48	0
4	LFA	A	247	5/20	0.93	0.09	46,46,46,46	0
2	RET	A	240	20/21	0.97	0.10	8,12,14,15	0

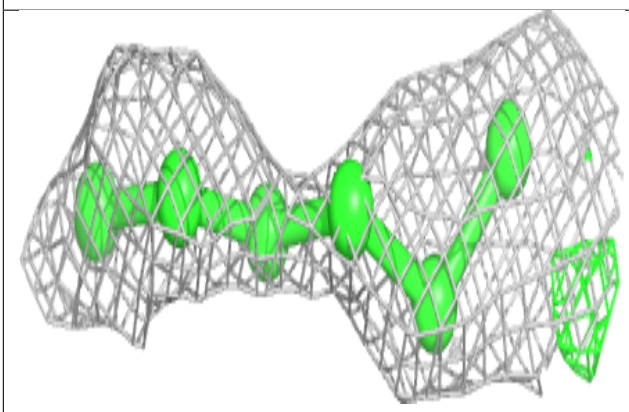
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

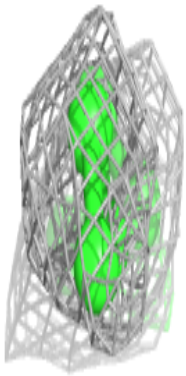
orientation to approximate a three-dimensional view.

Electron density around LFA A 262:

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

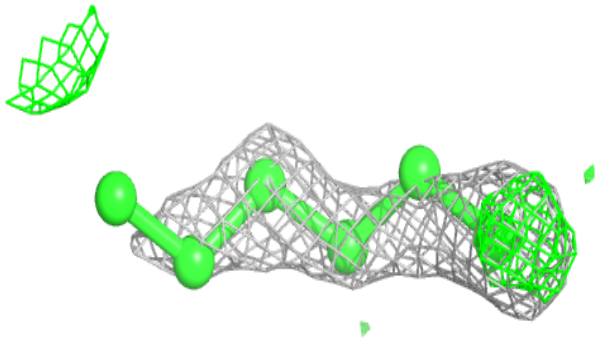


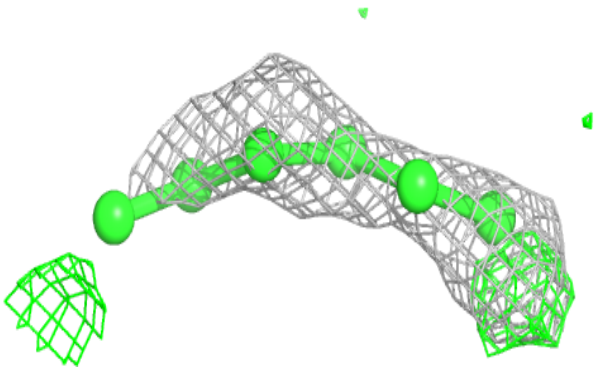


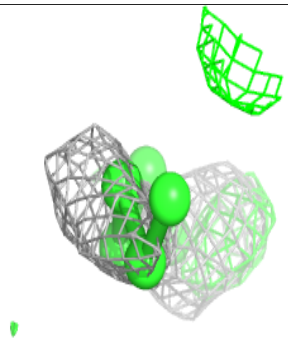


Electron density around LFA A 253:

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

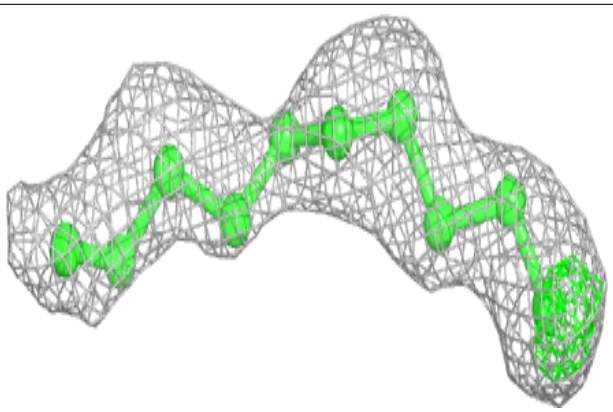


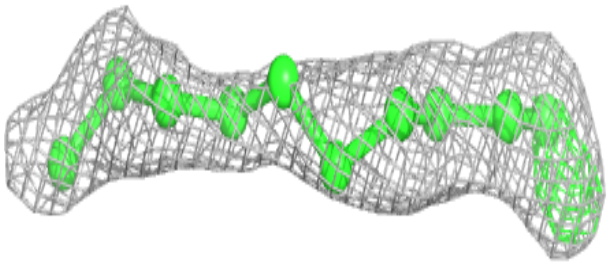


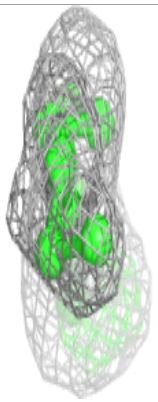


Electron density around LFA A 263:

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

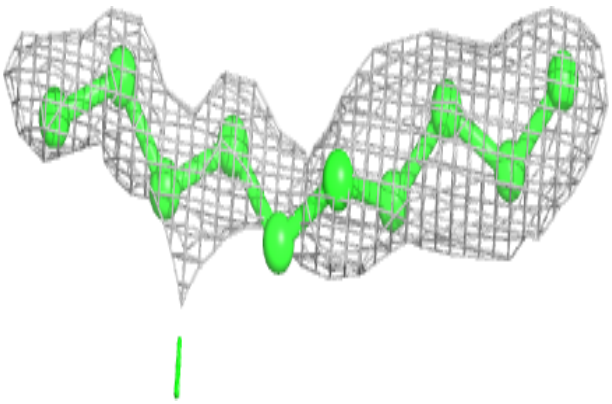


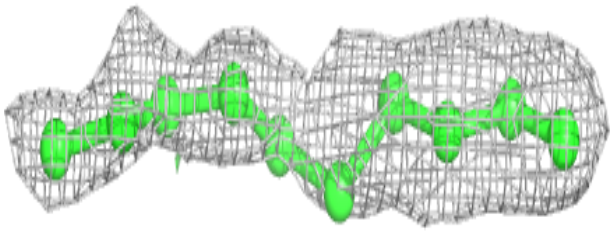


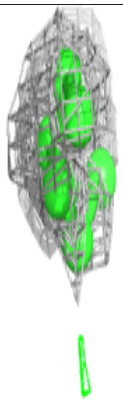


Electron density around LFA A 266:

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

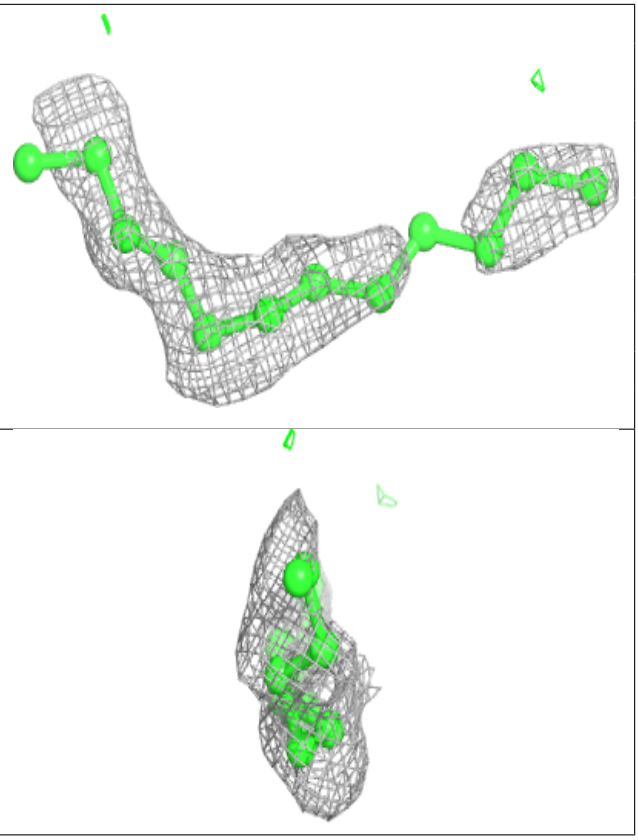


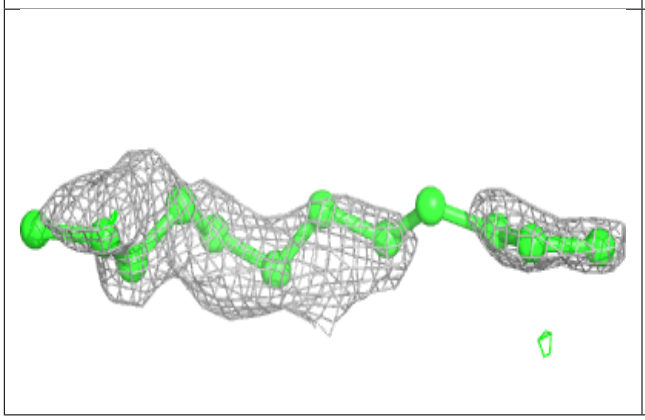




Electron density around LFA A 272:

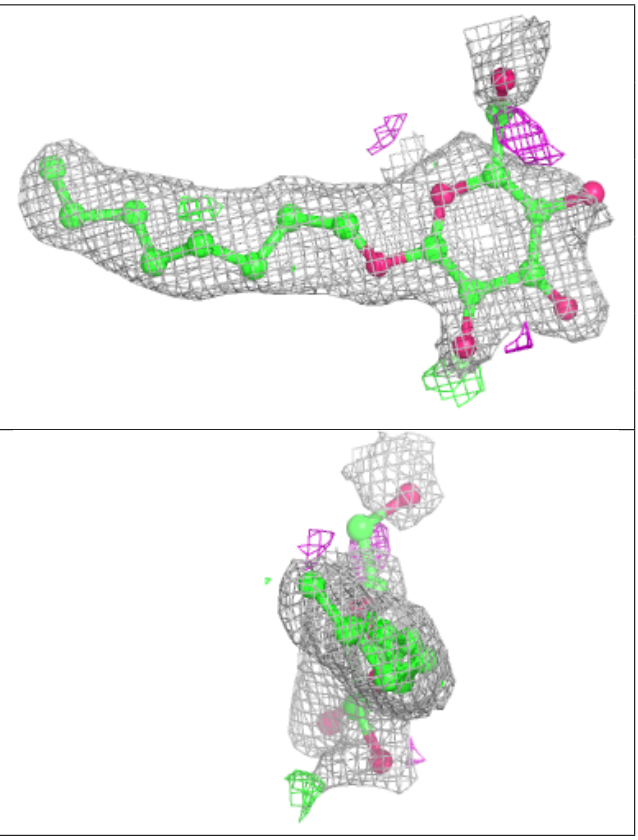
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

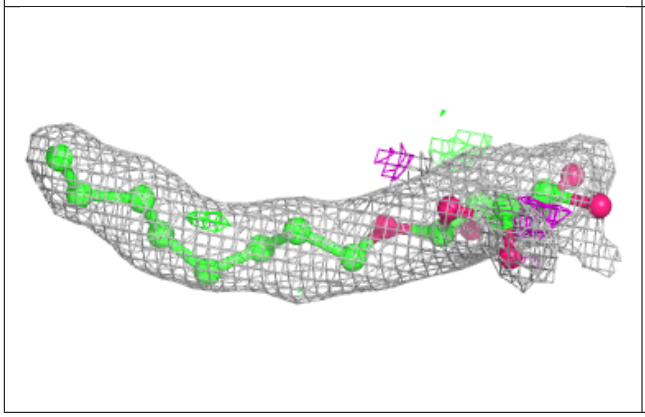




Electron density around BOG A 241:

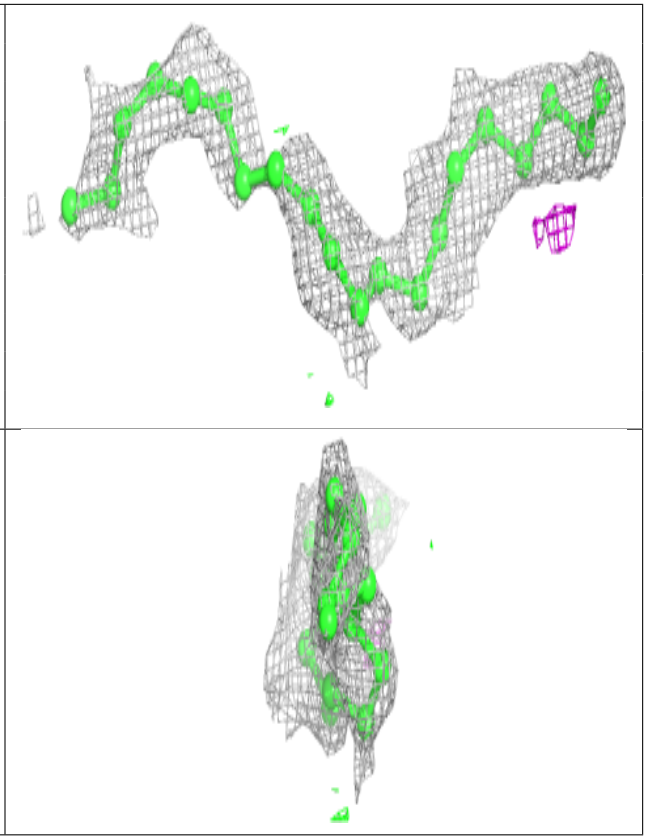
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





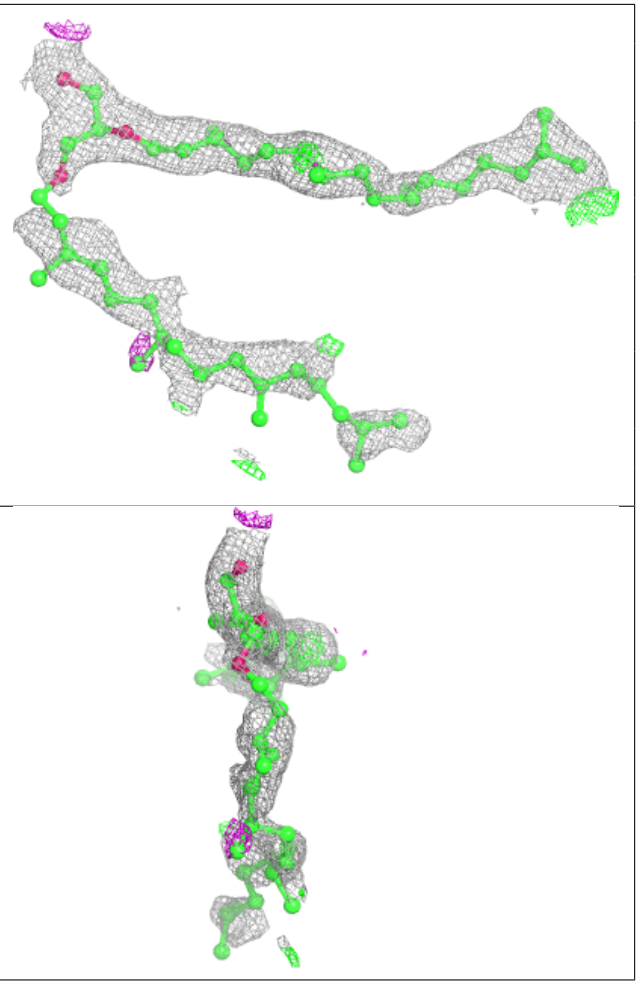
Electron density around LFA A 271:

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



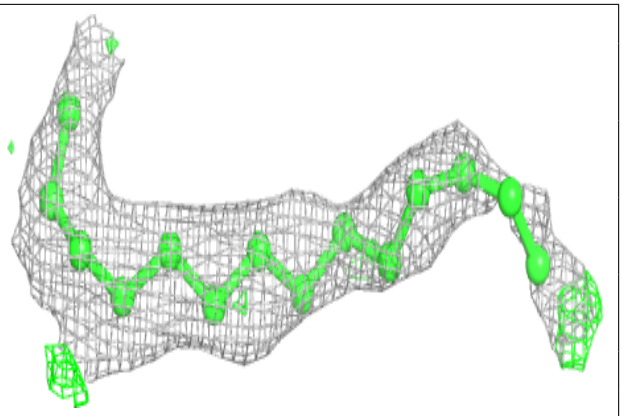
Electron density around L2P A 257:

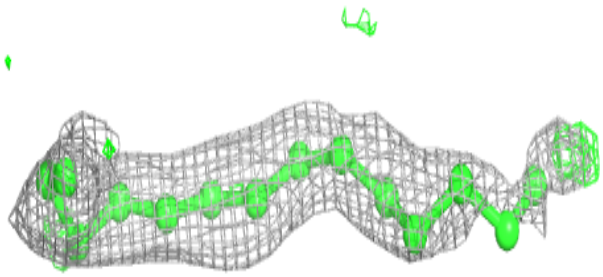
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

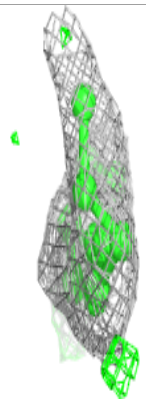


Electron density around LFA A 261:

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

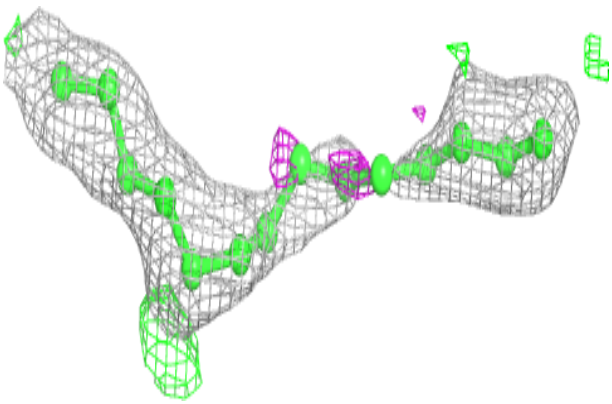


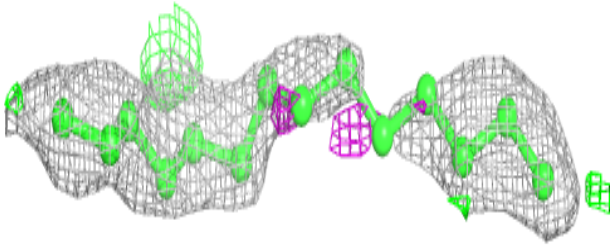


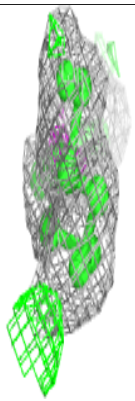


Electron density around LFA A 255:

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

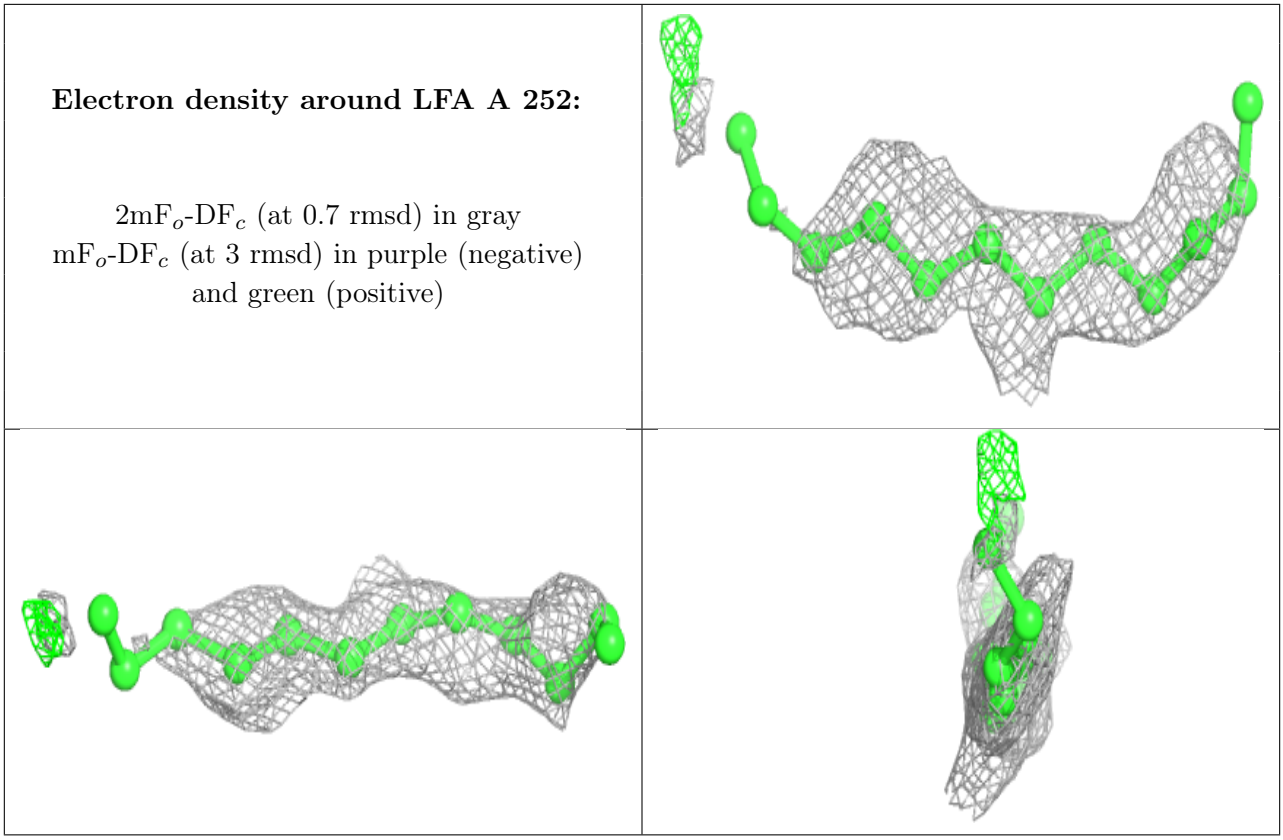






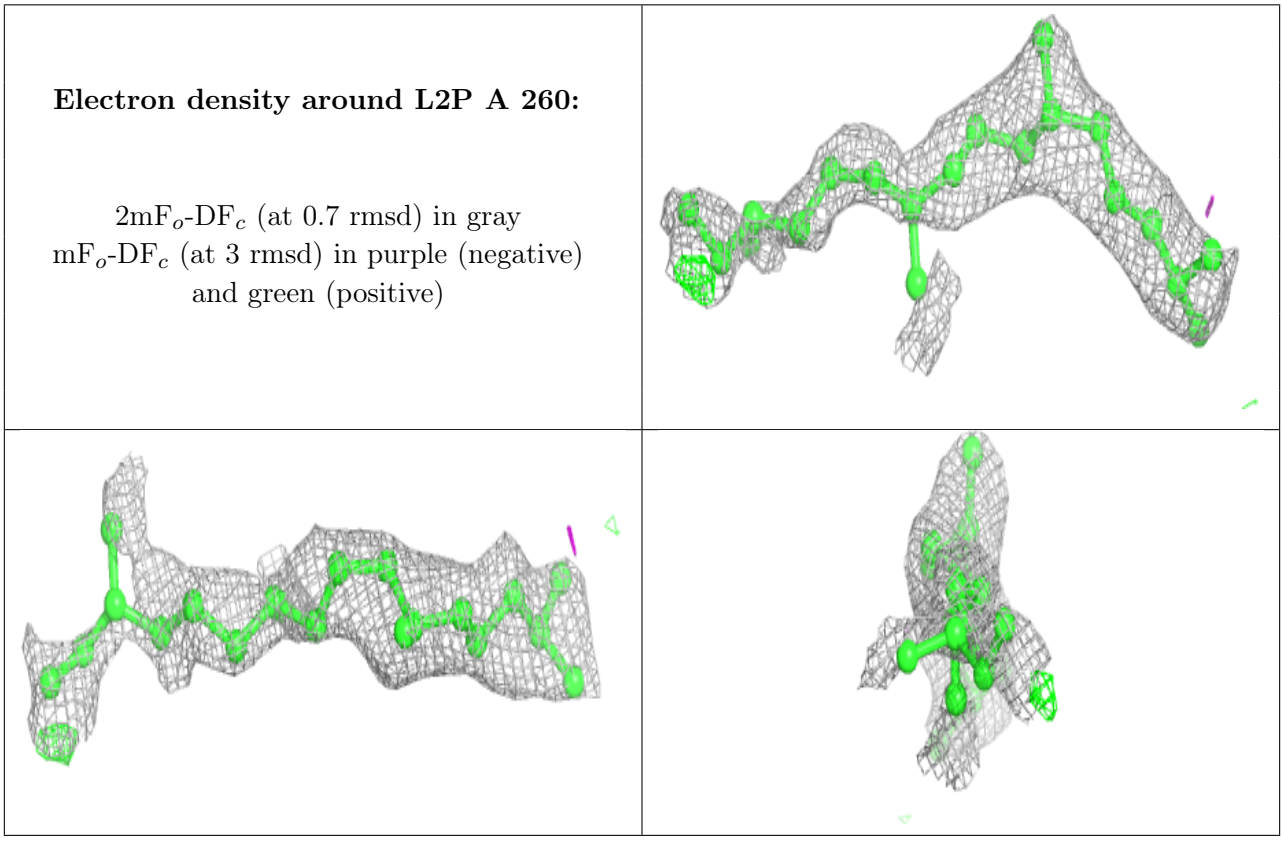
Electron density around LFA A 252:

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



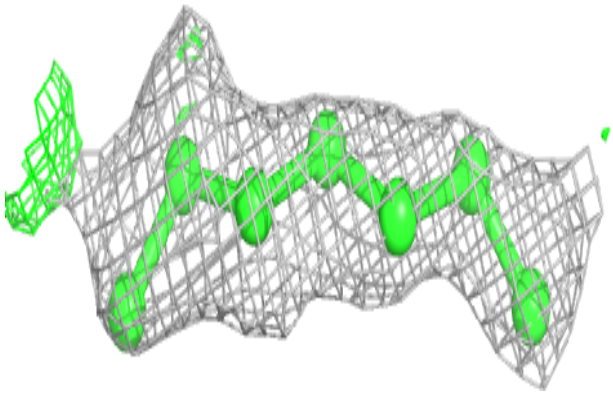
Electron density around L2P A 260:

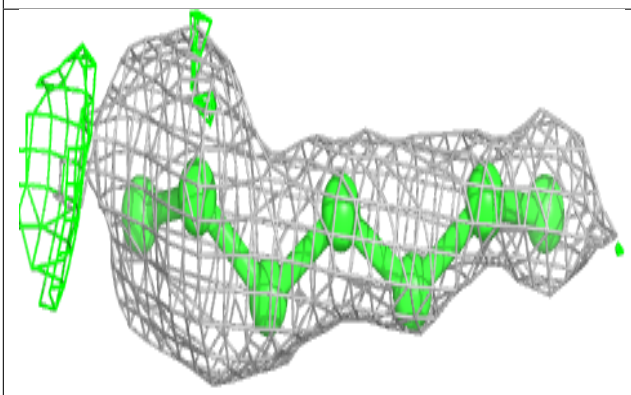
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

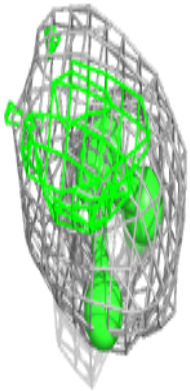


Electron density around LFA A 268:

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

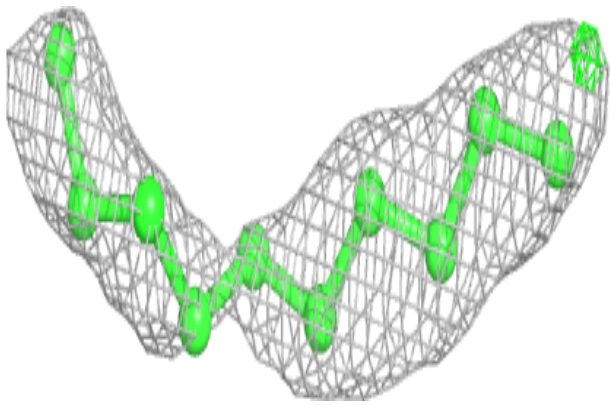


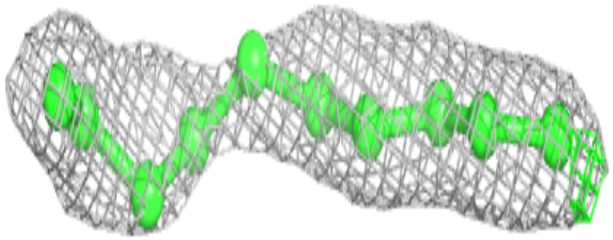


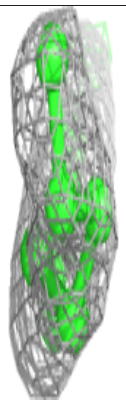


Electron density around LFA A 242:

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

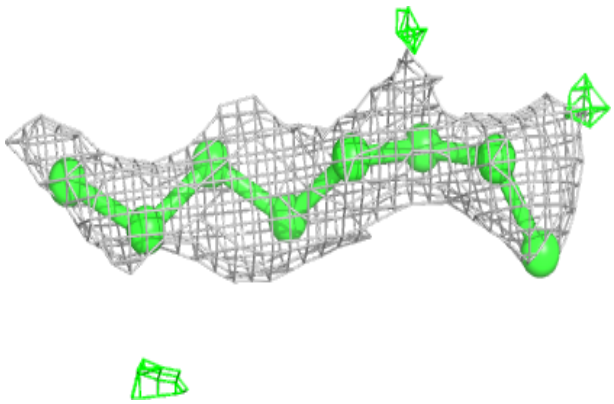


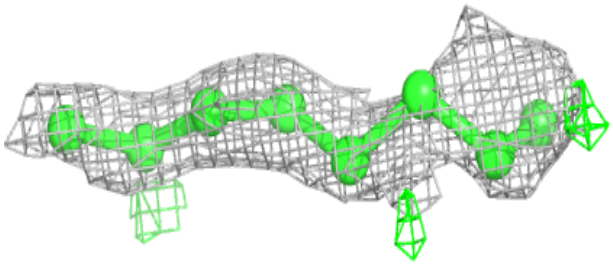


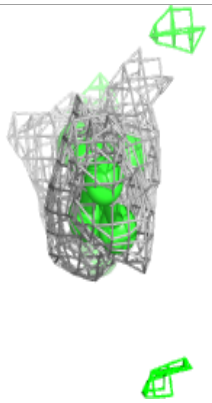


Electron density around LFA A 265:

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

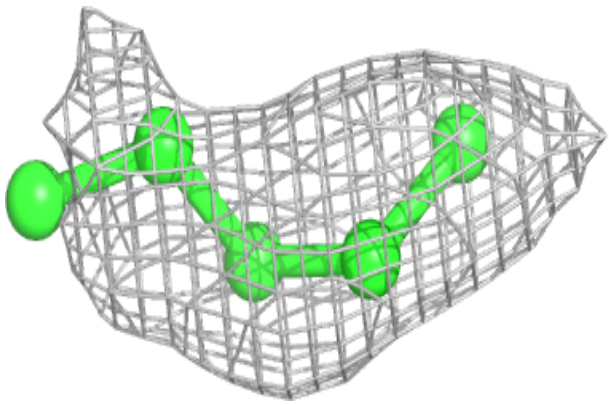


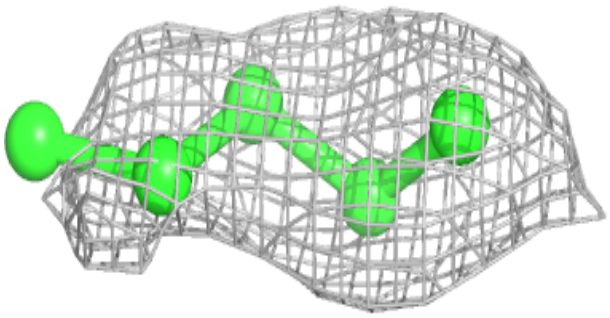


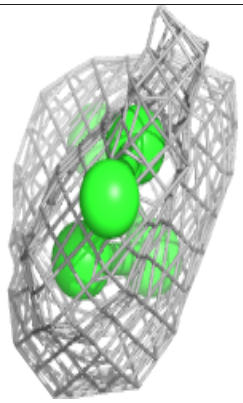


Electron density around LFA A 256:

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

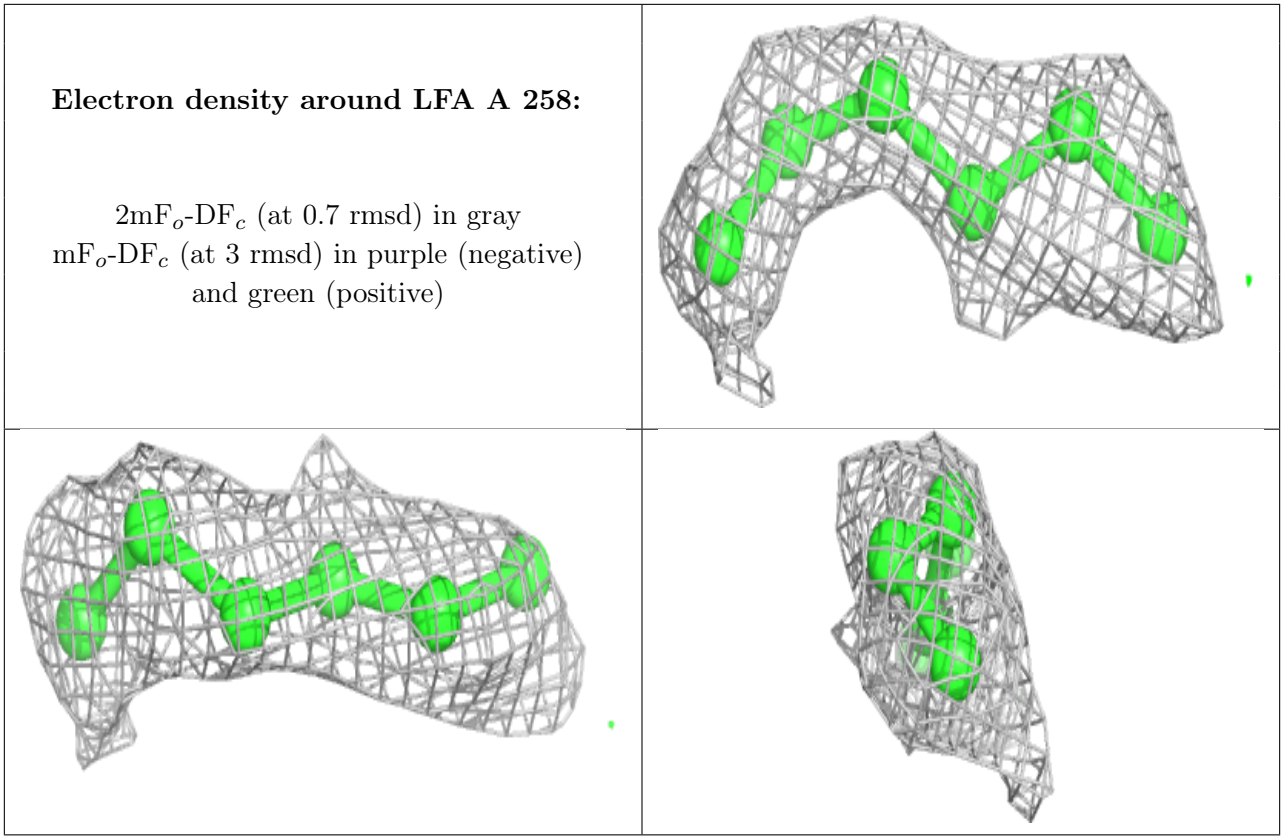






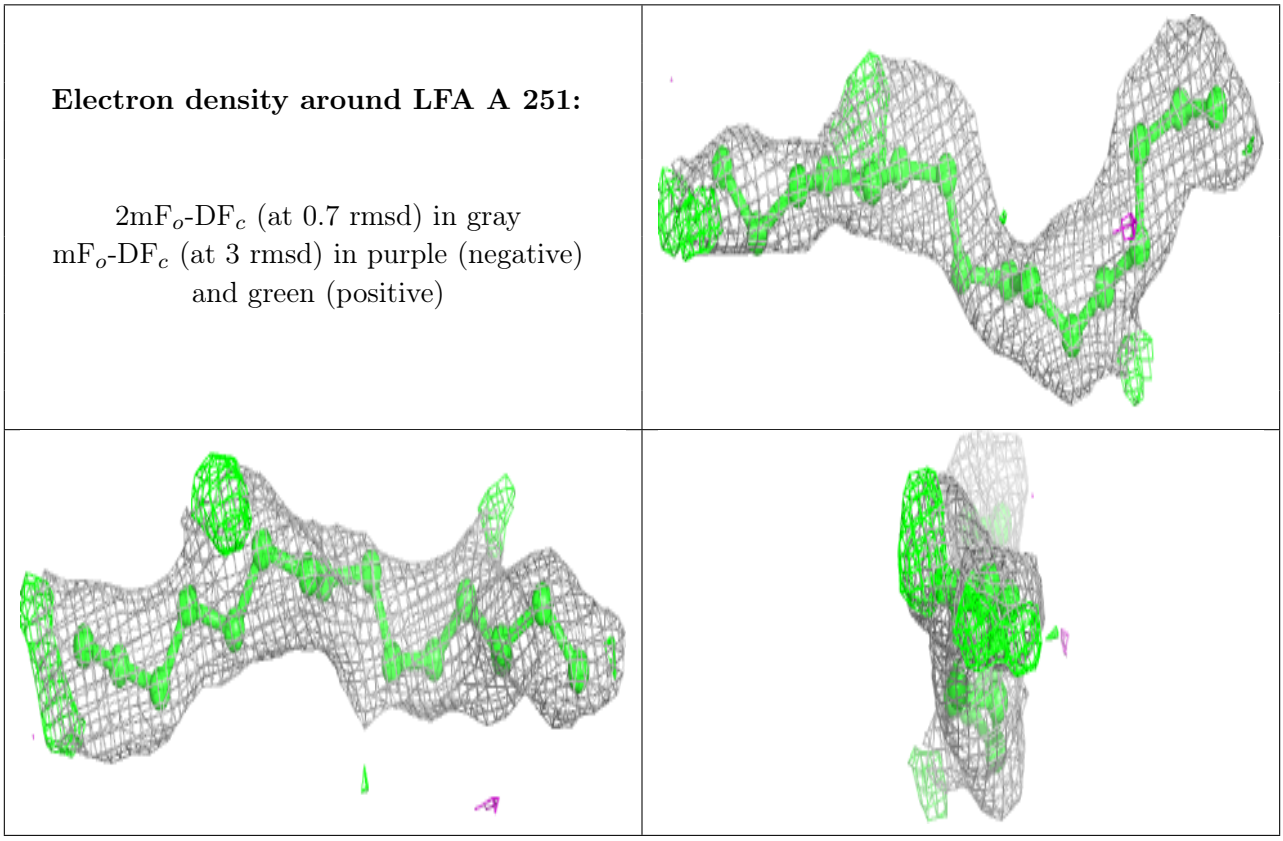
Electron density around LFA A 258:

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



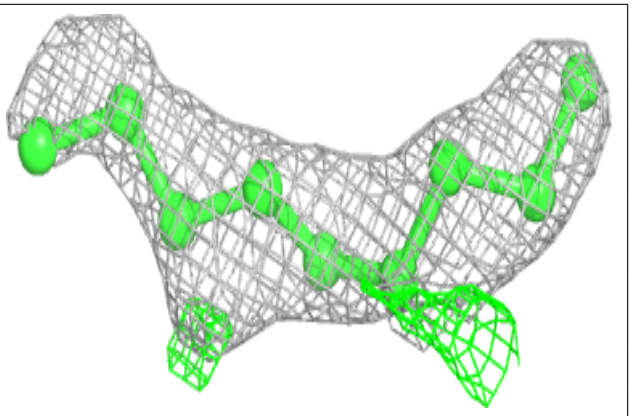
Electron density around LFA A 251:

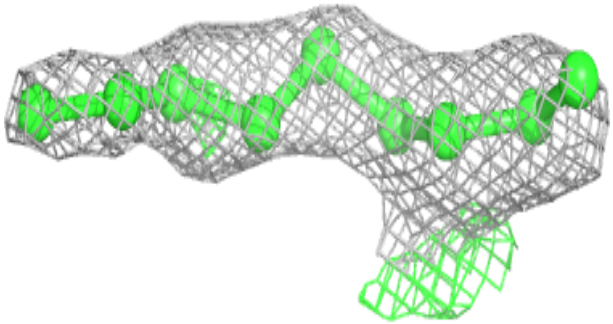
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

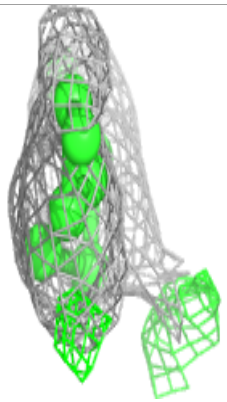


Electron density around LFA A 250:

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

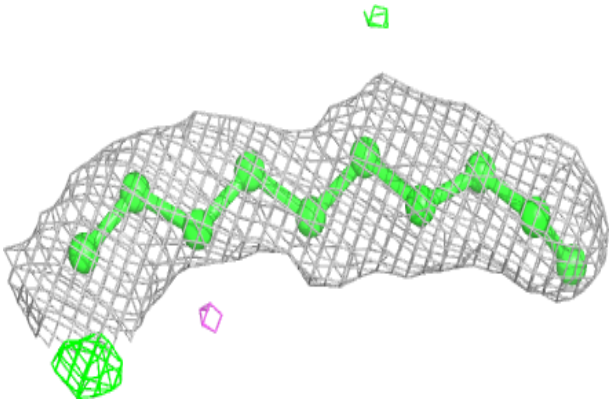


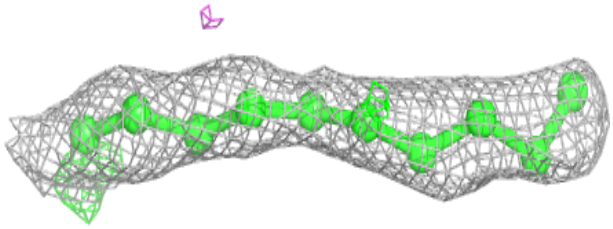


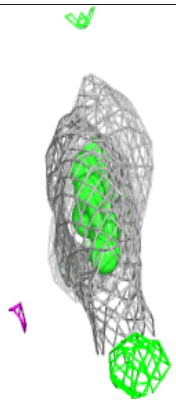


Electron density around LFA A 244:

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

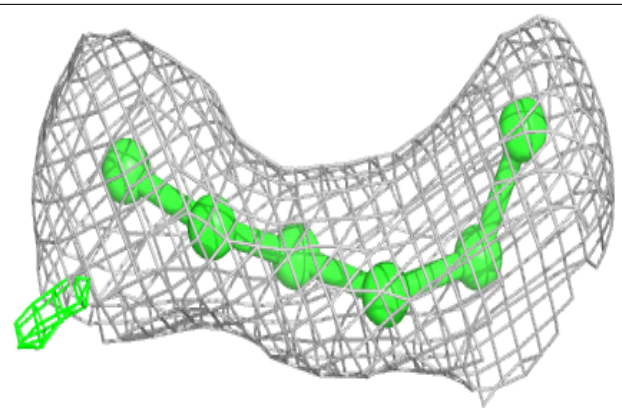


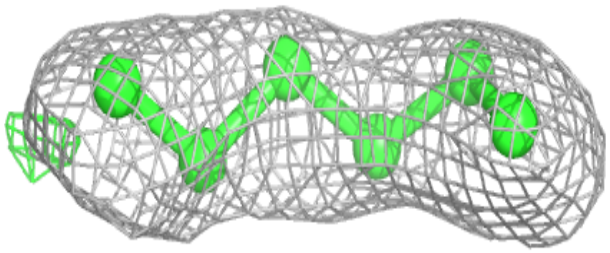


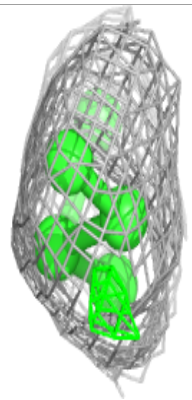


Electron density around LFA A 245:

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

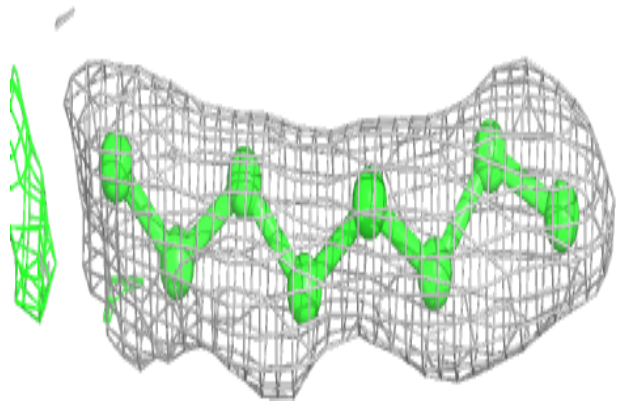


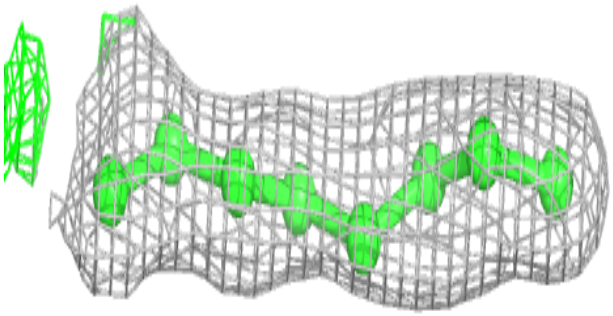


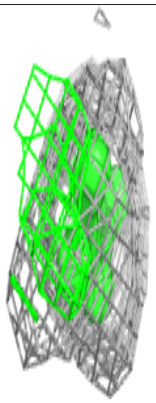


Electron density around LFA A 246:

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

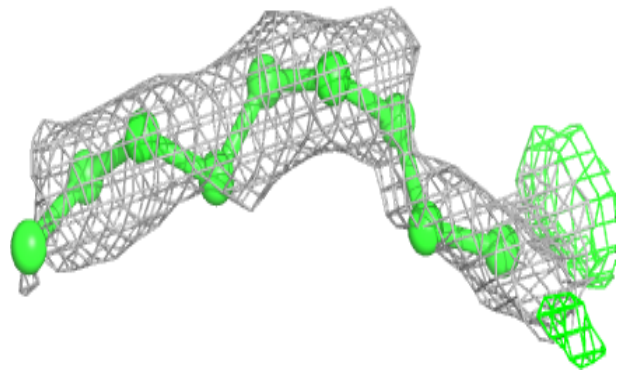


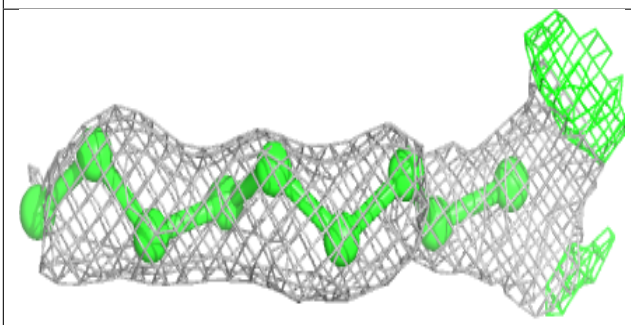


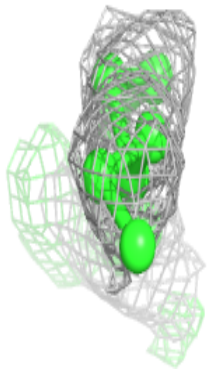


Electron density around LFA A 264:

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

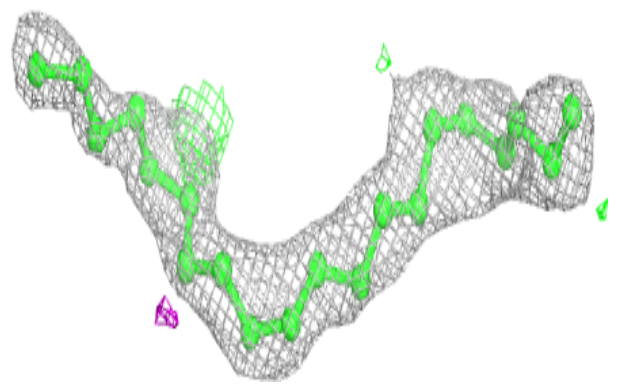


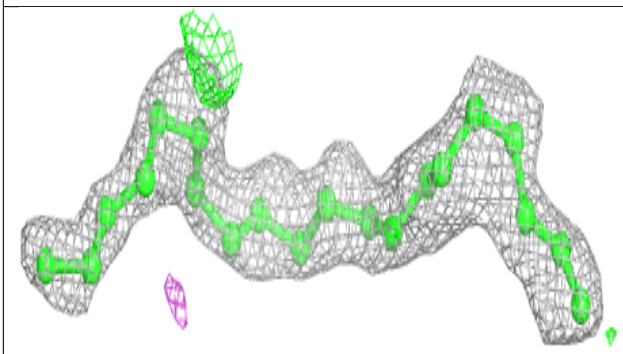


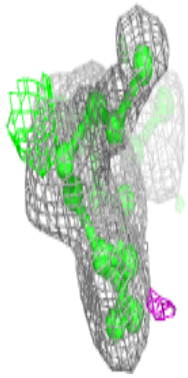


Electron density around LFA A 267:

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

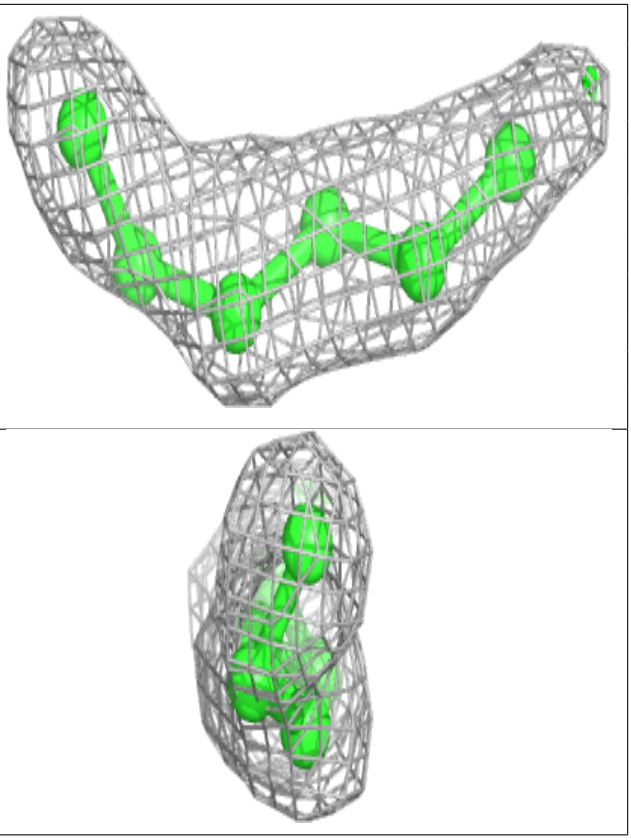


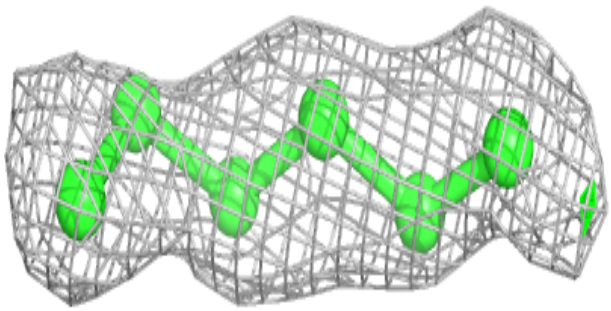




Electron density around LFA A 243:

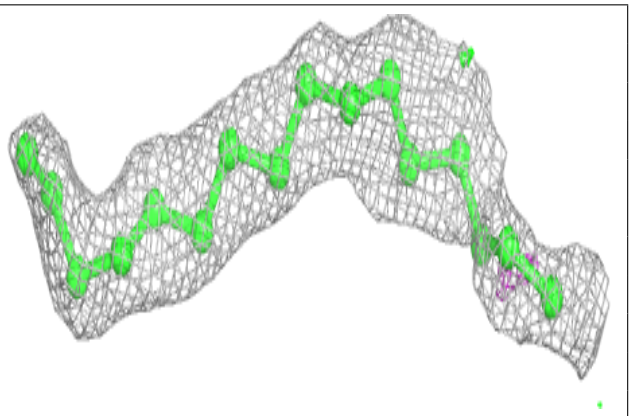
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

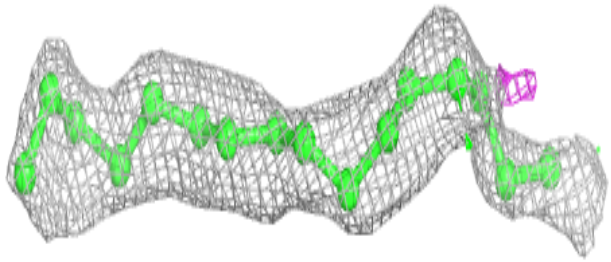


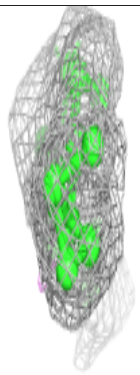


Electron density around LFA A 254:

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

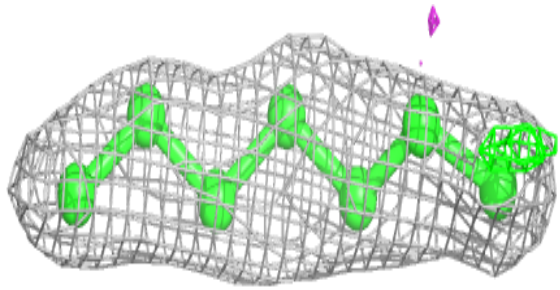


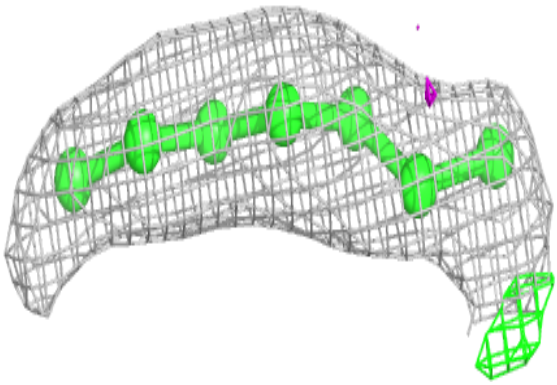


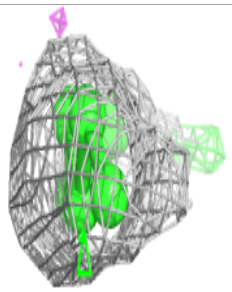


Electron density around LFA A 248:

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

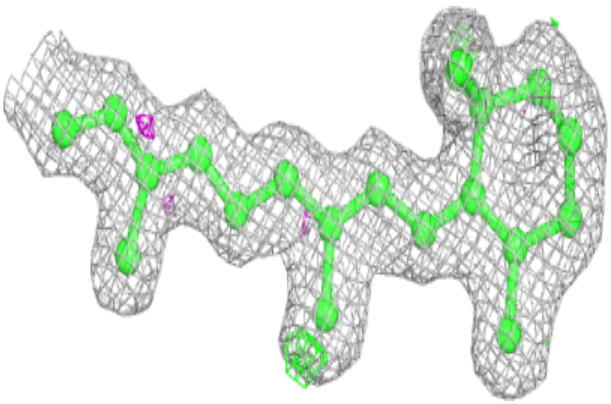


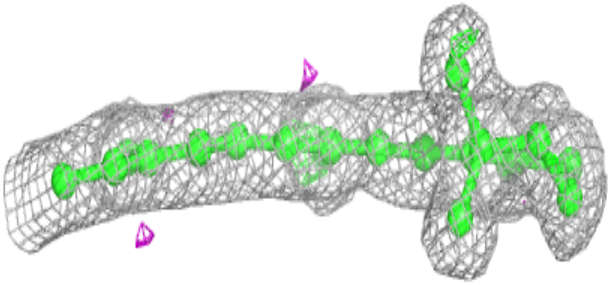


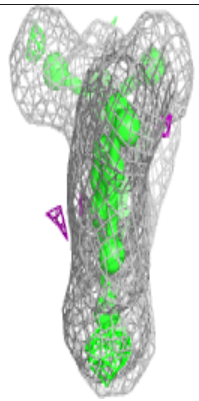


Electron density around RET A 240:

$2mF_o$-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.