Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 11:29 am GMT

PDB ID	:	6YBY
Title	:	Crystal structure of the D116N mutant of the light-driven sodium pump KR2 in the monomeric form, pH 4.6
Authors	:	Kovalev, K.; Gushchin, I.; Gordeliy, V.
Deposited on	:	2020-03-18
Resolution	:	1.80 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 ⓘ 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 ⓘ) were used in the production of this report:

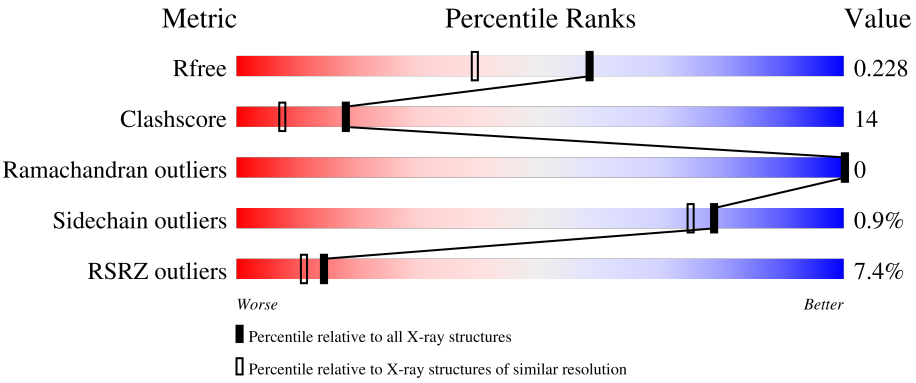
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	274	7% 80% 19%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LFA	A	331	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LFA	A	335	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2689 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 Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	18	0
			2228	1501	331	382	14			

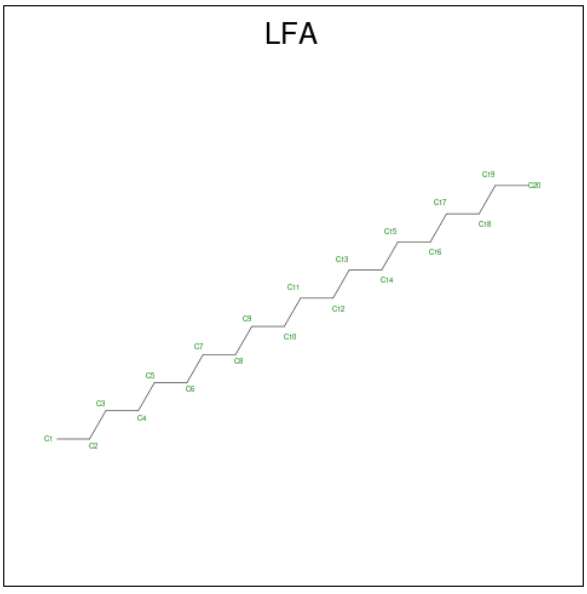
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ASN	ASP	engineered mutation	UNP N0DKS8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 16 16	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 4 4	0	0

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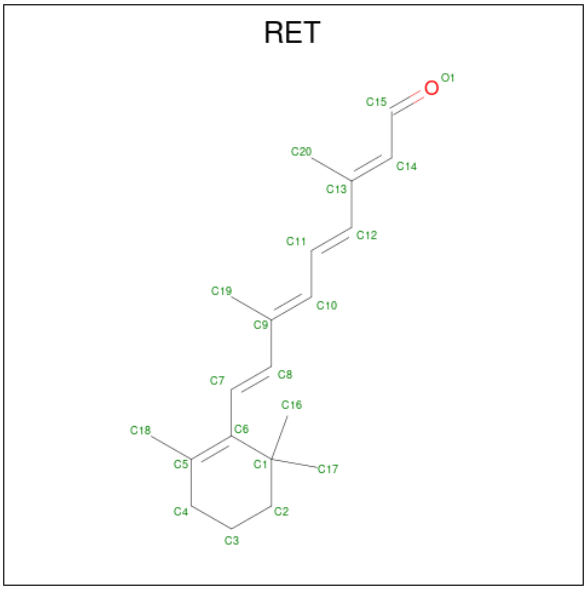
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 3 3	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 10 10	0	0

- Molecule 4 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 40 40	0	1

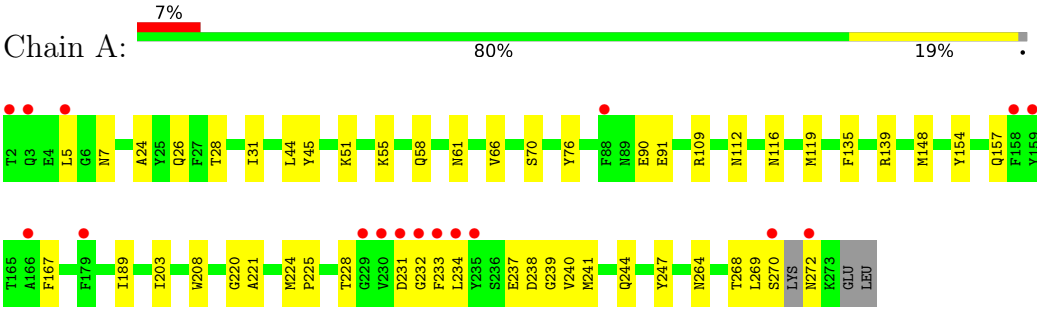
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	151	Total O 152 152	0	1

3 Residue-property plots (i)

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

• Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	40.89Å 83.60Å 233.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 1.80 40.28 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.83-1.80) 99.7 (40.28-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.201 , 0.220 0.212 , 0.228	Depositor DCC
R_{free} test set	1923 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 90.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2689	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, LFA, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.65	0/2337	0.62	0/3171

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2228	0	2246	41	0
2	A	1	0	0	0	0
3	A	268	0	478	26	0
4	A	40	0	54	12	0
5	A	152	0	0	12	1
All	All	2689	0	2778	72	1

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 14.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:305:LFA:H11	3:A:326:LFA:C10	1.69	1.21
3:A:302:LFA:H142	3:A:317:LFA:H101	1.21	1.16
3:A:305:LFA:C1	3:A:326:LFA:C10	2.22	1.16
3:A:318:LFA:H11	3:A:320:LFA:C6	1.95	0.96
1:A:58:GLN:OE1	5:A:401:HOH:O	1.86	0.93
3:A:302:LFA:C14	3:A:317:LFA:H101	2.03	0.89
3:A:305:LFA:H12	3:A:326:LFA:C10	2.02	0.88
3:A:314:LFA:H62	3:A:330:LFA:C8	2.05	0.87
3:A:314:LFA:H62	3:A:330:LFA:H82	1.58	0.84
1:A:90:GLU:CD	5:A:551:HOH:O	2.23	0.77
3:A:318:LFA:C1	3:A:320:LFA:C6	2.62	0.77
3:A:315:LFA:C2	3:A:316:LFA:C6	2.64	0.76
3:A:320:LFA:H12	5:A:421:HOH:O	1.90	0.72
1:A:51:LYS:HB2	5:A:441:HOH:O	1.91	0.70
1:A:154:TYR:O	1:A:157:GLN:HG3	1.94	0.68
4:A:336[A]:RET:H171	4:A:336[A]:RET:H8	1.78	0.66
4:A:336[B]:RET:H171	4:A:336[B]:RET:H8	1.79	0.65
1:A:240:VAL:O	1:A:244[B]:GLN:HG2	1.98	0.62
1:A:264:ASN:O	1:A:268[A]:THR:HG23	2.03	0.59
4:A:336[B]:RET:H8	4:A:336[B]:RET:H161	1.85	0.58
3:A:302:LFA:H142	3:A:317:LFA:C10	2.14	0.58
3:A:314:LFA:H62	3:A:330:LFA:C9	2.34	0.58
4:A:336[A]:RET:H8	4:A:336[A]:RET:H161	1.86	0.57
1:A:28:THR:O	1:A:31:ILE:HG22	2.05	0.56
1:A:91:GLU:CB	5:A:470:HOH:O	2.53	0.56
1:A:189:ILE:HD13	1:A:208:TRP:HB2	1.88	0.56
3:A:308:LFA:C10	3:A:317:LFA:C12	2.84	0.56
3:A:318:LFA:H11	3:A:320:LFA:C5	2.35	0.55
1:A:112:ASN:ND2	1:A:116:ASN:OD1	2.39	0.55
1:A:139:ARG:HH11	3:A:325:LFA:C6	2.21	0.54
1:A:224:MET:HB3	1:A:225:PRO:HD3	1.91	0.53
1:A:55:LYS:HE2	5:A:401:HOH:O	2.08	0.53
1:A:45:TYR:CD1	3:A:302:LFA:H71	2.46	0.51
1:A:270:SER:O	1:A:272:ASN:N	2.44	0.50
4:A:336[B]:RET:H161	4:A:336[B]:RET:C8	2.42	0.50
3:A:318:LFA:H11	3:A:320:LFA:H51	1.93	0.49
4:A:336[A]:RET:H161	4:A:336[A]:RET:C8	2.42	0.49
1:A:231:ASP:N	5:A:410:HOH:O	2.44	0.49
1:A:70[B]:SER:HB3	5:A:406:HOH:O	2.11	0.49
4:A:336[A]:RET:H171	4:A:336[A]:RET:C8	2.41	0.49
1:A:238:ASP:HA	1:A:241[B]:MET:HE2	1.94	0.49
4:A:336[B]:RET:H171	4:A:336[B]:RET:C8	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HD23	5:A:475:HOH:O	2.12	0.48
3:A:323:LFA:C4	5:A:538:HOH:O	2.62	0.47
3:A:311:LFA:H62	3:A:326:LFA:H51	1.95	0.47
1:A:7:ASN:C	1:A:7:ASN:N	2.67	0.47
1:A:163:ASN:HD21	3:A:304:LFA:C10	2.27	0.46
1:A:66:VAL:HG11	1:A:119[B]:MET:HE3	1.96	0.46
1:A:221:ALA:HB3	1:A:247:TYR:CE1	2.49	0.46
1:A:220:GLY:HA3	3:A:330:LFA:H92	1.98	0.46
1:A:76:TYR:CD2	3:A:303:LFA:H32	2.50	0.45
1:A:234:LEU:O	1:A:239:GLY:HA3	2.16	0.45
1:A:61:ASN:H	1:A:61:ASN:HD22	1.65	0.45
1:A:148[B]:MET:HA	1:A:148[B]:MET:CE	2.47	0.44
1:A:109[A]:ARG:HH21	1:A:109[A]:ARG:HG3	1.82	0.44
4:A:336[A]:RET:H7	4:A:336[A]:RET:H181	1.80	0.43
1:A:231:ASP:CA	5:A:410:HOH:O	2.66	0.43
4:A:336[B]:RET:H7	4:A:336[B]:RET:H181	1.80	0.43
1:A:24:ALA:HA	1:A:241[B]:MET:SD	2.59	0.43
1:A:272:ASN:N	1:A:272:ASN:HD22	2.17	0.43
1:A:26:GLN:HA	1:A:26:GLN:OE1	2.19	0.43
1:A:270:SER:CB	5:A:435:HOH:O	2.67	0.42
1:A:66:VAL:CG1	1:A:119[B]:MET:HE3	2.49	0.42
4:A:336[A]:RET:H11	4:A:336[A]:RET:H191	1.92	0.42
1:A:164:LEU:O	1:A:167:PHE:HB3	2.19	0.42
1:A:44[B]:LEU:HD23	3:A:308:LFA:H92	2.02	0.42
1:A:203:ILE:CD1	1:A:268[A]:THR:HG21	2.50	0.42
4:A:336[B]:RET:H11	4:A:336[B]:RET:H191	1.93	0.42
1:A:237:GLU:O	1:A:241[A]:MET:HG3	2.20	0.41
1:A:135:PHE:CE1	3:A:325:LFA:H41	2.56	0.41
1:A:228:THR:O	1:A:232:GLY:HA3	2.21	0.41
3:A:314:LFA:C6	3:A:330:LFA:H82	2.42	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:546:HOH:O	5:A:549:HOH:O[8_555]	2.14	0.06

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	285/274 (104%)	278 (98%)	7 (2%)	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	238/235 (101%)	236 (99%)	2 (1%)	81 78

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

Mol	Chain	Res	Type
1	A	5	LEU
1	A	233	PHE

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	112	ASN
1	A	116	ASN
1	A	206	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	LFA	A	329	-	4,4,19	0.14	0	3,3,18	0.24	0
3	LFA	A	313	-	4,4,19	0.14	0	3,3,18	0.21	0
3	LFA	A	303	-	7,7,19	0.11	0	6,6,18	0.08	0
3	LFA	A	323	-	3,3,19	0.24	0	2,2,18	0.44	0
3	LFA	A	316	-	4,4,19	0.14	0	3,3,18	0.27	0
3	LFA	A	306	-	4,4,19	0.15	0	3,3,18	0.21	0
3	LFA	A	333	-	9,9,19	0.10	0	8,8,18	0.07	0
4	RET	A	336[A]	1	20,20,21	1.56	4 (20%)	27,27,28	1.12	2 (7%)
3	LFA	A	327	-	6,6,19	0.12	0	5,5,18	0.08	0
3	LFA	A	318	-	11,11,19	0.08	0	10,10,18	0.08	0
3	LFA	A	315	-	3,3,19	0.21	0	2,2,18	0.44	0
3	LFA	A	335	-	9,9,19	0.10	0	8,8,18	0.06	0
3	LFA	A	311	-	9,9,19	0.09	0	8,8,18	0.08	0
3	LFA	A	332	-	4,4,19	0.13	0	3,3,18	0.24	0
3	LFA	A	317	-	10,10,19	0.09	0	9,9,18	0.08	0
3	LFA	A	310	-	7,7,19	0.11	0	6,6,18	0.08	0
3	LFA	A	325	-	5,5,19	0.11	0	4,4,18	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LFA	A	321	-	4,4,19	0.16	0	3,3,18	0.21	0
3	LFA	A	314	-	9,9,19	0.09	0	8,8,18	0.07	0
3	LFA	A	328	-	2,2,19	0.03	0	0,1,18	-	-
3	LFA	A	331	-	3,3,19	0.24	0	2,2,18	0.45	0
3	LFA	A	305	-	5,5,19	0.13	0	4,4,18	0.10	0
3	LFA	A	304	-	8,8,19	0.09	0	7,7,18	0.08	0
3	LFA	A	302	-	15,15,19	0.08	0	14,14,18	0.05	0
3	LFA	A	326	-	9,9,19	0.09	0	8,8,18	0.07	0
3	LFA	A	319	-	9,9,19	0.09	0	8,8,18	0.07	0
4	RET	A	336[B]	1	20,20,21	1.60	3 (15%)	27,27,28	1.13	2 (7%)
3	LFA	A	309	-	4,4,19	0.13	0	3,3,18	0.22	0
3	LFA	A	330	-	10,10,19	0.09	0	9,9,18	0.07	0
3	LFA	A	320	-	5,5,19	0.12	0	4,4,18	0.11	0
3	LFA	A	324	-	5,5,19	0.13	0	4,4,18	0.09	0
3	LFA	A	312	-	15,15,19	0.09	0	14,14,18	0.05	0
3	LFA	A	307	-	12,12,19	0.10	0	11,11,18	0.07	0
3	LFA	A	308	-	9,9,19	0.09	0	8,8,18	0.08	0
3	LFA	A	334	-	6,6,19	0.11	0	5,5,18	0.12	0
3	LFA	A	322	-	5,5,19	0.13	0	4,4,18	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
3	LFA	A	329	-	-	1/2/2/17	-
3	LFA	A	313	-	-	1/2/2/17	-
3	LFA	A	303	-	-	3/5/5/17	-
3	LFA	A	323	-	-	0/1/1/17	-
3	LFA	A	316	-	-	0/2/2/17	-
3	LFA	A	306	-	-	1/2/2/17	-
3	LFA	A	333	-	-	7/7/7/17	-
4	RET	A	336[A]	1	-	0/13/30/31	0/1/1/1
3	LFA	A	327	-	-	2/4/4/17	-
3	LFA	A	318	-	-	6/9/9/17	-
3	LFA	A	315	-	-	0/1/1/17	-
3	LFA	A	335	-	-	4/7/7/17	-
3	LFA	A	311	-	-	4/7/7/17	-
3	LFA	A	332	-	-	0/2/2/17	-
3	LFA	A	317	-	-	2/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	310	-	-	3/5/5/17	-
3	LFA	A	325	-	-	1/3/3/17	-
3	LFA	A	321	-	-	0/2/2/17	-
3	LFA	A	314	-	-	5/7/7/17	-
3	LFA	A	331	-	-	0/1/1/17	-
3	LFA	A	305	-	-	0/3/3/17	-
3	LFA	A	304	-	-	3/6/6/17	-
3	LFA	A	302	-	-	7/13/13/17	-
3	LFA	A	326	-	-	4/7/7/17	-
3	LFA	A	319	-	-	4/7/7/17	-
4	RET	A	336[B]	1	-	0/13/30/31	0/1/1/1
3	LFA	A	309	-	-	1/2/2/17	-
3	LFA	A	330	-	-	6/8/8/17	-
3	LFA	A	320	-	-	0/3/3/17	-
3	LFA	A	324	-	-	2/3/3/17	-
3	LFA	A	312	-	-	10/13/13/17	-
3	LFA	A	307	-	-	7/10/10/17	-
3	LFA	A	308	-	-	4/7/7/17	-
3	LFA	A	334	-	-	1/4/4/17	-
3	LFA	A	322	-	-	3/3/3/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	336[B]	RET	C10-C9	3.94	1.41	1.35
4	A	336[A]	RET	C10-C9	3.87	1.40	1.35
4	A	336[B]	RET	C14-C13	3.48	1.36	1.33
4	A	336[A]	RET	C14-C13	3.19	1.36	1.33
4	A	336[A]	RET	C8-C9	-2.46	1.40	1.45
4	A	336[B]	RET	C8-C9	-2.40	1.40	1.45
4	A	336[A]	RET	C12-C13	-2.00	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	336[A]	RET	C19-C9-C10	-4.12	117.15	122.92
4	A	336[B]	RET	C19-C9-C10	-4.08	117.21	122.92
4	A	336[B]	RET	C19-C9-C8	2.21	121.56	118.08
4	A	336[A]	RET	C19-C9-C8	2.20	121.55	118.08

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	330	LFA	C7-C8-C9-C10
3	A	333	LFA	C4-C5-C6-C7
3	A	307	LFA	C9-C10-C11-C12
3	A	314	LFA	C5-C6-C7-C8
3	A	333	LFA	C3-C4-C5-C6
3	A	302	LFA	C11-C12-C13-C14
3	A	314	LFA	C4-C5-C6-C7
3	A	324	LFA	C2-C3-C4-C5
3	A	311	LFA	C5-C6-C7-C8
3	A	335	LFA	C4-C5-C6-C7
3	A	302	LFA	C9-C10-C11-C12
3	A	330	LFA	C6-C7-C8-C9
3	A	307	LFA	C4-C5-C6-C7
3	A	333	LFA	C6-C7-C8-C9
3	A	318	LFA	C11-C10-C9-C8
3	A	333	LFA	C5-C6-C7-C8
3	A	318	LFA	C3-C4-C5-C6
3	A	319	LFA	C3-C4-C5-C6
3	A	326	LFA	C3-C4-C5-C6
3	A	333	LFA	C2-C3-C4-C5
3	A	330	LFA	C1-C2-C3-C4
3	A	329	LFA	C3-C4-C5-C6
3	A	311	LFA	C6-C7-C8-C9
3	A	318	LFA	C6-C7-C8-C9
3	A	317	LFA	C11-C10-C9-C8
3	A	307	LFA	C11-C10-C9-C8
3	A	335	LFA	C5-C6-C7-C8
3	A	304	LFA	C5-C6-C7-C8
3	A	314	LFA	C2-C3-C4-C5
3	A	308	LFA	C3-C4-C5-C6
3	A	326	LFA	C6-C7-C8-C9
3	A	312	LFA	C11-C10-C9-C8
3	A	304	LFA	C6-C7-C8-C9
3	A	314	LFA	C7-C8-C9-C10
3	A	312	LFA	C11-C12-C13-C14
3	A	309	LFA	C1-C2-C3-C4
3	A	311	LFA	C9-C10-C11-C12
3	A	312	LFA	C12-C13-C14-C15
3	A	322	LFA	C1-C2-C3-C4
3	A	308	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	308	LFA	C7-C8-C9-C10
3	A	307	LFA	C6-C7-C8-C9
3	A	317	LFA	C9-C10-C11-C12
3	A	312	LFA	C6-C7-C8-C9
3	A	318	LFA	C7-C8-C9-C10
3	A	333	LFA	C7-C8-C9-C10
3	A	310	LFA	C1-C2-C3-C4
3	A	307	LFA	C3-C4-C5-C6
3	A	304	LFA	C7-C8-C9-C10
3	A	326	LFA	C5-C6-C7-C8
3	A	312	LFA	C7-C8-C9-C10
3	A	314	LFA	C6-C7-C8-C9
3	A	312	LFA	C2-C3-C4-C5
3	A	324	LFA	C1-C2-C3-C4
3	A	326	LFA	C7-C8-C9-C10
3	A	303	LFA	C5-C6-C7-C8
3	A	312	LFA	C4-C5-C6-C7
3	A	327	LFA	C1-C2-C3-C4
3	A	302	LFA	C10-C11-C12-C13
3	A	325	LFA	C3-C4-C5-C6
3	A	312	LFA	C13-C14-C15-C16
3	A	322	LFA	C3-C4-C5-C6
3	A	303	LFA	C1-C2-C3-C4
3	A	302	LFA	C11-C10-C9-C8
3	A	312	LFA	C10-C11-C12-C13
3	A	319	LFA	C1-C2-C3-C4
3	A	330	LFA	C4-C5-C6-C7
3	A	310	LFA	C2-C3-C4-C5
3	A	318	LFA	C9-C10-C11-C12
3	A	312	LFA	C1-C2-C3-C4
3	A	318	LFA	C2-C3-C4-C5
3	A	333	LFA	C1-C2-C3-C4
3	A	335	LFA	C6-C7-C8-C9
3	A	313	LFA	C2-C3-C4-C5
3	A	319	LFA	C6-C7-C8-C9
3	A	303	LFA	C2-C3-C4-C5
3	A	308	LFA	C6-C7-C8-C9
3	A	327	LFA	C3-C4-C5-C6
3	A	307	LFA	C7-C8-C9-C10
3	A	311	LFA	C3-C4-C5-C6
3	A	319	LFA	C7-C8-C9-C10
3	A	330	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	307	LFA	C2-C3-C4-C5
3	A	302	LFA	C3-C4-C5-C6
3	A	322	LFA	C2-C3-C4-C5
3	A	335	LFA	C7-C8-C9-C10
3	A	310	LFA	C3-C4-C5-C6
3	A	302	LFA	C2-C3-C4-C5
3	A	306	LFA	C2-C3-C4-C5
3	A	302	LFA	C1-C2-C3-C4
3	A	330	LFA	C11-C10-C9-C8
3	A	334	LFA	C6-C7-C8-C9

There are no ring outliers.

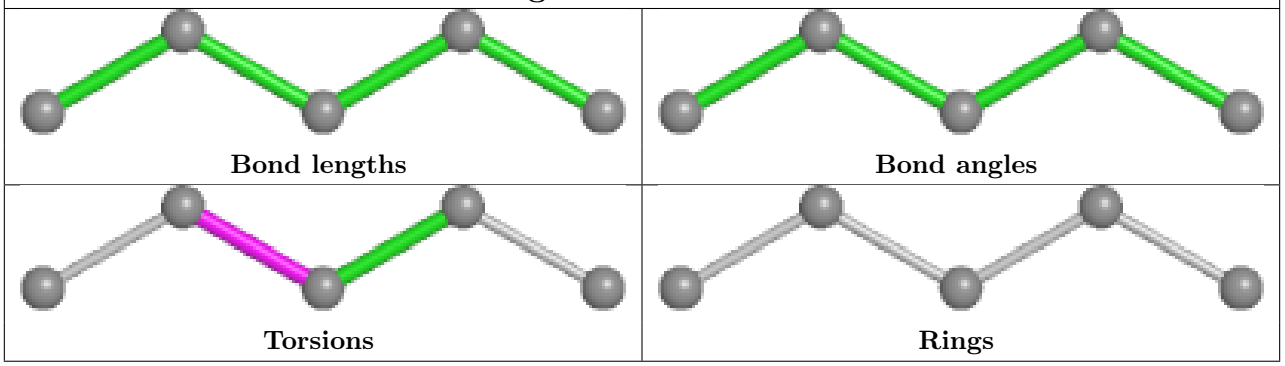
18 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	LFA	1	0
3	A	323	LFA	1	0
3	A	316	LFA	1	0
4	A	336[A]	RET	6	0
3	A	318	LFA	4	0
3	A	315	LFA	1	0
3	A	311	LFA	1	0
3	A	317	LFA	4	0
3	A	325	LFA	2	0
3	A	314	LFA	4	0
3	A	305	LFA	3	0
3	A	304	LFA	1	0
3	A	302	LFA	4	0
3	A	326	LFA	4	0
4	A	336[B]	RET	6	0
3	A	330	LFA	5	0
3	A	320	LFA	5	0
3	A	308	LFA	2	0

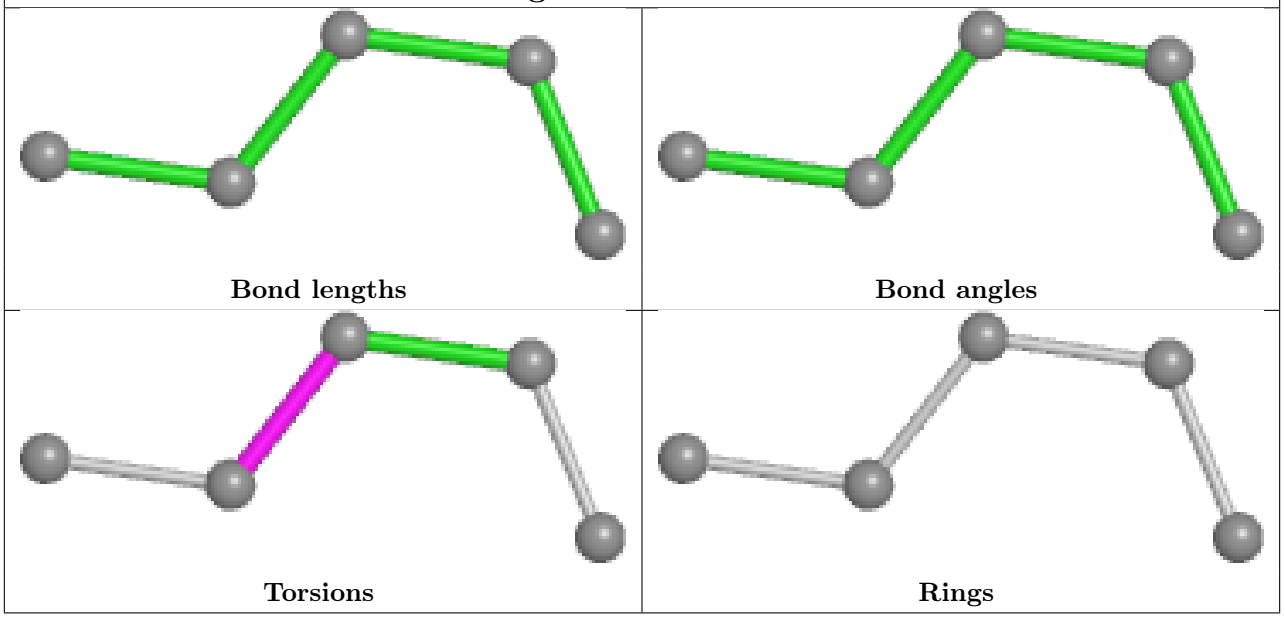
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

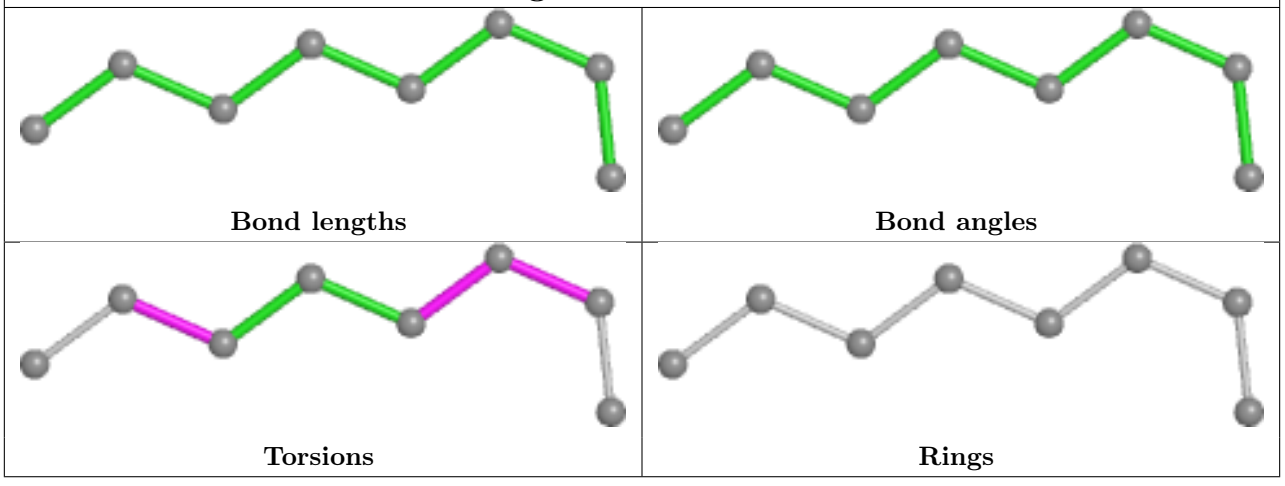
Ligand LFA A 329



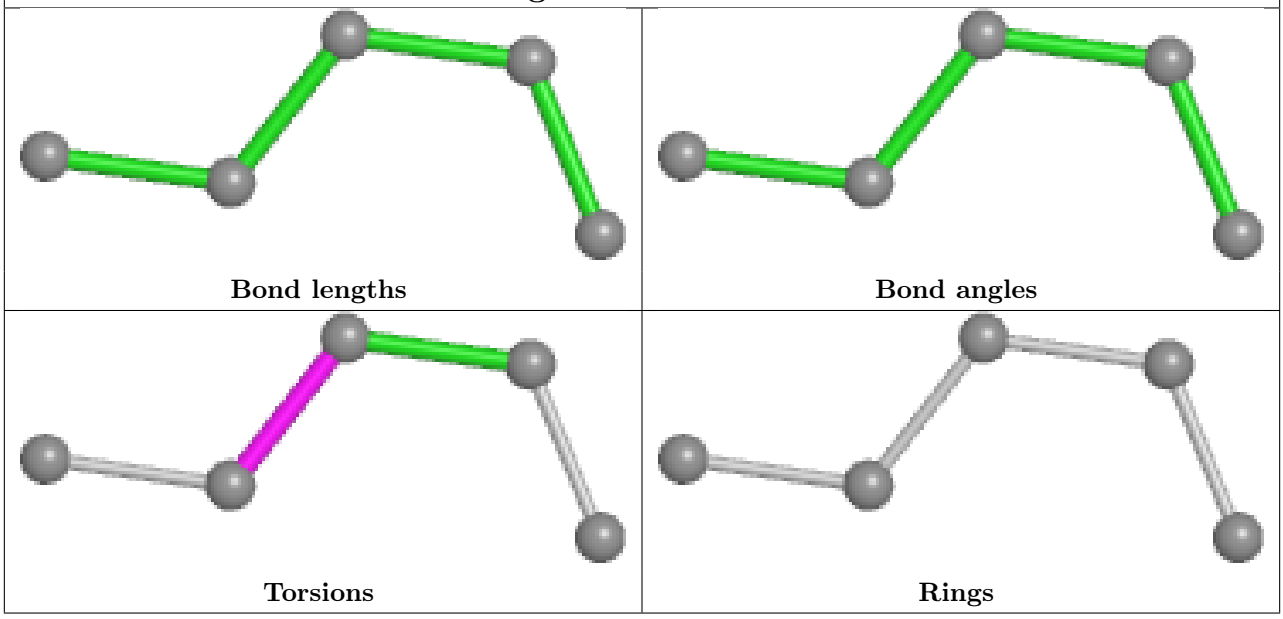
Ligand LFA A 313



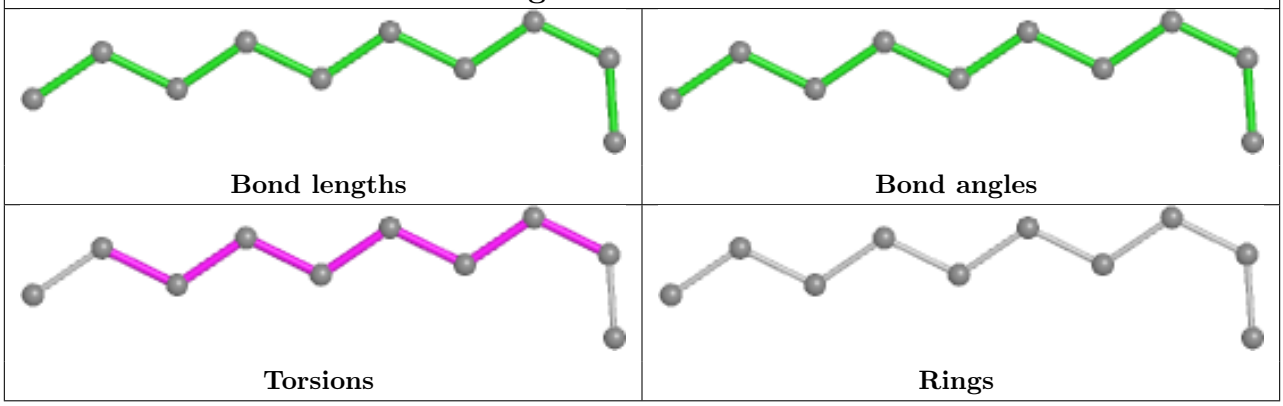
Ligand LFA A 303



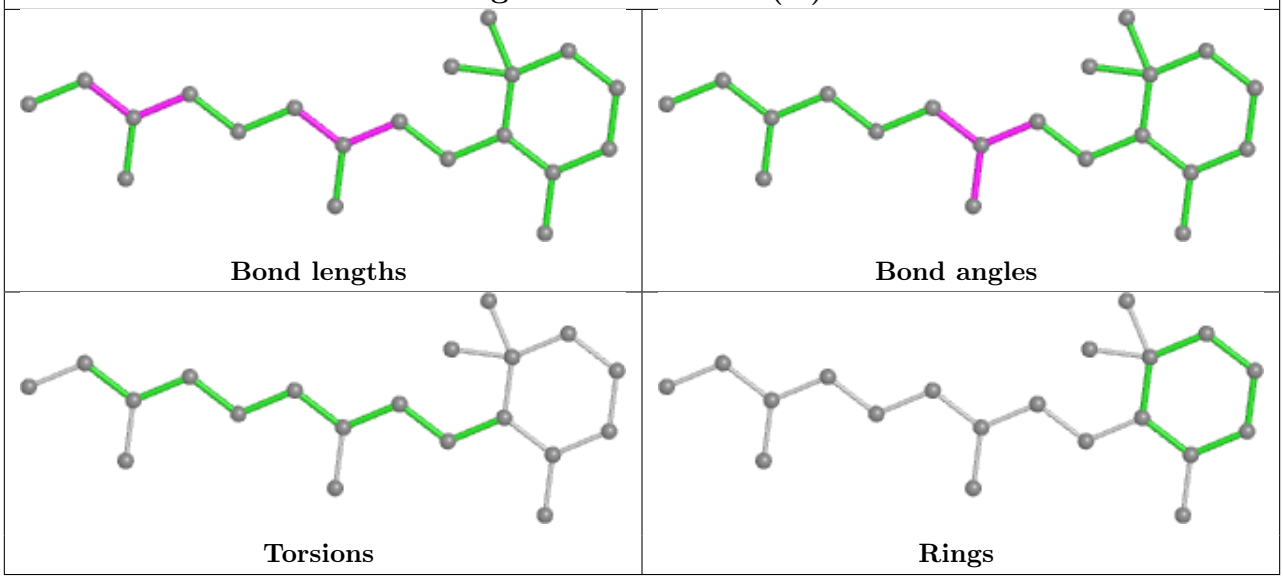
Ligand LFA A 306



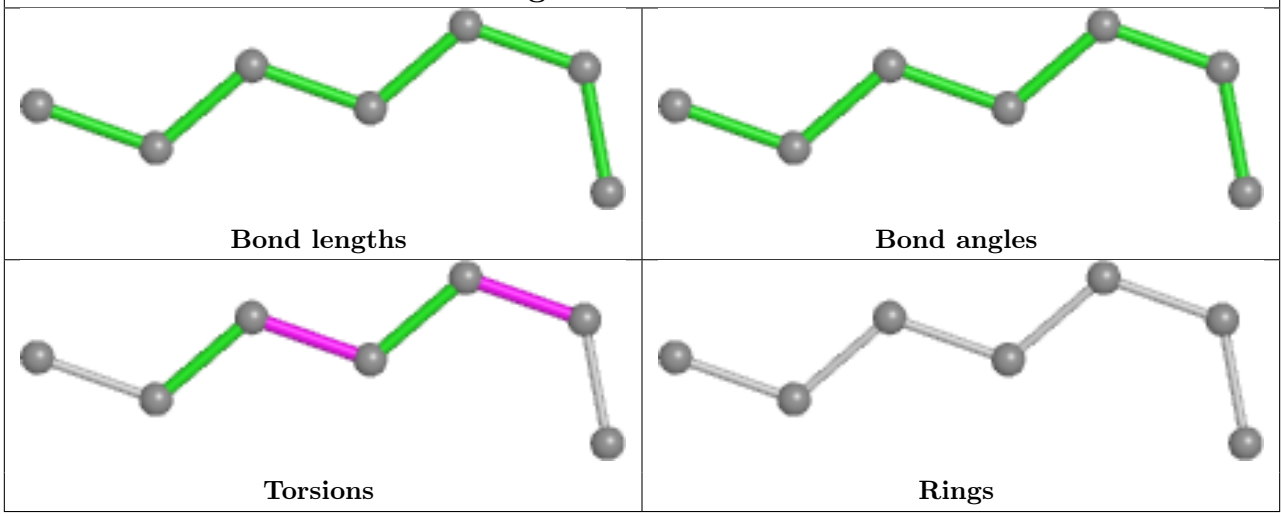
Ligand LFA A 333



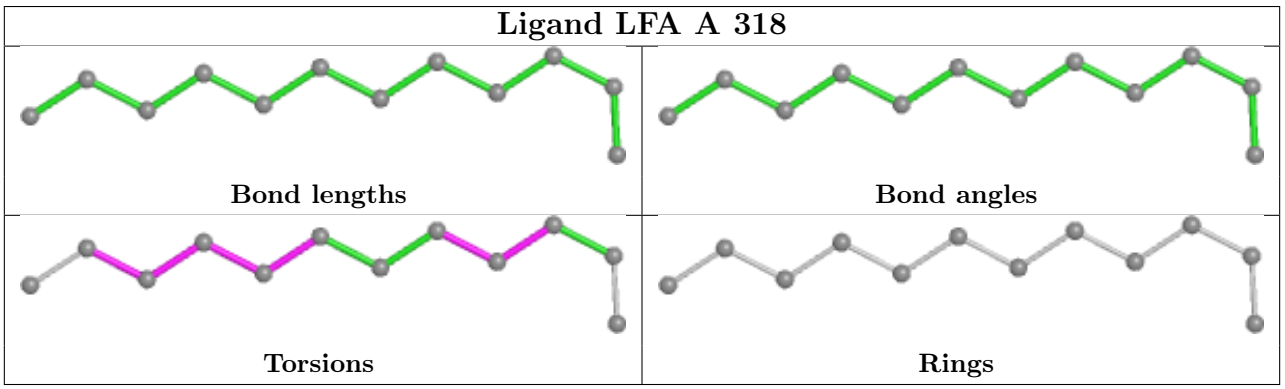
Ligand RET A 336 (A)



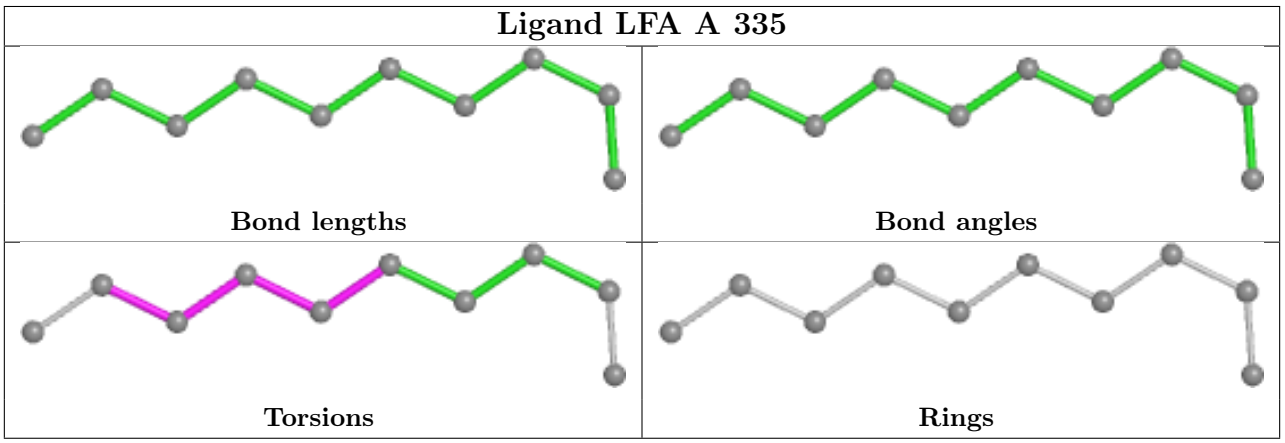
Ligand LFA A 327



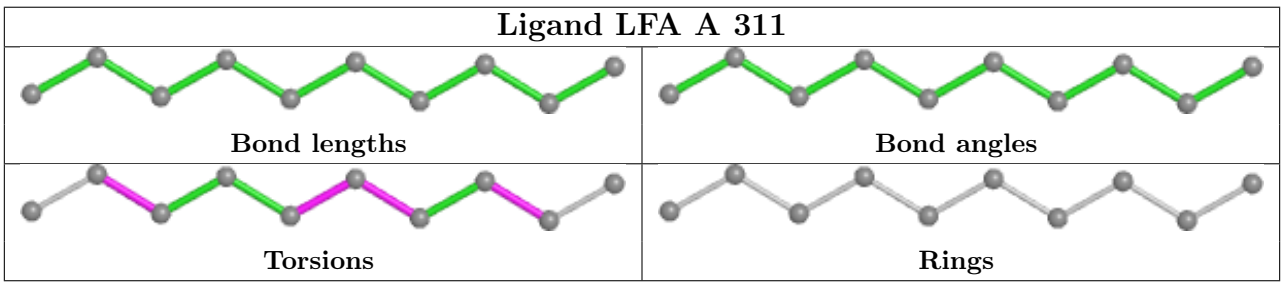
Ligand LFA A 318



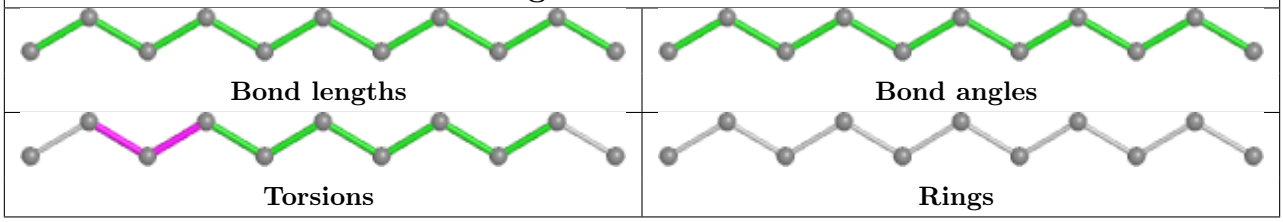
Ligand LFA A 335



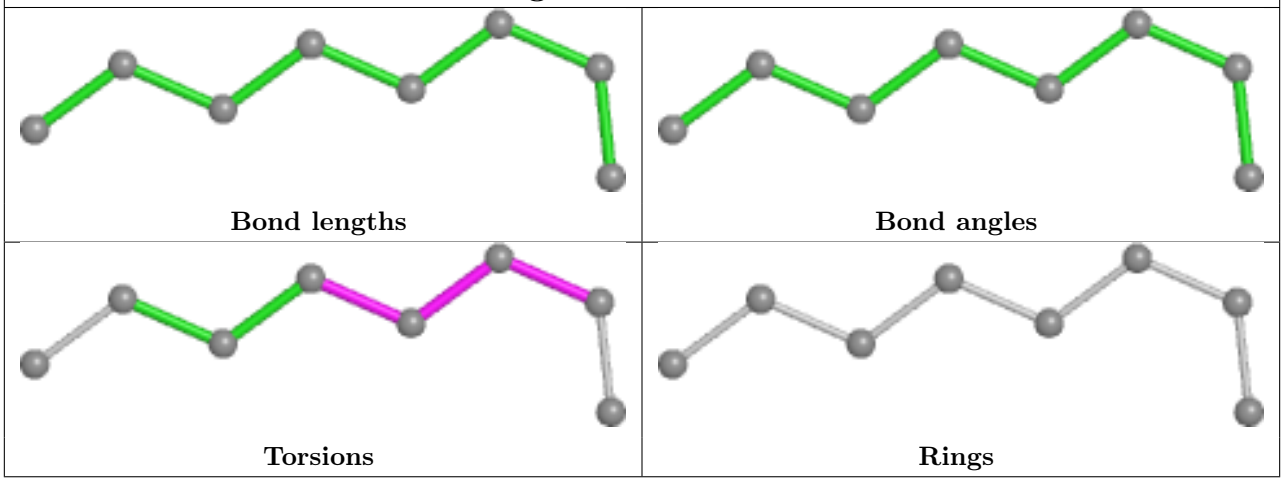
Ligand LFA A 311



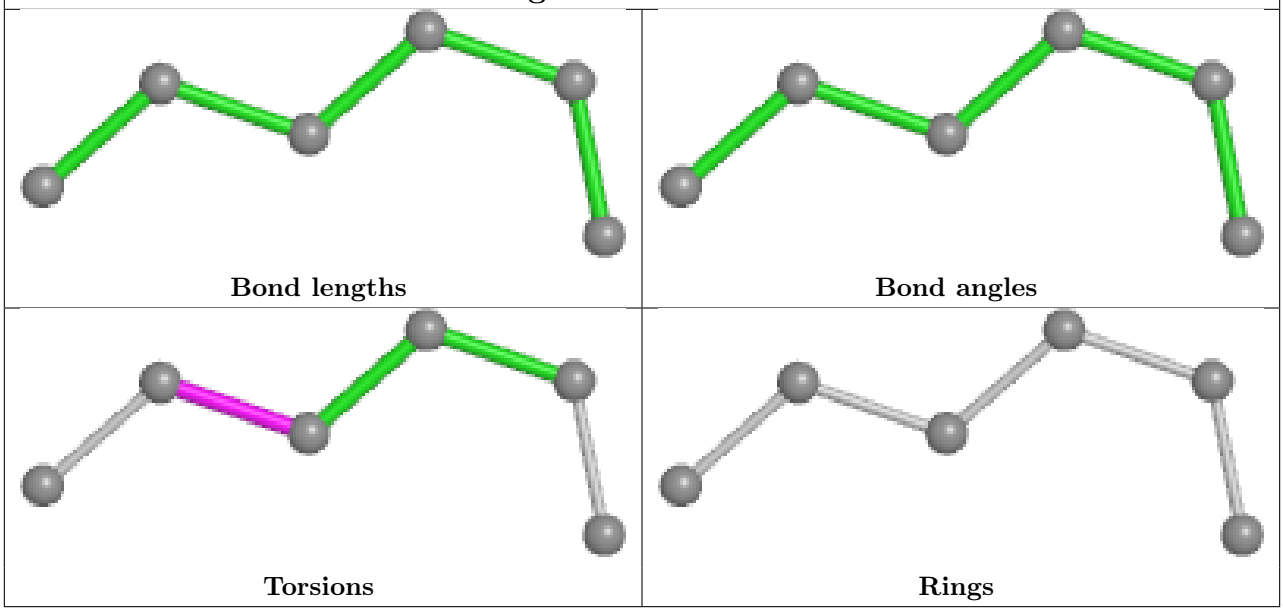
Ligand LFA A 317



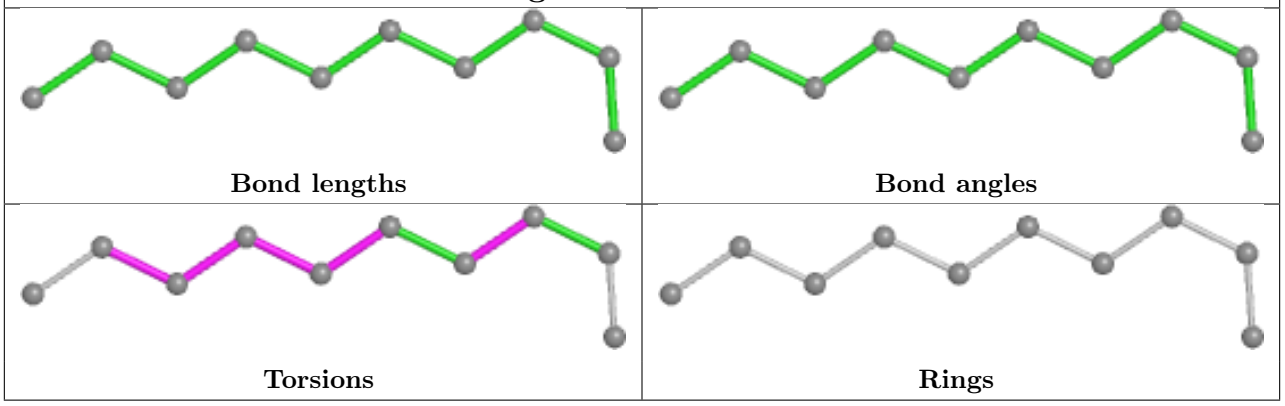
Ligand LFA A 310



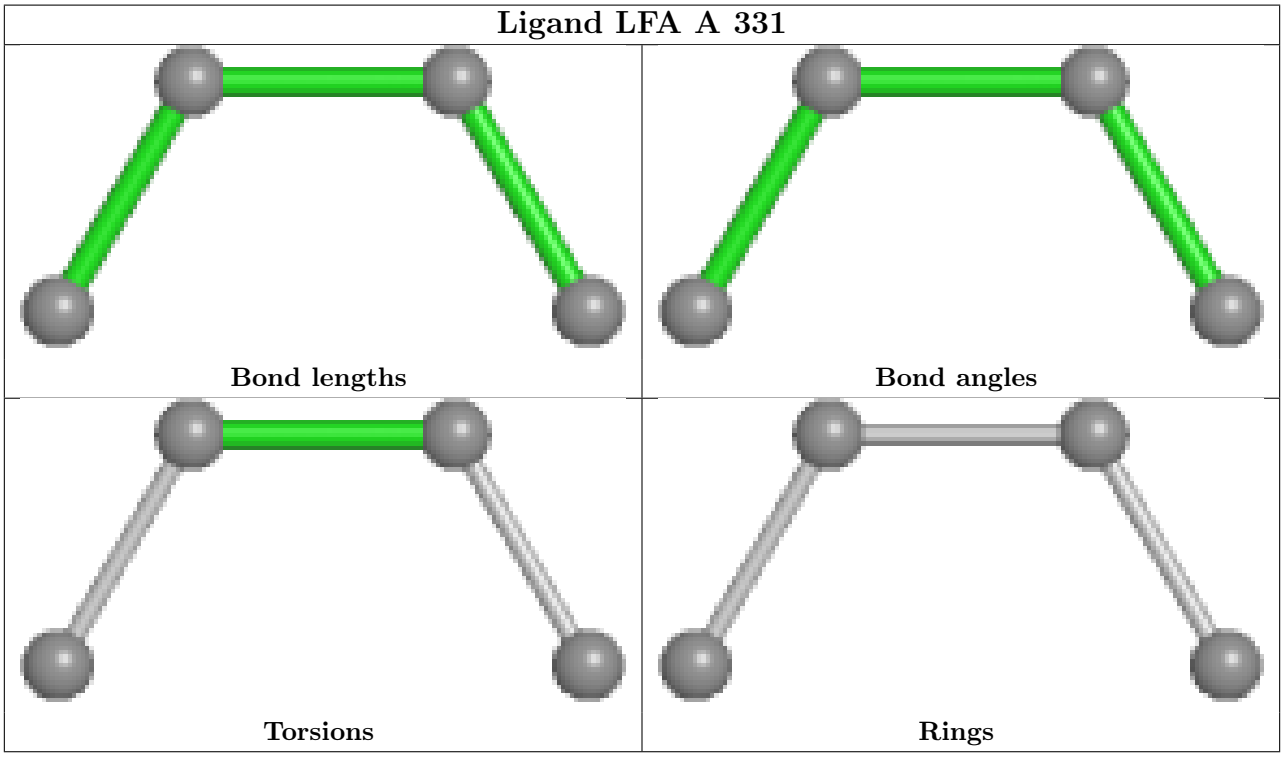
Ligand LFA A 325



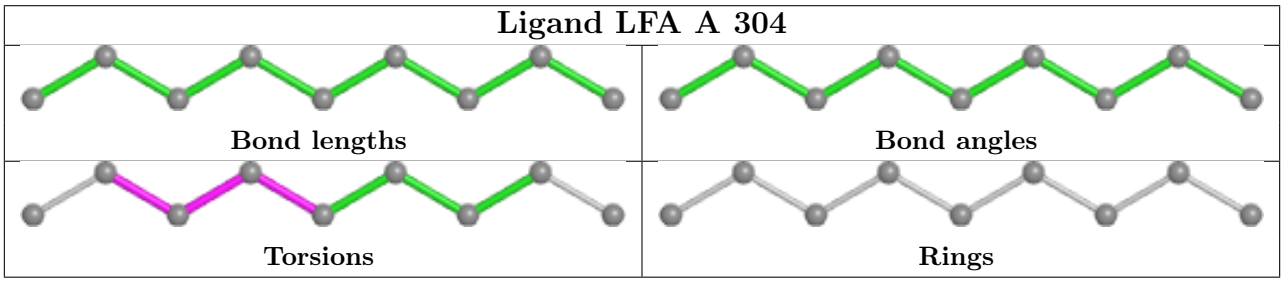
Ligand LFA A 314



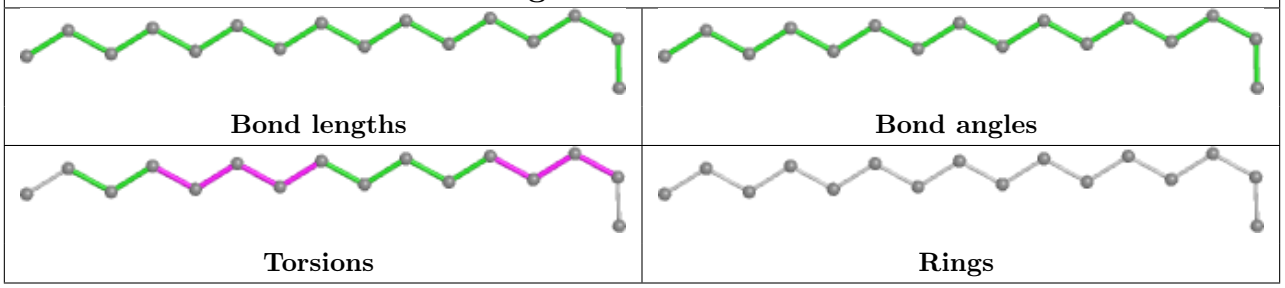
Ligand LFA A 331



Ligand LFA A 304



Ligand LFA A 302



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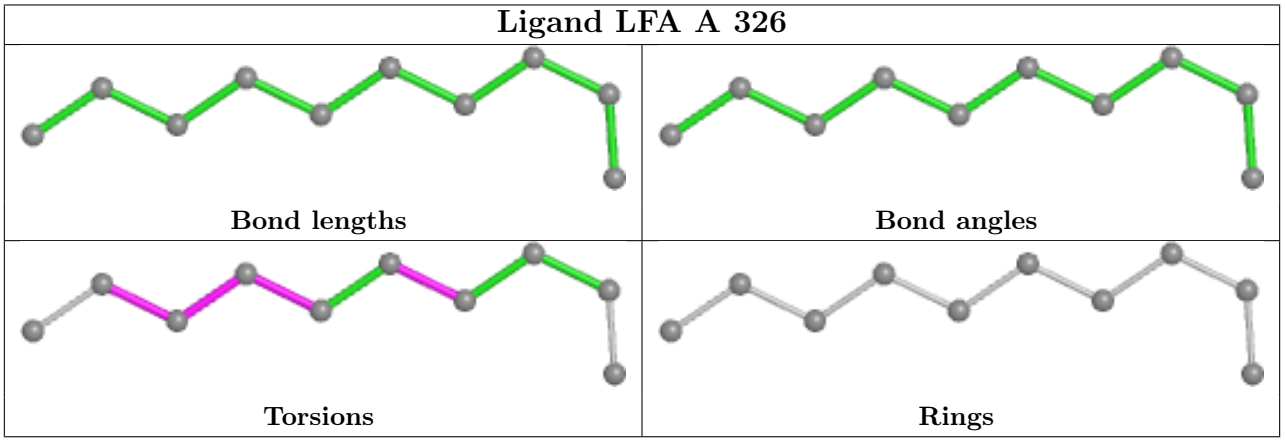
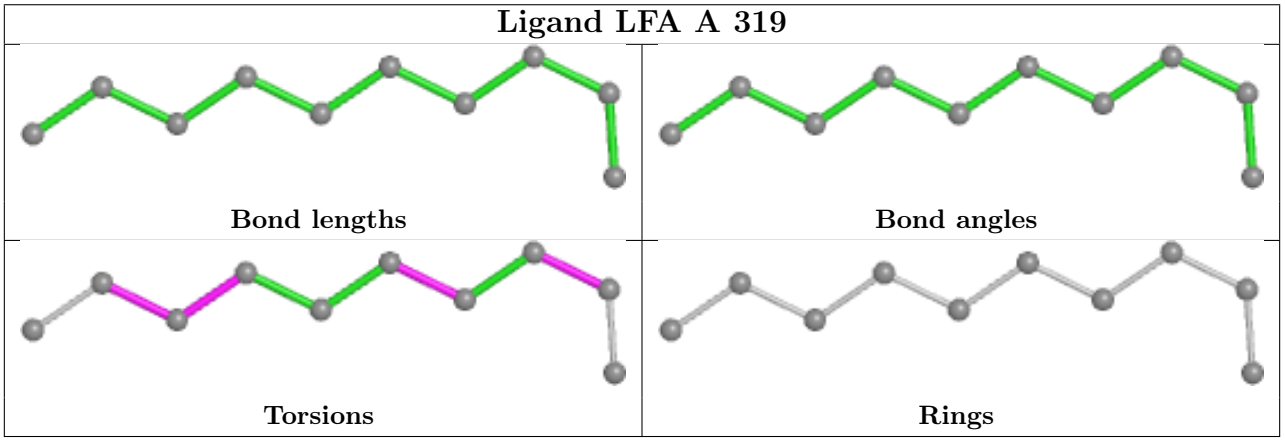
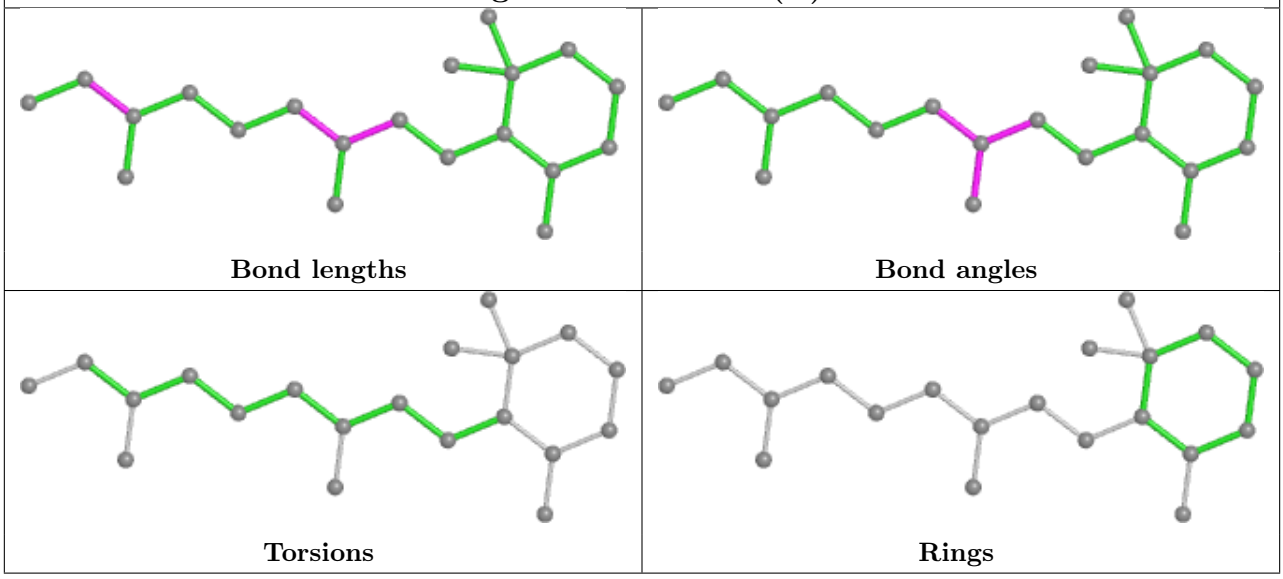


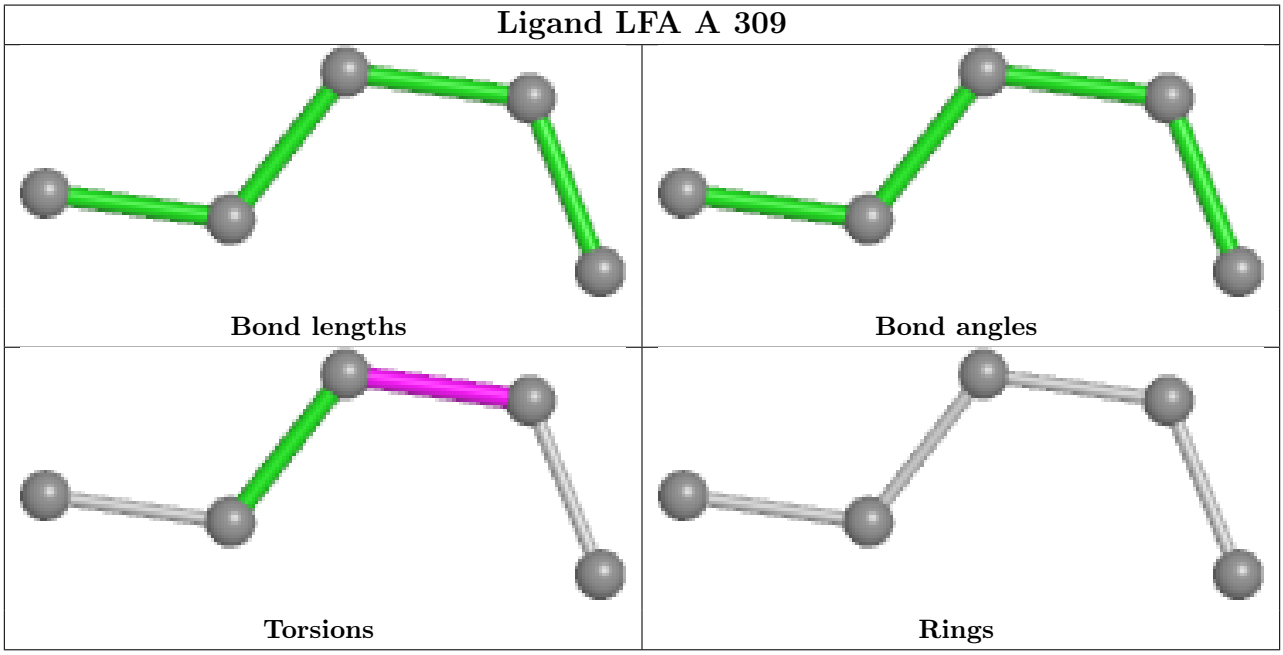
Ligand LFA A 319



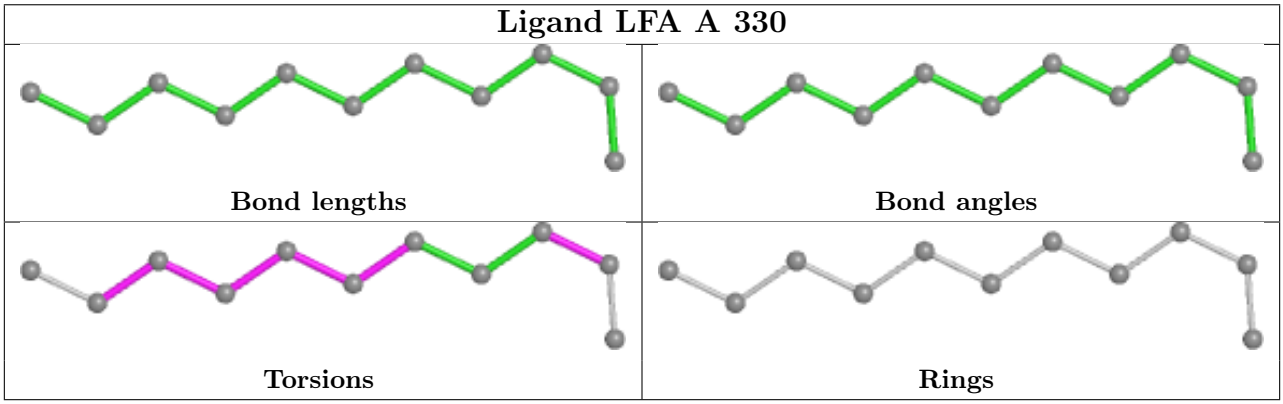
Ligand RET A 336 (B)



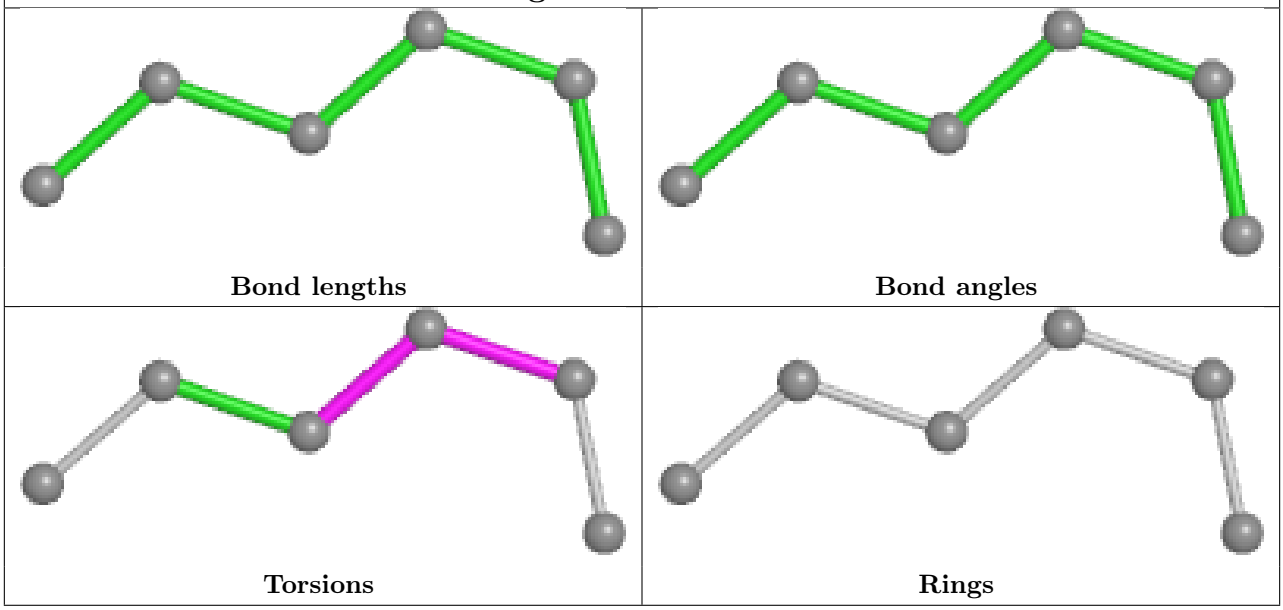
Ligand LFA A 309



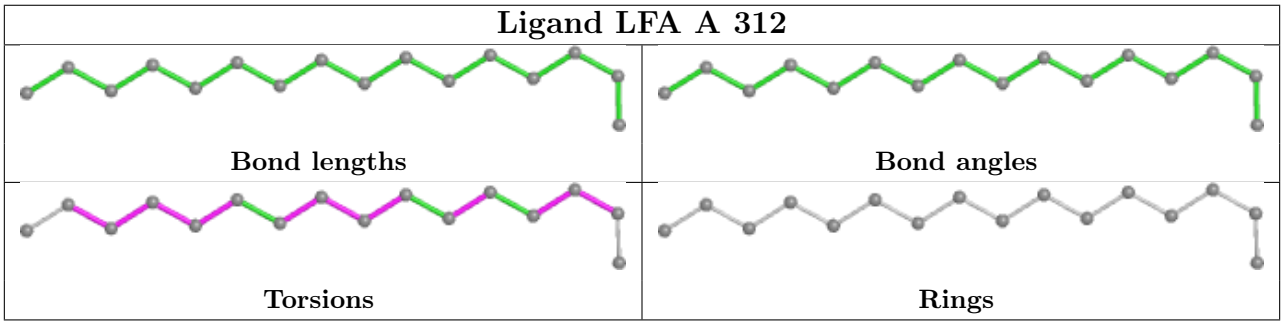
Ligand LFA A 330



Ligand LFA A 324



Ligand LFA A 312



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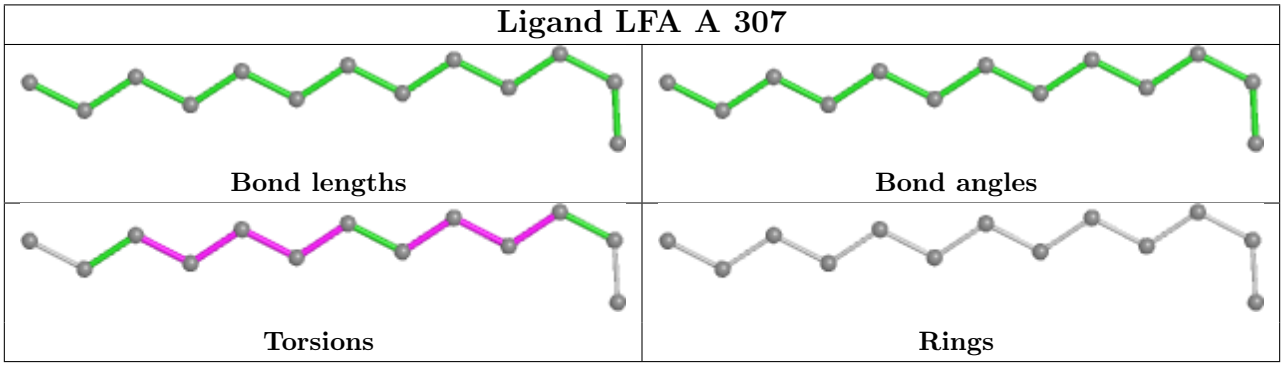
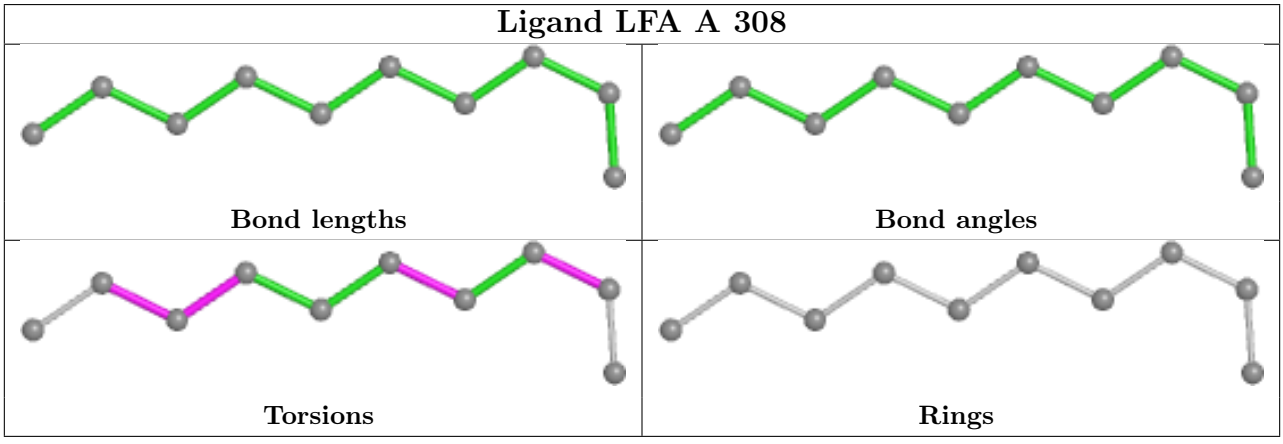
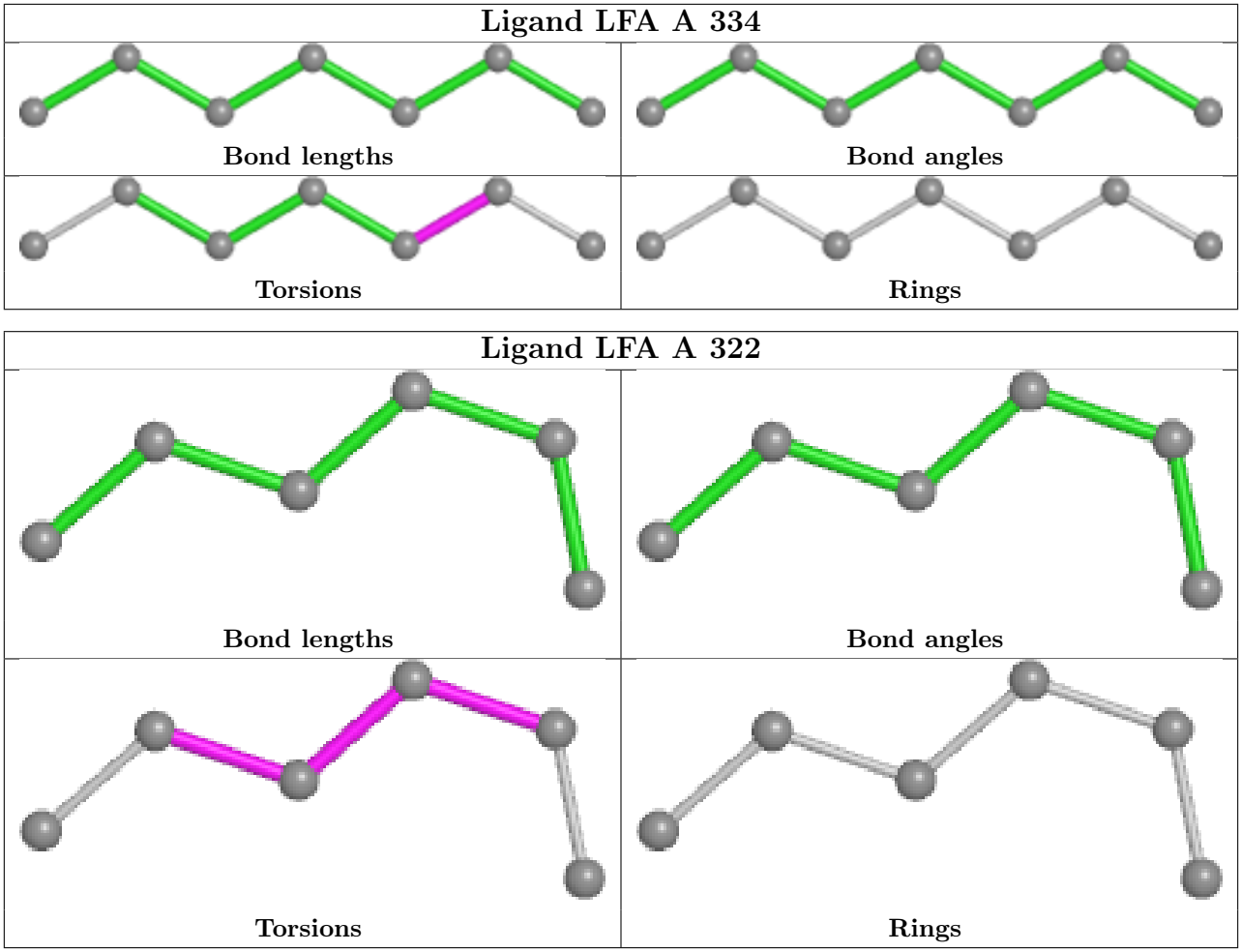


Ligand LFA A 308





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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	271/274 (98%)	0.34	20 (7%)	14	11	28, 42, 74, 130	3 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	6.5
1	A	230	VAL	6.0
1	A	232	GLY	4.0
1	A	272	ASN	3.7
1	A	164	LEU	3.5
1	A	233	PHE	3.5
1	A	163	ASN	3.2
1	A	235	TYR	3.1
1	A	5	LEU	3.0
1	A	162	SER	3.0
1	A	159	TYR	3.0
1	A	231	ASP	2.9
1	A	166	ALA	2.8
1	A	88	PHE	2.7
1	A	270	SER	2.7
1	A	3	GLN	2.5
1	A	234	LEU	2.3
1	A	229	GLY	2.2
1	A	179[A]	PHE	2.0
1	A	158	PHE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFA	A	335	10/20	-0.13	0.63	110,148,164,169	0
3	LFA	A	313	5/20	0.34	0.33	60,67,78,85	0
3	LFA	A	318	12/20	0.41	0.30	79,91,107,119	0
3	LFA	A	323	4/20	0.44	0.17	81,85,89,92	0
3	LFA	A	316	5/20	0.48	0.19	66,67,71,74	0
3	LFA	A	311	10/20	0.55	0.33	66,76,90,93	0
3	LFA	A	327	7/20	0.56	0.24	86,95,98,100	0
3	LFA	A	324	6/20	0.57	0.37	105,112,113,113	0
3	LFA	A	326	10/20	0.59	0.33	71,79,86,89	0
3	LFA	A	329	5/20	0.63	0.25	68,70,80,80	0
3	LFA	A	314	10/20	0.64	0.17	70,77,92,94	0
3	LFA	A	333	10/20	0.65	0.28	69,77,89,92	0
3	LFA	A	332	5/20	0.65	0.34	66,79,87,97	0
3	LFA	A	317	11/20	0.66	0.16	79,88,119,123	0
3	LFA	A	304	9/20	0.68	0.20	73,79,100,103	0
3	LFA	A	334	7/20	0.68	0.13	58,63,76,78	0
3	LFA	A	307	13/20	0.68	0.24	52,66,77,77	0
3	LFA	A	331	4/20	0.72	0.51	77,82,82,91	0
3	LFA	A	319	10/20	0.75	0.22	50,80,123,127	0
3	LFA	A	330	11/20	0.77	0.19	65,69,78,80	0
3	LFA	A	325	6/20	0.78	0.23	59,84,91,92	0
3	LFA	A	310	8/20	0.79	0.32	65,73,86,88	0
3	LFA	A	308	10/20	0.81	0.17	60,70,79,80	0
3	LFA	A	328	3/20	0.82	0.34	77,77,81,82	0
3	LFA	A	320	6/20	0.82	0.13	71,74,79,81	0
3	LFA	A	312	16/20	0.83	0.22	63,73,85,87	0
3	LFA	A	302	16/20	0.84	0.16	52,58,82,86	0
3	LFA	A	303	8/20	0.84	0.13	50,51,65,72	8
3	LFA	A	306	5/20	0.85	0.28	69,71,76,79	0
3	LFA	A	305	6/20	0.86	0.29	68,74,74,76	0
3	LFA	A	321	5/20	0.86	0.20	68,70,81,86	0
3	LFA	A	322	6/20	0.86	0.15	69,70,75,77	0

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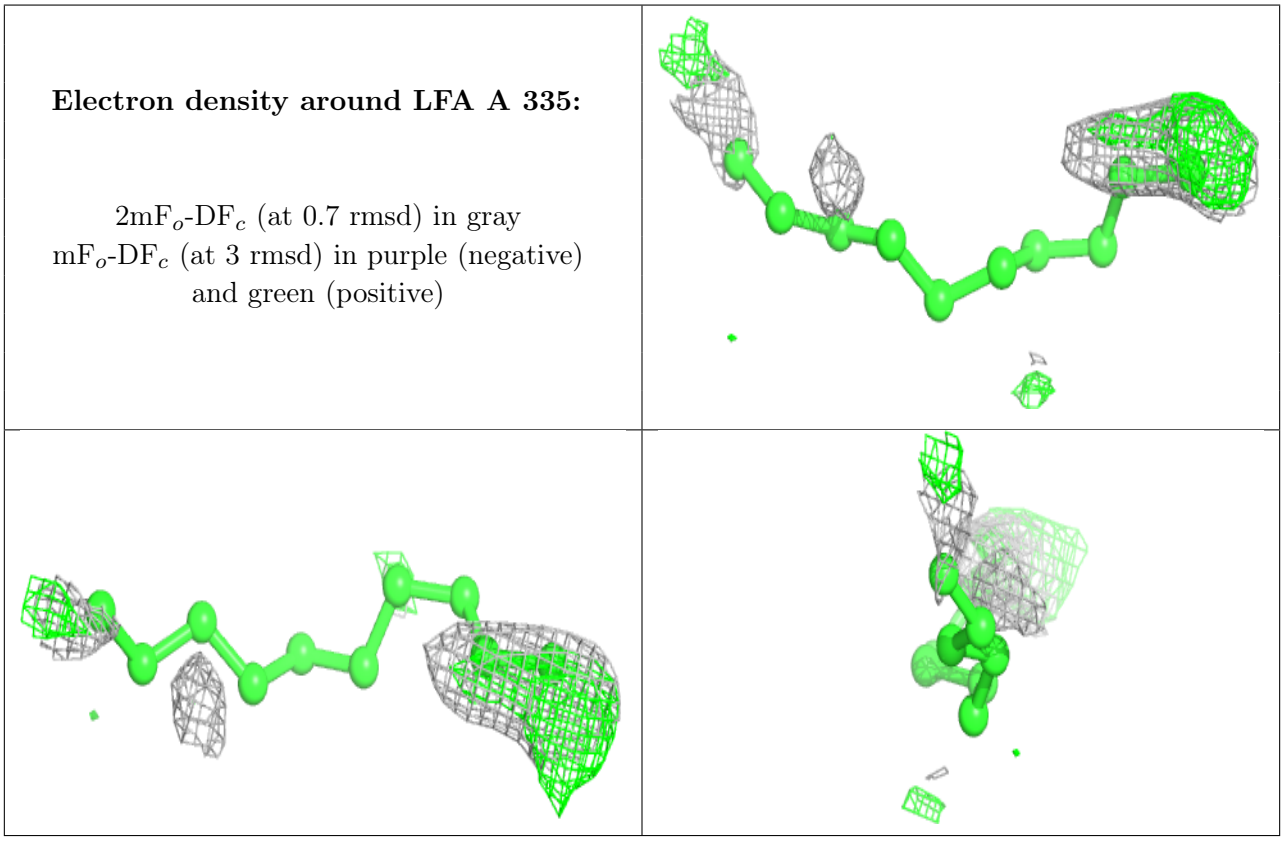
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFA	A	315	4/20	0.86	0.15	71,71,73,78	0
2	NA	A	301	1/1	0.88	0.28	55,55,55,55	0
3	LFA	A	309	5/20	0.91	0.33	96,99,102,105	0
4	RET	A	336[A]	20/21	0.91	0.10	29,35,45,46	20
4	RET	A	336[B]	20/21	0.91	0.10	29,35,45,46	20

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.

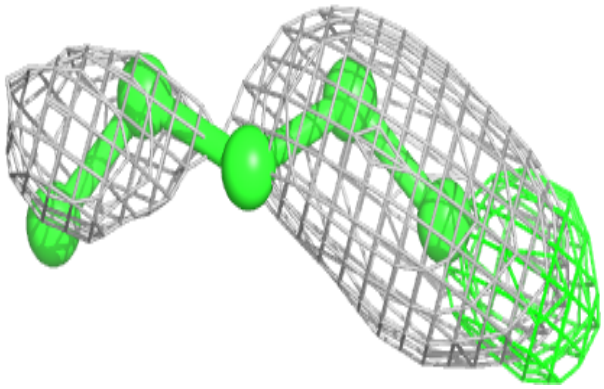
Electron density around LFA A 335:

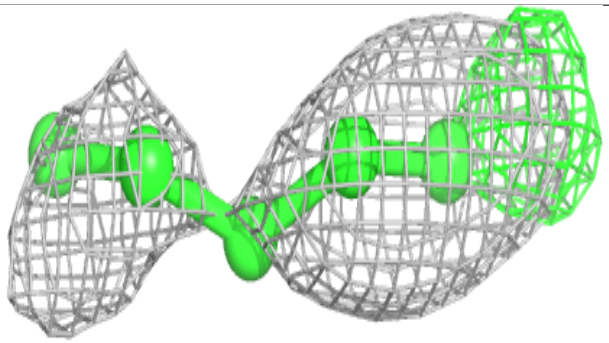
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

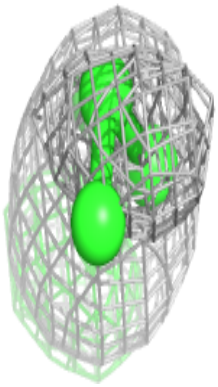


Electron density around LFA A 313:

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

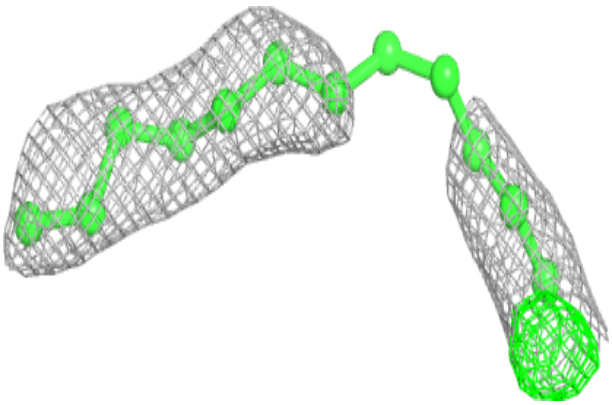


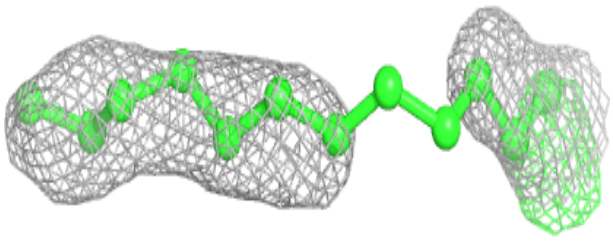


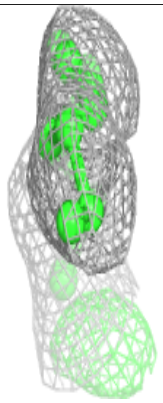


Electron density around LFA A 318:

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

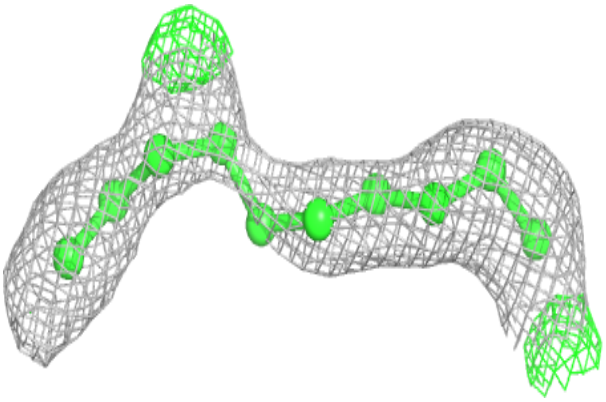


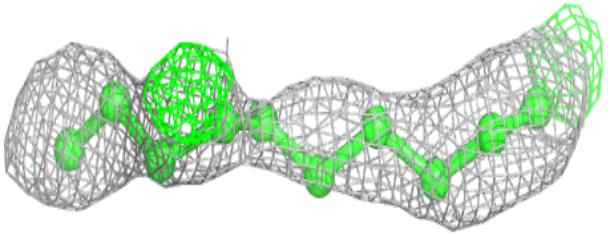


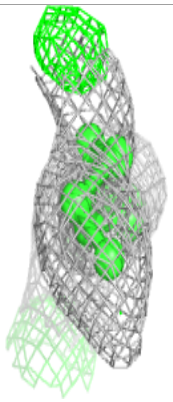


Electron density around LFA A 311:

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

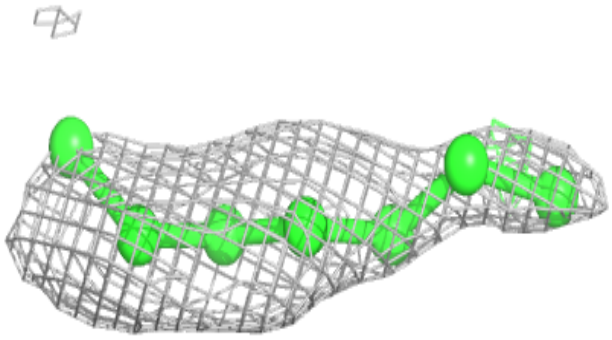


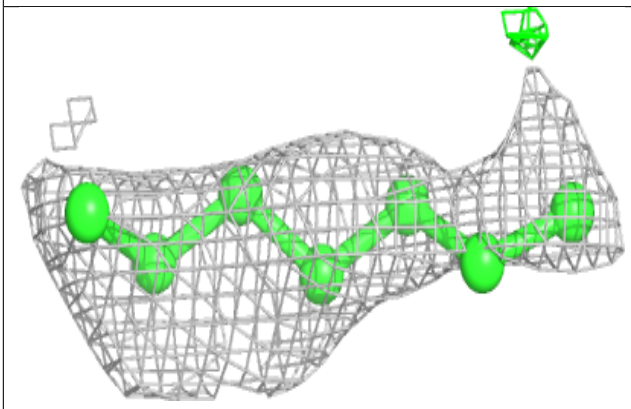


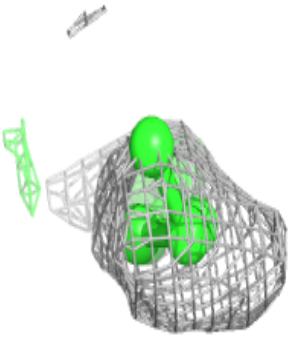


Electron density around LFA A 327:

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

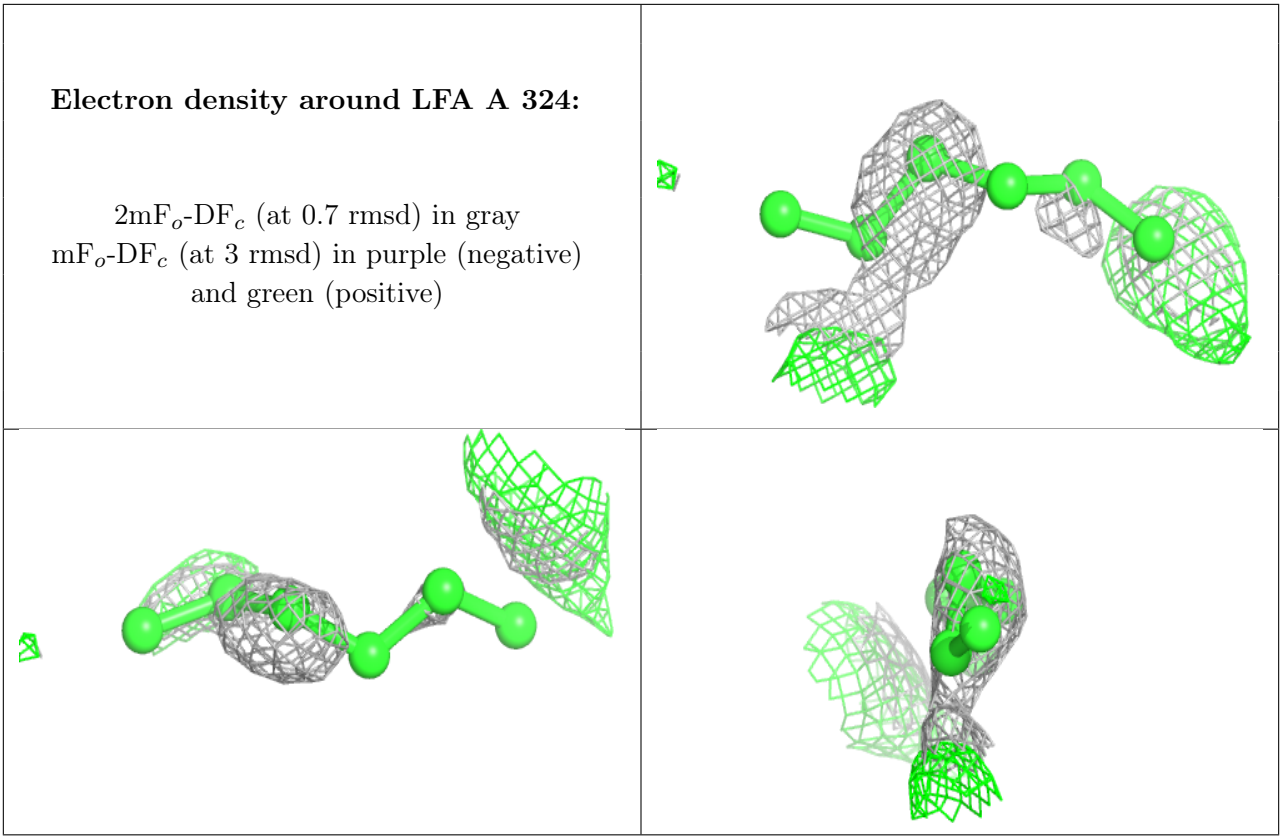






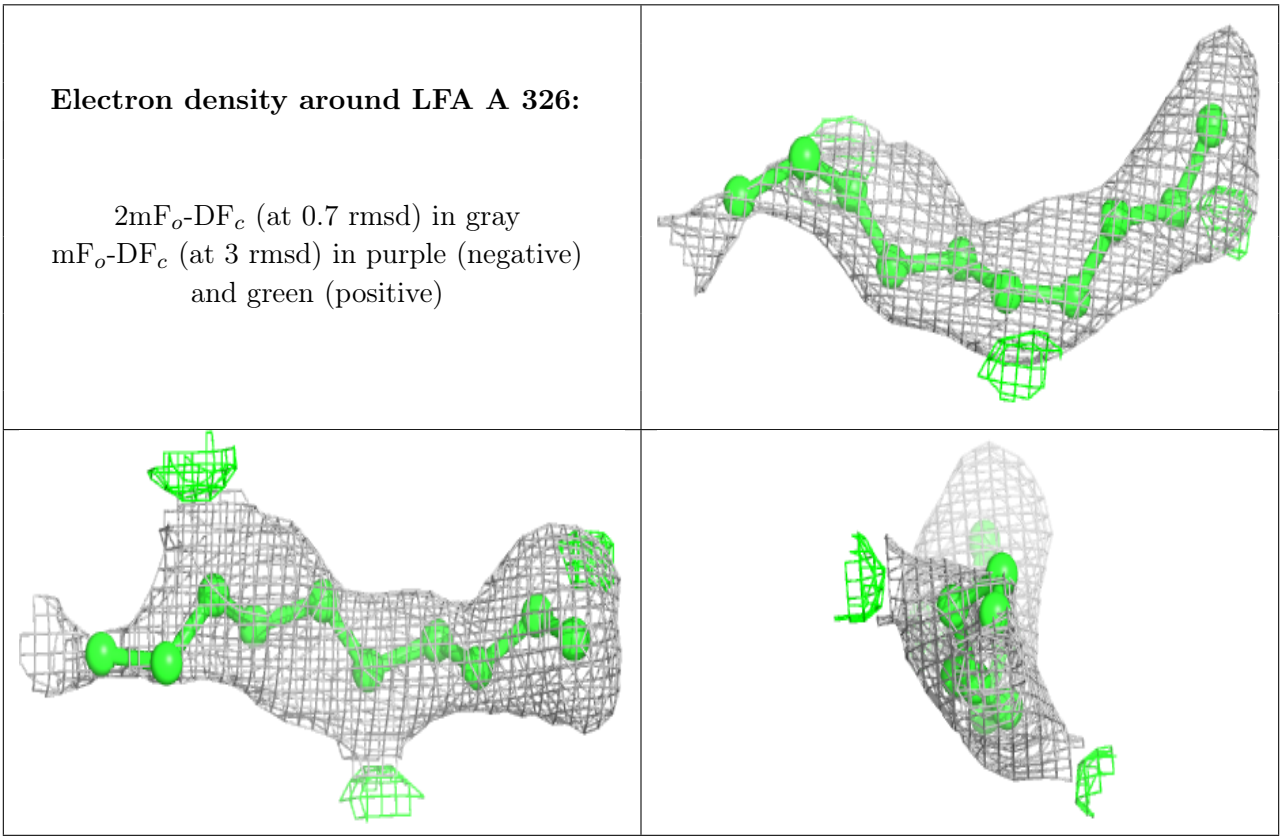
Electron density around LFA A 324:

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



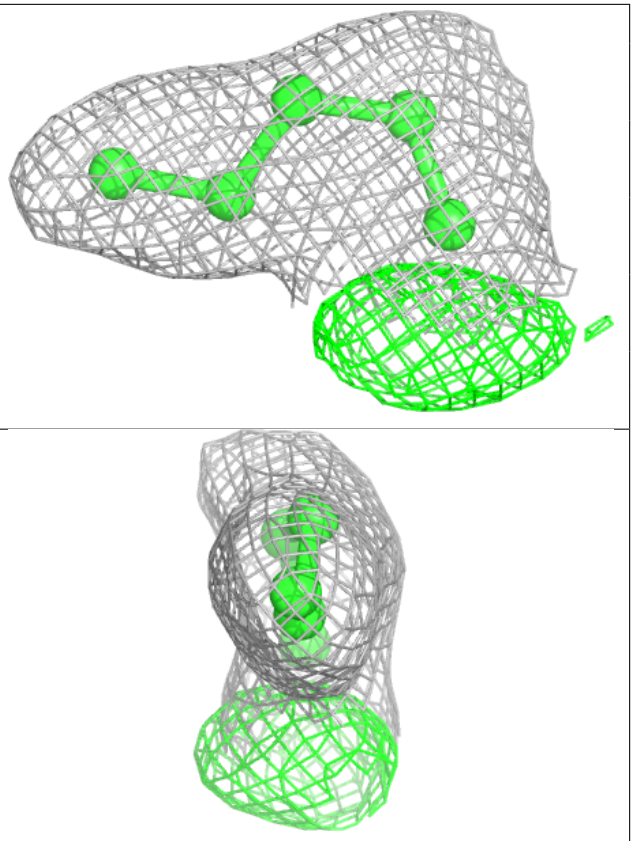
Electron density around LFA A 326:

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



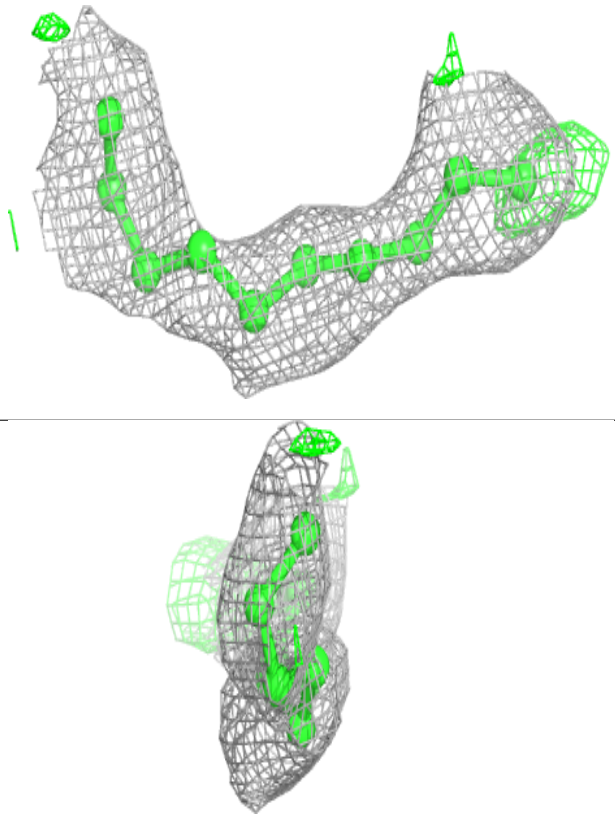
Electron density around LFA A 329:

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



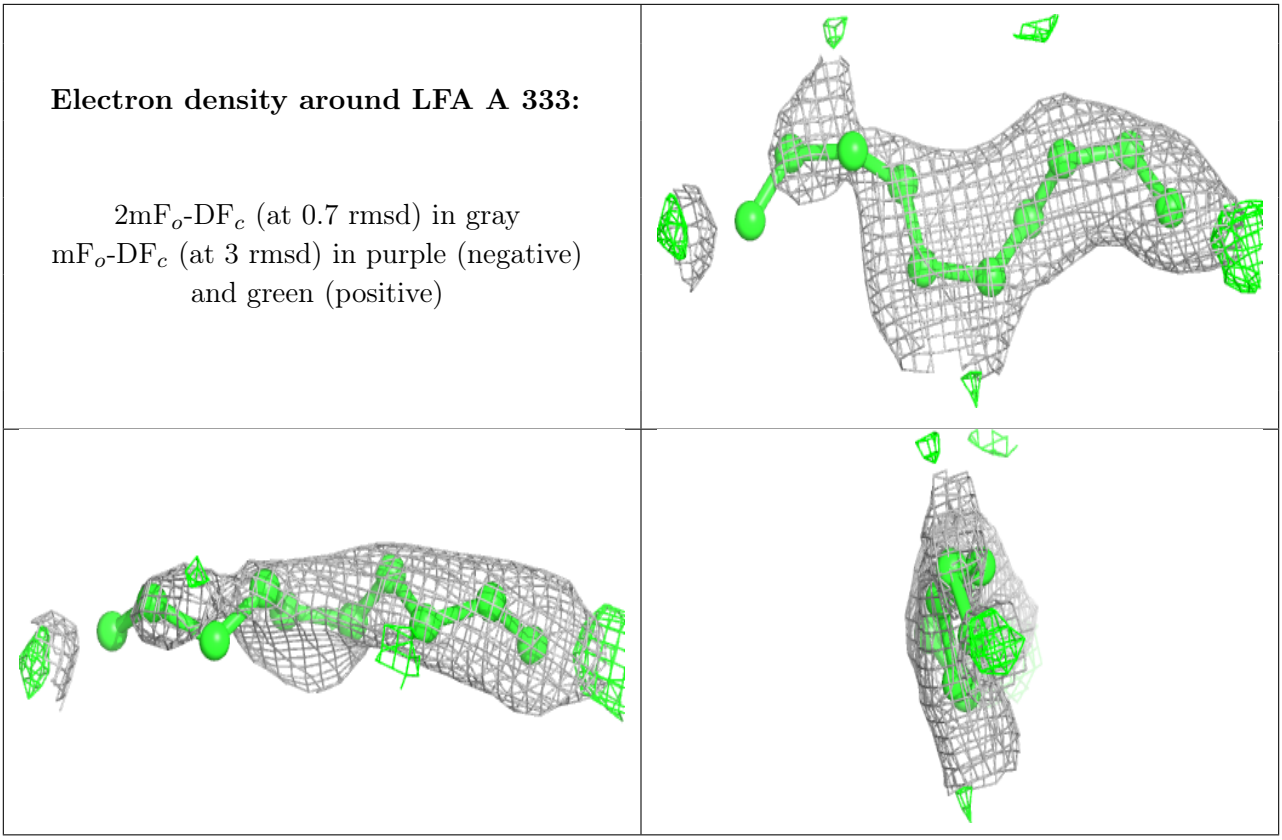
Electron density around LFA A 314:

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



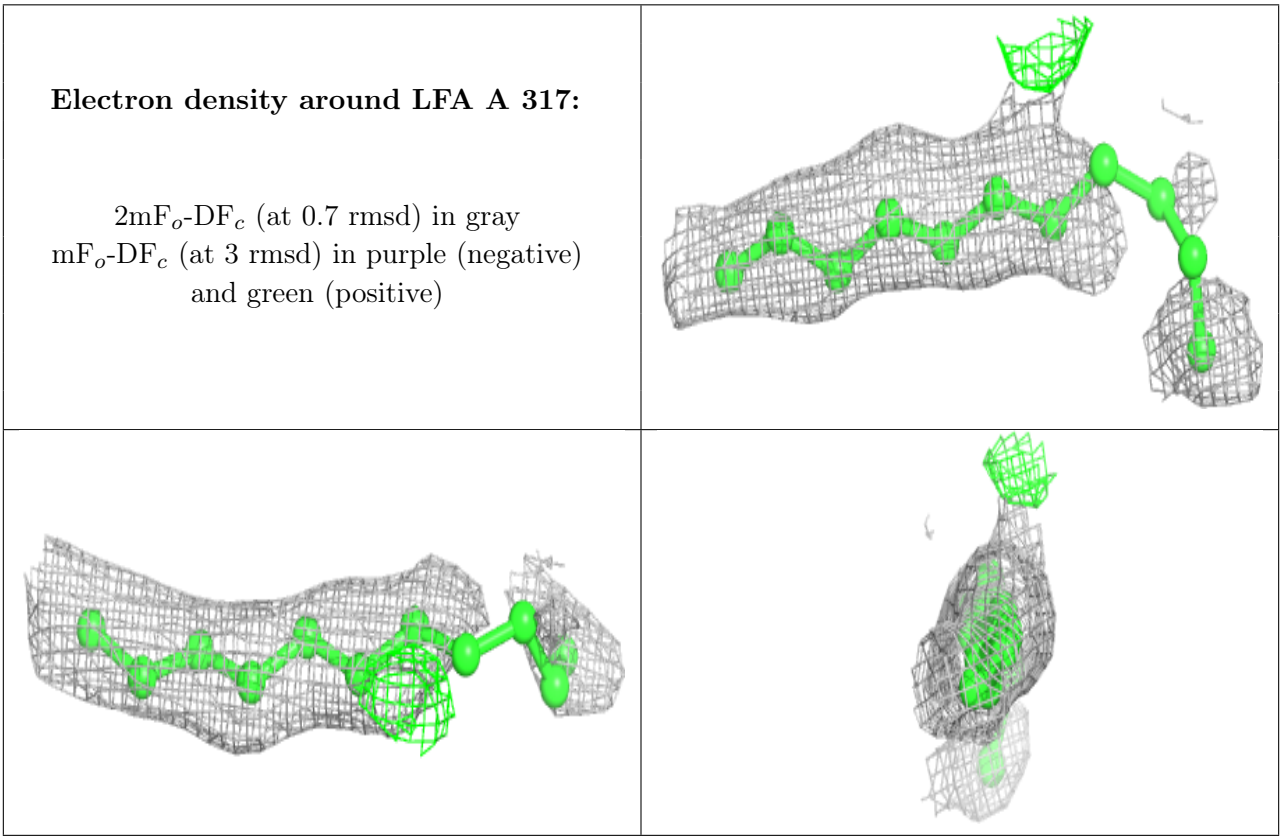
Electron density around LFA A 333:

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



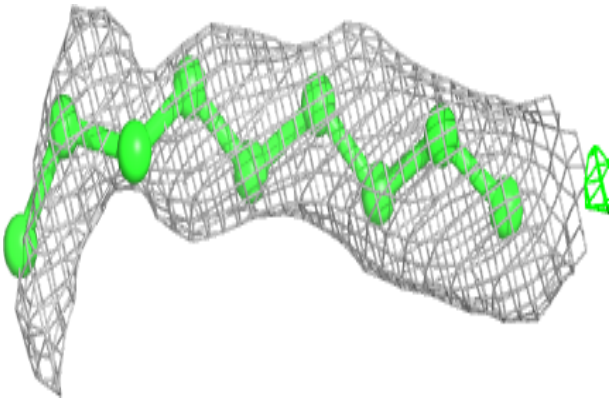
Electron density around LFA A 317:

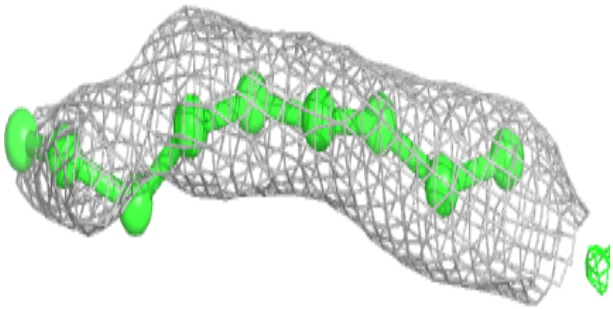
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

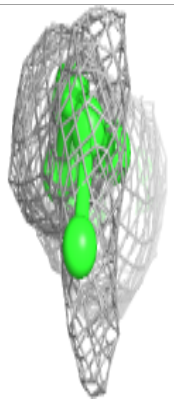


Electron density around LFA A 304:

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

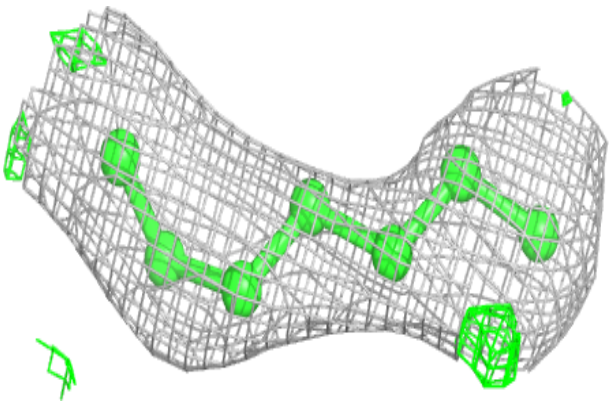


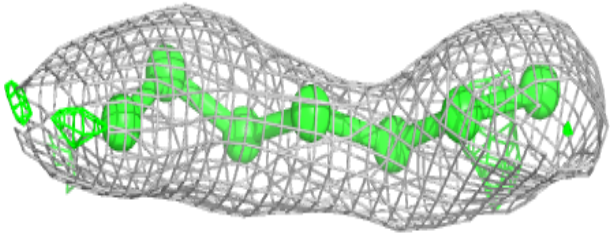


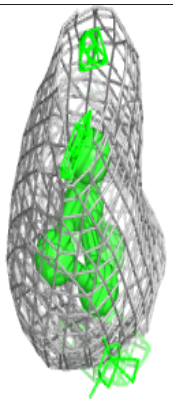


Electron density around LFA A 334:

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

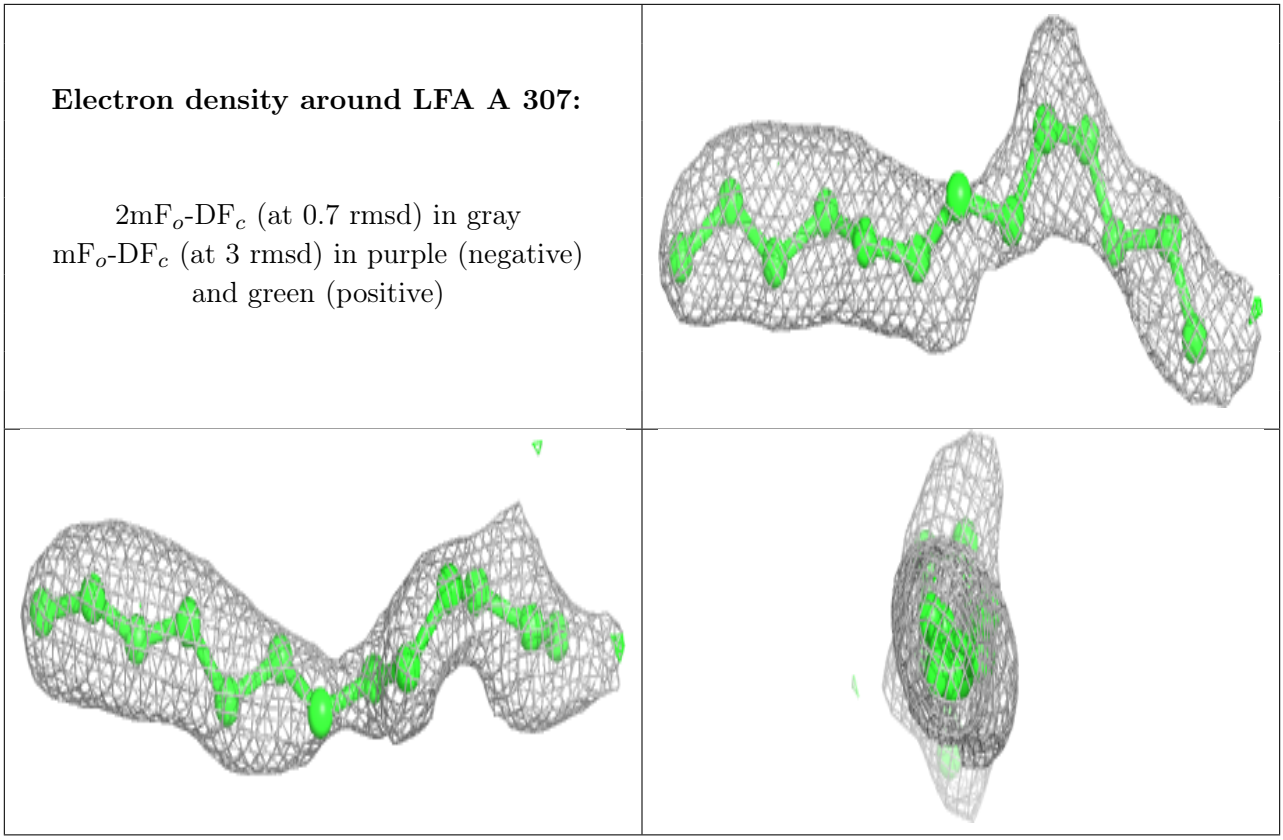






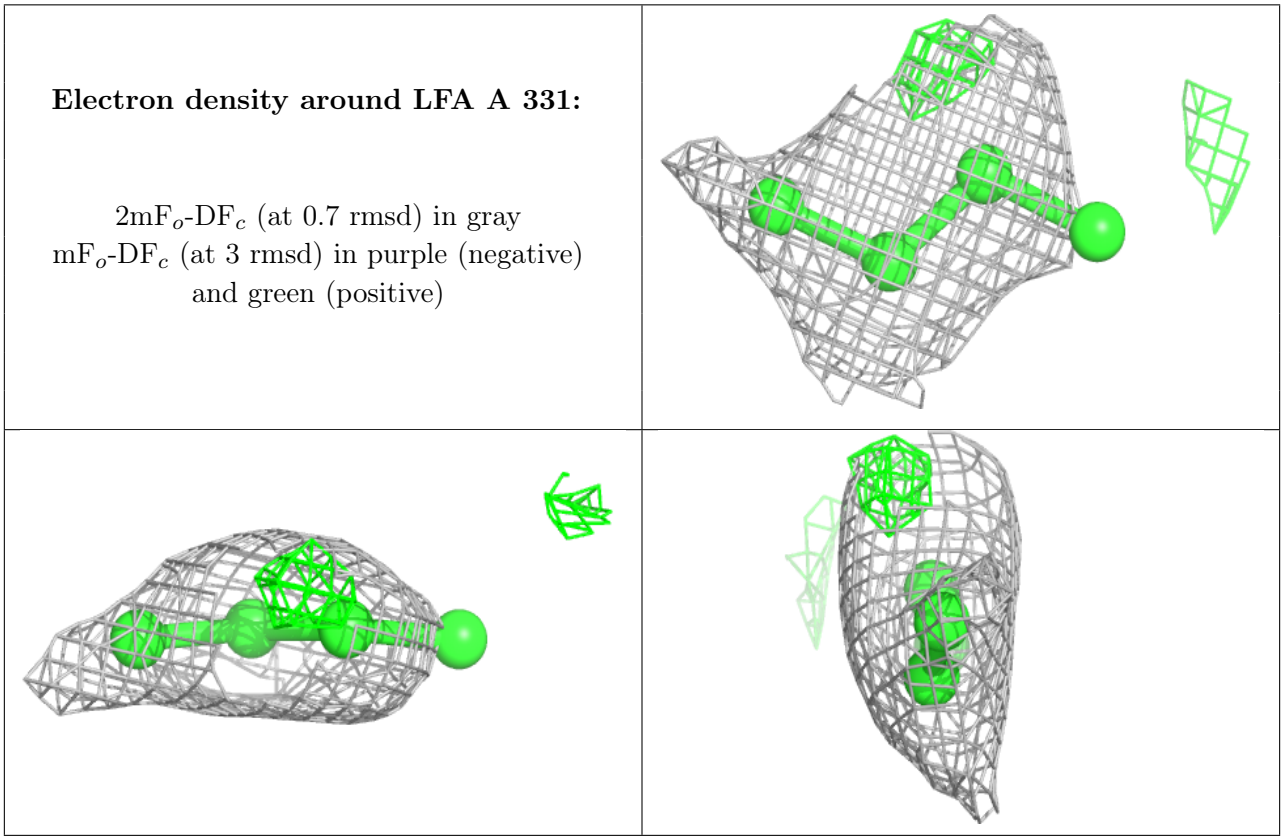
Electron density around LFA A 307:

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



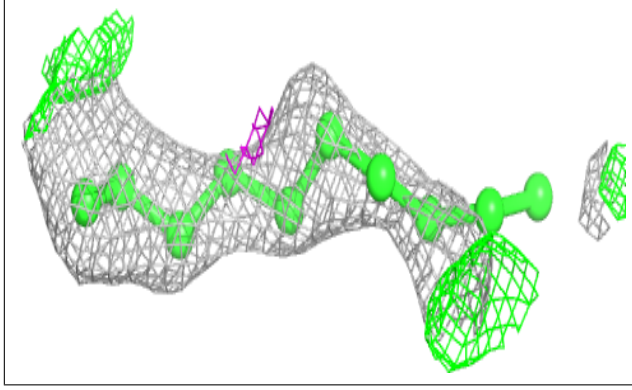
Electron density around LFA A 331:

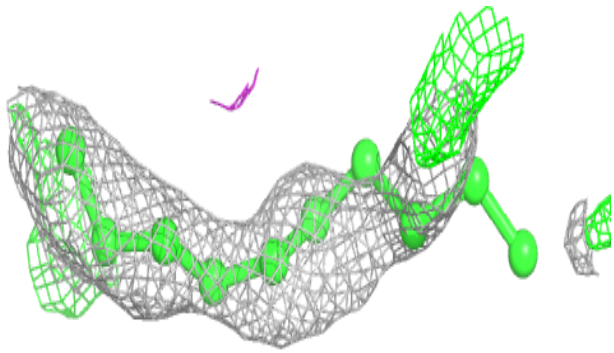
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

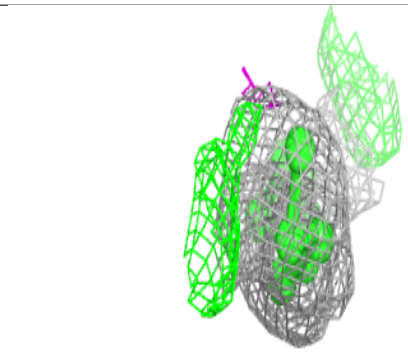


Electron density around LFA A 319:

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

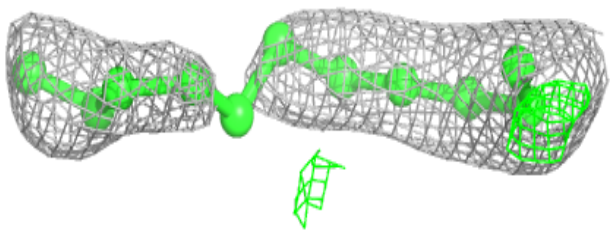


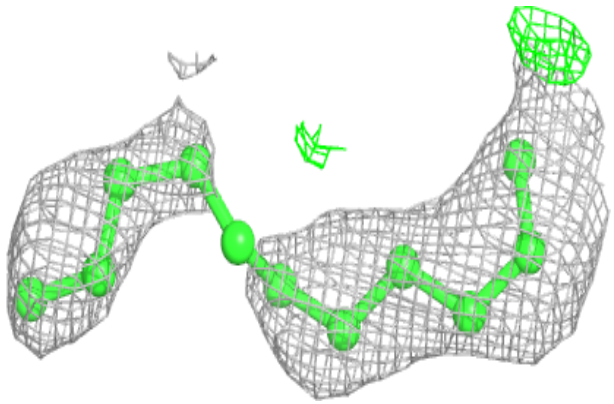


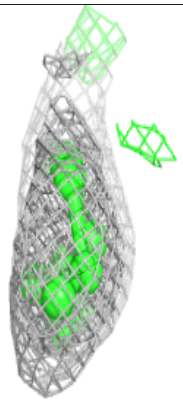


Electron density around LFA A 330:

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

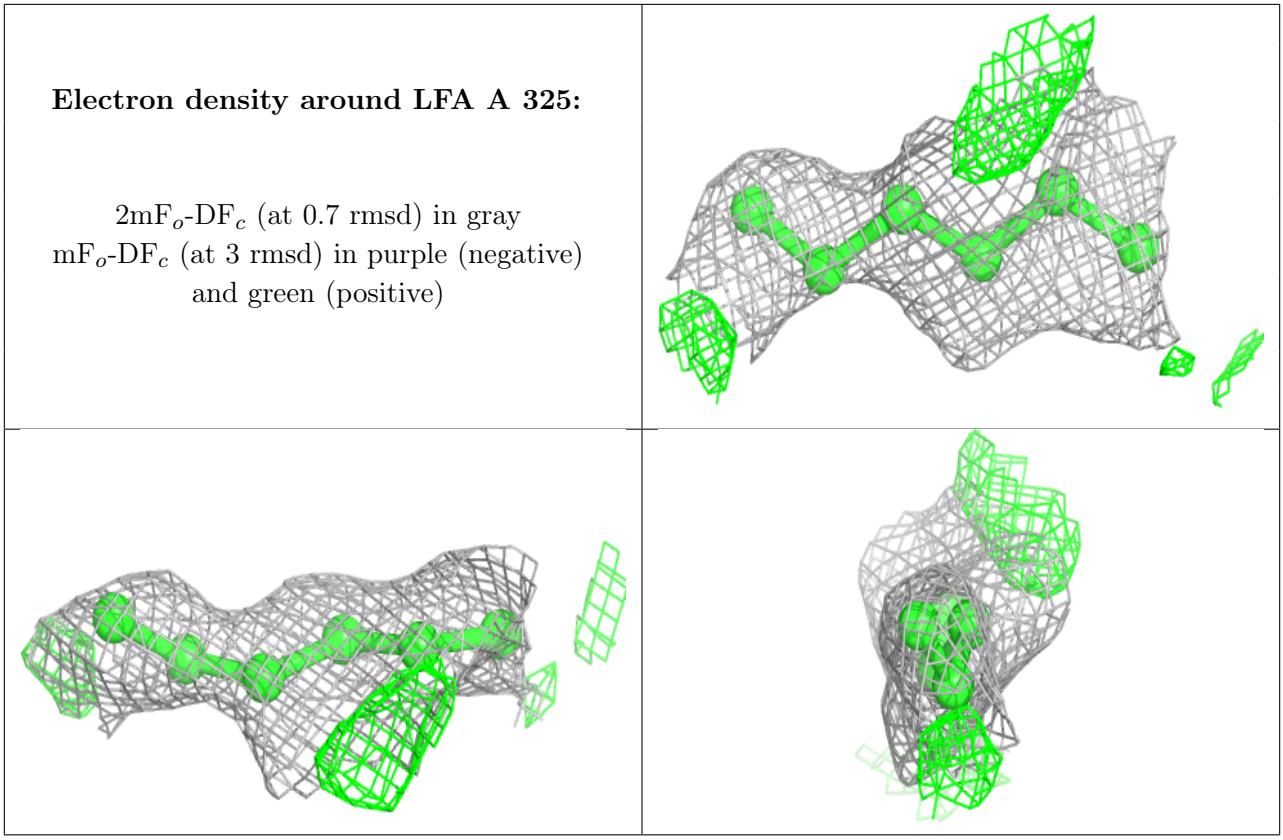






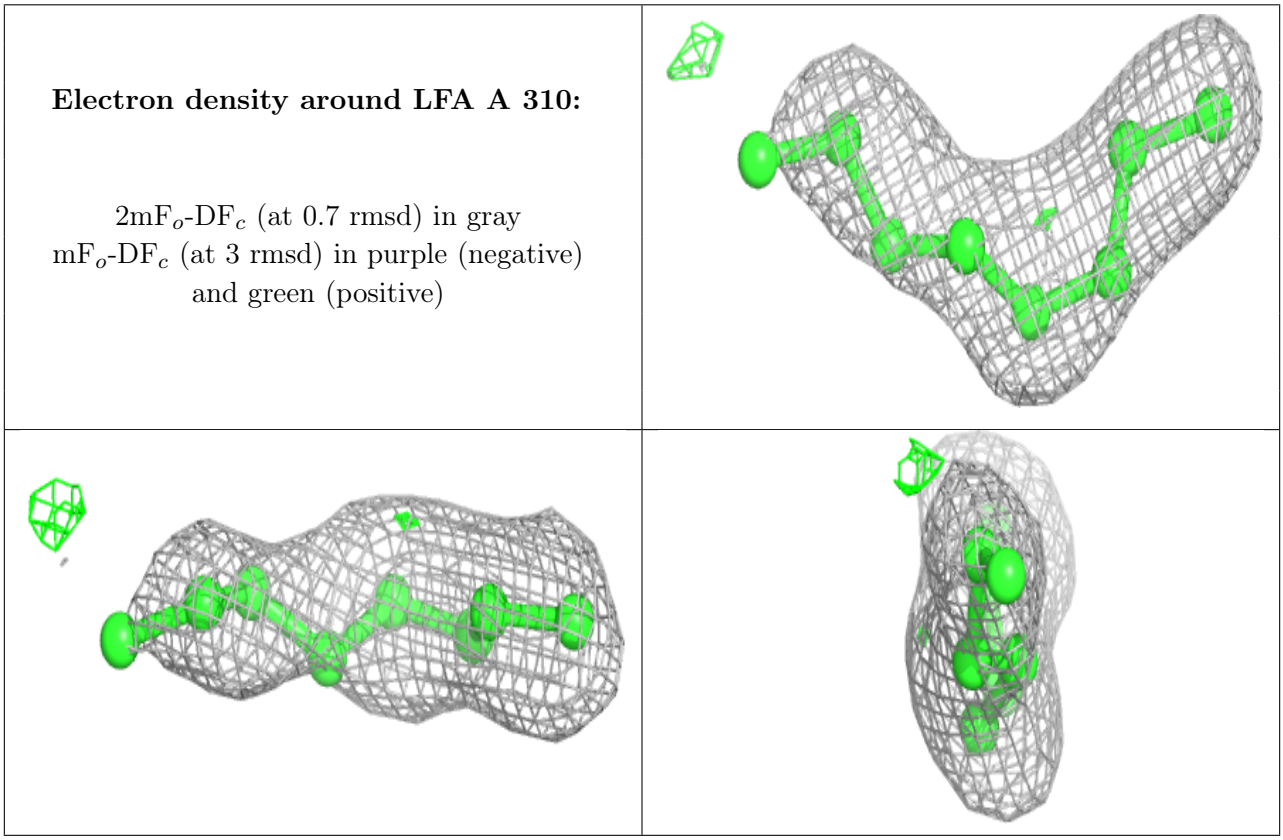
Electron density around LFA A 325:

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



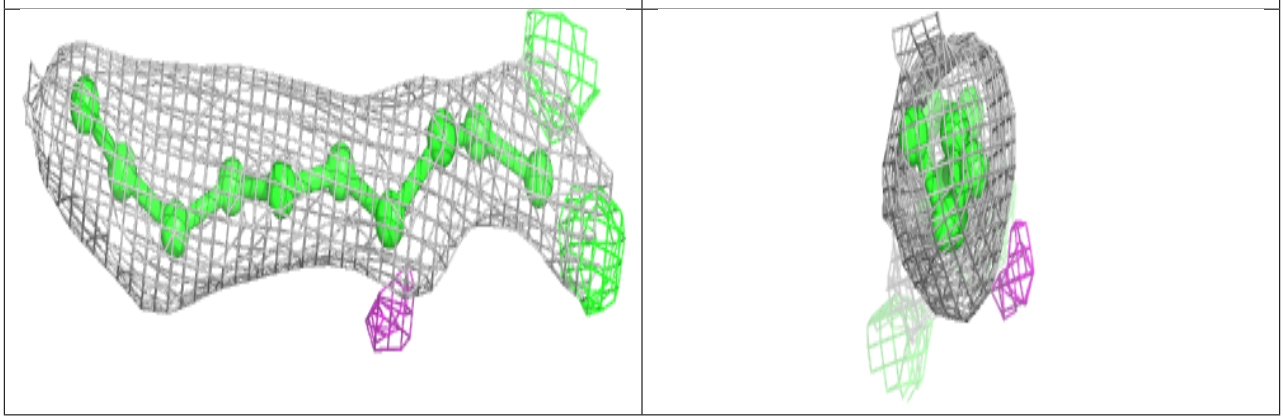
Electron density around LFA A 310:

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



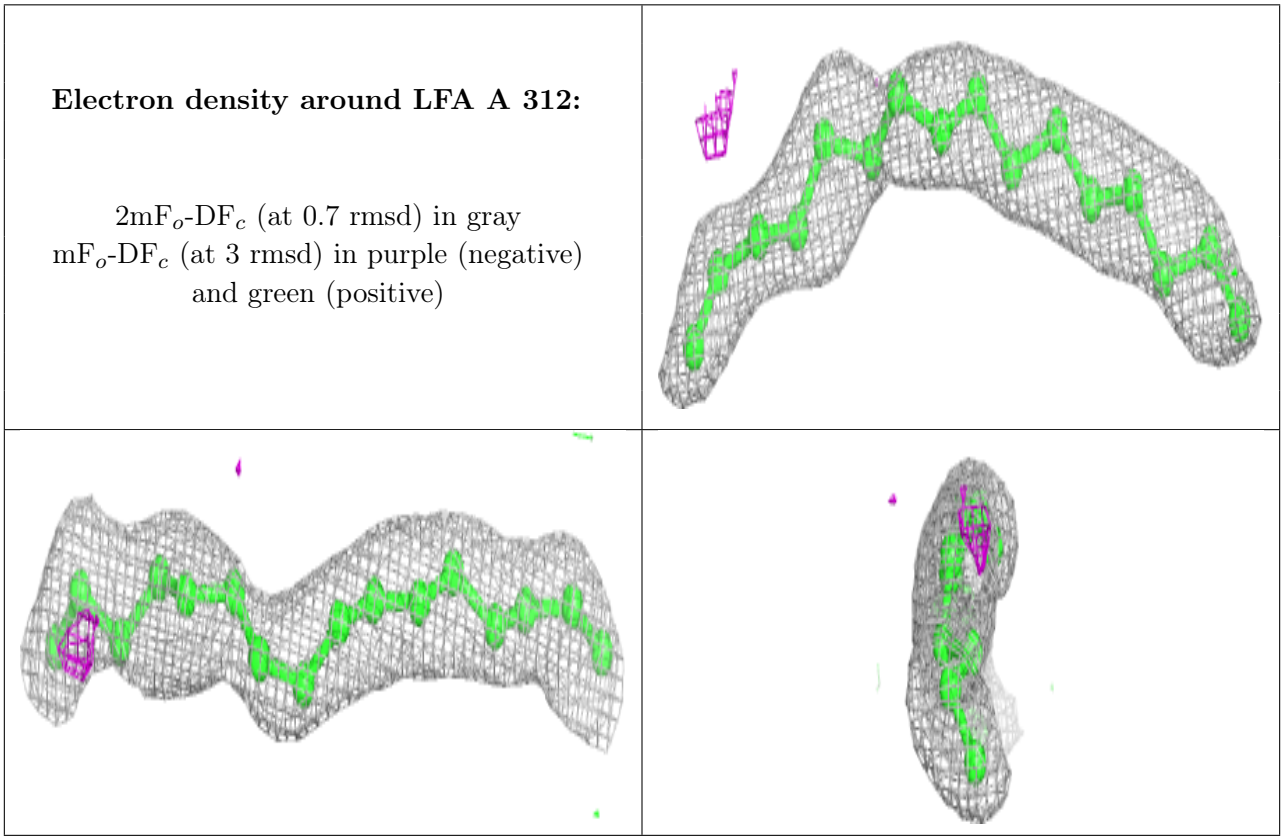
Electron density around LFA A 308:

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



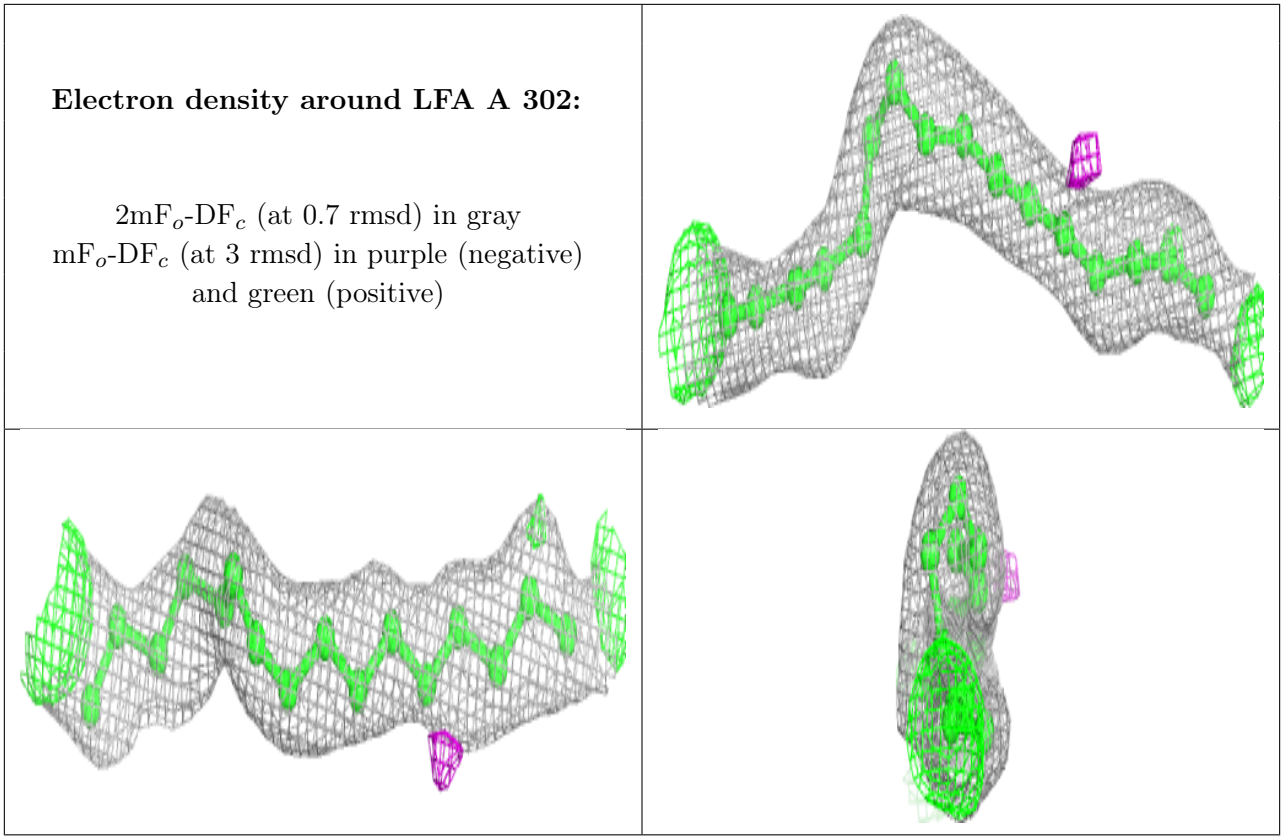
Electron density around LFA A 312:

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



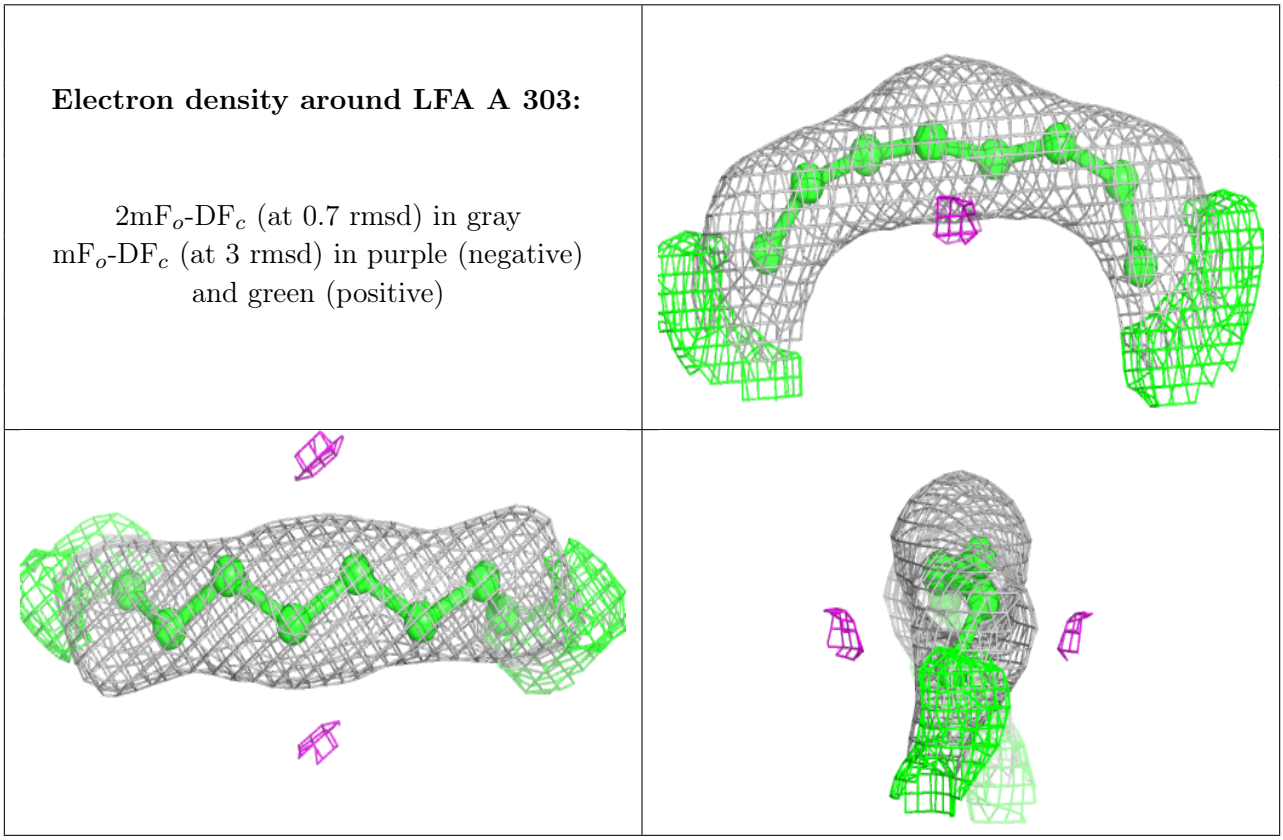
Electron density around LFA A 302:

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



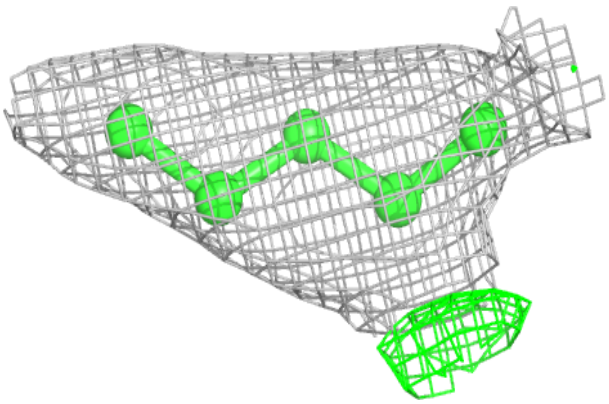
Electron density around LFA A 303:

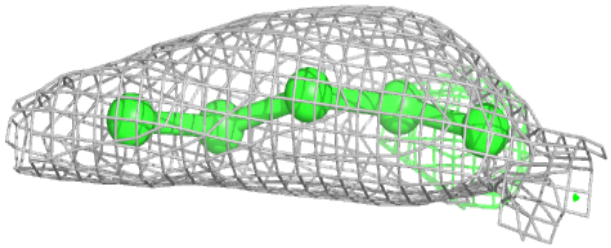
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

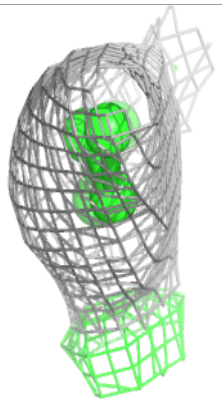


Electron density around LFA A 306:

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

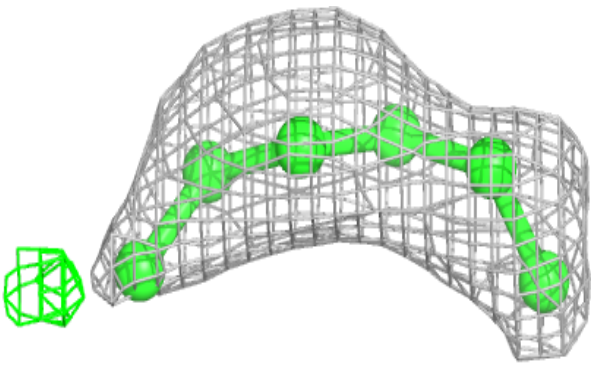


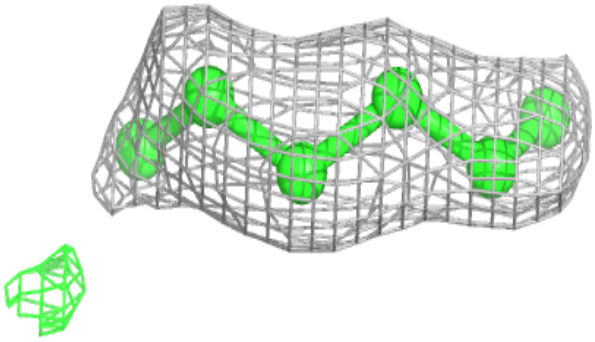


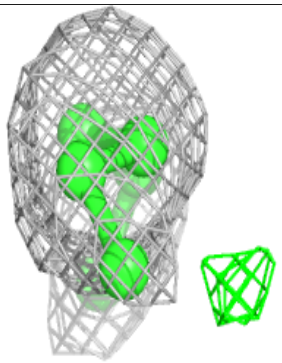


Electron density around LFA A 322:

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

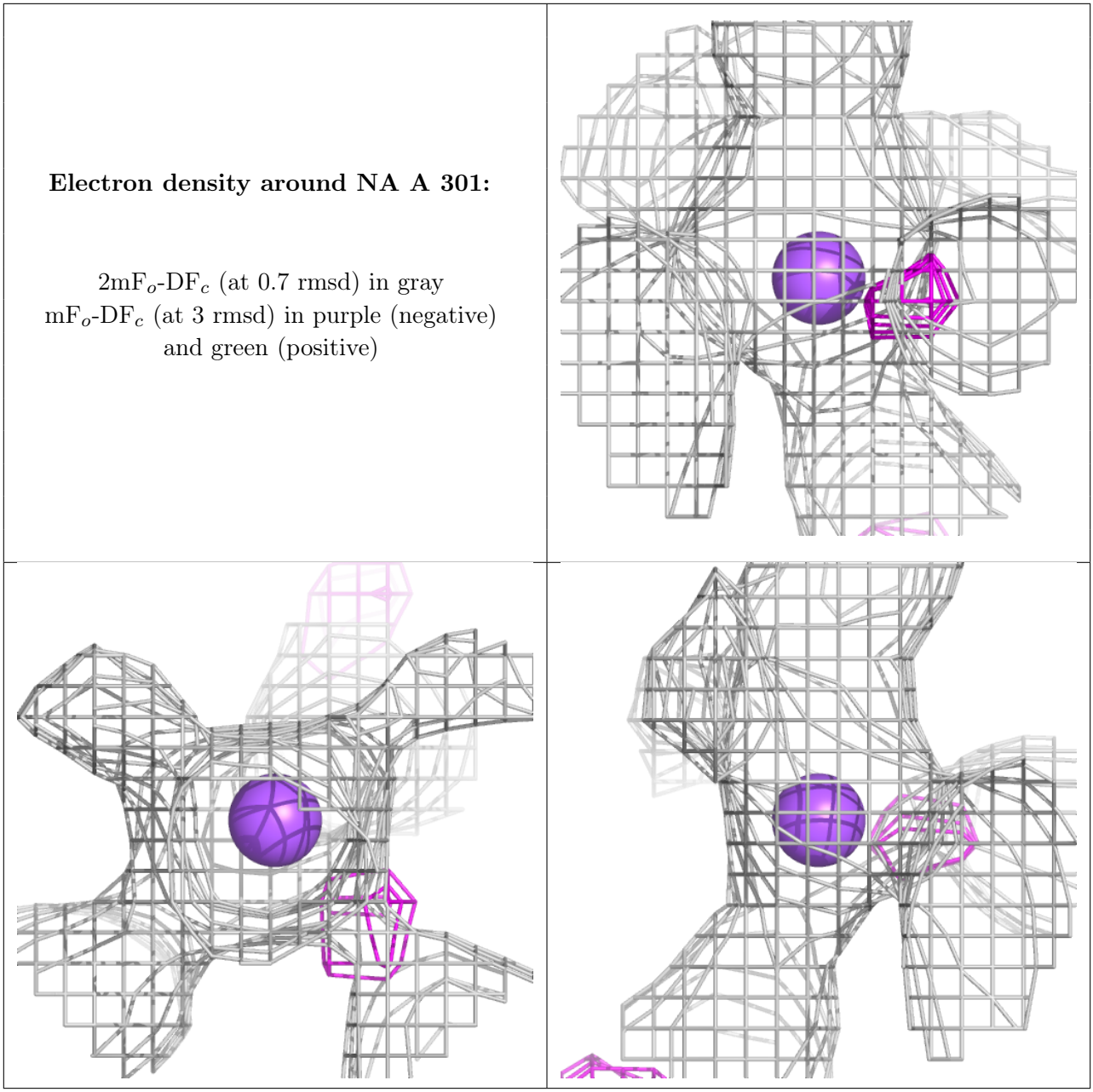






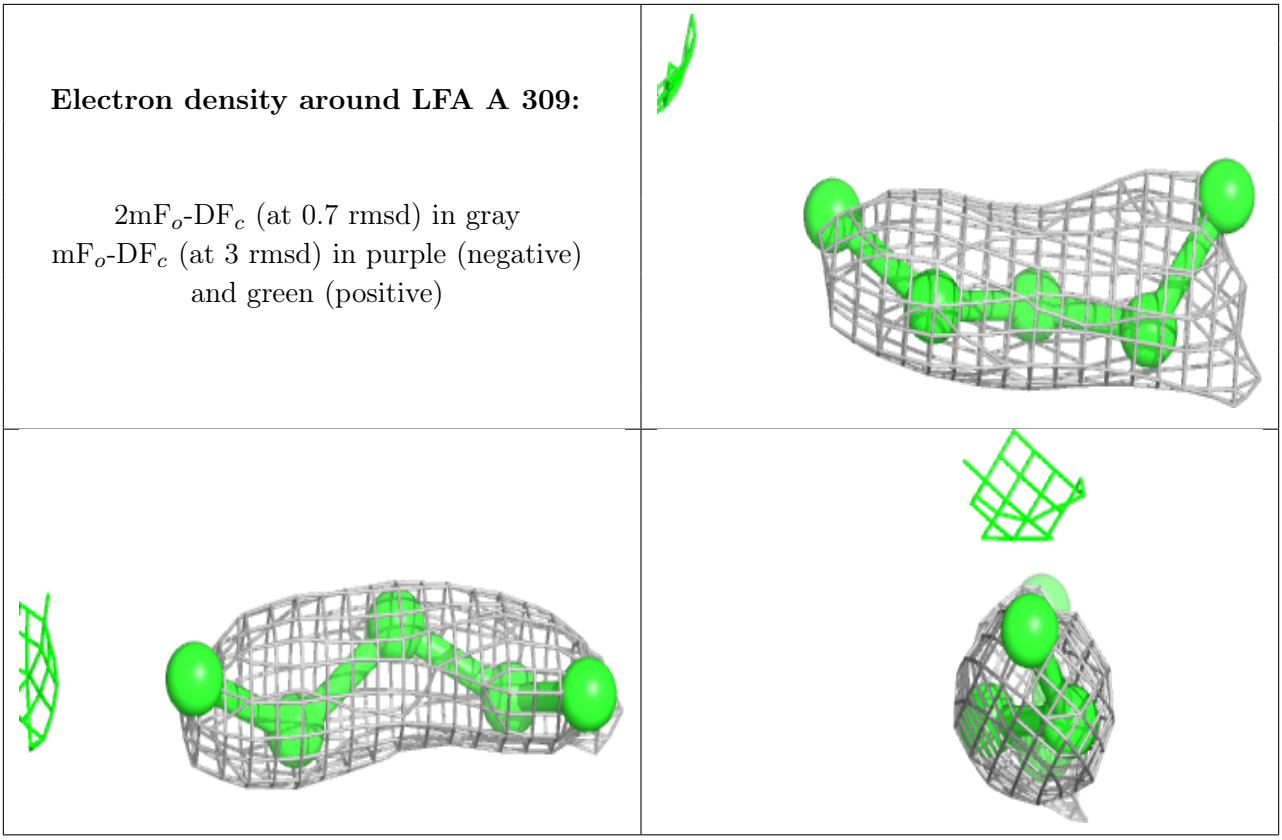
Electron density around NA A 301:

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



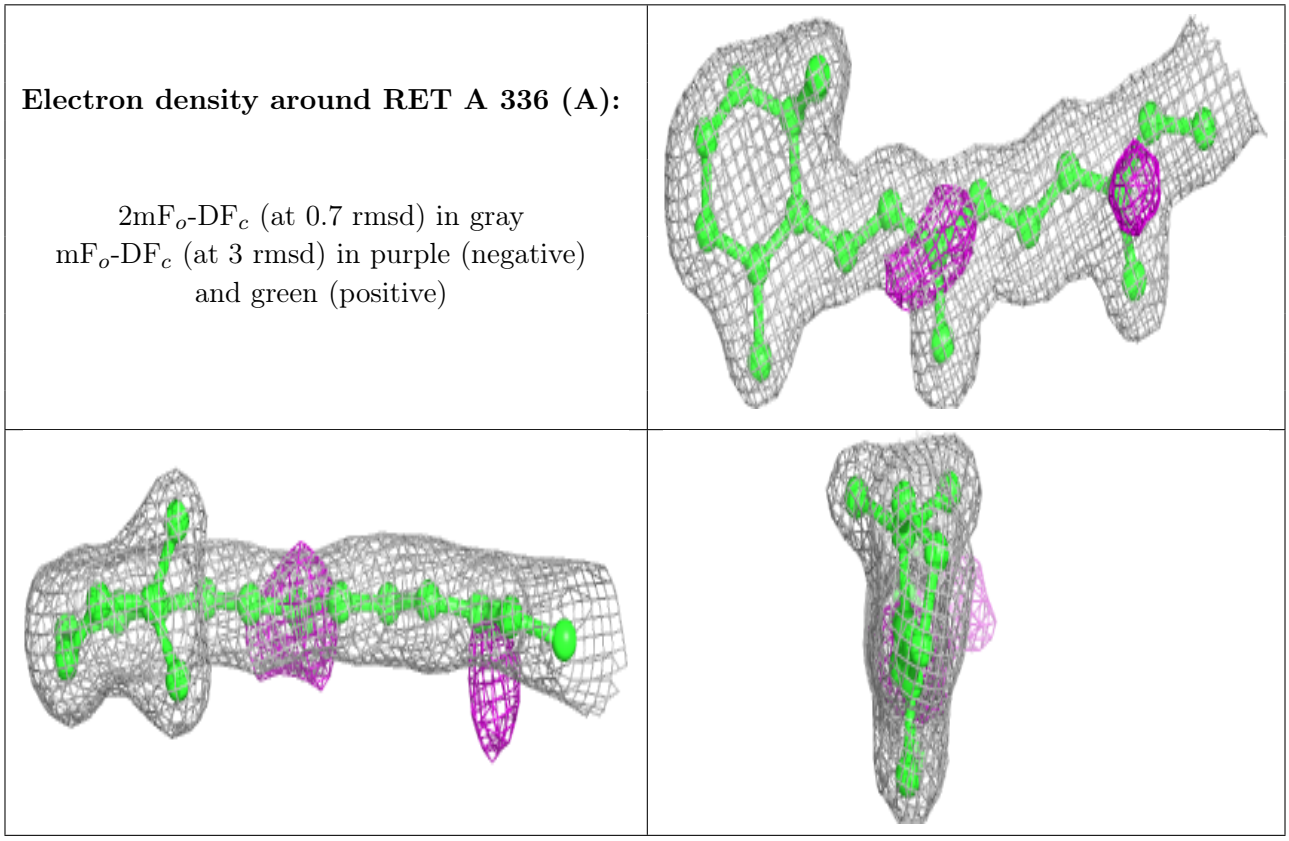
Electron density around LFA A 309:

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



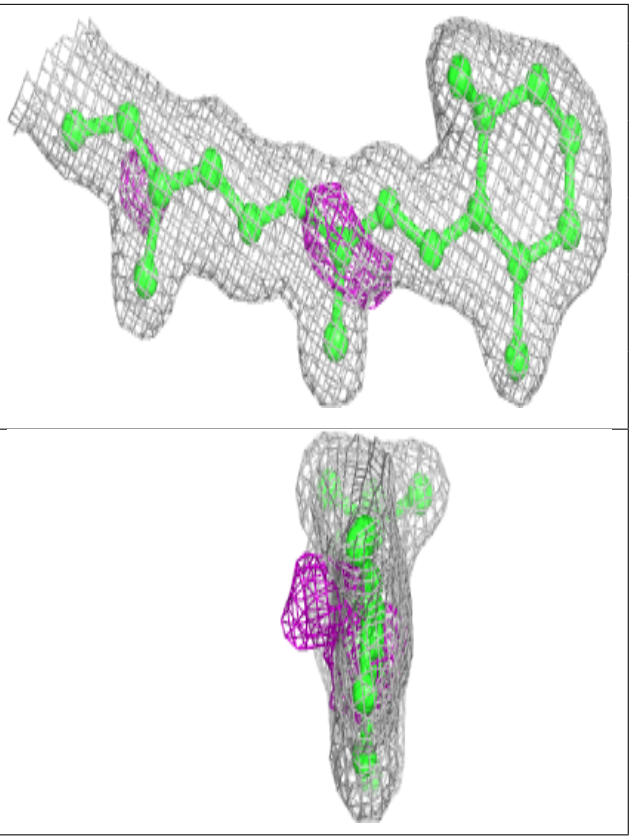
Electron density around RET A 336 (A):

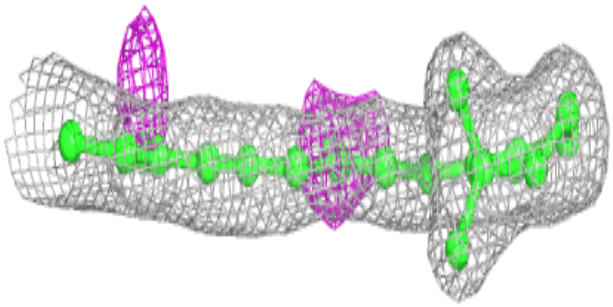
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around RET A 336 (B):

$2mF_o$-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.