



wwPDB X-ray Structure Validation Summary Report

Apr 25, 2026 – 04:28 PM EDT

PDB ID : 6RFA / pdb_00006rfa
Title : Crystal structure of the H30K mutant of the light-driven sodium pump KR2 in the monomeric form, pH 8.0
Authors : Kovalev, K.; Polovinkin, V.; Gushchin, I.; Borshchevskiy, V.; Gordeliy, V.
Deposited on : 2019-04-12
Resolution : 2.20 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

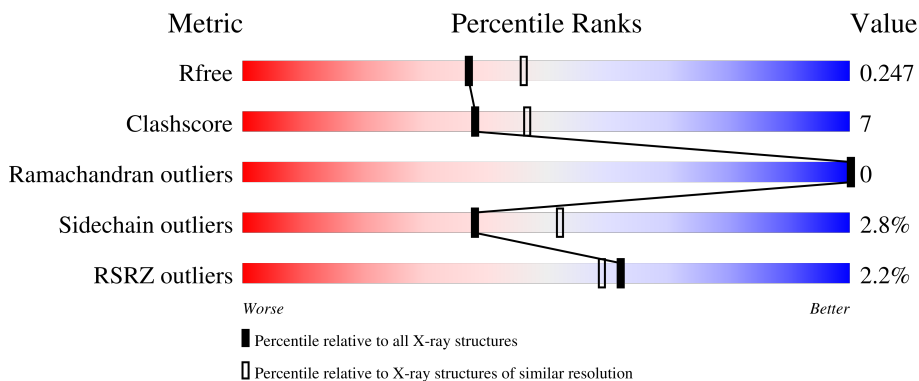
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	288	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2459 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
			Total	C	N	O	S			
1	A	269	2111	1414	318	370	9	0	0	0

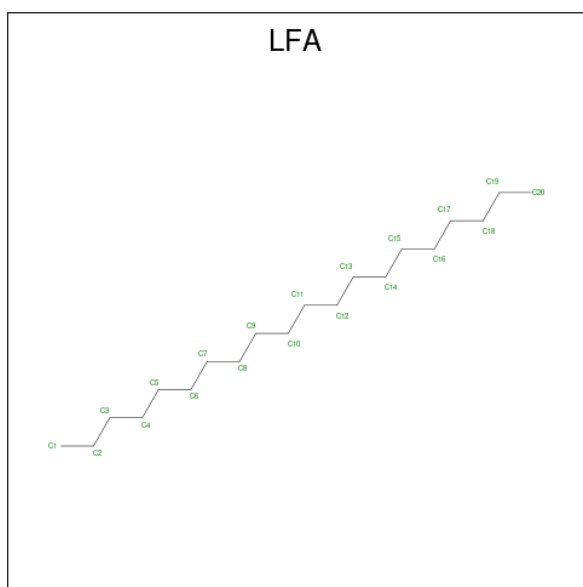
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	LYS	HIS	engineered mutation	UNP N0DKS8
A	281	LEU	-	expression tag	UNP N0DKS8
A	282	GLU	-	expression tag	UNP N0DKS8
A	283	HIS	-	expression tag	UNP N0DKS8
A	284	HIS	-	expression tag	UNP N0DKS8
A	285	HIS	-	expression tag	UNP N0DKS8
A	286	HIS	-	expression tag	UNP N0DKS8
A	287	HIS	-	expression tag	UNP N0DKS8
A	288	HIS	-	expression tag	UNP N0DKS8

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 12 12	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 5 5	0	0
3	A	1	Total C 5 5	0	0

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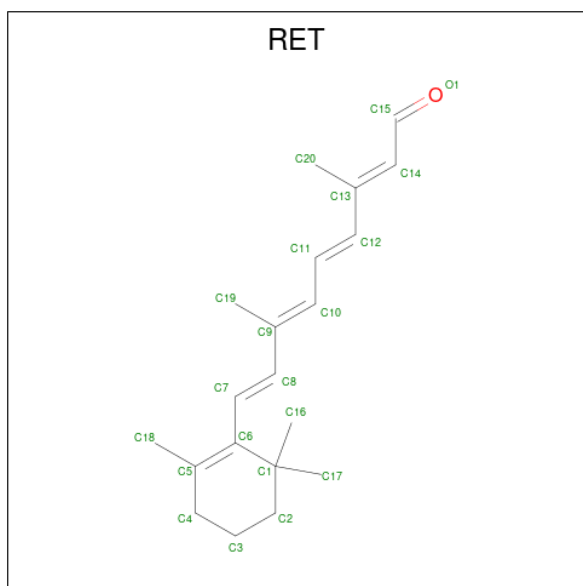
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 11 11	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total 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 12 12	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 20 20	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total 38	O 38	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	40.74Å 84.18Å 234.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.20 19.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.89-2.20) 99.6 (19.89-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.209 , 0.238 0.217 , 0.247	Depositor DCC
R_{free} test set	1013 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2459	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, LFA, GOL, RET

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	0.52	0/2167	0.90	0/2947

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	235	TYR	Peptide
1	A	243	ARG	Sidechain

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	2111	0	2080	21	0
2	A	1	0	0	0	0
3	A	283	0	517	11	0
4	A	6	0	8	0	0
5	A	20	0	27	7	0
6	A	38	0	0	3	0
All	All	2459	0	2632	35	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 7.

The worst 5 of 35 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:202:LYS:CB	6:A:436:HOH:O	2.13	0.97
1:A:230:VAL:HG23	3:A:308:LFA:C8	2.03	0.88
3:A:314:LFA:C2	3:A:315:LFA:C6	2.57	0.82
1:A:139:ARG:HH11	3:A:324:LFA:C6	1.97	0.77
5:A:337:RET:H161	5:A:337:RET:H8	1.68	0.74

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	266/288 (92%)	261 (98%)	5 (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	217/248 (88%)	211 (97%)	6 (3%)	38 52

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	137	SER
1	A	162	SER
1	A	22	GLU
1	A	18	GLU

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	3	GLN
1	A	61	ASN
1	A	112	ASN
1	A	180	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	319	-	5,5,19	0.30	0	4,4,18	0.34	0
5	RET	A	337	1	20,20,21	0.80	1 (5%)	27,27,28	1.74	7 (25%)
3	LFA	A	329	-	10,10,19	0.28	0	9,9,18	0.48	0
3	LFA	A	305	-	4,4,19	0.27	0	3,3,18	0.40	0
3	LFA	A	313	-	9,9,19	0.34	0	8,8,18	0.41	0
3	LFA	A	324	-	5,5,19	0.29	0	4,4,18	0.37	0
3	LFA	A	318	-	9,9,19	0.27	0	8,8,18	0.51	0
3	LFA	A	302	-	7,7,19	0.27	0	6,6,18	0.45	0
3	LFA	A	303	-	8,8,19	0.31	0	7,7,18	0.45	0
3	LFA	A	308	-	7,7,19	0.29	0	6,6,18	0.42	0
3	LFA	A	312	-	4,4,19	0.31	0	3,3,18	0.36	0
3	LFA	A	320	-	4,4,19	0.28	0	3,3,18	0.35	0
3	LFA	A	309	-	7,7,19	0.31	0	6,6,18	0.41	0
3	LFA	A	328	-	4,4,19	0.35	0	3,3,18	0.34	0
3	LFA	A	322	-	3,3,19	0.37	0	2,2,18	0.62	0
3	LFA	A	304	-	5,5,19	0.30	0	4,4,18	0.33	0
4	GOL	A	335	-	5,5,5	0.29	0	5,5,5	0.32	0
3	LFA	A	323	-	5,5,19	0.34	0	4,4,18	0.29	0
3	LFA	A	332	-	9,9,19	0.33	0	8,8,18	0.34	0
3	LFA	A	327	-	2,2,19	0.21	0	1,1,18	0.01	0
3	LFA	A	325	-	9,9,19	0.29	0	8,8,18	0.49	0
3	LFA	A	326	-	6,6,19	0.34	0	5,5,18	0.33	0
3	LFA	A	336	-	19,19,19	0.27	0	18,18,18	0.56	0
3	LFA	A	315	-	4,4,19	0.35	0	3,3,18	0.33	0
3	LFA	A	330	-	3,3,19	0.35	0	2,2,18	0.63	0
3	LFA	A	311	-	15,15,19	0.30	0	14,14,18	0.50	0
3	LFA	A	317	-	11,11,19	0.26	0	10,10,18	0.53	0
3	LFA	A	331	-	4,4,19	0.38	0	3,3,18	0.30	0
3	LFA	A	334	-	9,9,19	0.28	0	8,8,18	0.45	0
3	LFA	A	321	-	5,5,19	0.34	0	4,4,18	0.27	0
3	LFA	A	310	-	11,11,19	0.31	0	10,10,18	0.39	0
3	LFA	A	314	-	4,4,19	0.35	0	3,3,18	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	A	333	-	11,11,19	0.29	0	10,10,18	0.48	0
3	LFA	A	316	-	10,10,19	0.33	0	9,9,18	0.42	0
3	LFA	A	306	-	12,12,19	0.26	0	11,11,18	0.53	0
3	LFA	A	307	-	9,9,19	0.29	0	8,8,18	0.45	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	319	-	-	1/3/3/17	-
5	RET	A	337	1	-	0/13/30/31	0/1/1/1
3	LFA	A	329	-	-	5/8/8/17	-
3	LFA	A	305	-	-	0/2/2/17	-
3	LFA	A	313	-	-	3/7/7/17	-
3	LFA	A	324	-	-	1/3/3/17	-
3	LFA	A	318	-	-	3/7/7/17	-
3	LFA	A	302	-	-	4/5/5/17	-
3	LFA	A	303	-	-	1/6/6/17	-
3	LFA	A	308	-	-	2/5/5/17	-
3	LFA	A	312	-	-	2/2/2/17	-
3	LFA	A	320	-	-	0/2/2/17	-
3	LFA	A	309	-	-	1/5/5/17	-
3	LFA	A	328	-	-	0/2/2/17	-
3	LFA	A	322	-	-	0/1/1/17	-
3	LFA	A	304	-	-	2/3/3/17	-
4	GOL	A	335	-	-	2/4/4/4	-
3	LFA	A	323	-	-	3/3/3/17	-
3	LFA	A	332	-	-	6/7/7/17	-
3	LFA	A	325	-	-	4/7/7/17	-
3	LFA	A	326	-	-	3/4/4/17	-
3	LFA	A	336	-	-	9/17/17/17	-
3	LFA	A	315	-	-	1/2/2/17	-
3	LFA	A	330	-	-	0/1/1/17	-
3	LFA	A	311	-	-	6/13/13/17	-
3	LFA	A	317	-	-	4/9/9/17	-
3	LFA	A	331	-	-	1/2/2/17	-
3	LFA	A	334	-	-	4/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	321	-	-	2/3/3/17	-
3	LFA	A	310	-	-	5/9/9/17	-
3	LFA	A	314	-	-	1/2/2/17	-
3	LFA	A	333	-	-	6/9/9/17	-
3	LFA	A	316	-	-	2/8/8/17	-
3	LFA	A	306	-	-	4/10/10/17	-
3	LFA	A	307	-	-	4/7/7/17	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	337	RET	C14-C13	2.30	1.35	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	337	RET	C18-C5-C6	-4.99	119.03	124.48
5	A	337	RET	C7-C8-C9	-2.90	121.95	126.23
5	A	337	RET	C11-C10-C9	-2.75	123.42	127.28
5	A	337	RET	C10-C11-C12	-2.27	116.61	123.20
5	A	337	RET	C19-C9-C8	2.23	121.50	118.09

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	335	GOL	O1-C1-C2-C3
3	A	310	LFA	C4-C5-C6-C7
3	A	317	LFA	C3-C4-C5-C6
3	A	321	LFA	C2-C3-C4-C5
3	A	329	LFA	C4-C5-C6-C7

There are no ring outliers.

14 monomers are involved in 18 short contacts:

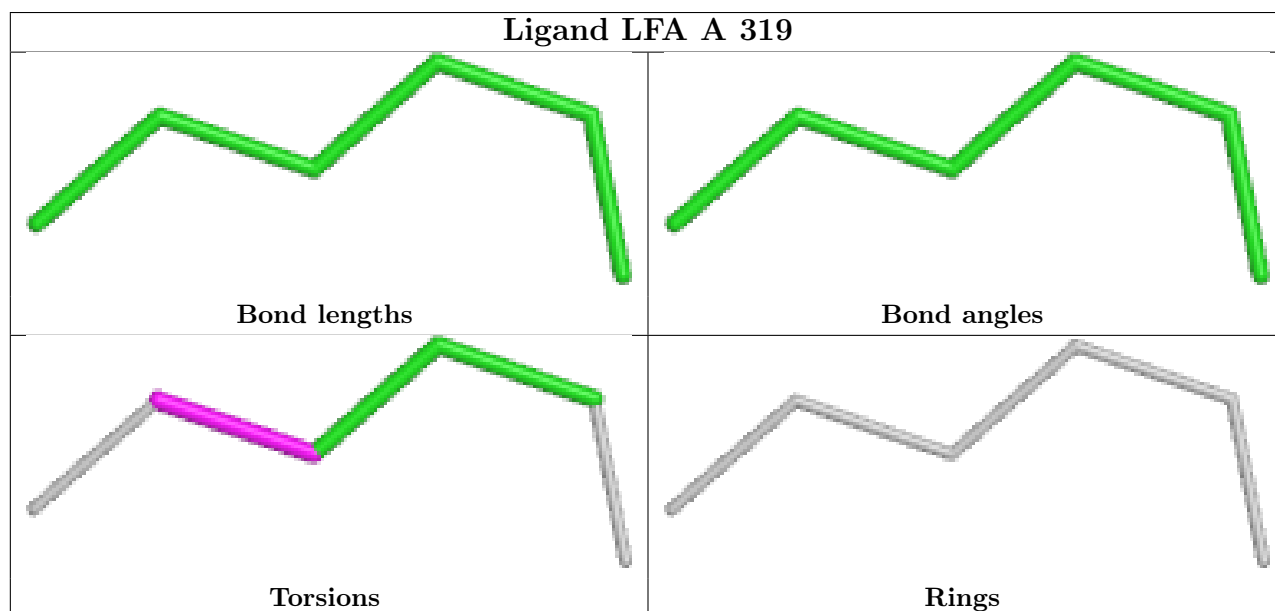
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3	A	319	LFA	1	0
5	A	337	RET	7	0
3	A	324	LFA	2	0

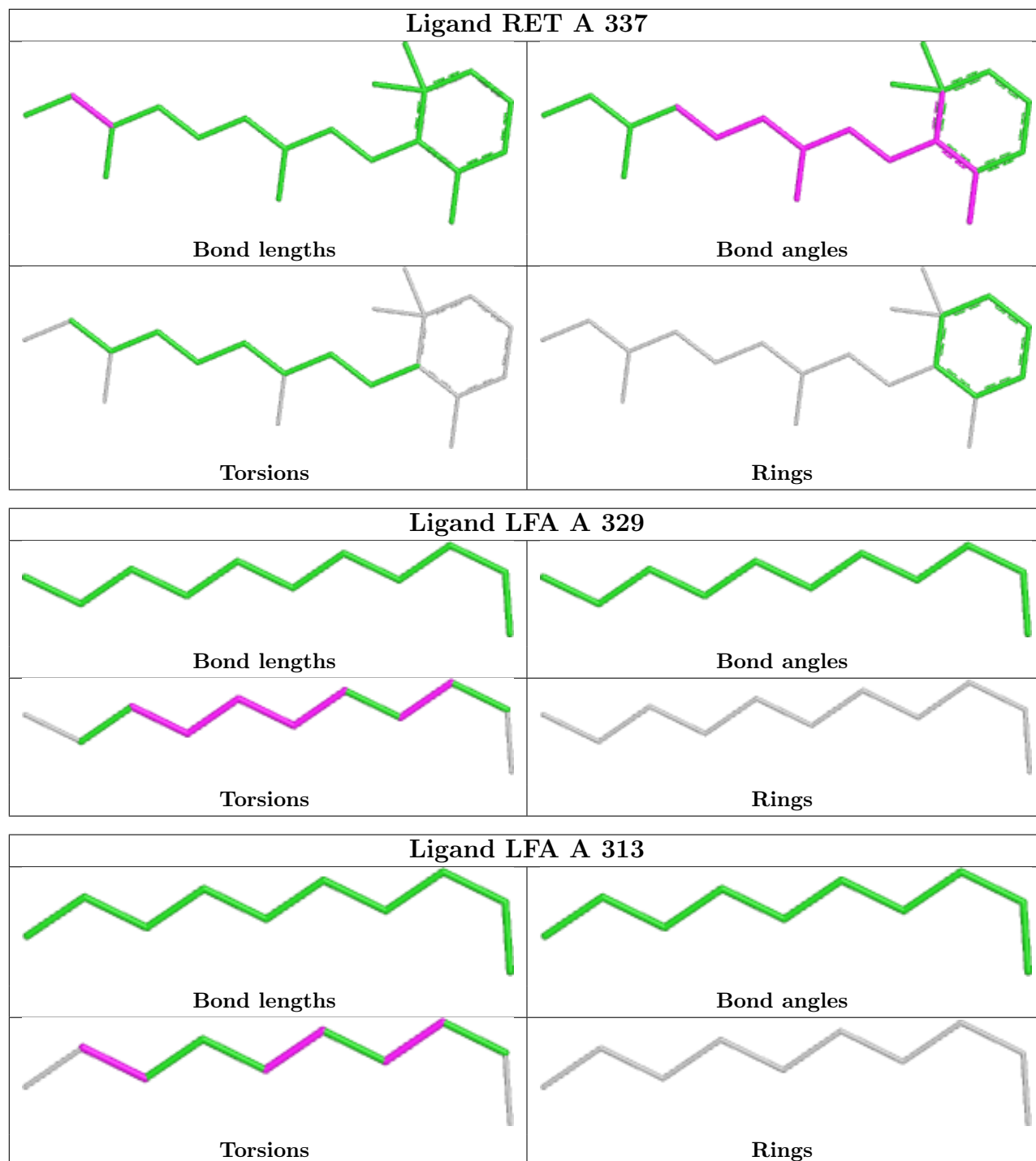
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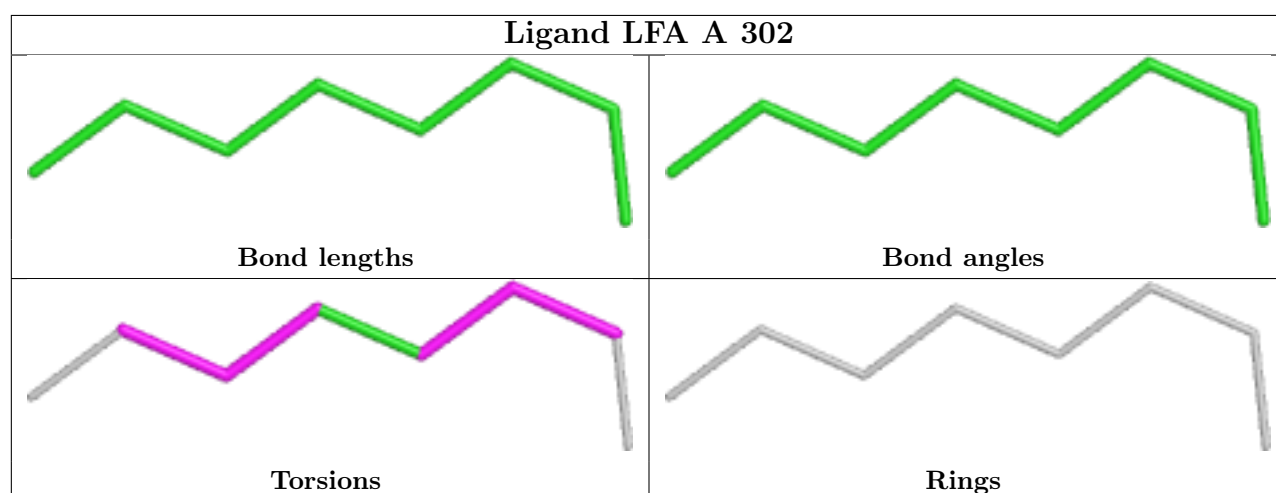
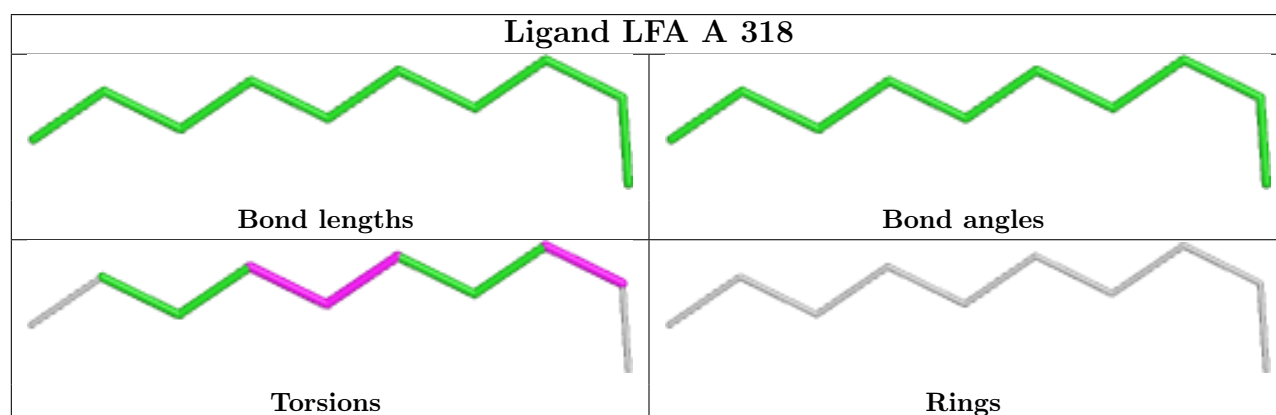
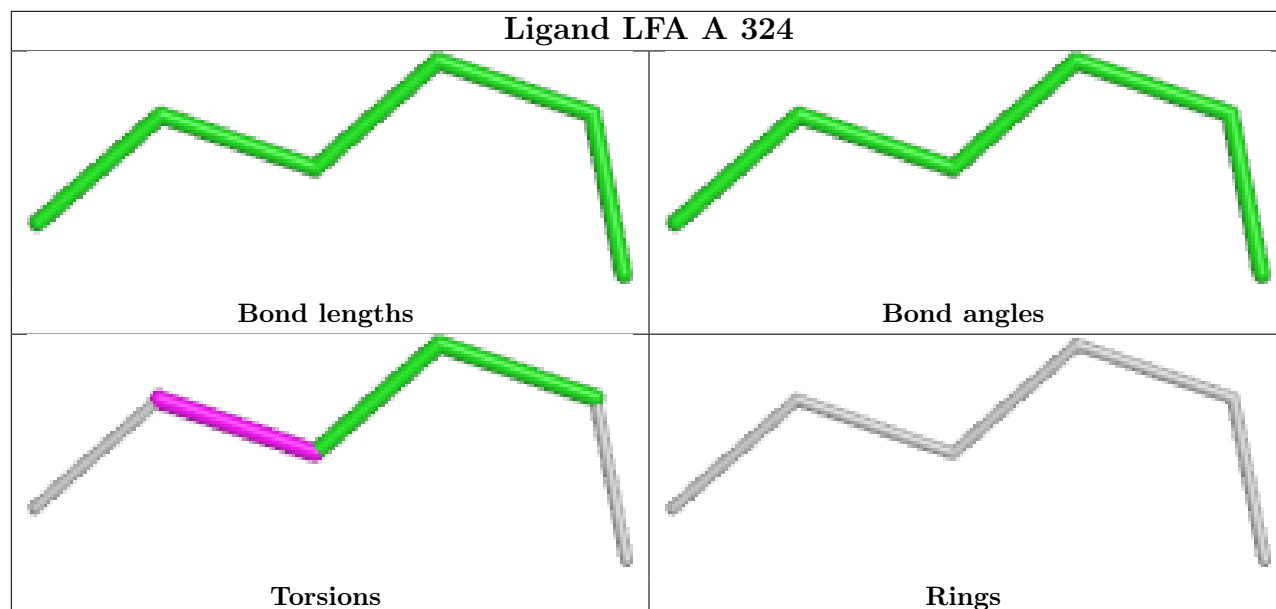
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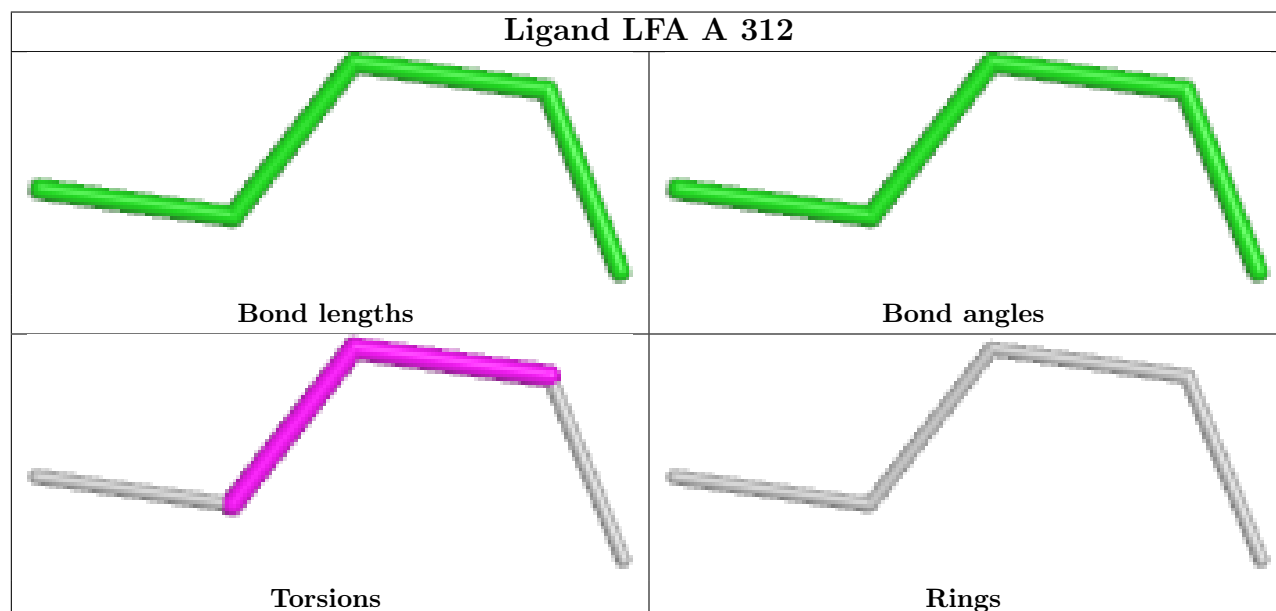
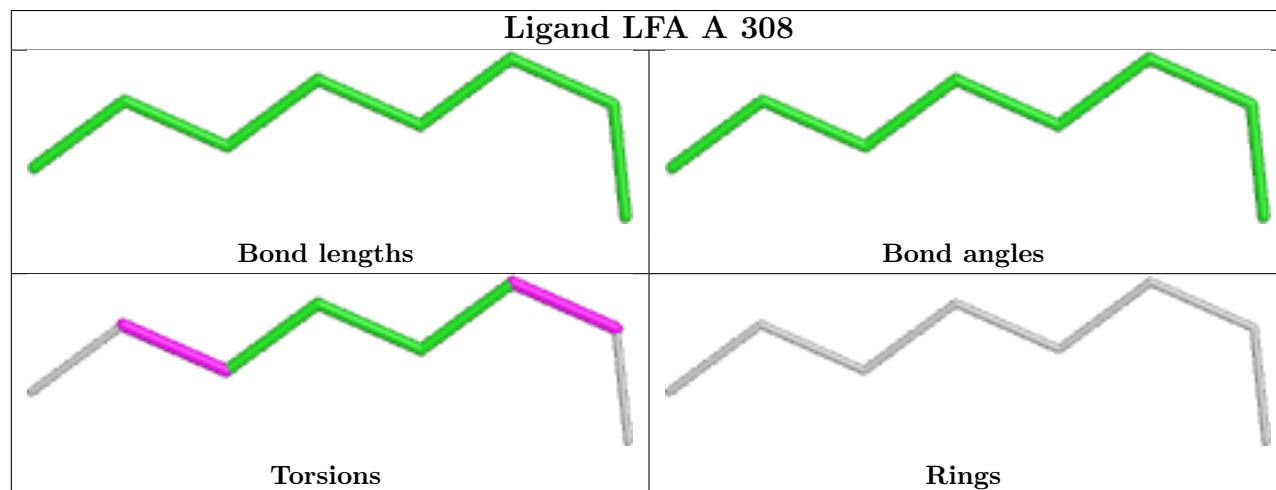
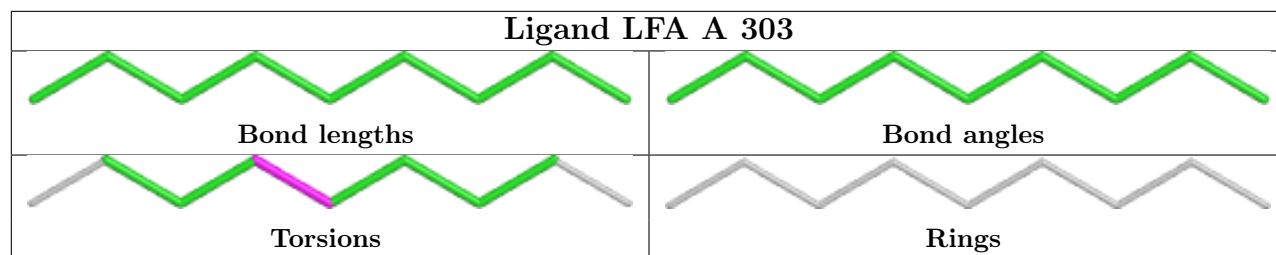
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	308	LFA	1	0
3	A	304	LFA	2	0
3	A	325	LFA	2	0
3	A	336	LFA	2	0
3	A	315	LFA	1	0
3	A	330	LFA	1	0
3	A	317	LFA	1	0
3	A	331	LFA	1	0
3	A	321	LFA	2	0
3	A	310	LFA	1	0
3	A	314	LFA	1	0

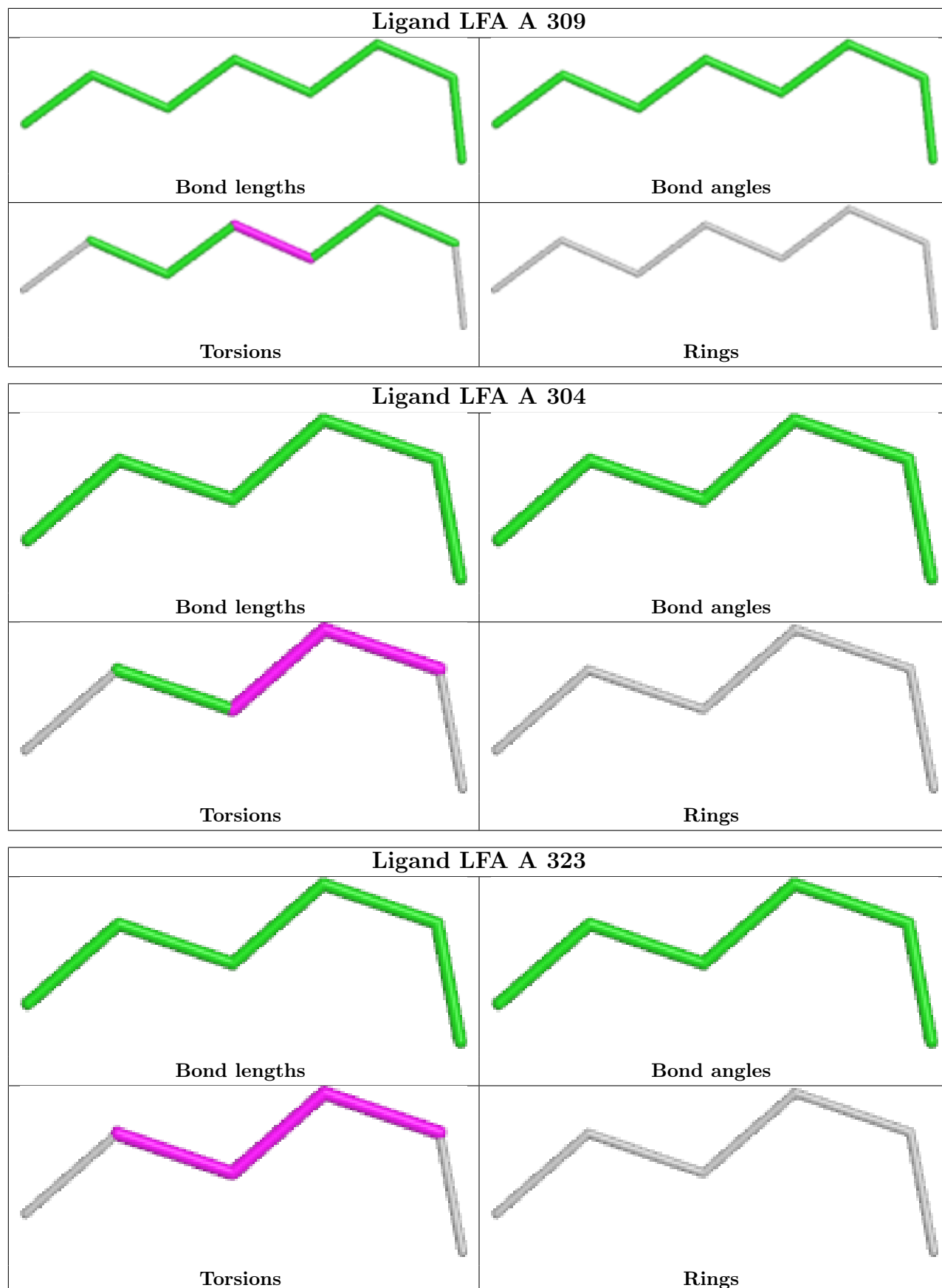
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

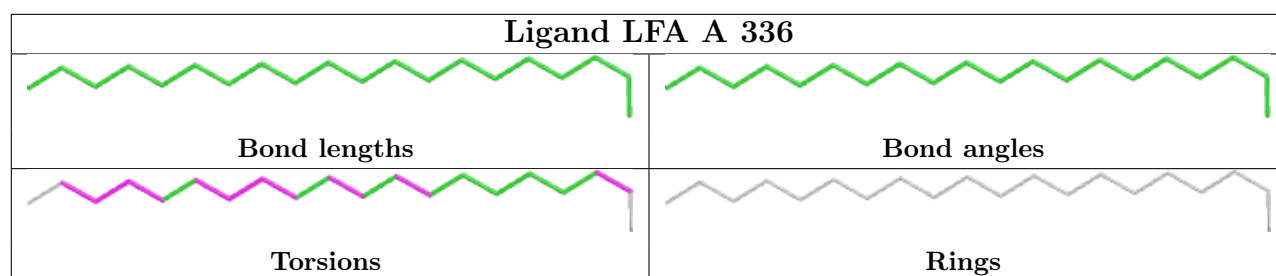
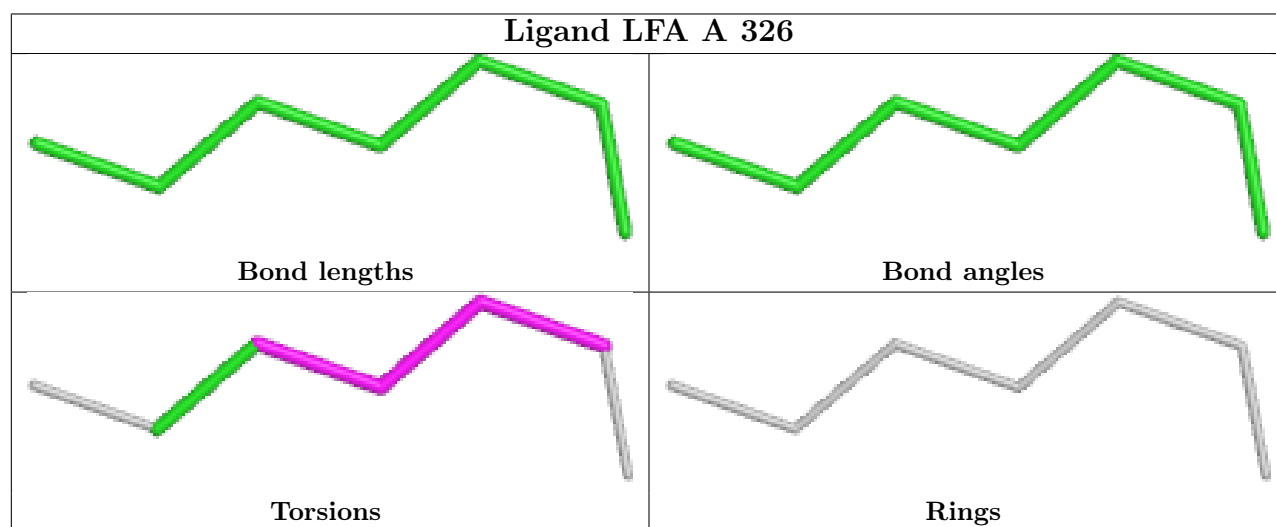
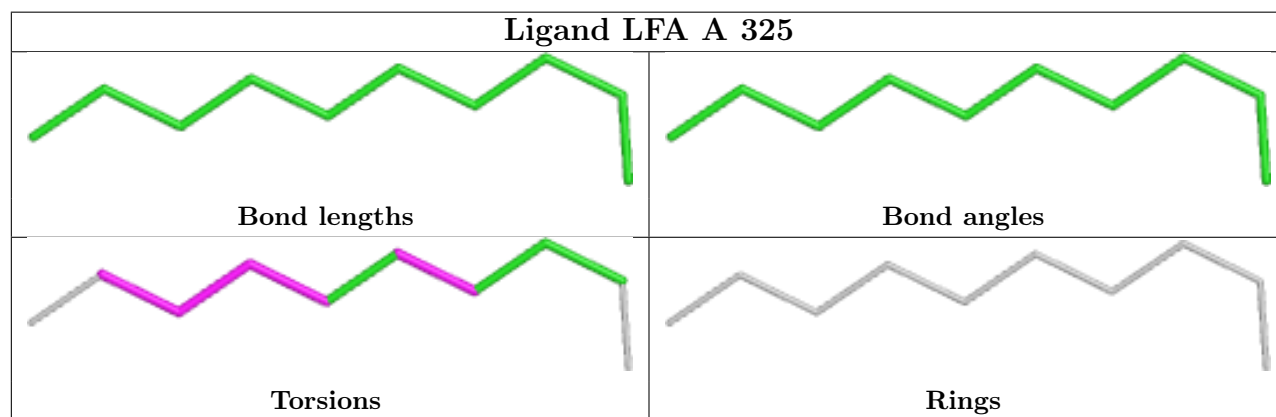
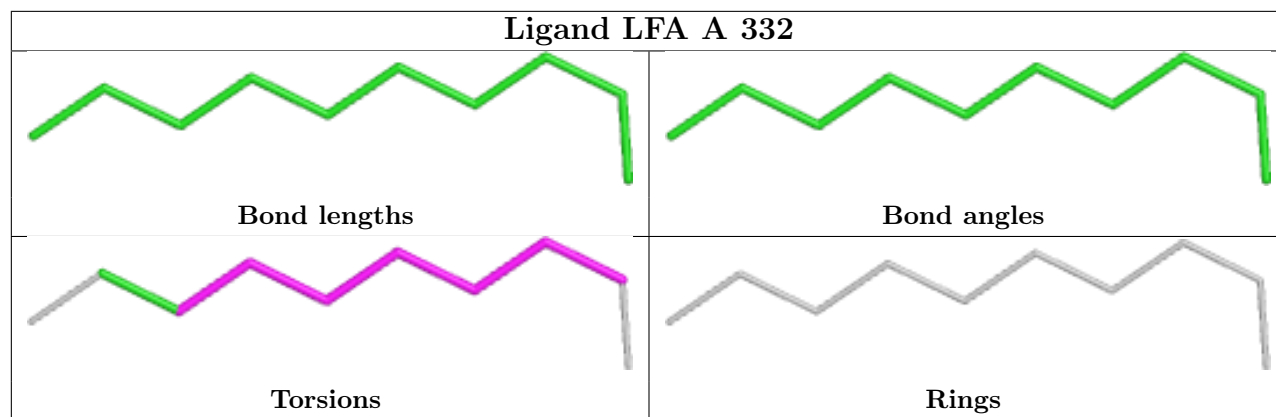


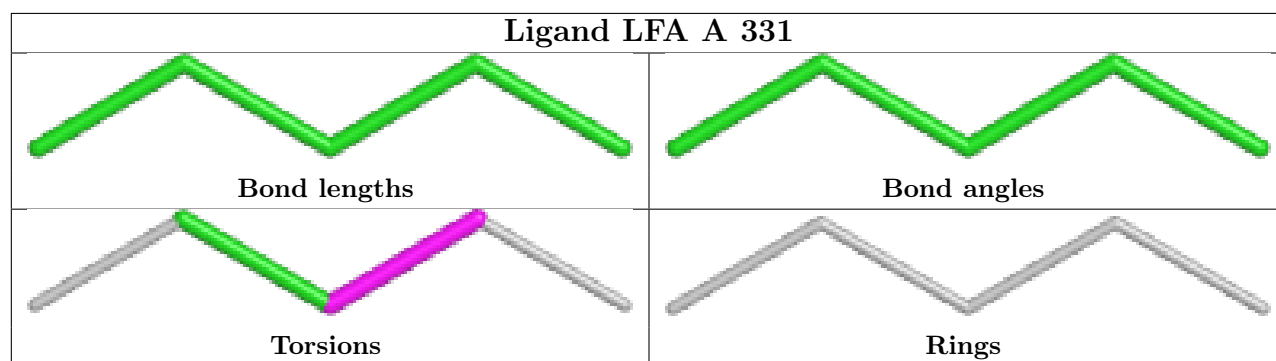
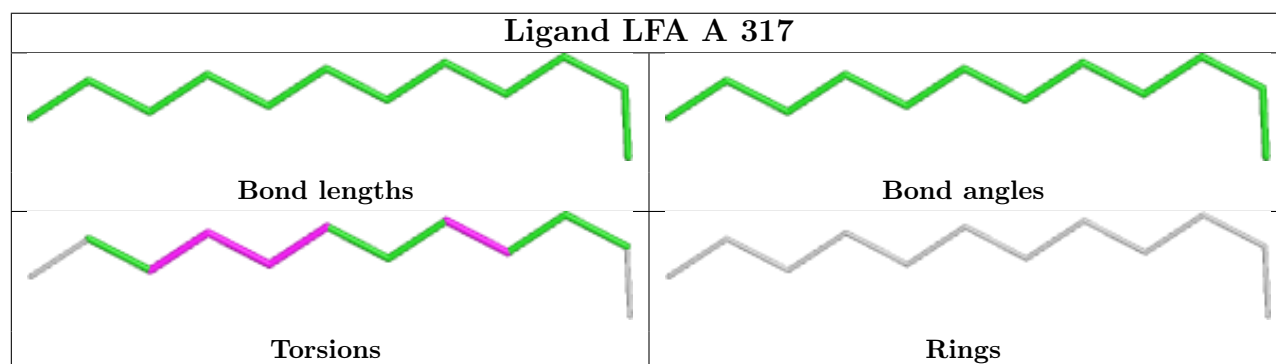
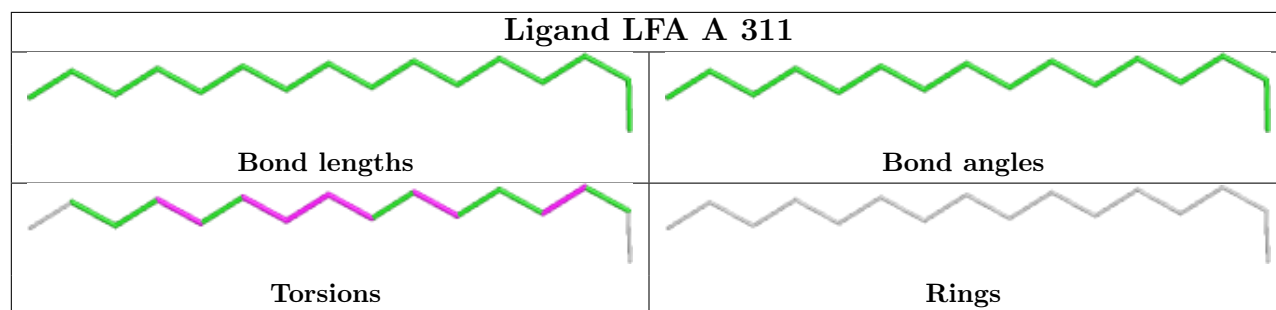
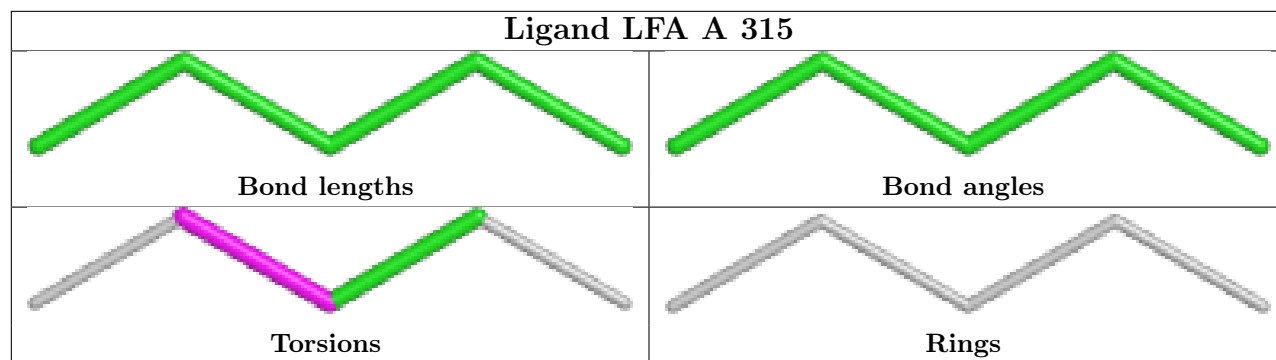


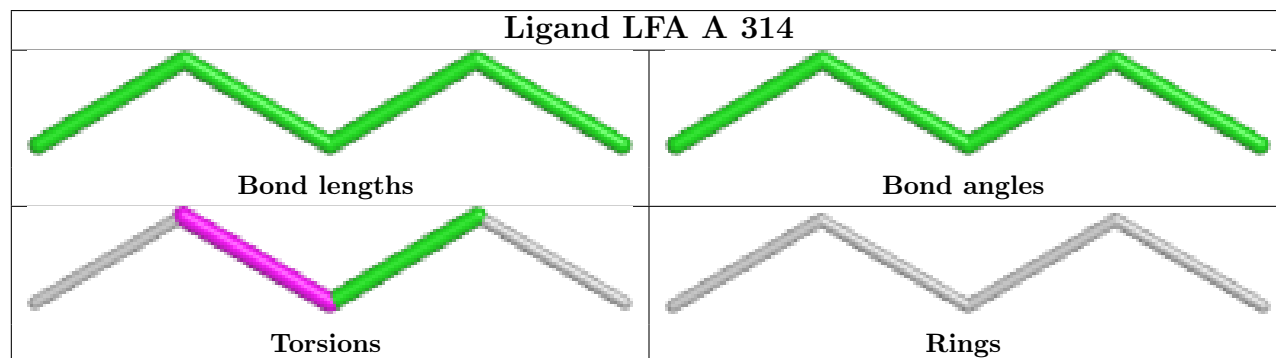
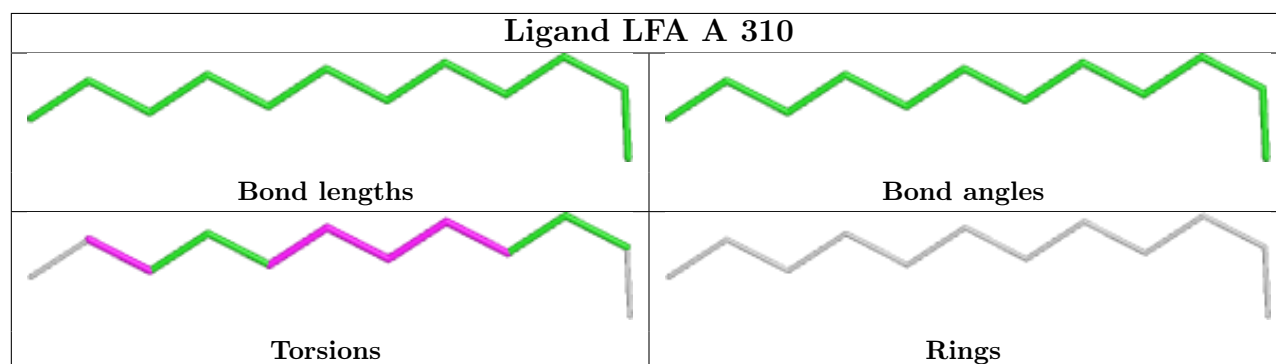
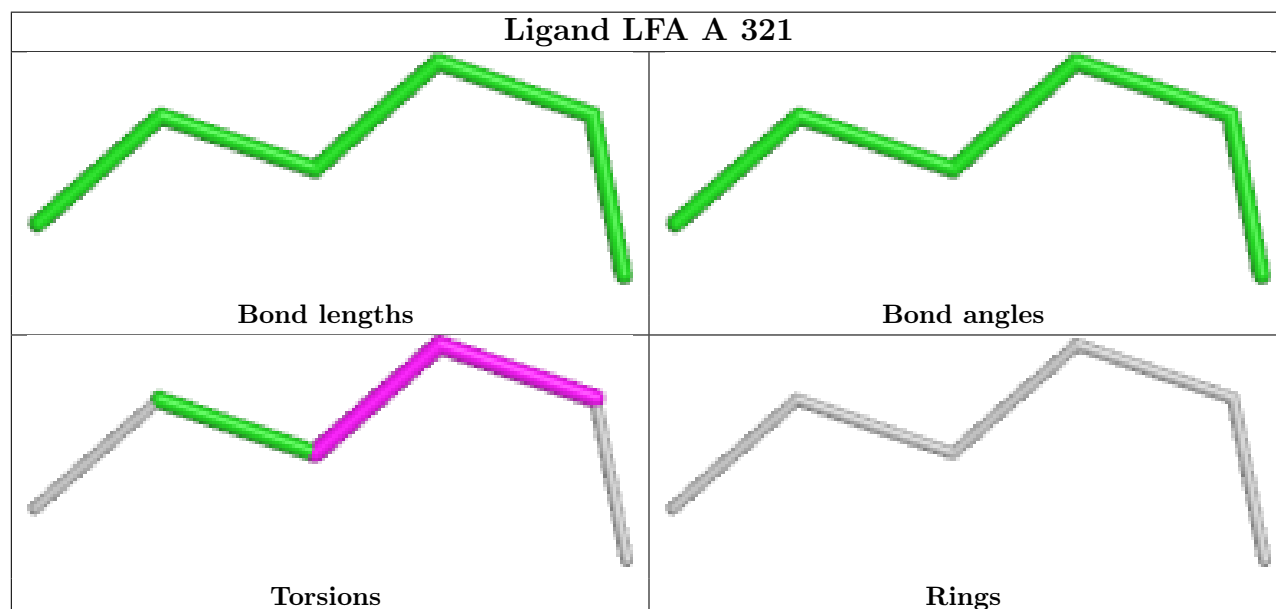
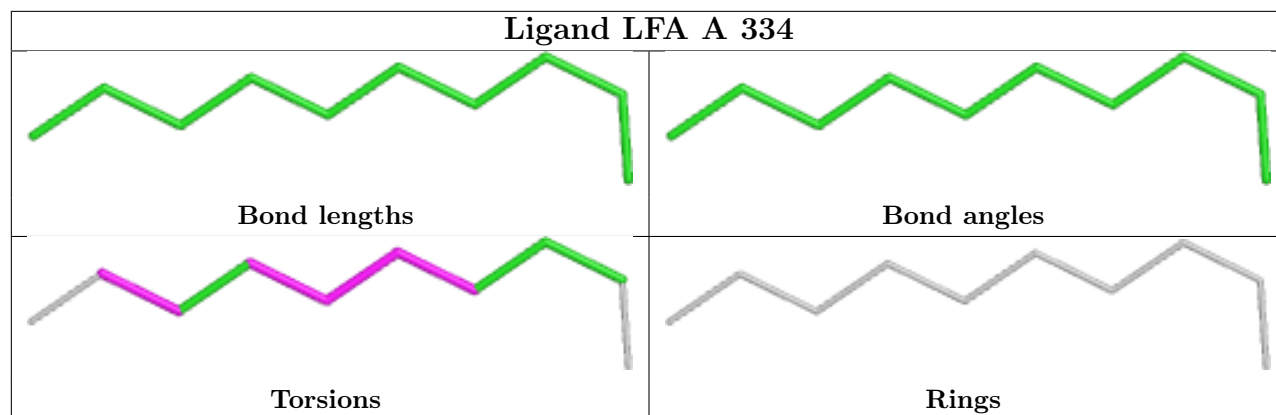


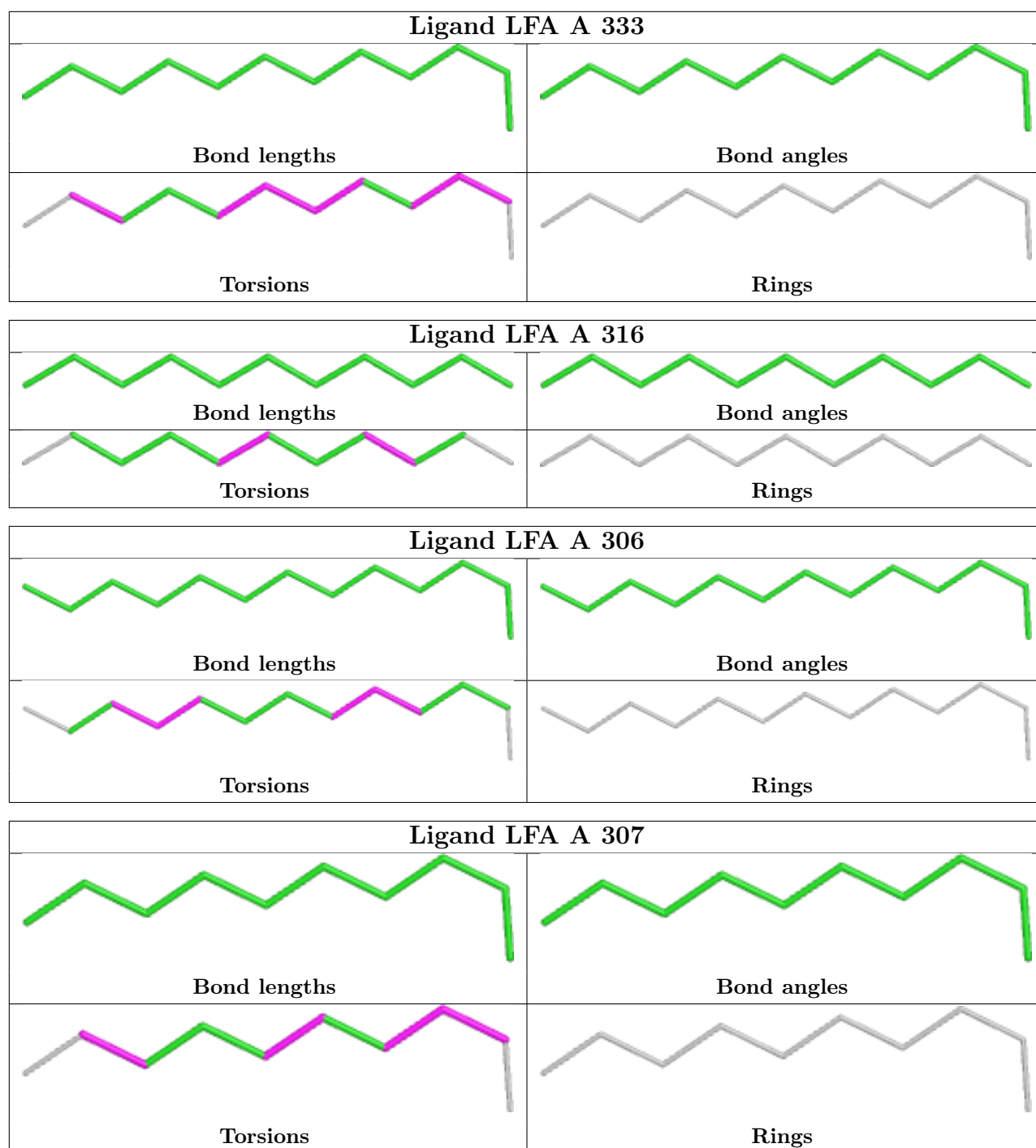












5.7 Other polymers [i](#)

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	269/288 (93%)	-0.24	6 (2%) 62 59	22, 35, 63, 87	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	3.5
1	A	270	SER	2.6
1	A	5	LEU	2.5
1	A	230	VAL	2.5
1	A	158	PHE	2.2

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 oligosaccharides 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
3	LFA	A	324	6/20	0.39	0.25	46,82,85,86	0
3	LFA	A	331	5/20	0.52	0.21	65,66,82,83	0

Continued on next page...

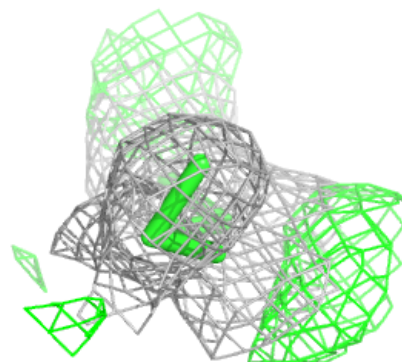
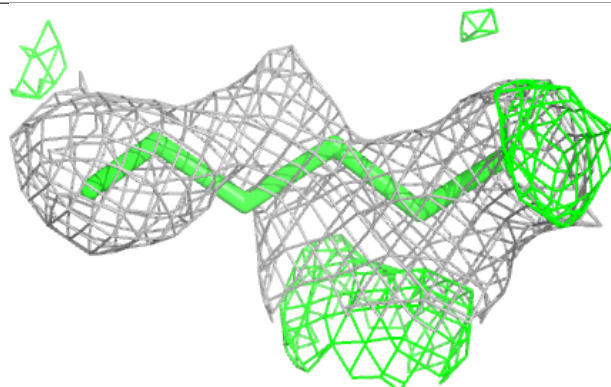
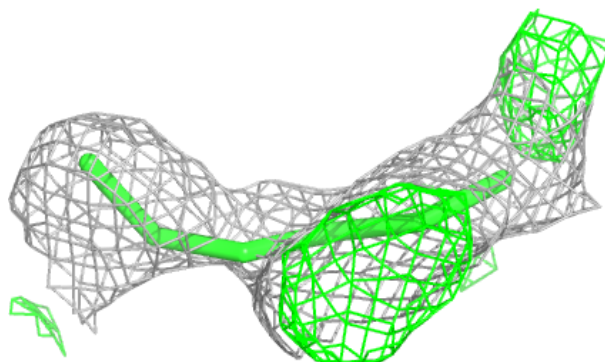
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	335	6/6	0.53	0.18	100,125,137,140	0
3	LFA	A	328	5/20	0.57	0.23	71,72,76,79	0
3	LFA	A	326	7/20	0.60	0.21	67,75,81,82	0
3	LFA	A	330	4/20	0.61	0.22	78,82,82,84	0
3	LFA	A	316	11/20	0.65	0.17	72,80,93,104	0
3	LFA	A	321	6/20	0.65	0.20	66,72,78,80	0
3	LFA	A	334	10/20	0.67	0.20	65,91,106,110	0
3	LFA	A	332	10/20	0.68	0.23	71,81,92,96	0
3	LFA	A	322	4/20	0.69	0.21	49,60,60,65	0
3	LFA	A	325	10/20	0.71	0.17	66,81,89,95	0
3	LFA	A	318	10/20	0.71	0.18	76,85,88,91	0
3	LFA	A	323	6/20	0.72	0.17	57,65,71,71	0
3	LFA	A	313	10/20	0.72	0.23	56,77,98,106	0
3	LFA	A	319	6/20	0.74	0.20	51,59,66,71	0
3	LFA	A	327	3/20	0.74	0.21	63,63,73,73	0
3	LFA	A	308	8/20	0.75	0.17	61,66,88,88	0
3	LFA	A	310	12/20	0.75	0.18	58,83,93,102	0
3	LFA	A	317	12/20	0.75	0.22	81,91,116,120	0
3	LFA	A	320	5/20	0.76	0.20	75,78,82,86	0
3	LFA	A	311	16/20	0.77	0.14	64,69,90,92	0
3	LFA	A	309	8/20	0.78	0.14	55,62,70,75	0
3	LFA	A	303	9/20	0.79	0.15	58,64,67,67	0
3	LFA	A	314	5/20	0.79	0.16	55,57,62,66	0
3	LFA	A	304	6/20	0.80	0.14	50,68,72,76	0
3	LFA	A	305	5/20	0.81	0.14	67,70,72,75	0
3	LFA	A	336	20/20	0.82	0.13	43,69,83,85	0
3	LFA	A	312	5/20	0.83	0.14	57,58,64,65	0
3	LFA	A	307	10/20	0.83	0.13	41,51,78,81	0
3	LFA	A	333	12/20	0.84	0.15	63,68,78,79	0
3	LFA	A	329	11/20	0.84	0.14	55,60,76,77	0
3	LFA	A	315	5/20	0.85	0.13	53,55,60,60	0
2	NA	A	301	1/1	0.86	0.16	60,60,60,60	0
3	LFA	A	302	8/20	0.88	0.20	31,33,75,272	8
3	LFA	A	306	13/20	0.88	0.16	48,51,76,77	0
5	RET	A	337	20/21	0.92	0.09	27,31,35,37	0

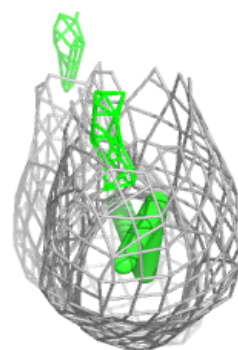
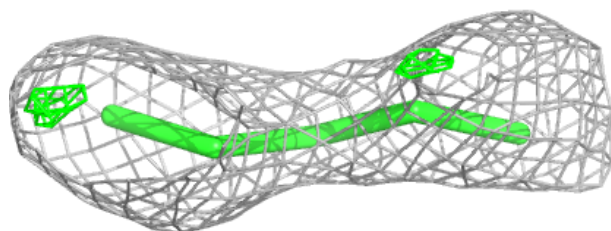
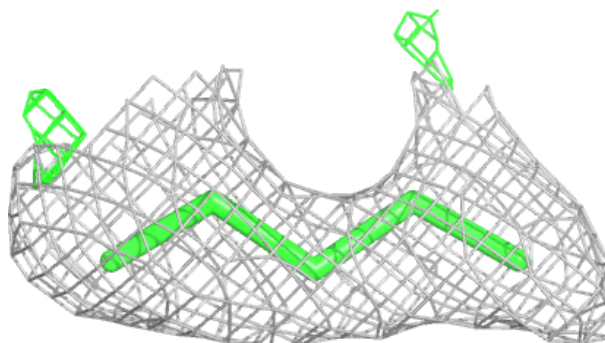
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA A 324:

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

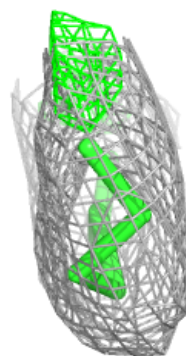
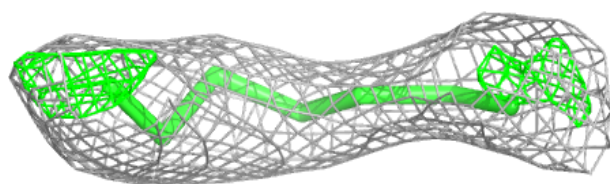
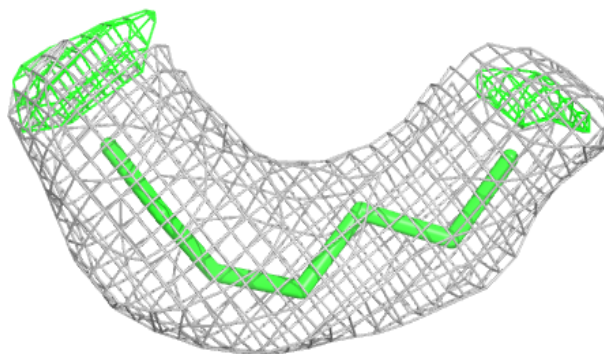
**Electron density around LFA A 331:**

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

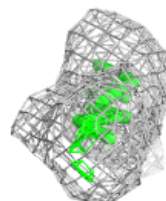
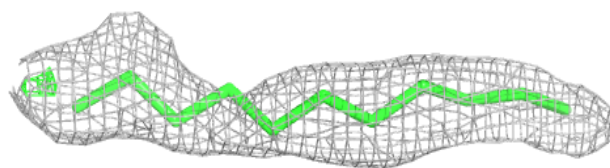
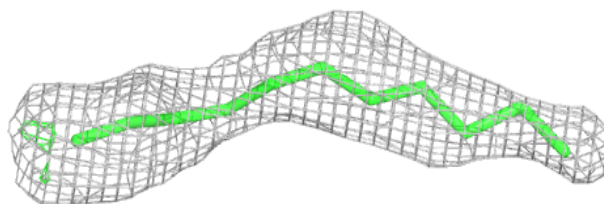


Electron density around LFA A 326:

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

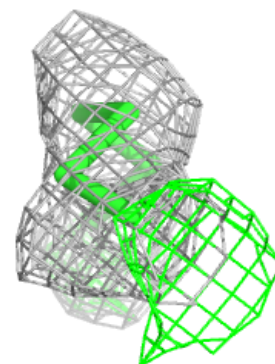
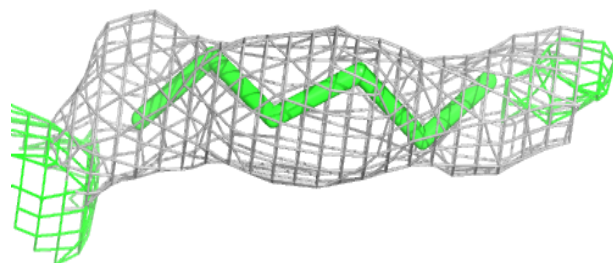
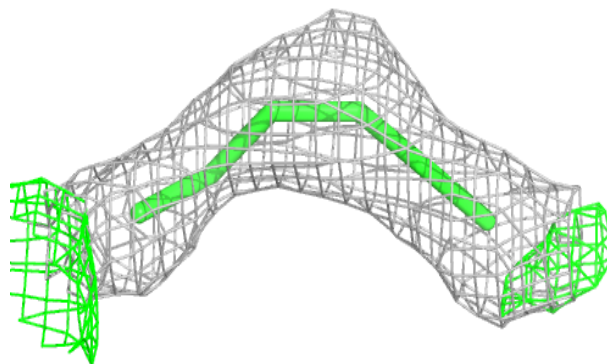
**Electron density around LFA A 316:**

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

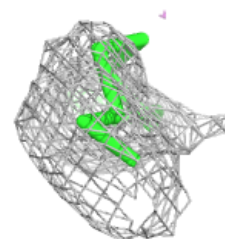
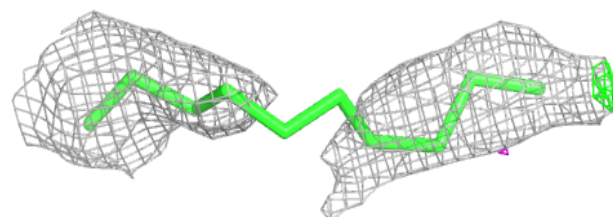
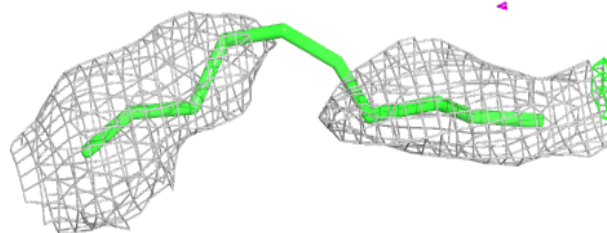


Electron density around LFA A 321:

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

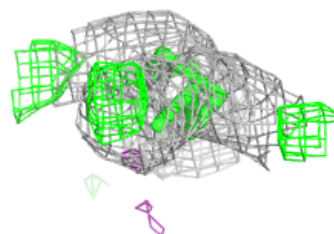
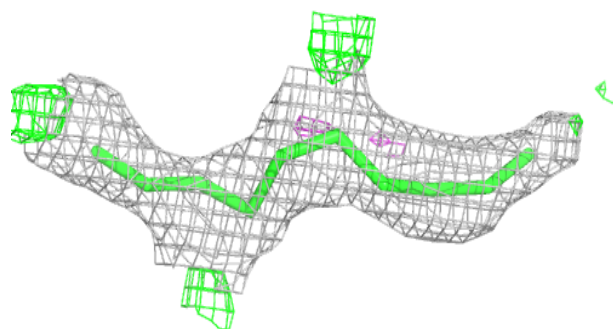
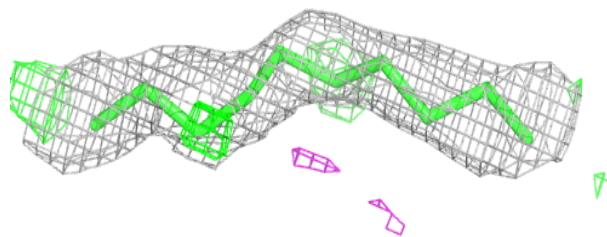
**Electron density around LFA A 334:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

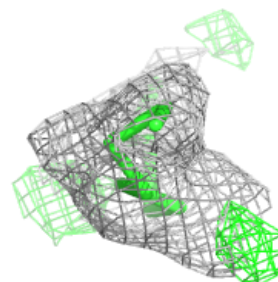
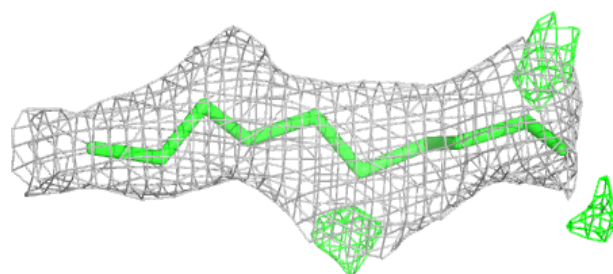
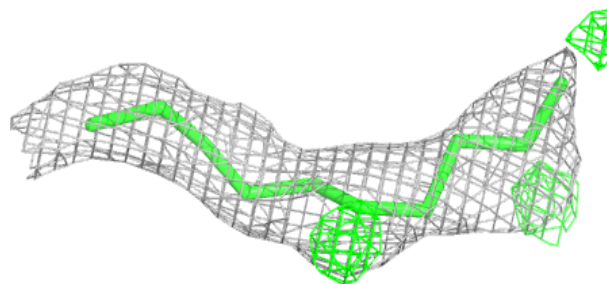


Electron density around LFA A 332:

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

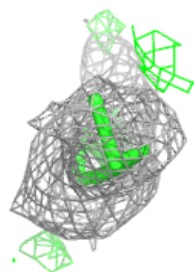
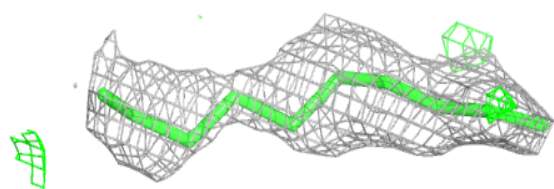
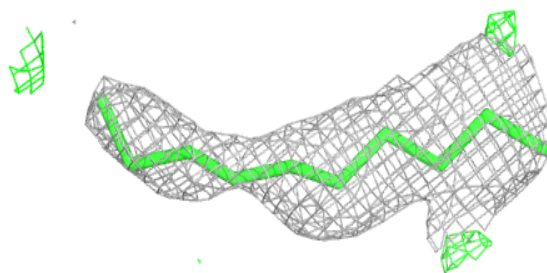
**Electron density around LFA A 325:**

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

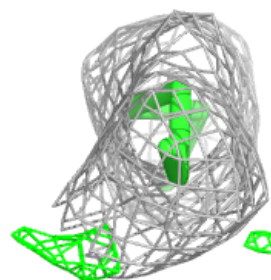
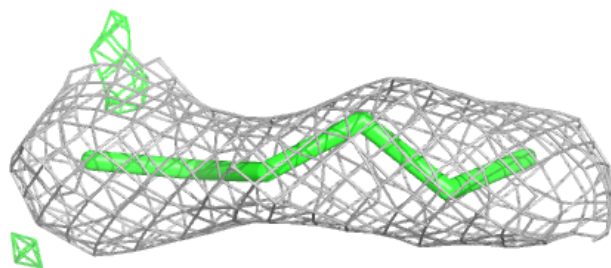
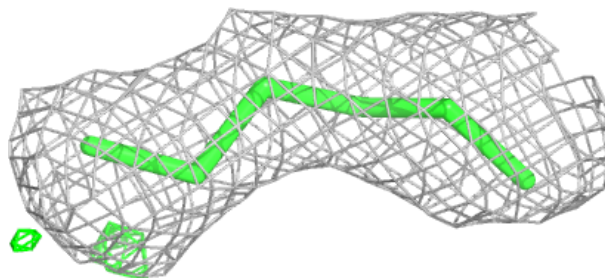


Electron density around LFA A 318:

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

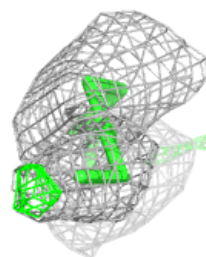
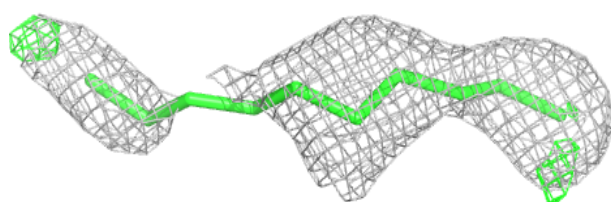
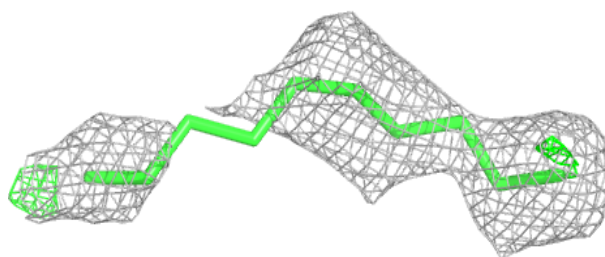
**Electron density around LFA A 323:**

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

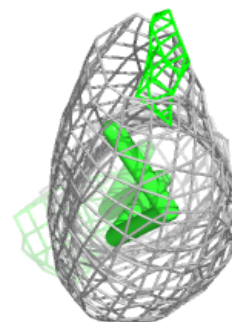
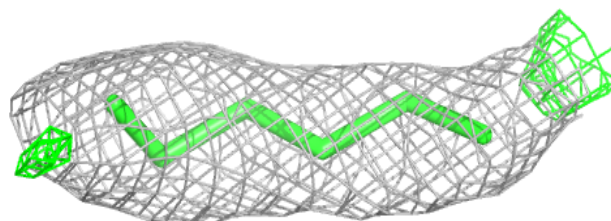
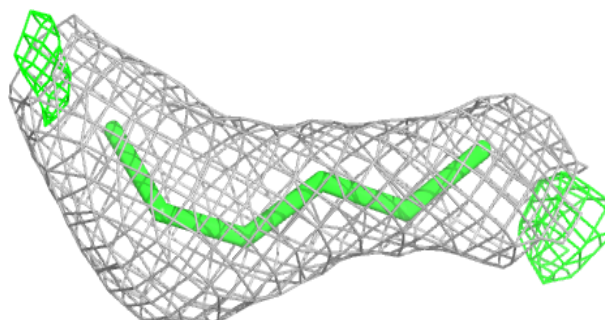


Electron density around LFA A 313:

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

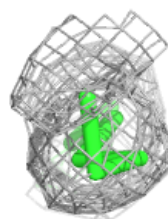
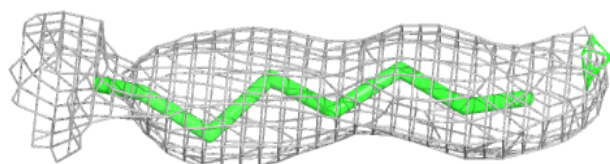
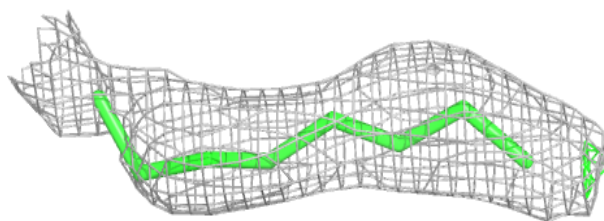
**Electron density around LFA A 319:**

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

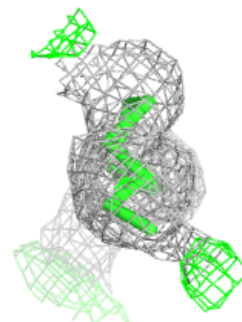
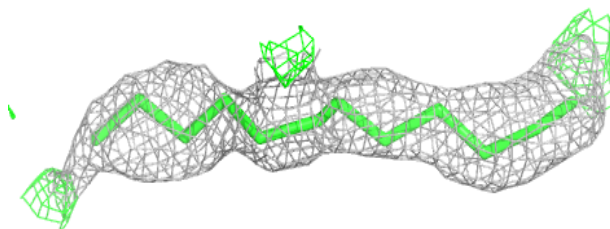
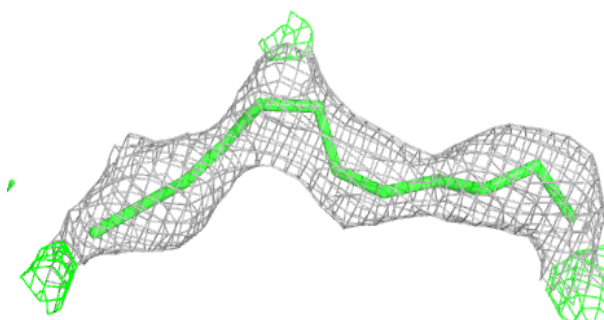


Electron density around LFA A 308:

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

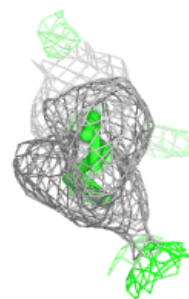
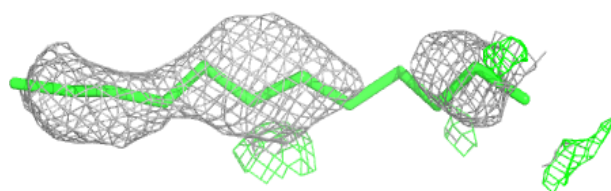
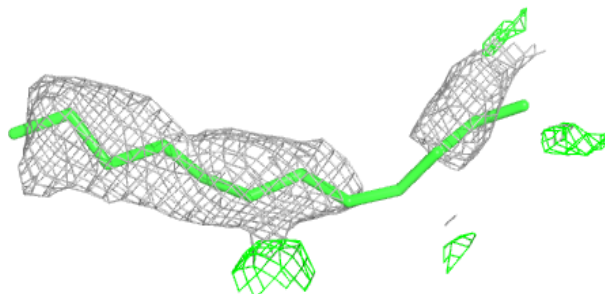
**Electron density around LFA A 310:**

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

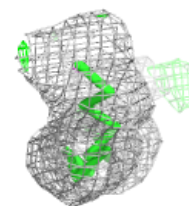
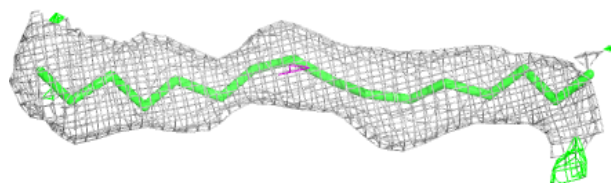
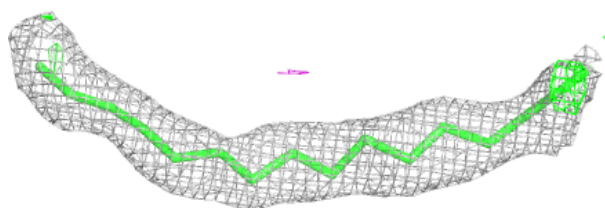


Electron density around LFA A 317:

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

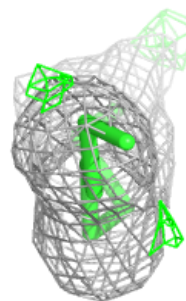
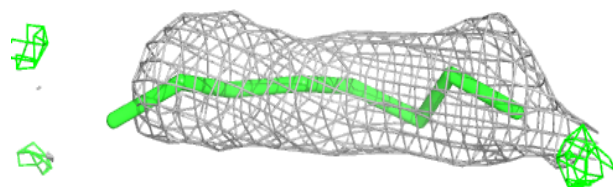
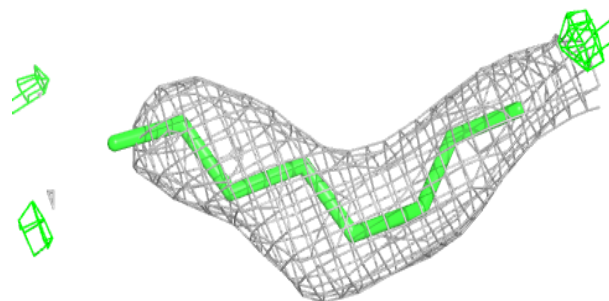
**Electron density around LFA A 311:**

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

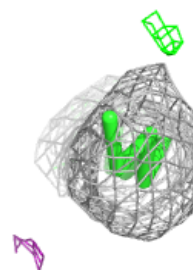
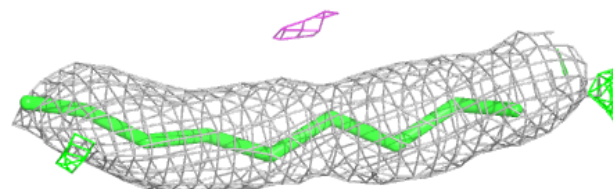
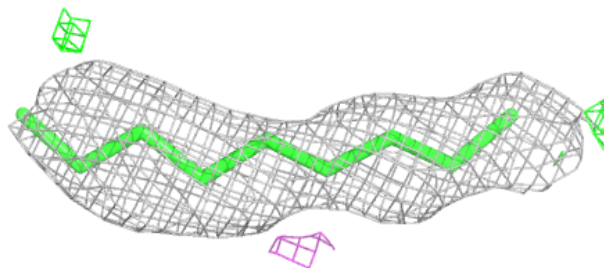


Electron density around LFA A 309:

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

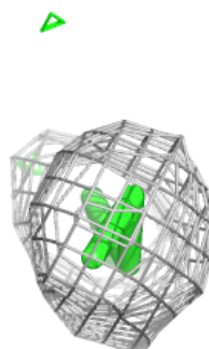
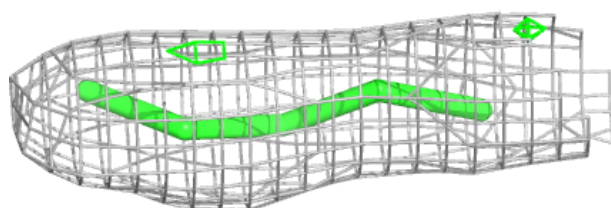
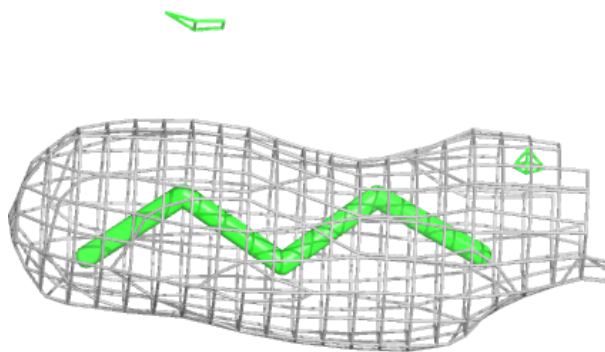
**Electron density around LFA A 303:**

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

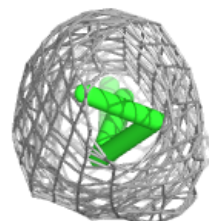
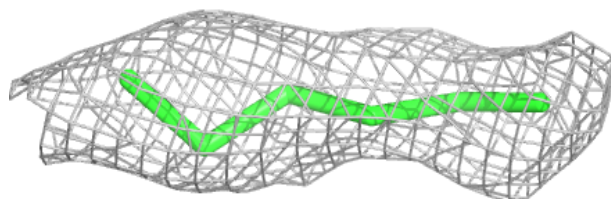
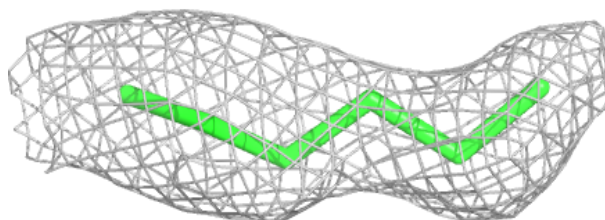


Electron density around LFA A 314:

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

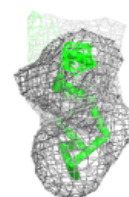
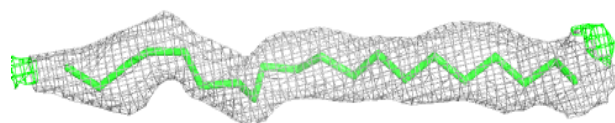
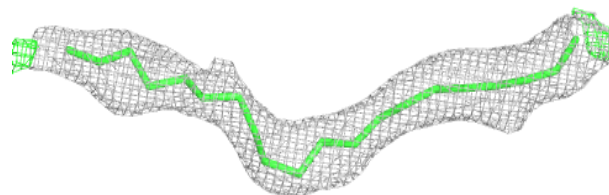
**Electron density around LFA A 304:**

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

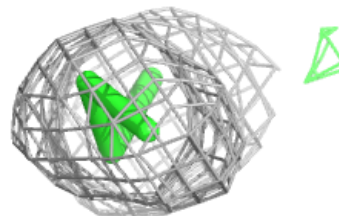
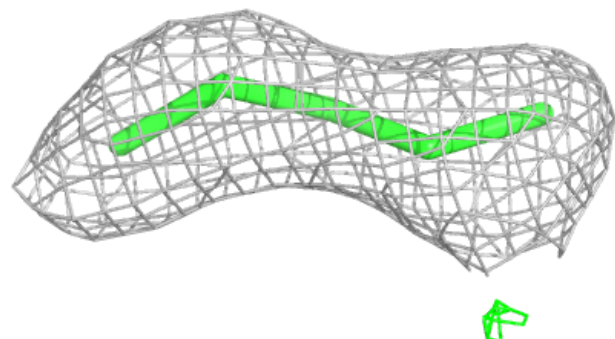
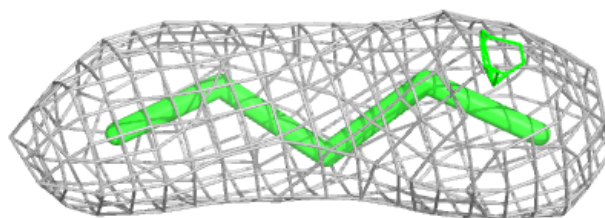


Electron density around LFA A 336:

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

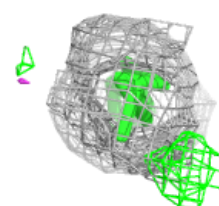
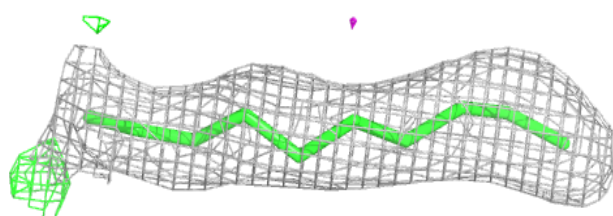
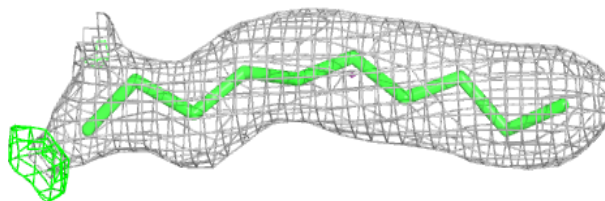
**Electron density around LFA A 312:**

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

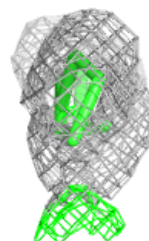
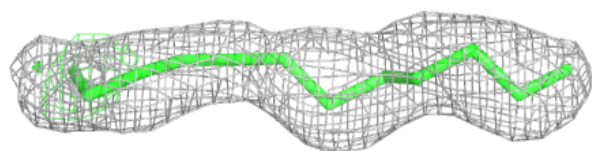
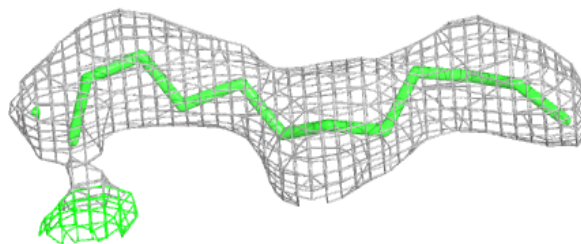


Electron density around LFA A 307:

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

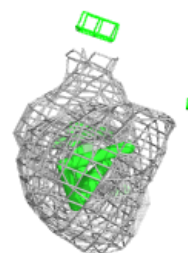
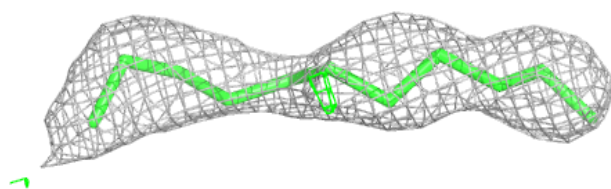
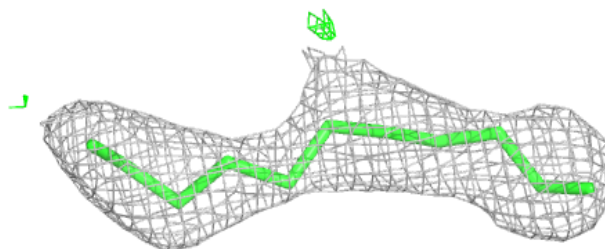
**Electron density around LFA A 333:**

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

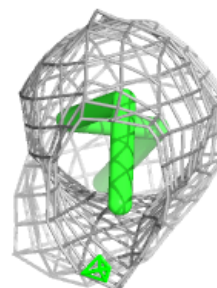
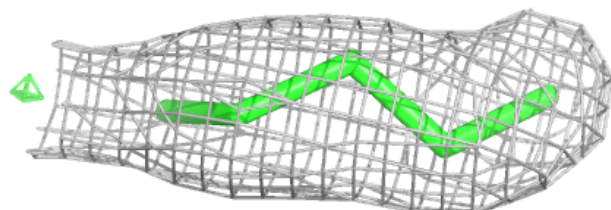
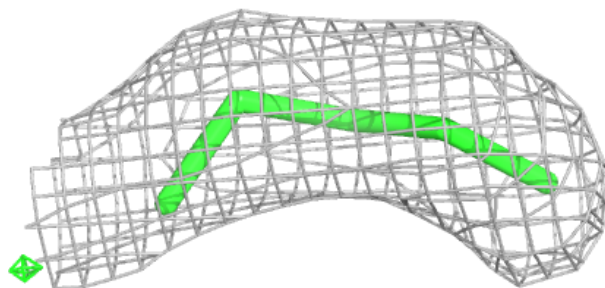


Electron density around LFA A 329:

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

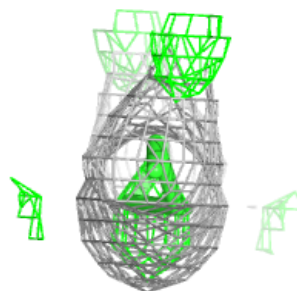
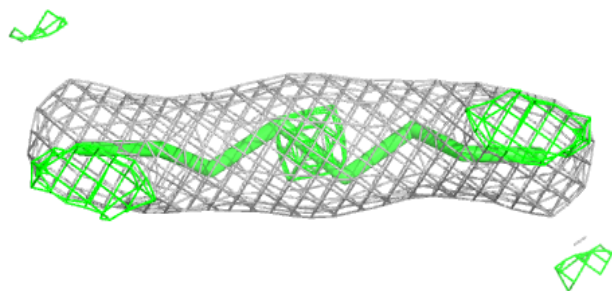
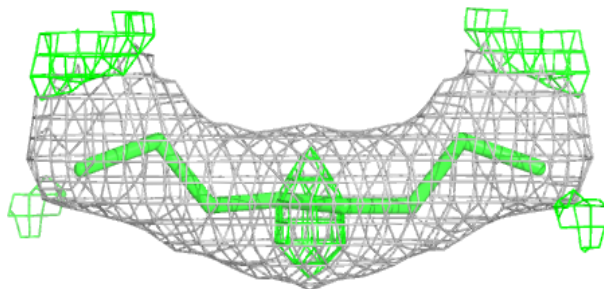
**Electron density around LFA A 315:**

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

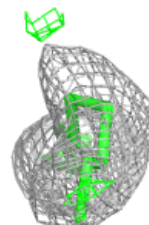
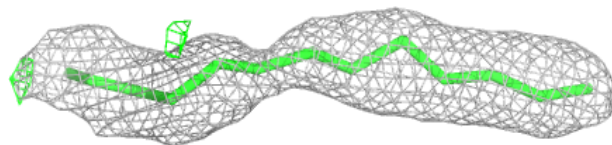
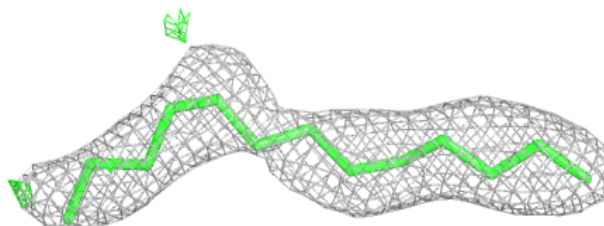


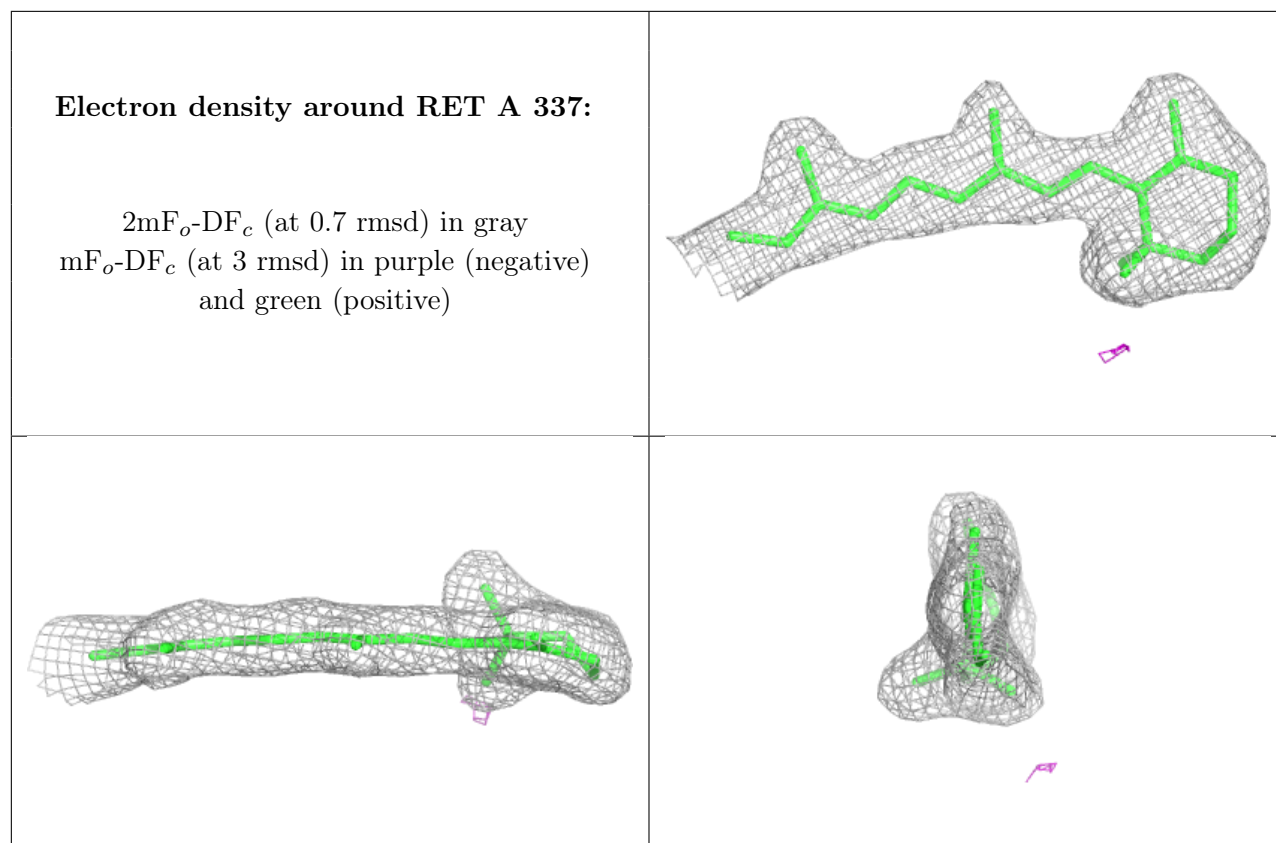
Electron density around LFA A 302:

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

**Electron density around LFA A 306:**

$2mF_o-DF_c$ (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.