



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:48 PM UTC

PDB ID : 6RFB / pdb_00006rfb
Title : Crystal structure of the potassium-pumping S254A mutant of the light-driven sodium pump KR2 in the monomeric form, pH 4.3
Authors : Kovalev, K.; Polovinkin, V.; Gushchin, I.; Borshchevskiy, V.; Gordeliy, V.
Deposited on : 2019-04-12
Resolution : 2.10 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 : 4-5-2 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

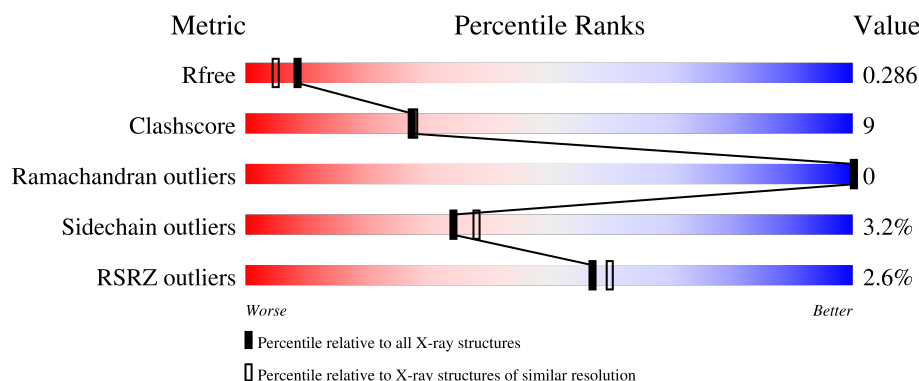
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

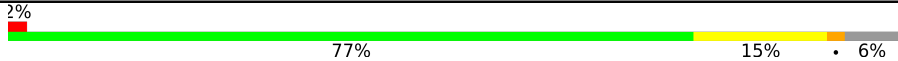
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	

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
5	RET	A	338	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2467 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	0	0
			2126	1422	323	372	9			

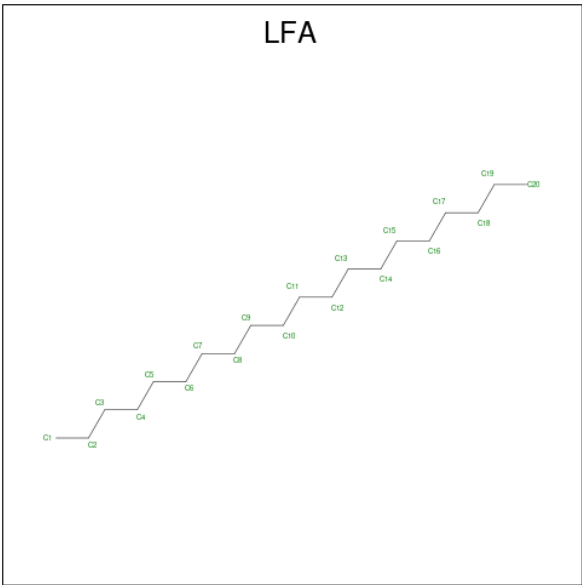
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	SER	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).



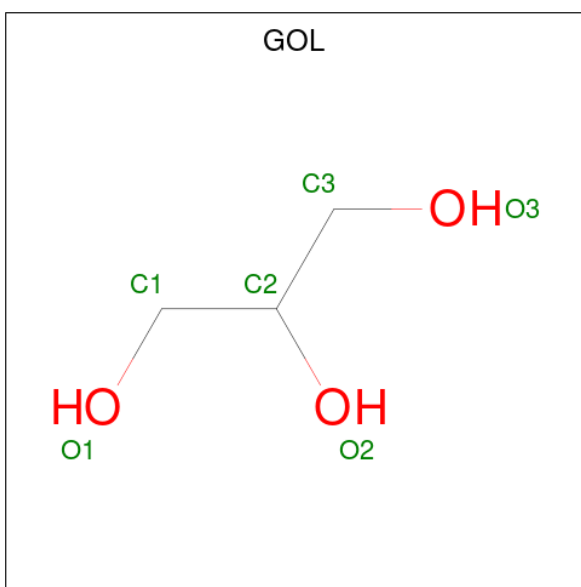
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 16 16	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total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

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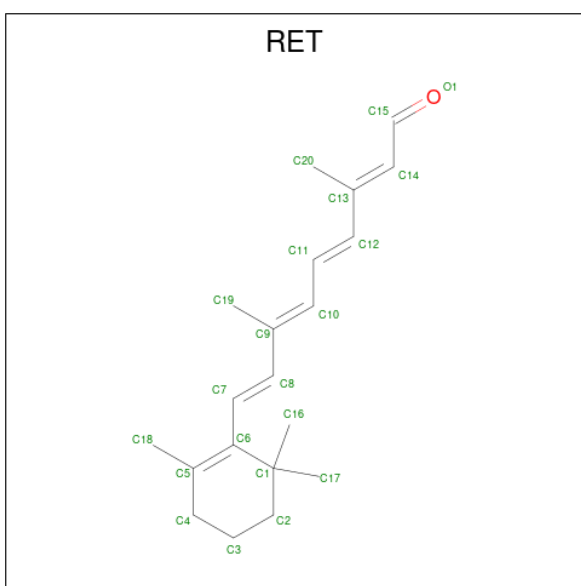
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 5 5	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

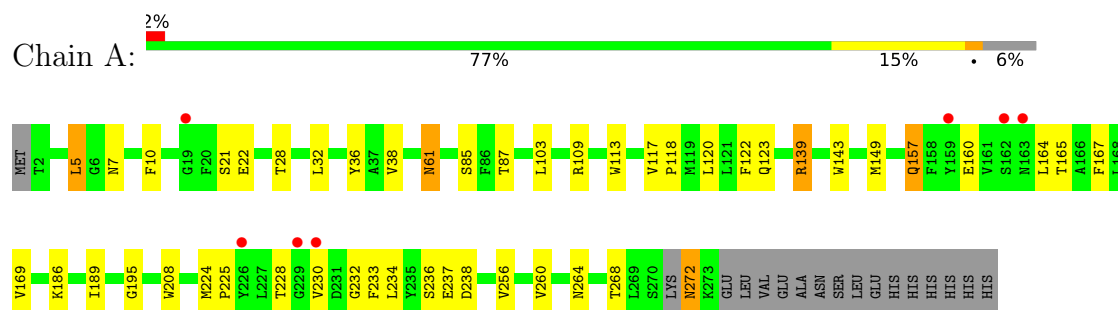
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		

3 Residue-property plots

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	40.80Å 83.00Å 234.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.10) 99.0 (20.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.226 , 0.279 0.238 , 0.286	Depositor DCC
R_{free} test set	1096 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2467	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.48	0/2182	0.94	0/2967

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	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	139	ARG	Sidechain
1	A	195	GLY	Peptide
1	A	232	GLY	Peptide

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	2126	0	2088	32	0
2	A	1	0	0	0	0
3	A	279	0	506	10	0
4	A	12	0	16	2	0
5	A	20	0	27	9	0
6	A	29	0	0	2	0
All	All	2467	0	2637	46	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 9.

All (46) 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:318:LFA:H11	3:A:320:LFA:C6	1.44	1.44
3:A:318:LFA:C1	3:A:320:LFA:C6	2.38	1.01
5:A:338:RET:H161	5:A:338:RET:H8	1.56	0.87
1:A:230:VAL:HG23	3:A:309:LFA:C8	2.08	0.84
3:A:320:LFA:H12	6:A:405:HOH:O	1.77	0.83
3:A:305:LFA:C1	3:A:326:LFA:C10	2.64	0.76
3:A:315:LFA:C2	3:A:316:LFA:C6	2.65	0.74
3:A:305:LFA:H11	3:A:326:LFA:C10	2.18	0.73
3:A:305:LFA:H12	3:A:326:LFA:C10	2.28	0.64
1:A:272:ASN:HD22	1:A:272:ASN:N	1.97	0.61
5:A:338:RET:H161	5:A:338:RET:C8	2.26	0.61
1:A:85:SER:HA	6:A:418:HOH:O	2.05	0.57
1:A:186:LYS:HD3	4:A:337:GOL:H32	1.86	0.56
1:A:165:THR:O	1:A:169:VAL:HG23	2.07	0.55
1:A:113:TRP:CD1	5:A:338:RET:H14	2.44	0.53
1:A:186:LYS:HD3	4:A:337:GOL:C3	2.39	0.52
1:A:122:PHE:CE1	1:A:139:ARG:HG3	2.45	0.52
1:A:21:SER:OG	1:A:237:GLU:OE1	2.28	0.52
1:A:264:ASN:O	1:A:268:THR:HG23	2.11	0.50
5:A:338:RET:H8	5:A:338:RET:H171	1.95	0.49
1:A:28:THR:O	1:A:32:LEU:HG	2.13	0.48
1:A:224:MET:N	1:A:225:PRO:CD	2.77	0.48
1:A:5:LEU:HD23	1:A:5:LEU:HA	1.77	0.46
1:A:164:LEU:O	1:A:167:PHE:HB3	2.16	0.46
1:A:189:ILE:HD13	1:A:208:TRP:HB2	1.98	0.46
1:A:120:LEU:O	1:A:123:GLN:HG2	2.16	0.45
5:A:338:RET:H8	5:A:338:RET:C16	2.34	0.45
1:A:149:MET:CE	5:A:338:RET:H192	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASN:C	1:A:7:ASN:N	2.75	0.45
1:A:61:ASN:H	1:A:61:ASN:HD22	1.65	0.44
5:A:338:RET:H181	5:A:338:RET:H7	1.62	0.44
1:A:38:VAL:HG22	3:A:302:LFA:H152	2.00	0.43
1:A:224:MET:HB3	1:A:225:PRO:HD3	2.00	0.43
1:A:236:SER:C	1:A:238:ASP:H	2.26	0.43
1:A:139:ARG:HH11	3:A:325:LFA:C6	2.32	0.43
1:A:85:SER:OG	1:A:103:LEU:C	2.62	0.42
5:A:338:RET:H11	5:A:338:RET:H191	1.82	0.42
1:A:139:ARG:HD2	1:A:143:TRP:CH2	2.54	0.42
1:A:157:GLN:HE21	1:A:157:GLN:HB3	1.57	0.42
5:A:338:RET:C8	5:A:338:RET:H171	2.49	0.41
1:A:61:ASN:HD22	1:A:61:ASN:N	2.18	0.41
1:A:256:VAL:O	1:A:260:VAL:HG23	2.20	0.41
1:A:117:VAL:HB	1:A:118:PRO:HD3	2.03	0.41
1:A:10:PHE:HB2	1:A:160:GLU:OE1	2.20	0.41
1:A:36:TYR:CD1	1:A:36:TYR:C	2.99	0.40
1:A:228:THR:OG1	1:A:234:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	266/288 (92%)	253 (95%)	13 (5%)	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	218/247 (88%)	211 (97%)	7 (3%)	34	38

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	22	GLU
1	A	61	ASN
1	A	87	THR
1	A	157	GLN
1	A	233	PHE
1	A	272	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	26	GLN
1	A	61	ASN
1	A	80	GLN
1	A	157	GLN
1	A	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 38 ligands modelled in this entry, 1 is monoatomic - leaving 37 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	315	-	4,4,19	0.33	0	3,3,18	0.35	0
3	LFA	A	331	-	3,3,19	0.35	0	2,2,18	0.62	0
3	LFA	A	311	-	11,11,19	0.29	0	10,10,18	0.44	0
4	GOL	A	336	-	5,5,5	0.29	0	5,5,5	0.18	0
5	RET	A	338	1	20,20,21	0.62	0	27,27,28	1.89	6 (22%)
3	LFA	A	318	-	11,11,19	0.26	0	10,10,18	0.50	0
3	LFA	A	314	-	9,9,19	0.29	0	8,8,18	0.44	0
3	LFA	A	306	-	4,4,19	0.29	0	3,3,18	0.36	0
3	LFA	A	332	-	4,4,19	0.33	0	3,3,18	0.35	0
3	LFA	A	309	-	7,7,19	0.27	0	6,6,18	0.44	0
3	LFA	A	321	-	4,4,19	0.27	0	3,3,18	0.36	0
3	LFA	A	307	-	12,12,19	0.24	0	11,11,18	0.57	0
3	LFA	A	302	-	15,15,19	0.29	0	14,14,18	0.49	0
3	LFA	A	310	-	7,7,19	0.25	0	6,6,18	0.49	0
3	LFA	A	308	-	9,9,19	0.29	0	8,8,18	0.46	0
3	LFA	A	304	-	8,8,19	0.31	0	7,7,18	0.44	0
3	LFA	A	328	-	2,2,19	0.17	0	1,1,18	0.03	0
3	LFA	A	334	-	11,11,19	0.27	0	10,10,18	0.49	0
3	LFA	A	323	-	3,3,19	0.34	0	2,2,18	0.64	0
3	LFA	A	324	-	5,5,19	0.28	0	4,4,18	0.36	0
3	LFA	A	325	-	5,5,19	0.26	0	4,4,18	0.42	0
3	LFA	A	326	-	9,9,19	0.23	0	8,8,18	0.52	0
3	LFA	A	327	-	6,6,19	0.29	0	5,5,18	0.39	0
3	LFA	A	305	-	5,5,19	0.28	0	4,4,18	0.39	0
3	LFA	A	322	-	5,5,19	0.28	0	4,4,18	0.35	0
3	LFA	A	329	-	4,4,19	0.32	0	3,3,18	0.38	0
3	LFA	A	333	-	9,9,19	0.28	0	8,8,18	0.44	0
3	LFA	A	319	-	9,9,19	0.26	0	8,8,18	0.51	0
3	LFA	A	316	-	4,4,19	0.34	0	3,3,18	0.34	0
3	LFA	A	335	-	9,9,19	0.26	0	8,8,18	0.50	0
3	LFA	A	320	-	5,5,19	0.25	0	4,4,18	0.41	0
4	GOL	A	337	-	5,5,5	0.27	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	A	303	-	7,7,19	0.27	0	6,6,18	0.46	0
3	LFA	A	317	-	10,10,19	0.30	0	9,9,18	0.47	0
3	LFA	A	330	-	10,10,19	0.28	0	9,9,18	0.46	0
3	LFA	A	313	-	4,4,19	0.28	0	3,3,18	0.36	0
3	LFA	A	312	-	15,15,19	0.26	0	14,14,18	0.53	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	315	-	-	0/2/2/17	-
3	LFA	A	331	-	-	0/1/1/17	-
3	LFA	A	311	-	-	6/9/9/17	-
4	GOL	A	336	-	-	2/4/4/4	-
5	RET	A	338	1	-	0/13/30/31	0/1/1/1
3	LFA	A	318	-	-	4/9/9/17	-
3	LFA	A	314	-	-	3/7/7/17	-
3	LFA	A	306	-	-	1/2/2/17	-
3	LFA	A	332	-	-	0/2/2/17	-
3	LFA	A	309	-	-	2/5/5/17	-
3	LFA	A	321	-	-	1/2/2/17	-
3	LFA	A	307	-	-	6/10/10/17	-
3	LFA	A	302	-	-	5/13/13/17	-
3	LFA	A	310	-	-	3/5/5/17	-
3	LFA	A	308	-	-	3/7/7/17	-
3	LFA	A	304	-	-	2/6/6/17	-
3	LFA	A	334	-	-	5/9/9/17	-
3	LFA	A	323	-	-	0/1/1/17	-
3	LFA	A	324	-	-	1/3/3/17	-
3	LFA	A	325	-	-	0/3/3/17	-
3	LFA	A	326	-	-	4/7/7/17	-
3	LFA	A	327	-	-	2/4/4/17	-
3	LFA	A	305	-	-	0/3/3/17	-
3	LFA	A	322	-	-	2/3/3/17	-
3	LFA	A	329	-	-	0/2/2/17	-
3	LFA	A	333	-	-	6/7/7/17	-
3	LFA	A	319	-	-	3/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	316	-	-	0/2/2/17	-
3	LFA	A	335	-	-	3/7/7/17	-
3	LFA	A	320	-	-	1/3/3/17	-
4	GOL	A	337	-	-	2/4/4/4	-
3	LFA	A	303	-	-	3/5/5/17	-
3	LFA	A	317	-	-	2/8/8/17	-
3	LFA	A	330	-	-	7/8/8/17	-
3	LFA	A	313	-	-	0/2/2/17	-
3	LFA	A	312	-	-	8/13/13/17	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	338	RET	C18-C5-C6	-4.99	119.04	124.48
5	A	338	RET	C11-C10-C9	-4.04	121.61	127.28
5	A	338	RET	C7-C8-C9	-3.62	120.88	126.23
5	A	338	RET	C20-C13-C12	2.96	122.62	118.09
5	A	338	RET	C10-C11-C12	-2.55	115.82	123.20
5	A	338	RET	C19-C9-C8	2.01	121.15	118.09

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	336	GOL	O1-C1-C2-C3
4	A	337	GOL	C1-C2-C3-O3
3	A	312	LFA	C11-C10-C9-C8
3	A	319	LFA	C5-C6-C7-C8
3	A	330	LFA	C5-C6-C7-C8
4	A	337	GOL	O2-C2-C3-O3
3	A	333	LFA	C6-C7-C8-C9
3	A	335	LFA	C4-C5-C6-C7
3	A	322	LFA	C2-C3-C4-C5
3	A	311	LFA	C5-C6-C7-C8
3	A	330	LFA	C4-C5-C6-C7
3	A	311	LFA	C3-C4-C5-C6
3	A	326	LFA	C3-C4-C5-C6
3	A	333	LFA	C5-C6-C7-C8
3	A	312	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	307	LFA	C4-C5-C6-C7
3	A	334	LFA	C4-C5-C6-C7
3	A	330	LFA	C7-C8-C9-C10
3	A	335	LFA	C6-C7-C8-C9
3	A	303	LFA	C2-C3-C4-C5
3	A	334	LFA	C6-C7-C8-C9
3	A	307	LFA	C9-C10-C11-C12
3	A	319	LFA	C3-C4-C5-C6
3	A	333	LFA	C4-C5-C6-C7
3	A	311	LFA	C6-C7-C8-C9
3	A	314	LFA	C5-C6-C7-C8
3	A	318	LFA	C7-C8-C9-C10
3	A	307	LFA	C3-C4-C5-C6
3	A	334	LFA	C5-C6-C7-C8
3	A	330	LFA	C2-C3-C4-C5
3	A	304	LFA	C5-C6-C7-C8
3	A	317	LFA	C6-C7-C8-C9
3	A	334	LFA	C2-C3-C4-C5
3	A	311	LFA	C2-C3-C4-C5
3	A	326	LFA	C6-C7-C8-C9
3	A	312	LFA	C9-C10-C11-C12
3	A	333	LFA	C1-C2-C3-C4
3	A	334	LFA	C1-C2-C3-C4
3	A	309	LFA	C5-C6-C7-C8
4	A	336	GOL	O1-C1-C2-O2
3	A	318	LFA	C6-C7-C8-C9
3	A	312	LFA	C6-C7-C8-C9
3	A	309	LFA	C3-C4-C5-C6
3	A	317	LFA	C9-C10-C11-C12
3	A	311	LFA	C9-C10-C11-C12
3	A	303	LFA	C1-C2-C3-C4
3	A	320	LFA	C3-C4-C5-C6
3	A	333	LFA	C3-C4-C5-C6
3	A	324	LFA	C2-C3-C4-C5
3	A	302	LFA	C12-C13-C14-C15
3	A	314	LFA	C4-C5-C6-C7
3	A	322	LFA	C3-C4-C5-C6
3	A	318	LFA	C11-C10-C9-C8
3	A	310	LFA	C4-C5-C6-C7
3	A	330	LFA	C1-C2-C3-C4
3	A	314	LFA	C7-C8-C9-C10
3	A	330	LFA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	A	302	LFA	C10-C11-C12-C13
3	A	326	LFA	C5-C6-C7-C8
3	A	303	LFA	C5-C6-C7-C8
3	A	302	LFA	C11-C12-C13-C14
3	A	312	LFA	C3-C4-C5-C6
3	A	302	LFA	C11-C10-C9-C8
3	A	312	LFA	C11-C12-C13-C14
3	A	335	LFA	C5-C6-C7-C8
3	A	307	LFA	C6-C7-C8-C9
3	A	321	LFA	C2-C3-C4-C5
3	A	318	LFA	C3-C4-C5-C6
3	A	307	LFA	C11-C10-C9-C8
3	A	308	LFA	C7-C8-C9-C10
3	A	306	LFA	C2-C3-C4-C5
3	A	310	LFA	C2-C3-C4-C5
3	A	302	LFA	C2-C3-C4-C5
3	A	304	LFA	C6-C7-C8-C9
3	A	319	LFA	C2-C3-C4-C5
3	A	327	LFA	C3-C4-C5-C6
3	A	330	LFA	C6-C7-C8-C9
3	A	308	LFA	C2-C3-C4-C5
3	A	308	LFA	C1-C2-C3-C4
3	A	333	LFA	C2-C3-C4-C5
3	A	326	LFA	C7-C8-C9-C10
3	A	311	LFA	C11-C10-C9-C8
3	A	307	LFA	C7-C8-C9-C10
3	A	327	LFA	C2-C3-C4-C5
3	A	312	LFA	C7-C8-C9-C10
3	A	312	LFA	C13-C14-C15-C16
3	A	310	LFA	C1-C2-C3-C4

There are no ring outliers.

11 monomers are involved in 21 short contacts:

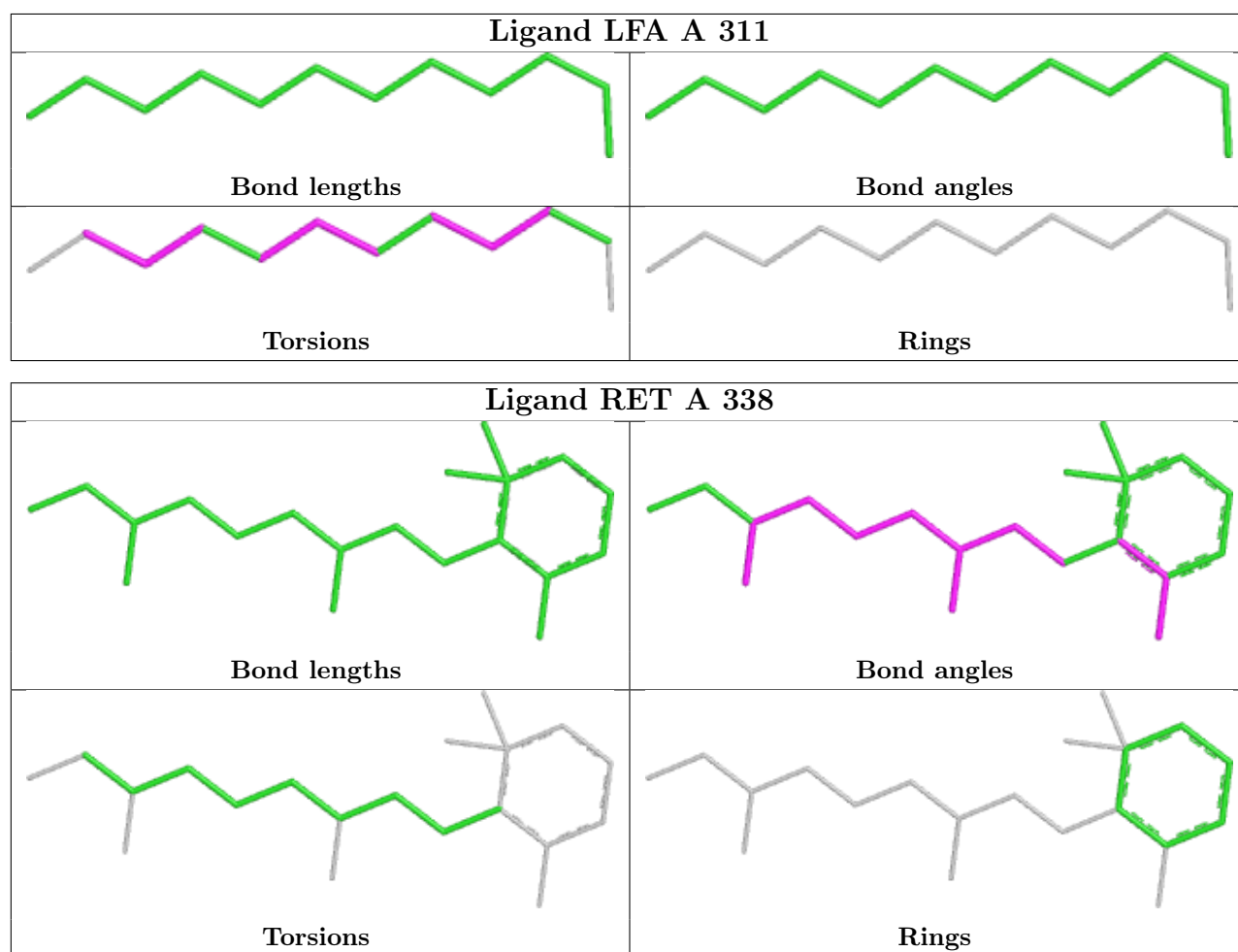
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	315	LFA	1	0
5	A	338	RET	9	0
3	A	318	LFA	2	0
3	A	309	LFA	1	0
3	A	302	LFA	1	0
3	A	325	LFA	1	0
3	A	326	LFA	3	0

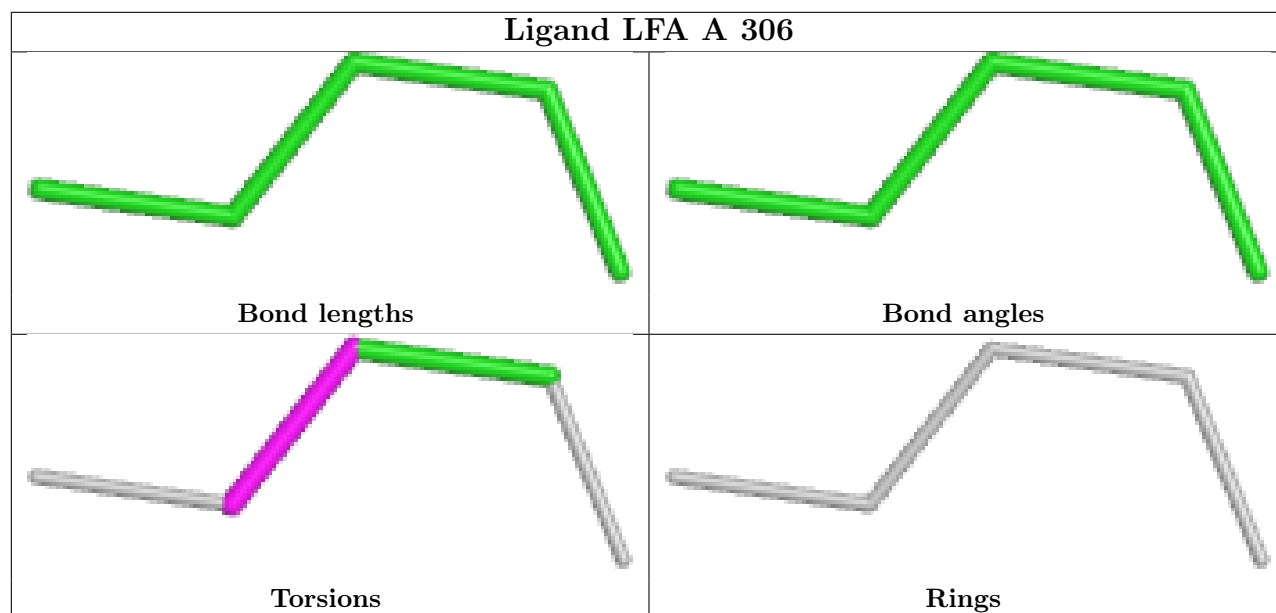
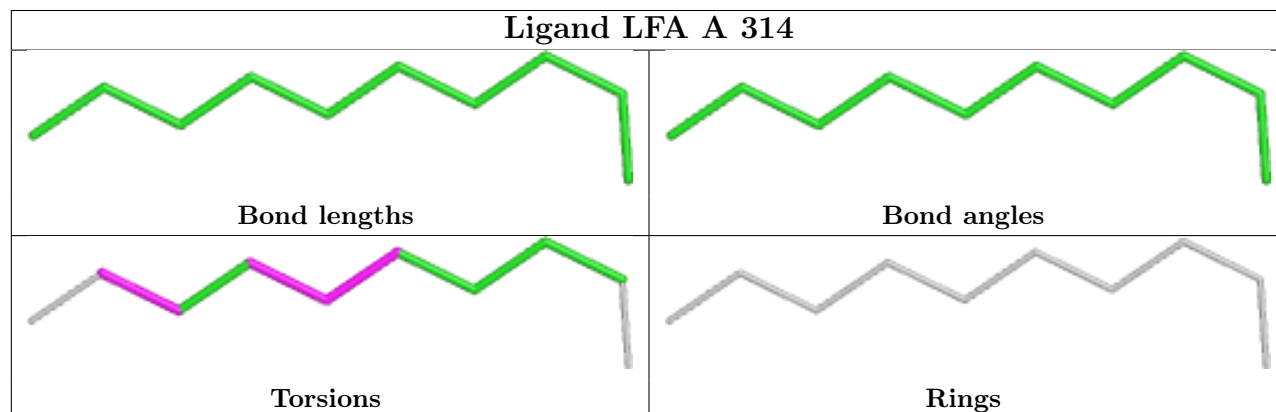
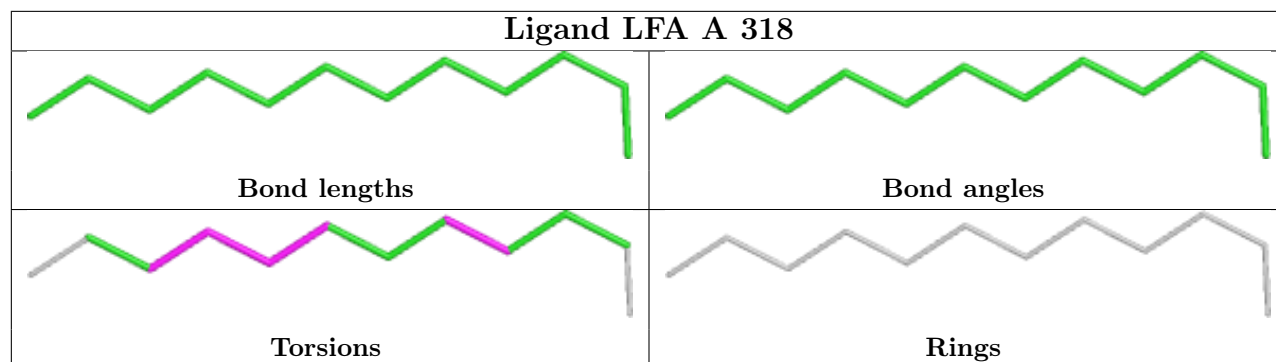
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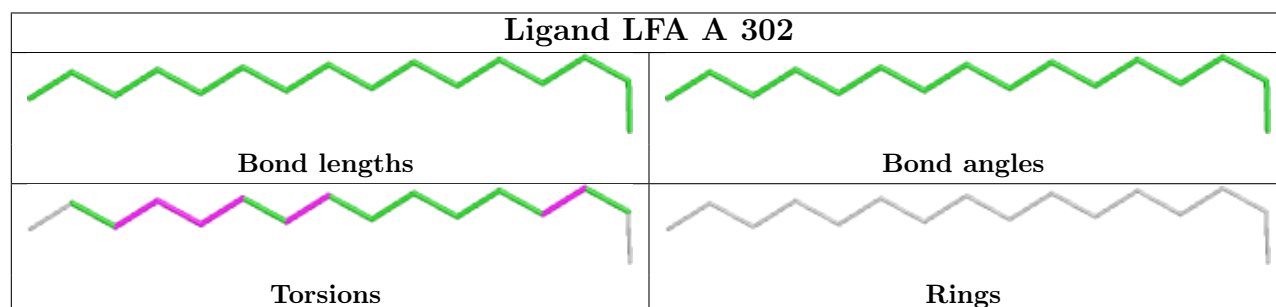
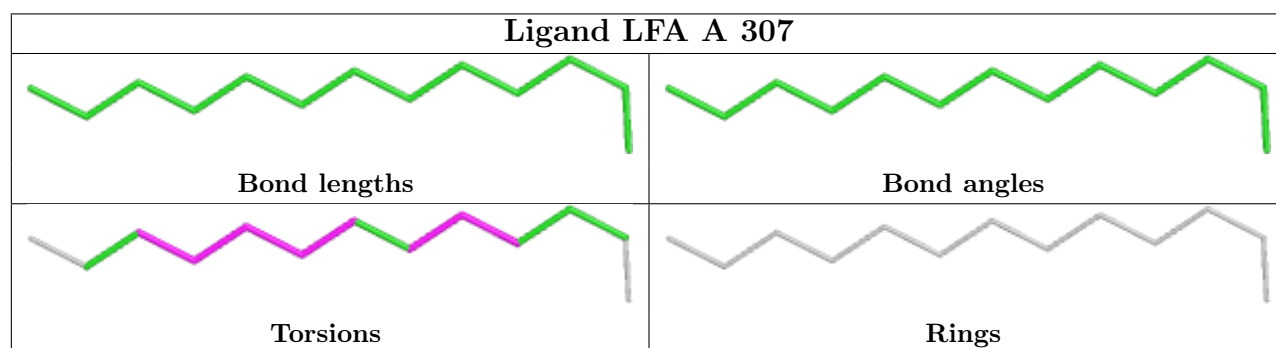
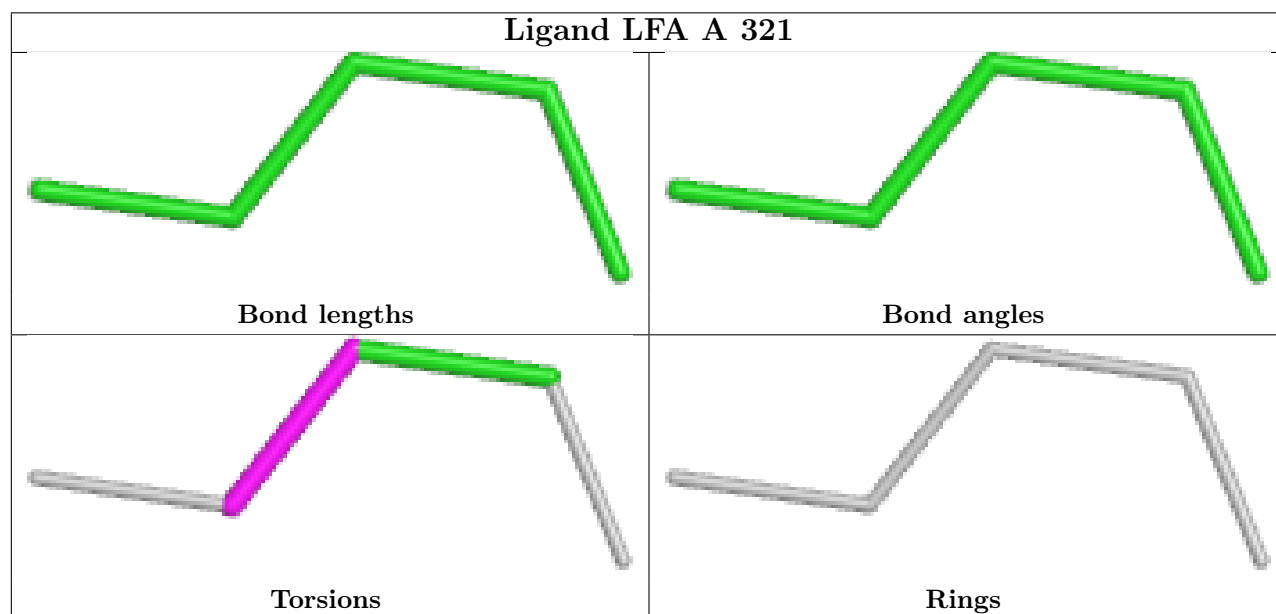
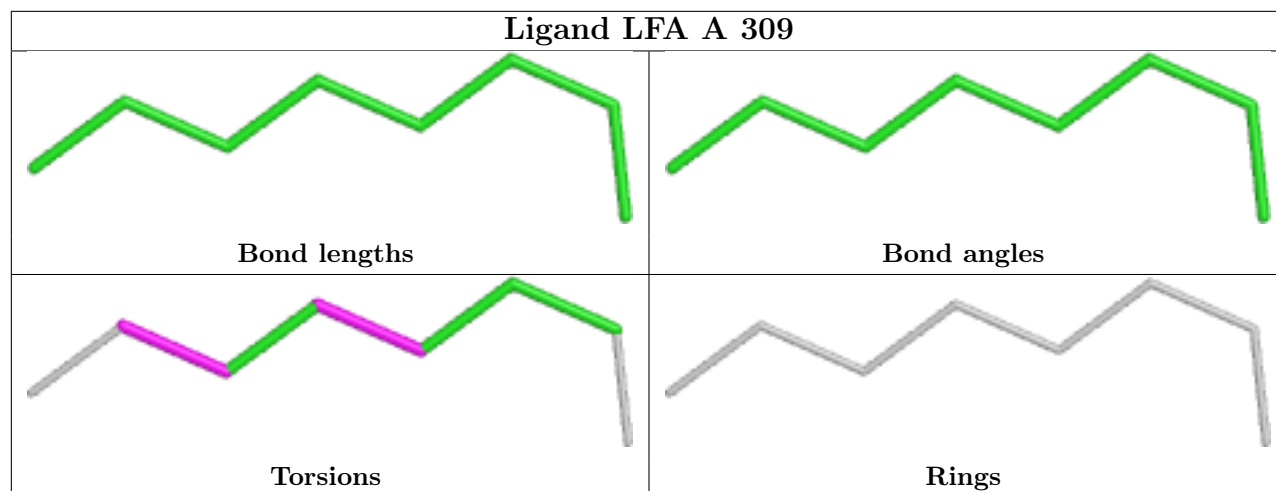
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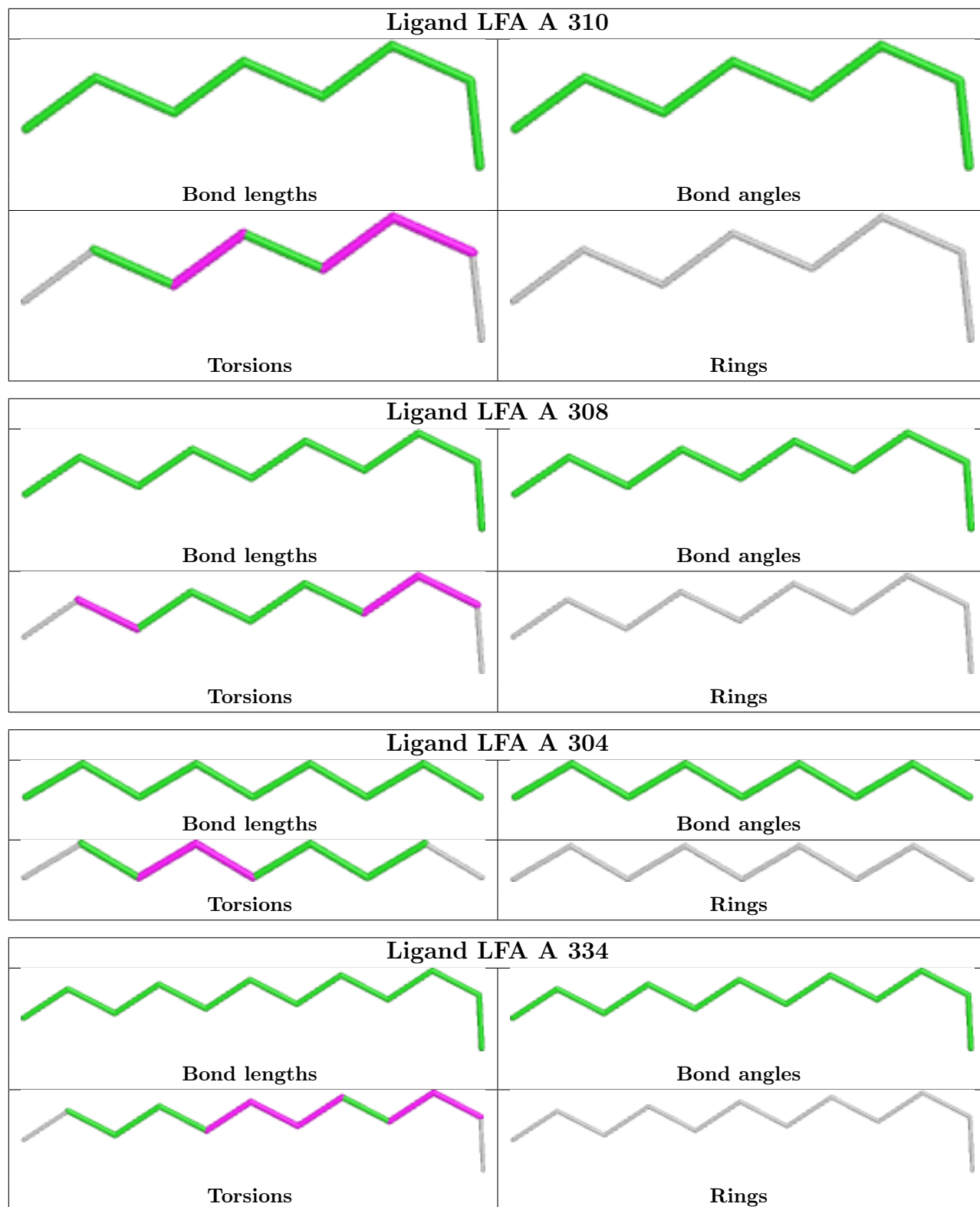
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	305	LFA	3	0
3	A	316	LFA	1	0
3	A	320	LFA	3	0
4	A	337	GOL	2	0

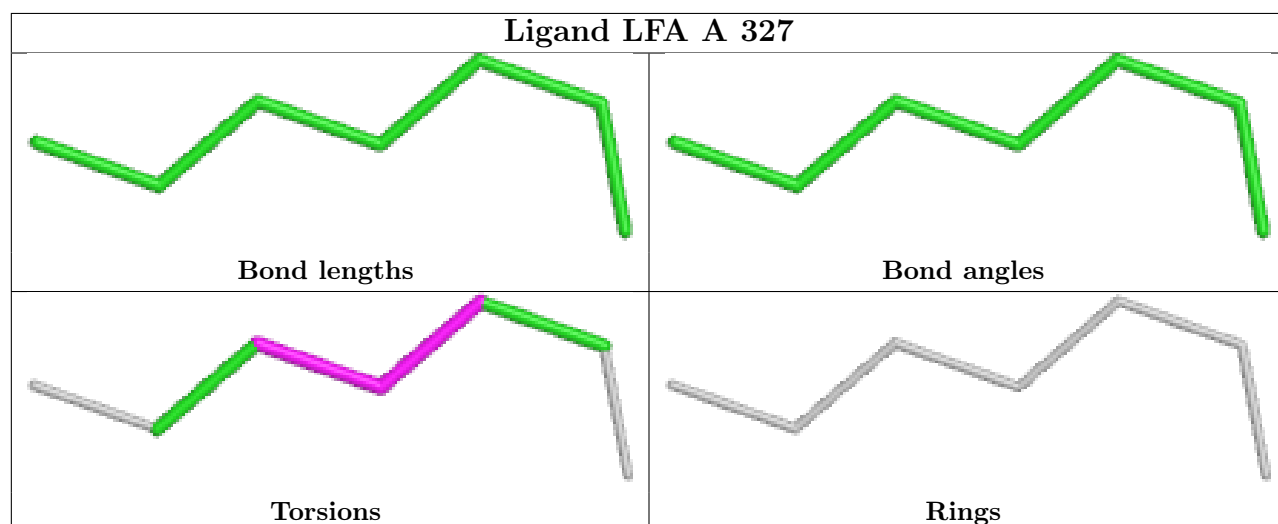
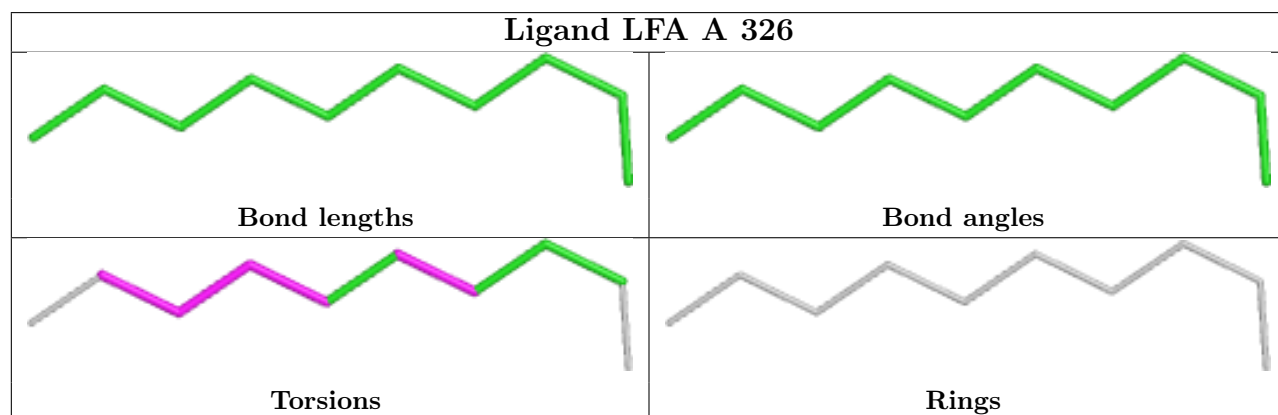
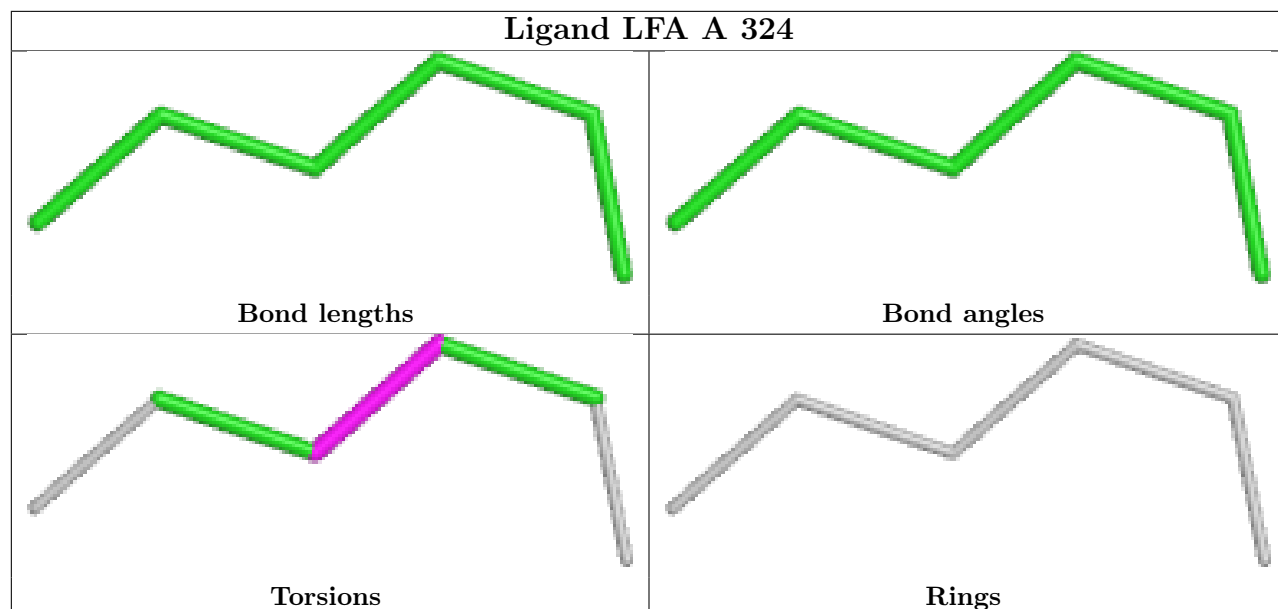
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

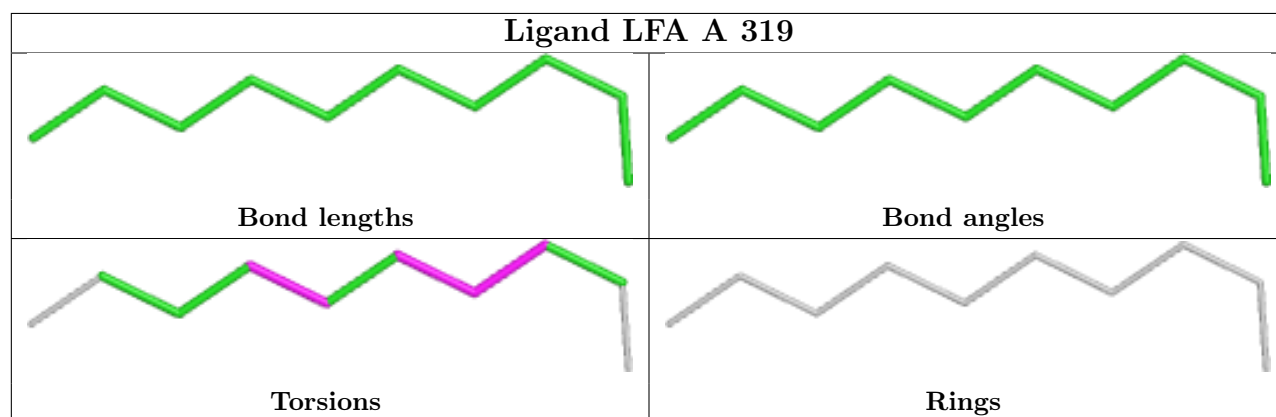
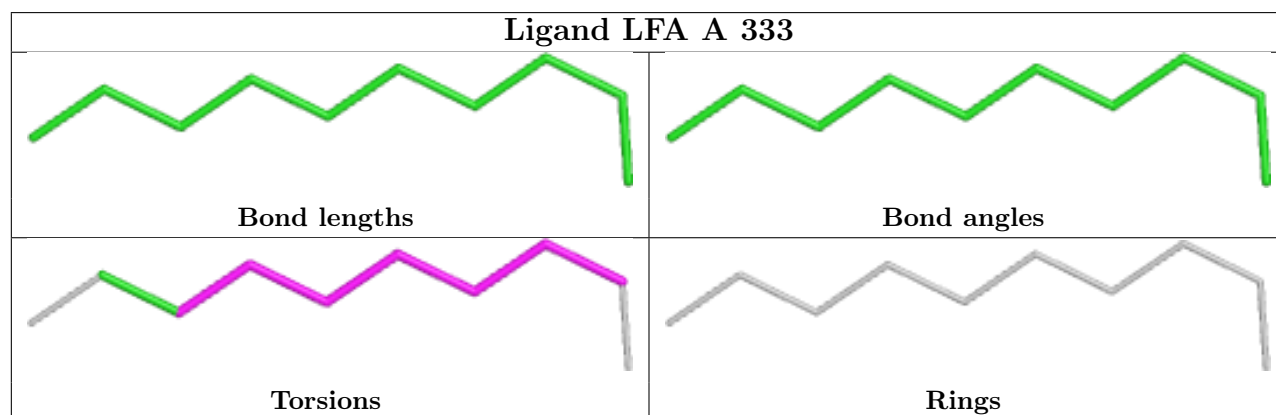
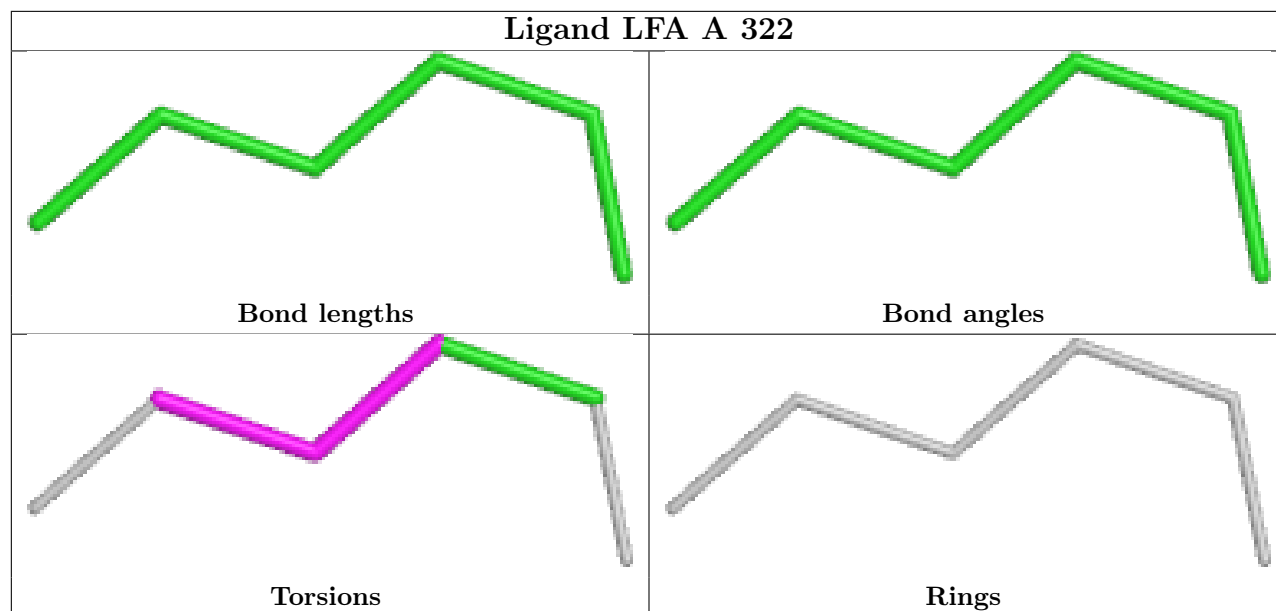


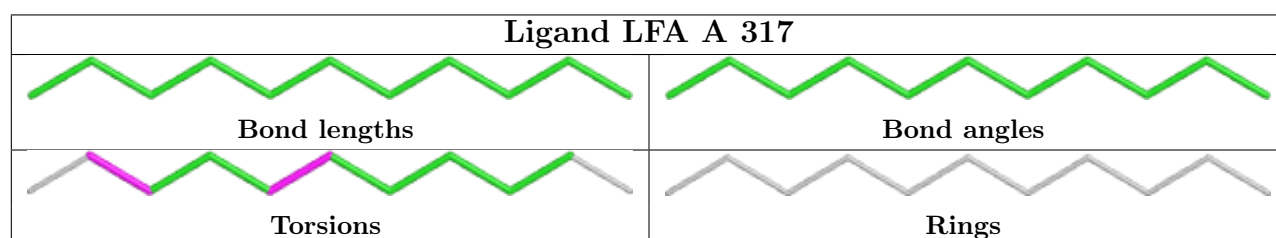
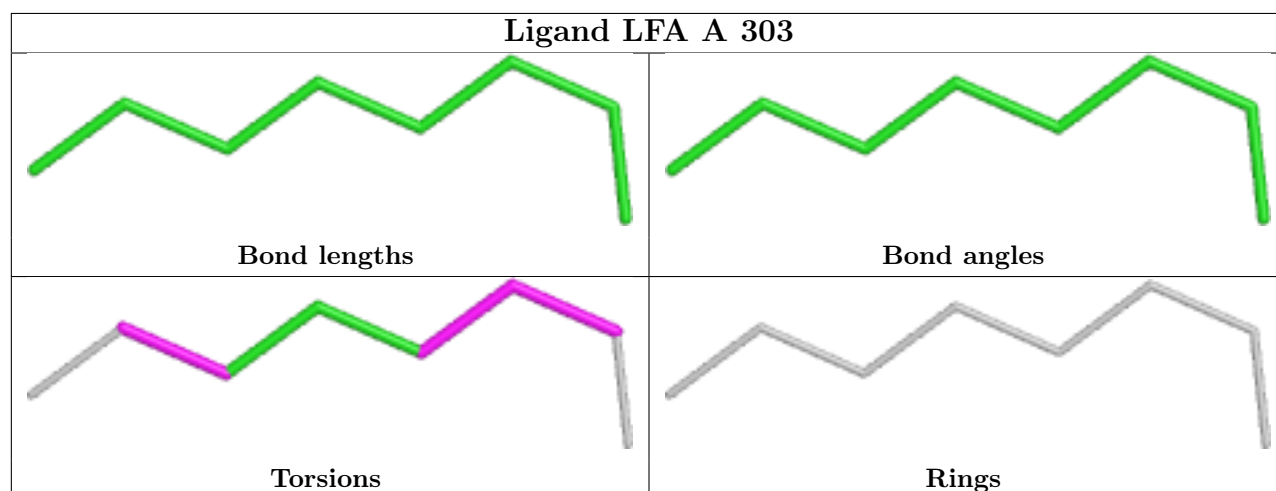
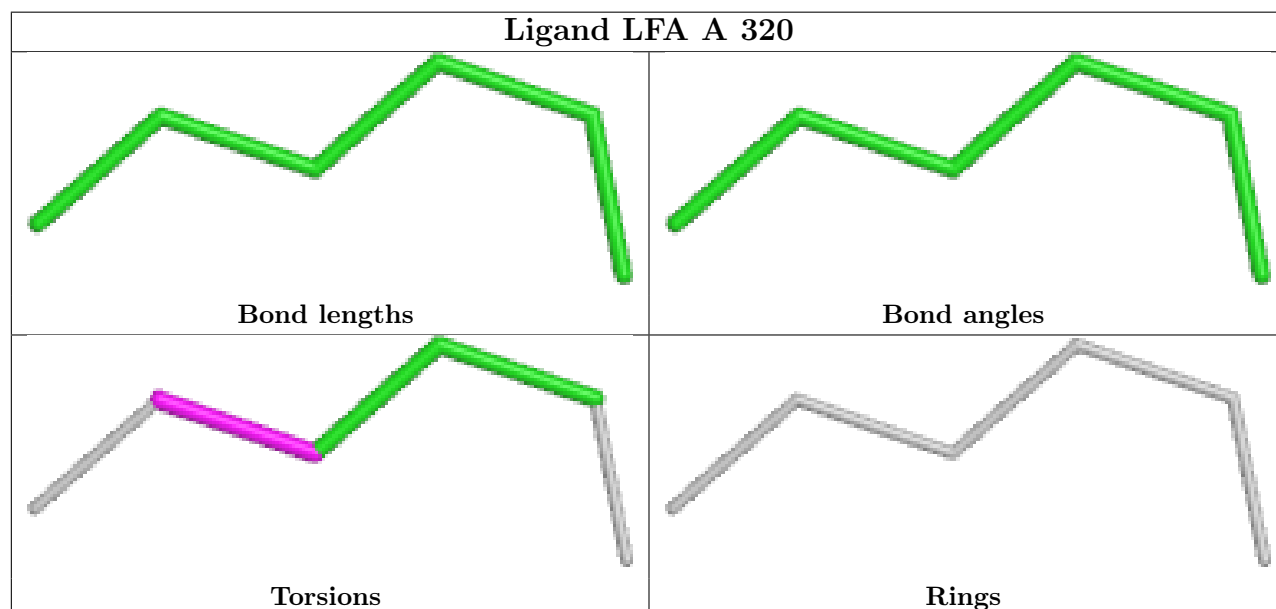
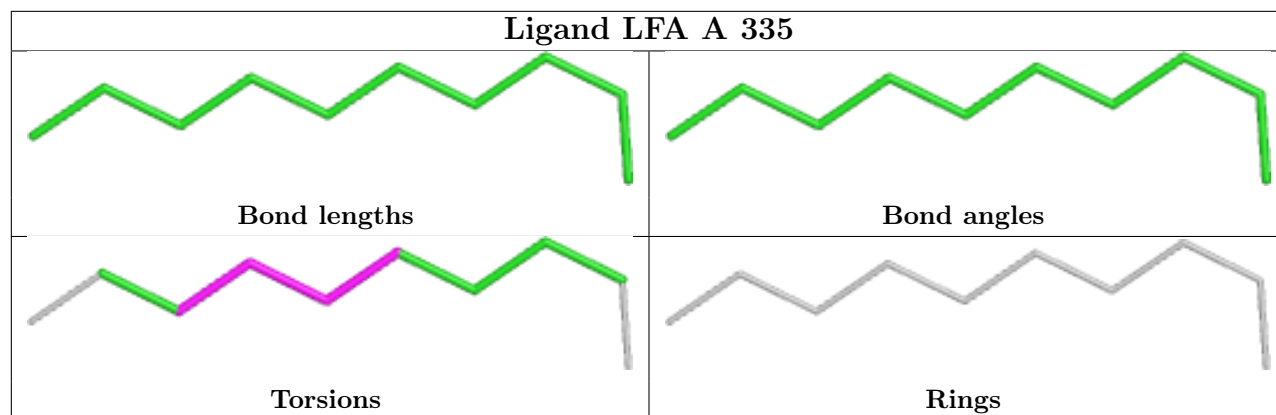


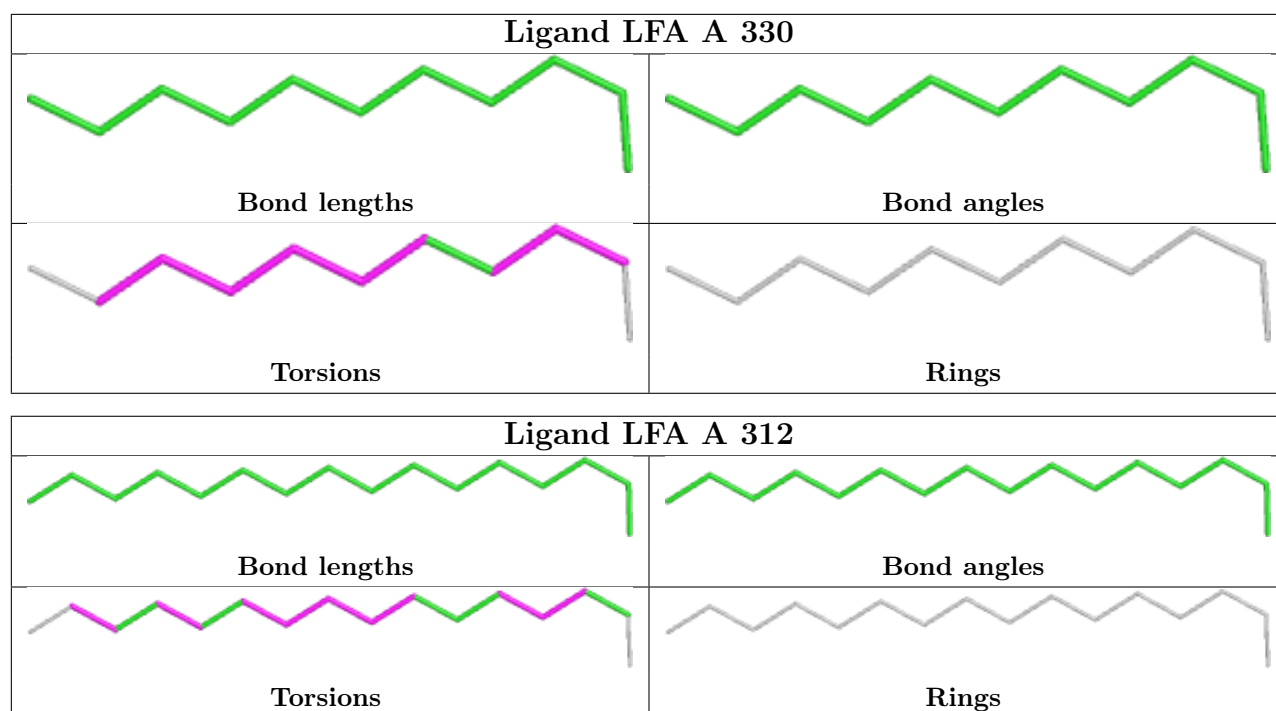












5.7 Other polymers [i](#)

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	271/288 (94%)	0.13	7 (2%) 57 60	30, 48, 84, 122	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	VAL	3.7
1	A	229	GLY	2.6
1	A	226	TYR	2.6
1	A	159	TYR	2.4
1	A	19	GLY	2.4
1	A	163	ASN	2.3
1	A	162	SER	2.1

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	0.38	0.25	84,93,103,104	0

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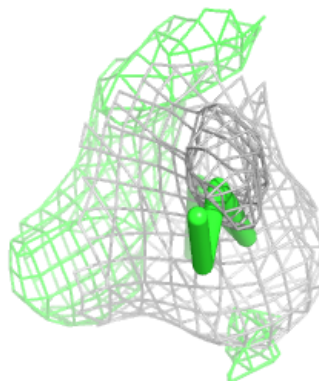
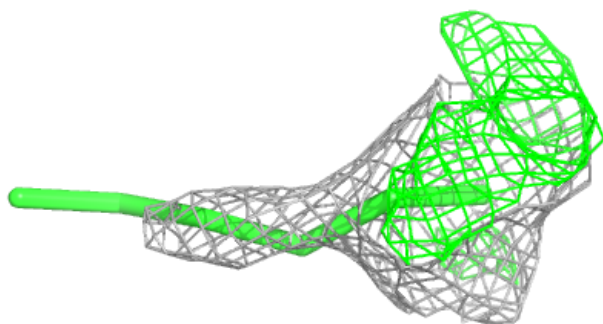
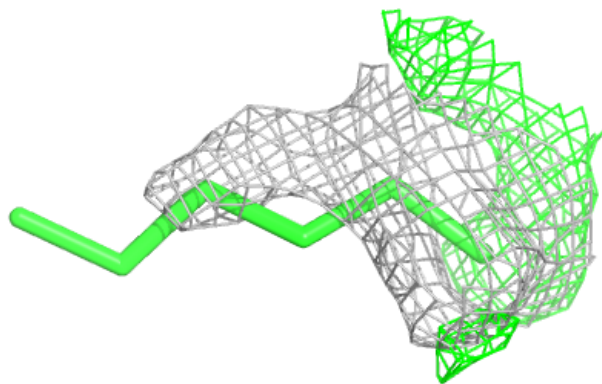
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LFA	A	323	4/20	0.49	0.29	70,80,85,87	0
3	LFA	A	331	4/20	0.60	0.17	90,93,95,101	0
3	LFA	A	317	11/20	0.64	0.17	72,101,109,115	0
4	GOL	A	336	6/6	0.64	0.17	95,112,121,147	0
3	LFA	A	327	7/20	0.65	0.16	80,94,108,114	0
3	LFA	A	309	8/20	0.65	0.22	98,108,118,118	0
3	LFA	A	335	10/20	0.65	0.19	96,126,153,153	0
3	LFA	A	306	5/20	0.65	0.18	78,80,86,92	0
3	LFA	A	314	10/20	0.68	0.19	70,92,103,107	0
3	LFA	A	311	12/20	0.71	0.18	64,84,98,100	0
3	LFA	A	319	10/20	0.72	0.16	50,80,111,114	0
3	LFA	A	308	10/20	0.73	0.18	57,77,101,104	0
3	LFA	A	332	5/20	0.73	0.14	65,75,86,96	0
3	LFA	A	315	5/20	0.75	0.17	73,80,82,87	0
3	LFA	A	316	5/20	0.76	0.13	61,69,74,75	0
3	LFA	A	330	11/20	0.76	0.17	67,81,104,107	0
3	LFA	A	325	6/20	0.76	0.17	73,75,81,85	0
3	LFA	A	312	16/20	0.77	0.16	84,91,98,101	0
3	LFA	A	328	3/20	0.78	0.25	75,75,77,78	0
3	LFA	A	333	10/20	0.79	0.17	72,84,87,90	0
3	LFA	A	329	5/20	0.79	0.15	69,72,77,78	0
3	LFA	A	310	8/20	0.79	0.15	44,68,80,84	0
3	LFA	A	318	12/20	0.81	0.18	61,79,103,109	0
3	LFA	A	334	12/20	0.82	0.17	72,78,97,102	0
3	LFA	A	326	10/20	0.82	0.14	72,77,81,87	0
3	LFA	A	304	9/20	0.82	0.12	63,71,78,80	0
4	GOL	A	337	6/6	0.82	0.12	75,84,89,105	0
3	LFA	A	321	5/20	0.83	0.15	75,77,79,80	0
3	LFA	A	313	5/20	0.83	0.13	58,63,69,70	0
3	LFA	A	322	6/20	0.85	0.15	82,84,87,90	0
3	LFA	A	303	8/20	0.85	0.11	49,52,57,58	8
3	LFA	A	307	13/20	0.86	0.14	49,59,78,79	0
3	LFA	A	305	6/20	0.87	0.13	62,75,83,84	0
3	LFA	A	302	16/20	0.87	0.13	51,63,85,86	0
3	LFA	A	320	6/20	0.90	0.11	56,64,65,70	0
2	NA	A	301	1/1	0.91	0.10	69,69,69,69	0
5	RET	A	338	20/21	0.92	0.10	33,42,50,52	0

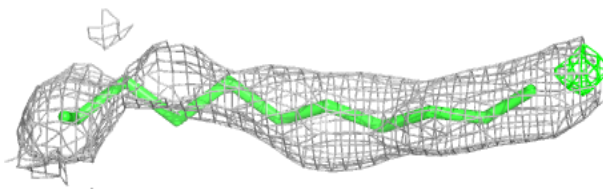
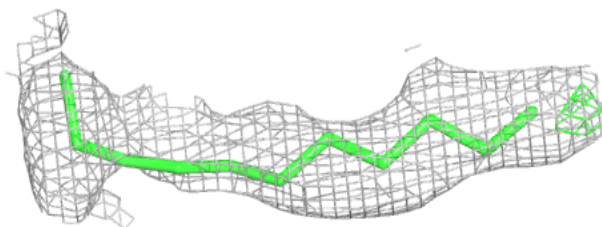
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

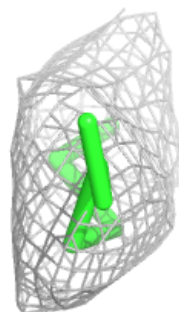
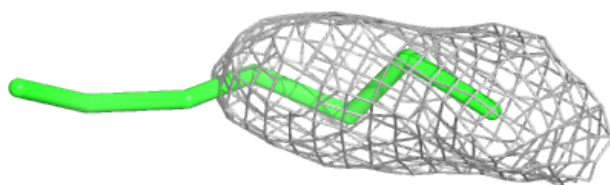
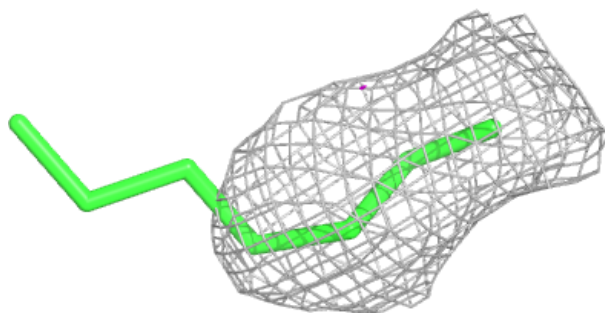
**Electron density around LFA A 317:**

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

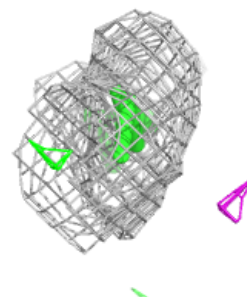
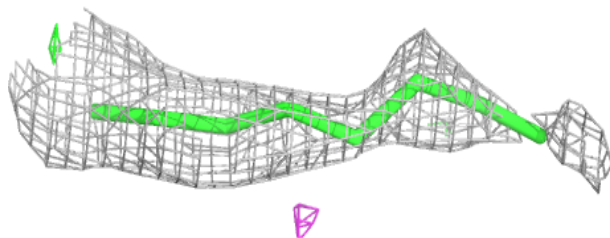
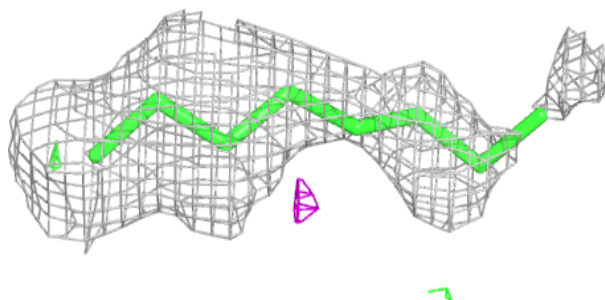


Electron density around LFA A 327:

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

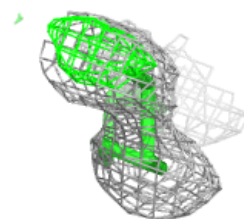
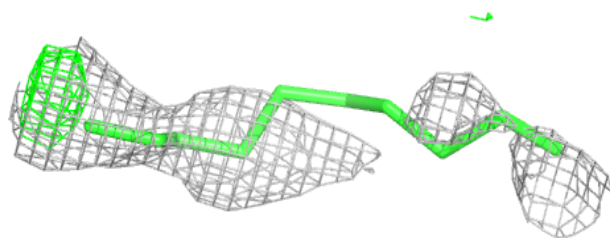
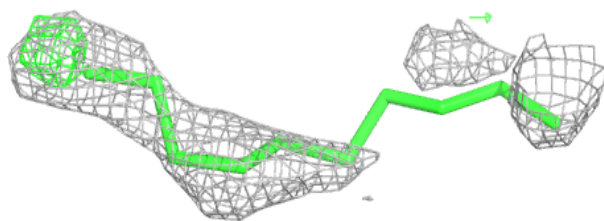
**Electron density around LFA A 309:**

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

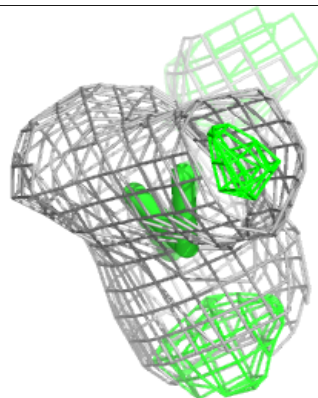
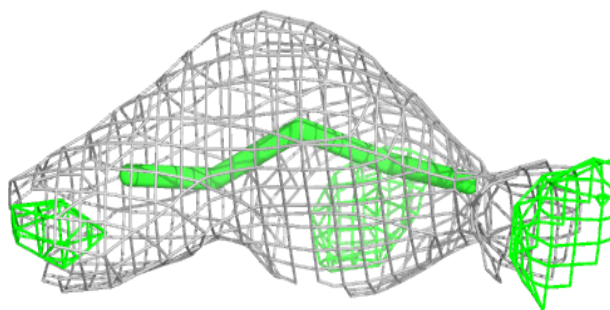
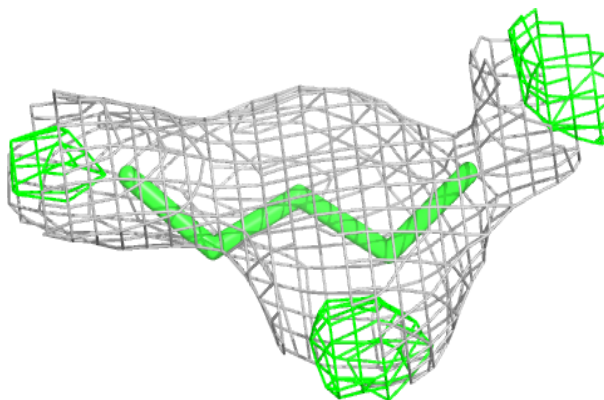


Electron density around LFA A 335:

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

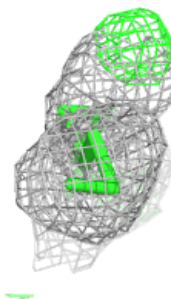
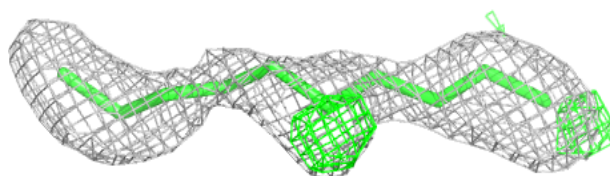
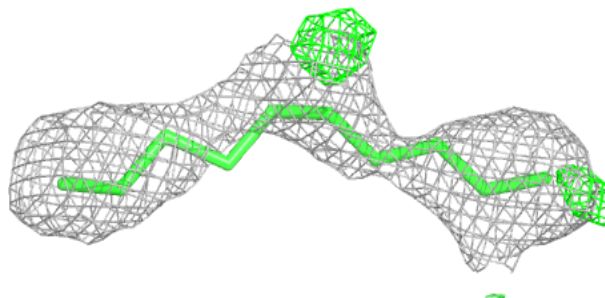
**Electron density around LFA A 306:**

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

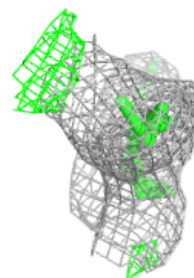
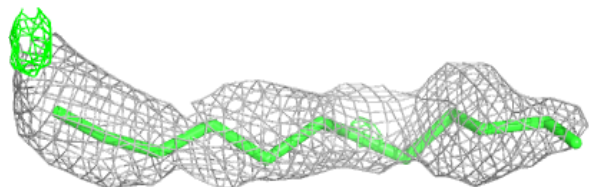
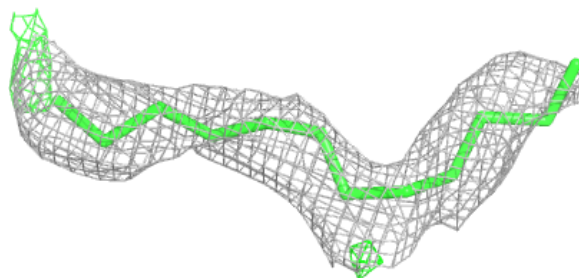


Electron density around LFA A 314:

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

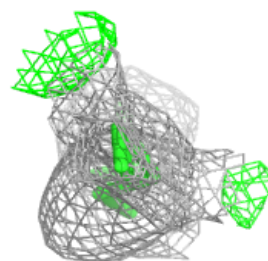
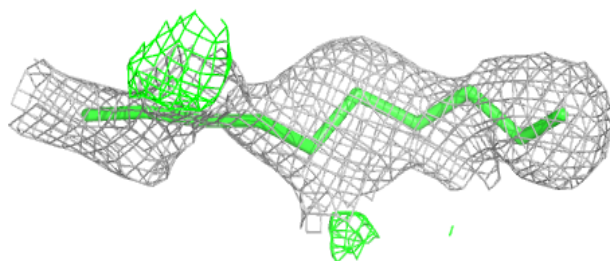
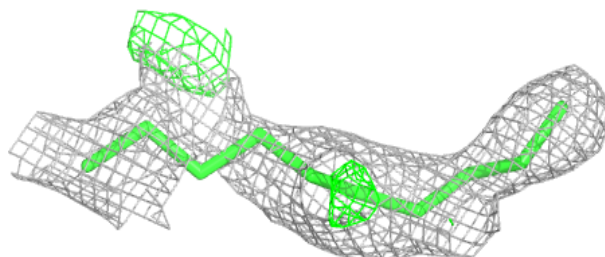
**Electron density around LFA A 311:**

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

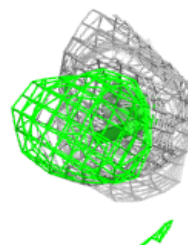
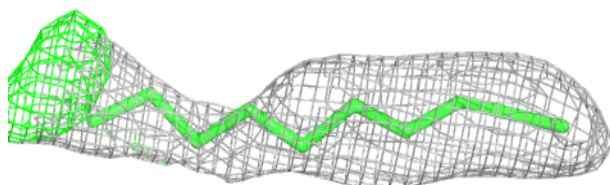
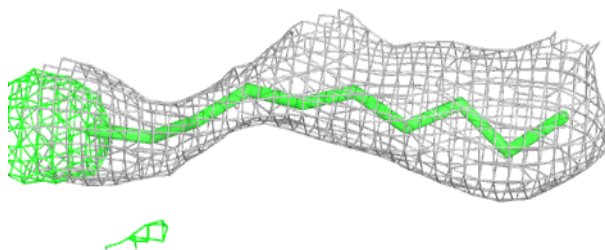


Electron density around LFA A 319:

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

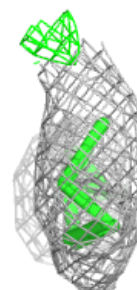
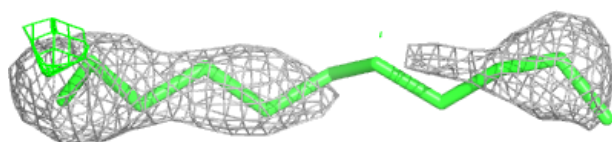
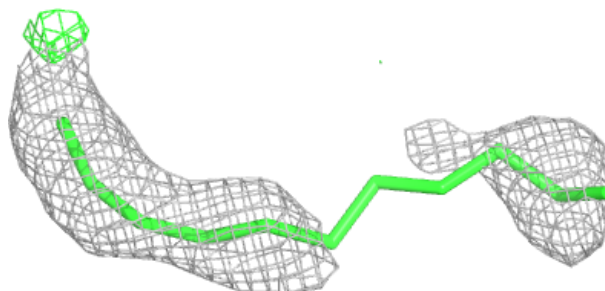
**Electron density around LFA A 308:**

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

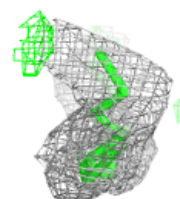
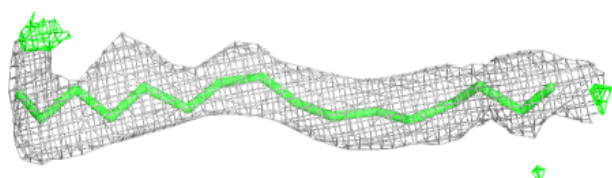
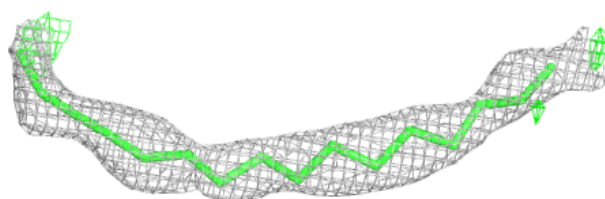


Electron density around LFA A 330:

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

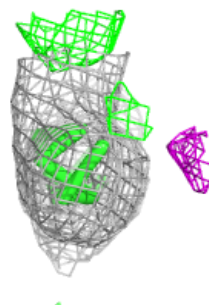
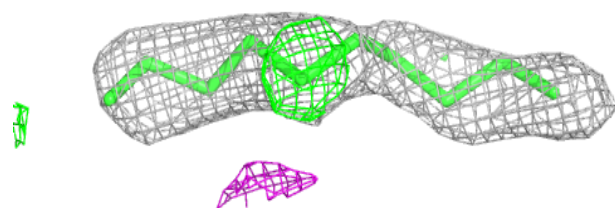
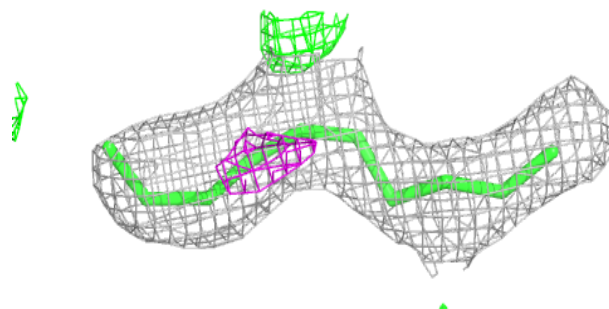
**Electron density around LFA A 312:**

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

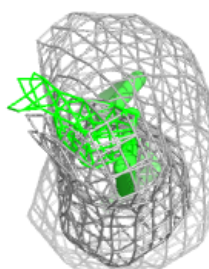
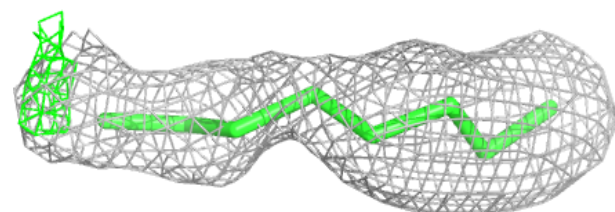
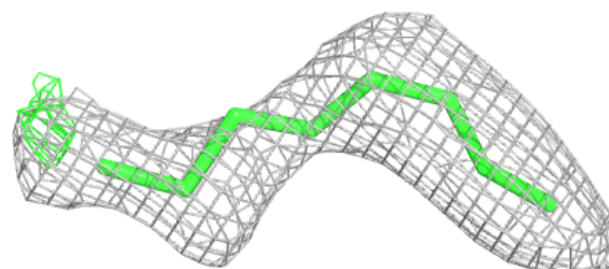


Electron density around LFA A 333:

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

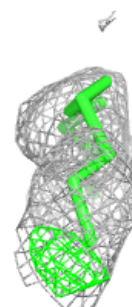
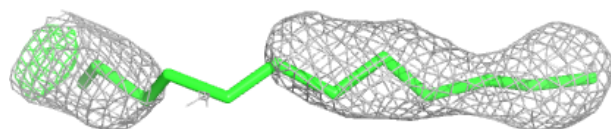
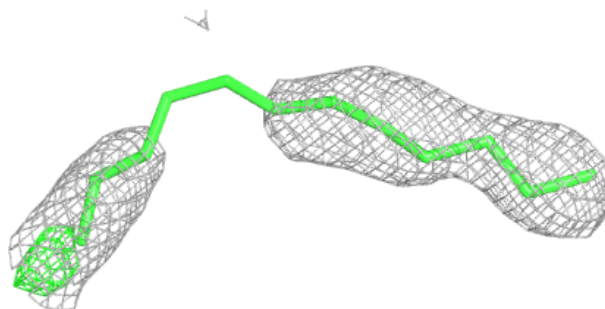
**Electron density around LFA A 310:**

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

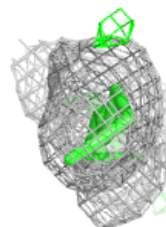
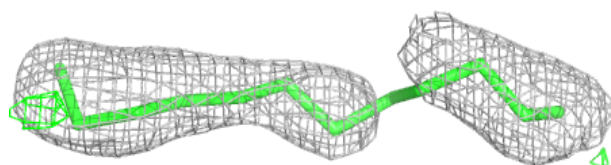
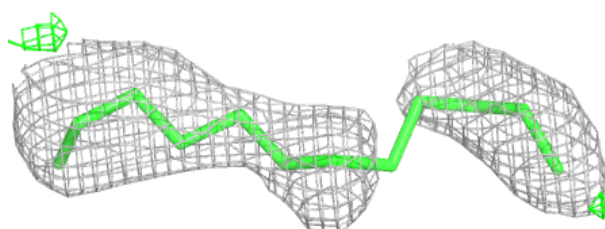


Electron density around LFA A 318:

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

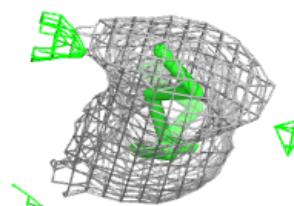
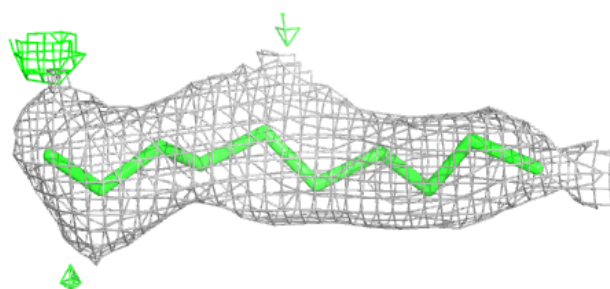
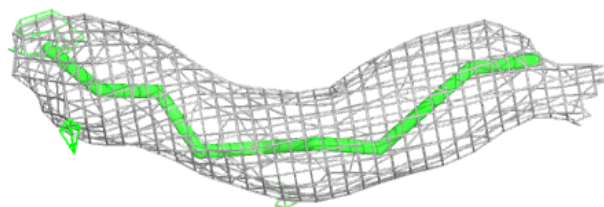
**Electron density around LFA A 334:**

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

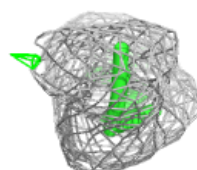
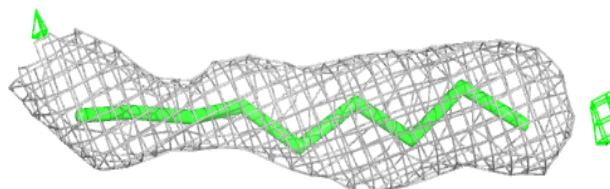
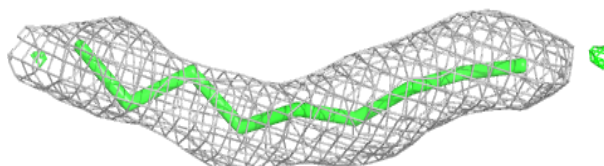


Electron density around LFA A 326:

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

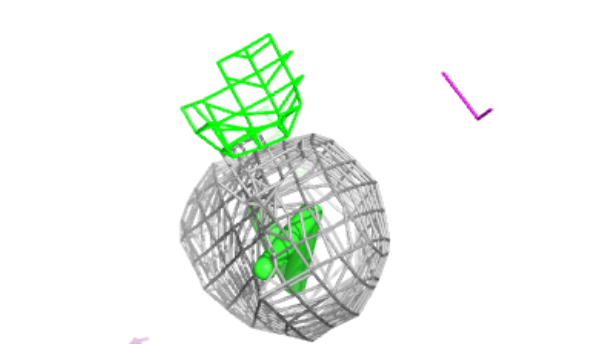
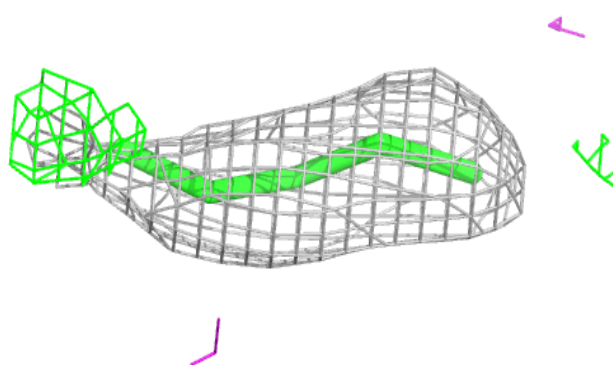
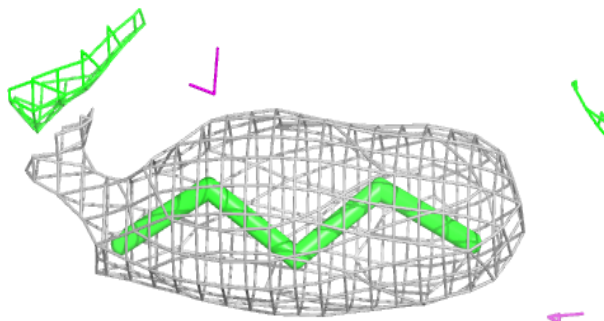
**Electron density around LFA A 304:**

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

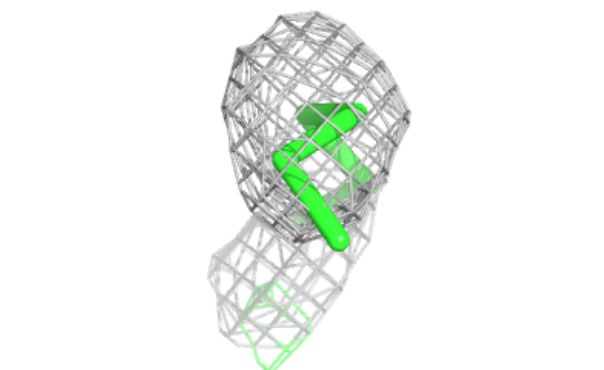
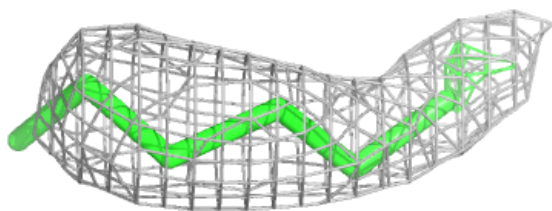
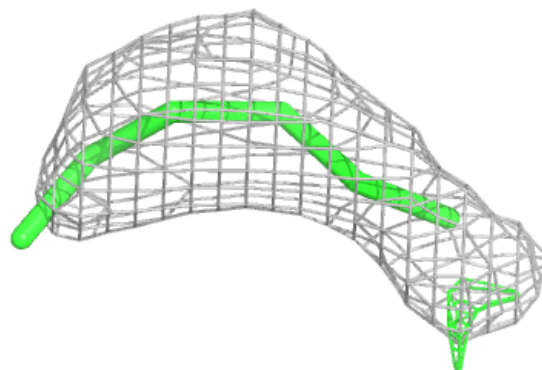


Electron density around LFA A 321:

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

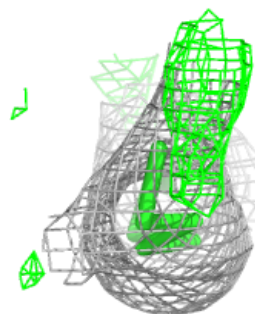
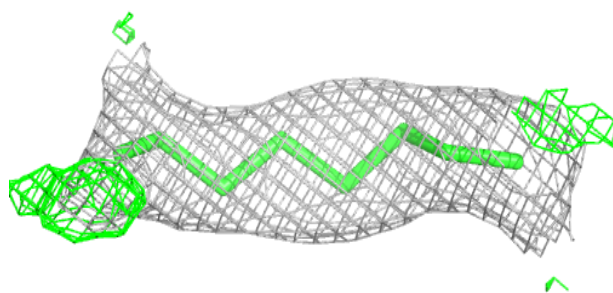
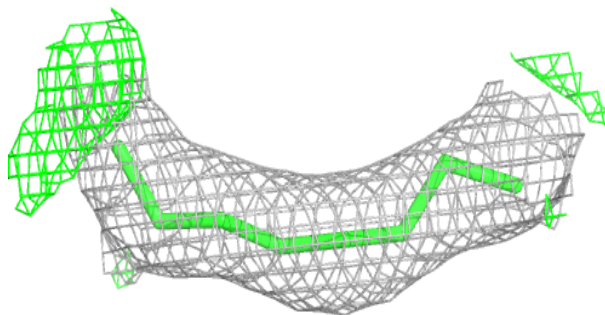
**Electron density around LFA A 322:**

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

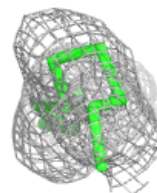
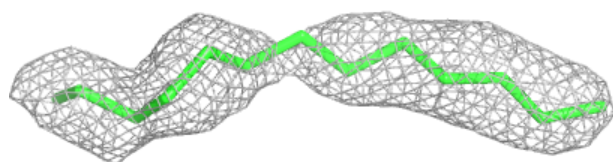
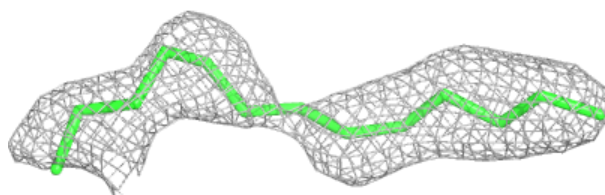


Electron density around LFA A 303:

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

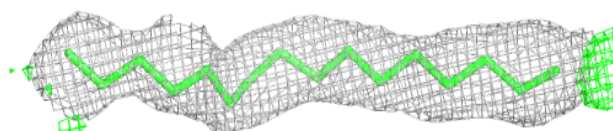
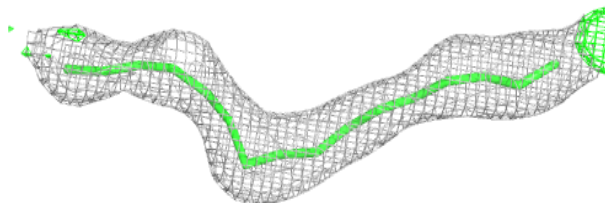
**Electron density around LFA A 307:**

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

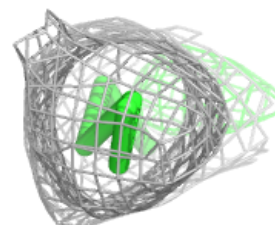
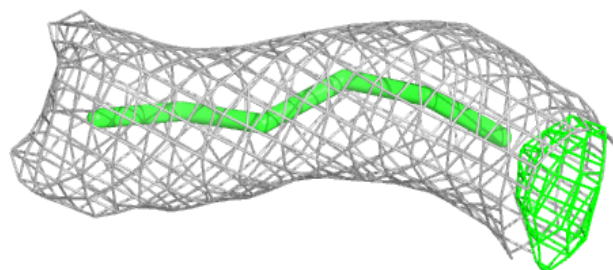
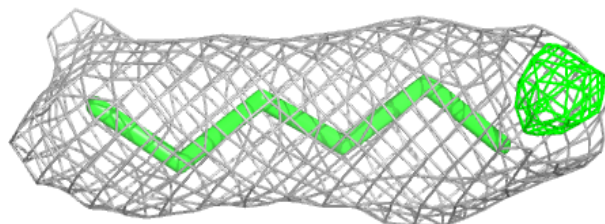


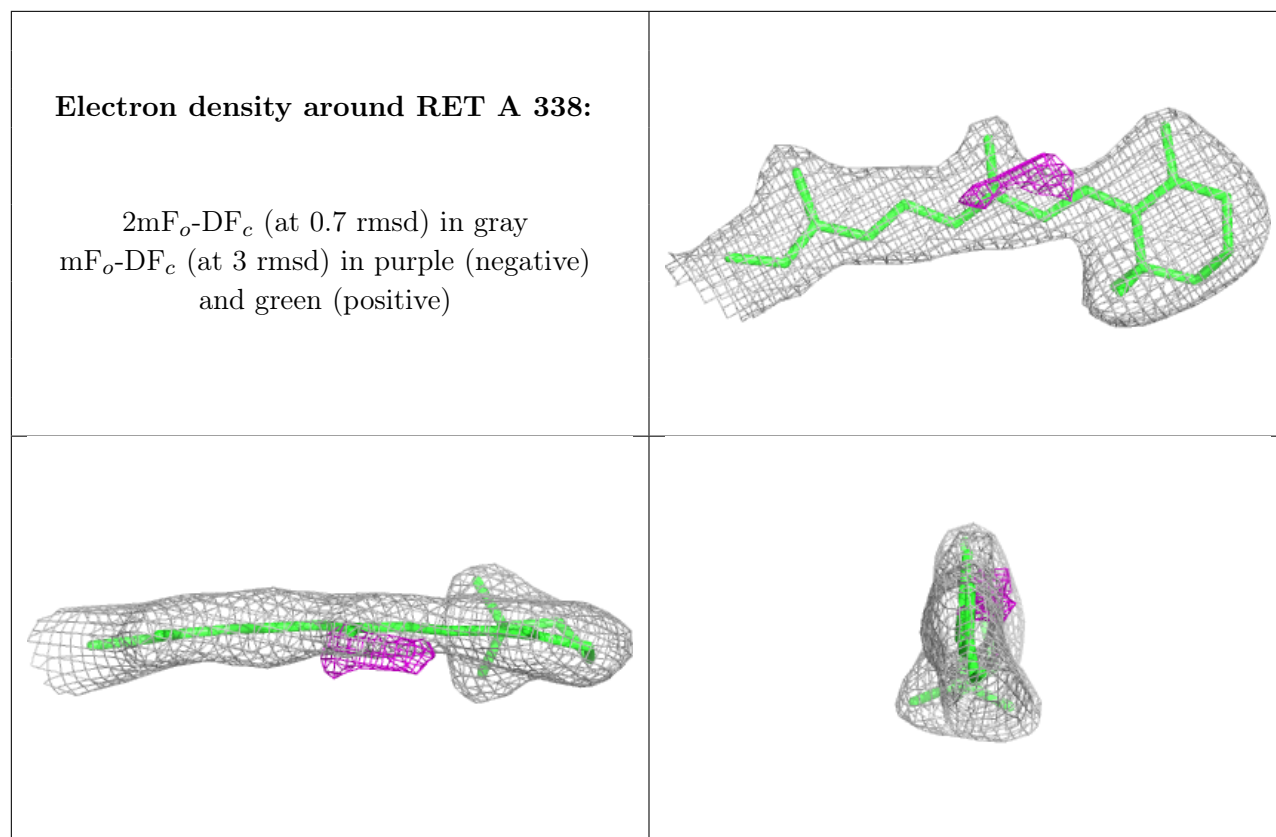
Electron density around LFA A 302:

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

**Electron density around LFA A 320:**

$2mF_o-DF_c$ (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.