



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:46 AM UTC

PDB ID : 3QAP / pdb_00003qap
Title : Crystal structure of Natronomonas pharaonis sensory rhodopsin II in the ground state
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Deposited on : 2011-01-11
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

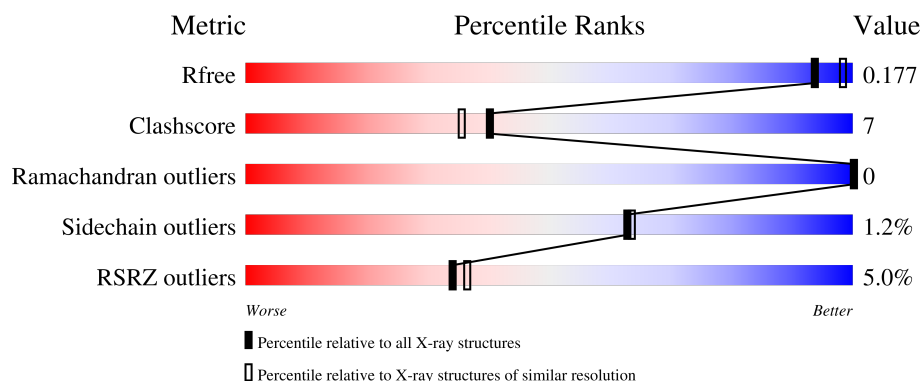
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	239	5% 83% 8% 8%

2 Entry composition [i](#)

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sensory rhodopsin-2.

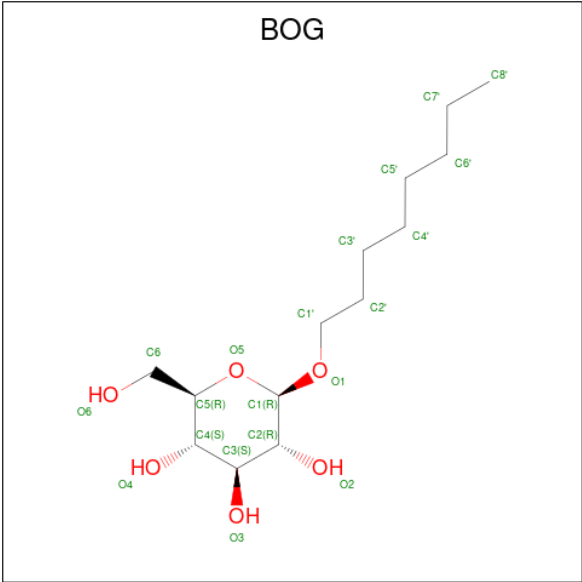
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	2	11	0
			1694	1153	261	274	6			

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



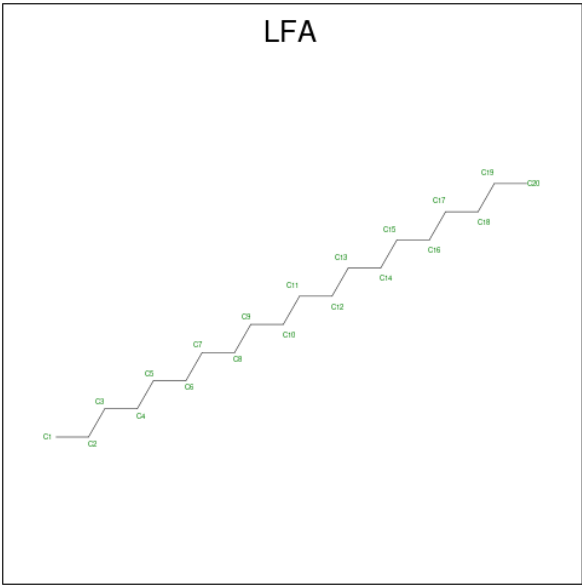
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

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



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

- Molecule 4 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



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

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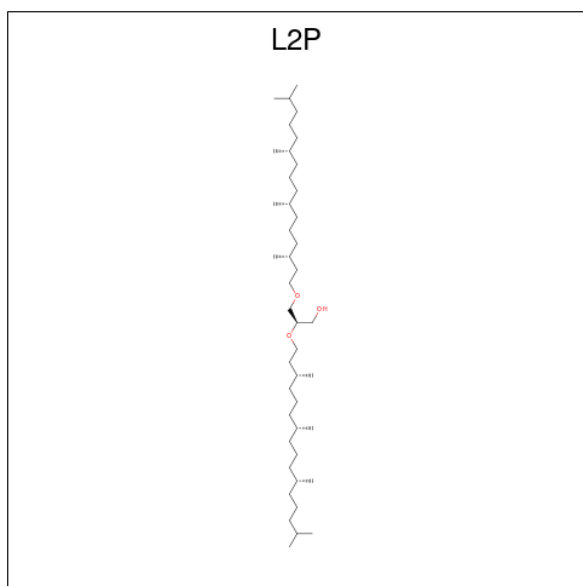
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 6 6	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 14 14	0	0
4	A	1	Total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

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

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



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

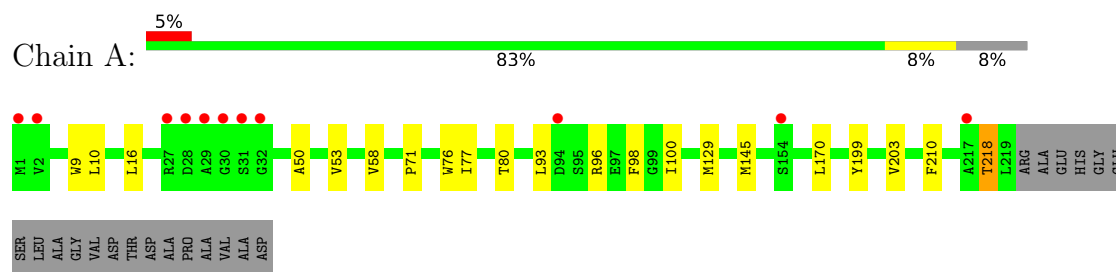
- Molecule 6 is water.

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

3 Residue-property plots

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

• Molecule 1: Sensory rhodopsin-2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	86.99Å 128.09Å 50.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.00 – 1.90 22.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (22.00-1.90) 95.8 (22.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.152 , 0.173 0.166 , 0.177	Depositor DCC
R_{free} test set	1107 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 94.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2142	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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: RET, L2P, LFA, BOG

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	0.89	2/1767 (0.1%)	0.90	3/2422 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	THR	CB-OG1	-17.34	1.16	1.43
1	A	218	THR	CB-CG2	-5.84	1.33	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	THR	OG1-CB-CG2	16.52	142.34	109.30
1	A	80	THR	CA-C-N	-6.58	112.92	119.56
1	A	80	THR	C-N-CA	-6.58	112.92	119.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	218	THR	CB

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1694	0	1806	21	0
2	A	20	0	27	3	0
3	A	20	0	28	0	0
4	A	269	0	515	12	0
5	A	66	0	127	7	0
6	A	73	0	0	0	0
All	All	2142	0	2503	30	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.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210[B]:PHE:HD2	4:A:255:LFA:H92	1.51	0.76
4:A:252:LFA:H11	4:A:261:LFA:H61	1.67	0.75
4:A:259:LFA:H21	4:A:261:LFA:H111	1.73	0.70
1:A:16[B]:LEU:HD23	4:A:261:LFA:H12	1.78	0.65
1:A:96[B]:ARG:HH11	1:A:100:ILE:HD11	1.62	0.65
1:A:210[B]:PHE:CD2	4:A:255:LFA:H92	2.33	0.63
1:A:50:ALA:HB2	5:A:257:L2P:H491	1.80	0.62
1:A:9:TRP:HZ3	4:A:252:LFA:H13	1.70	0.56
1:A:170:LEU:HD13	1:A:203[B]:VAL:HG13	1.86	0.55
2:A:240:RET:H8	2:A:240:RET:H171	1.91	0.52
1:A:10:LEU:HB3	4:A:267:LFA:H121	1.91	0.52
1:A:77:ILE:HG21	5:A:257:L2P:H241	1.92	0.52
1:A:53:VAL:HG13	1:A:58:VAL:HB	1.92	0.51
1:A:96[B]:ARG:NH1	1:A:100:ILE:HD11	2.25	0.50
1:A:93[B]:LEU:HD21	1:A:145:MET:HG2	1.94	0.49
1:A:76:TRP:CD1	2:A:240:RET:H14	2.51	0.46
1:A:129:MET:HA	1:A:129:MET:HE3	1.98	0.46
1:A:199:TYR:HB2	4:A:267:LFA:H161	1.98	0.46
4:A:245:LFA:H21	5:A:257:L2P:H243	1.98	0.45
1:A:16[A]:LEU:HD23	1:A:16[A]:LEU:HA	1.83	0.45
4:A:255:LFA:H12	4:A:267:LFA:H152	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:257:L2P:H492	5:A:257:L2P:H462	1.85	0.43
1:A:50:ALA:CB	5:A:257:L2P:H491	2.47	0.43
4:A:252:LFA:C1	4:A:261:LFA:H61	2.42	0.43
2:A:240:RET:H8	2:A:240:RET:H161	2.01	0.43
1:A:71:PRO:HG3	5:A:257:L2P:H421	2.00	0.42
1:A:16[B]:LEU:CD2	4:A:261:LFA:H12	2.48	0.42
1:A:93[B]:LEU:HD11	1:A:145:MET:HG2	2.02	0.42
5:A:257:L2P:H542	5:A:257:L2P:H512	1.89	0.42
1:A:170:LEU:HD13	1:A:203[B]:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/239 (95%)	226 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/180 (96%)	170 (99%)	2 (1%)	63	63

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	151	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	LFA	A	267	-	19,19,19	0.40	0	18,18,18	0.53	0
4	LFA	A	261	-	13,13,19	0.37	0	12,12,18	0.60	0
4	LFA	A	251	-	15,15,19	0.41	0	14,14,18	0.51	0
4	LFA	A	259	-	3,3,19	0.45	0	2,2,18	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LFA	A	269	-	3,3,19	0.48	0	2,2,18	0.63	0
4	LFA	A	258	-	5,5,19	0.41	0	4,4,18	0.38	0
4	LFA	A	265	-	7,7,19	0.43	0	6,6,18	0.47	0
4	LFA	A	255	-	13,13,19	0.37	0	12,12,18	0.56	0
4	LFA	A	264	-	8,8,19	0.35	0	7,7,18	0.51	0
4	LFA	A	245	-	5,5,19	0.42	0	4,4,18	0.35	0
4	LFA	A	266	-	9,9,19	0.43	0	8,8,18	0.47	0
4	LFA	A	243	-	5,5,19	0.43	0	4,4,18	0.35	0
4	LFA	A	248	-	6,6,19	0.35	0	5,5,18	0.50	0
4	LFA	A	242	-	9,9,19	0.44	0	8,8,18	0.53	0
4	LFA	A	246	-	7,7,19	0.37	0	6,6,18	0.55	0
2	RET	A	240	-	20,20,21	2.62	12 (60%)	27,27,28	1.86	8 (29%)
4	LFA	A	270	-	3,3,19	0.43	0	2,2,18	0.63	0
4	LFA	A	252	-	11,11,19	0.35	0	10,10,18	0.61	0
4	LFA	A	249	-	4,4,19	0.38	0	3,3,18	0.47	0
4	LFA	A	253	-	5,5,19	0.43	0	4,4,18	0.34	0
4	LFA	A	250	-	8,8,19	0.41	0	7,7,18	0.44	0
4	LFA	A	268	-	6,6,19	0.40	0	5,5,18	0.48	0
5	L2P	A	260	-	19,19,45	0.33	0	22,22,53	0.61	0
3	BOG	A	241	-	20,20,20	0.61	0	25,25,25	1.02	2 (8%)
4	LFA	A	247	-	4,4,19	0.41	0	3,3,18	0.45	0
4	LFA	A	272	-	11,11,19	0.42	0	10,10,18	0.46	0
4	LFA	A	256	-	4,4,19	0.41	0	3,3,18	0.36	0
4	LFA	A	271	-	19,19,19	0.39	0	18,18,18	0.56	0
4	LFA	A	244	-	9,9,19	0.44	0	8,8,18	0.52	0
4	LFA	A	254	-	15,15,19	0.39	0	14,14,18	0.56	0
5	L2P	A	257	-	45,45,45	0.50	0	51,53,53	0.73	0
4	LFA	A	262	-	5,5,19	0.42	0	4,4,18	0.36	0
4	LFA	A	263	-	9,9,19	0.41	0	8,8,18	0.48	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
4	LFA	A	267	-	-	9/17/17/17	-
4	LFA	A	261	-	-	7/11/11/17	-
4	LFA	A	251	-	-	8/13/13/17	-
4	LFA	A	259	-	-	0/1/1/17	-
4	LFA	A	269	-	-	0/1/1/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LFA	A	258	-	-	1/3/3/17	-
4	LFA	A	265	-	-	4/5/5/17	-
4	LFA	A	255	-	-	5/11/11/17	-
4	LFA	A	264	-	-	5/6/6/17	-
4	LFA	A	245	-	-	2/3/3/17	-
4	LFA	A	266	-	-	4/7/7/17	-
4	LFA	A	243	-	-	1/3/3/17	-
4	LFA	A	248	-	-	1/4/4/17	-
4	LFA	A	242	-	-	4/7/7/17	-
4	LFA	A	246	-	-	3/5/5/17	-
2	RET	A	240	-	-	0/13/30/31	0/1/1/1
4	LFA	A	270	-	-	0/1/1/17	-
4	LFA	A	252	-	-	6/9/9/17	-
4	LFA	A	249	-	-	0/2/2/17	-
4	LFA	A	253	-	-	1/3/3/17	-
4	LFA	A	250	-	-	3/6/6/17	-
4	LFA	A	268	-	-	2/4/4/17	-
5	L2P	A	260	-	-	10/20/20/51	-
3	BOG	A	241	-	-	6/11/31/31	0/1/1/1
4	LFA	A	247	-	-	0/2/2/17	-
4	LFA	A	272	-	-	4/9/9/17	-
4	LFA	A	256	-	-	1/2/2/17	-
4	LFA	A	271	-	-	14/17/17/17	-
4	LFA	A	244	-	-	2/7/7/17	-
4	LFA	A	254	-	-	10/13/13/17	-
5	L2P	A	257	-	-	25/51/51/51	-
4	LFA	A	262	-	-	1/3/3/17	-
4	LFA	A	263	-	-	5/7/7/17	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	240	RET	C14-C13	5.54	1.37	1.33
2	A	240	RET	C1-C6	4.70	1.59	1.53
2	A	240	RET	C5-C6	4.26	1.41	1.34
2	A	240	RET	C15-C14	-3.03	1.38	1.49
2	A	240	RET	C18-C5	2.77	1.55	1.50
2	A	240	RET	C8-C7	2.71	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	240	RET	C19-C9	2.57	1.56	1.50
2	A	240	RET	C12-C13	-2.55	1.40	1.46
2	A	240	RET	C20-C13	2.38	1.55	1.50
2	A	240	RET	C8-C9	-2.26	1.41	1.46
2	A	240	RET	C10-C9	2.22	1.40	1.35
2	A	240	RET	C17-C1	2.15	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	240	RET	C10-C11-C12	-3.89	111.94	123.20
2	A	240	RET	C11-C10-C9	-3.25	122.72	127.28
3	A	241	BOG	C1'-O1-C1	-3.11	108.36	113.68
2	A	240	RET	C3-C4-C5	-2.94	108.82	114.06
2	A	240	RET	C20-C13-C12	2.84	122.42	118.09
2	A	240	RET	C1-C6-C7	2.54	122.54	115.65
2	A	240	RET	C18-C5-C6	-2.45	121.81	124.48
2	A	240	RET	C7-C8-C9	-2.37	122.73	126.23
2	A	240	RET	C2-C3-C4	-2.21	106.43	111.28
3	A	241	BOG	O1-C1-C2	2.07	111.42	108.27

There are no chirality outliers.

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	257	L2P	C1-C2-C3-O3
5	A	257	L2P	O2-C2-C3-O3
5	A	257	L2P	C41-C42-C43-C44
3	A	241	BOG	O5-C5-C6-O6
3	A	241	BOG	C4-C5-C6-O6
5	A	257	L2P	C16-C17-C18-C19
5	A	257	L2P	C43-C45-C46-C47
5	A	257	L2P	C45-C46-C47-C48
5	A	257	L2P	O2-C41-C42-C43
4	A	271	LFA	C9-C10-C11-C12
5	A	260	L2P	C45-C46-C47-C48
5	A	257	L2P	C50-C51-C52-C53
5	A	257	L2P	C26-C27-C28-C29
5	A	260	L2P	C48-C50-C51-C52
4	A	264	LFA	C5-C6-C7-C8
4	A	264	LFA	C2-C3-C4-C5
4	A	254	LFA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	242	LFA	C6-C7-C8-C9
4	A	251	LFA	C4-C5-C6-C7
4	A	255	LFA	C4-C5-C6-C7
4	A	261	LFA	C2-C3-C4-C5
5	A	257	L2P	C26-C27-C28-C30
3	A	241	BOG	C2'-C3'-C4'-C5'
4	A	261	LFA	C3-C4-C5-C6
4	A	251	LFA	C3-C4-C5-C6
4	A	271	LFA	C2-C3-C4-C5
4	A	263	LFA	C3-C4-C5-C6
4	A	266	LFA	C4-C5-C6-C7
4	A	251	LFA	C2-C3-C4-C5
3	A	241	BOG	C3'-C4'-C5'-C6'
4	A	254	LFA	C11-C10-C9-C8
4	A	264	LFA	C3-C4-C5-C6
4	A	267	LFA	C6-C7-C8-C9
5	A	257	L2P	C23-C25-C26-C27
3	A	241	BOG	C1'-C2'-C3'-C4'
5	A	260	L2P	C41-C42-C43-C45
4	A	254	LFA	C9-C10-C11-C12
4	A	264	LFA	C4-C5-C6-C7
4	A	272	LFA	C3-C4-C5-C6
4	A	261	LFA	C5-C6-C7-C8
4	A	267	LFA	C3-C4-C5-C6
4	A	267	LFA	C11-C12-C13-C14
4	A	271	LFA	C15-C16-C17-C18
4	A	271	LFA	C4-C5-C6-C7
4	A	254	LFA	C4-C5-C6-C7
4	A	261	LFA	C10-C11-C12-C13
4	A	255	LFA	C7-C8-C9-C10
4	A	251	LFA	C7-C8-C9-C10
4	A	265	LFA	C3-C4-C5-C6
4	A	271	LFA	C6-C7-C8-C9
4	A	265	LFA	C2-C3-C4-C5
4	A	271	LFA	C12-C13-C14-C15
4	A	271	LFA	C5-C6-C7-C8
4	A	263	LFA	C5-C6-C7-C8
5	A	260	L2P	C47-C48-C50-C51
5	A	260	L2P	C49-C48-C50-C51
4	A	242	LFA	C5-C6-C7-C8
5	A	257	L2P	C18-C20-C21-C22
4	A	271	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
4	A	242	LFA	C4-C5-C6-C7
4	A	255	LFA	C6-C7-C8-C9
4	A	267	LFA	C10-C11-C12-C13
4	A	262	LFA	C1-C2-C3-C4
4	A	252	LFA	C11-C10-C9-C8
4	A	271	LFA	C3-C4-C5-C6
4	A	261	LFA	C1-C2-C3-C4
4	A	264	LFA	C6-C7-C8-C9
4	A	250	LFA	C5-C6-C7-C8
4	A	265	LFA	C4-C5-C6-C7
4	A	244	LFA	C7-C8-C9-C10
4	A	265	LFA	C5-C6-C7-C8
4	A	252	LFA	C7-C8-C9-C10
4	A	271	LFA	C10-C11-C12-C13
4	A	255	LFA	C5-C6-C7-C8
4	A	272	LFA	C1-C2-C3-C4
4	A	245	LFA	C3-C4-C5-C6
4	A	271	LFA	C14-C15-C16-C17
4	A	263	LFA	C7-C8-C9-C10
3	A	241	BOG	C4'-C5'-C6'-C7'
4	A	261	LFA	C11-C12-C13-C14
5	A	257	L2P	O1-C1-C2-C3
4	A	243	LFA	C3-C4-C5-C6
4	A	252	LFA	C1-C2-C3-C4
4	A	263	LFA	C4-C5-C6-C7
4	A	251	LFA	C13-C14-C15-C16
4	A	256	LFA	C2-C3-C4-C5
5	A	257	L2P	O1-C1-C2-O2
4	A	258	LFA	C1-C2-C3-C4
4	A	252	LFA	C6-C7-C8-C9
4	A	248	LFA	C2-C3-C4-C5
4	A	255	LFA	C3-C4-C5-C6
4	A	252	LFA	C9-C10-C11-C12
4	A	254	LFA	C11-C12-C13-C14
5	A	260	L2P	C41-C42-C43-C44
4	A	266	LFA	C2-C3-C4-C5
4	A	244	LFA	C5-C6-C7-C8
4	A	251	LFA	C12-C13-C14-C15
5	A	257	L2P	C49-C48-C50-C51
4	A	254	LFA	C10-C11-C12-C13
5	A	257	L2P	C15-C16-C17-C18
4	A	261	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	A	250	LFA	C2-C3-C4-C5
4	A	254	LFA	C7-C8-C9-C10
4	A	272	LFA	C11-C10-C9-C8
4	A	267	LFA	C5-C6-C7-C8
4	A	246	LFA	C3-C4-C5-C6
4	A	253	LFA	C2-C3-C4-C5
4	A	254	LFA	C13-C14-C15-C16
5	A	257	L2P	C41-C42-C43-C45
4	A	242	LFA	C7-C8-C9-C10
4	A	250	LFA	C3-C4-C5-C6
4	A	268	LFA	C1-C2-C3-C4
4	A	254	LFA	C3-C4-C5-C6
5	A	257	L2P	C47-C48-C50-C51
4	A	266	LFA	C6-C7-C8-C9
4	A	267	LFA	C11-C10-C9-C8
5	A	257	L2P	C16-C17-C18-C20
4	A	245	LFA	C2-C3-C4-C5
4	A	267	LFA	C15-C16-C17-C18
4	A	272	LFA	C6-C7-C8-C9
4	A	246	LFA	C1-C2-C3-C4
5	A	257	L2P	C44-C43-C45-C46
4	A	263	LFA	C2-C3-C4-C5
4	A	267	LFA	C4-C5-C6-C7
4	A	267	LFA	C1-C2-C3-C4
4	A	266	LFA	C5-C6-C7-C8
4	A	268	LFA	C4-C5-C6-C7
4	A	271	LFA	C17-C18-C19-C20
5	A	260	L2P	C46-C47-C48-C50
5	A	260	L2P	C53-C55-C56-C57
4	A	246	LFA	C2-C3-C4-C5
4	A	271	LFA	C1-C2-C3-C4
4	A	251	LFA	C6-C7-C8-C9
4	A	271	LFA	C11-C12-C13-C14
5	A	257	L2P	C12-C11-O1-C1
4	A	251	LFA	C9-C10-C11-C12
4	A	254	LFA	C1-C2-C3-C4
5	A	257	L2P	C42-C43-C45-C46
5	A	260	L2P	C56-C57-C58-C59
5	A	257	L2P	C22-C23-C25-C26
5	A	257	L2P	C54-C53-C55-C56
5	A	260	L2P	C46-C47-C48-C49
5	A	257	L2P	C13-C15-C16-C17

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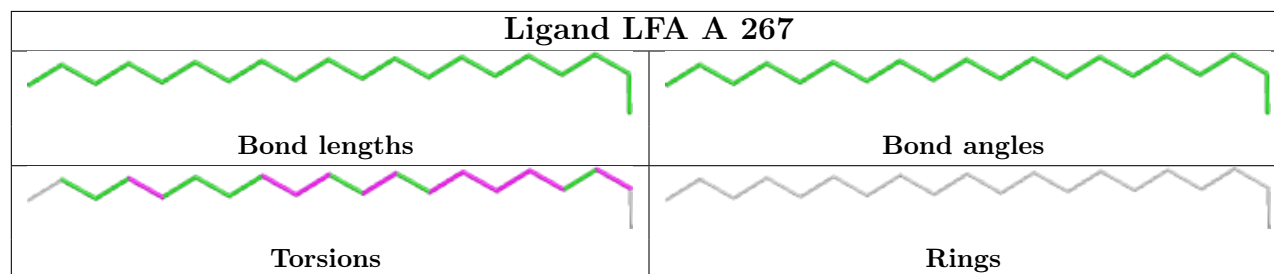
Mol	Chain	Res	Type	Atoms
4	A	252	LFA	C5-C6-C7-C8

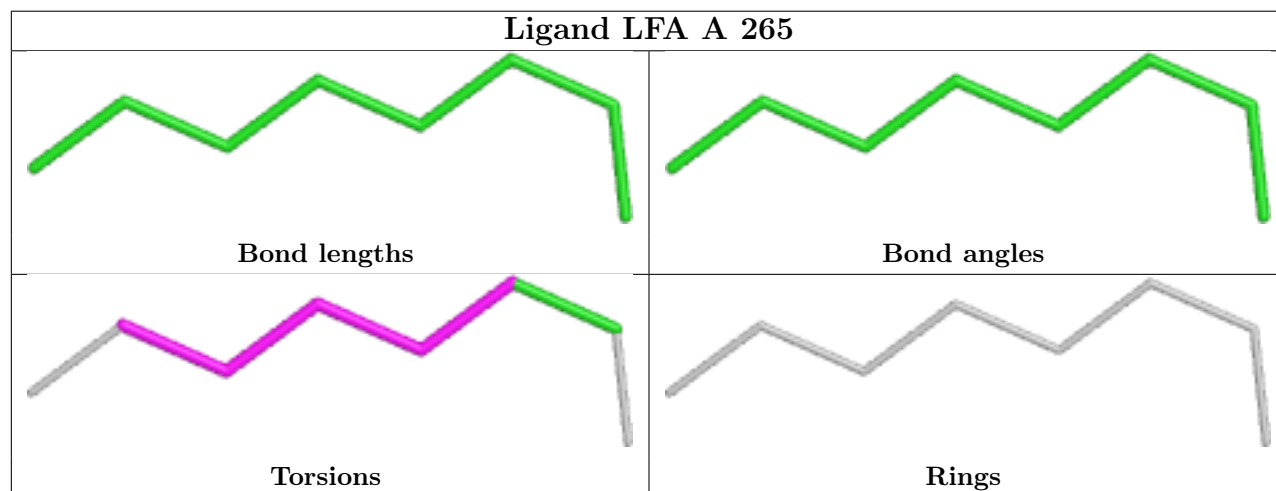
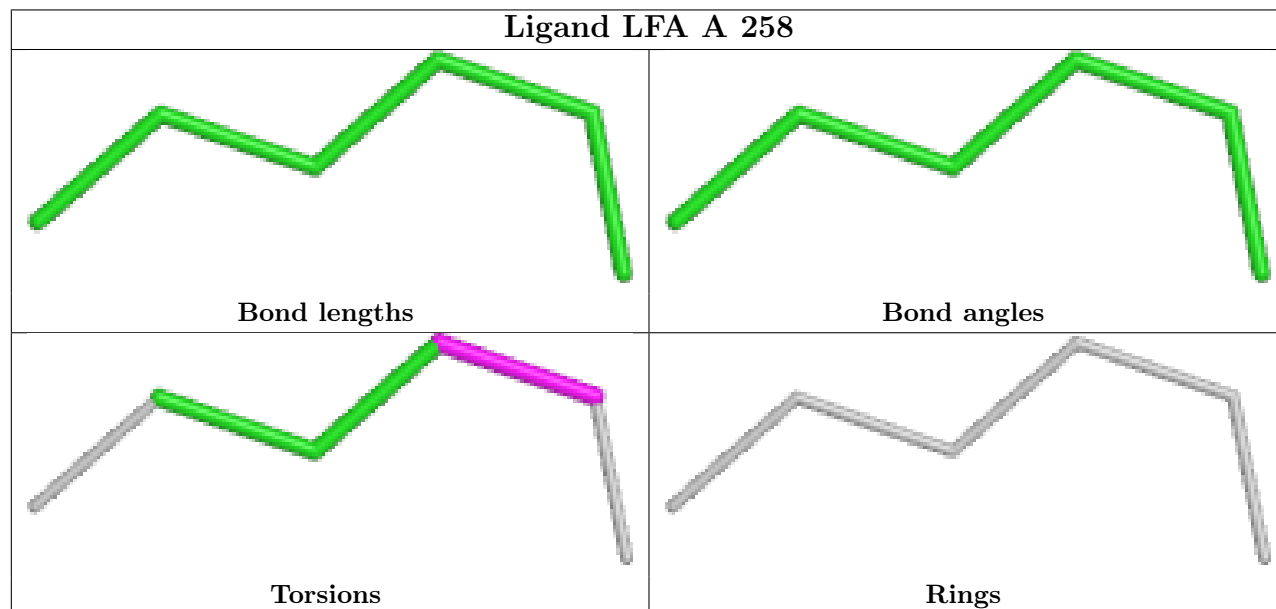
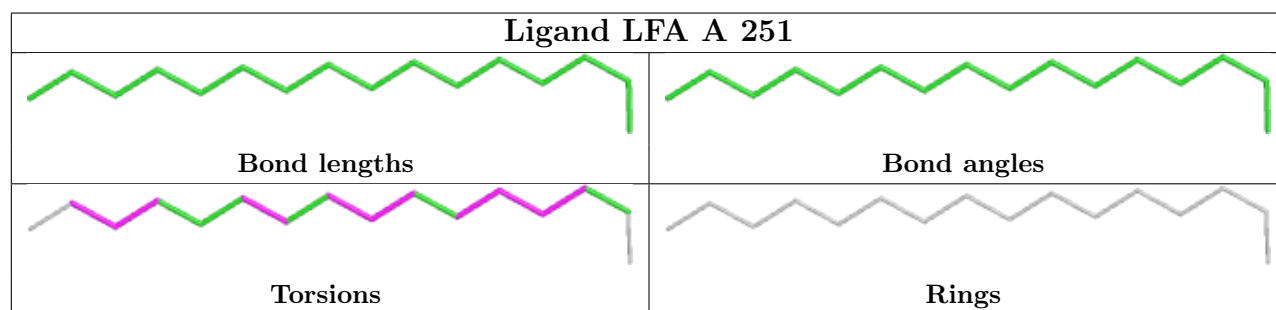
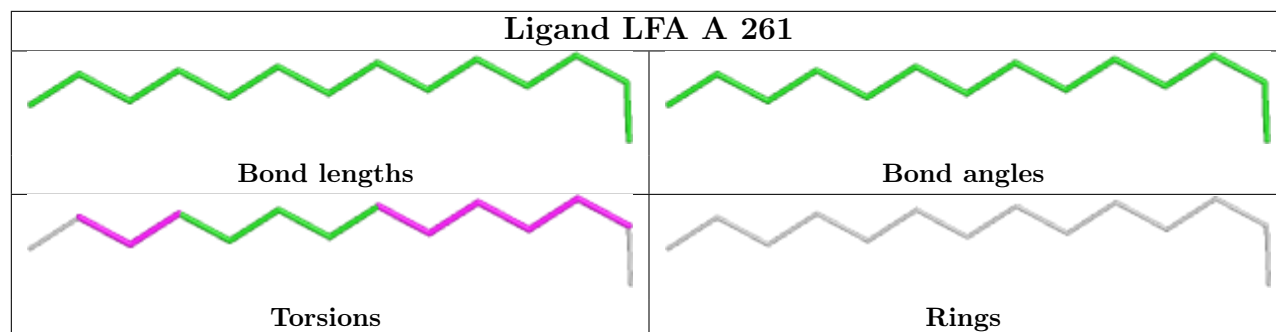
There are no ring outliers.

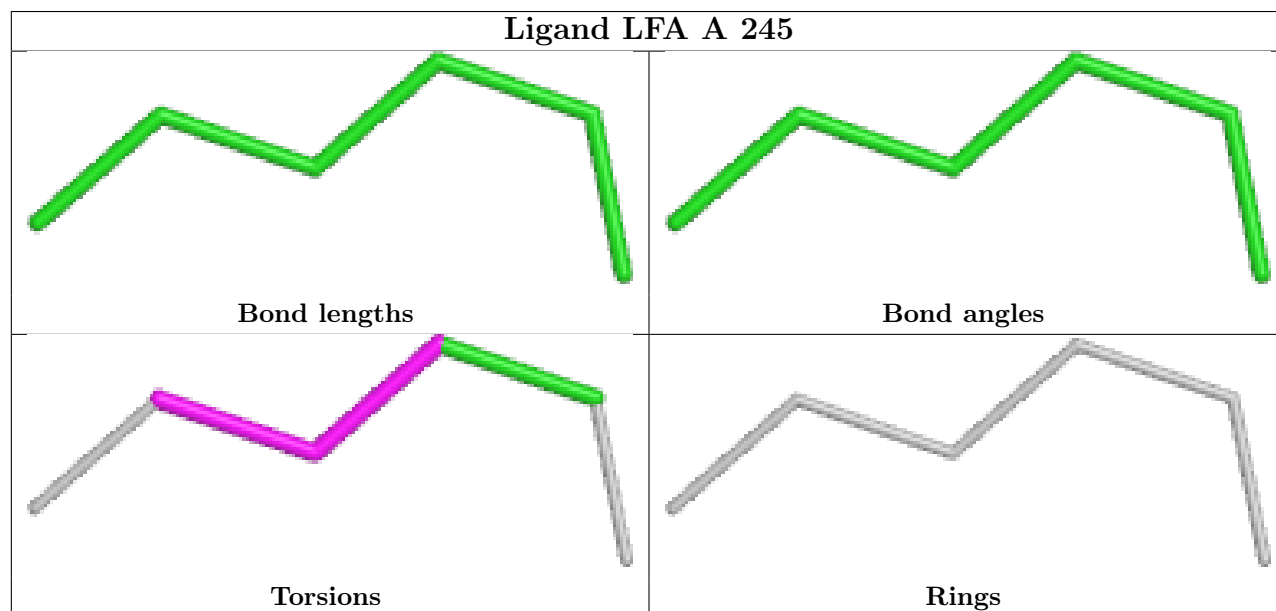
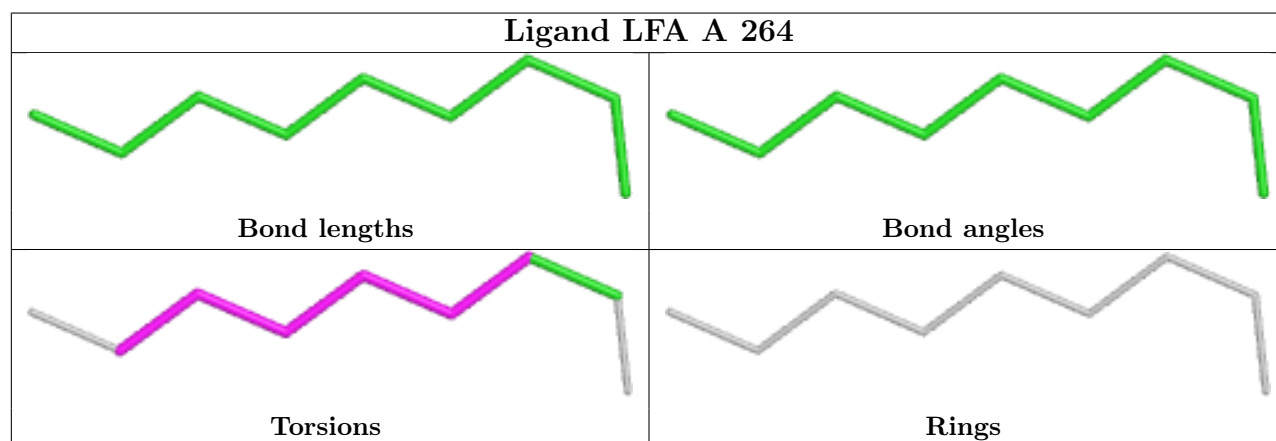
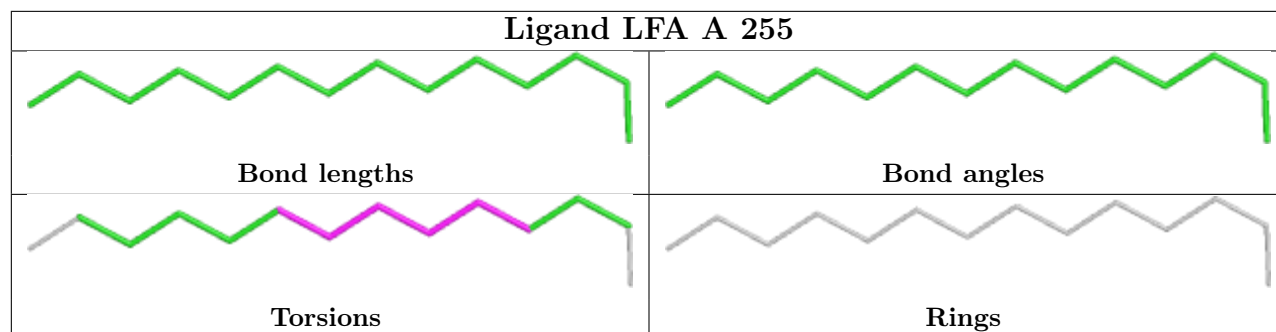
8 monomers are involved in 21 short contacts:

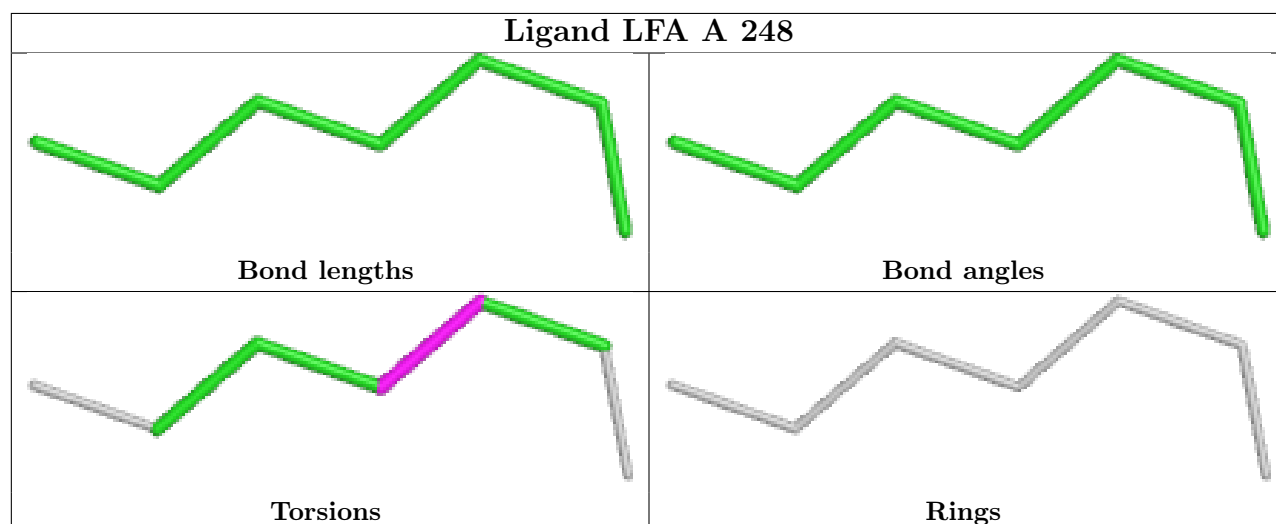
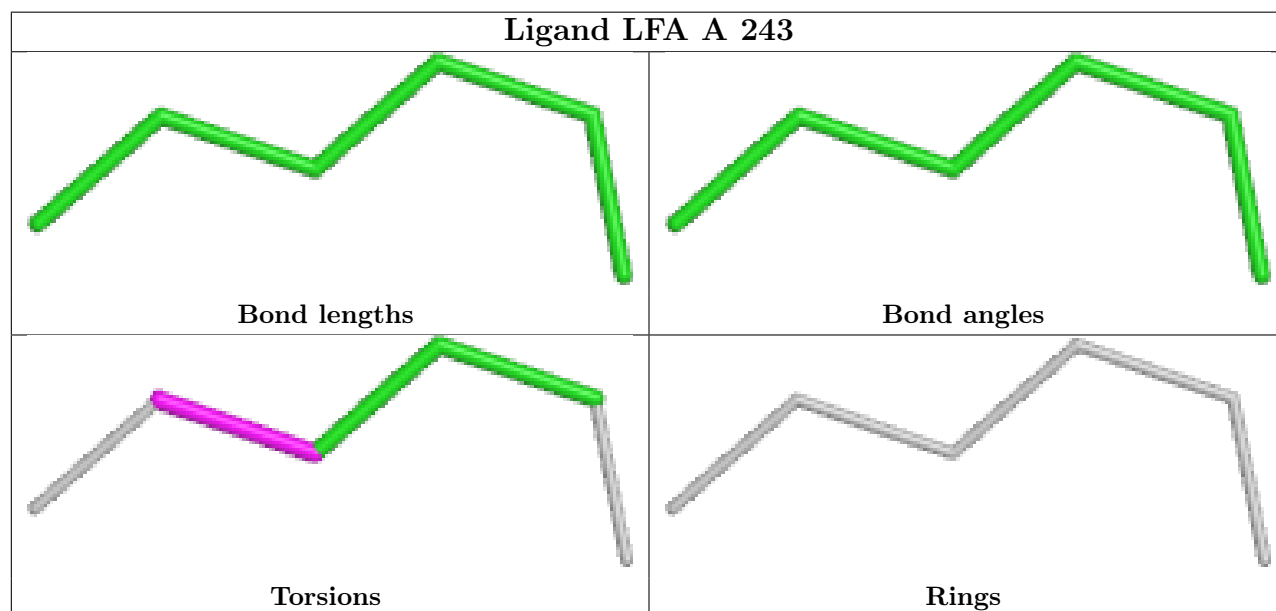
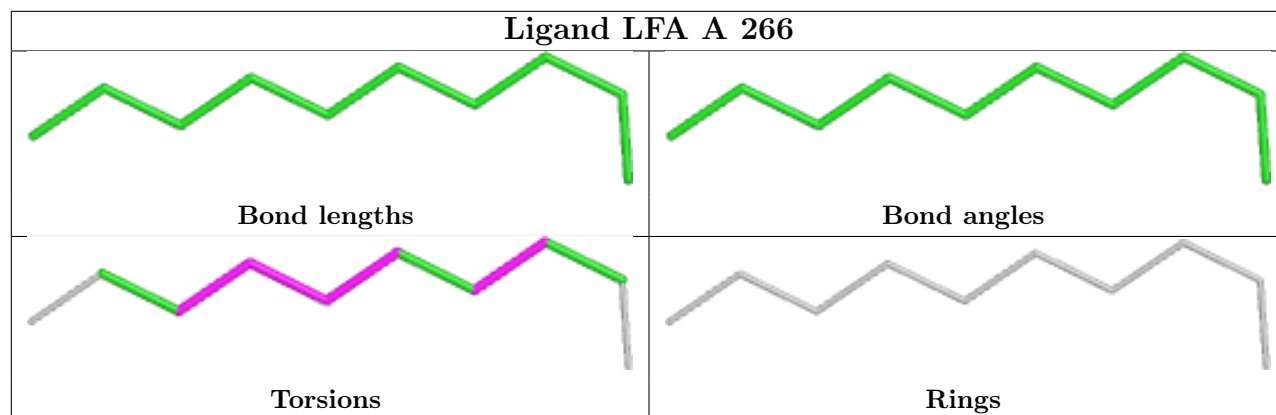
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	267	LFA	3	0
4	A	261	LFA	5	0
4	A	259	LFA	1	0
4	A	255	LFA	3	0
4	A	245	LFA	1	0
2	A	240	RET	3	0
4	A	252	LFA	3	0
5	A	257	L2P	7	0

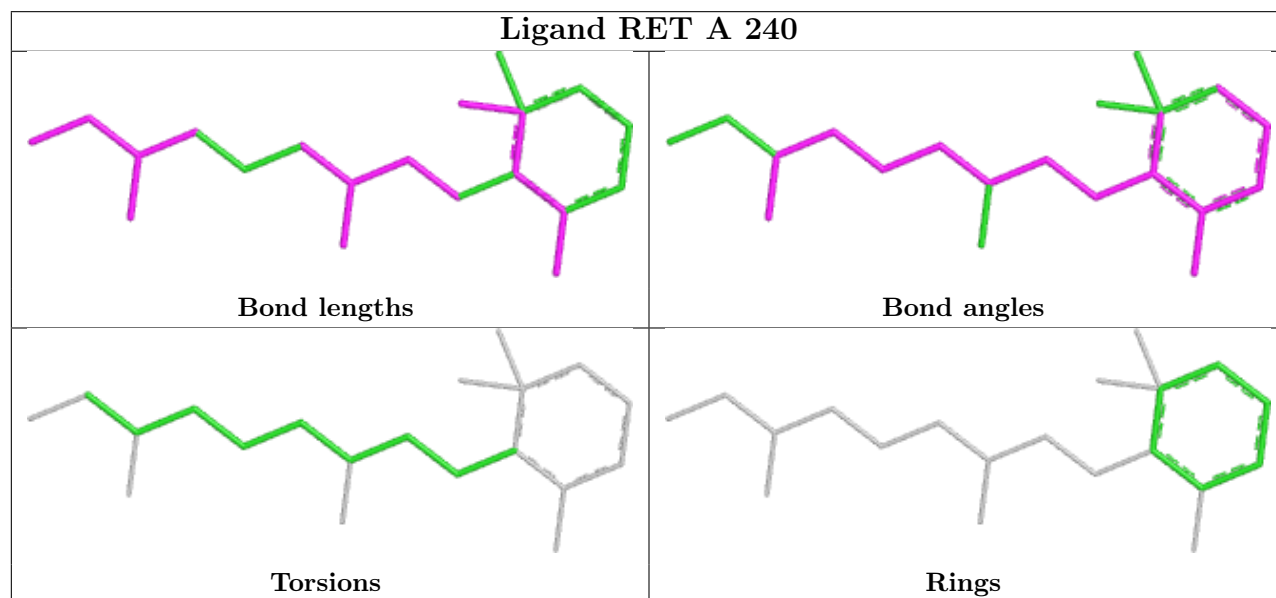
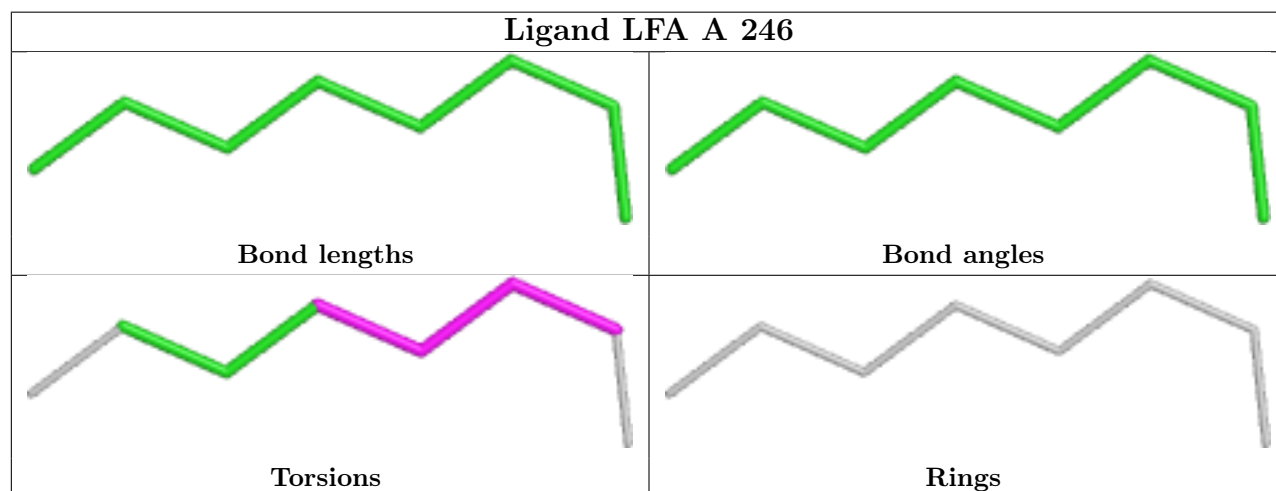
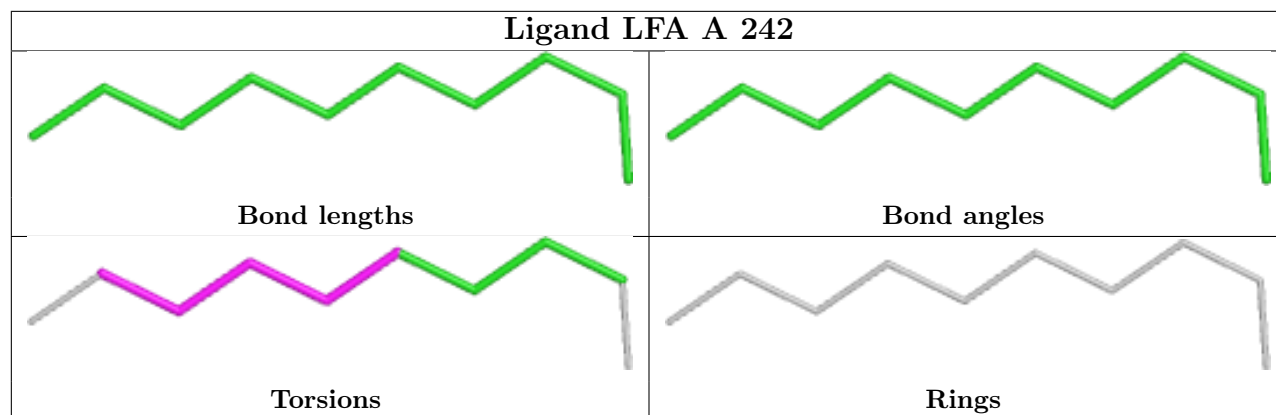
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

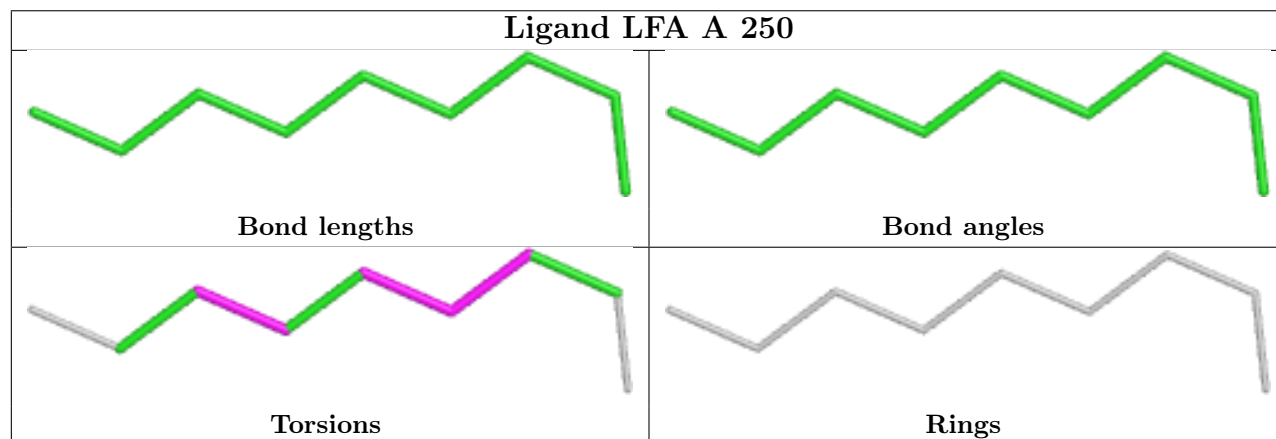
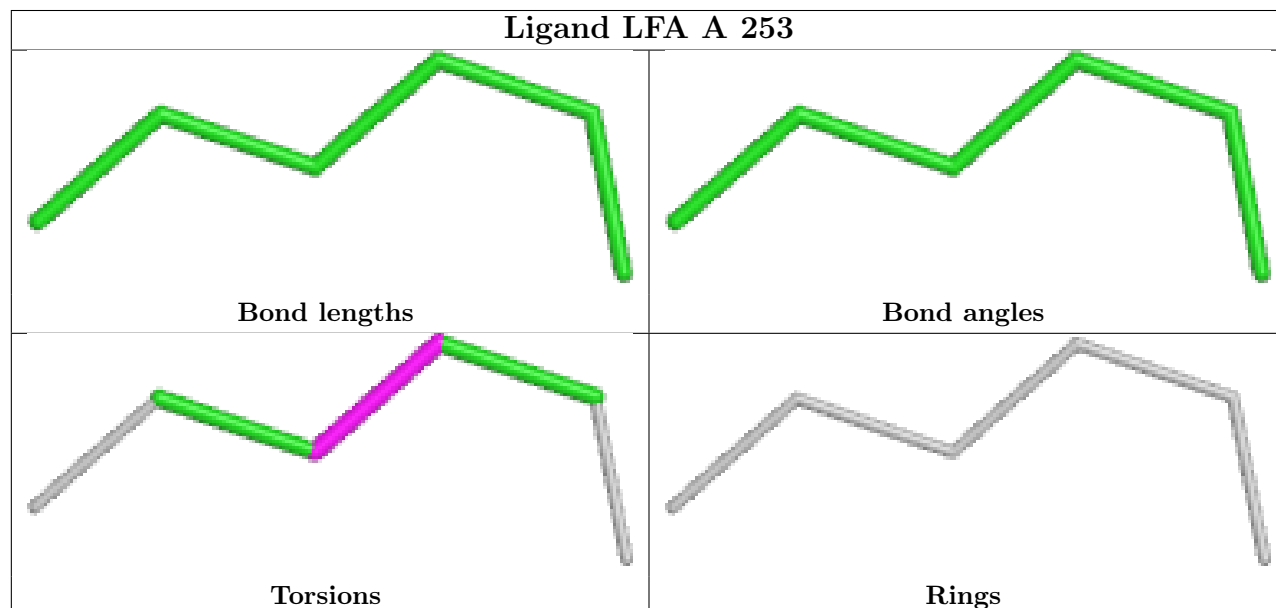
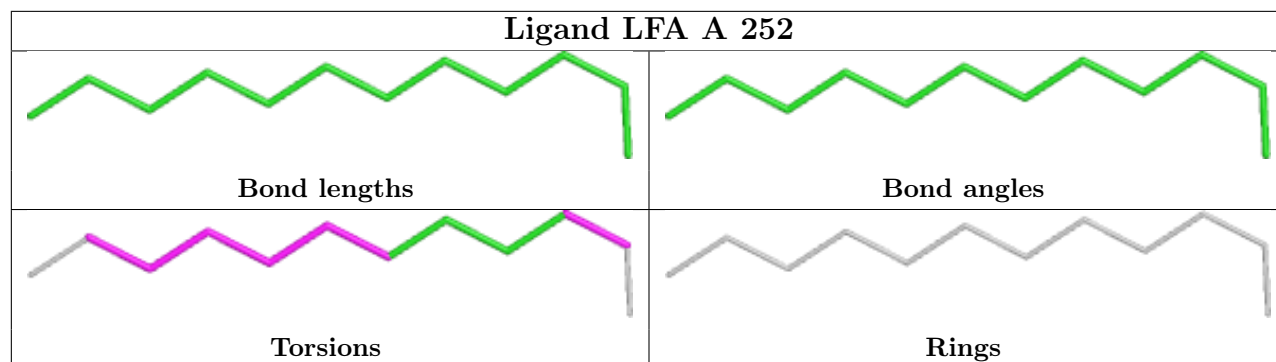


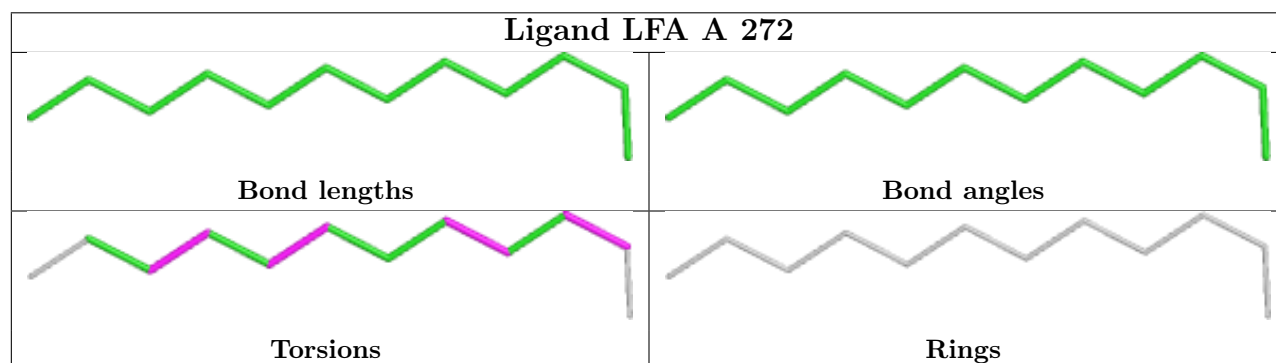
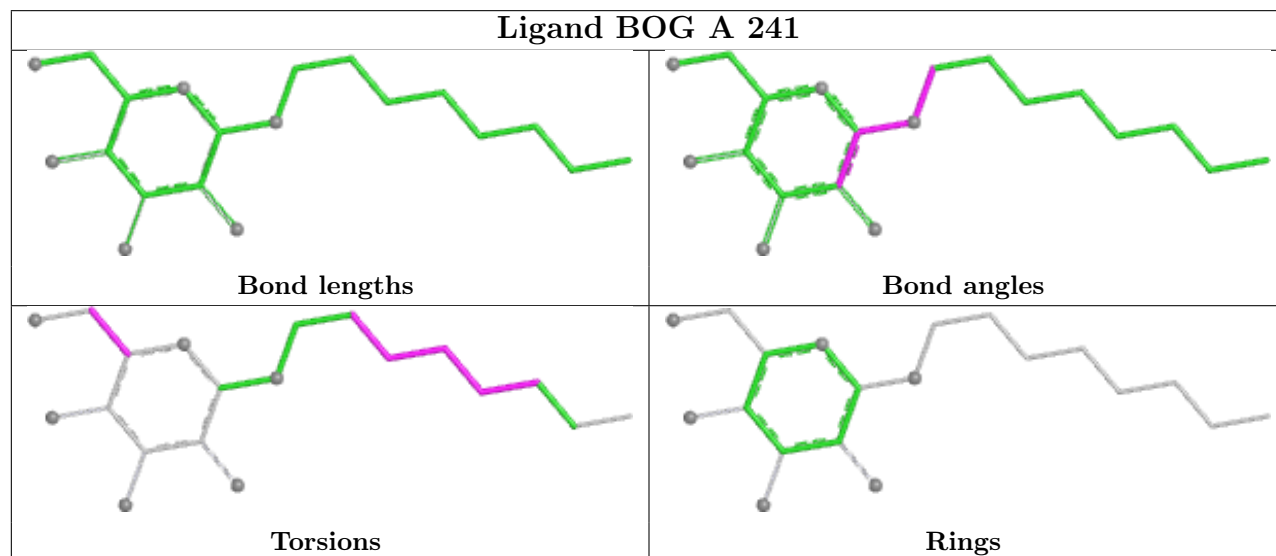
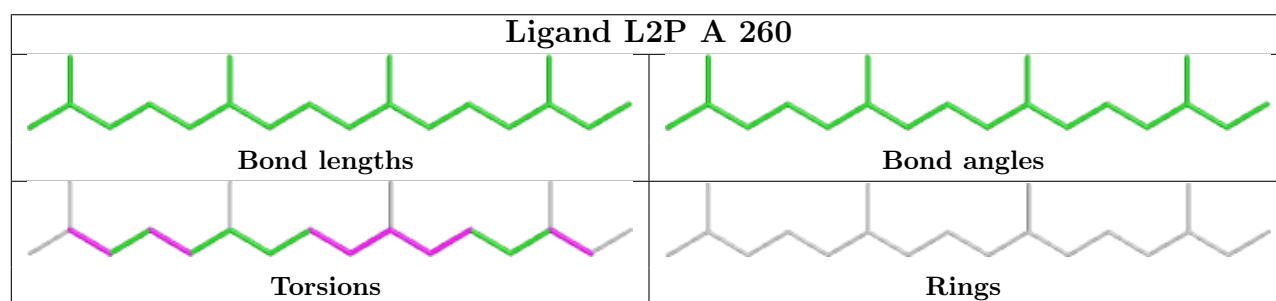
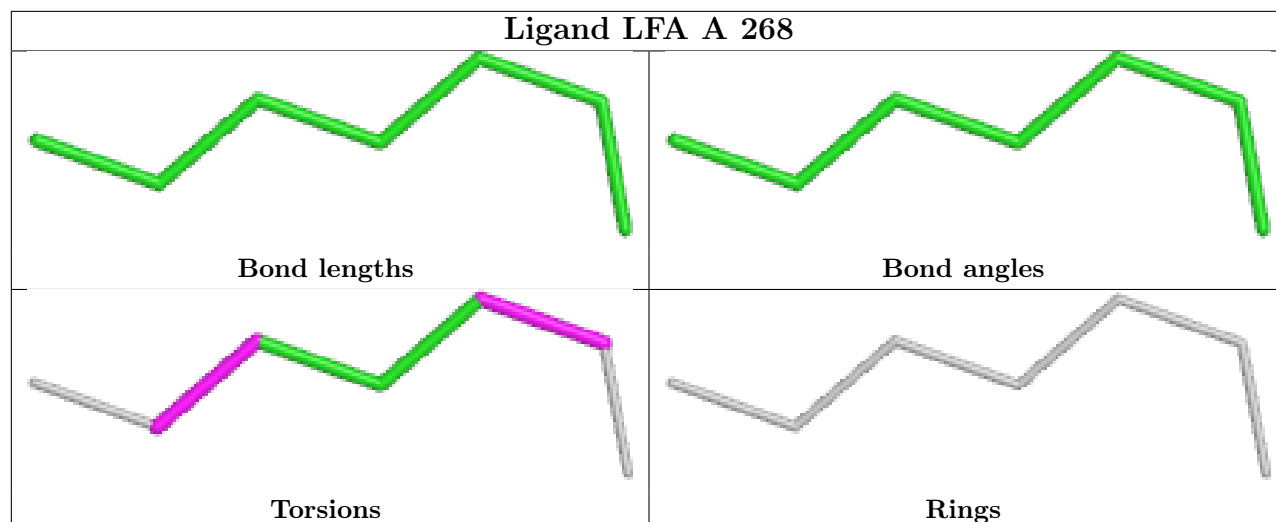


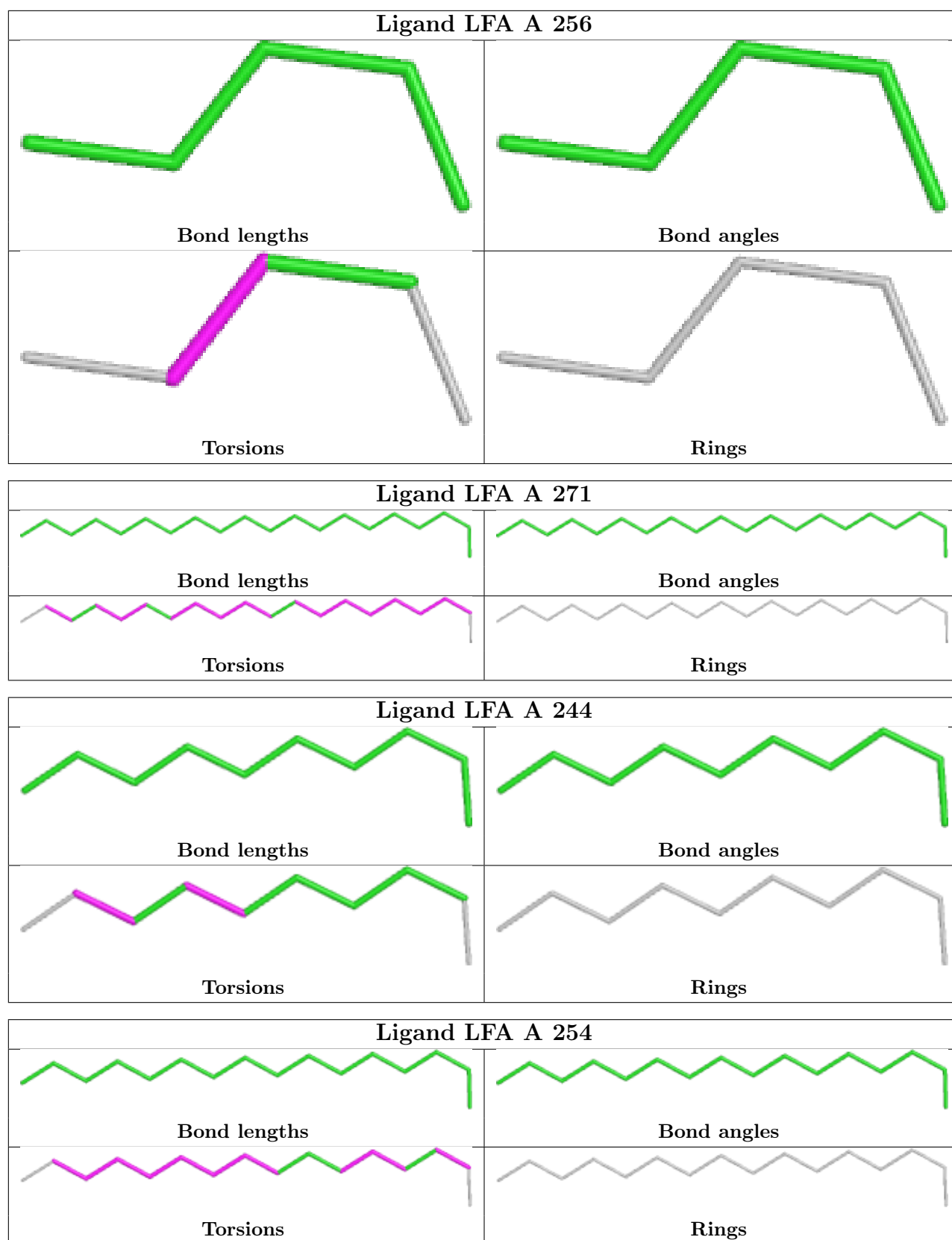




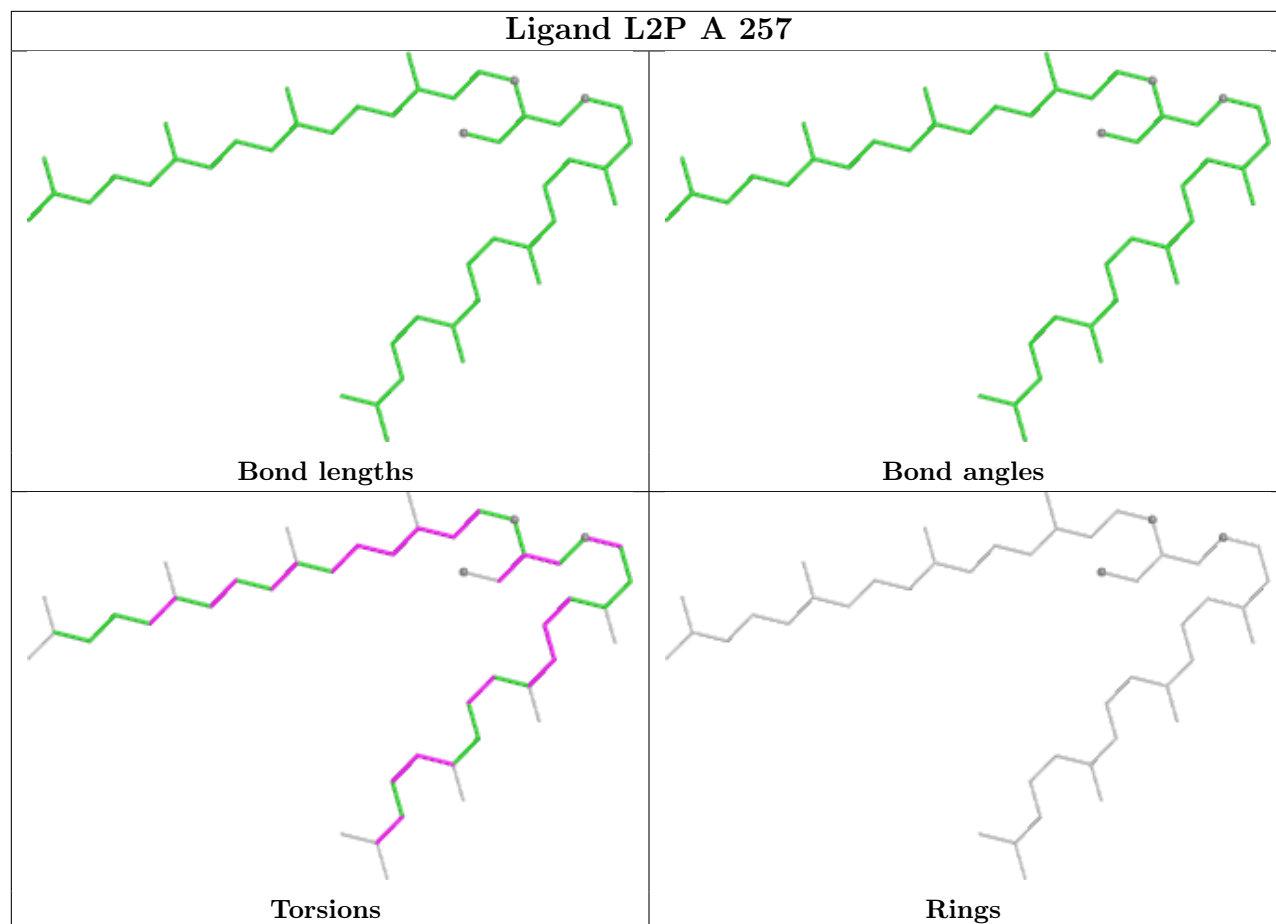




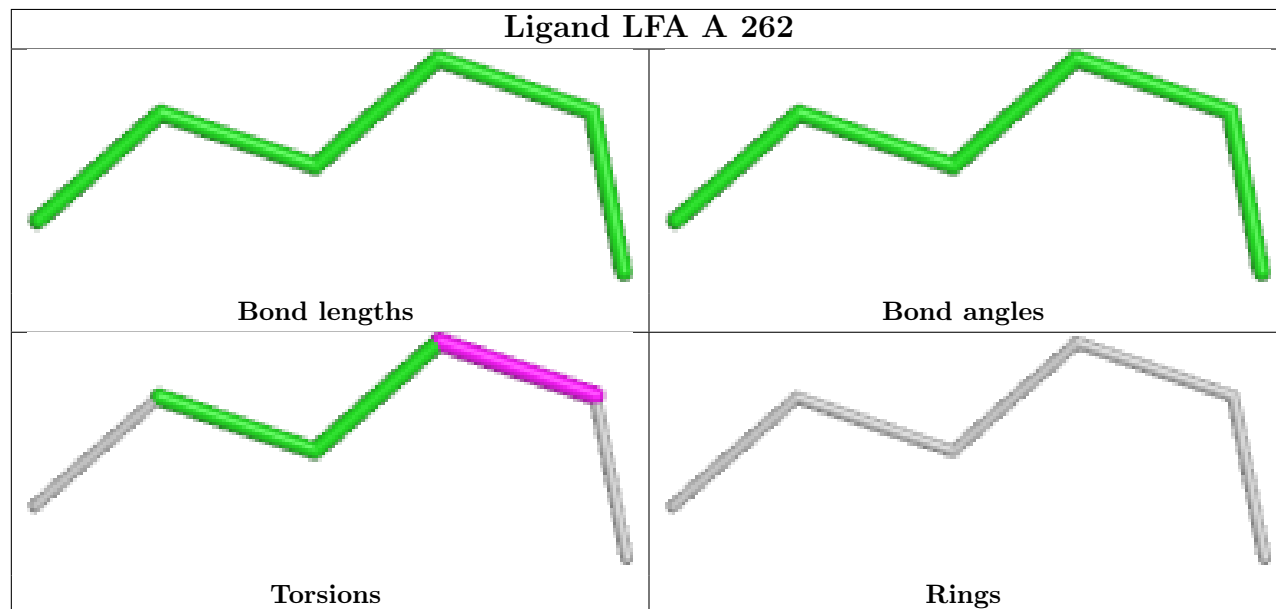


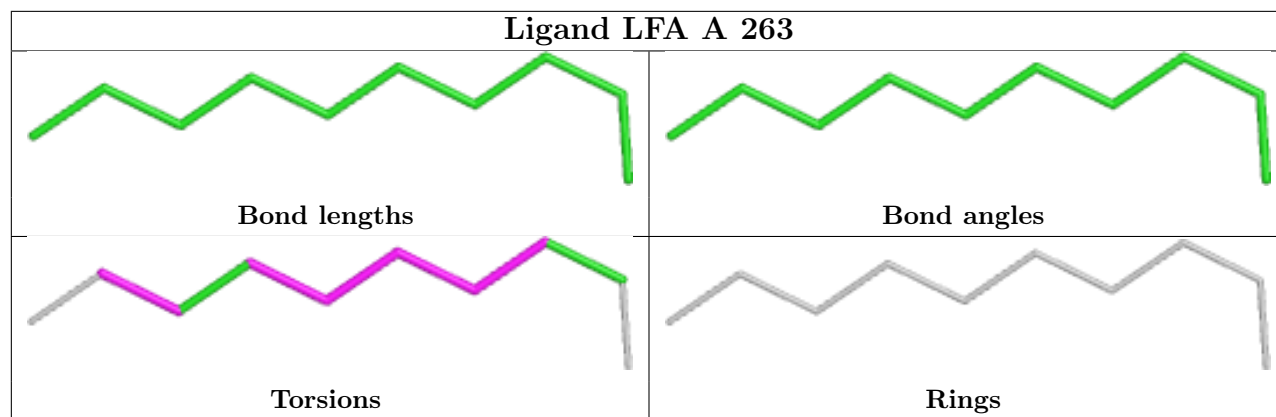


Ligand L2P A 257



Ligand LFA A 262





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/239 (91%)	-0.12	11 (5%) 34 36	9, 20, 40, 66	22 (10%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	ASP	3.7
1	A	29	ALA	3.6
1	A	1	MET	3.5
1	A	30	GLY	3.4
1	A	2	VAL	3.3
1	A	154	SER	3.3
1	A	28	ASP	3.2
1	A	32	GLY	3.1
1	A	31	SER	2.6
1	A	27	ARG	2.4
1	A	217	ALA	2.3

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,

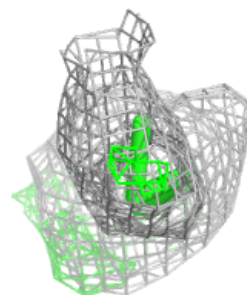
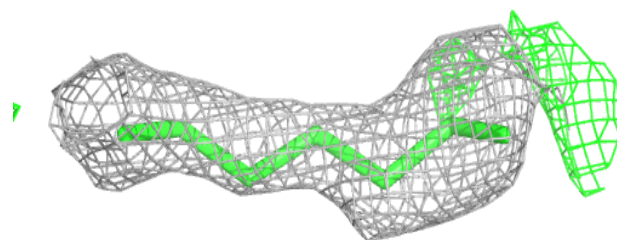
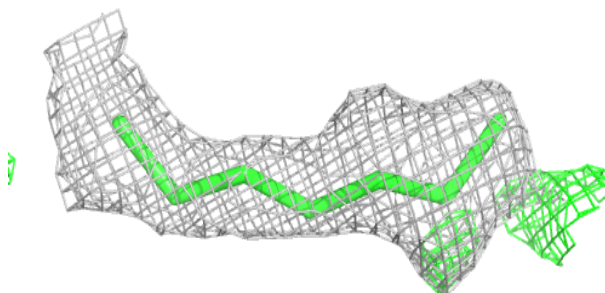
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LFA	A	268	7/20	0.66	0.19	56,57,57,57	0
4	LFA	A	269	4/20	0.67	0.20	68,68,69,69	0
4	LFA	A	272	12/20	0.70	0.23	77,78,79,79	0
4	LFA	A	253	6/20	0.71	0.19	67,68,68,68	0
4	LFA	A	262	6/20	0.72	0.14	69,69,70,70	0
4	LFA	A	259	4/20	0.72	0.22	64,64,65,65	0
4	LFA	A	265	8/20	0.73	0.14	60,62,63,63	0
4	LFA	A	255	14/20	0.74	0.18	43,46,50,50	0
4	LFA	A	245	6/20	0.75	0.12	57,57,58,58	0
4	LFA	A	261	14/20	0.76	0.17	58,59,65,66	0
4	LFA	A	264	9/20	0.76	0.15	69,69,71,71	0
4	LFA	A	263	10/20	0.77	0.17	50,56,58,59	0
4	LFA	A	251	16/20	0.77	0.14	55,57,58,58	0
4	LFA	A	270	4/20	0.77	0.17	59,60,60,60	0
4	LFA	A	244	10/20	0.77	0.16	54,55,56,56	0
5	L2P	A	260	20/46	0.77	0.16	59,64,70,70	0
4	LFA	A	256	5/20	0.78	0.19	63,63,63,63	0
4	LFA	A	252	12/20	0.79	0.14	78,79,79,79	0
4	LFA	A	242	10/20	0.79	0.14	46,50,55,55	0
5	L2P	A	257	46/46	0.79	0.14	59,69,80,81	0
3	BOG	A	241	20/20	0.79	0.14	37,60,64,65	0
4	LFA	A	271	20/20	0.80	0.15	66,71,75,75	0
4	LFA	A	266	10/20	0.82	0.11	56,61,61,61	0
4	LFA	A	250	9/20	0.83	0.14	59,59,60,60	0
4	LFA	A	243	6/20	0.83	0.09	50,52,52,52	0
4	LFA	A	254	16/20	0.84	0.14	45,50,59,60	0
4	LFA	A	258	6/20	0.84	0.13	70,70,71,71	0
4	LFA	A	246	8/20	0.86	0.10	47,49,50,51	0
4	LFA	A	267	20/20	0.86	0.13	47,51,57,57	0
4	LFA	A	248	7/20	0.86	0.10	46,46,47,48	0
4	LFA	A	249	5/20	0.87	0.12	34,35,37,40	0
4	LFA	A	247	5/20	0.91	0.09	46,46,46,46	0
2	RET	A	240	20/21	0.96	0.04	8,12,14,15	0

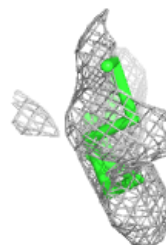
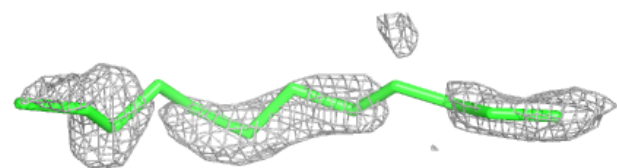
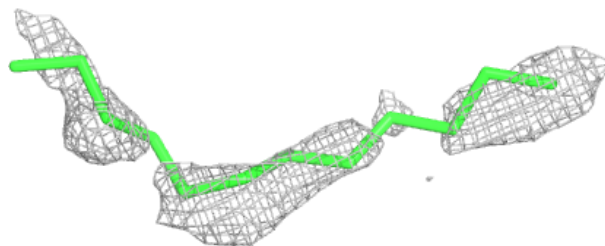
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA A 268:

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

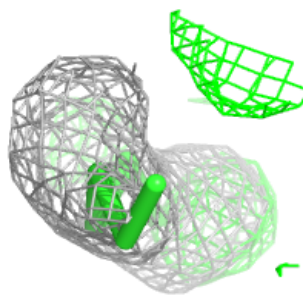
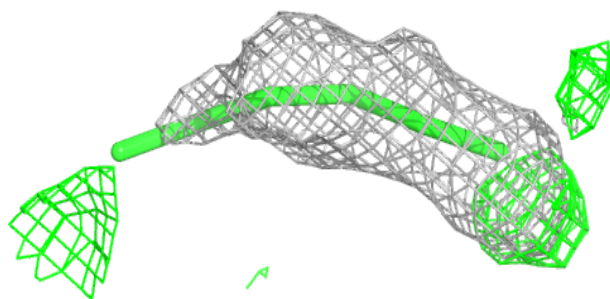
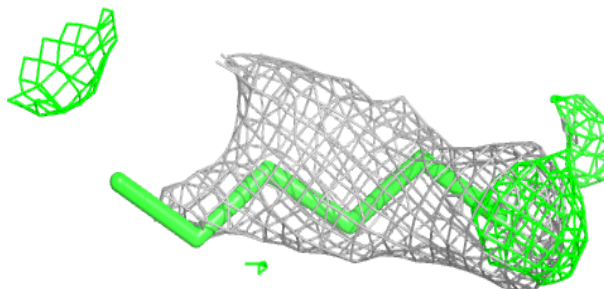
**Electron density around LFA A 272:**

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

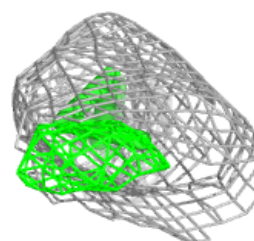
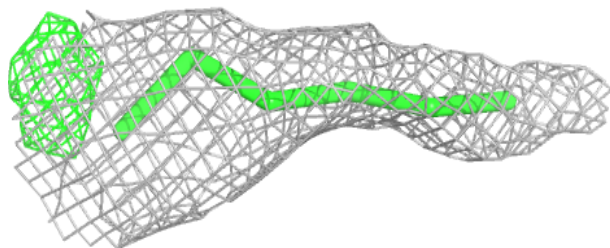
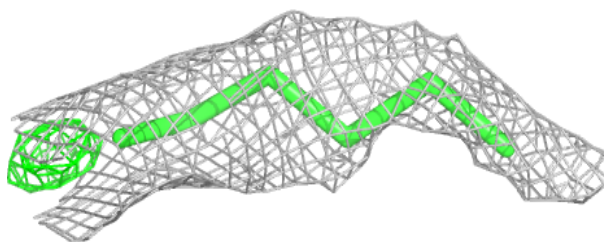


Electron density around LFA A 253:

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

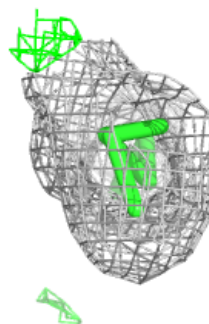
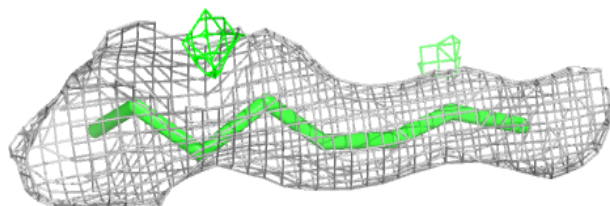
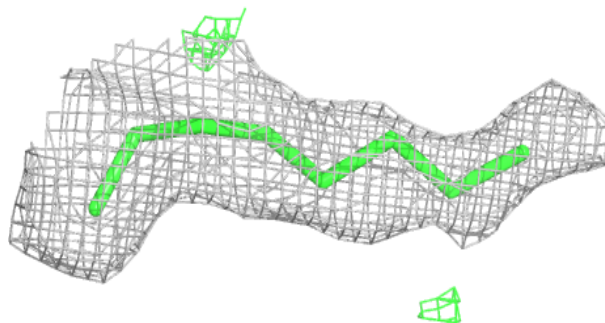
**Electron density around LFA A 262:**

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

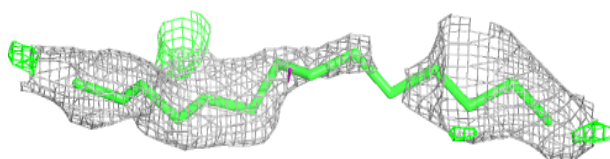
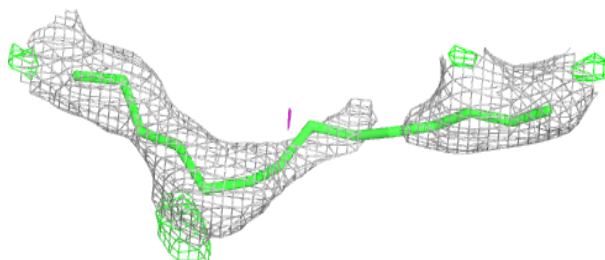


Electron density around LFA A 265:

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

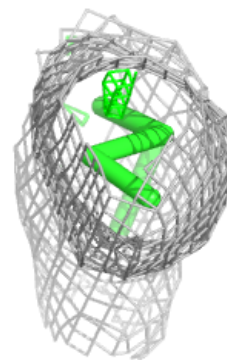
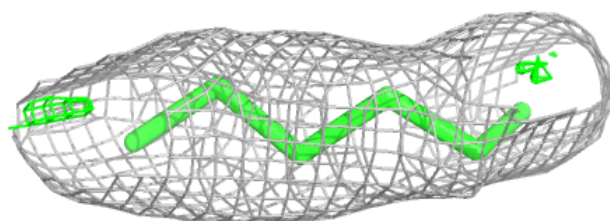
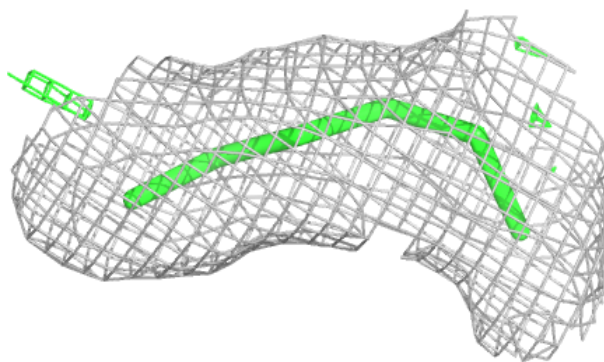
**Electron density around LFA A 255:**

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

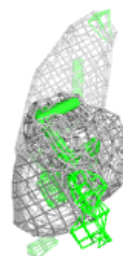
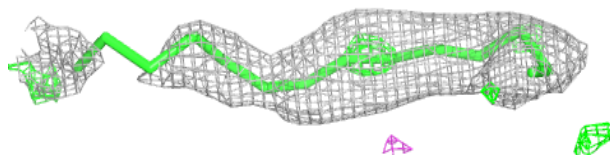
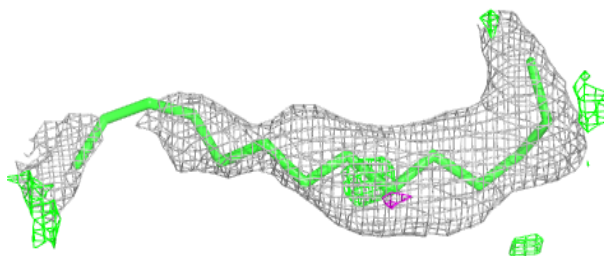


Electron density around LFA A 245:

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

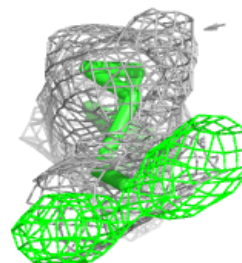
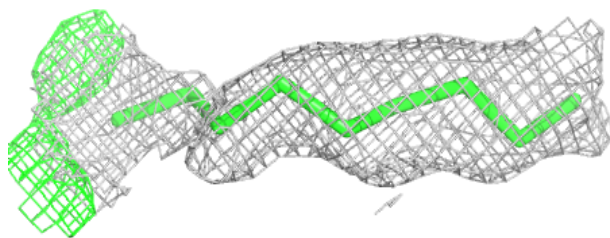
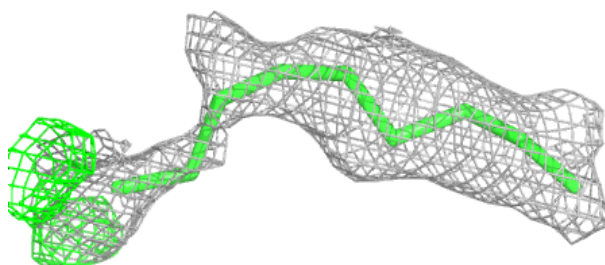
**Electron density around LFA A 261:**

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

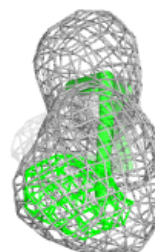
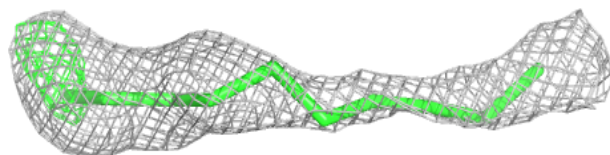
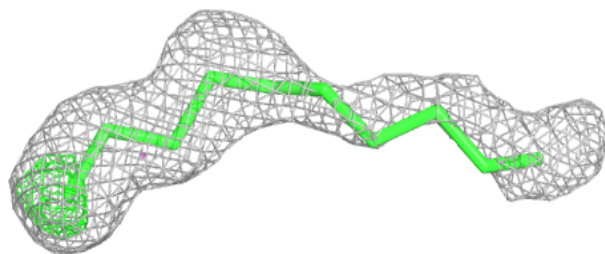


Electron density around LFA A 264:

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

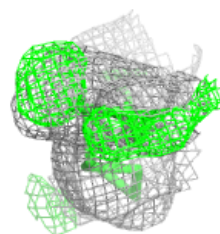
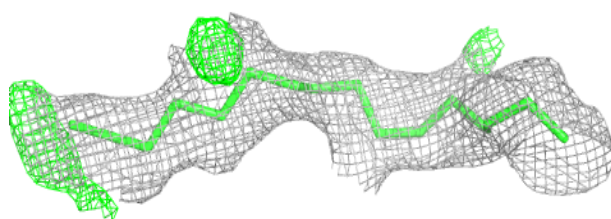
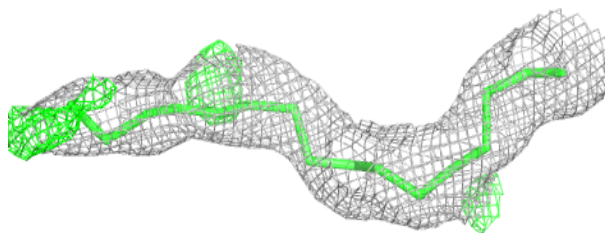
**Electron density around LFA A 263:**

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

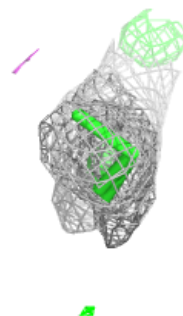
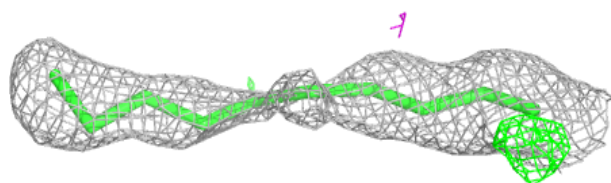
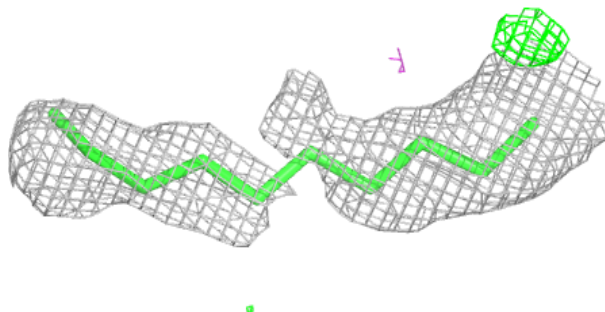


Electron density around LFA A 251:

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

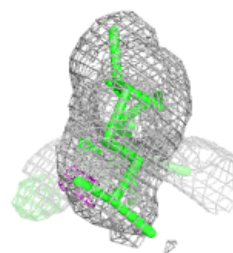
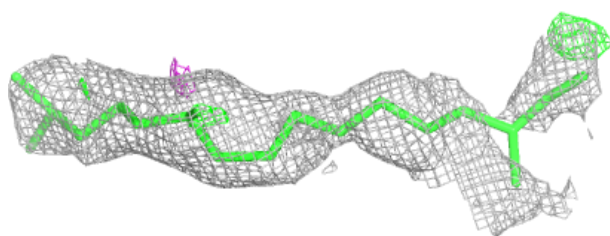
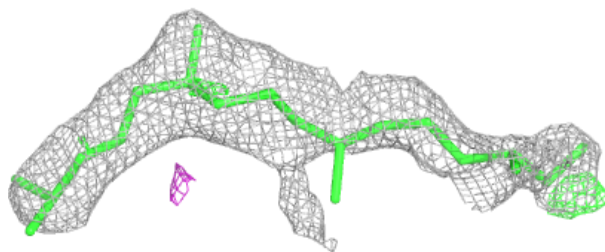
**Electron density around LFA A 244:**

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

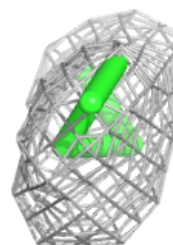
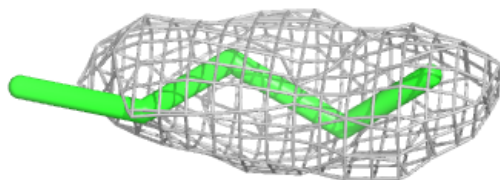
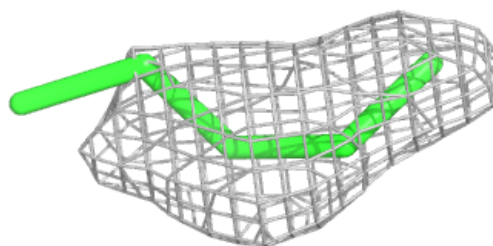


Electron density around L2P A 260:

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

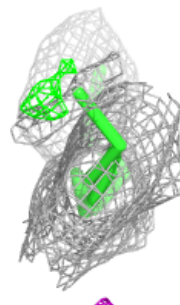
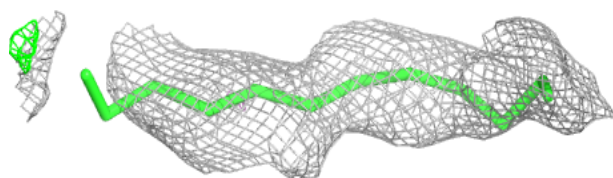
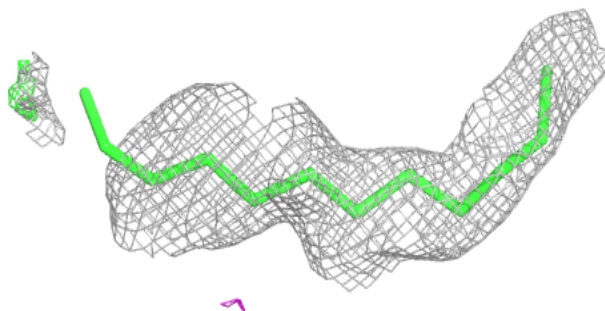
**Electron density around LFA A 256:**

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

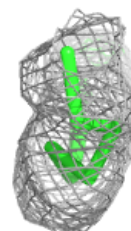
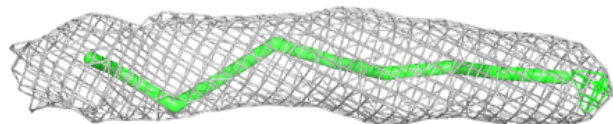
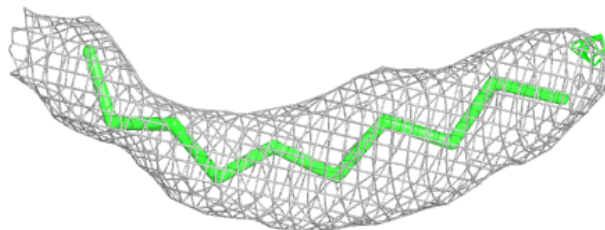


Electron density around LFA A 252:

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

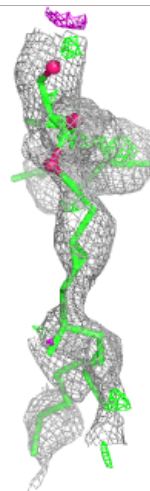
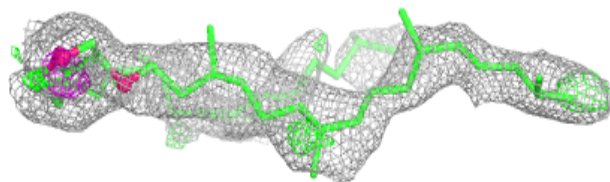
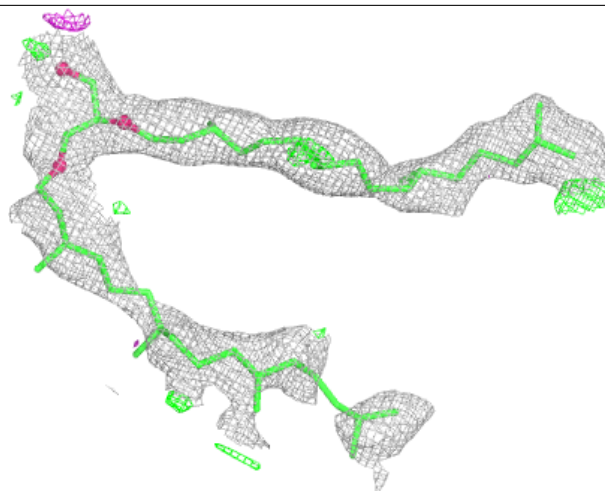
**Electron density around LFA A 242:**

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



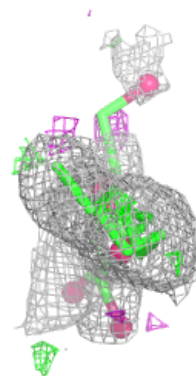
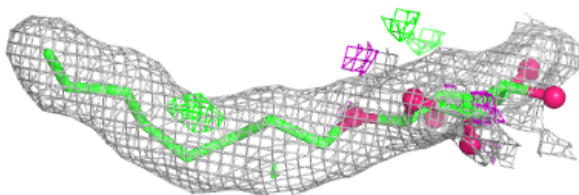
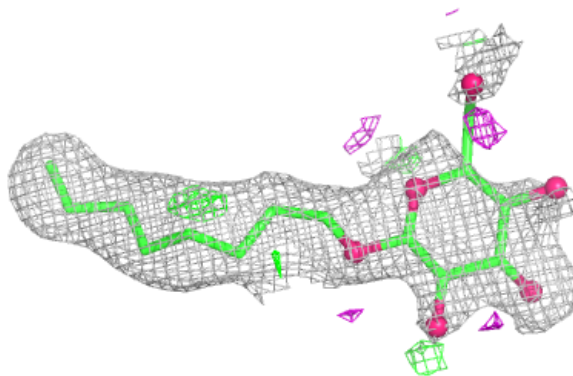
Electron density around L2P A 257:

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

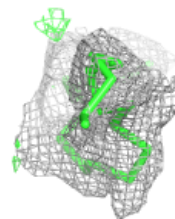
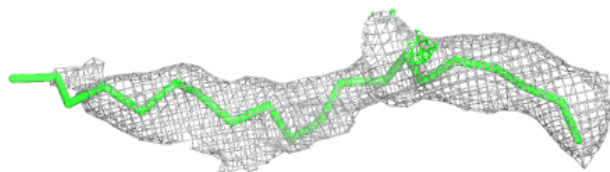
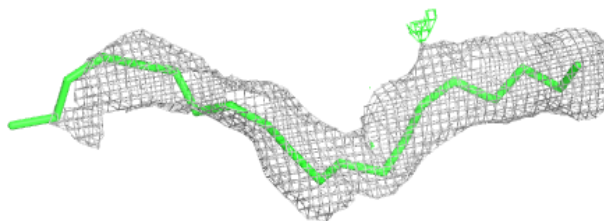


Electron density around BOG A 241:

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

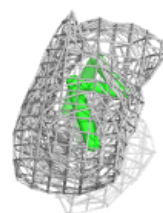
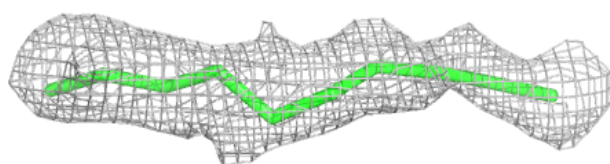
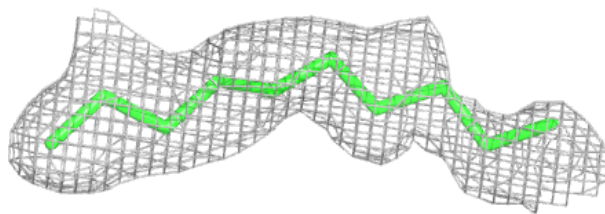
**Electron density around LFA A 271:**

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

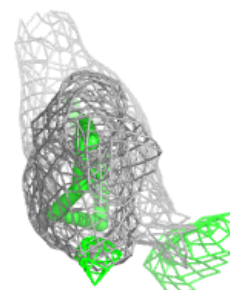
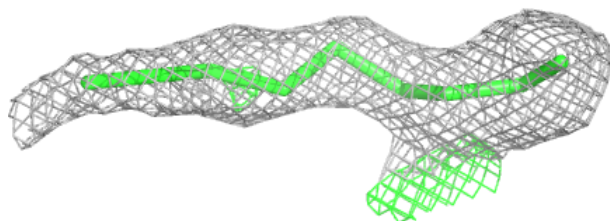
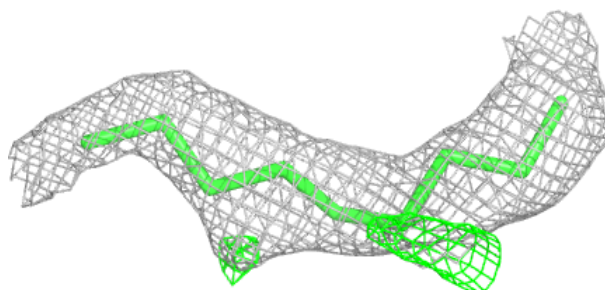


Electron density around LFA A 266:

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

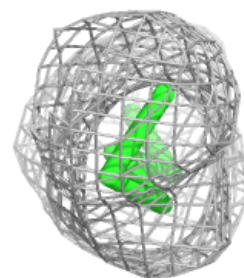
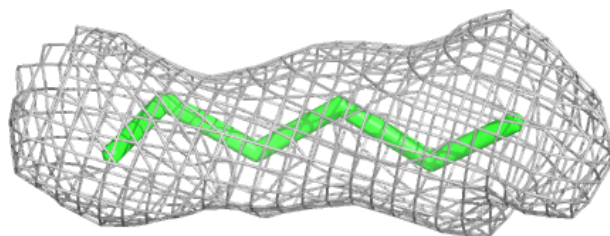
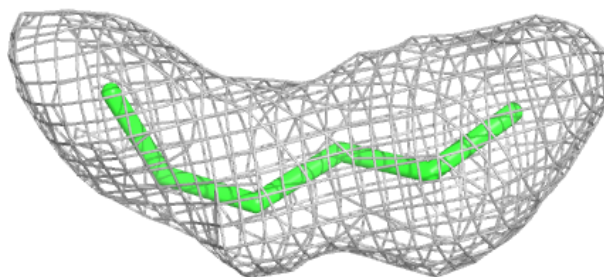
**Electron density around LFA A 250:**

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

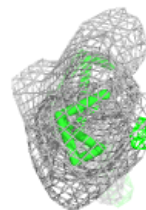
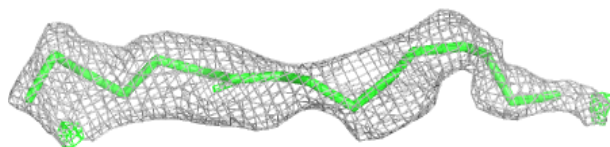
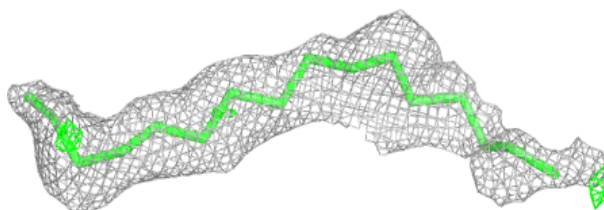


Electron density around LFA A 243:

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

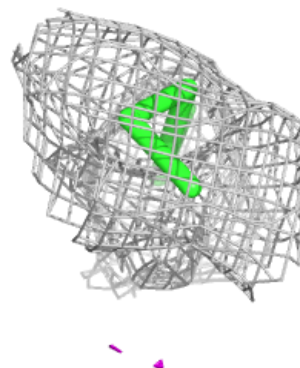
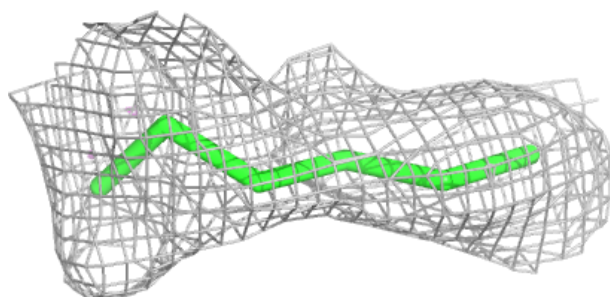
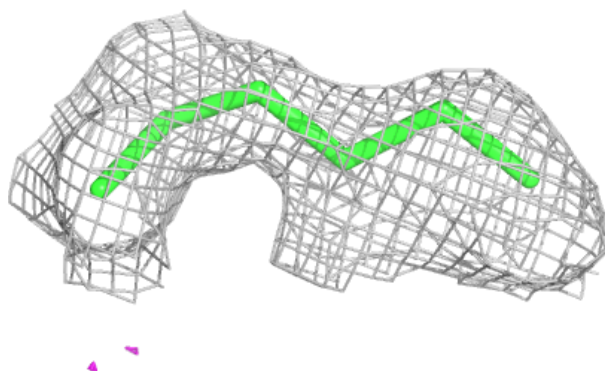
**Electron density around LFA A 254:**

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

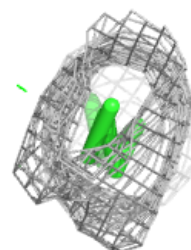
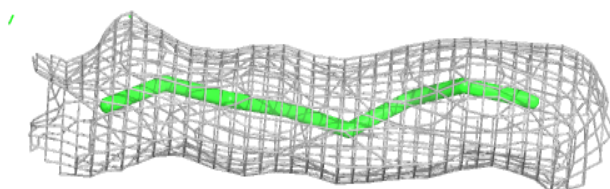
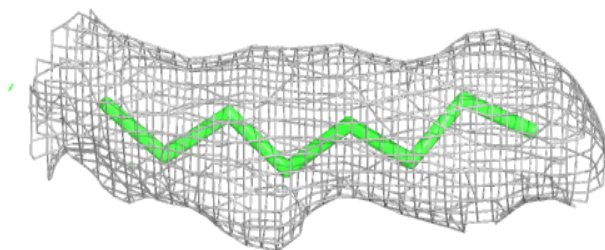


Electron density around LFA A 258:

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

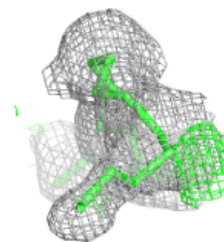
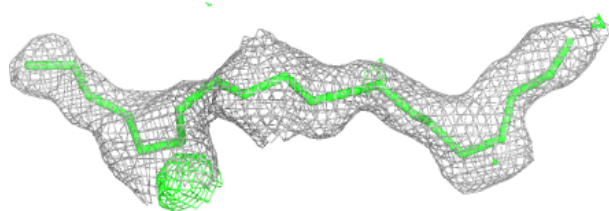
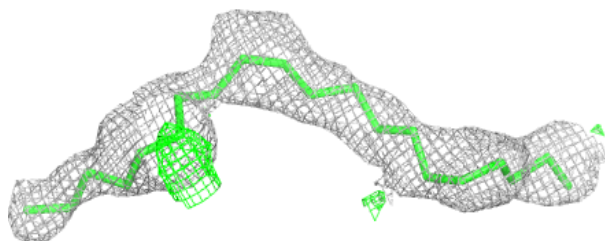
**Electron density around LFA A 246:**

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

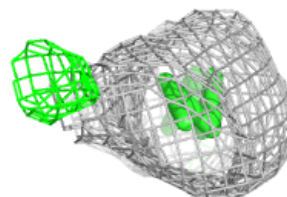
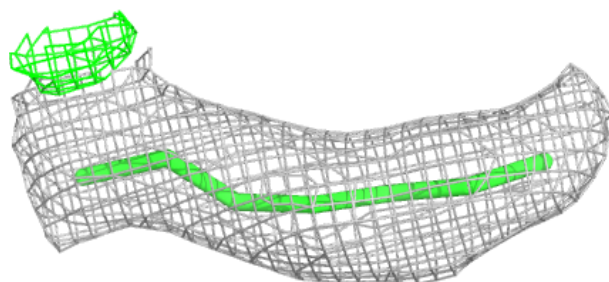
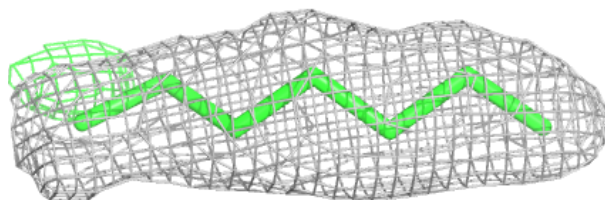


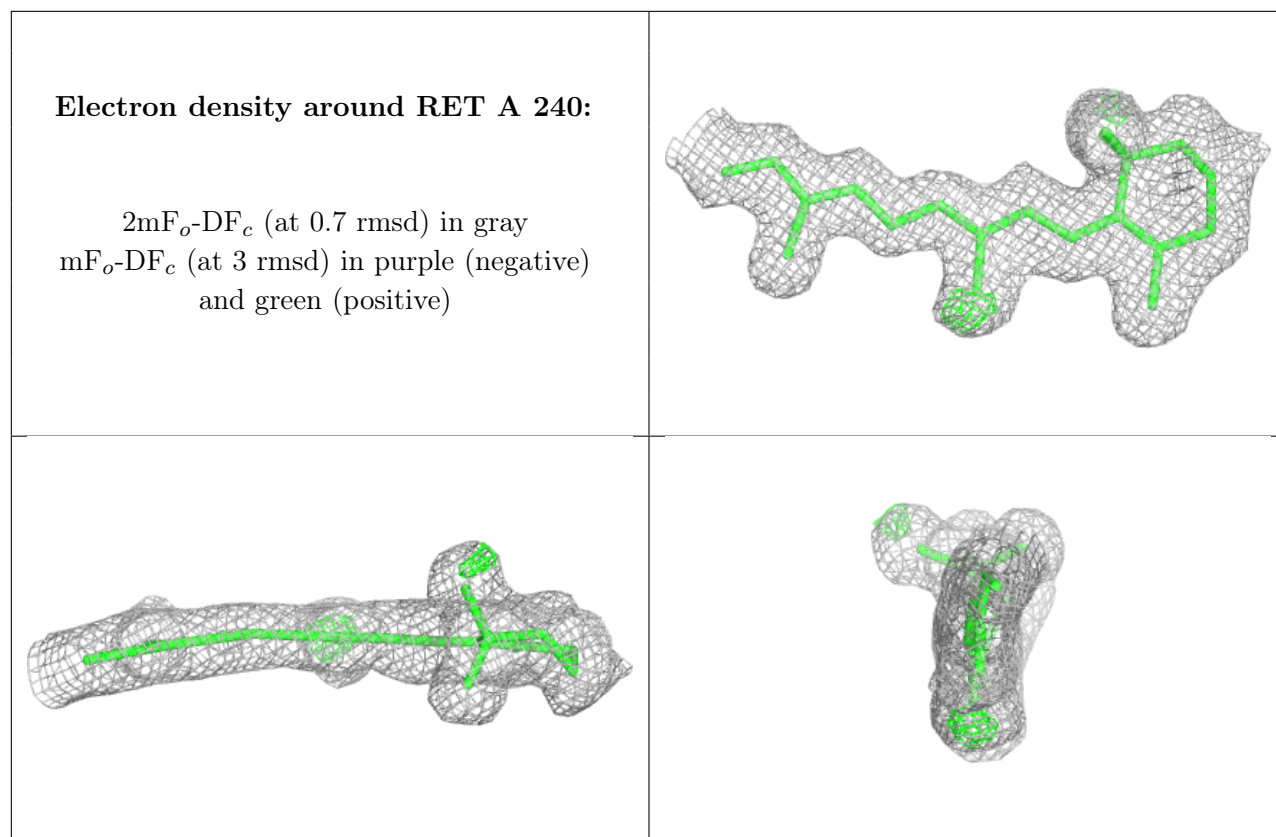
Electron density around LFA A 267:

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

**Electron density around LFA A 248:**

$2mF_o-DF_c$ (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.