



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:16 AM UTC

PDB ID : 7BMH / pdb_00007bmh
Title : Crystal structure of a light-driven proton pump LR (Mac) from *Leptosphaeria maculans*
Authors : Kovalev, K.; Zabelskii, D.; Dmitrieva, N.; Volkov, O.; Shevchenko, V.; Astashkin, R.; Zinovev, E.; Gordeliy, V.
Deposited on : 2021-01-20
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

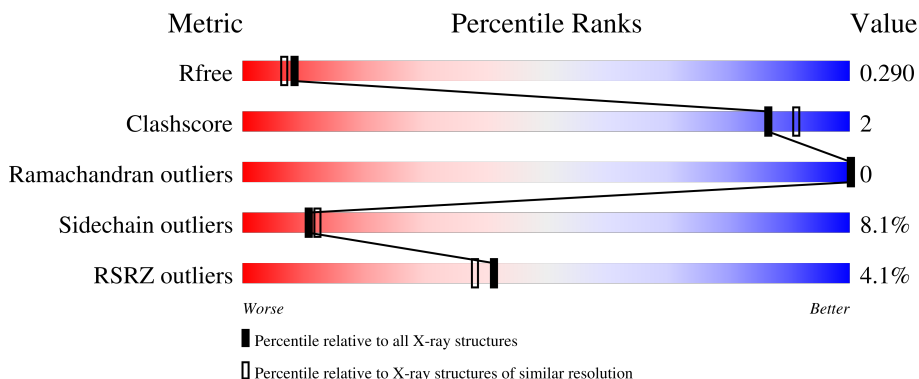
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	324	3% 69% 6% 24%
1	B	324	3% 67% 6% 26%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4213 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.

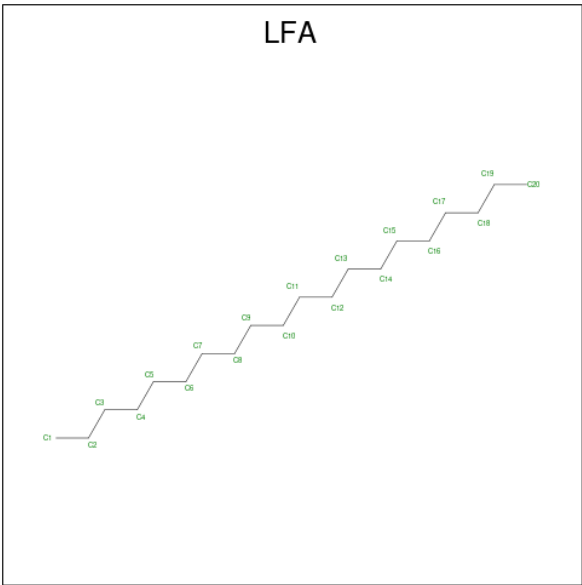
- Molecule 1 is a protein called Opsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1881	1266	294	315	6			
1	B	239	Total	C	N	O	S	0	0	0
			1809	1218	282	303	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	GLY	-	expression tag	UNP Q9HGT7
A	315	THR	-	expression tag	UNP Q9HGT7
A	316	HIS	-	expression tag	UNP Q9HGT7
A	317	HIS	-	expression tag	UNP Q9HGT7
A	318	HIS	-	expression tag	UNP Q9HGT7
A	319	HIS	-	expression tag	UNP Q9HGT7
A	320	HIS	-	expression tag	UNP Q9HGT7
A	321	HIS	-	expression tag	UNP Q9HGT7
A	322	HIS	-	expression tag	UNP Q9HGT7
A	323	HIS	-	expression tag	UNP Q9HGT7
A	324	HIS	-	expression tag	UNP Q9HGT7
B	314	GLY	-	expression tag	UNP Q9HGT7
B	315	THR	-	expression tag	UNP Q9HGT7
B	316	HIS	-	expression tag	UNP Q9HGT7
B	317	HIS	-	expression tag	UNP Q9HGT7
B	318	HIS	-	expression tag	UNP Q9HGT7
B	319	HIS	-	expression tag	UNP Q9HGT7
B	320	HIS	-	expression tag	UNP Q9HGT7
B	321	HIS	-	expression tag	UNP Q9HGT7
B	322	HIS	-	expression tag	UNP Q9HGT7
B	323	HIS	-	expression tag	UNP Q9HGT7
B	324	HIS	-	expression tag	UNP Q9HGT7

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 16 16	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 5 5	0	0

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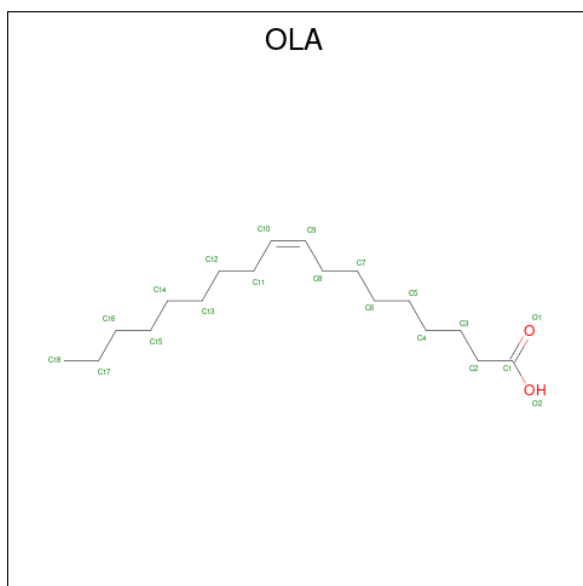
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 3 3	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 12 12	0	0
2	B	1	Total C 15 15	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 3 3	0	0
2	B	1	Total C 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 7 7	0	0
2	B	1	Total C 3 3	0	0
2	B	1	Total C 4 4	0	0
2	B	1	Total C 3 3	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 14 2	0	0
3	A	1	Total C O 14 12 2	0	0
3	A	1	Total C O 10 8 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			16	14	2		
3	B	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			16	14	2		

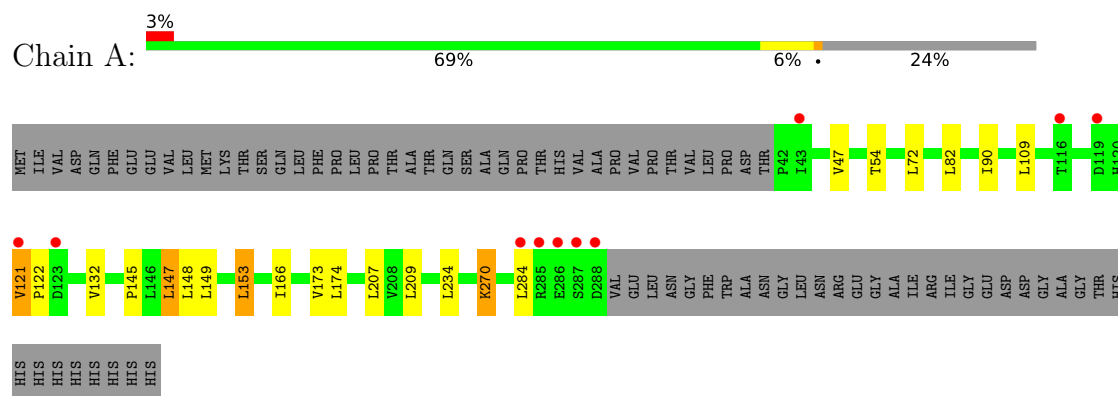
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	1
			51	51		
4	B	52	Total	O	0	1
			53	53		

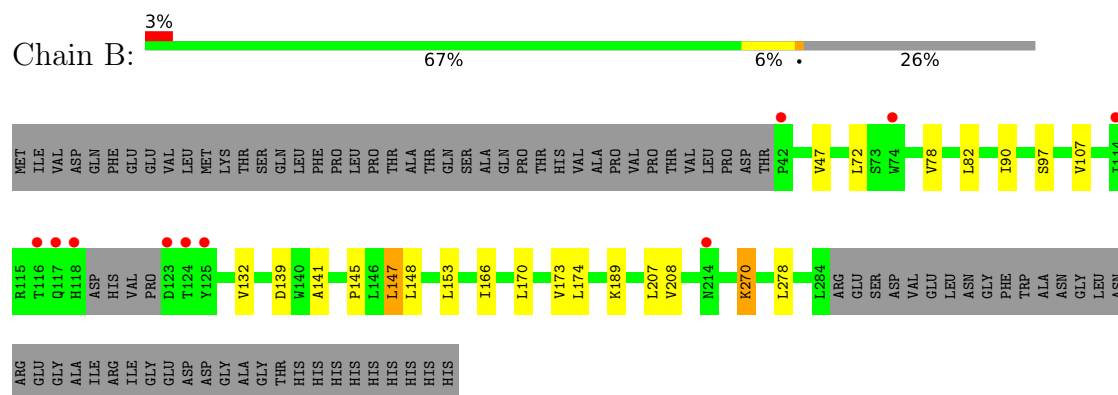
3 Residue-property plots [i](#)

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

• Molecule 1: Opsin



• Molecule 1: Opsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.54Å 70.78Å 148.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.20 19.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.92-2.20) 82.5 (19.92-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.236 , 0.285 0.241 , 0.290	Depositor DCC
R_{free} test set	1650 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4213	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9188e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/1904	0.54	0/2614
1	B	0.28	0/1827	0.46	0/2506
All	All	0.31	0/3731	0.50	0/5120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1881	0	1877	10	0
1	B	1809	0	1800	7	0
2	A	168	0	308	3	0
2	B	168	0	306	3	0
3	A	40	0	52	0	0
3	B	43	0	58	0	0
4	A	51	0	0	0	0
4	B	53	0	0	0	0
All	All	4213	0	4401	18	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 2.

The worst 5 of 18 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:90:ILE:HD13	1:A:147:LEU:HD13	1.69	0.74
1:B:270:LYR:H9	1:B:270:LYR:H183	1.69	0.74
1:B:90:ILE:HD13	1:B:147:LEU:HD13	1.70	0.72
1:B:72:LEU:HD21	2:B:410:LFA:H162	1.83	0.60
1:A:72:LEU:HD23	2:A:422:LFA:H41	1.85	0.58

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	244/324 (75%)	239 (98%)	5 (2%)	0	100	100
1	B	234/324 (72%)	232 (99%)	2 (1%)	0	100	100
All	All	478/648 (74%)	471 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/259 (68%)	164 (93%)	13 (7%)	13	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	167/259 (64%)	152 (91%)	15 (9%)	9	9
All	All	344/518 (66%)	316 (92%)	28 (8%)	11	12

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	78	VAL
1	B	278	LEU
1	B	107	VAL
1	B	174	LEU
1	B	97	SER

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

Mol	Chain	Res	Type
1	A	105	HIS
1	A	161	HIS
1	B	110	ASN
1	B	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	LYR	B	270	1	27,29,30	1.23	3 (11%)	30,37,39	1.31	4 (13%)
1	LYR	A	270	1	27,29,30	1.13	3 (11%)	30,37,39	1.27	3 (10%)

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
1	LYR	B	270	1	-	1/22/40/42	0/1/1/1
1	LYR	A	270	1	-	0/22/40/42	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	LYR	O-C	3.09	1.31	1.20
1	A	270	LYR	C9-C80	-2.66	1.40	1.46
1	A	270	LYR	C4-C3	-2.39	1.46	1.50
1	B	270	LYR	C4-C3	-2.29	1.46	1.50
1	B	270	LYR	C9-C80	-2.25	1.41	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	LYR	C8-C80-C7	-3.81	116.65	122.82
1	A	270	LYR	C8-C80-C7	-3.58	117.02	122.82
1	B	270	LYR	C1-NZ-CE	3.00	118.93	112.85
1	A	270	LYR	C6-C7-C80	2.14	130.28	127.28
1	A	270	LYR	C17-C11-C10	2.08	121.30	115.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	270	LYR	CD-CE-NZ-C1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	270	LYR	1	0
1	A	270	LYR	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

49 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	$\# Z > 2$
2	LFA	A	411	-	2,2,19	0.31	0	1,1,18	0.20	0
2	LFA	A	420	-	3,3,19	0.42	0	2,2,18	0.68	0
2	LFA	B	424	-	6,6,19	0.33	0	5,5,18	0.65	0
2	LFA	A	418	-	2,2,19	0.37	0	1,1,18	0.07	0
3	OLA	A	413	-	9,9,19	0.72	0	9,9,19	0.78	0
2	LFA	A	401	-	15,15,19	0.37	0	14,14,18	0.85	0
2	LFA	A	406	-	13,13,19	0.32	0	12,12,18	0.88	0
2	LFA	B	411	-	9,9,19	0.30	0	8,8,18	0.80	0
2	LFA	B	407	-	9,9,19	0.31	0	8,8,18	0.97	0
2	LFA	A	422	-	5,5,19	0.37	0	4,4,18	0.57	0
2	LFA	A	416	-	3,3,19	0.38	0	2,2,18	0.79	0
2	LFA	A	425	-	11,11,19	0.40	0	10,10,18	0.69	0
2	LFA	B	408	-	6,6,19	0.36	0	5,5,18	0.70	0
2	LFA	B	415	-	2,2,19	0.28	0	1,1,18	0.03	0
2	LFA	B	403	-	15,15,19	0.33	0	14,14,18	0.94	0
2	LFA	B	420	-	2,2,19	0.38	0	1,1,18	0.03	0
2	LFA	A	415	-	5,5,19	0.36	0	4,4,18	0.47	0
2	LFA	A	423	-	6,6,19	0.36	0	5,5,18	0.61	0
2	LFA	B	418	-	2,2,19	0.31	0	1,1,18	0.18	0
2	LFA	A	405	-	9,9,19	0.32	0	8,8,18	0.87	0
2	LFA	A	424	-	4,4,19	0.41	0	3,3,18	0.50	0
2	LFA	B	404	-	9,9,19	0.34	0	8,8,18	0.70	0
3	OLA	B	401	-	15,15,19	0.59	0	15,15,19	0.57	0
2	LFA	A	404	-	13,13,19	0.33	0	12,12,18	0.91	0
2	LFA	B	409	-	10,10,19	0.35	0	9,9,18	0.88	0
2	LFA	B	422	-	6,6,19	0.37	0	5,5,18	0.58	0
2	LFA	A	417	-	4,4,19	0.31	0	3,3,18	0.65	0
3	OLA	A	412	-	13,13,19	0.64	0	13,13,19	0.55	0
2	LFA	A	403	-	7,7,19	0.37	0	6,6,18	0.84	0
2	LFA	A	408	-	11,11,19	0.35	0	10,10,18	0.74	0
2	LFA	B	419	-	3,3,19	0.42	0	2,2,18	0.69	0
2	LFA	B	406	-	7,7,19	0.35	0	6,6,18	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	B	421	-	6,6,19	0.33	0	5,5,18	0.67	0
2	LFA	A	407	-	6,6,19	0.34	0	5,5,18	0.57	0
2	LFA	B	412	-	5,5,19	0.36	0	4,4,18	0.59	0
3	OLA	B	413	-	10,10,19	0.70	0	10,10,19	0.61	0
2	LFA	B	402	-	14,14,19	0.28	0	13,13,18	0.94	0
3	OLA	B	414	-	15,15,19	0.61	0	15,15,19	0.54	0
2	LFA	B	417	-	6,6,19	0.34	0	5,5,18	0.67	0
2	LFA	A	409	-	9,9,19	0.33	0	8,8,18	0.79	0
2	LFA	A	414	-	2,2,19	0.27	0	1,1,18	0.07	0
2	LFA	B	423	-	8,8,19	0.40	0	7,7,18	0.69	0
2	LFA	B	405	-	7,7,19	0.30	0	6,6,18	0.83	0
3	OLA	A	402	-	15,15,19	0.61	0	15,15,19	0.62	0
2	LFA	A	419	-	2,2,19	0.26	0	1,1,18	0.12	0
2	LFA	B	410	-	7,7,19	0.36	0	6,6,18	0.63	0
2	LFA	A	410	-	11,11,19	0.38	0	10,10,18	0.68	0
2	LFA	A	421	-	3,3,19	0.43	0	2,2,18	0.74	0
2	LFA	B	416	-	8,8,19	0.32	0	7,7,18	0.76	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
2	LFA	A	420	-	-	1/1/1/17	-
2	LFA	B	424	-	-	1/4/4/17	-
3	OLA	A	413	-	-	2/7/7/17	-
2	LFA	A	401	-	-	6/13/13/17	-
2	LFA	A	406	-	-	6/11/11/17	-
2	LFA	B	411	-	-	5/7/7/17	-
2	LFA	B	407	-	-	2/7/7/17	-
2	LFA	A	422	-	-	1/3/3/17	-
2	LFA	A	416	-	-	0/1/1/17	-
2	LFA	A	425	-	-	3/9/9/17	-
2	LFA	B	408	-	-	3/4/4/17	-
2	LFA	B	403	-	-	6/13/13/17	-
2	LFA	A	415	-	-	1/3/3/17	-
2	LFA	A	423	-	-	1/4/4/17	-
2	LFA	A	405	-	-	3/7/7/17	-
2	LFA	A	424	-	-	0/2/2/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	B	404	-	-	3/7/7/17	-
3	OLA	B	401	-	-	0/13/13/17	-
2	LFA	A	404	-	-	5/11/11/17	-
2	LFA	B	409	-	-	4/8/8/17	-
2	LFA	B	422	-	-	1/4/4/17	-
2	LFA	A	417	-	-	0/2/2/17	-
3	OLA	A	412	-	-	5/11/11/17	-
2	LFA	A	403	-	-	1/5/5/17	-
2	LFA	A	408	-	-	3/9/9/17	-
2	LFA	B	419	-	-	1/1/1/17	-
2	LFA	B	406	-	-	0/5/5/17	-
2	LFA	B	421	-	-	1/4/4/17	-
2	LFA	A	407	-	-	2/4/4/17	-
2	LFA	B	412	-	-	1/3/3/17	-
3	OLA	B	413	-	-	4/8/8/17	-
2	LFA	B	402	-	-	9/12/12/17	-
3	OLA	B	414	-	-	3/13/13/17	-
2	LFA	B	417	-	-	2/4/4/17	-
2	LFA	A	409	-	-	3/7/7/17	-
2	LFA	B	423	-	-	0/6/6/17	-
2	LFA	B	405	-	-	3/5/5/17	-
3	OLA	A	402	-	-	3/13/13/17	-
2	LFA	B	410	-	-	4/5/5/17	-
2	LFA	A	410	-	-	5/9/9/17	-
2	LFA	A	421	-	-	1/1/1/17	-
2	LFA	B	416	-	-	2/6/6/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 107 torsion outliers are listed below:

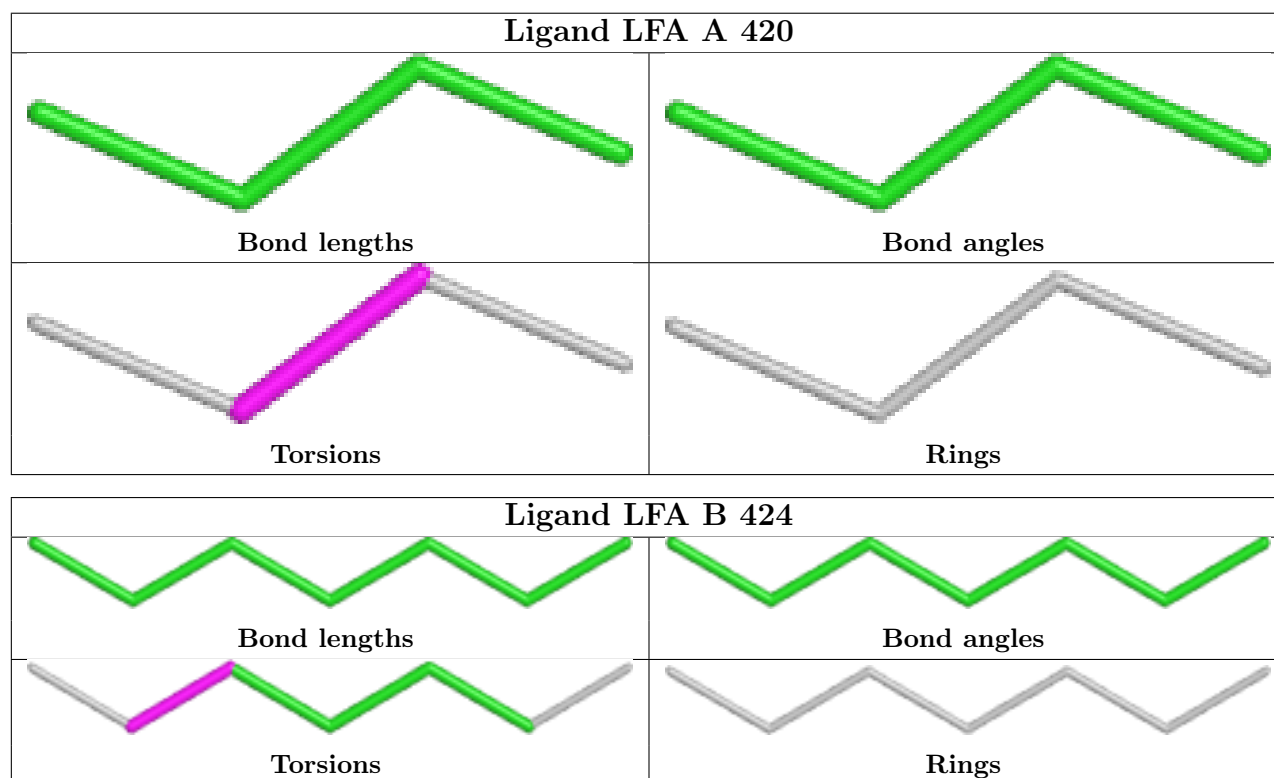
Mol	Chain	Res	Type	Atoms
2	B	402	LFA	C7-C8-C9-C10
2	B	409	LFA	C7-C8-C9-C10
2	B	404	LFA	C6-C7-C8-C9
2	B	409	LFA	C5-C6-C7-C8
2	B	411	LFA	C2-C3-C4-C5

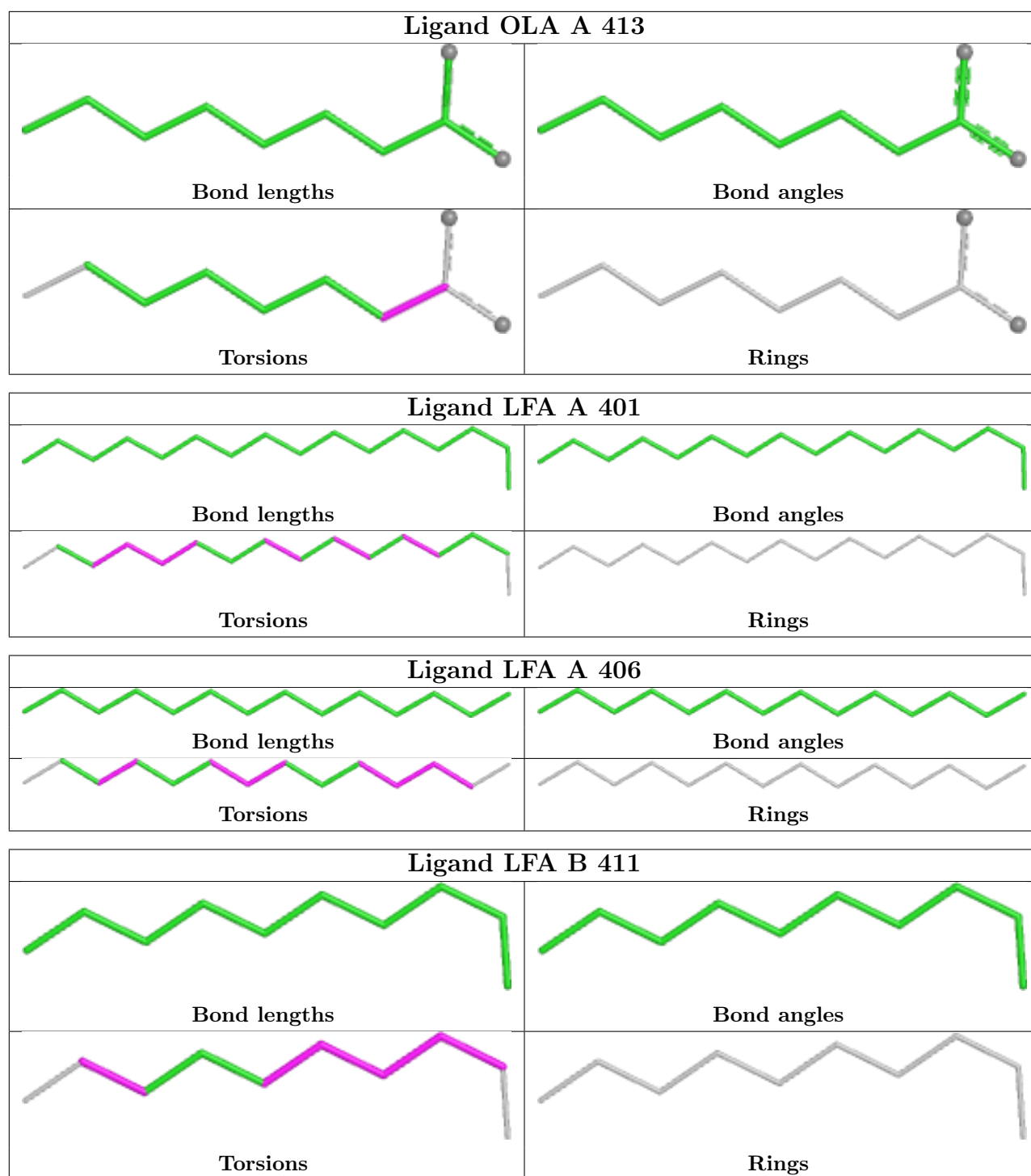
There are no ring outliers.

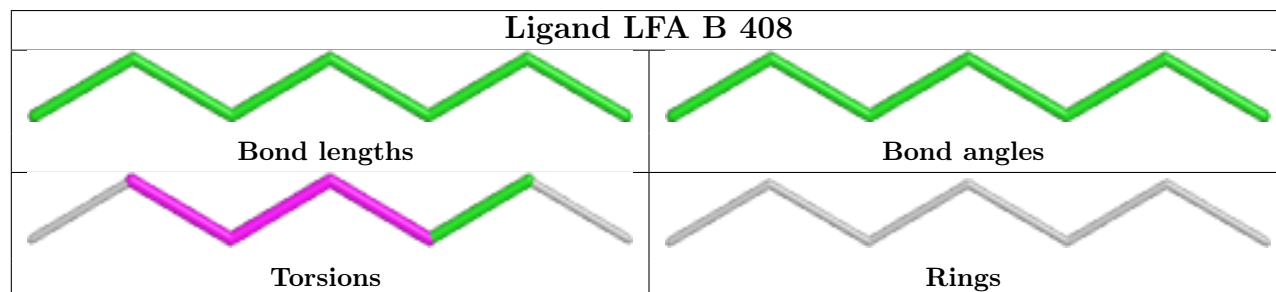
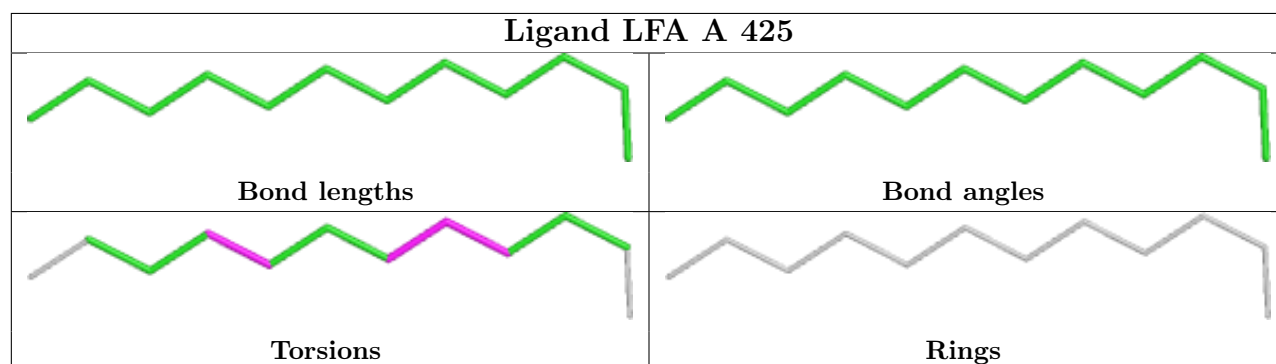
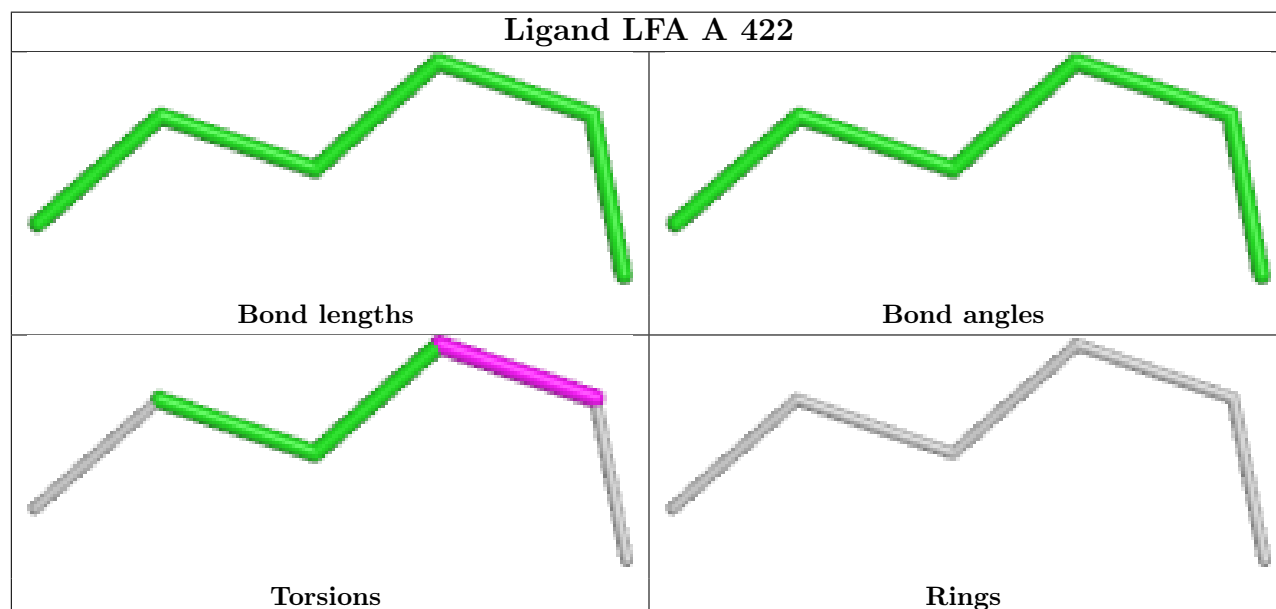
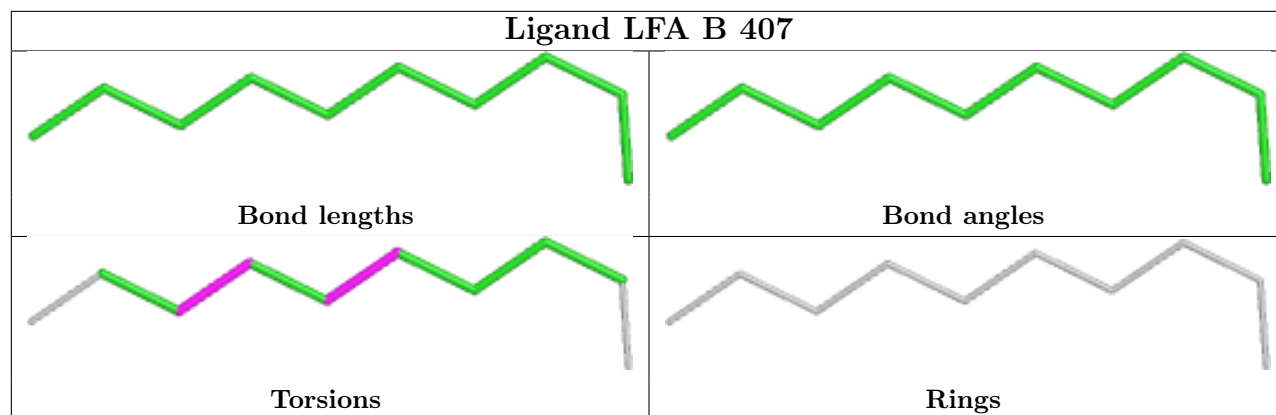
7 monomers are involved in 6 short contacts:

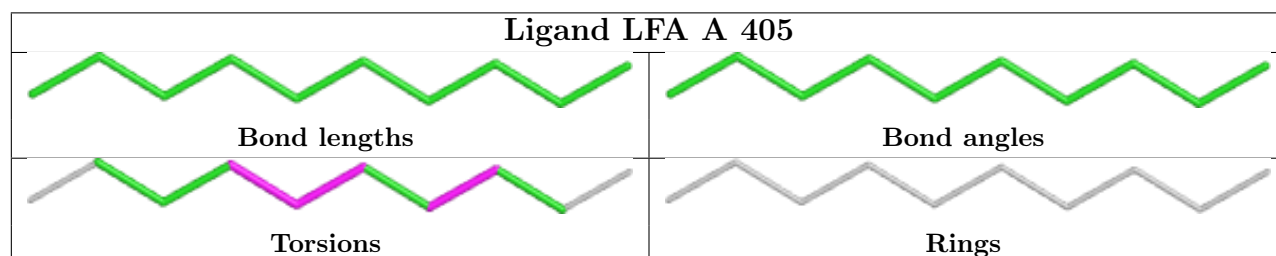
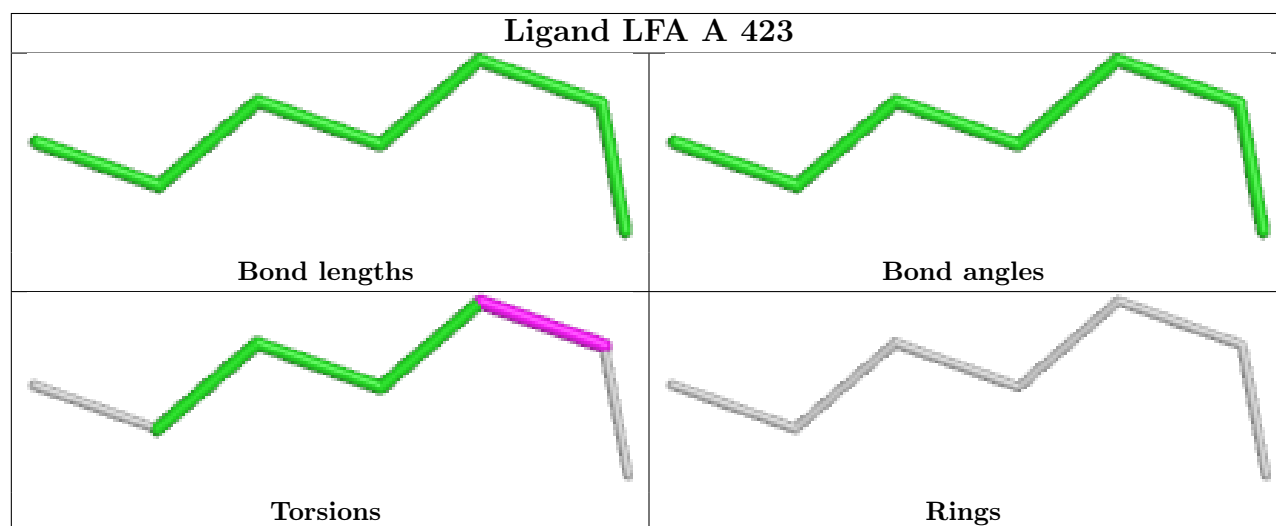
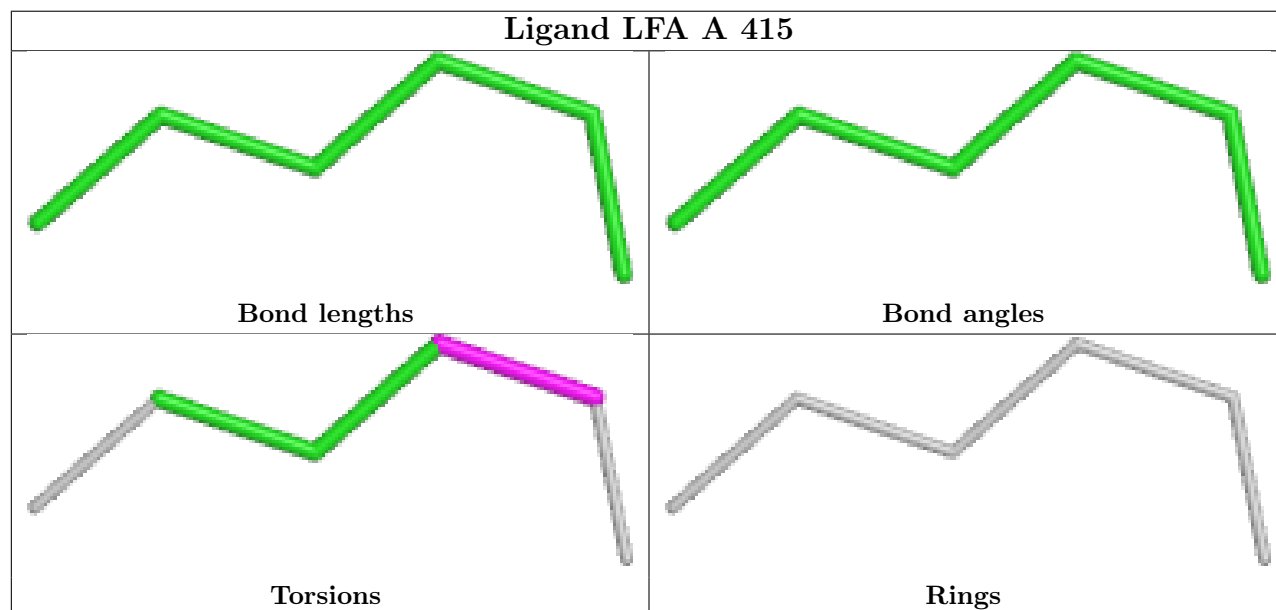
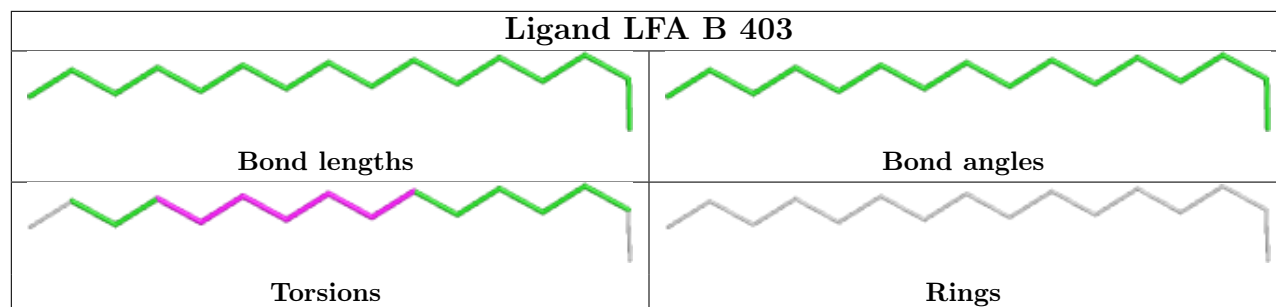
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	424	LFA	1	0
2	A	406	LFA	1	0
2	A	422	LFA	1	0
2	A	416	LFA	1	0
2	A	417	LFA	1	0
2	B	412	LFA	1	0
2	B	410	LFA	1	0

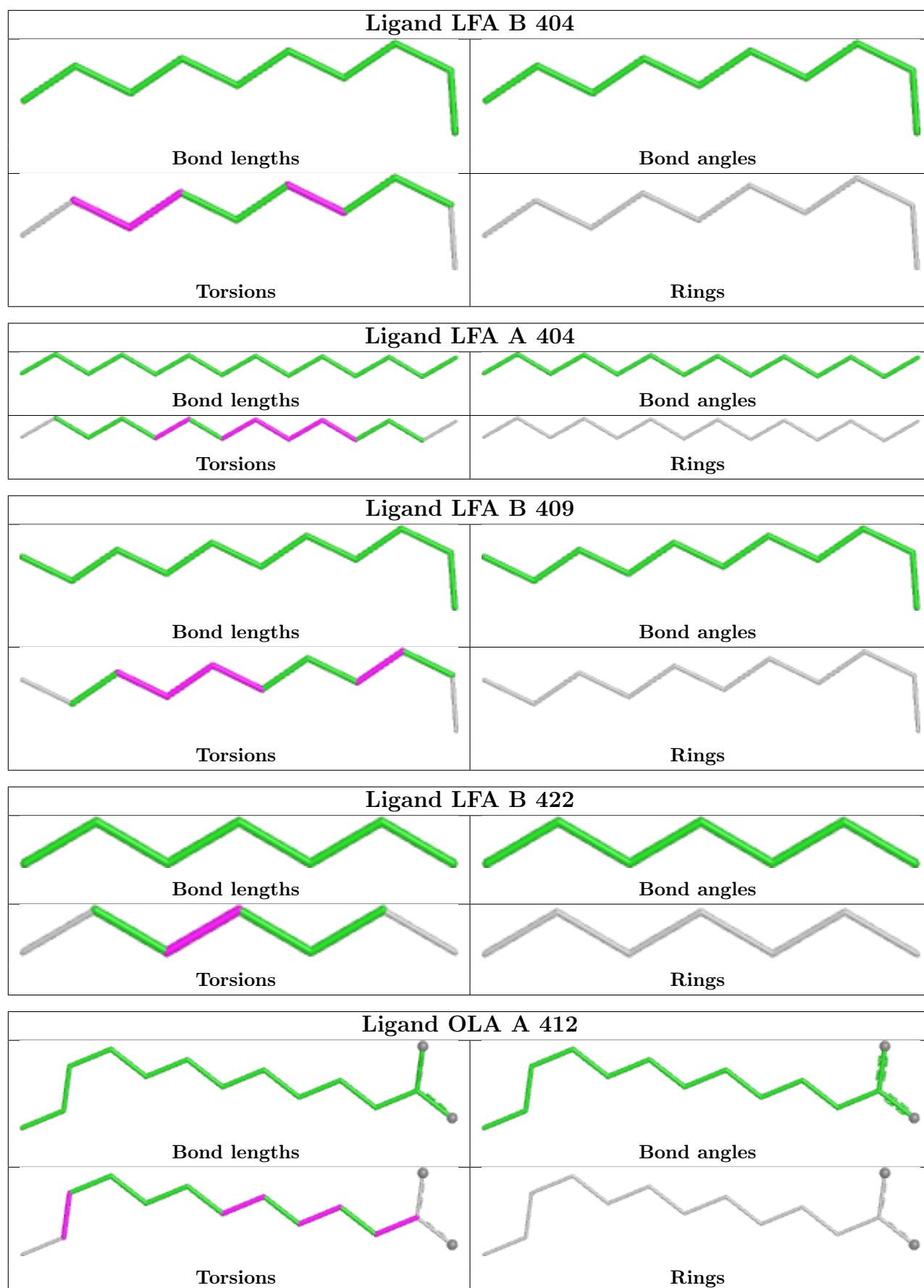
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

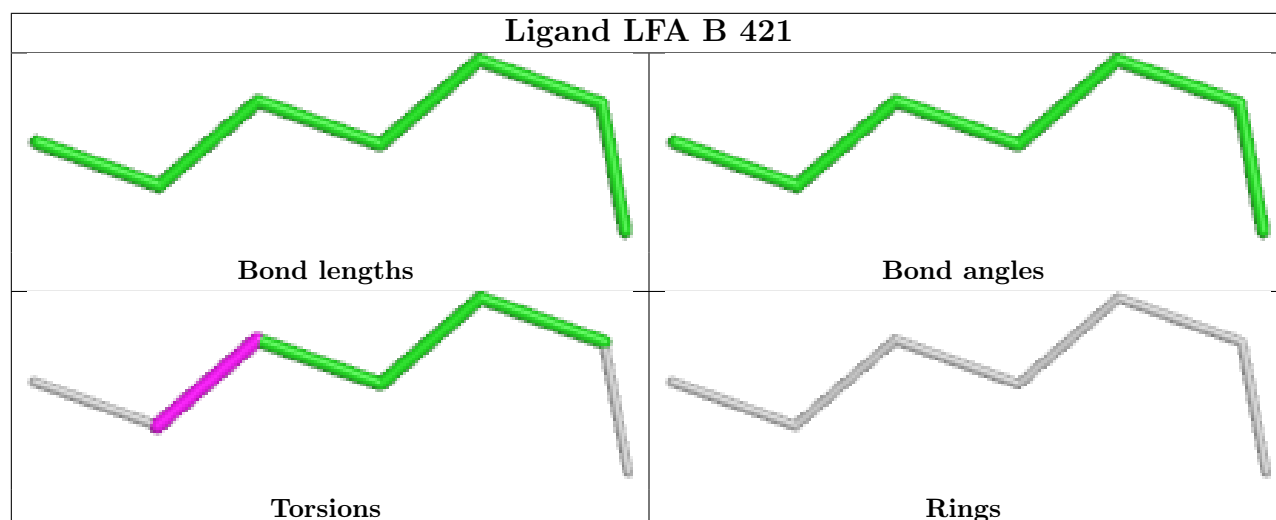
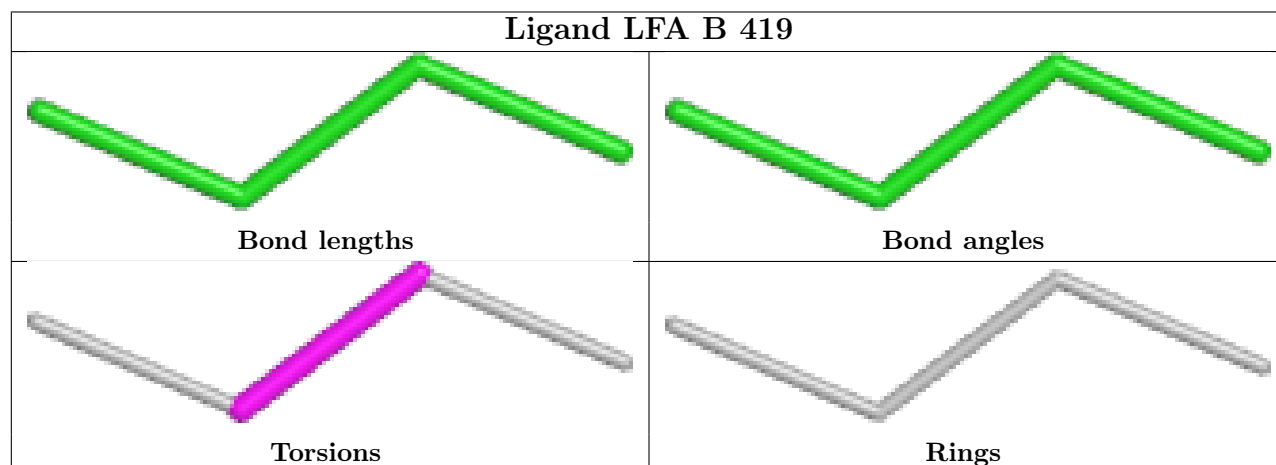
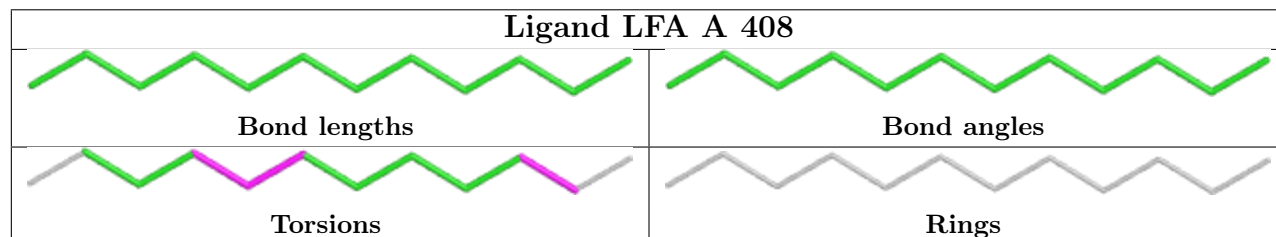
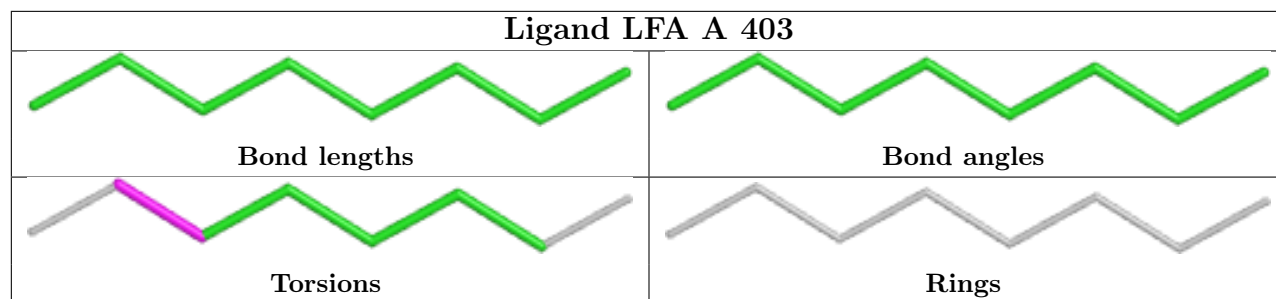


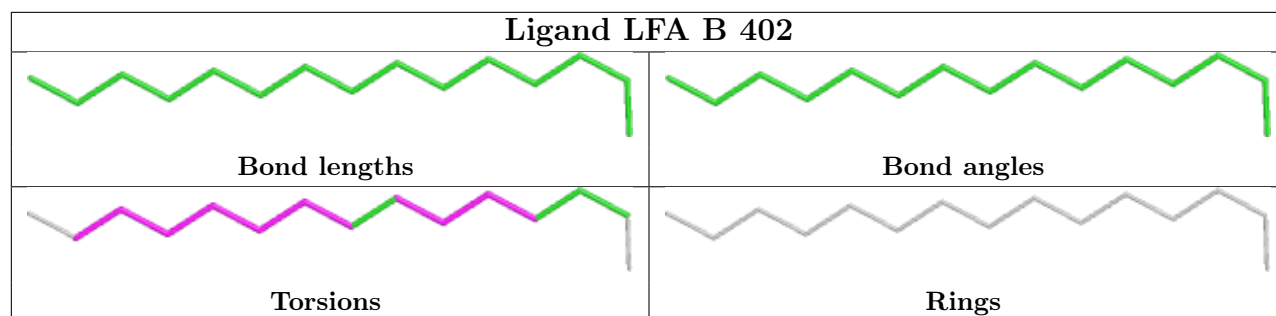
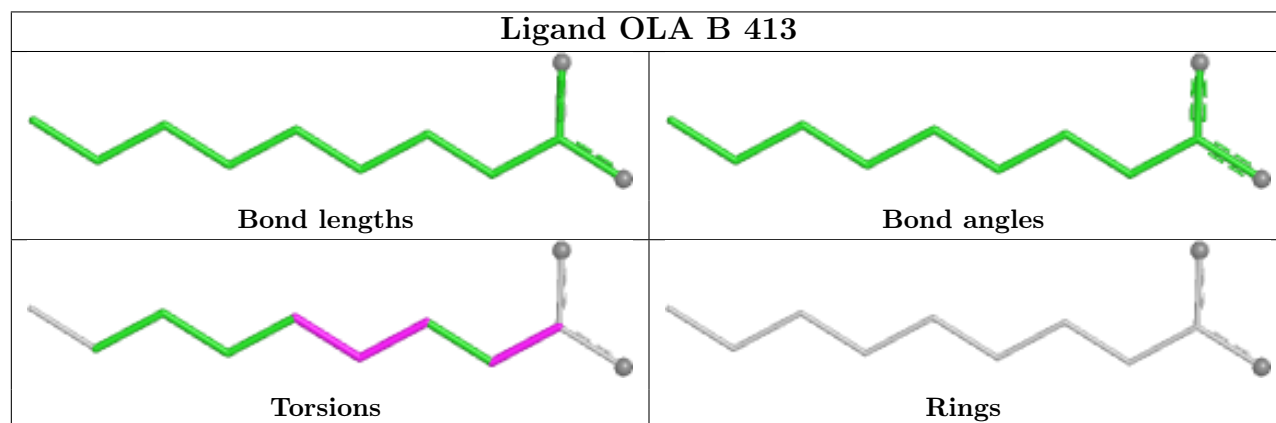
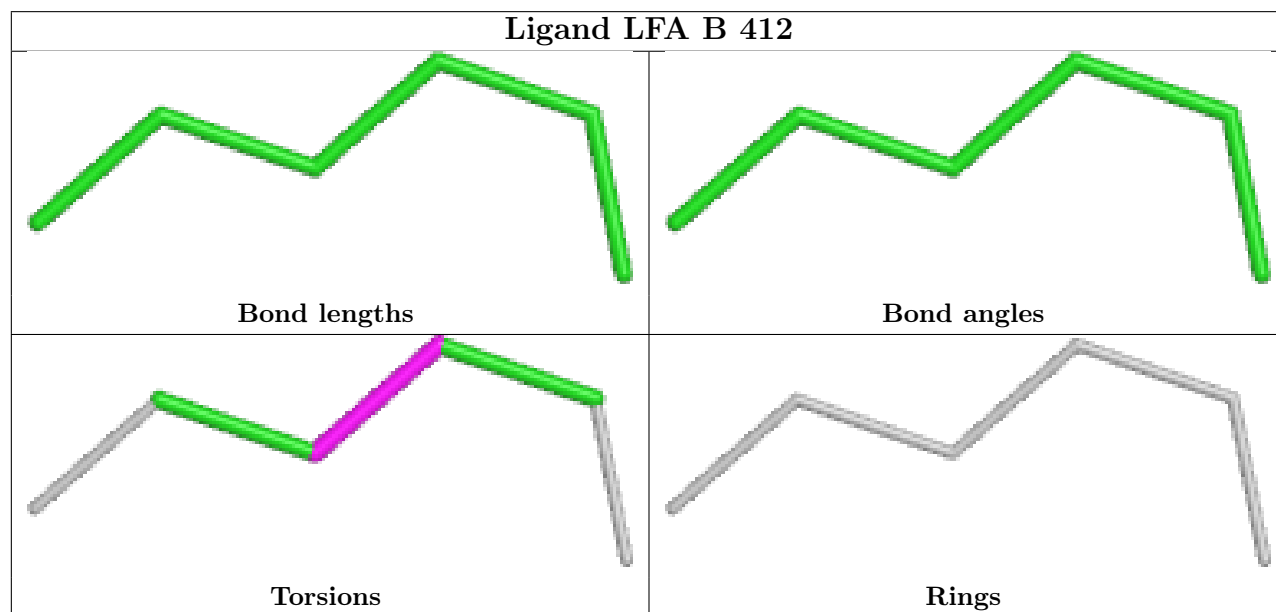
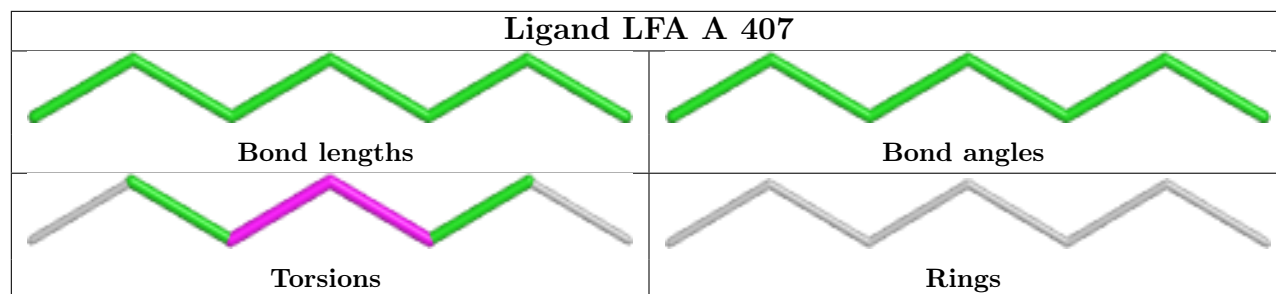


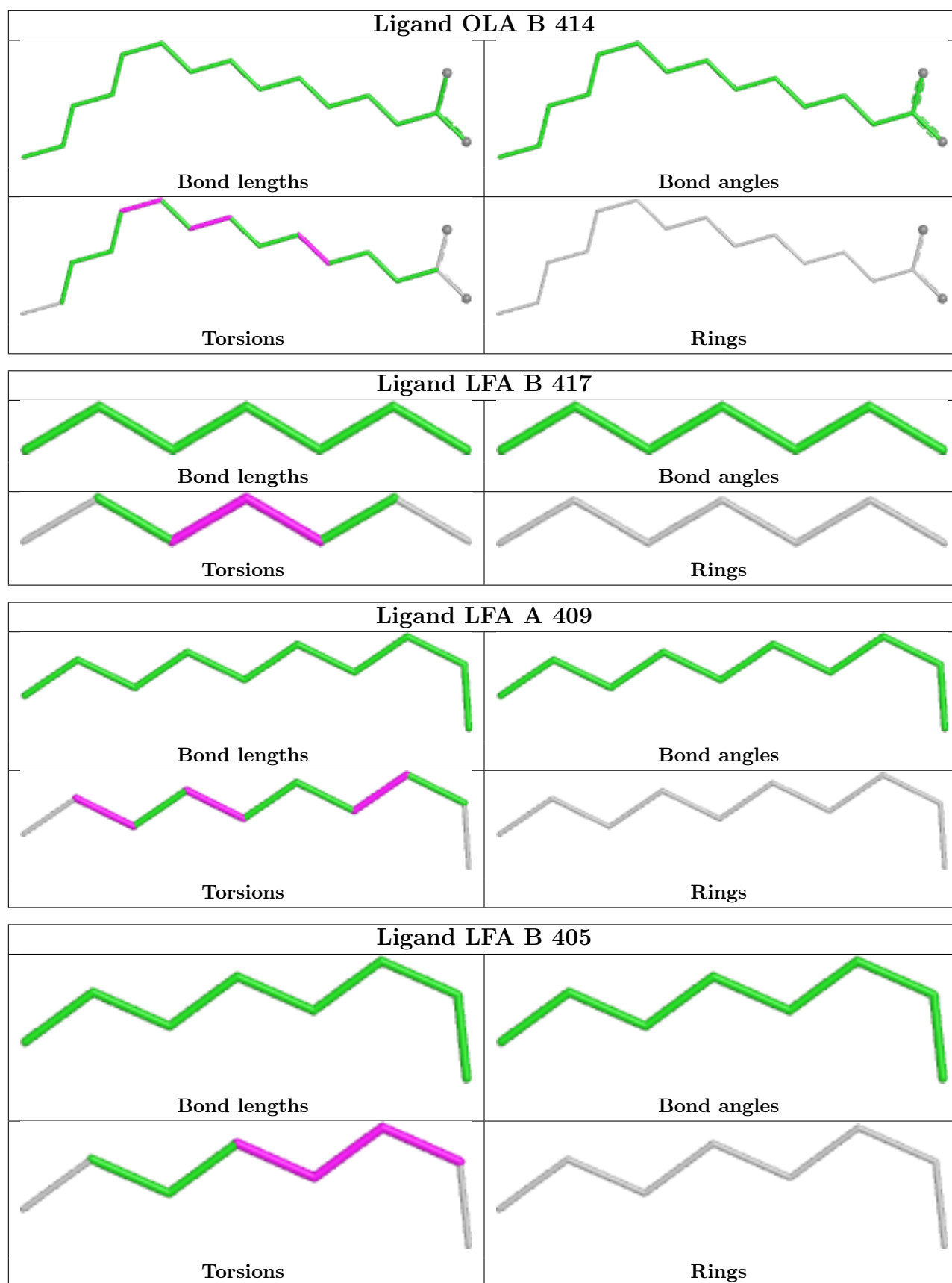


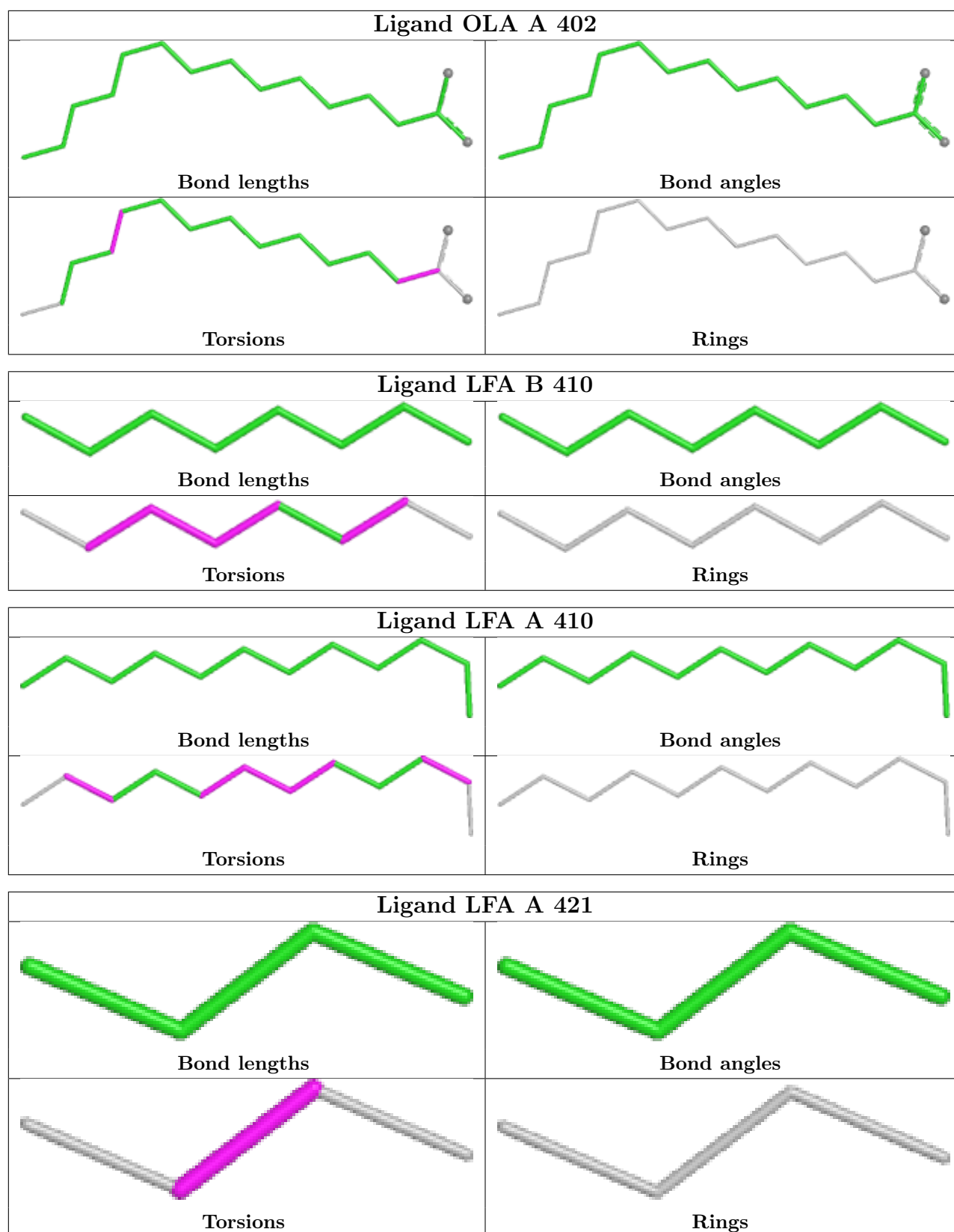












Ligand LFA B 416	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	246/324 (75%)	0.46	10 (4%) 41 38	23, 31, 70, 97	0
1	B	238/324 (73%)	0.34	10 (4%) 40 37	23, 30, 63, 108	0
All	All	484/648 (74%)	0.40	20 (4%) 41 38	23, 30, 67, 108	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	SER	6.2
1	A	286	GLU	4.8
1	A	288	ASP	4.7
1	A	119	ASP	4.5
1	B	125	TYR	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LYR	A	270	29/30	0.88	0.11	21,28,32,34	0
1	LYR	B	270	29/30	0.90	0.10	22,26,32,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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
2	LFA	A	423	7/20	0.55	0.25	51,51,55,60	0
2	LFA	B	423	9/20	0.55	0.19	43,49,54,56	0
2	LFA	A	415	6/20	0.60	0.20	33,38,42,43	0
2	LFA	A	416	4/20	0.62	0.24	43,45,47,47	0
2	LFA	A	410	12/20	0.64	0.16	38,47,53,56	0
2	LFA	A	422	6/20	0.65	0.21	41,45,50,52	0
2	LFA	B	424	7/20	0.65	0.18	39,45,50,53	0
2	LFA	B	422	7/20	0.67	0.16	44,52,56,56	0
2	LFA	B	421	7/20	0.68	0.19	49,50,55,55	0
2	LFA	A	420	4/20	0.68	0.19	40,43,47,51	0
3	OLA	A	412	14/20	0.68	0.14	38,45,53,66	0
2	LFA	B	412	6/20	0.70	0.15	34,45,47,50	0
2	LFA	A	424	5/20	0.72	0.15	28,31,43,50	0
2	LFA	B	417	7/20	0.72	0.18	32,38,41,49	0
2	LFA	B	419	4/20	0.72	0.14	33,34,44,45	0
2	LFA	B	409	11/20	0.72	0.17	33,41,51,52	0
3	OLA	A	413	10/20	0.73	0.14	44,50,62,63	0
2	LFA	B	410	8/20	0.76	0.15	31,44,49,51	0
2	LFA	A	409	10/20	0.76	0.14	43,45,50,53	0
3	OLA	B	414	16/20	0.76	0.15	34,43,53,60	0
2	LFA	A	417	5/20	0.77	0.17	38,39,41,49	0
2	LFA	A	418	3/20	0.77	0.15	31,31,35,39	0
2	LFA	B	403	16/20	0.77	0.14	43,49,55,57	0
2	LFA	A	401	16/20	0.77	0.15	32,43,48,58	0
2	LFA	A	404	14/20	0.77	0.12	44,47,52,55	0
2	LFA	B	408	7/20	0.78	0.14	39,40,46,49	0
2	LFA	A	419	3/20	0.78	0.23	34,34,46,50	0
2	LFA	B	416	9/20	0.78	0.12	33,39,43,44	0
2	LFA	B	407	10/20	0.79	0.13	30,32,42,43	0
2	LFA	B	415	3/20	0.79	0.14	32,32,32,40	0
2	LFA	B	406	8/20	0.79	0.14	34,42,49,49	0
3	OLA	B	413	11/20	0.80	0.14	45,47,59,65	0
2	LFA	B	404	10/20	0.80	0.12	37,48,51,52	0
2	LFA	A	408	12/20	0.81	0.13	32,42,53,58	0
2	LFA	B	402	15/20	0.82	0.17	39,47,58,61	0
2	LFA	A	414	3/20	0.82	0.16	35,35,36,44	0
2	LFA	A	406	14/20	0.82	0.13	32,41,47,48	0

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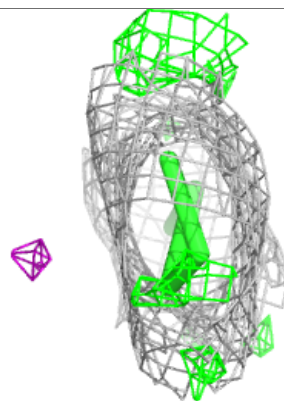
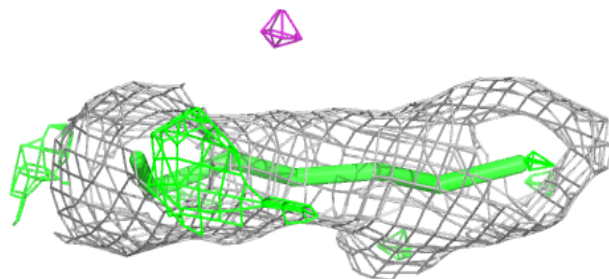
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LFA	B	405	8/20	0.83	0.10	33,39,40,45	0
2	LFA	A	407	7/20	0.84	0.12	35,41,44,48	0
2	LFA	B	420	3/20	0.85	0.14	33,33,35,36	0
3	OLA	B	401	16/20	0.85	0.13	25,33,51,56	0
3	OLA	A	402	16/20	0.85	0.13	22,36,47,50	0
2	LFA	A	405	10/20	0.85	0.11	31,47,51,54	0
2	LFA	A	403	8/20	0.86	0.11	30,36,46,46	0
2	LFA	B	411	10/20	0.86	0.10	36,45,47,48	0
2	LFA	A	411	3/20	0.87	0.20	24,24,31,34	0
2	LFA	B	418	3/20	0.87	0.16	33,33,40,42	0
2	LFA	A	421	4/20	0.88	0.10	31,39,40,40	0
2	LFA	A	425	12/20	0.89	0.11	31,38,49,52	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.

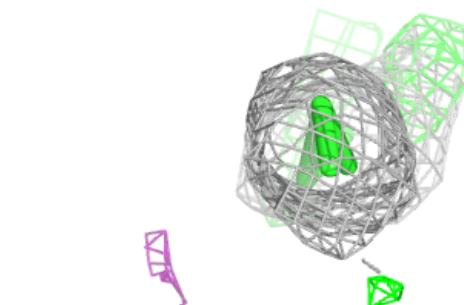
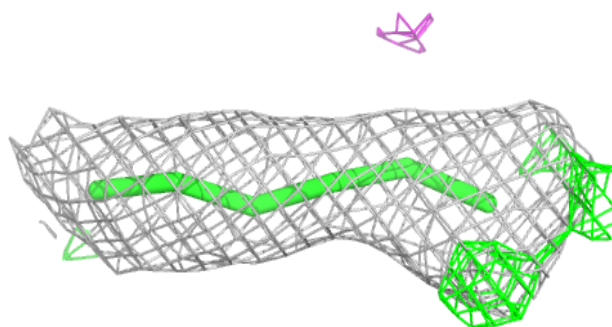
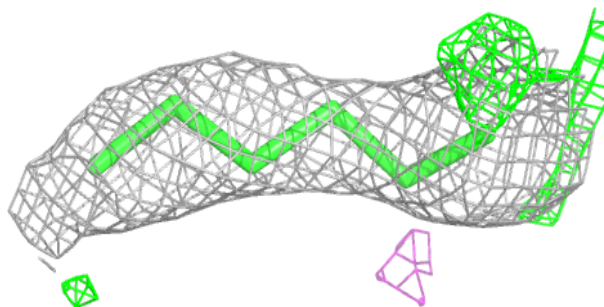
Electron density around LFA A 423:

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

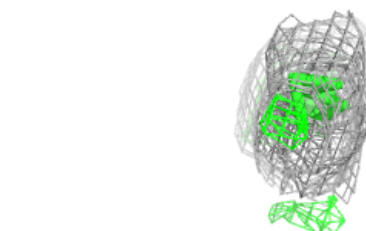
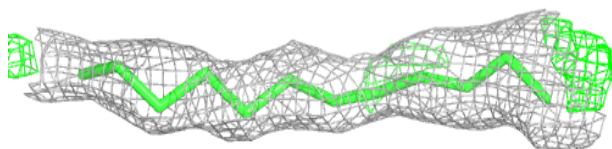
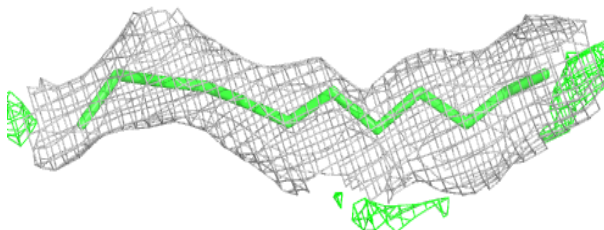


Electron density around LFA A 415:

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

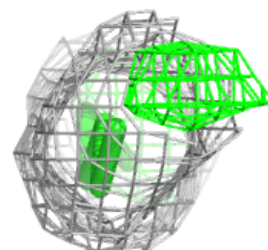
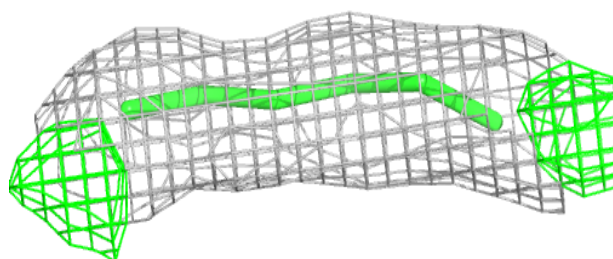
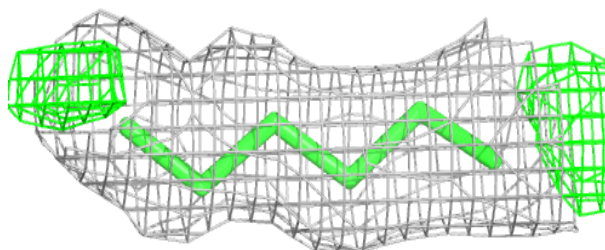
**Electron density around LFA A 410:**

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

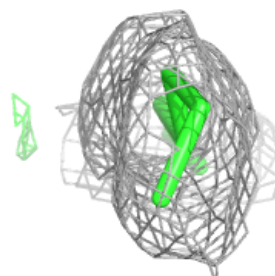
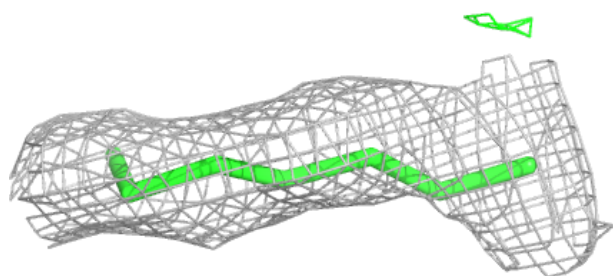
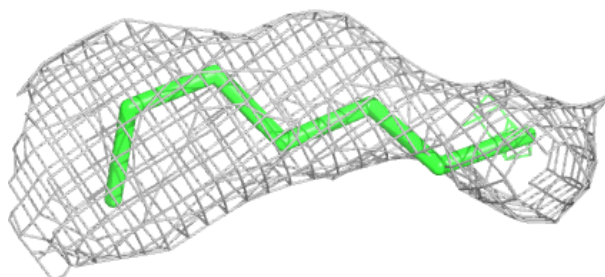


Electron density around LFA A 422:

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

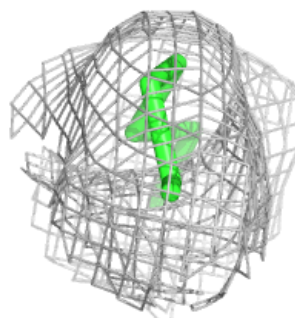
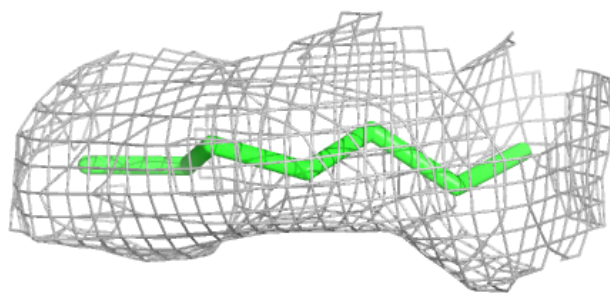
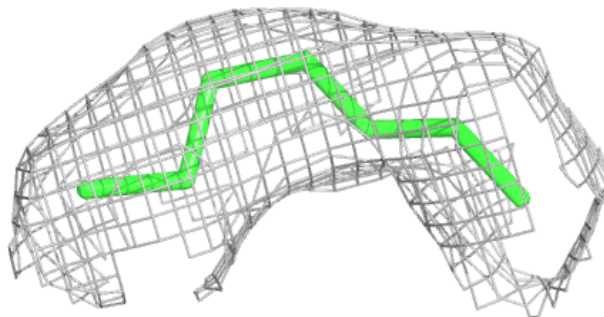
**Electron density around LFA B 424:**

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

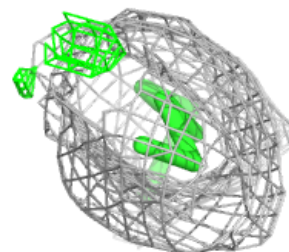
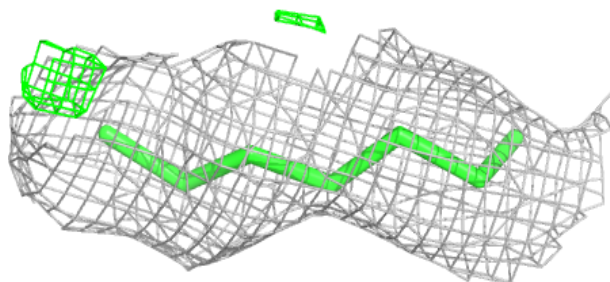
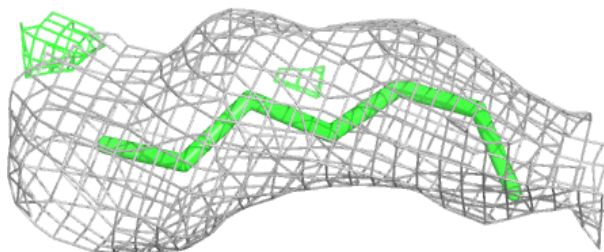


Electron density around LFA B 422:

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

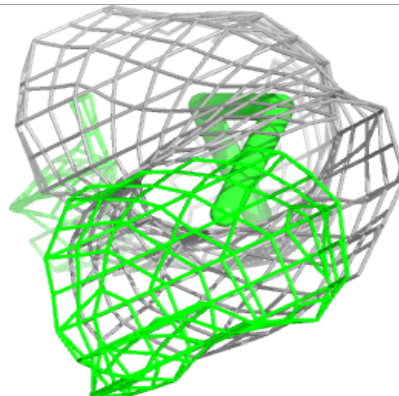
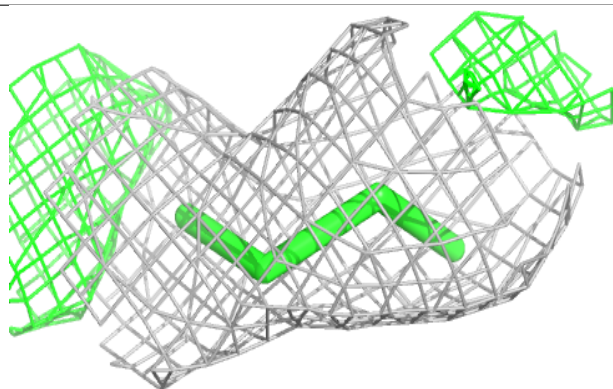
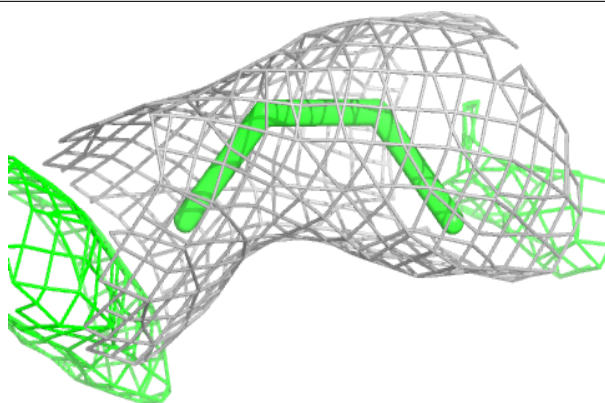
**Electron density around LFA B 421:**

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

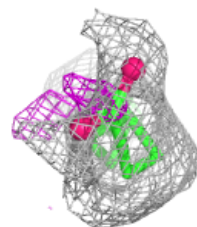
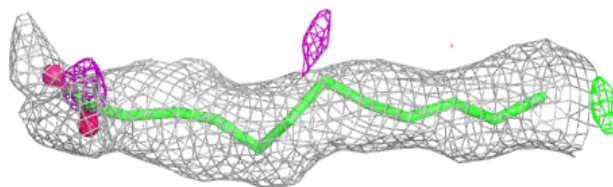
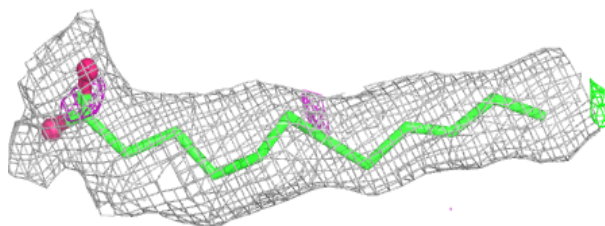


Electron density around LFA A 420:

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

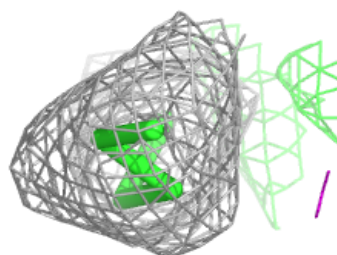
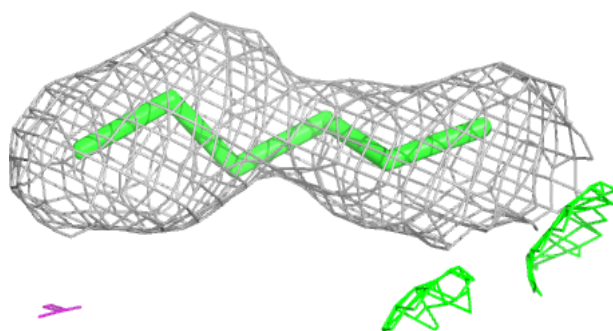
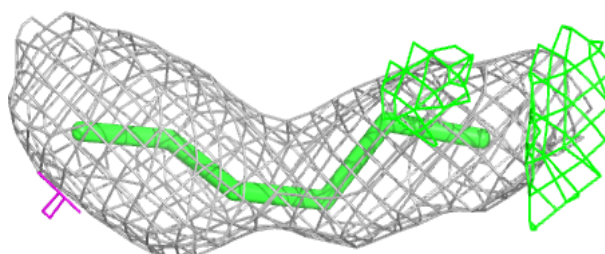
**Electron density around OLA A 412:**

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

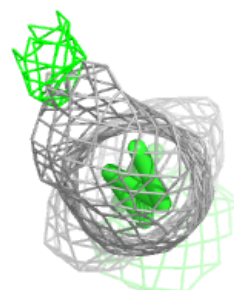
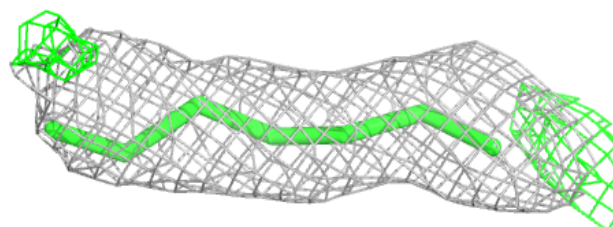
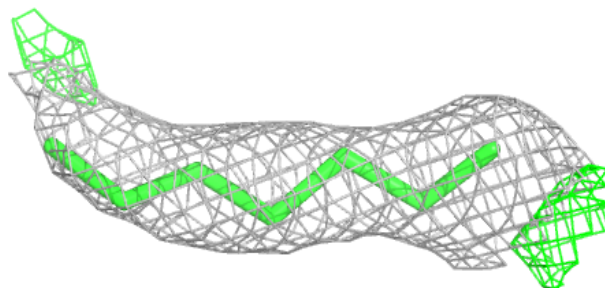


Electron density around LFA B 412:

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

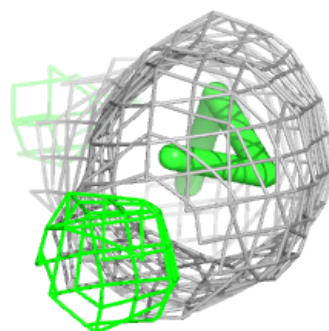
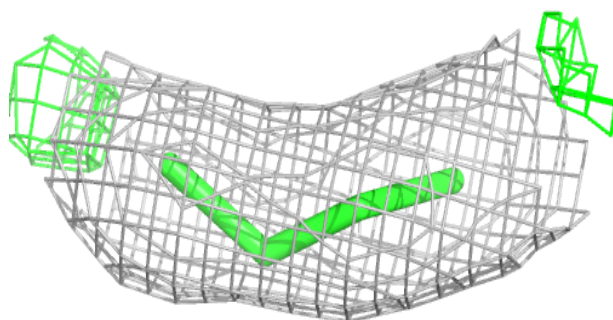
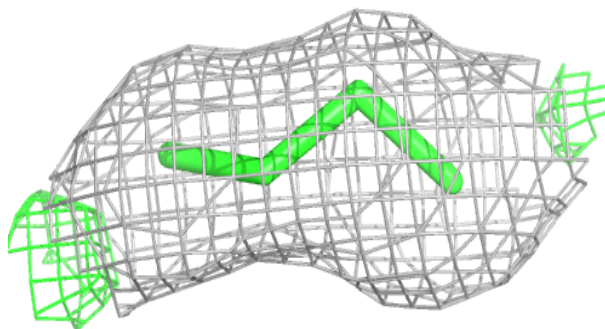
**Electron density around LFA B 417:**

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

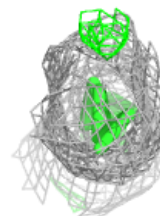
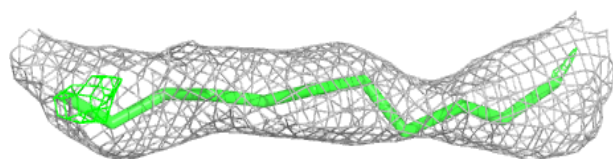
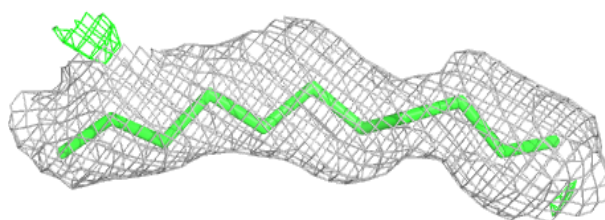


Electron density around LFA B 419:

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

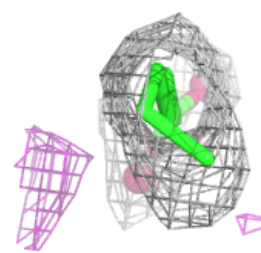
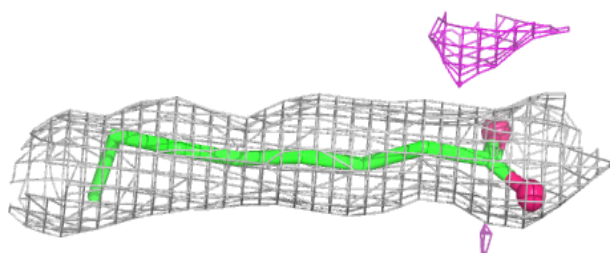
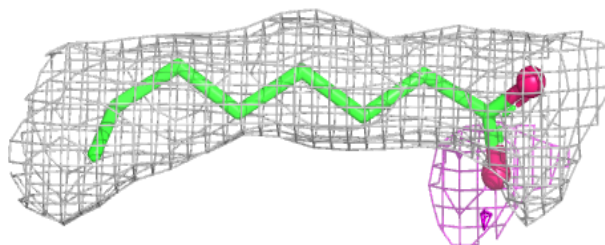
**Electron density around LFA B 409:**

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

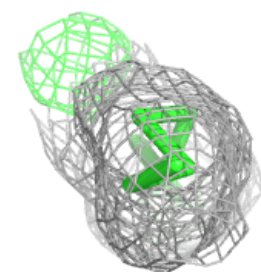
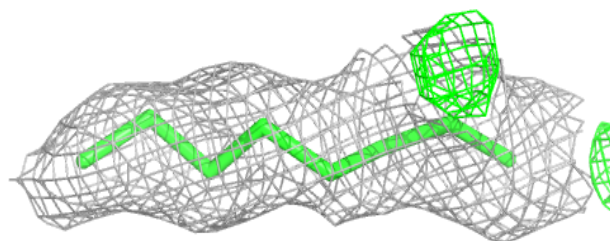
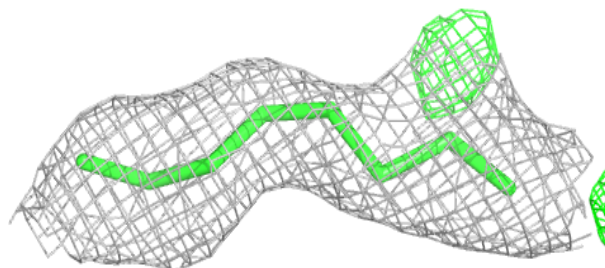


Electron density around OLA A 413:

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

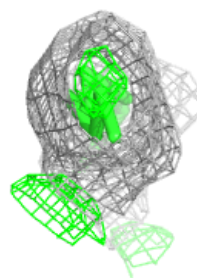
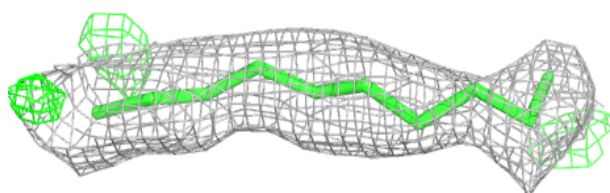
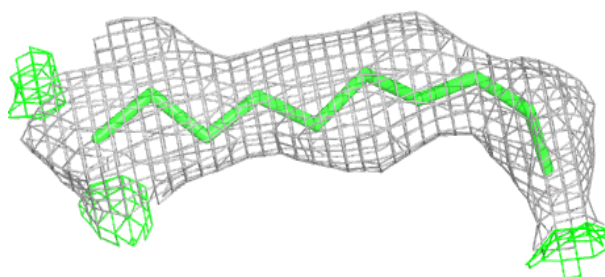
**Electron density around LFA B 410:**

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

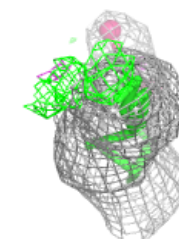
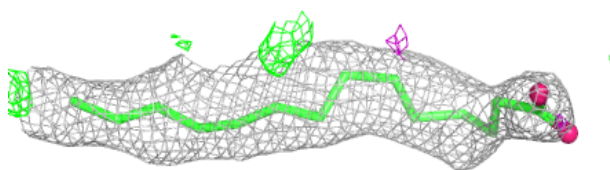
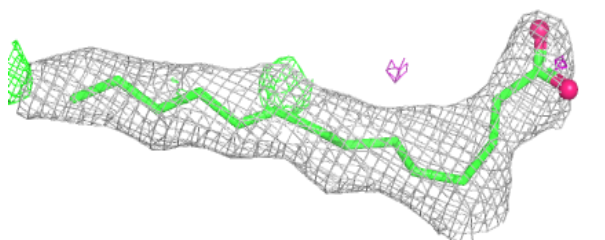


Electron density around LFA A 409:

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

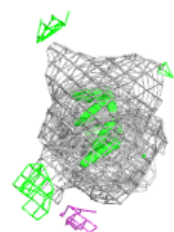
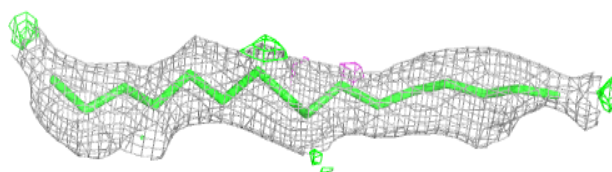
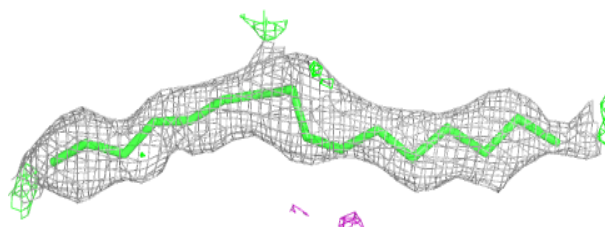
**Electron density around OLA B 414:**

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

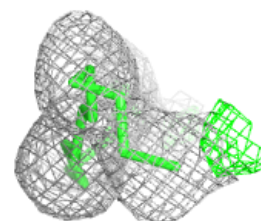
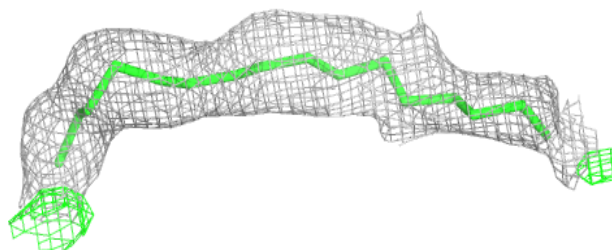
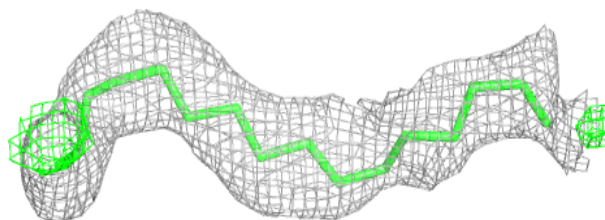


Electron density around LFA B 403:

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

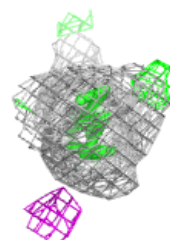
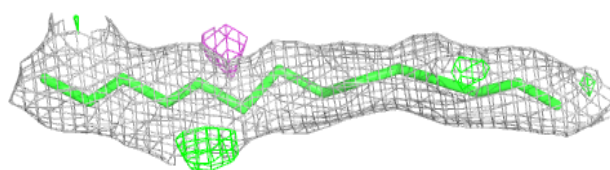
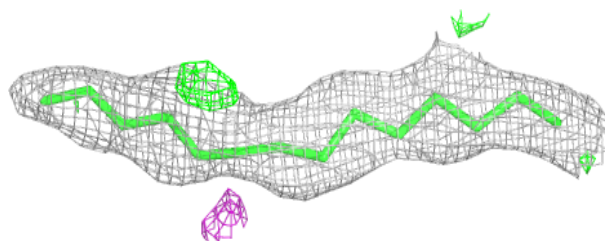
**Electron density around LFA A 401:**

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

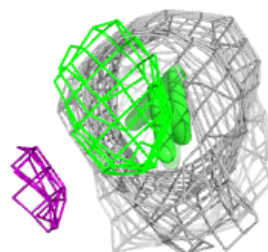
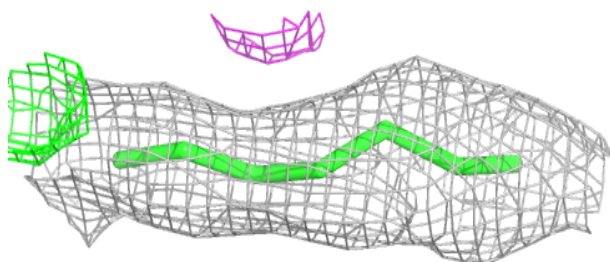
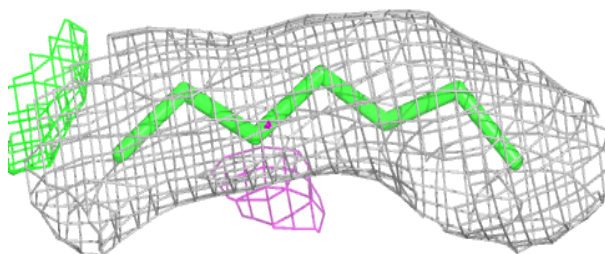


Electron density around LFA A 404:

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

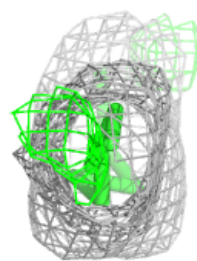
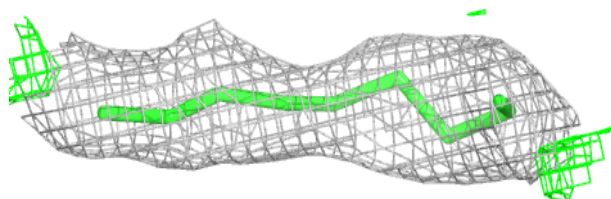
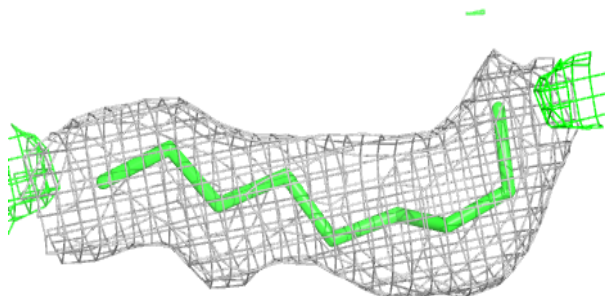
**Electron density around LFA B 408:**

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

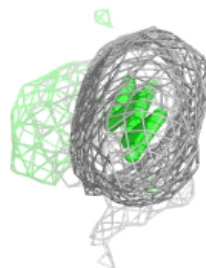
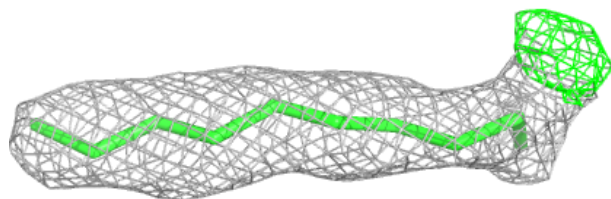
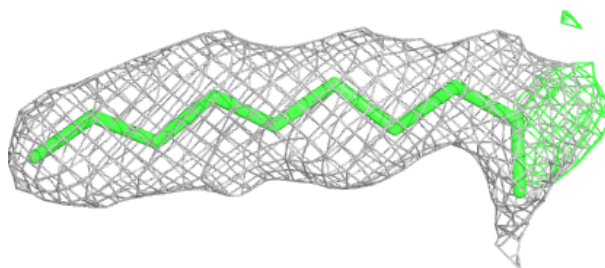


Electron density around LFA B 416:

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

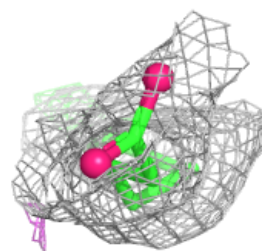
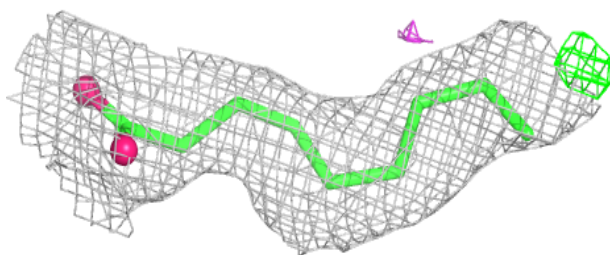
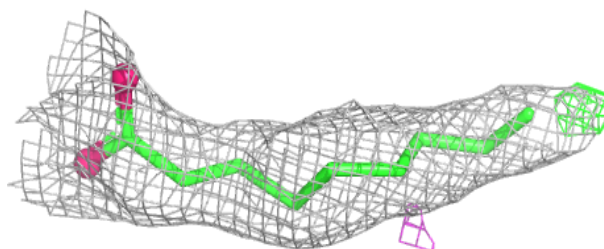
**Electron density around LFA B 407:**

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

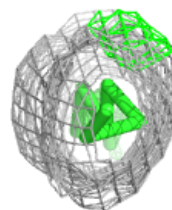
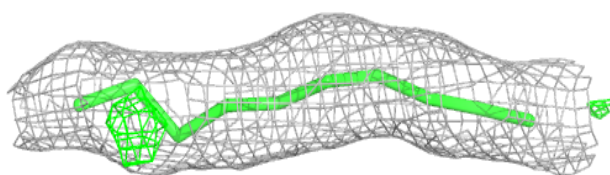
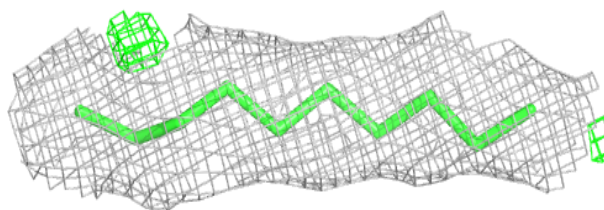


Electron density around OLA B 413:

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

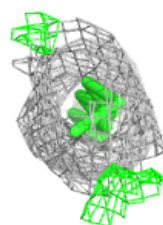
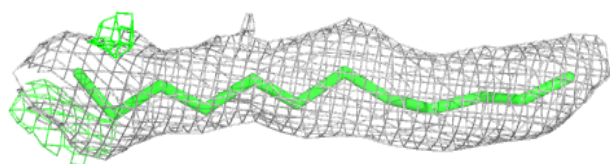
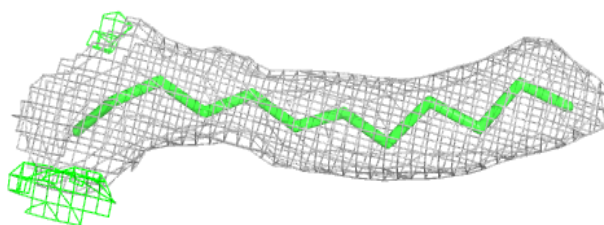
**Electron density around LFA B 404:**

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

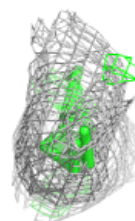
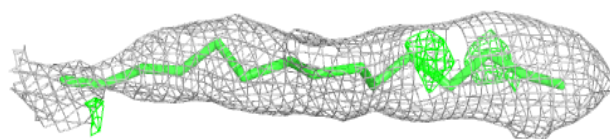
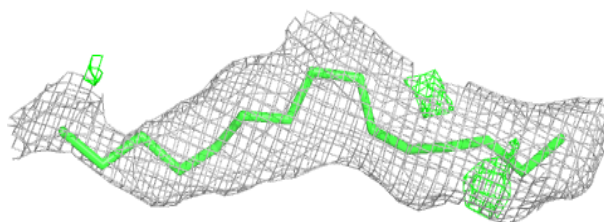


Electron density around LFA A 408:

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

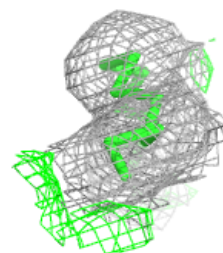
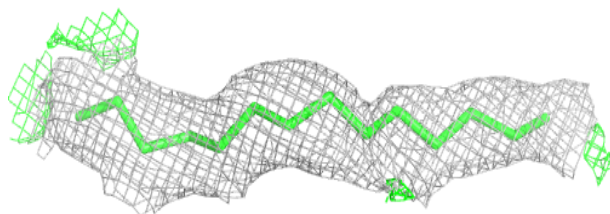
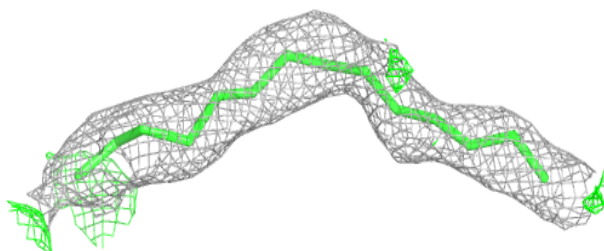
**Electron density around LFA B 402:**

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

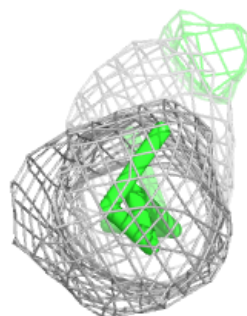
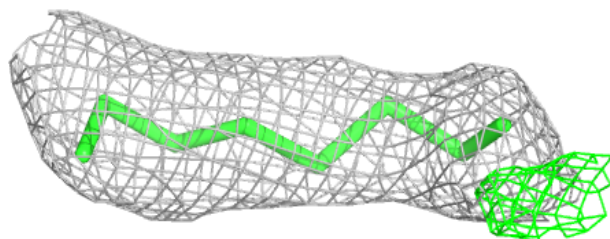
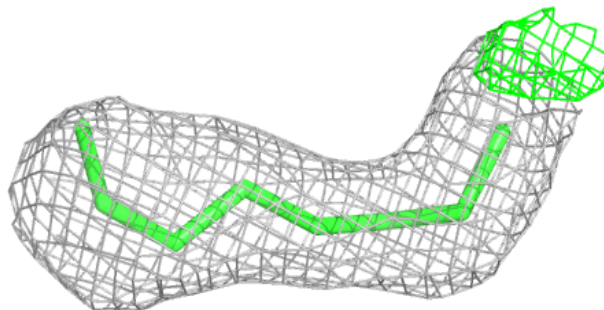


Electron density around LFA A 406:

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

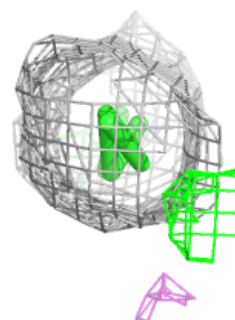
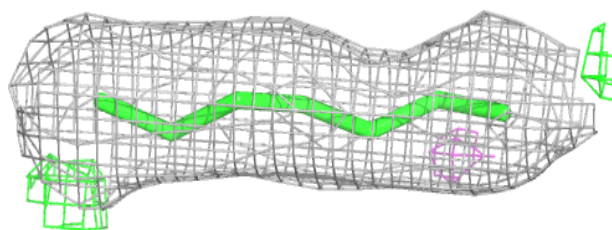
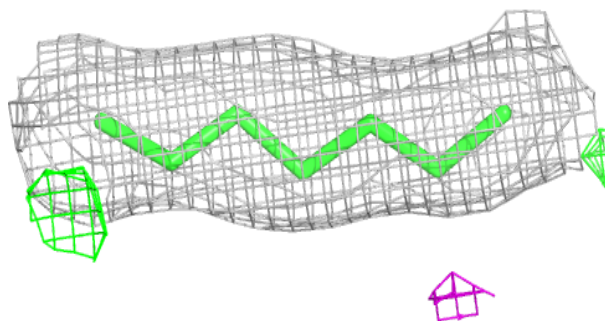
**Electron density around LFA B 405:**

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

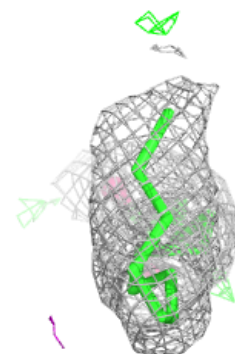
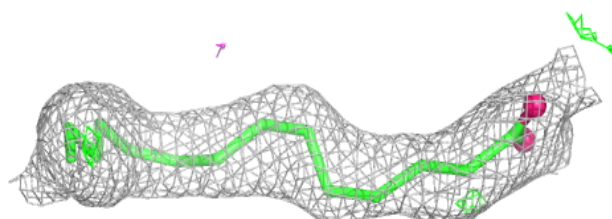
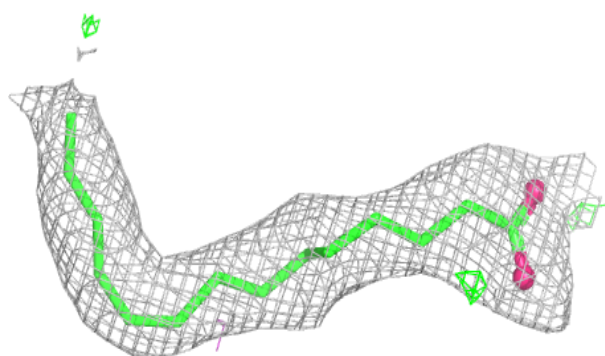


Electron density around LFA A 407:

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

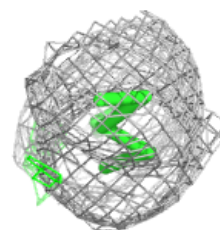
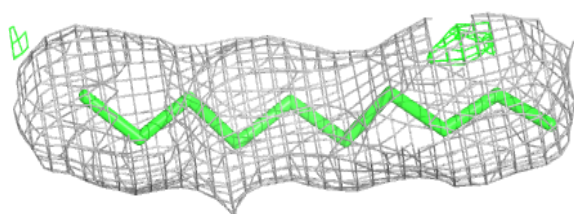
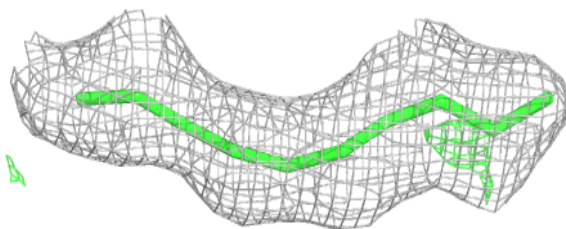
**Electron density around OLA A 402:**

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

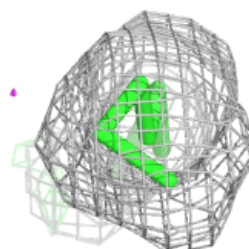
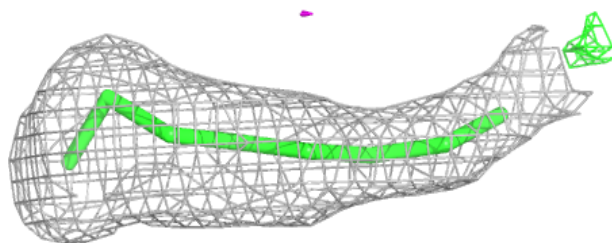
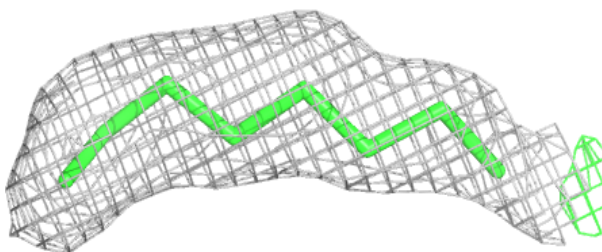


Electron density around LFA A 405:

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

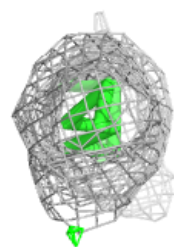
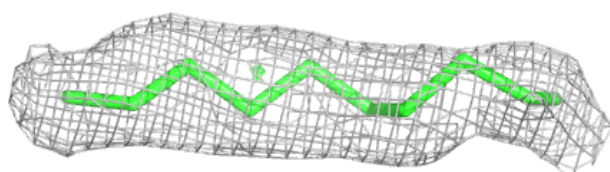
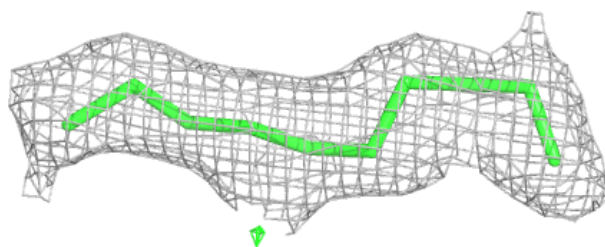
**Electron density around LFA A 403:**

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

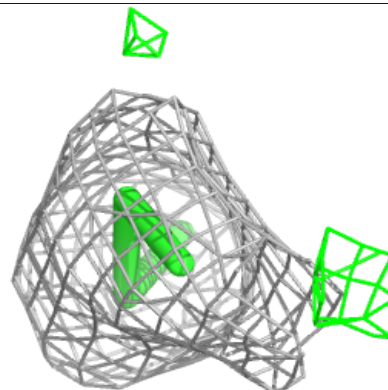
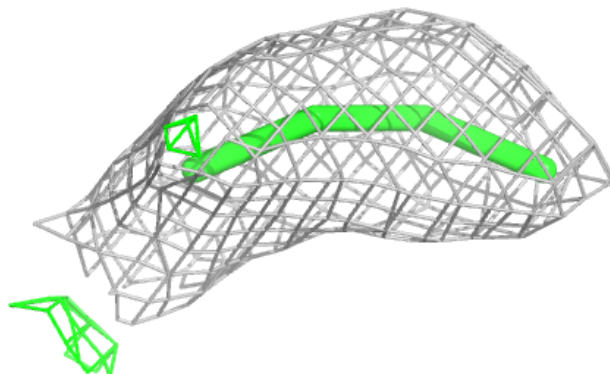
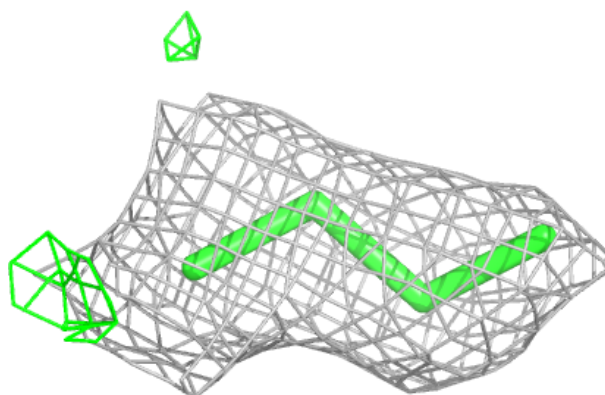


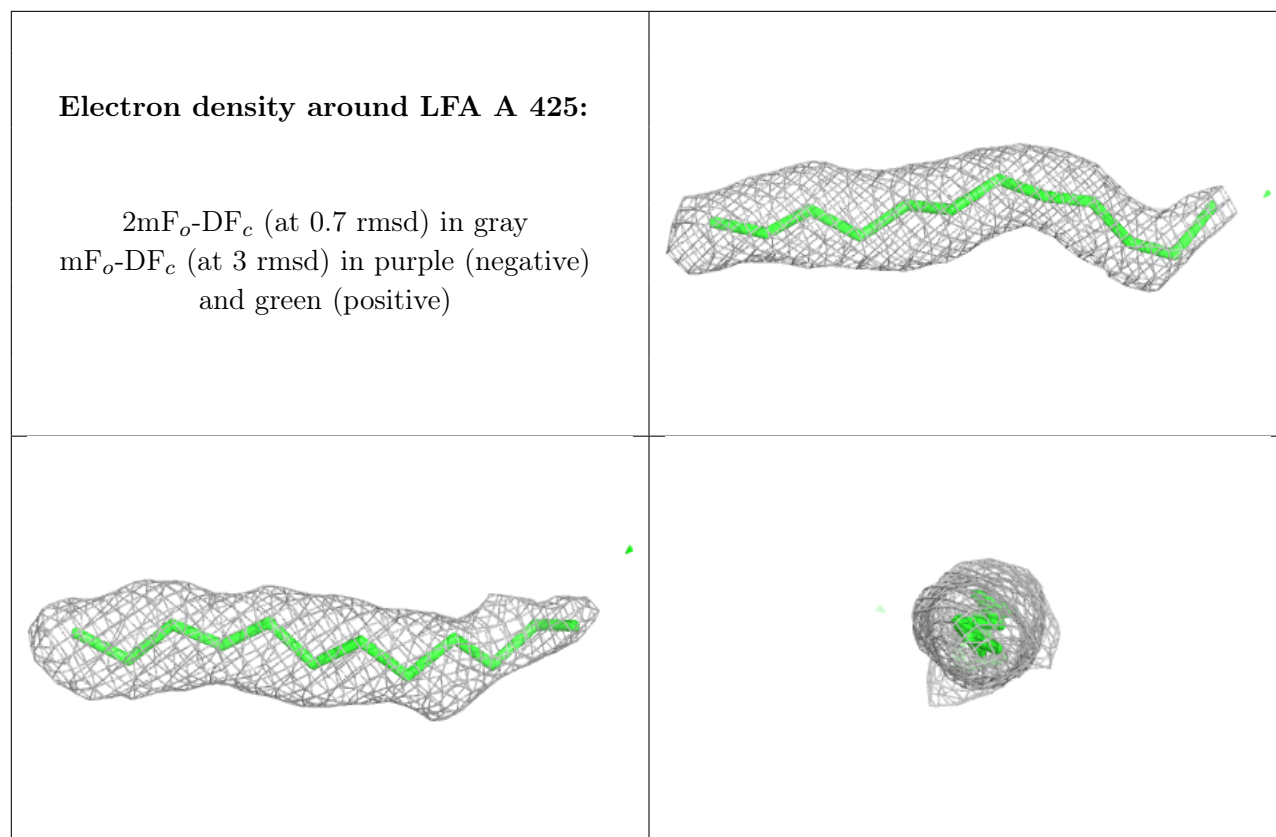
Electron density around LFA B 411:

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

**Electron density around LFA A 421:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.