



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:35 PM UTC

PDB ID : 7Z0C / pdb_00007z0c
Title : Crystal structure of the K state of bacteriorhodopsin at 1.53 Angstrom resolution
Authors : Borshchevskiy, V.; Kovalev, K.; Round, E.; Efremov, R.; Bourenkov, G.; Gordeliy, V.
Deposited on : 2022-02-22
Resolution : 1.53 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

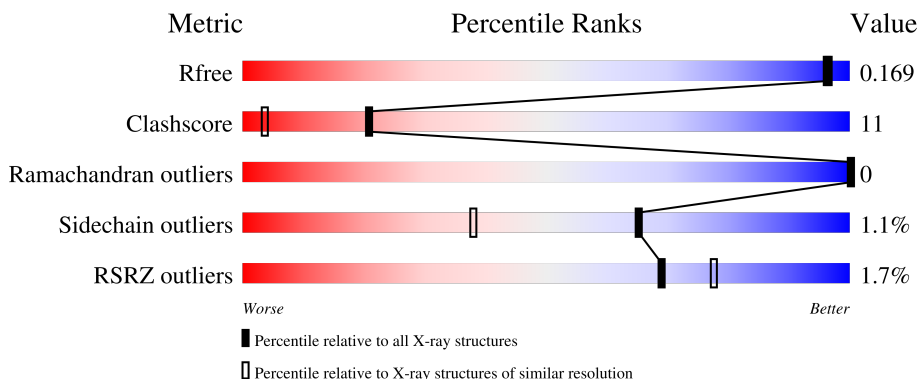
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

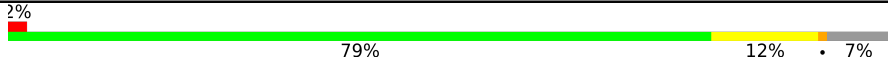
The reported resolution of this entry is 1.53 Å.

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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	248	

2 Entry composition [i](#)

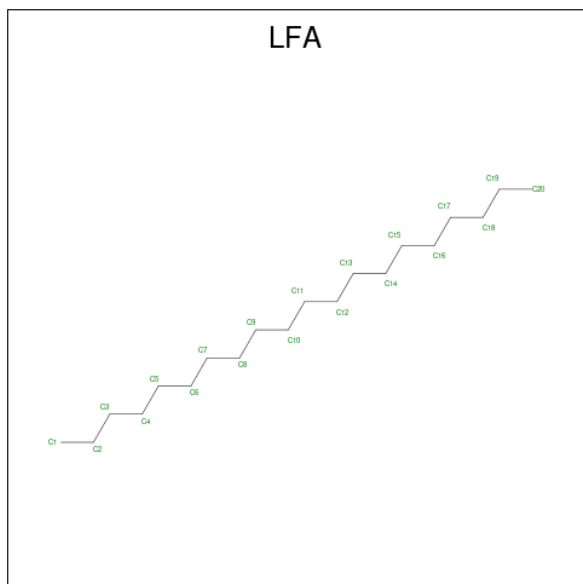
There are 5 unique types of molecules in this entry. The entry contains 4825 atoms, of which 2470 are hydrogens and 0 are deuteriums.

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 Bacteriorhodopsin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	44	0
			4102	1362	2093	297	338	12			

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



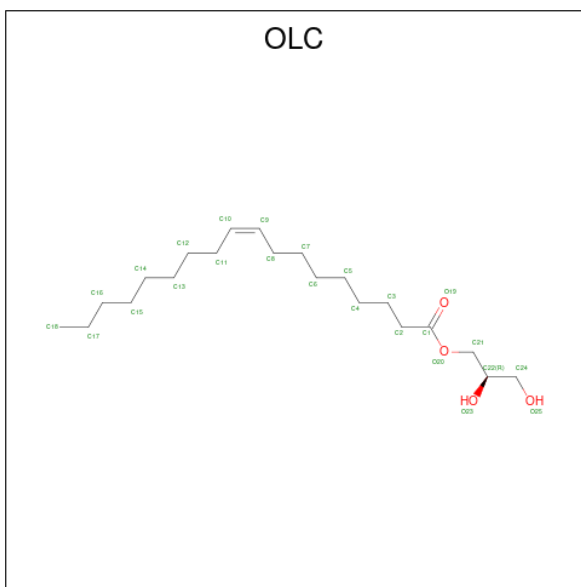
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C		0	0
			7	7			
2	A	1	Total	C	H	0	0
			19	6	13		
2	A	1	Total	C	H	0	0
			25	8	17		
2	A	1	Total	C	H	0	0
			19	6	13		
2	A	1	Total	C	H	0	0
			28	10	18		

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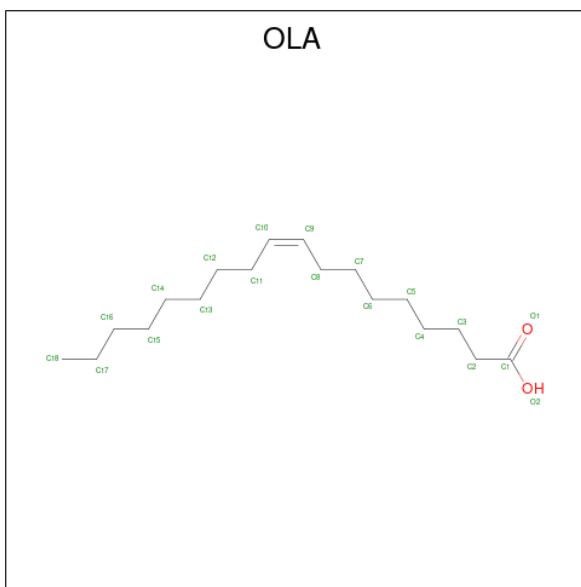
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H 31 10 21	0	0
2	A	1	Total C H 13 4 9	0	0
2	A	1	Total C H 31 10 21	0	0
2	A	1	Total C H 34 11 23	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C H 25 8 17	0	0
2	A	1	Total C H 13 4 9	0	0
2	A	1	Total C H 31 10 21	0	0
2	A	1	Total C H 25 8 17	0	0
2	A	1	Total C H 43 14 29	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C H 49 16 33	0	0
2	A	1	Total C H 19 6 13	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 2 2	0	0
2	A	1	Total C H 13 4 9	0	0

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			65	21	40	4		
3	A	1	Total	C	H	O	0	0
			46	16	26	4		
3	A	1	Total	C	H	O	0	0
			17	9	4	4		

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			40	14	24	2		

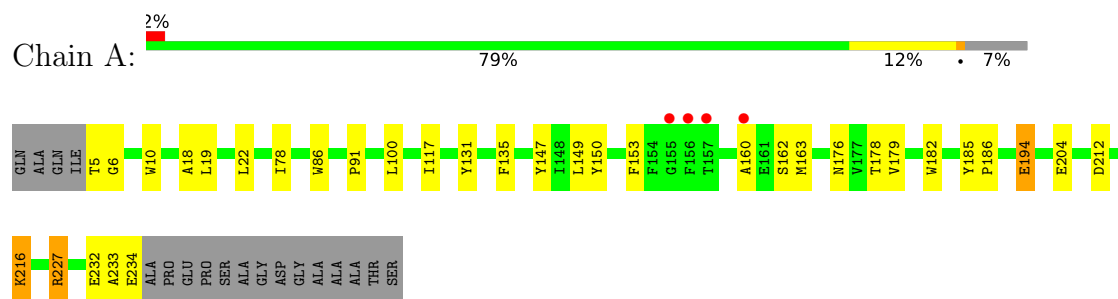
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total 89	O 89	0	7

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: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	60.99Å 60.99Å 110.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.11 – 1.53 38.11 – 1.53	Depositor EDS
% Data completeness (in resolution range)	85.1 (38.11-1.53) 85.1 (38.11-1.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.53Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.149 , 0.171 0.149 , 0.169	Depositor DCC
R_{free} test set	1031 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4825	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLC, LFA, 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	0.59	6/2139 (0.3%)	0.74	6/2923 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86[A]	TRP	C-O	6.78	1.32	1.24
1	A	86[D]	TRP	C-O	6.78	1.32	1.24
1	A	212[A]	ASP	C-O	6.05	1.31	1.24
1	A	212[D]	ASP	C-O	6.05	1.31	1.24
1	A	185[A]	TYR	C-O	5.29	1.29	1.24
1	A	185[D]	TYR	C-O	5.29	1.29	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185[A]	TYR	CA-C-O	11.91	129.89	118.34
1	A	185[D]	TYR	CA-C-O	11.91	129.89	118.34
1	A	185[A]	TYR	N-CA-C	7.85	124.31	113.16
1	A	185[D]	TYR	N-CA-C	7.85	124.31	113.16
1	A	212[A]	ASP	N-CA-C	5.30	117.06	111.28
1	A	212[D]	ASP	N-CA-C	5.30	117.06	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194[A]	GLU	Mainchain
1	A	6	GLY	Mainchain

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	2009	2093	1939	38	0
2	A	183	283	333	17	0
3	A	58	70	82	9	0
4	A	16	24	22	3	0
5	A	89	0	0	6	0
All	All	2355	2470	2376	53	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 11.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:811:OLC:H5A	3:A:811:OLC:H9	1.50	0.93
2:A:814:LFA:H11	2:A:828:LFA:H22	1.48	0.93
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.38	0.88
1:A:216[D]:LYR:H192	1:A:216[D]:LYR:H9	1.54	0.87
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.11	0.84
1:A:216[D]:LYR:H192	1:A:216[D]:LYR:C9	2.17	0.74
2:A:810:LFA:C11	2:A:812:LFA:H162	2.17	0.73
3:A:803:OLC:O25	5:A:901:HOH:O	2.08	0.71
3:A:811:OLC:H9	3:A:811:OLC:C5	2.20	0.71
1:A:232:GLU:HA	5:A:912:HOH:O	1.91	0.70
2:A:821:LFA:C14	2:A:827:LFA:C3	2.71	0.68
1:A:160:ALA:HA	1:A:163:MET:HE3	1.77	0.67
2:A:814:LFA:H11	2:A:828:LFA:C2	2.23	0.67
1:A:232:GLU:OE2	5:A:902:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:SER:OG	5:A:903:HOH:O	2.15	0.64
2:A:806:LFA:H81	2:A:813:LFA:H41	1.84	0.58
3:A:811:OLC:H5A	3:A:811:OLC:C9	2.30	0.58
2:A:818:LFA:C19	2:A:819:LFA:C15	2.83	0.57
1:A:149:LEU:HD22	1:A:179:VAL:HG22	1.88	0.54
1:A:18:ALA:HA	2:A:807:LFA:H72	1.90	0.53
2:A:822:LFA:C16	3:A:824:OLC:C6	2.87	0.53
1:A:176:ASN:OD1	2:A:806:LFA:C3	2.58	0.52
1:A:5:THR:HG23	1:A:10:TRP:NE1	2.25	0.52
1:A:176:ASN:OD1	2:A:806:LFA:H31	2.10	0.52
1:A:78:ILE:HD12	1:A:194[B]:GLU:HG2	1.93	0.51
1:A:182[D]:TRP:NE1	1:A:216[D]:LYR:H43	2.26	0.51
1:A:194[A]:GLU:OE1	1:A:204[A]:GLU:OE2	2.30	0.49
1:A:216[D]:LYR:C9	1:A:216[D]:LYR:C19	2.88	0.49
1:A:147:TYR:HE1	2:A:819:LFA:H202	1.77	0.48
1:A:178:THR:O	1:A:182[D]:TRP:HB2	2.13	0.48
1:A:91:PRO:HB2	2:A:812:LFA:H181	1.95	0.48
1:A:131:TYR:OH	4:A:826:OLA:H31	2.14	0.48
1:A:216[D]:LYR:H6	1:A:216[D]:LYR:H41	1.77	0.46
1:A:117:ILE:HG21	3:A:803:OLC:H11A	1.98	0.46
1:A:19:LEU:HD22	3:A:811:OLC:H8	1.97	0.45
1:A:216[A]:LYR:H192	1:A:216[A]:LYR:H9	1.96	0.45
1:A:100[A]:LEU:HD23	1:A:100[A]:LEU:HA	1.86	0.45
2:A:814:LFA:H22	2:A:828:LFA:H11	1.99	0.45
1:A:150:TYR:HE2	2:A:819:LFA:H182	1.81	0.45
1:A:234:GLU:HG3	1:A:234:GLU:O	2.16	0.45
1:A:216[D]:LYR:HE3	5:A:920[D]:HOH:O	2.17	0.44
1:A:227:ARG:HD2	1:A:227:ARG:HA	1.49	0.44
3:A:811:OLC:C5	3:A:811:OLC:C9	2.91	0.43
3:A:803:OLC:H8A	3:A:803:OLC:H11	1.48	0.42
1:A:131:TYR:CE2	4:A:826:OLA:H31	2.55	0.42
1:A:100[B]:LEU:HD12	1:A:100[B]:LEU:HA	1.89	0.41
1:A:150:TYR:CE2	2:A:819:LFA:H182	2.54	0.41
1:A:233:ALA:N	5:A:912:HOH:O	2.52	0.41
1:A:135:PHE:CZ	4:A:826:OLA:H42	2.56	0.41
1:A:176:ASN:OD1	2:A:806:LFA:H32	2.21	0.40
1:A:216[A]:LYR:H9	1:A:216[A]:LYR:H183	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	271/248 (109%)	269 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	215/193 (111%)	212 (99%)	3 (1%)	59	29

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22[A]	LEU
1	A	22[B]	LEU
1	A	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	A	216[D]	1	27,29,30	1.12	2 (7%)	30,37,39	1.37	5 (16%)
1	LYR	A	216[A]	1	27,29,30	0.67	0	30,37,39	1.10	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	A	216[D]	1	-	3/22/40/42	0/1/1/1
1	LYR	A	216[A]	1	-	3/22/40/42	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216[D]	LYR	C9-C80	-2.73	1.40	1.46
1	A	216[D]	LYR	C7-C80	2.19	1.40	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216[D]	LYR	C8-C80-C7	-3.68	116.85	122.82
1	A	216[D]	LYR	C9-C80-C7	2.91	123.59	119.01
1	A	216[A]	LYR	C19-C17-C11	2.80	114.64	110.24
1	A	216[D]	LYR	C1-NZ-CE	2.75	118.42	112.85
1	A	216[D]	LYR	C7-C6-C5	2.71	131.06	123.20
1	A	216[D]	LYR	C5-C3-C2	2.56	122.05	118.49
1	A	216[A]	LYR	C16-C17-C11	2.13	113.53	110.44
1	A	216[A]	LYR	C9-C80-C7	-2.04	115.80	119.01

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	216[A]	LYR	C1-C2-C3-C4
1	A	216[A]	LYR	C1-C2-C3-C5
1	A	216[D]	LYR	C1-C2-C3-C5
1	A	216[D]	LYR	CG-CD-CE-NZ
1	A	216[D]	LYR	C1-C2-C3-C4
1	A	216[A]	LYR	CD-CE-NZ-C1

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	216[D]	LYR	6	0
1	A	216[A]	LYR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 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	809	-	9,9,19	0.23	0	8,8,18	0.21	0
2	LFA	A	808	-	3,3,19	0.15	0	2,2,18	0.45	0
2	LFA	A	806	-	9,9,19	0.12	0	8,8,18	0.12	0
2	LFA	A	801	-	6,6,19	0.18	0	5,5,18	0.23	0
2	LFA	A	812	-	9,9,19	0.18	0	8,8,18	0.12	0
2	LFA	A	823	-	5,5,19	0.16	0	4,4,18	0.06	0
2	LFA	A	819	-	5,5,19	0.15	0	4,4,18	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	A	816	-	7,7,19	0.14	0	6,6,18	0.10	0
2	LFA	A	814	-	3,3,19	0.16	0	2,2,18	0.47	0
2	LFA	A	802	-	5,5,19	0.15	0	4,4,18	0.11	0
2	LFA	A	817	-	13,13,19	0.30	0	12,12,18	0.85	0
2	LFA	A	825	-	4,4,19	0.16	0	3,3,18	0.27	0
2	LFA	A	820	-	2,2,19	0.25	0	1,1,18	0.10	0
2	LFA	A	805	-	5,5,19	0.17	0	4,4,18	0.14	0
2	LFA	A	822	-	15,15,19	0.30	0	14,14,18	0.82	0
2	LFA	A	815	-	9,9,19	0.18	0	8,8,18	0.12	0
3	OLC	A	824	-	12,12,24	1.21	1 (8%)	13,13,25	1.35	2 (15%)
2	LFA	A	807	-	9,9,19	0.29	0	8,8,18	0.79	0
3	OLC	A	811	-	19,19,24	1.04	1 (5%)	20,20,25	0.94	2 (10%)
2	LFA	A	804	-	7,7,19	0.18	0	6,6,18	0.18	0
2	LFA	A	821	-	6,6,19	0.15	0	5,5,18	0.13	0
4	OLA	A	826	-	15,15,19	0.60	0	15,15,19	0.56	0
3	OLC	A	803	-	24,24,24	0.83	1 (4%)	25,25,25	1.05	2 (8%)
2	LFA	A	818	-	7,7,19	0.20	0	6,6,18	0.12	0
2	LFA	A	827	-	1,1,19	0.04	0	-	-	-
2	LFA	A	828	-	3,3,19	0.39	0	2,2,18	0.74	0
2	LFA	A	810	-	10,10,19	0.29	0	9,9,18	0.10	0
2	LFA	A	813	-	7,7,19	0.13	0	6,6,18	0.07	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	809	-	-	5/7/7/17	-
2	LFA	A	808	-	-	1/1/1/17	-
2	LFA	A	806	-	-	6/7/7/17	-
2	LFA	A	801	-	-	0/4/4/17	-
2	LFA	A	812	-	-	5/7/7/17	-
2	LFA	A	823	-	-	1/3/3/17	-
2	LFA	A	819	-	-	2/3/3/17	-
2	LFA	A	816	-	-	3/5/5/17	-
2	LFA	A	814	-	-	1/1/1/17	-
2	LFA	A	802	-	-	1/3/3/17	-
2	LFA	A	817	-	-	6/11/11/17	-
2	LFA	A	825	-	-	2/2/2/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	805	-	-	0/3/3/17	-
2	LFA	A	822	-	-	4/13/13/17	-
2	LFA	A	815	-	-	4/7/7/17	-
3	OLC	A	824	-	-	9/12/12/24	-
2	LFA	A	807	-	-	4/7/7/17	-
3	OLC	A	811	-	-	7/19/19/24	-
2	LFA	A	804	-	-	2/5/5/17	-
2	LFA	A	821	-	-	2/4/4/17	-
4	OLA	A	826	-	-	9/13/13/17	-
3	OLC	A	803	-	-	6/24/24/24	-
2	LFA	A	818	-	-	3/5/5/17	-
2	LFA	A	828	-	-	1/1/1/17	-
2	LFA	A	810	-	-	4/8/8/17	-
2	LFA	A	813	-	-	4/5/5/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	811	OLC	O20-C1	4.20	1.45	1.33
3	A	824	OLC	O20-C1	3.91	1.44	1.33
3	A	803	OLC	O20-C1	3.43	1.43	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	824	OLC	O20-C1-C2	3.44	122.32	111.83
3	A	803	OLC	O20-C1-C2	3.00	120.97	111.83
3	A	811	OLC	O20-C1-C2	2.78	120.31	111.83
3	A	824	OLC	O20-C1-O19	-2.47	117.46	123.63
3	A	803	OLC	O20-C1-O19	-2.15	118.26	123.63
3	A	811	OLC	O20-C1-O19	-2.01	118.60	123.63

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	808	LFA	C1-C2-C3-C4
2	A	814	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	828	LFA	C1-C2-C3-C4
3	A	811	OLC	C10-C11-C12-C13
3	A	824	OLC	C21-C22-C24-O25
3	A	824	OLC	O20-C21-C22-O23
3	A	824	OLC	O19-C1-O20-C21
3	A	824	OLC	C2-C1-O20-C21
3	A	824	OLC	O23-C22-C24-O25
4	A	826	OLA	C1-C2-C3-C4
3	A	811	OLC	C21-C22-C24-O25
2	A	810	LFA	C3-C4-C5-C6
2	A	806	LFA	C3-C4-C5-C6
2	A	807	LFA	C4-C5-C6-C7
2	A	812	LFA	C16-C17-C18-C19
2	A	822	LFA	C11-C10-C9-C8
3	A	824	OLC	C1-C2-C3-C4
3	A	811	OLC	C4-C5-C6-C7
4	A	826	OLA	C4-C5-C6-C7
2	A	813	LFA	C3-C4-C5-C6
2	A	804	LFA	C3-C4-C5-C6
2	A	802	LFA	C2-C3-C4-C5
2	A	822	LFA	C2-C3-C4-C5
2	A	817	LFA	C9-C10-C11-C12
2	A	825	LFA	C16-C17-C18-C19
3	A	811	OLC	O20-C21-C22-C24
2	A	809	LFA	C7-C8-C9-C10
2	A	818	LFA	C13-C14-C15-C16
3	A	803	OLC	C11-C12-C13-C14
4	A	826	OLA	C3-C4-C5-C6
3	A	811	OLC	O20-C21-C22-O23
2	A	806	LFA	C5-C6-C7-C8
4	A	826	OLA	C10-C11-C12-C13
2	A	816	LFA	C3-C4-C5-C6
2	A	817	LFA	C10-C11-C12-C13
2	A	807	LFA	C2-C3-C4-C5
2	A	819	LFA	C17-C18-C19-C20
2	A	806	LFA	C7-C8-C9-C10
2	A	822	LFA	C9-C10-C11-C12
2	A	813	LFA	C2-C3-C4-C5
2	A	807	LFA	C3-C4-C5-C6
2	A	818	LFA	C14-C15-C16-C17
2	A	818	LFA	C15-C16-C17-C18
3	A	803	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	825	LFA	C17-C18-C19-C20
2	A	816	LFA	C1-C2-C3-C4
3	A	824	OLC	C3-C4-C5-C6
2	A	810	LFA	C2-C3-C4-C5
2	A	815	LFA	C2-C3-C4-C5
4	A	826	OLA	C2-C3-C4-C5
2	A	816	LFA	C5-C6-C7-C8
2	A	815	LFA	C1-C2-C3-C4
2	A	806	LFA	C4-C5-C6-C7
3	A	803	OLC	C12-C13-C14-C15
3	A	824	OLC	O20-C21-C22-C24
2	A	815	LFA	C7-C8-C9-C10
2	A	821	LFA	C14-C15-C16-C17
2	A	815	LFA	C6-C7-C8-C9
2	A	810	LFA	C11-C10-C9-C8
2	A	817	LFA	C6-C7-C8-C9
2	A	817	LFA	C3-C4-C5-C6
2	A	822	LFA	C7-C8-C9-C10
3	A	811	OLC	O23-C22-C24-O25
2	A	804	LFA	C5-C6-C7-C8
2	A	823	LFA	C1-C2-C3-C4
2	A	813	LFA	C4-C5-C6-C7
2	A	812	LFA	C13-C14-C15-C16
4	A	826	OLA	C11-C12-C13-C14
3	A	803	OLC	C4-C5-C6-C7
2	A	809	LFA	C2-C3-C4-C5
2	A	809	LFA	C1-C2-C3-C4
2	A	806	LFA	C2-C3-C4-C5
2	A	813	LFA	C1-C2-C3-C4
2	A	819	LFA	C15-C16-C17-C18
2	A	821	LFA	C17-C18-C19-C20
2	A	809	LFA	C3-C4-C5-C6
3	A	803	OLC	C5-C6-C7-C8
4	A	826	OLA	O2-C1-C2-C3
2	A	812	LFA	C12-C13-C14-C15
2	A	817	LFA	C11-C12-C13-C14
2	A	810	LFA	C4-C5-C6-C7
4	A	826	OLA	O1-C1-C2-C3
2	A	812	LFA	C15-C16-C17-C18
3	A	824	OLC	C2-C3-C4-C5
4	A	826	OLA	C7-C8-C9-C10
3	A	811	OLC	C7-C8-C9-C10

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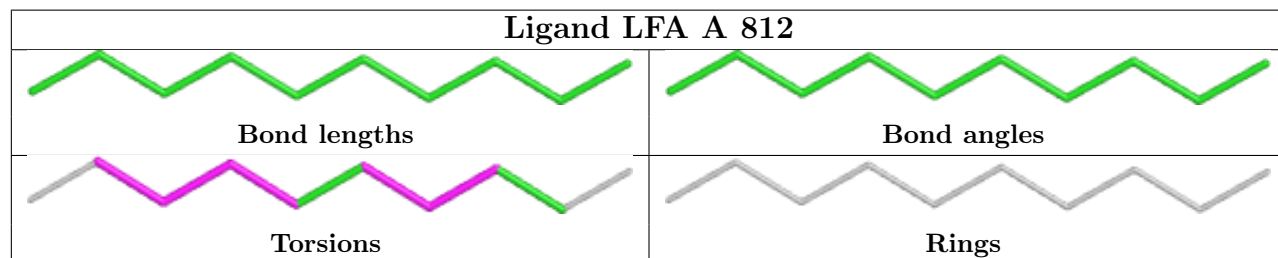
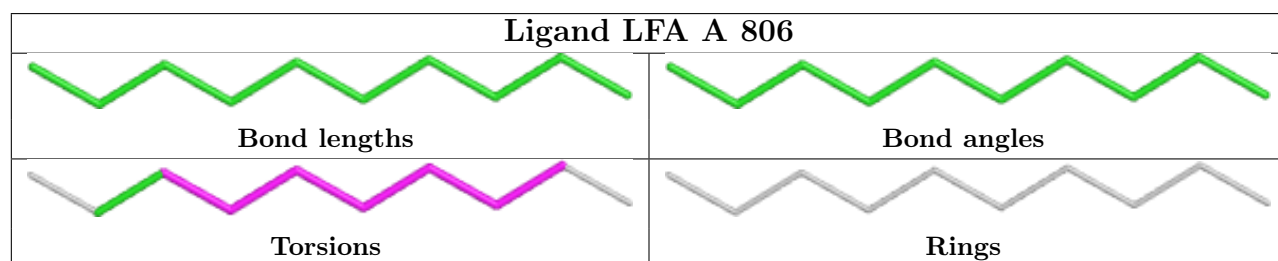
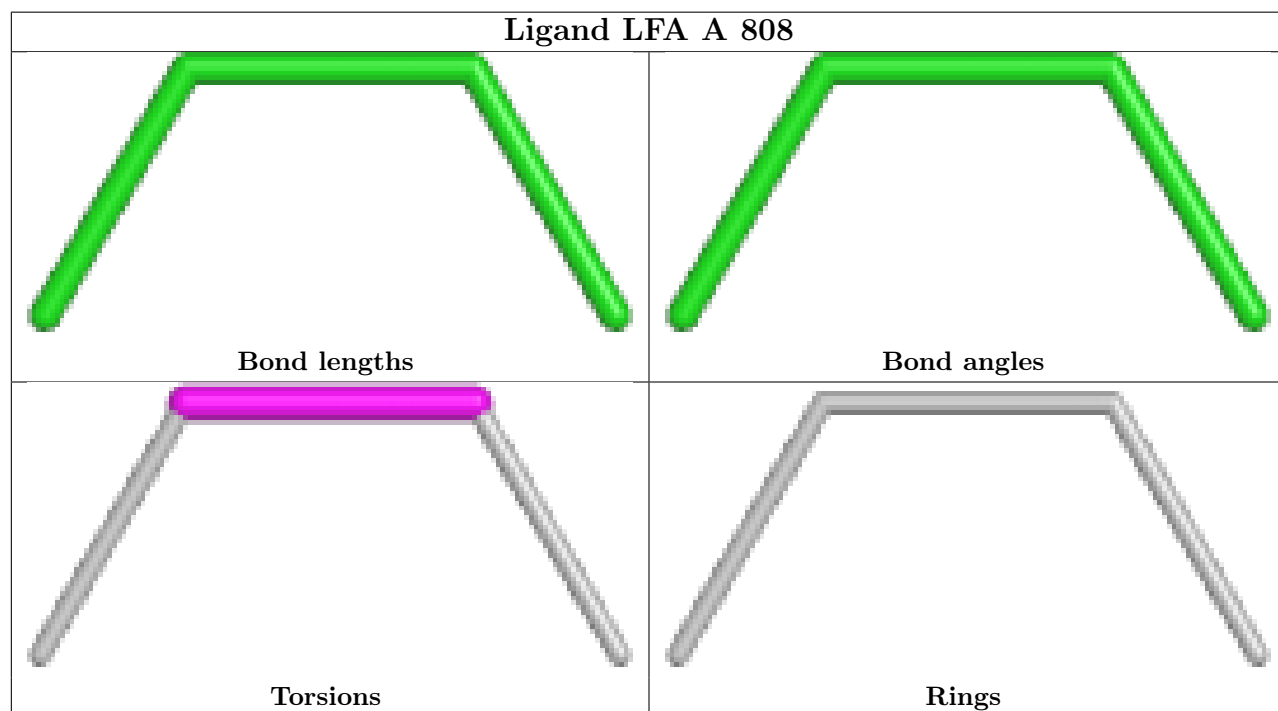
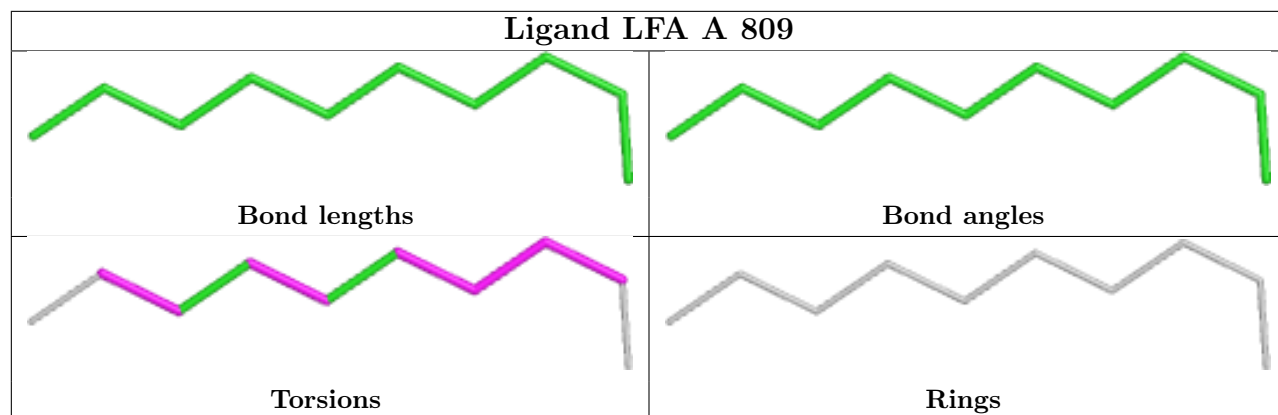
Mol	Chain	Res	Type	Atoms
2	A	807	LFA	C5-C6-C7-C8
3	A	803	OLC	C14-C15-C16-C17
2	A	817	LFA	C7-C8-C9-C10
2	A	809	LFA	C5-C6-C7-C8
2	A	806	LFA	C6-C7-C8-C9
2	A	812	LFA	C17-C18-C19-C20

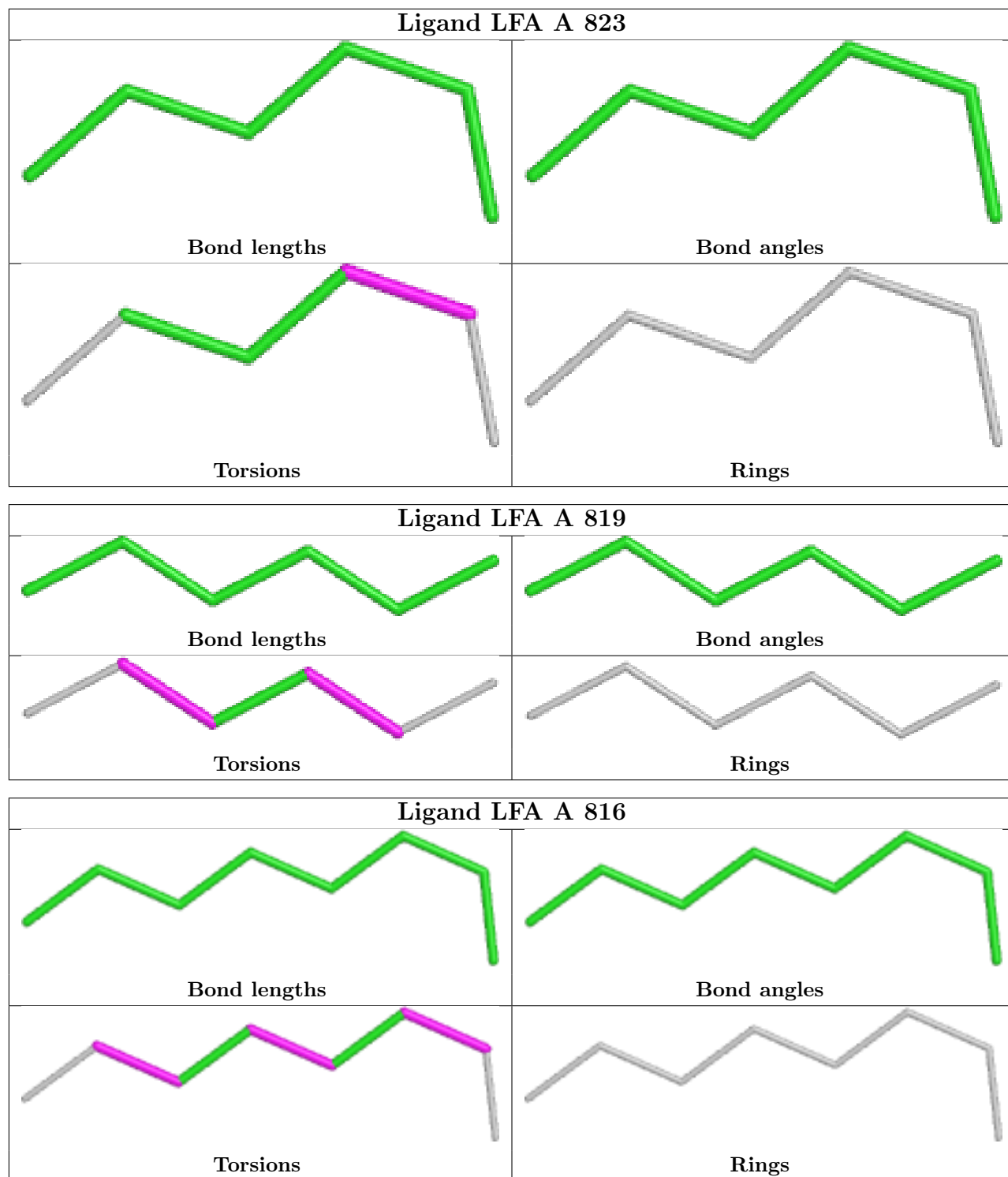
There are no ring outliers.

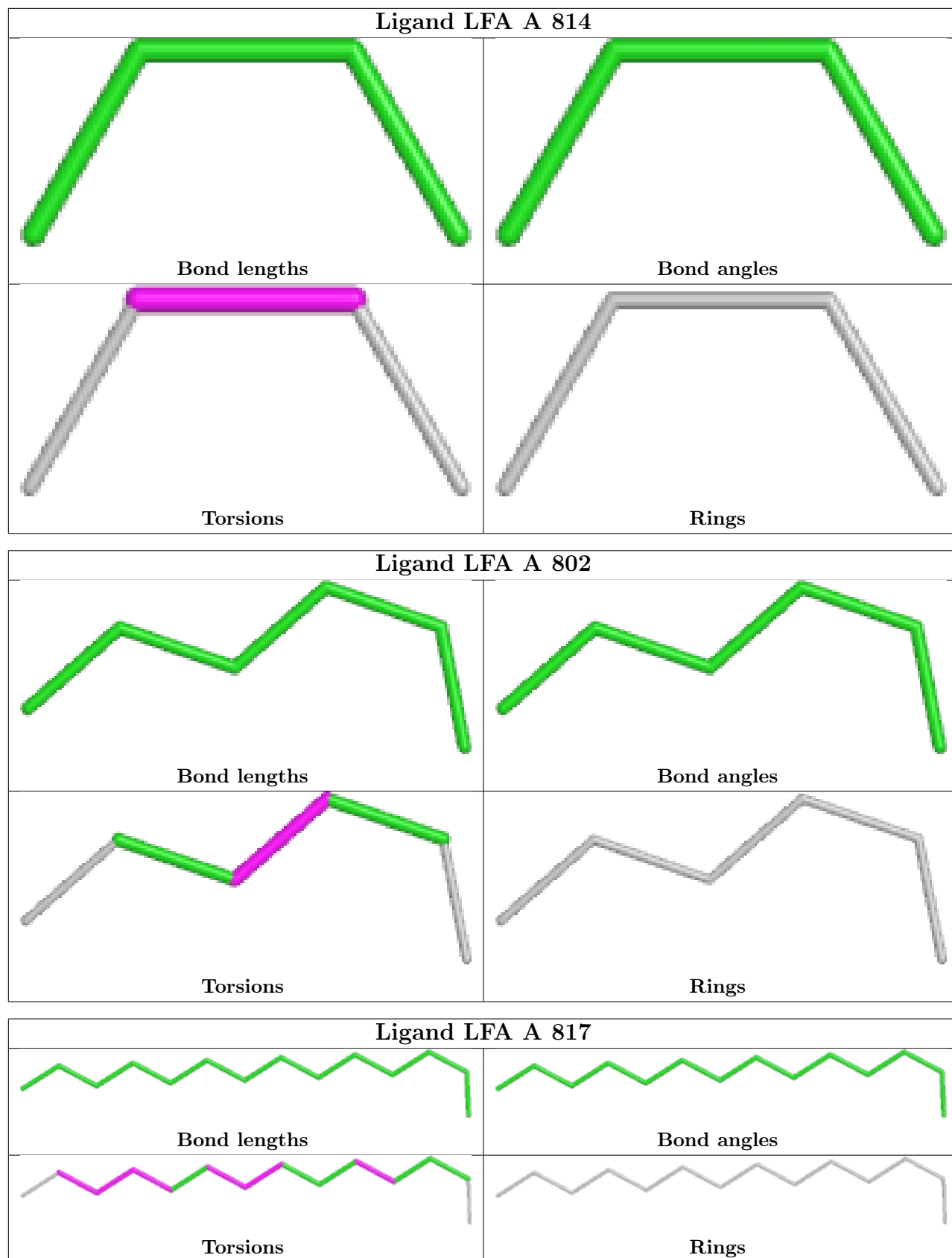
16 monomers are involved in 28 short contacts:

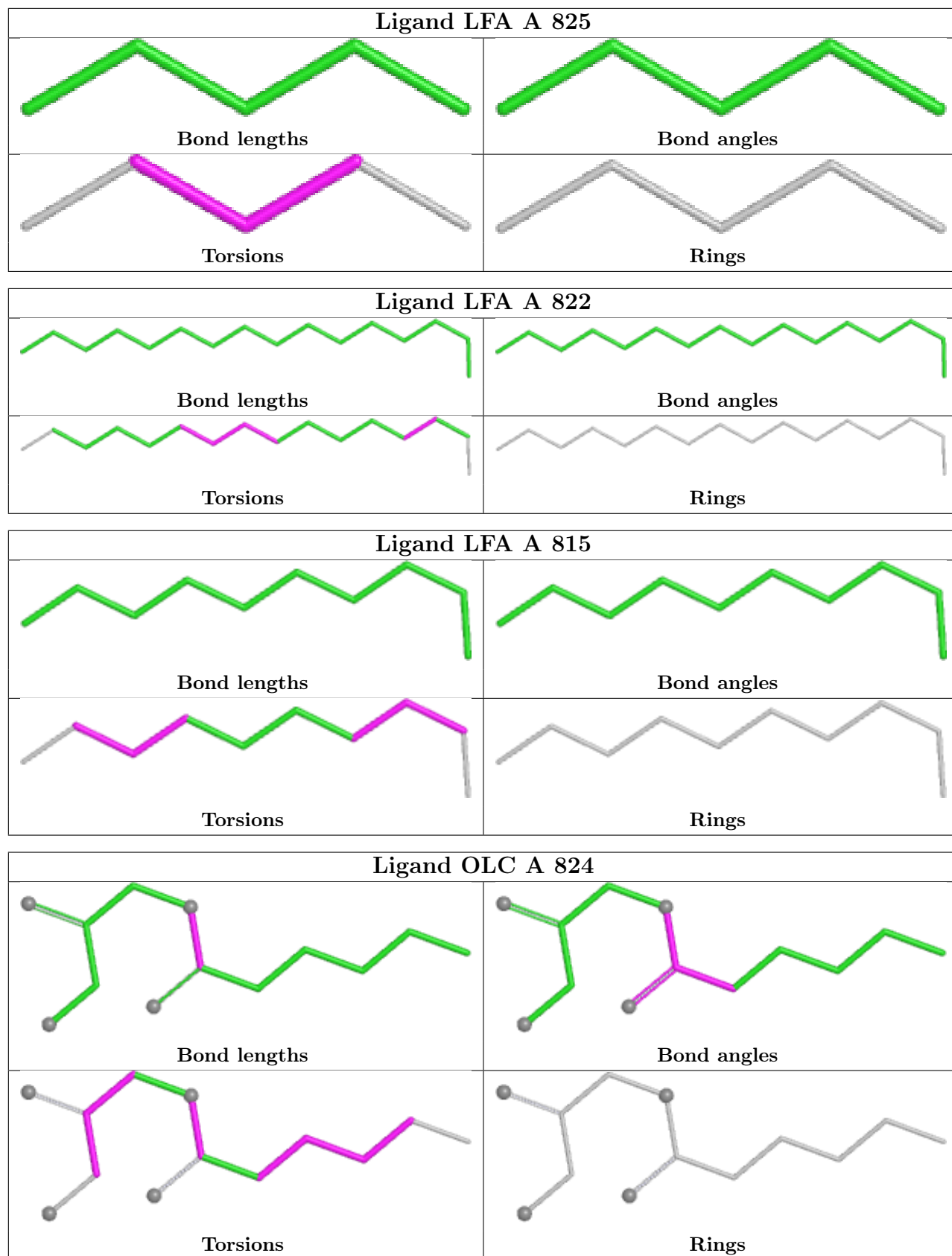
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	806	LFA	4	0
2	A	812	LFA	2	0
2	A	819	LFA	4	0
2	A	814	LFA	4	0
2	A	822	LFA	1	0
3	A	824	OLC	1	0
2	A	807	LFA	1	0
3	A	811	OLC	5	0
2	A	821	LFA	1	0
4	A	826	OLA	3	0
3	A	803	OLC	3	0
2	A	818	LFA	1	0
2	A	827	LFA	1	0
2	A	828	LFA	3	0
2	A	810	LFA	1	0
2	A	813	LFA	1	0

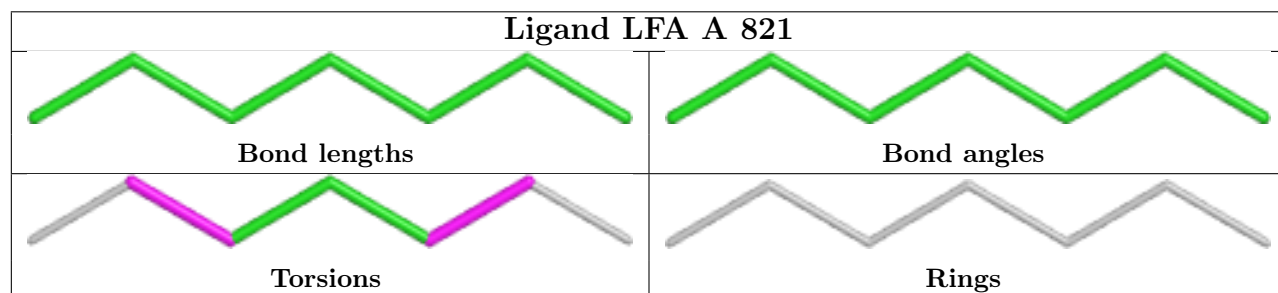
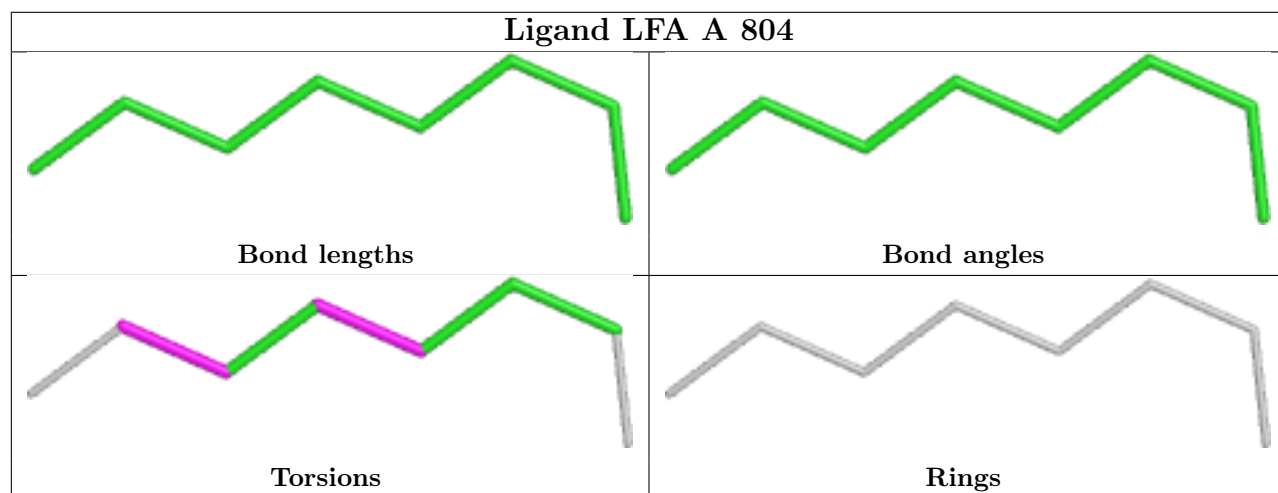
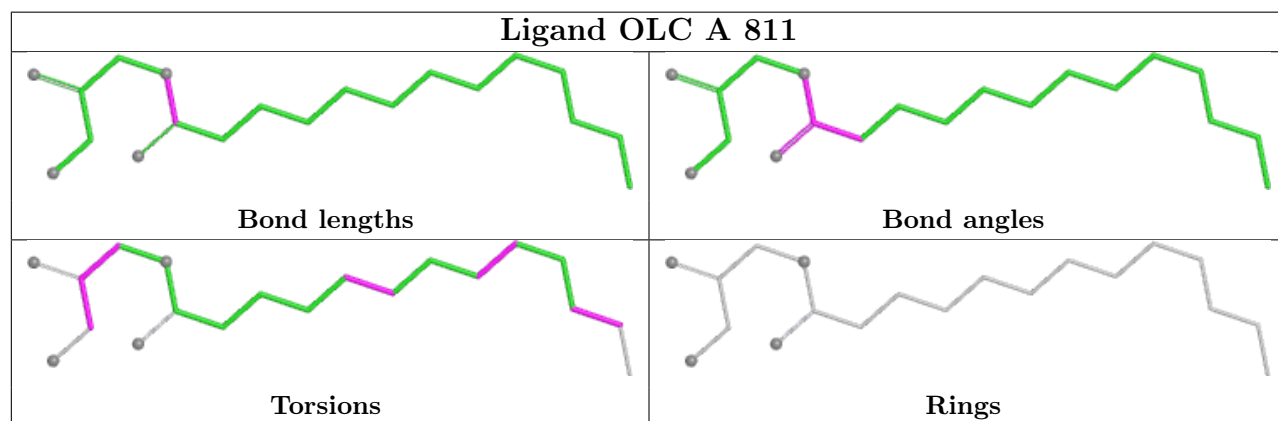
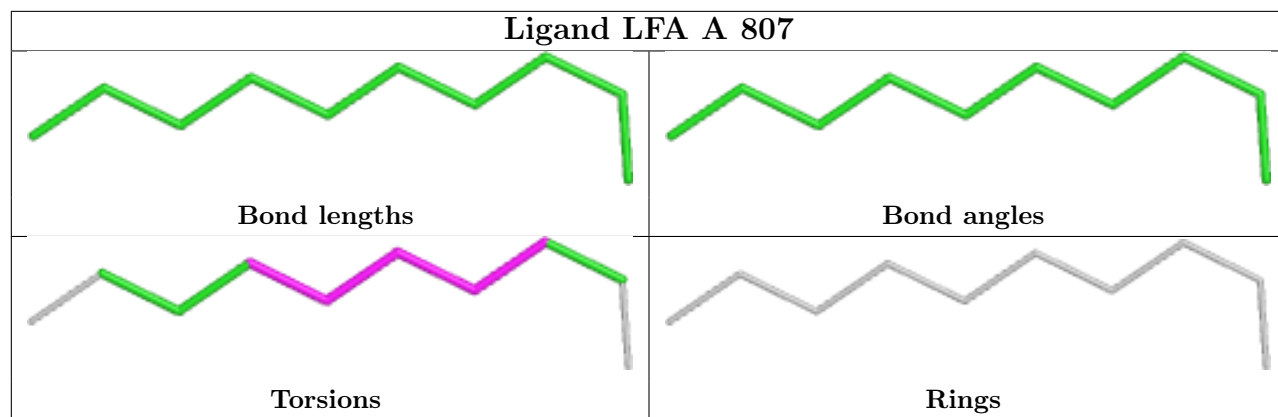
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

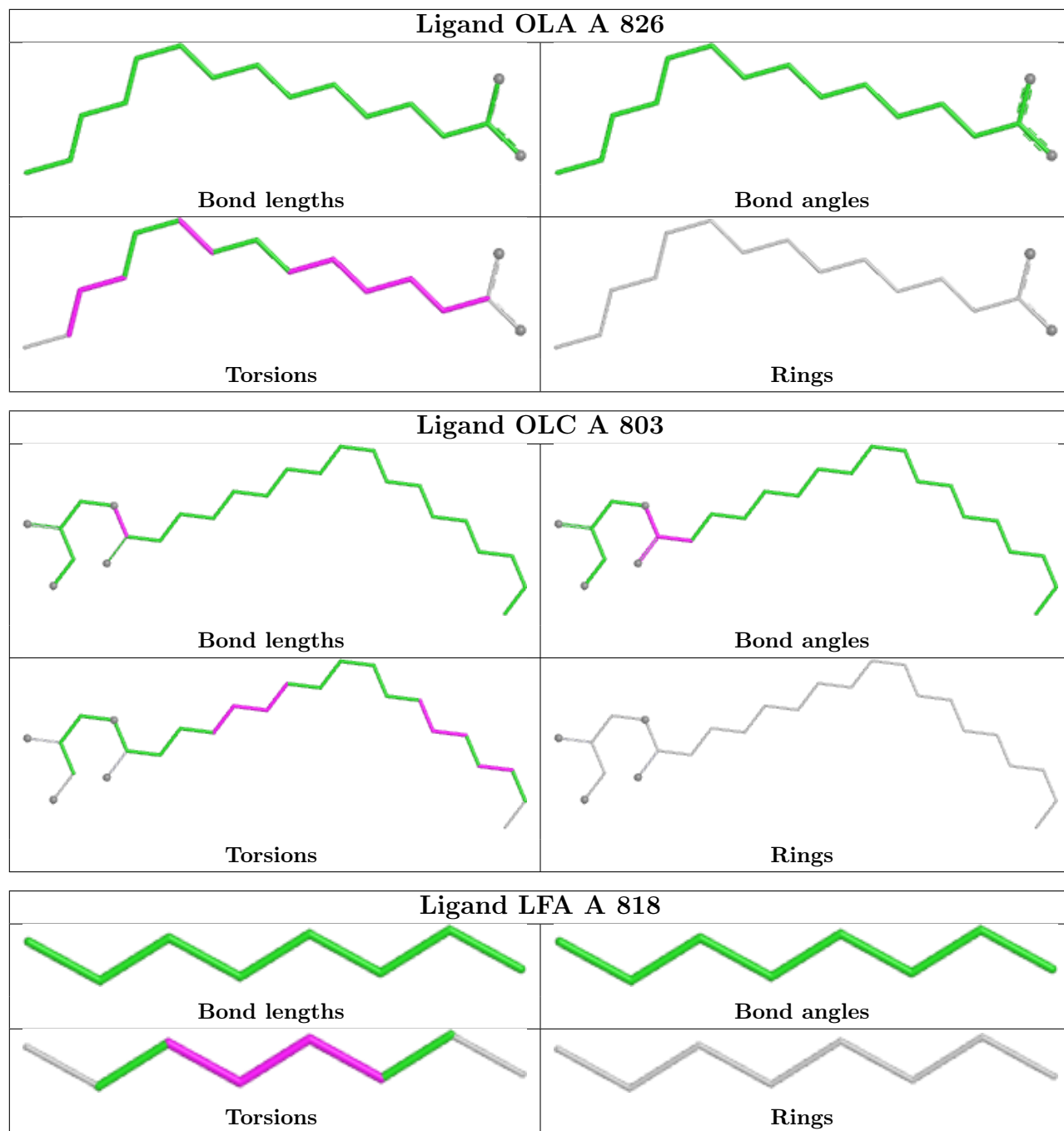


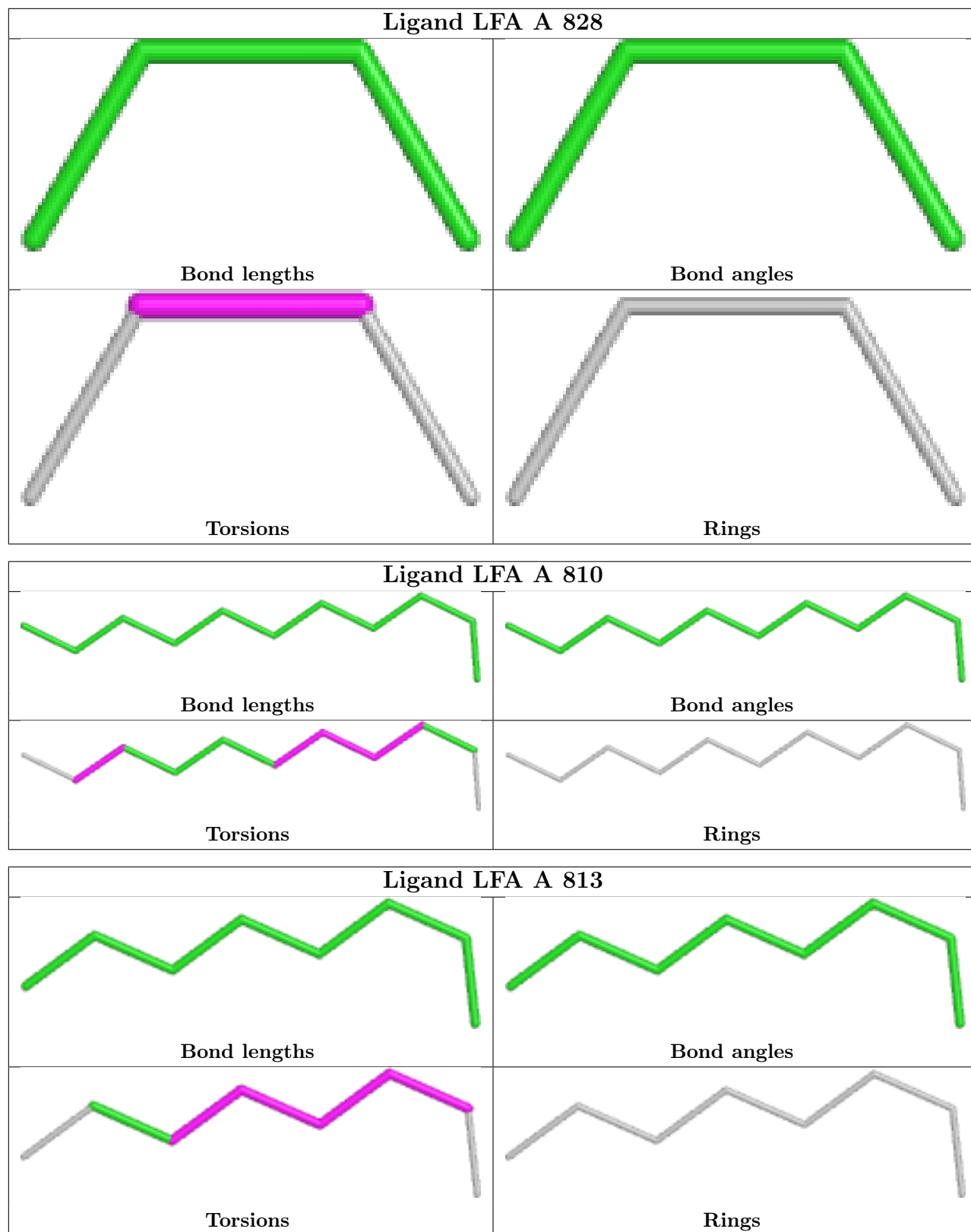












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	229/248 (92%)	-0.04	4 (1%) 69 77	11, 27, 59, 93	26 (11%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	THR	4.1
1	A	156	PHE	3.4
1	A	155	GLY	3.3
1	A	160	ALA	2.2

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	216[A]	29/30	0.96	0.05	19,24,29,30	68
1	LYR	A	216[D]	29/30	0.96	0.05	19,24,29,30	68

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,

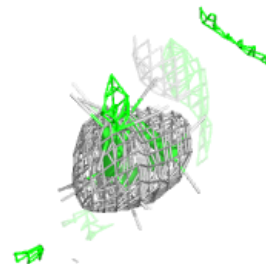
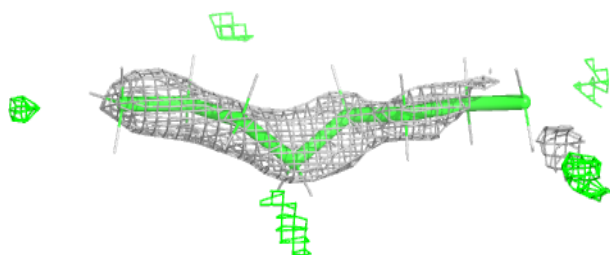
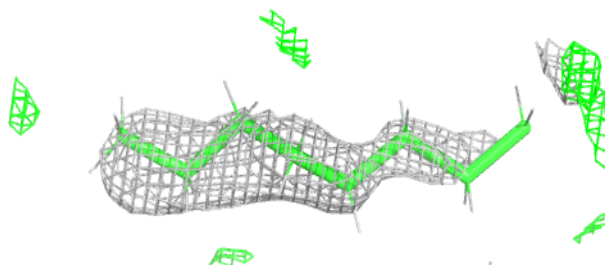
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LFA	A	813	8/20	0.71	0.12	58,70,72,72	0
2	LFA	A	816	8/20	0.73	0.14	61,74,81,81	0
2	LFA	A	828	4/20	0.74	0.13	58,70,71,71	0
2	LFA	A	817	14/20	0.76	0.11	67,82,83,83	0
2	LFA	A	806	10/20	0.76	0.15	53,64,66,66	0
3	OLC	A	811	20/25	0.80	0.12	54,66,78,79	0
2	LFA	A	808	4/20	0.81	0.10	55,66,66,66	0
3	OLC	A	824	13/25	0.81	0.10	58,59,77,77	0
2	LFA	A	814	4/20	0.82	0.11	54,65,66,66	0
2	LFA	A	815	10/20	0.83	0.14	65,79,84,84	0
2	LFA	A	804	8/20	0.83	0.12	52,63,70,70	0
2	LFA	A	821	7/20	0.84	0.08	47,48,50,50	0
2	LFA	A	822	16/20	0.84	0.11	48,59,65,65	0
2	LFA	A	827	2/20	0.84	0.20	45,45,45,45	0
2	LFA	A	812	10/20	0.85	0.12	47,48,49,49	0
2	LFA	A	825	5/20	0.86	0.11	48,48,50,50	0
4	OLA	A	826	16/20	0.86	0.11	49,61,69,72	0
2	LFA	A	807	10/20	0.87	0.11	47,59,70,71	0
2	LFA	A	805	6/20	0.87	0.13	50,60,62,62	0
2	LFA	A	823	6/20	0.87	0.11	49,60,64,64	0
2	LFA	A	809	10/20	0.88	0.11	46,56,61,61	0
2	LFA	A	819	6/20	0.89	0.11	48,49,49,49	0
2	LFA	A	818	8/20	0.89	0.12	51,52,53,53	0
3	OLC	A	803	25/25	0.90	0.09	40,49,60,62	0
2	LFA	A	801	7/20	0.90	0.09	44,44,45,45	0
2	LFA	A	802	6/20	0.90	0.07	46,55,58,58	0
2	LFA	A	820	3/20	0.90	0.10	44,44,44,44	0
2	LFA	A	810	11/20	0.92	0.08	45,55,58,58	0

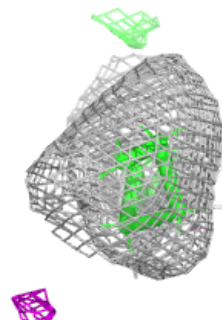
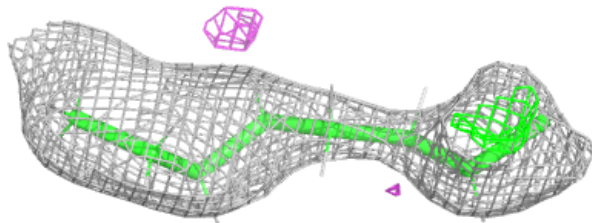
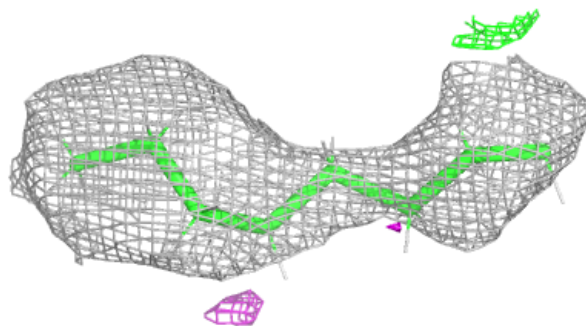
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA A 813:

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

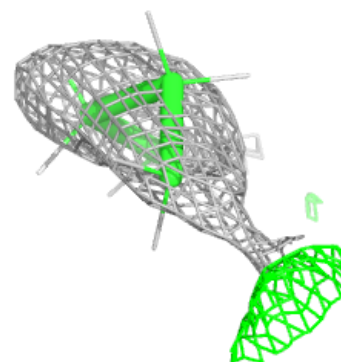
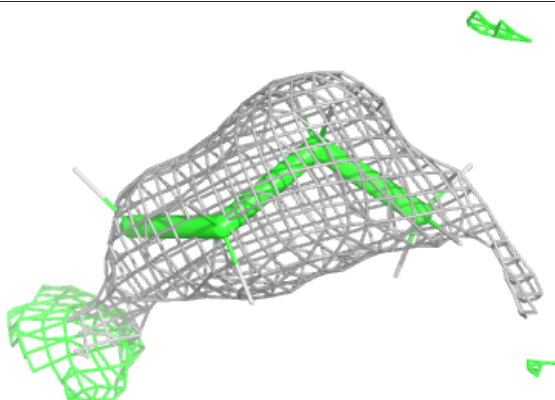
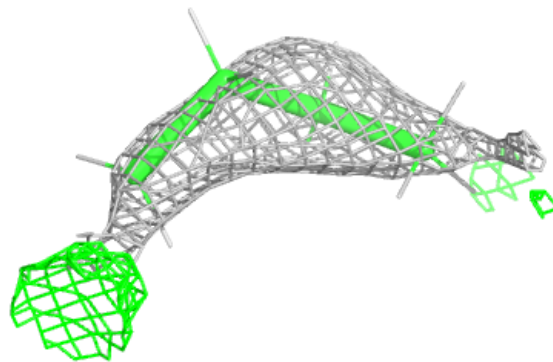
**Electron density around LFA A 816:**

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

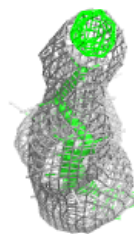
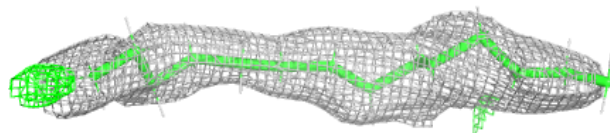
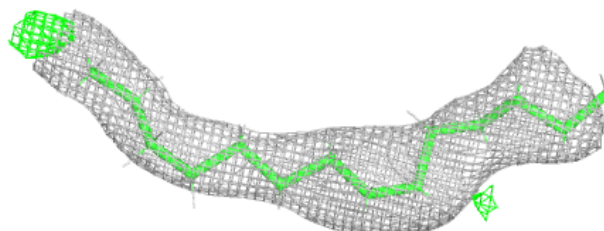


Electron density around LFA A 828:

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

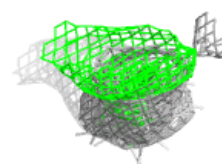
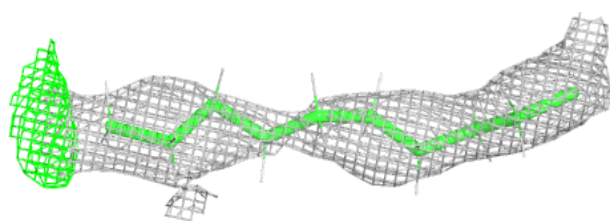
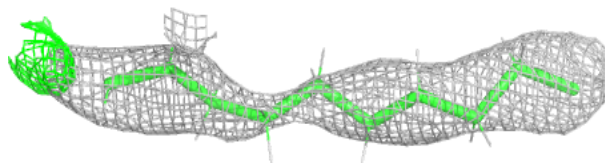
**Electron density around LFA A 817:**

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

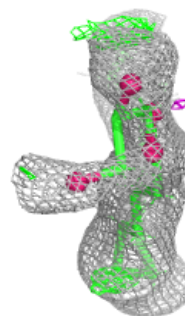
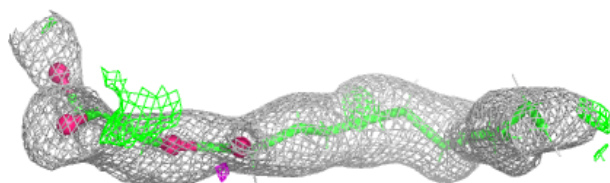
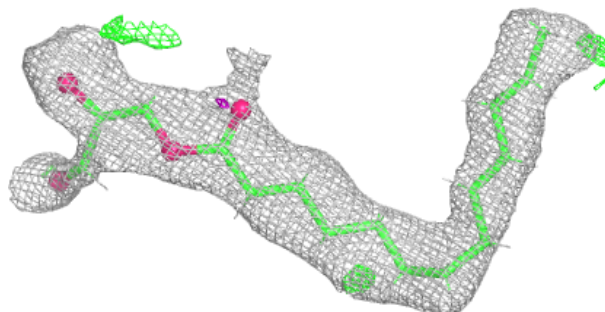


Electron density around LFA A 806:

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

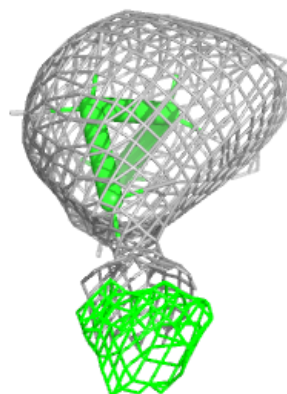
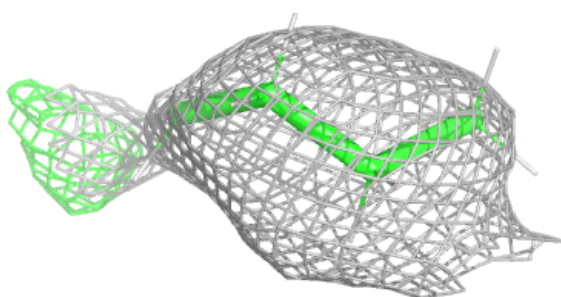
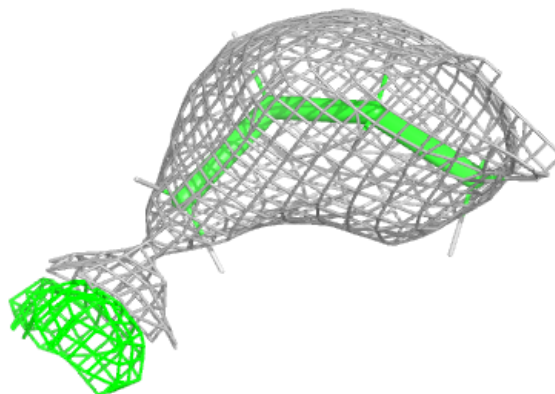
**Electron density around OLC A 811:**

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

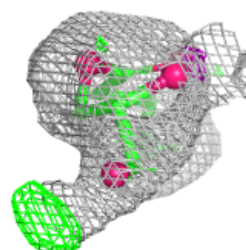
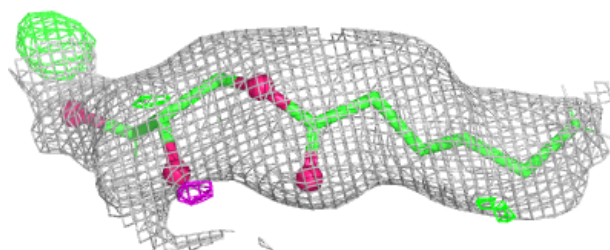
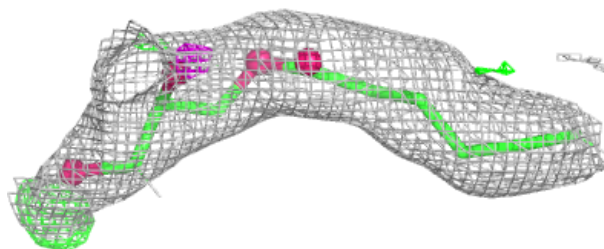


Electron density around LFA A 808:

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

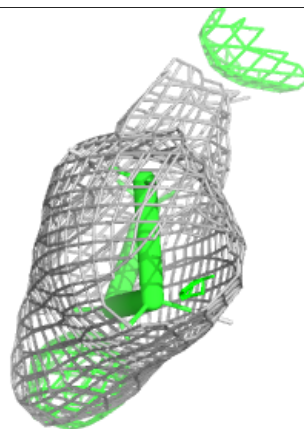
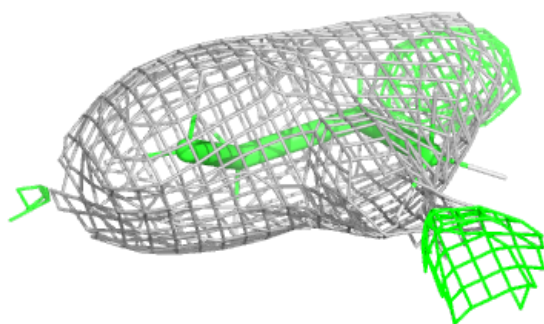
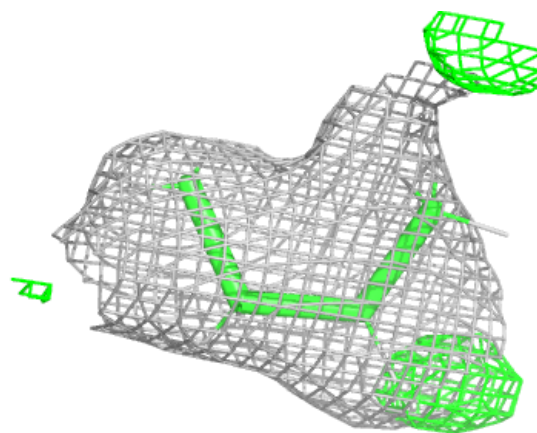
**Electron density around OLC A 824:**

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

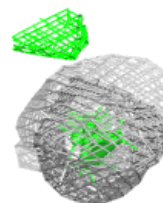
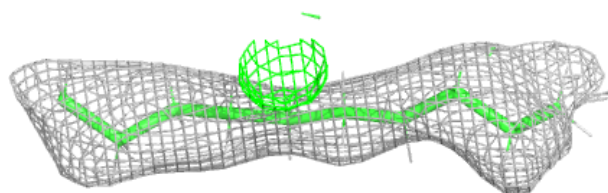
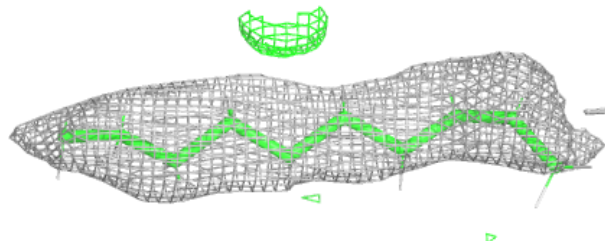


Electron density around LFA A 814:

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

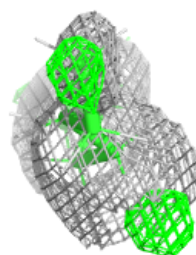
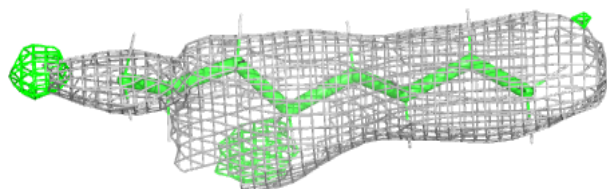
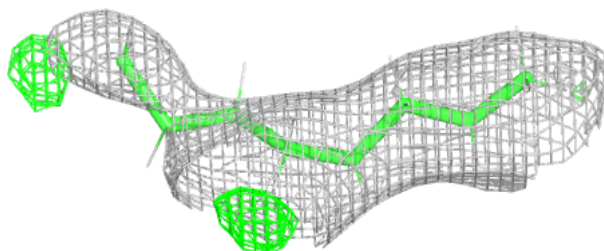
**Electron density around LFA A 815:**

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

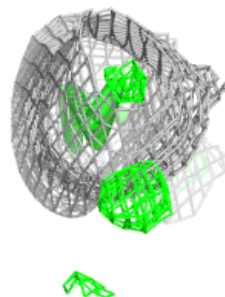
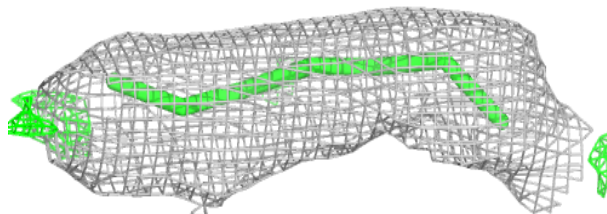
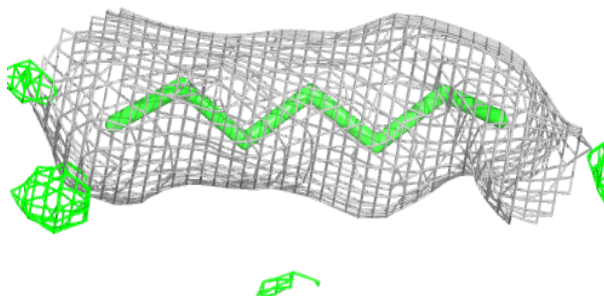


Electron density around LFA A 804:

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

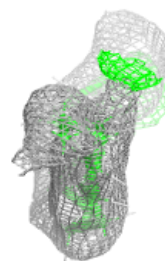
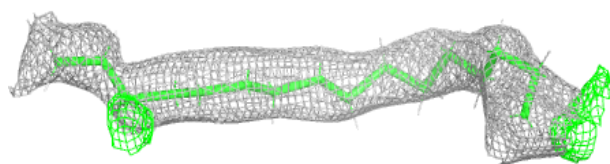
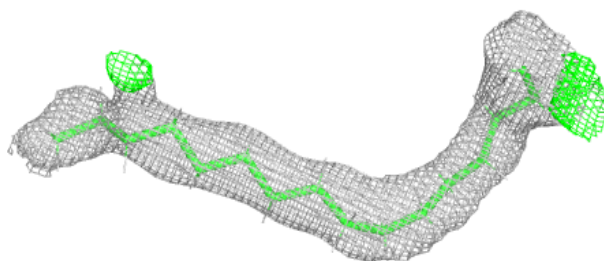
**Electron density around LFA A 821:**

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

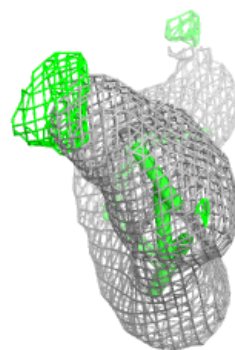
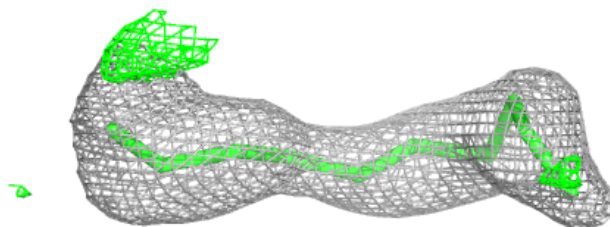
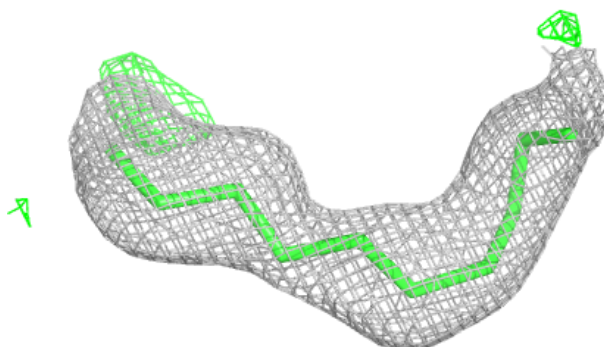


Electron density around LFA A 822:

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

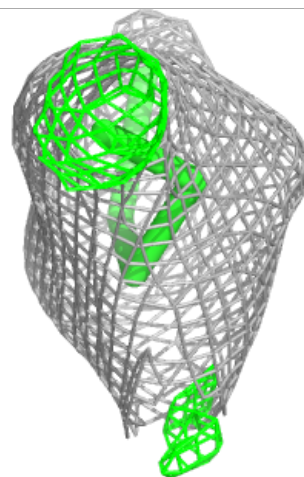
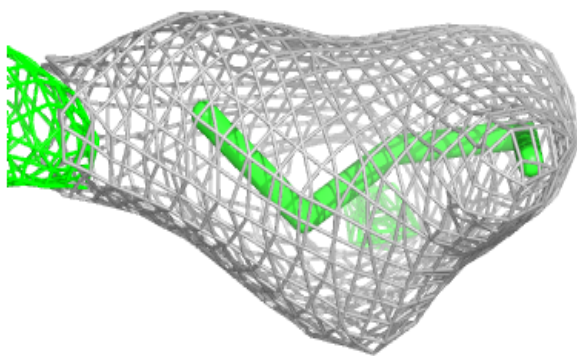
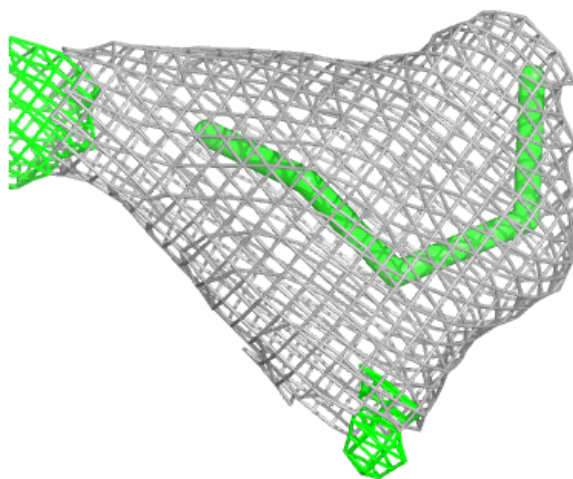
**Electron density around LFA A 812:**

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



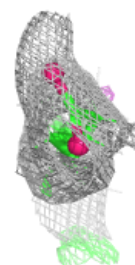
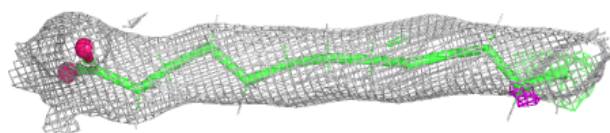
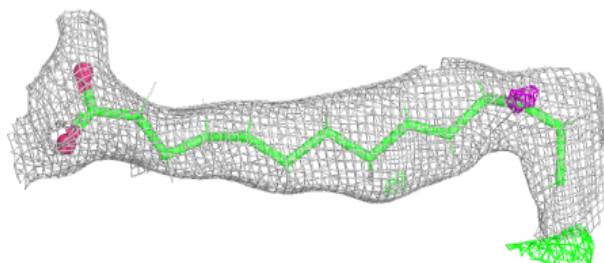
Electron density around LFA A 825:

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

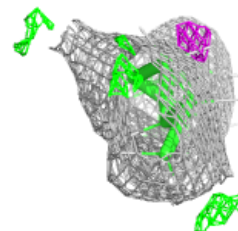
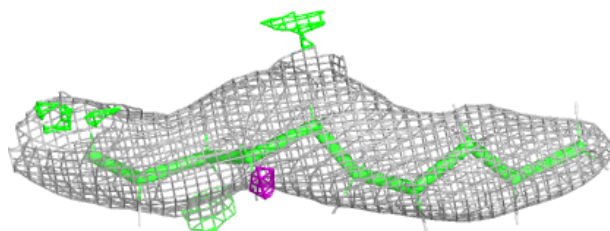
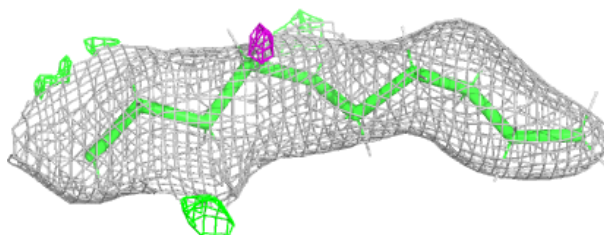


Electron density around OLA A 826:

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

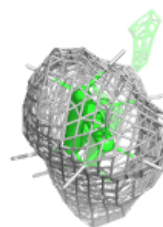
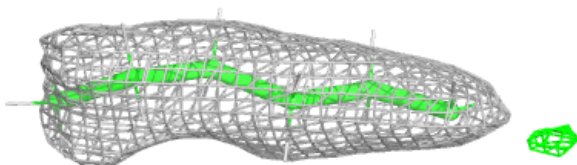
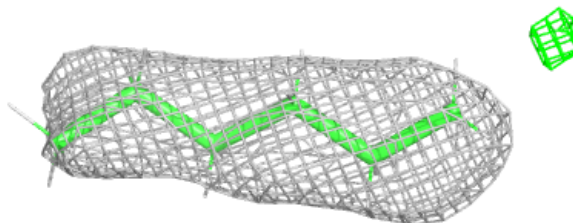
**Electron density around LFA A 807:**

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

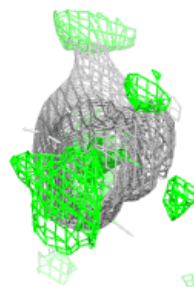
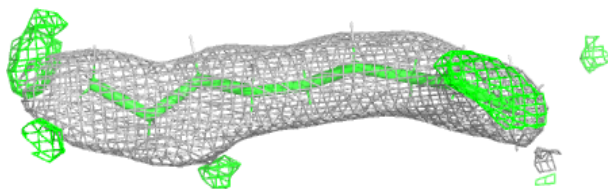
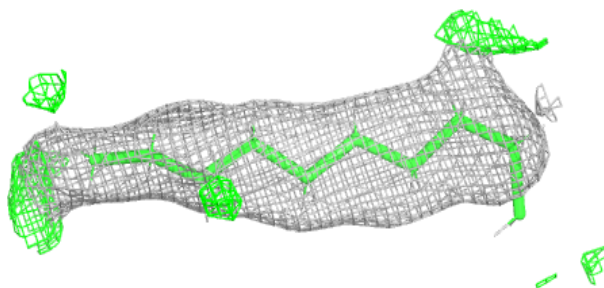


Electron density around LFA A 823:

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

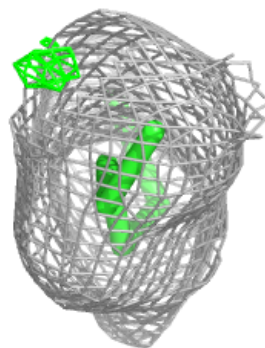
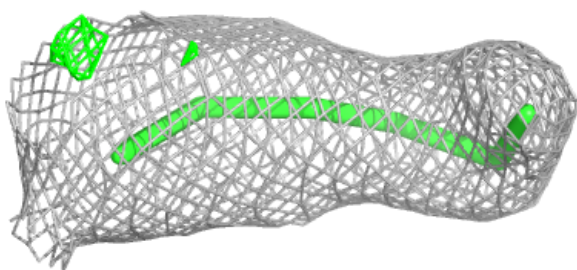
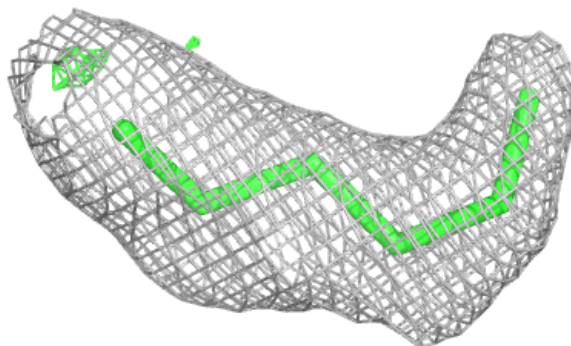
**Electron density around LFA A 809:**

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

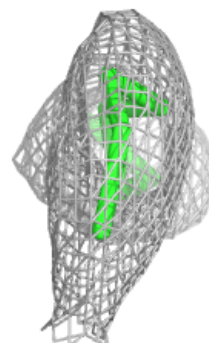
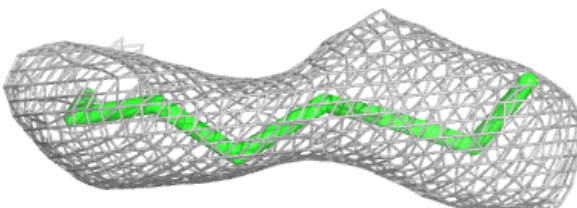
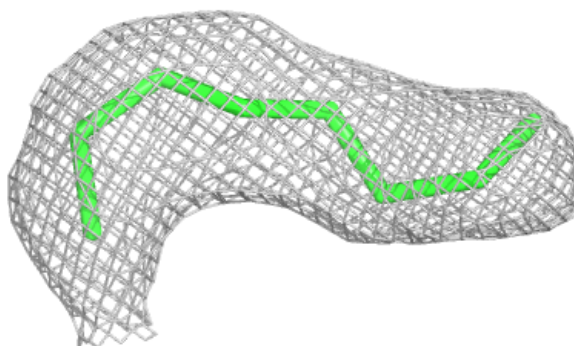


Electron density around LFA A 819:

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

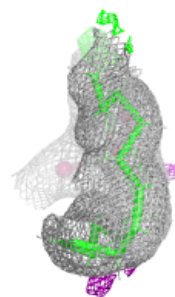
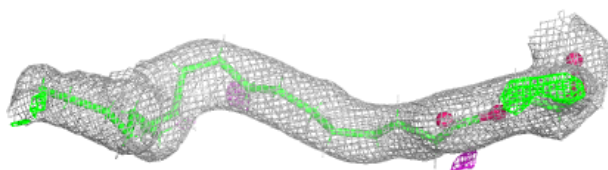
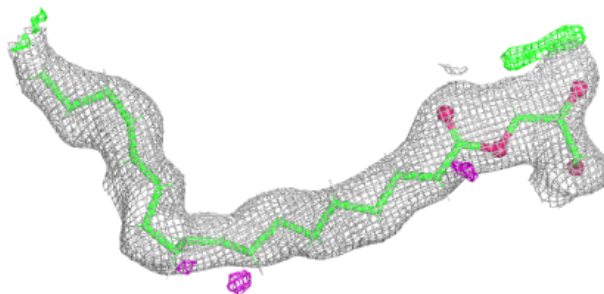
**Electron density around LFA A 818:**

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

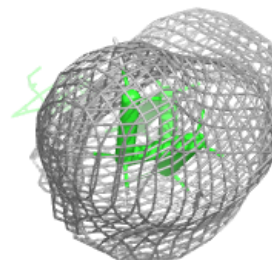
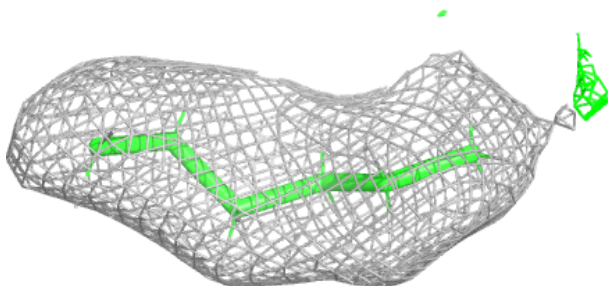
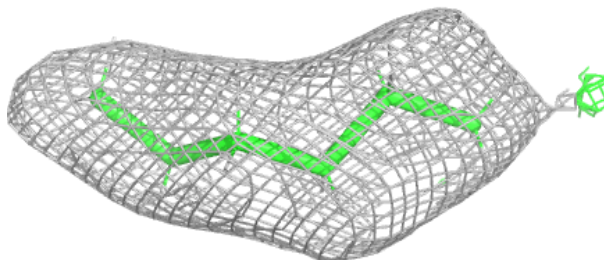


Electron density around OLC A 803:

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

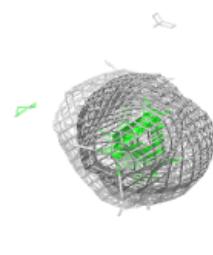
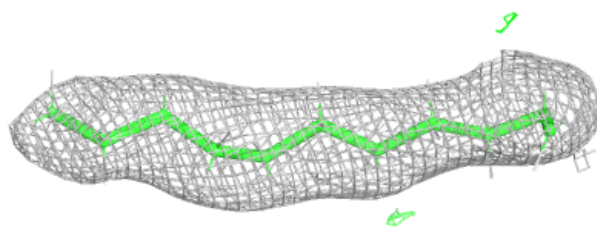
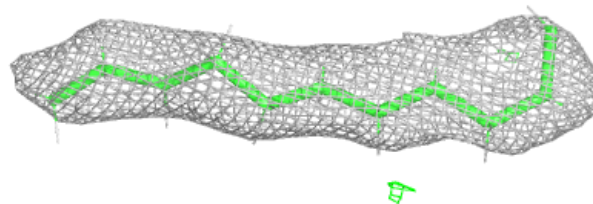
**Electron density around LFA A 802:**

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



Electron density around LFA A 810:

$2mF_o-DF_c$ (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.