



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:52 AM UTC

PDB ID : 7ZNH / pdb_00007znh
Title : Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the activated state at pH 8.2 at room temperature, 250-750-mks-snapshot
Authors : Kovalev, K.; Tsybrov, F.; Alekseev, A.; Bourenkov, G.; Gordeliy, V.
Deposited on : 2022-04-20
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

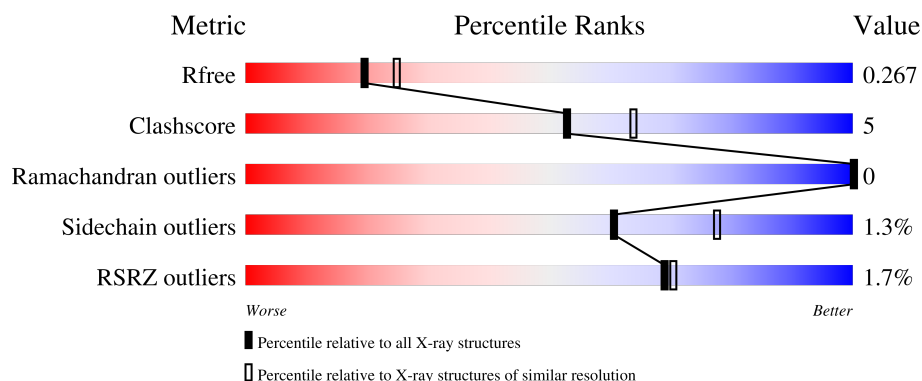
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	229	0% 87% 10% .
1	B	229	0% 86% 10% .
1	C	229	2% 89% 7% ..

2 Entry composition [i](#)

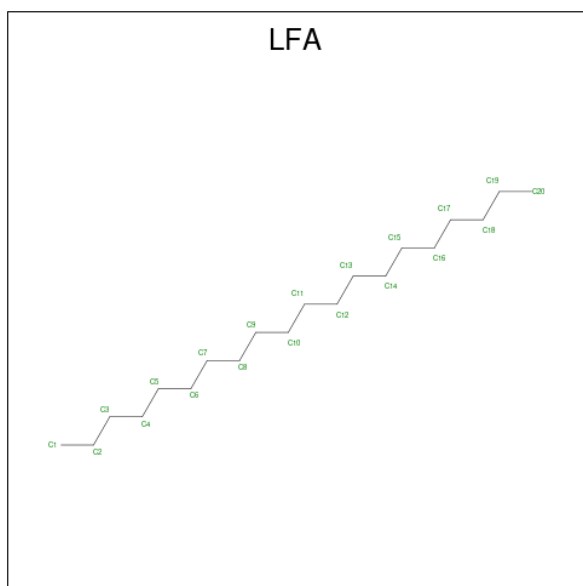
There are 5 unique types of molecules in this entry. The entry contains 6123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 xenorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	8	0
			1835	1260	271	298	6			
1	B	221	Total	C	N	O	S	0	9	0
			1829	1254	273	297	5			
1	C	223	Total	C	N	O	S	0	8	0
			1839	1262	273	298	6			

- 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	0	0
			13	13		
2	A	1	Total	C	0	0
			11	11		

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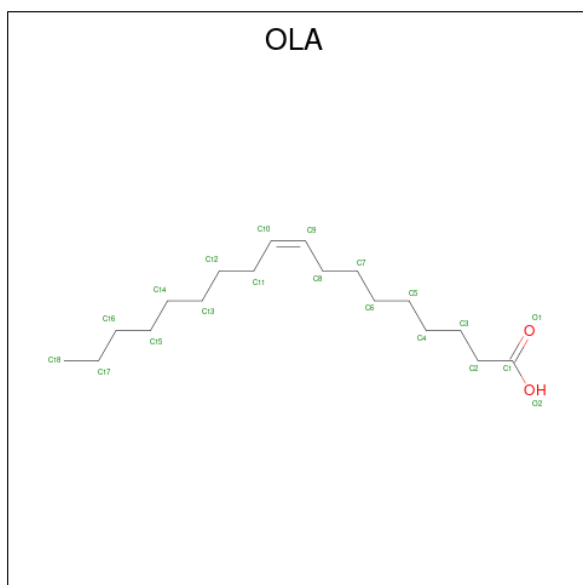
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 15 15	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 6 6	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 15 15	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 9 9	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 5 5	0	0
2	B	1	Total C 14 14	0	0
2	C	1	Total C 17 17	0	0

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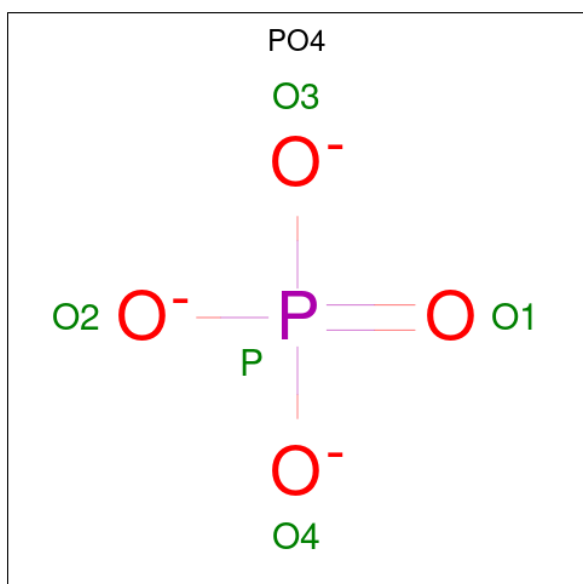
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 9 9	0	0
2	C	1	Total C 13 13	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 17 17	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C 4 4	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0

- 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 11 9 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 16 14 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 19 17 2	0	0
3	B	1	Total C O 20 18 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 16 14 2	0	0
3	B	1	Total C O 11 9 2	0	0
3	C	1	Total C O 20 18 2	0	0
3	C	1	Total C O 16 14 2	0	0
3	C	1	Total C O 14 12 2	0	0
3	C	1	Total C O 16 14 2	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

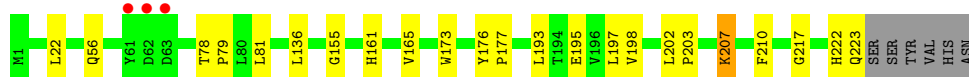
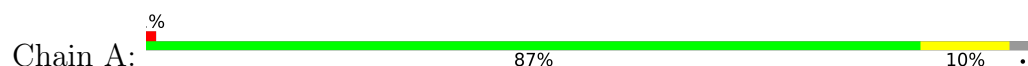
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	1
			28	28		
5	B	21	Total	O	0	1
			22	22		
5	C	24	Total	O	0	1
			25	25		

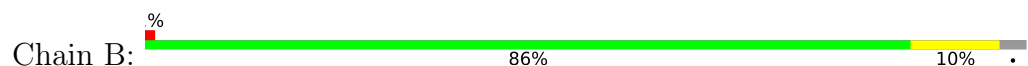
3 Residue-property plots [i](#)

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.

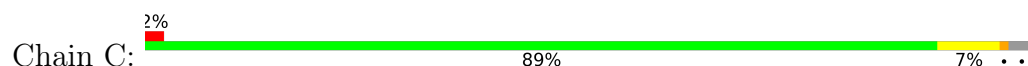
- Molecule 1: xenorhodopsin



- Molecule 1: xenorhodopsin



- Molecule 1: xenorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.91Å 111.86Å 119.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.30) 82.6 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.31 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.220 , 0.248 0.232 , 0.267	Depositor DCC
R_{free} test set	2154 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 86.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6123	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FME, LFA, LYR, PO4, OLA

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	1.01	0/1814	1.45	1/2479 (0.0%)
1	B	1.01	0/1810	1.43	1/2471 (0.0%)
1	C	1.00	0/1819	1.45	1/2487 (0.0%)
All	All	1.00	0/5443	1.45	3/7437 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	GLY	CA-C-O	-6.35	118.09	122.22
1	C	155	GLY	CA-C-O	-5.74	118.49	122.22
1	A	155	GLY	CA-C-O	-5.03	118.95	122.22

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	1835	0	1909	23	0
1	B	1829	0	1904	22	0
1	C	1839	0	1914	18	0
2	A	96	0	176	2	0
2	B	124	0	229	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	116	0	214	1	0
3	A	77	0	111	1	0
3	B	61	0	87	3	0
3	C	66	0	95	0	0
4	C	5	0	0	0	0
5	A	28	0	0	1	0
5	B	22	0	0	1	0
5	C	25	0	0	1	0
All	All	6123	0	6639	64	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 5.

All (64) 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:B:81[C]:LEU:HD21	5:B:406:HOH:O	1.66	0.95
1:C:81[C]:LEU:HD21	5:C:423:HOH:O	1.70	0.89
1:A:222:HIS:C	1:A:223:GLN:N	2.33	0.87
1:A:81[C]:LEU:HD21	5:A:918:HOH:O	1.75	0.85
2:C:311:LFA:C12	2:C:313:LFA:H131	2.23	0.69
1:C:207[C]:LYR:H9	1:C:207[C]:LYR:H192	1.80	0.63
1:B:207[C]:LYR:H192	1:B:207[C]:LYR:H9	1.80	0.62
1:C:207[C]:LYR:H9	1:C:207[C]:LYR:H183	1.81	0.62
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.35	0.62
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.36	0.61
1:A:207[C]:LYR:H192	1:A:207[C]:LYR:H9	1.83	0.61
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.35	0.60
1:C:207[C]:LYR:H192	1:C:207[C]:LYR:C9	2.32	0.59
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.85	0.59
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.85	0.58
1:C:207[A]:LYR:H9	1:C:207[A]:LYR:H183	1.84	0.58
1:B:207[C]:LYR:H192	1:B:207[C]:LYR:C9	2.32	0.57
1:A:207[C]:LYR:H192	1:A:207[C]:LYR:C9	2.34	0.57
1:A:207[C]:LYR:H9	1:A:207[C]:LYR:H183	1.87	0.57
1:B:207[C]:LYR:H9	1:B:207[C]:LYR:H183	1.87	0.57
1:A:136[C]:LEU:C	1:A:136[C]:LEU:HD23	2.29	0.56
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.87	0.56
1:B:198:VAL:HG22	2:B:313:LFA:H81	1.87	0.56
1:B:207[A]:LYR:H183	1:B:207[A]:LYR:H9	1.88	0.56
1:A:165:VAL:HG13	1:A:210:PHE:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136[C]:LEU:C	1:C:136[C]:LEU:HD23	2.31	0.55
1:A:207[A]:LYR:H183	1:A:207[A]:LYR:H9	1.88	0.55
1:B:136[C]:LEU:C	1:B:136[C]:LEU:HD23	2.33	0.53
1:A:56:GLN:HB3	3:A:804:OLA:H52	1.90	0.52
1:B:207[A]:LYR:H192	1:B:207[A]:LYR:C9	2.41	0.51
1:B:207[A]:LYR:H9	1:B:207[A]:LYR:H192	1.92	0.51
1:C:207[A]:LYR:H192	1:C:207[A]:LYR:C9	2.41	0.50
1:A:207[A]:LYR:H9	1:A:207[A]:LYR:H192	1.93	0.50
1:A:207[A]:LYR:H192	1:A:207[A]:LYR:C9	2.41	0.50
1:C:207[A]:LYR:H9	1:C:207[A]:LYR:H192	1.94	0.50
1:A:198:VAL:HG21	2:A:810:LFA:H161	1.94	0.49
1:B:97:LEU:HB2	3:B:301:OLA:H32	1.97	0.46
1:B:194:THR:HG21	3:B:308:OLA:C2	2.46	0.46
1:B:194:THR:HG21	3:B:308:OLA:H22	1.98	0.45
1:A:78:THR:N	1:A:79:PRO:HD2	2.33	0.44
1:B:21:TYR:CZ	1:B:25:LYS:HE2	2.53	0.44
1:A:195:GLU:HB2	2:A:810:LFA:C18	2.48	0.43
1:B:78:THR:N	1:B:79:PRO:HD2	2.34	0.43
1:C:81[C]:LEU:HD23	1:C:173[C]:TRP:HZ3	1.83	0.43
1:A:81[C]:LEU:CD1	1:A:210:PHE:CD2	3.03	0.42
1:C:78:THR:N	1:C:79:PRO:HD2	2.34	0.42
1:A:165:VAL:CG1	1:A:210:PHE:CE1	3.02	0.42
1:B:176:TYR:N	1:B:177:PRO:HD2	2.35	0.42
1:B:81[C]:LEU:HD23	1:B:173[C]:TRP:HZ3	1.83	0.42
1:A:81[C]:LEU:HD11	1:A:210:PHE:CD2	2.55	0.42
1:C:207[C]:LYR:H6	1:C:207[C]:LYR:H41	1.78	0.42
1:A:81[C]:LEU:HD23	1:A:173[C]:TRP:HZ3	1.85	0.41
1:B:81[C]:LEU:CD1	1:B:210:PHE:CD2	3.02	0.41
1:C:81[C]:LEU:HD11	1:C:210:PHE:CD2	2.55	0.41
1:A:176:TYR:N	1:A:177:PRO:HD2	2.35	0.41
1:A:207[C]:LYR:H10	1:A:207[C]:LYR:H81	1.87	0.41
1:B:207[C]:LYR:H41	1:B:207[C]:LYR:H6	1.77	0.41
1:C:193:LEU:O	1:C:197:LEU:HD23	2.20	0.41
1:C:207[C]:LYR:H10	1:C:207[C]:LYR:H81	1.76	0.41
1:B:81[C]:LEU:HD11	1:B:210:PHE:CD2	2.55	0.41
1:B:193:LEU:O	1:B:197:LEU:HD23	2.21	0.41
1:C:176:TYR:N	1:C:177:PRO:HD2	2.36	0.41
1:A:193:LEU:O	1:A:197:LEU:HD23	2.20	0.40
1:C:207[C]:LYR:H183	1:C:207[C]:LYR:C9	2.49	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	226/229 (99%)	222 (98%)	4 (2%)	0	100	100
1	B	224/229 (98%)	223 (100%)	1 (0%)	0	100	100
1	C	227/229 (99%)	225 (99%)	2 (1%)	0	100	100
All	All	677/687 (98%)	670 (99%)	7 (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	182/189 (96%)	181 (100%)	1 (0%)	81	90
1	B	182/189 (96%)	180 (99%)	2 (1%)	65	81
1	C	182/189 (96%)	178 (98%)	4 (2%)	45	65
All	All	546/567 (96%)	539 (99%)	7 (1%)	61	77

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

Mol	Chain	Res	Type
1	A	22	LEU
1	B	22	LEU
1	B	121	ILE
1	C	18	LEU
1	C	22	LEU

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Mol	Chain	Res	Type
1	C	152	LEU
1	C	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	154	ASN
1	A	161	HIS
1	A	191	GLN
1	A	222	HIS
1	B	60	GLN
1	B	154	ASN
1	B	191	GLN
1	B	222	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	207[C]	1	27,29,30	1.07	2 (7%)	30,37,39	1.35	5 (16%)
1	FME	A	1	1	8,9,10	0.36	0	8,9,11	0.79	0
1	LYR	B	207[C]	1	27,29,30	1.06	2 (7%)	30,37,39	1.28	4 (13%)
1	LYR	C	207[A]	1	27,29,30	1.22	3 (11%)	30,37,39	1.09	3 (10%)
1	FME	B	1	1	5,6,10	0.71	0	4,6,11	1.07	0
1	LYR	C	207[C]	1	27,29,30	1.12	2 (7%)	30,37,39	1.30	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LYR	A	207[A]	1	27,29,30	1.12	3 (11%)	30,37,39	1.13	4 (13%)
1	FME	C	1	1	8,9,10	0.52	0	8,9,11	0.65	0
1	LYR	B	207[A]	1	27,29,30	1.11	3 (11%)	30,37,39	1.03	2 (6%)

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	207[C]	1	-	5/22/40/42	0/1/1/1
1	FME	A	1	1	-	1/7/9/11	-
1	LYR	B	207[C]	1	-	5/22/40/42	0/1/1/1
1	LYR	C	207[A]	1	-	2/22/40/42	0/1/1/1
1	FME	B	1	1	-	0/3/5/11	-
1	LYR	C	207[C]	1	-	5/22/40/42	0/1/1/1
1	LYR	A	207[A]	1	-	2/22/40/42	0/1/1/1
1	FME	C	1	1	-	2/7/9/11	-
1	LYR	B	207[A]	1	-	2/22/40/42	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207[A]	LYR	C9-C80	-2.91	1.39	1.46
1	A	207[C]	LYR	C9-C80	-2.74	1.40	1.46
1	C	207[C]	LYR	C9-C80	-2.70	1.40	1.46
1	B	207[A]	LYR	C9-C80	-2.66	1.40	1.46
1	C	207[A]	LYR	C4-C3	-2.61	1.45	1.50
1	A	207[A]	LYR	C9-C80	-2.58	1.40	1.46
1	B	207[C]	LYR	C9-C80	-2.57	1.40	1.46
1	C	207[A]	LYR	C5-C3	-2.53	1.40	1.46
1	B	207[C]	LYR	C7-C80	2.45	1.41	1.35
1	A	207[C]	LYR	C7-C80	2.30	1.41	1.35
1	C	207[C]	LYR	C7-C80	2.27	1.41	1.35
1	B	207[A]	LYR	C5-C3	-2.21	1.41	1.46
1	B	207[A]	LYR	C7-C80	2.20	1.40	1.35
1	A	207[A]	LYR	C5-C3	-2.05	1.41	1.46
1	A	207[A]	LYR	C4-C3	-2.03	1.46	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207[C]	LYR	C8-C80-C7	-3.88	116.53	122.82
1	A	207[C]	LYR	C5-C3-C2	3.83	123.83	118.49
1	B	207[C]	LYR	C8-C80-C7	-3.68	116.86	122.82
1	C	207[C]	LYR	C9-C80-C7	3.52	124.55	119.01
1	A	207[C]	LYR	C8-C80-C7	-3.46	117.22	122.82
1	C	207[A]	LYR	C8-C80-C7	-3.13	117.75	122.82
1	A	207[A]	LYR	C8-C80-C7	-3.05	117.87	122.82
1	B	207[C]	LYR	C9-C80-C7	2.94	123.63	119.01
1	B	207[A]	LYR	C8-C80-C7	-2.92	118.09	122.82
1	A	207[A]	LYR	C8-C80-C9	2.88	122.48	118.09
1	B	207[C]	LYR	C7-C6-C5	2.80	131.30	123.20
1	B	207[C]	LYR	C5-C3-C2	2.78	122.36	118.49
1	C	207[A]	LYR	C8-C80-C9	2.67	122.17	118.09
1	C	207[C]	LYR	C5-C3-C2	2.59	122.10	118.49
1	B	207[A]	LYR	C8-C80-C9	2.58	122.02	118.09
1	A	207[C]	LYR	C7-C6-C5	2.56	130.61	123.20
1	A	207[A]	LYR	C6-C7-C80	2.38	130.62	127.28
1	C	207[C]	LYR	C7-C6-C5	2.35	130.00	123.20
1	A	207[C]	LYR	C4-C3-C2	-2.11	120.08	123.73
1	C	207[A]	LYR	C6-C7-C80	2.06	130.16	127.28
1	A	207[C]	LYR	C9-C80-C7	2.06	122.24	119.01
1	A	207[A]	LYR	C1-NZ-CE	2.04	117.00	112.85

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	207[C]	LYR	C1-C2-C3-C4
1	A	207[C]	LYR	C1-C2-C3-C5
1	B	207[C]	LYR	C1-C2-C3-C4
1	B	207[C]	LYR	C1-C2-C3-C5
1	C	207[C]	LYR	C1-C2-C3-C4
1	C	207[C]	LYR	C1-C2-C3-C5
1	A	207[C]	LYR	CD-CE-NZ-C1
1	B	207[C]	LYR	CD-CE-NZ-C1
1	B	207[C]	LYR	CG-CD-CE-NZ
1	C	1	FME	CB-CG-SD-CE
1	A	207[C]	LYR	CG-CD-CE-NZ
1	A	207[C]	LYR	C2-C1-NZ-CE
1	A	1	FME	N-CA-CB-CG
1	C	207[C]	LYR	CD-CE-NZ-C1
1	C	207[C]	LYR	CG-CD-CE-NZ
1	C	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	C	207[C]	LYR	C2-C1-NZ-CE
1	B	207[C]	LYR	C2-C1-NZ-CE
1	B	207[A]	LYR	C2-C1-NZ-CE
1	A	207[A]	LYR	C2-C1-NZ-CE
1	C	207[A]	LYR	C2-C1-NZ-CE
1	A	207[A]	LYR	CD-CE-NZ-C1
1	B	207[A]	LYR	CD-CE-NZ-C1
1	C	207[A]	LYR	CD-CE-NZ-C1

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	207[C]	LYR	4	0
1	B	207[C]	LYR	4	0
1	C	207[A]	LYR	3	0
1	C	207[C]	LYR	6	0
1	A	207[A]	LYR	3	0
1	B	207[A]	LYR	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	303	-	14,14,19	0.22	0	13,13,18	0.19	0
2	LFA	B	314	-	6,6,19	0.36	0	5,5,18	0.19	0
2	LFA	C	307	-	8,8,19	0.22	0	7,7,18	0.21	0
3	OLA	A	804	-	15,15,19	0.57	0	15,15,19	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OLA	B	307	-	15,15,19	0.63	0	15,15,19	0.55	0
2	LFA	C	308	-	12,12,19	0.18	0	11,11,18	0.12	0
2	LFA	A	809	-	14,14,19	0.20	0	13,13,18	0.12	0
2	LFA	A	801	-	6,6,19	0.24	0	5,5,18	0.36	0
2	LFA	C	309	-	5,5,19	0.20	0	4,4,18	0.18	0
3	OLA	C	301	-	19,19,19	0.54	0	19,19,19	0.55	0
2	LFA	A	810	-	8,8,19	0.17	0	7,7,18	0.15	0
2	LFA	C	316	-	5,5,19	0.22	0	4,4,18	0.19	0
3	OLA	A	806	-	18,18,19	0.58	0	18,18,19	0.49	0
2	LFA	C	303	-	16,16,19	0.16	0	15,15,18	0.08	0
3	OLA	C	305	-	15,15,19	0.58	0	15,15,19	0.71	0
3	OLA	A	805	-	10,10,19	0.83	0	10,10,19	0.63	0
2	LFA	A	815	-	5,5,19	0.26	0	4,4,18	0.15	0
2	LFA	B	317	-	13,13,19	0.13	0	12,12,18	0.15	0
2	LFA	C	317	-	5,5,19	0.17	0	4,4,18	0.12	0
2	LFA	B	316	-	4,4,19	0.19	0	3,3,18	0.24	0
2	LFA	B	313	-	8,8,19	0.23	0	7,7,18	0.21	0
2	LFA	C	311	-	8,8,19	0.15	0	7,7,18	0.19	0
2	LFA	B	305	-	6,6,19	0.28	0	5,5,18	0.16	0
3	OLA	C	304	-	13,13,19	0.62	0	13,13,19	0.57	0
2	LFA	A	811	-	8,8,19	0.16	0	7,7,18	0.13	0
2	LFA	A	807	-	12,12,19	0.14	0	11,11,18	0.15	0
2	LFA	A	812	-	5,5,19	0.29	0	4,4,18	0.29	0
2	LFA	C	315	-	7,7,19	0.11	0	6,6,18	0.10	0
3	OLA	A	803	-	19,19,19	0.53	0	19,19,19	0.51	0
2	LFA	C	313	-	10,10,19	0.17	0	9,9,18	0.13	0
2	LFA	C	312	-	16,16,19	0.21	0	15,15,18	0.17	0
2	LFA	B	311	-	13,13,19	0.14	0	12,12,18	0.19	0
2	LFA	C	314	-	3,3,19	0.32	0	2,2,18	0.43	0
3	OLA	B	301	-	19,19,19	0.48	0	19,19,19	0.56	0
2	LFA	A	813	-	11,11,19	0.17	0	10,10,18	0.14	0
2	LFA	B	310	-	7,7,19	0.09	0	6,6,18	0.11	0
2	LFA	B	309	-	9,9,19	0.11	0	8,8,18	0.12	0
2	LFA	B	312	-	11,11,19	0.21	0	10,10,18	0.18	0
3	OLA	A	802	-	10,10,19	0.74	0	10,10,19	0.71	0
3	OLA	C	302	-	15,15,19	0.62	0	15,15,19	0.51	0
2	LFA	B	302	-	6,6,19	0.15	0	5,5,18	0.29	0
2	LFA	B	304	-	8,8,19	0.26	0	7,7,18	0.17	0
2	LFA	B	315	-	6,6,19	0.26	0	5,5,18	0.17	0
4	PO4	C	306	-	4,4,4	0.85	0	6,6,6	0.43	0
2	LFA	A	814	-	7,7,19	0.11	0	6,6,18	0.10	0
3	OLA	B	306	-	13,13,19	0.70	0	13,13,19	0.47	0
2	LFA	C	310	-	9,9,19	0.18	0	8,8,18	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OLA	B	308	-	10,10,19	0.70	0	10,10,19	0.80	0
2	LFA	A	808	-	10,10,19	0.19	0	9,9,18	0.19	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	B	303	-	-	5/12/12/17	-
2	LFA	B	314	-	-	1/4/4/17	-
2	LFA	C	307	-	-	0/6/6/17	-
3	OLA	A	804	-	-	4/13/13/17	-
3	OLA	B	307	-	-	8/13/13/17	-
2	LFA	C	308	-	-	4/10/10/17	-
2	LFA	A	809	-	-	7/12/12/17	-
2	LFA	A	801	-	-	0/4/4/17	-
2	LFA	C	309	-	-	0/3/3/17	-
3	OLA	C	301	-	-	3/17/17/17	-
2	LFA	A	810	-	-	3/6/6/17	-
2	LFA	C	316	-	-	1/3/3/17	-
3	OLA	A	806	-	-	2/16/16/17	-
2	LFA	C	303	-	-	5/14/14/17	-
3	OLA	C	305	-	-	2/13/13/17	-
3	OLA	A	805	-	-	3/8/8/17	-
2	LFA	A	815	-	-	1/3/3/17	-
2	LFA	B	317	-	-	3/11/11/17	-
2	LFA	C	317	-	-	3/3/3/17	-
2	LFA	B	316	-	-	1/2/2/17	-
2	LFA	B	313	-	-	0/6/6/17	-
2	LFA	C	311	-	-	2/6/6/17	-
2	LFA	B	305	-	-	0/4/4/17	-
3	OLA	C	304	-	-	6/11/11/17	-
2	LFA	A	811	-	-	3/6/6/17	-
2	LFA	A	807	-	-	4/10/10/17	-
2	LFA	A	812	-	-	0/3/3/17	-
2	LFA	C	315	-	-	0/5/5/17	-
3	OLA	A	803	-	-	10/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	313	-	-	2/8/8/17	-
2	LFA	C	312	-	-	2/14/14/17	-
2	LFA	B	311	-	-	2/11/11/17	-
2	LFA	C	314	-	-	0/1/1/17	-
3	OLA	B	301	-	-	7/17/17/17	-
2	LFA	A	813	-	-	2/9/9/17	-
2	LFA	B	310	-	-	1/5/5/17	-
2	LFA	B	309	-	-	3/7/7/17	-
2	LFA	B	312	-	-	0/9/9/17	-
3	OLA	A	802	-	-	2/8/8/17	-
3	OLA	C	302	-	-	7/13/13/17	-
2	LFA	B	302	-	-	1/4/4/17	-
2	LFA	B	304	-	-	0/6/6/17	-
2	LFA	B	315	-	-	2/4/4/17	-
2	LFA	A	814	-	-	1/5/5/17	-
3	OLA	B	306	-	-	8/11/11/17	-
2	LFA	C	310	-	-	2/7/7/17	-
3	OLA	B	308	-	-	5/8/8/17	-
2	LFA	A	808	-	-	3/8/8/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	307	OLA	C11-C10-C9-C8
3	B	308	OLA	C1-C2-C3-C4
3	C	304	OLA	C11-C10-C9-C8
3	A	804	OLA	C11-C10-C9-C8
3	C	302	OLA	C1-C2-C3-C4
3	A	805	OLA	C4-C5-C6-C7
2	A	810	LFA	C11-C12-C13-C14
3	B	301	OLA	C11-C12-C13-C14
2	B	317	LFA	C11-C10-C9-C8
2	A	811	LFA	C4-C5-C6-C7
3	A	803	OLA	C5-C6-C7-C8
2	A	808	LFA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
2	A	809	LFA	C2-C3-C4-C5
2	A	807	LFA	C7-C8-C9-C10
2	B	303	LFA	C4-C5-C6-C7
2	C	303	LFA	C9-C10-C11-C12
3	B	307	OLA	C5-C6-C7-C8
3	B	307	OLA	C6-C7-C8-C9
2	B	315	LFA	C3-C4-C5-C6
2	C	303	LFA	C11-C10-C9-C8
2	C	308	LFA	C9-C10-C11-C12
2	C	303	LFA	C5-C6-C7-C8
3	A	803	OLA	C3-C4-C5-C6
3	B	306	OLA	C5-C6-C7-C8
3	A	806	OLA	C6-C7-C8-C9
2	B	311	LFA	C12-C13-C14-C15
3	B	306	OLA	C3-C4-C5-C6
3	B	306	OLA	C1-C2-C3-C4
2	B	303	LFA	C3-C4-C5-C6
2	B	303	LFA	C6-C7-C8-C9
3	C	301	OLA	C5-C6-C7-C8
2	C	312	LFA	C11-C10-C9-C8
3	A	803	OLA	C4-C5-C6-C7
3	C	302	OLA	C3-C4-C5-C6
3	B	301	OLA	C6-C7-C8-C9
2	B	317	LFA	C7-C8-C9-C10
3	C	305	OLA	C4-C5-C6-C7
3	A	803	OLA	C10-C11-C12-C13
3	B	306	OLA	C11-C10-C9-C8
3	B	308	OLA	C2-C3-C4-C5
2	A	810	LFA	C14-C15-C16-C17
2	C	311	LFA	C15-C16-C17-C18
2	A	810	LFA	C13-C14-C15-C16
2	A	808	LFA	C10-C11-C12-C13
3	B	301	OLA	C1-C2-C3-C4
2	B	302	LFA	C13-C14-C15-C16
2	A	813	LFA	C5-C6-C7-C8
2	B	315	LFA	C2-C3-C4-C5
2	C	308	LFA	C6-C7-C8-C9
2	C	316	LFA	C4-C5-C6-C7
2	B	314	LFA	C2-C3-C4-C5
3	A	804	OLA	C11-C12-C13-C14
2	C	303	LFA	C10-C11-C12-C13
3	C	304	OLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	C	313	LFA	C10-C11-C12-C13
3	B	307	OLA	C3-C4-C5-C6
3	A	805	OLA	C5-C6-C7-C8
2	C	308	LFA	C11-C10-C9-C8
2	C	310	LFA	C3-C4-C5-C6
2	C	317	LFA	C3-C4-C5-C6
3	C	304	OLA	C9-C10-C11-C12
2	A	809	LFA	C10-C11-C12-C13
3	A	804	OLA	C5-C6-C7-C8
2	A	809	LFA	C4-C5-C6-C7
3	C	301	OLA	C2-C3-C4-C5
2	B	310	LFA	C2-C3-C4-C5
2	B	317	LFA	C5-C6-C7-C8
3	A	805	OLA	C3-C4-C5-C6
2	A	814	LFA	C3-C4-C5-C6
2	A	809	LFA	C11-C12-C13-C14
2	C	311	LFA	C17-C18-C19-C20
2	A	813	LFA	C9-C10-C11-C12
3	C	302	OLA	C5-C6-C7-C8
3	B	306	OLA	C7-C8-C9-C10
2	C	313	LFA	C11-C12-C13-C14
3	A	803	OLA	C13-C14-C15-C16
3	B	301	OLA	C15-C16-C17-C18
2	C	310	LFA	C5-C6-C7-C8
2	A	809	LFA	C6-C7-C8-C9
2	A	811	LFA	C5-C6-C7-C8
2	A	811	LFA	C6-C7-C8-C9
3	B	306	OLA	C9-C10-C11-C12
2	A	809	LFA	C1-C2-C3-C4
3	B	308	OLA	C6-C7-C8-C9
2	A	815	LFA	C2-C3-C4-C5
2	A	809	LFA	C9-C10-C11-C12
3	B	301	OLA	O2-C1-C2-C3
3	A	803	OLA	C12-C13-C14-C15
2	A	807	LFA	C9-C10-C11-C12
2	C	303	LFA	C7-C8-C9-C10
2	A	807	LFA	C3-C4-C5-C6
3	B	301	OLA	O1-C1-C2-C3
2	B	303	LFA	C7-C8-C9-C10
3	B	301	OLA	C9-C10-C11-C12
3	B	308	OLA	O1-C1-C2-C3
3	C	302	OLA	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	307	OLA	C7-C8-C9-C10
3	B	307	OLA	O1-C1-C2-C3
2	B	311	LFA	C11-C10-C9-C8
3	C	304	OLA	O2-C1-C2-C3
3	A	803	OLA	C14-C15-C16-C17
3	C	302	OLA	O2-C1-C2-C3
3	C	304	OLA	O1-C1-C2-C3
2	B	309	LFA	C4-C5-C6-C7
3	C	305	OLA	C2-C3-C4-C5
2	C	317	LFA	C1-C2-C3-C4
2	B	316	LFA	C16-C17-C18-C19
2	B	309	LFA	C5-C6-C7-C8
3	C	302	OLA	C2-C3-C4-C5
3	B	308	OLA	O2-C1-C2-C3
3	C	302	OLA	C11-C10-C9-C8
3	B	307	OLA	O2-C1-C2-C3
3	A	803	OLA	C7-C8-C9-C10
2	A	807	LFA	C5-C6-C7-C8
3	A	802	OLA	O2-C1-C2-C3
3	B	306	OLA	O2-C1-C2-C3
3	C	301	OLA	C7-C8-C9-C10
3	A	804	OLA	C4-C5-C6-C7
3	A	803	OLA	O1-C1-C2-C3
3	A	803	OLA	O2-C1-C2-C3
3	B	306	OLA	O1-C1-C2-C3
2	C	317	LFA	C2-C3-C4-C5
2	A	808	LFA	C16-C17-C18-C19
3	A	806	OLA	C11-C12-C13-C14
3	A	802	OLA	O1-C1-C2-C3
2	B	303	LFA	C11-C10-C9-C8
2	C	308	LFA	C4-C5-C6-C7
3	C	304	OLA	C2-C3-C4-C5
3	B	307	OLA	C1-C2-C3-C4
2	C	312	LFA	C6-C7-C8-C9
2	B	309	LFA	C6-C7-C8-C9

There are no ring outliers.

7 monomers are involved in 8 short contacts:

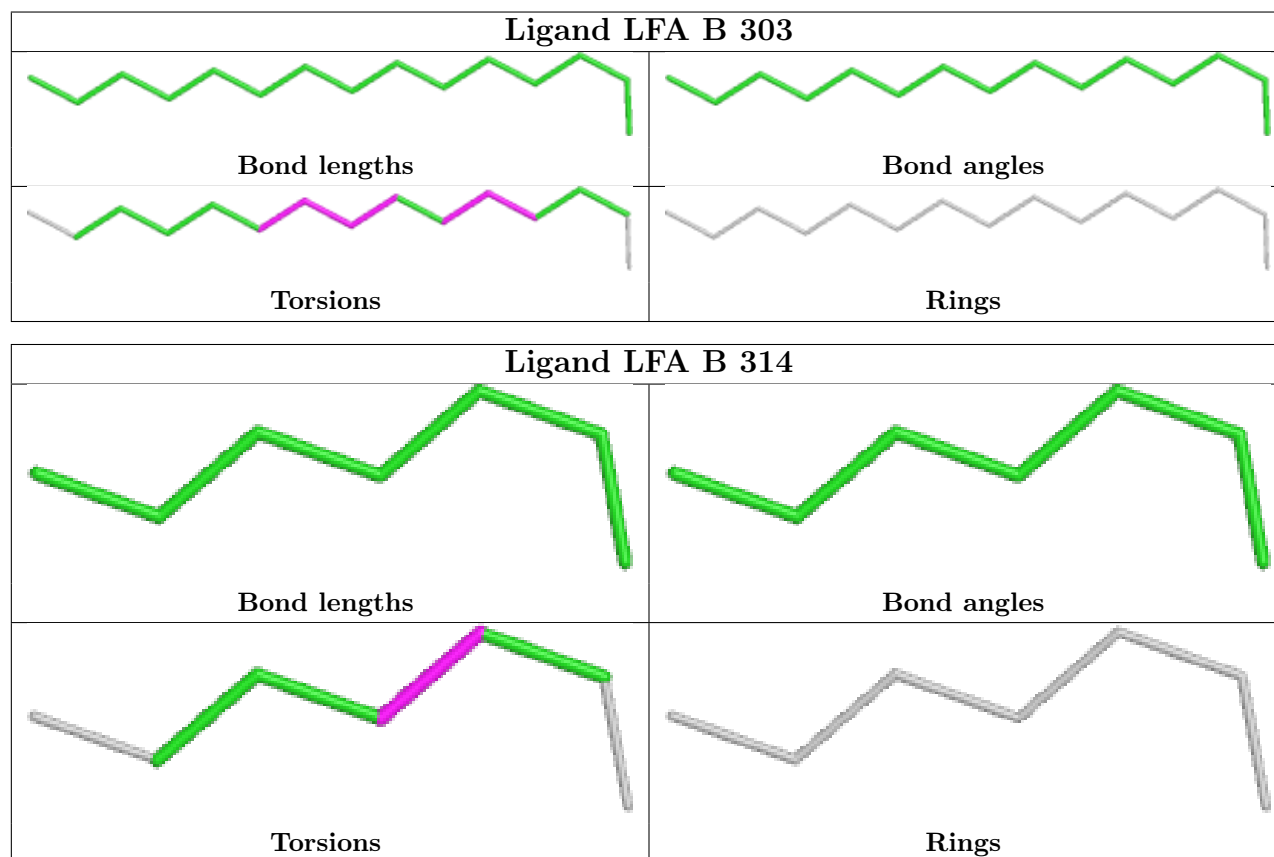
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	OLA	1	0
2	A	810	LFA	2	0

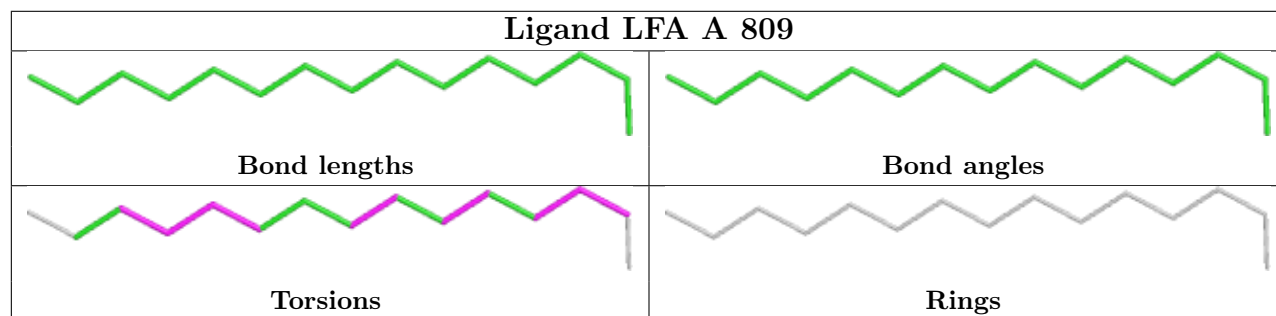
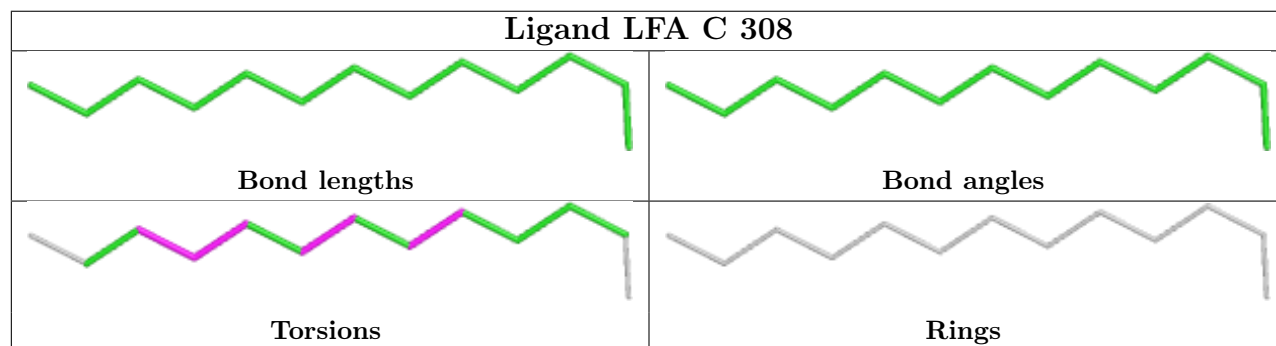
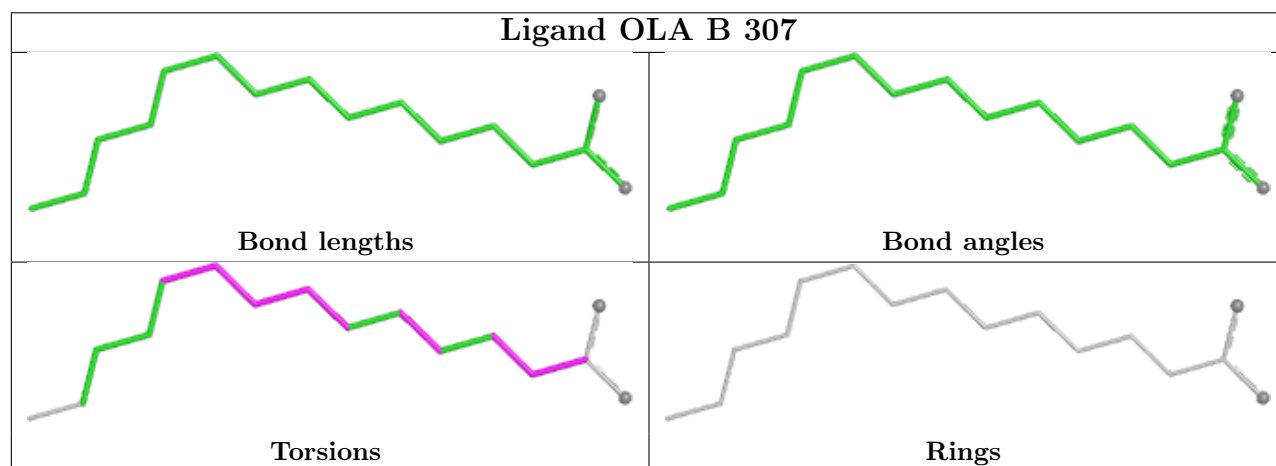
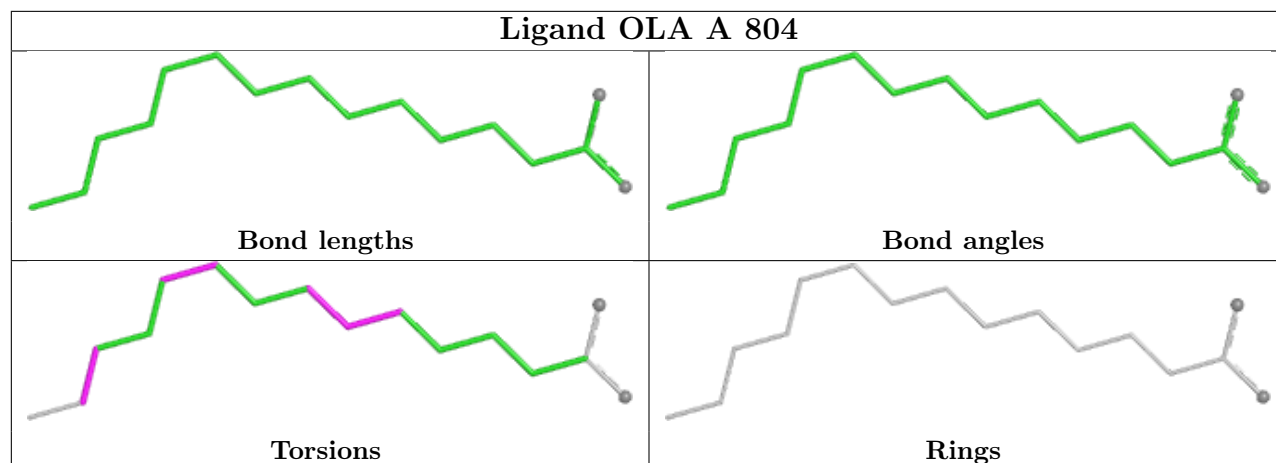
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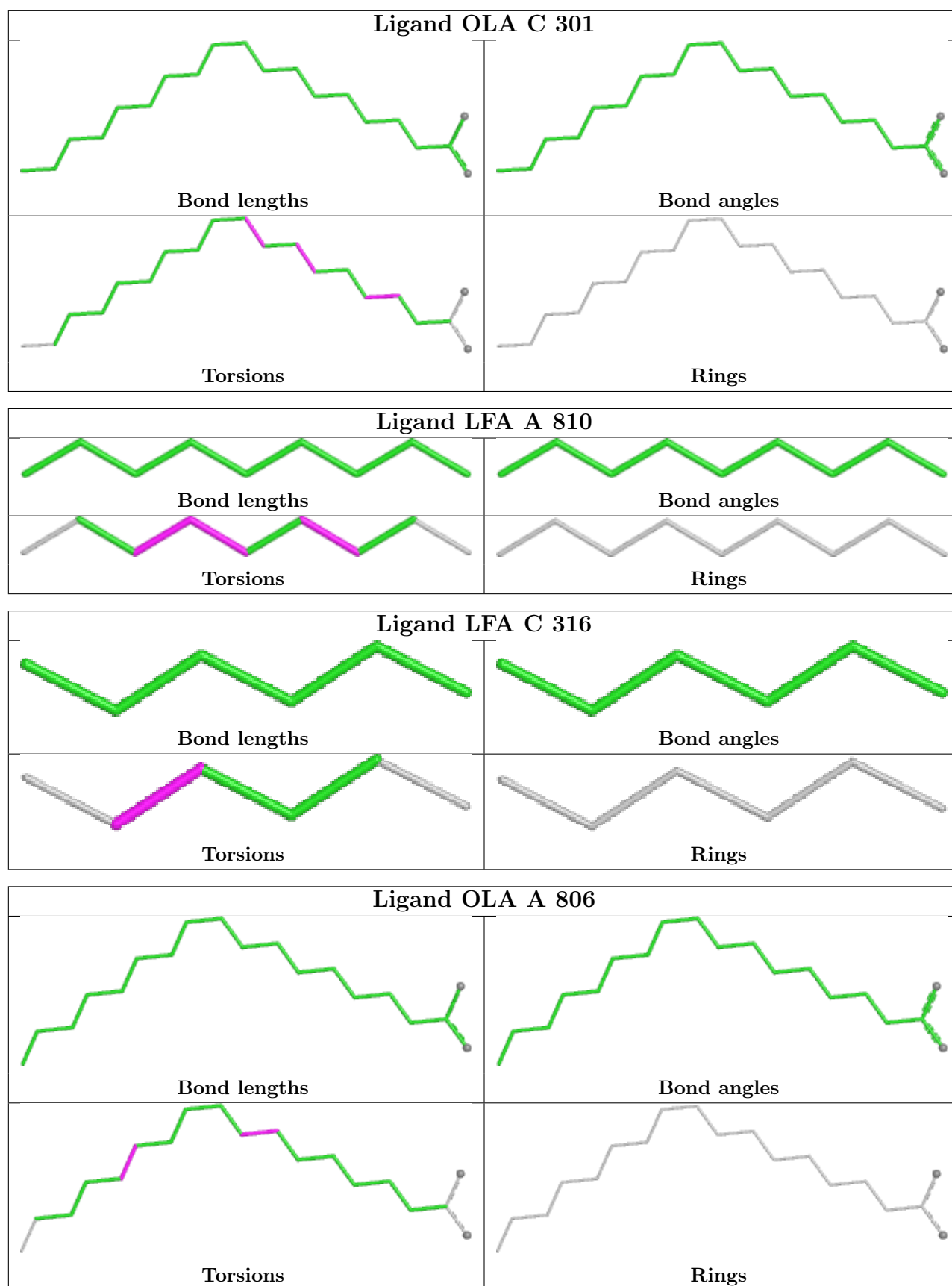
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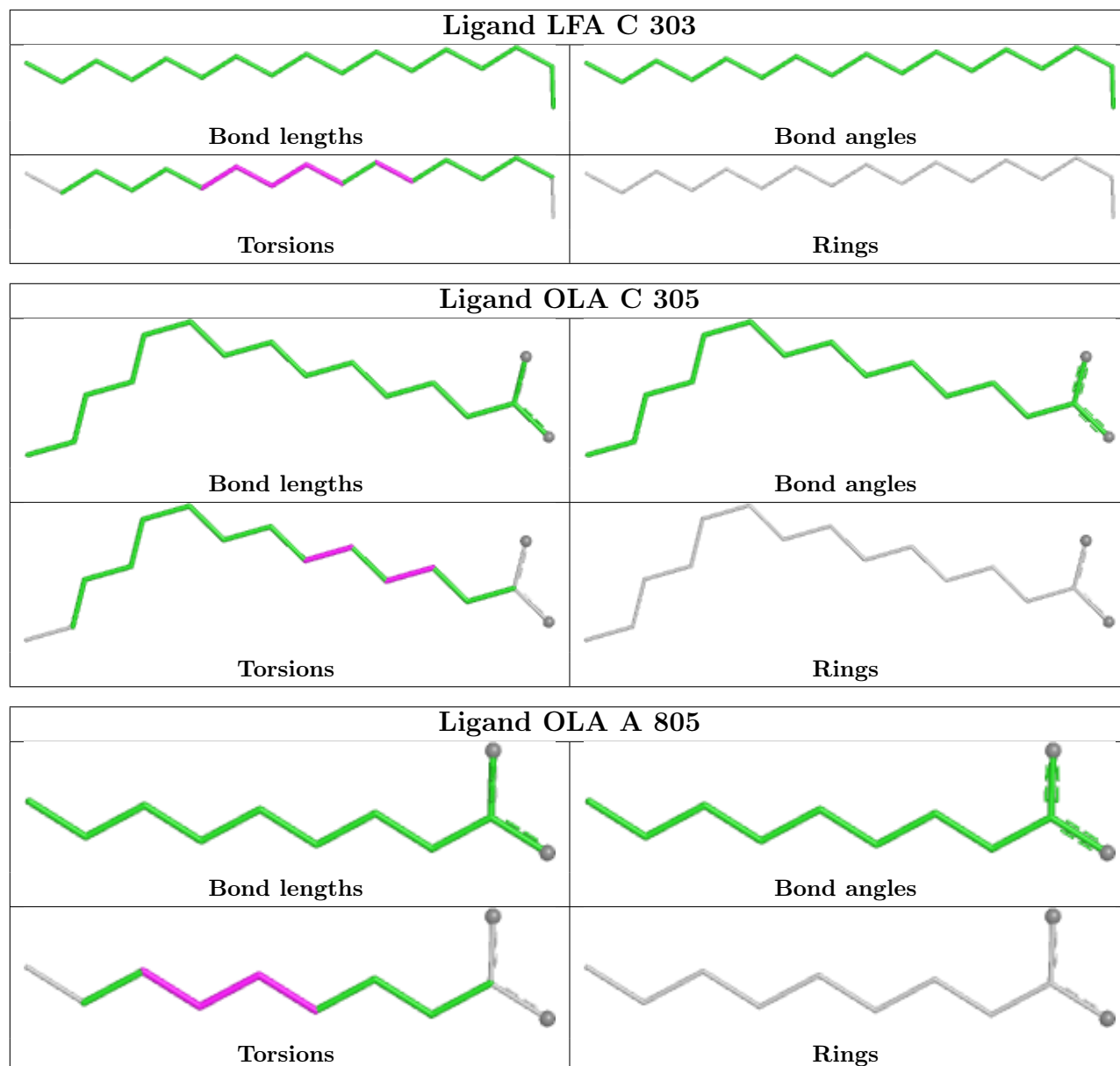
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	313	LFA	1	0
2	C	311	LFA	1	0
2	C	313	LFA	1	0
3	B	301	OLA	1	0
3	B	308	OLA	2	0

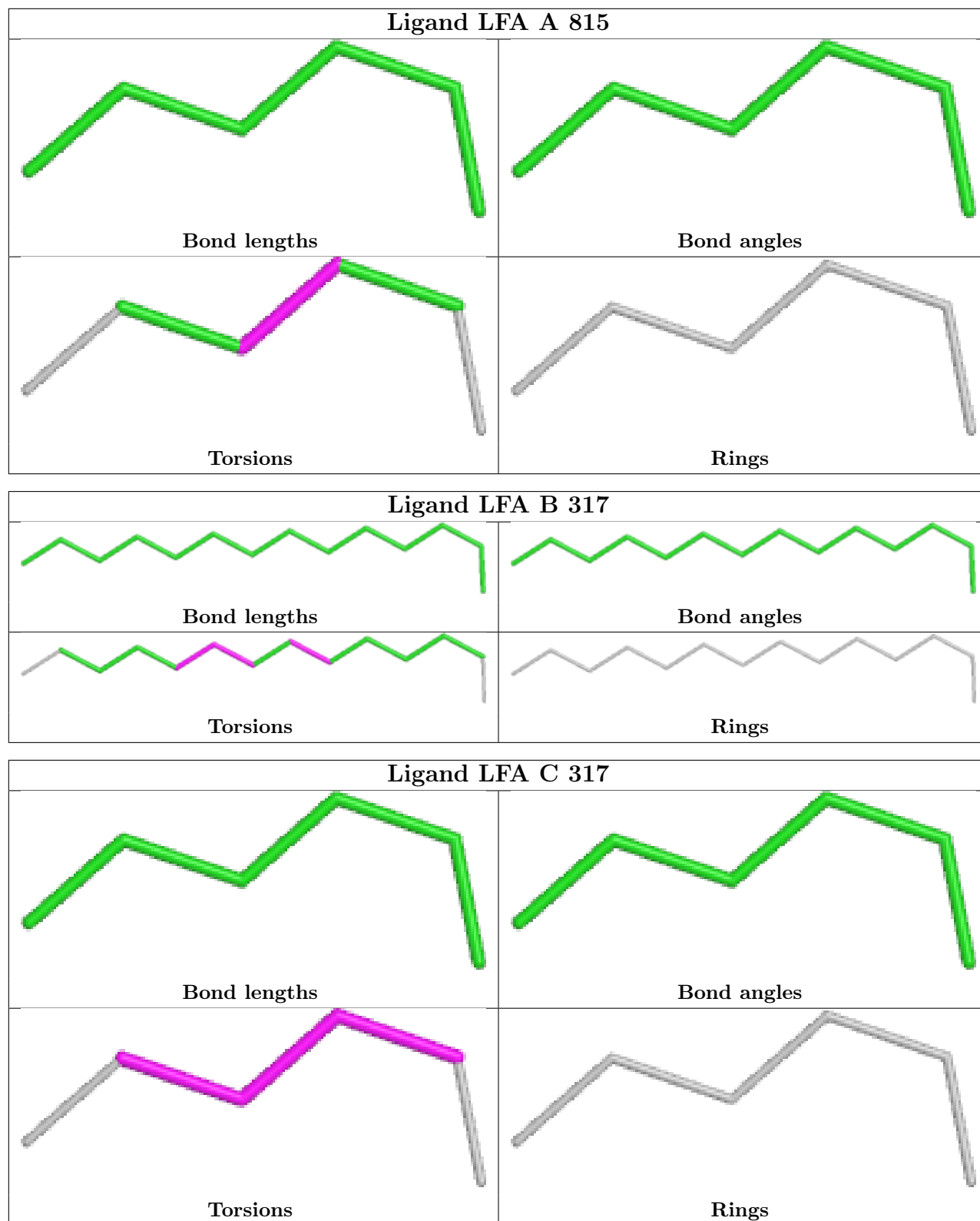
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

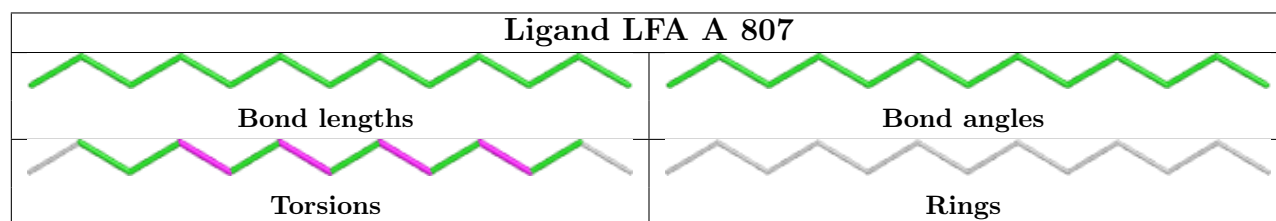
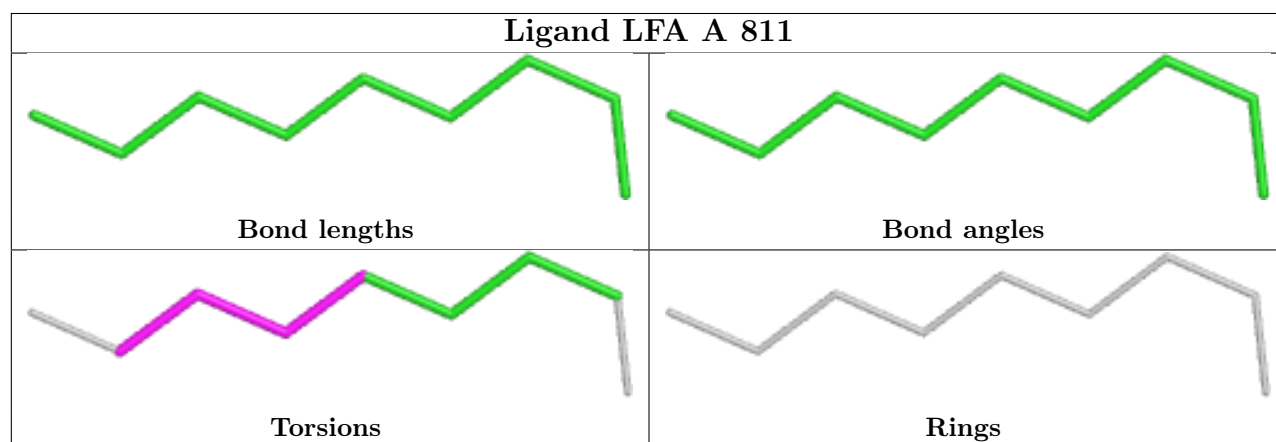
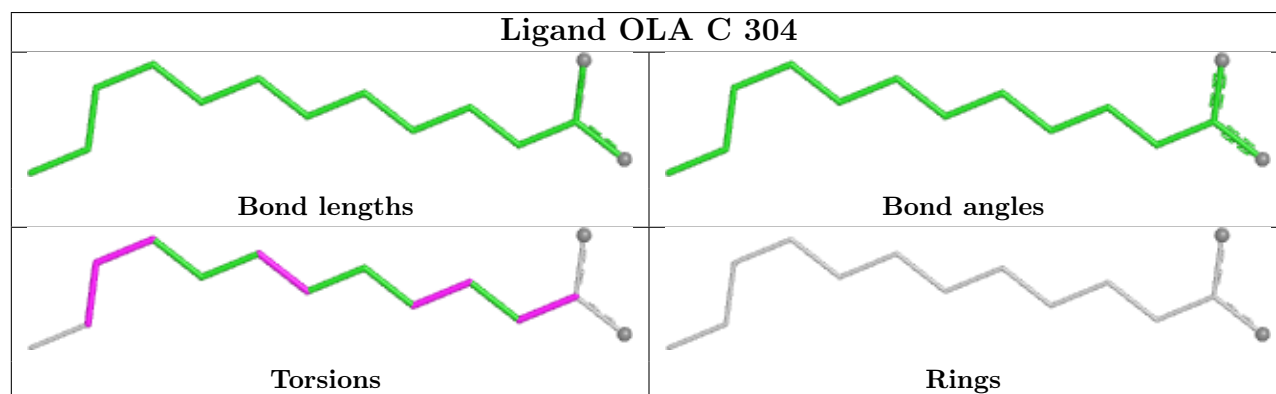
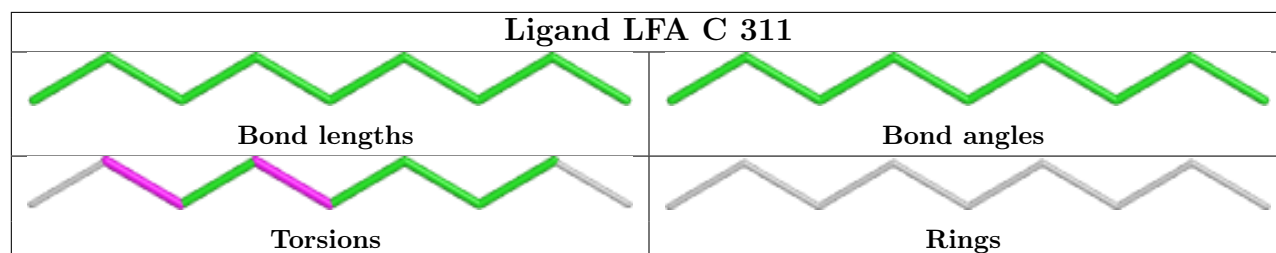
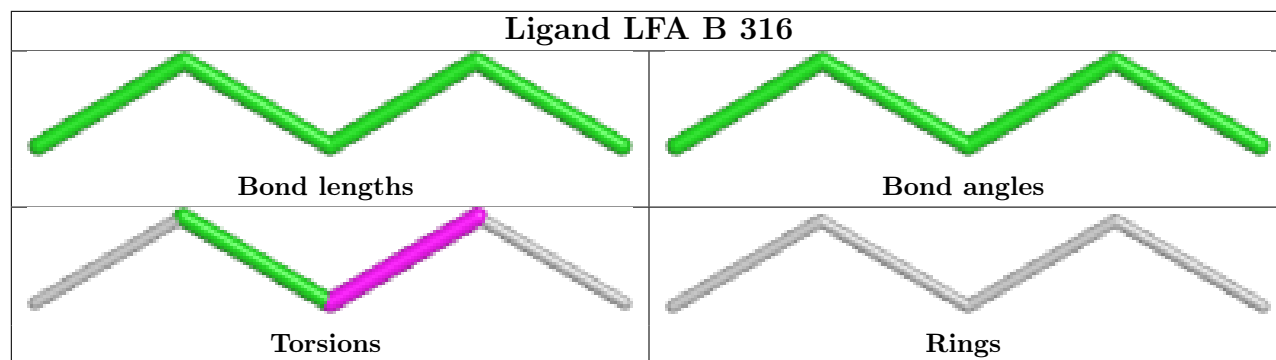


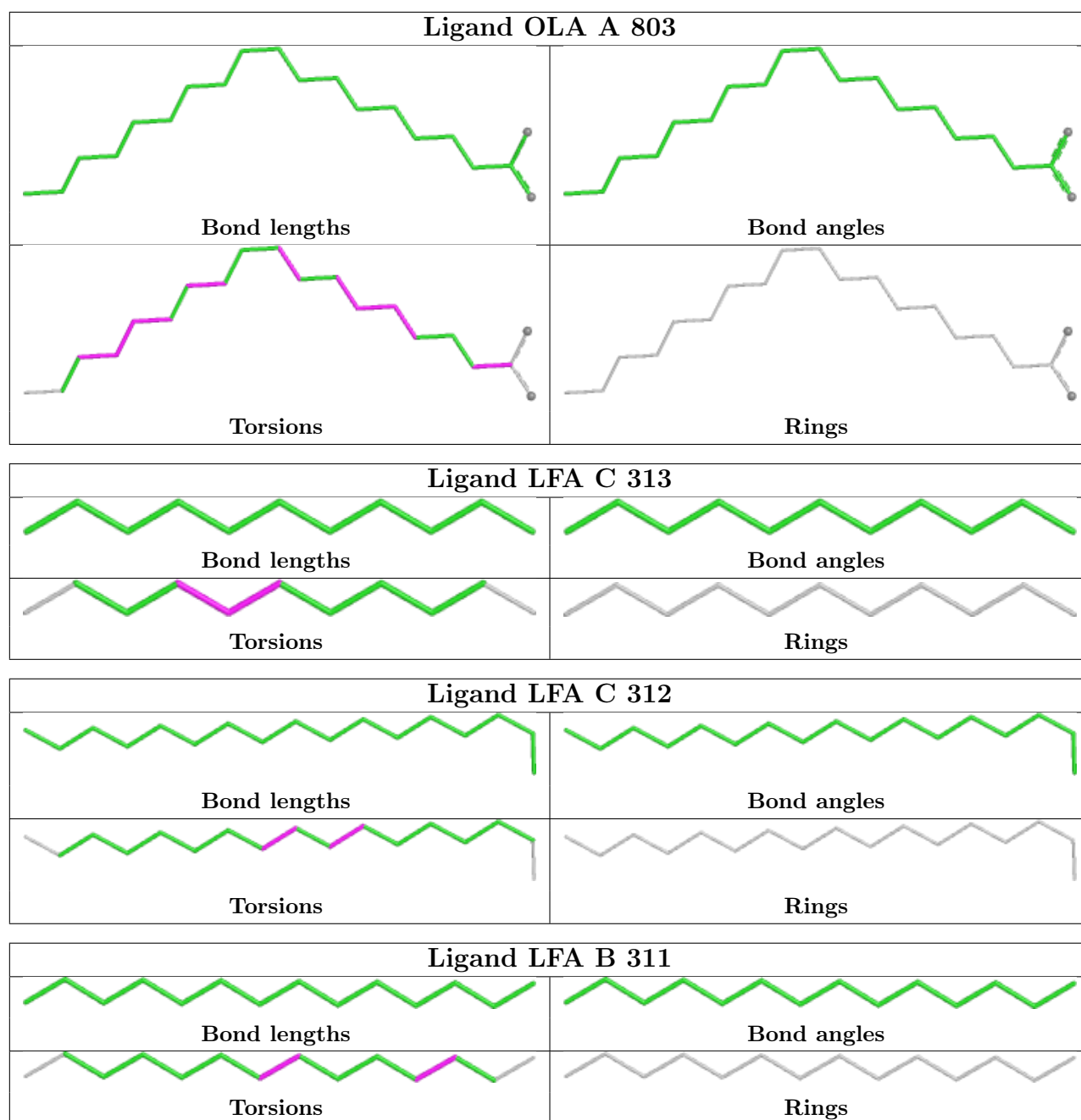


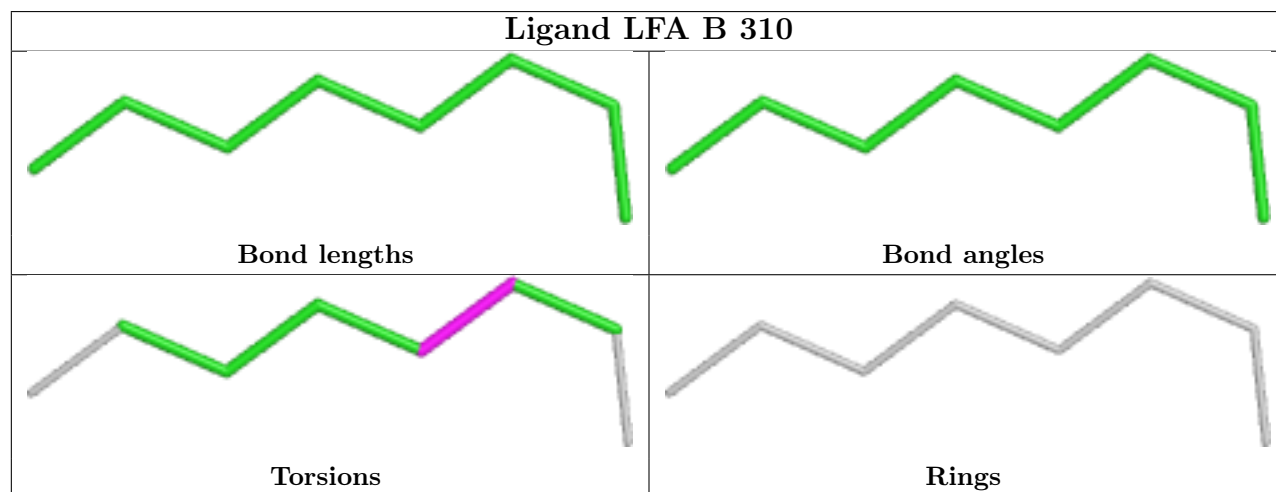
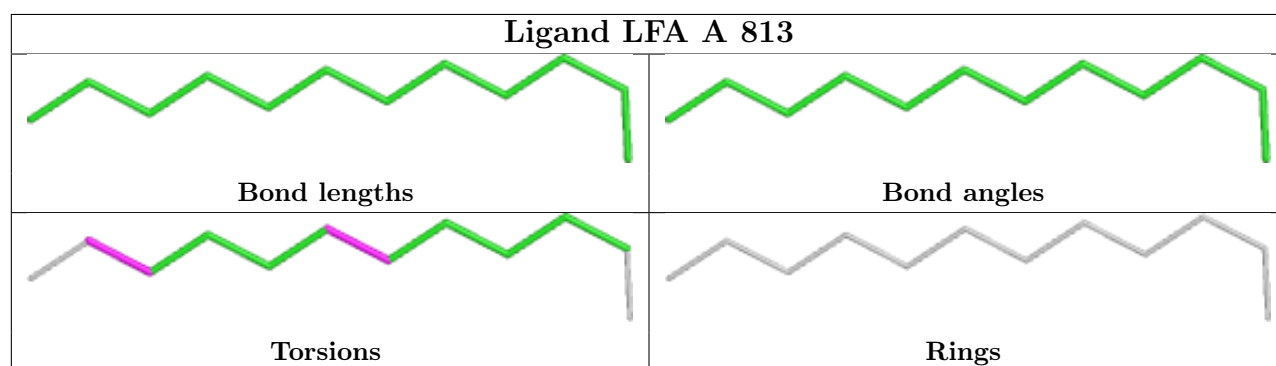
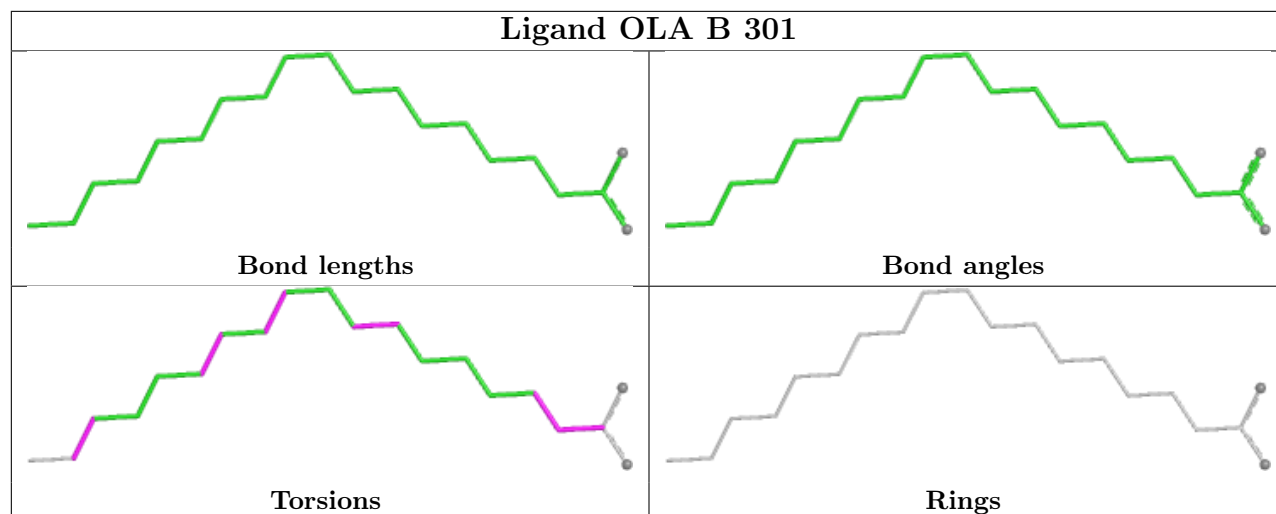


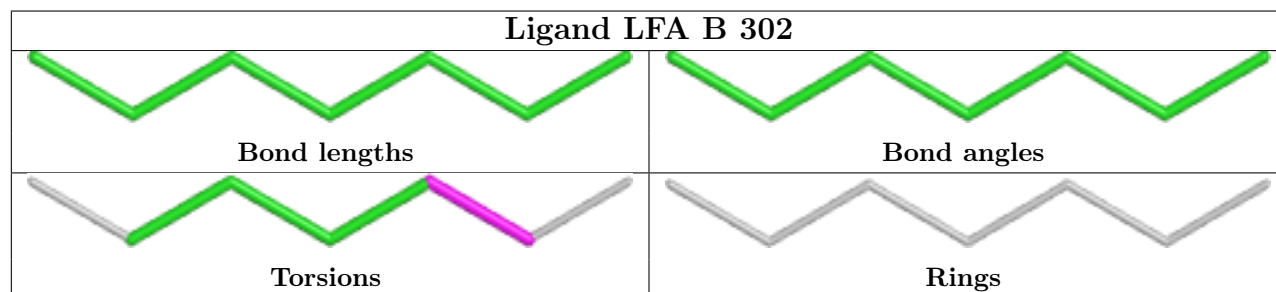
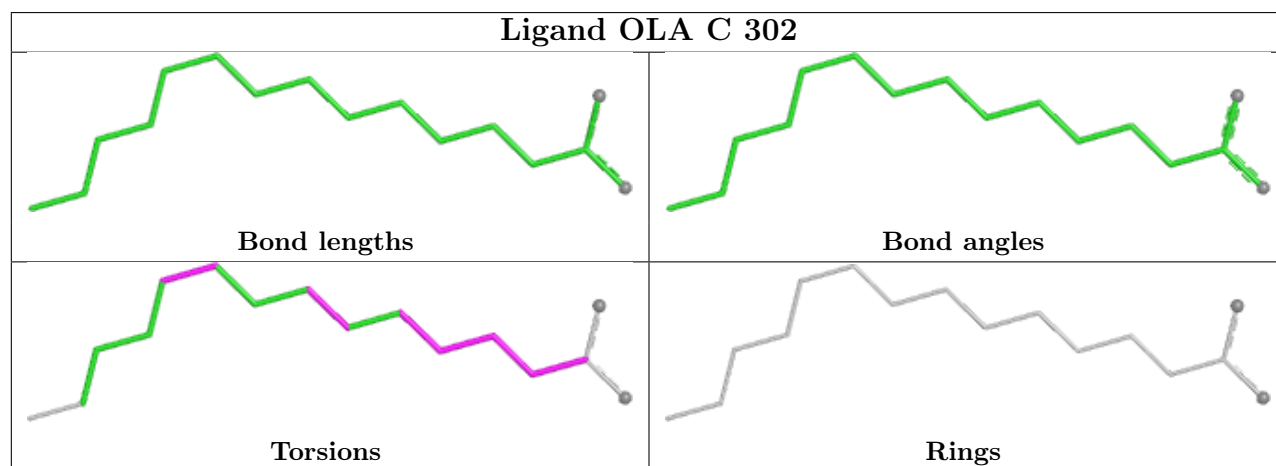
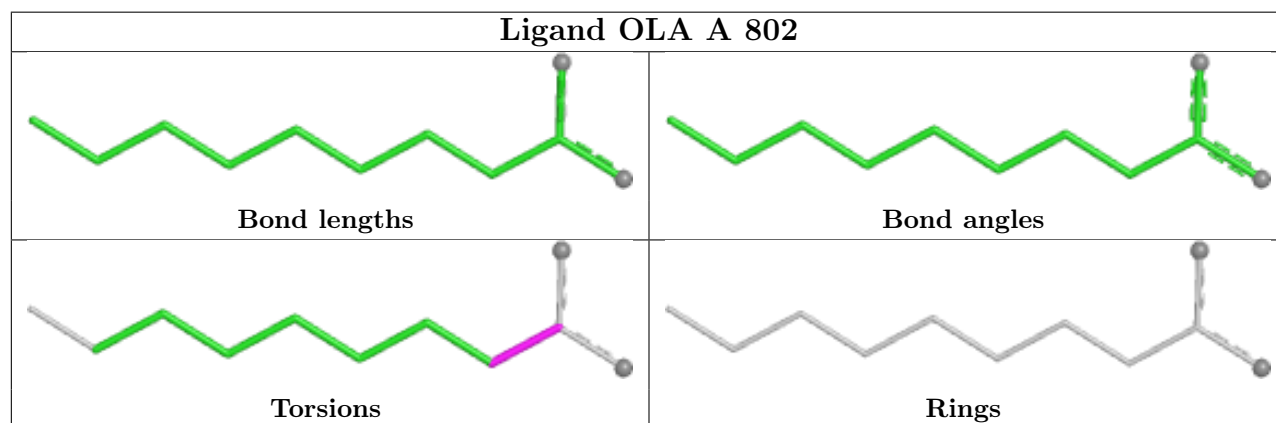
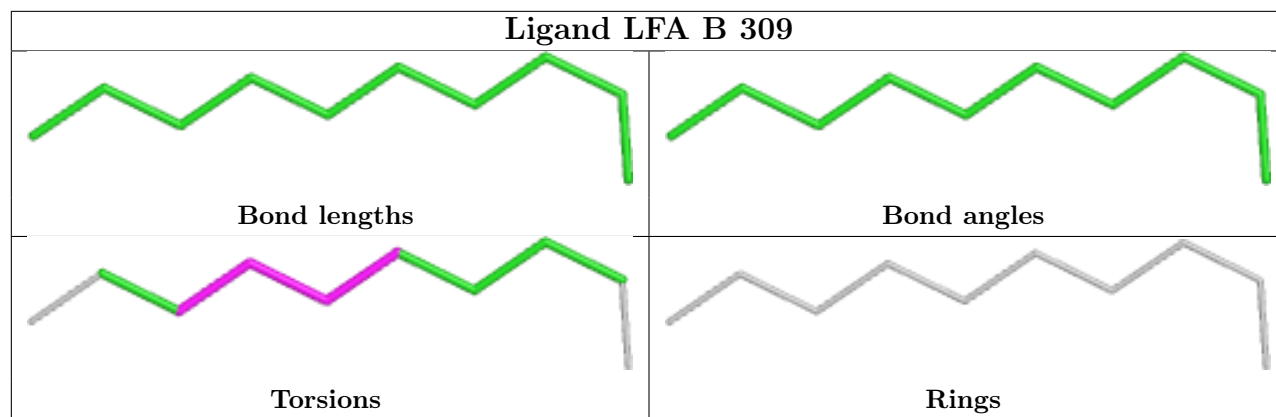


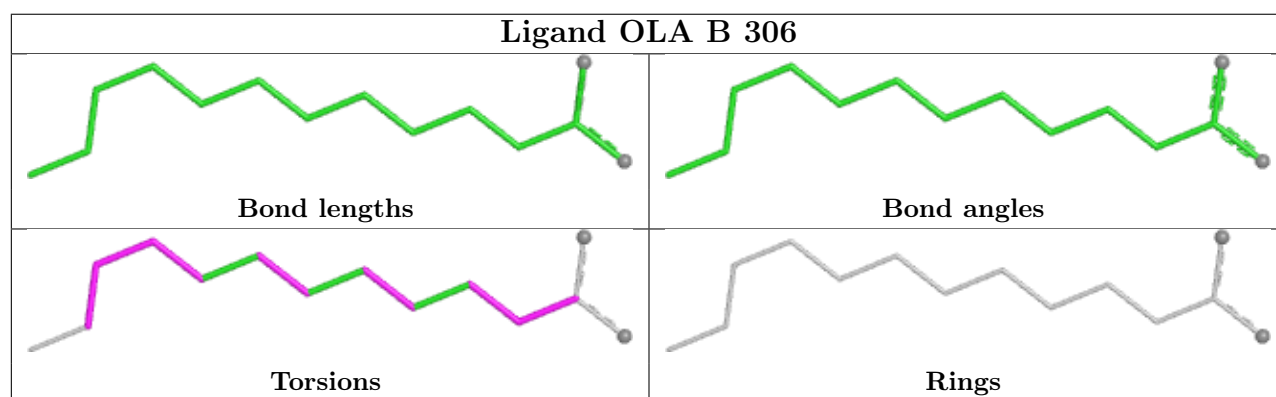
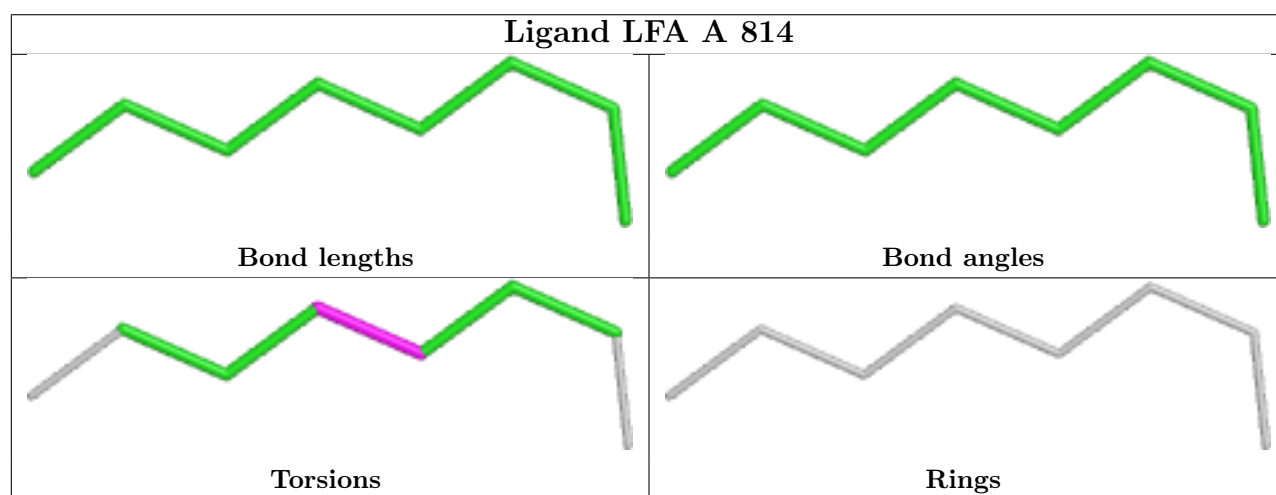
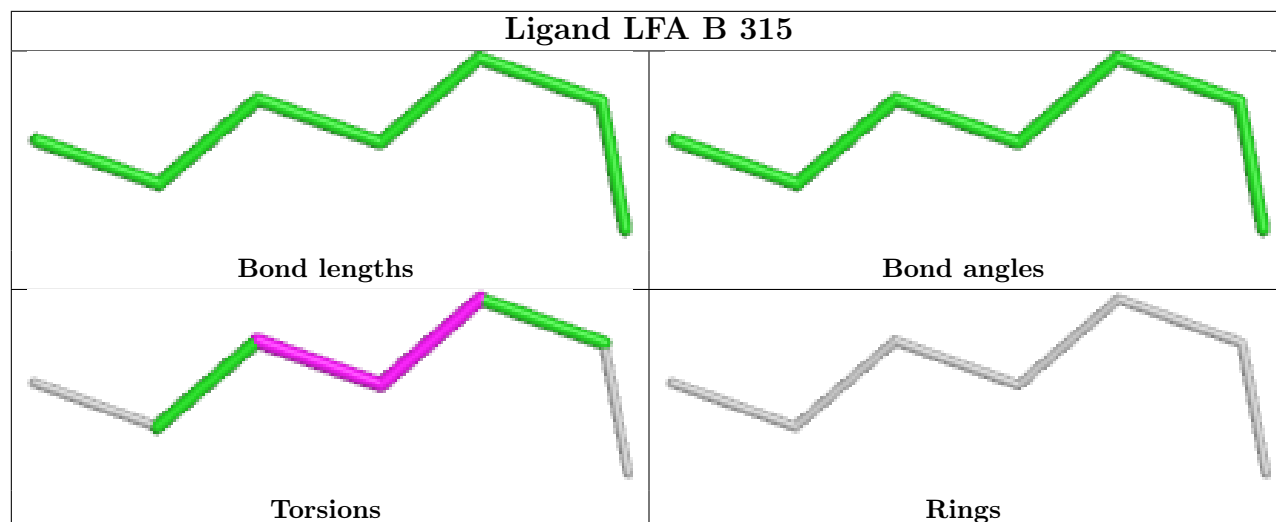


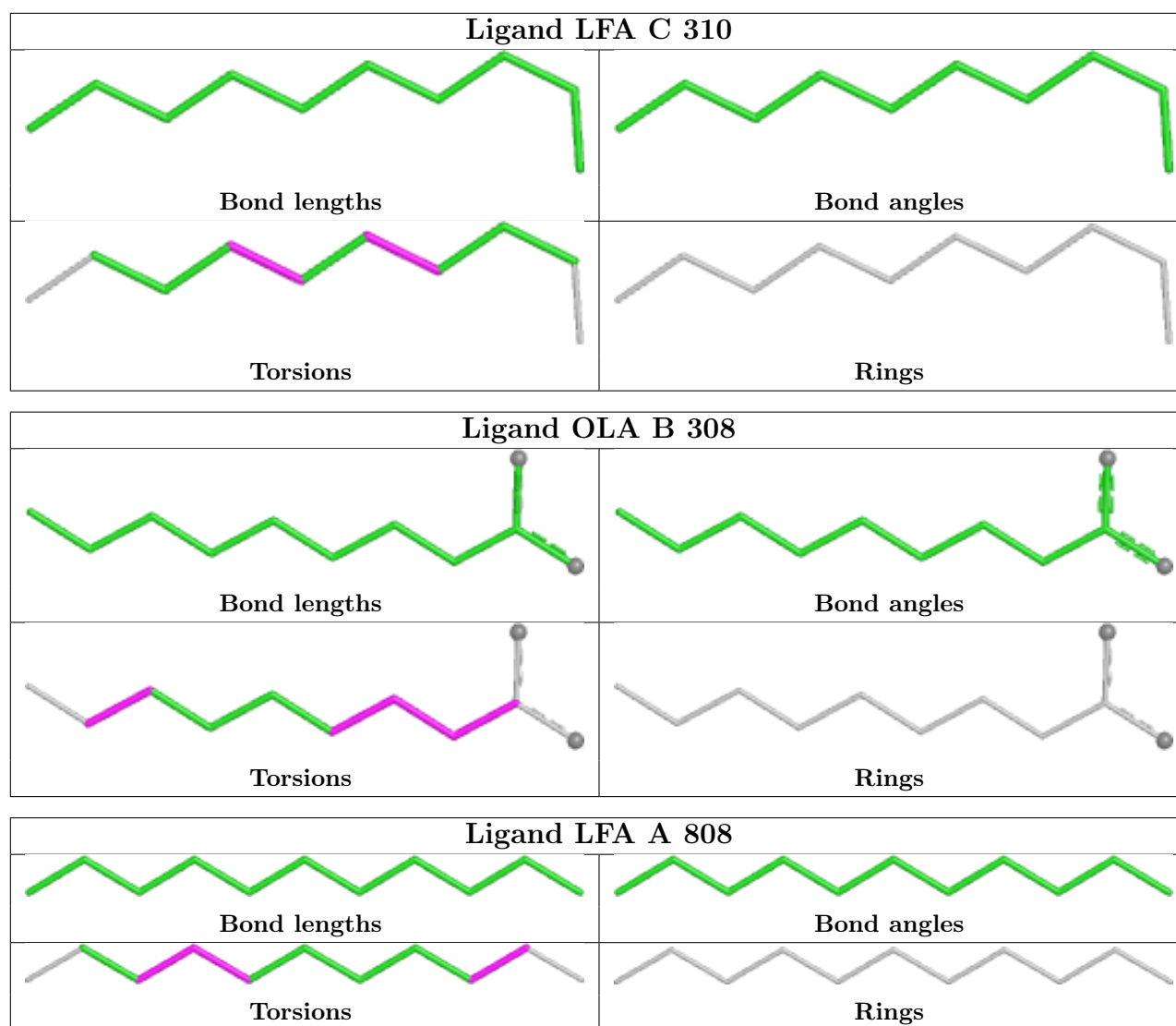












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	222:HIS	C	223:GLN	N	2.33

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	221/229 (96%)	0.07	3 (1%) 73 75	18, 45, 69, 117	7 (3%)
1	B	219/229 (95%)	0.14	3 (1%) 73 75	18, 48, 75, 112	8 (3%)
1	C	221/229 (96%)	0.10	5 (2%) 61 63	19, 47, 77, 122	7 (3%)
All	All	661/687 (96%)	0.10	11 (1%) 69 70	18, 47, 75, 122	22 (3%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	ASP	3.0
1	A	62	ASP	2.9
1	B	223	GLN	2.8
1	C	62	ASP	2.7
1	C	222	HIS	2.3
1	C	63	ASP	2.3
1	C	193	LEU	2.2
1	C	223	GLN	2.2
1	A	61	TYR	2.2
1	B	121	ILE	2.2
1	B	63	ASP	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	FME	B	1	7/11	0.60	0.15	81,85,90,92	0
1	FME	C	1	10/11	0.74	0.14	70,81,114,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	FME	A	1	10/11	0.75	0.16	73,85,115,117	0
1	LYR	B	207[A]	29/30	0.91	0.10	36,38,47,55	29
1	LYR	B	207[C]	29/30	0.91	0.10	29,30,37,38	29
1	LYR	C	207[A]	29/30	0.91	0.11	38,46,50,60	29
1	LYR	C	207[C]	29/30	0.91	0.11	29,31,36,36	29
1	LYR	A	207[A]	29/30	0.92	0.11	37,40,45,50	29
1	LYR	A	207[C]	29/30	0.92	0.11	30,31,35,35	29

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($\text{\AA}^2$)	Q<0.9
2	LFA	C	316	6/20	0.57	0.17	99,109,112,113	0
2	LFA	A	811	9/20	0.61	0.16	106,110,112,113	0
2	LFA	C	315	8/20	0.63	0.19	100,105,106,106	0
4	PO4	C	306	5/5	0.64	0.12	122,125,132,133	0
2	LFA	C	312	17/20	0.71	0.18	66,89,102,102	0
2	LFA	C	314	4/20	0.72	0.21	73,78,80,81	0
2	LFA	B	314	7/20	0.72	0.14	61,71,76,79	0
2	LFA	B	316	5/20	0.72	0.16	80,81,85,88	0
2	LFA	A	814	8/20	0.72	0.20	113,123,131,131	0
2	LFA	C	313	11/20	0.73	0.19	97,110,120,121	0
2	LFA	A	808	11/20	0.74	0.18	82,87,91,92	0
2	LFA	B	315	7/20	0.75	0.18	81,84,87,89	0
2	LFA	C	309	6/20	0.75	0.16	82,86,91,93	0
2	LFA	B	305	7/20	0.76	0.20	79,82,95,97	0
3	OLA	A	805	11/20	0.77	0.16	72,87,91,99	0
2	LFA	A	813	12/20	0.77	0.19	71,102,109,109	0
3	OLA	B	308	11/20	0.78	0.17	89,94,101,105	0
2	LFA	B	313	9/20	0.79	0.17	86,93,99,102	0
3	OLA	C	305	16/20	0.79	0.16	80,99,102,103	0
2	LFA	C	311	9/20	0.79	0.19	90,94,99,104	0
2	LFA	A	815	6/20	0.80	0.15	66,74,79,82	0

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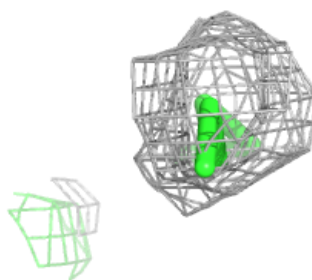
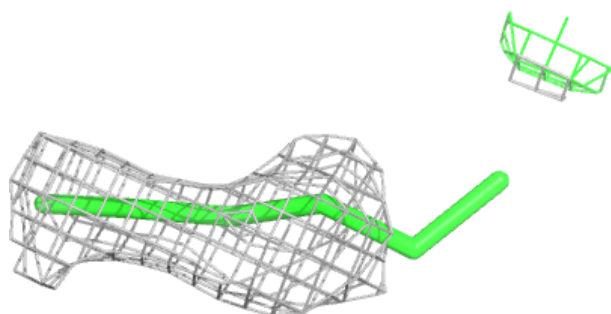
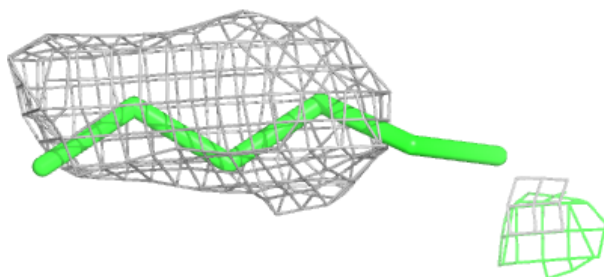
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LFA	C	317	6/20	0.81	0.15	54,58,62,64	0
3	OLA	A	802	11/20	0.81	0.13	61,75,94,103	0
2	LFA	B	311	14/20	0.81	0.16	78,96,104,105	0
2	LFA	A	810	9/20	0.81	0.17	78,83,87,88	0
2	LFA	B	304	9/20	0.81	0.12	60,68,74,75	0
2	LFA	A	812	6/20	0.81	0.16	54,62,65,67	0
3	OLA	A	803	20/20	0.82	0.15	68,79,91,95	0
2	LFA	C	310	10/20	0.83	0.12	77,84,89,90	0
2	LFA	A	801	7/20	0.83	0.13	65,67,70,70	0
2	LFA	B	302	7/20	0.84	0.15	71,76,82,84	0
2	LFA	B	312	12/20	0.84	0.16	71,81,89,89	0
2	LFA	C	303	17/20	0.84	0.12	61,67,77,79	0
2	LFA	B	310	8/20	0.85	0.21	73,85,93,93	0
2	LFA	A	807	13/20	0.85	0.17	83,89,106,108	0
3	OLA	B	306	14/20	0.85	0.12	77,84,100,101	0
2	LFA	A	809	15/20	0.86	0.16	72,96,115,117	0
2	LFA	C	307	9/20	0.86	0.11	66,70,79,80	0
3	OLA	C	301	20/20	0.86	0.13	66,78,93,96	0
3	OLA	A	806	19/20	0.86	0.12	61,73,97,98	0
3	OLA	B	301	20/20	0.86	0.14	62,68,110,123	0
2	LFA	B	309	10/20	0.87	0.17	74,101,103,106	0
2	LFA	B	317	14/20	0.88	0.15	64,73,102,107	0
3	OLA	A	804	16/20	0.88	0.14	67,80,108,108	0
2	LFA	B	303	15/20	0.89	0.10	52,58,90,90	0
3	OLA	B	307	16/20	0.90	0.12	60,78,93,95	0
3	OLA	C	304	14/20	0.91	0.11	55,80,110,111	0
3	OLA	C	302	16/20	0.92	0.12	61,75,87,90	0
2	LFA	C	308	13/20	0.92	0.12	60,66,82,82	0

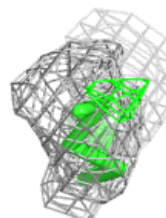
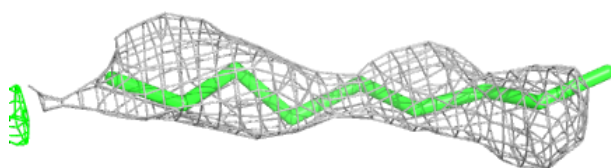
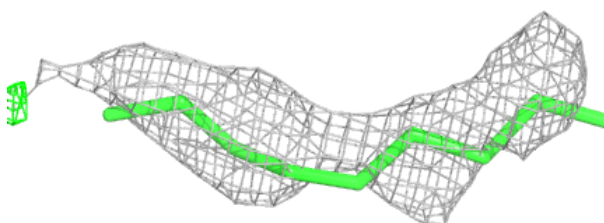
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA C 316:

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

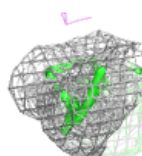
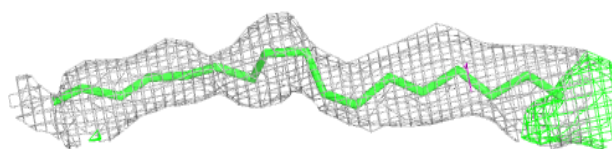
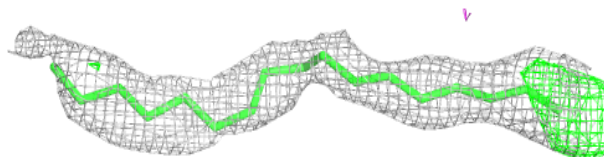
**Electron density around LFA A 811:**

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

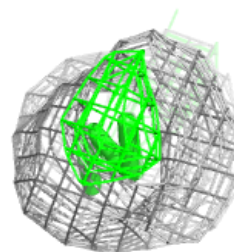
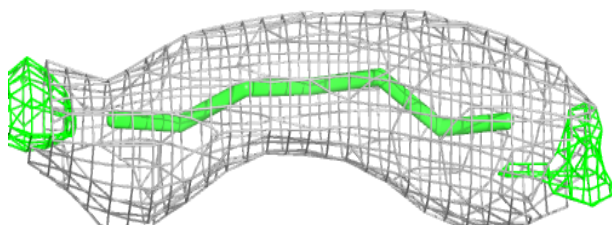
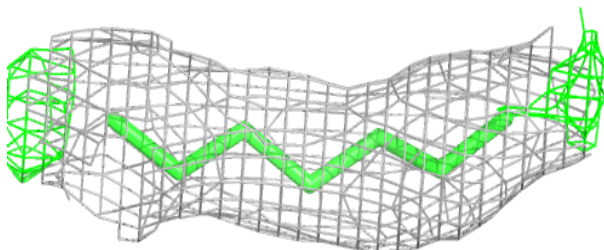


Electron density around LFA C 312:

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

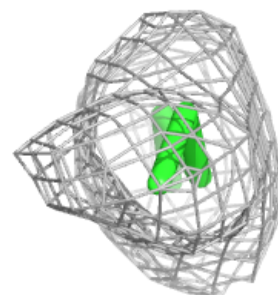
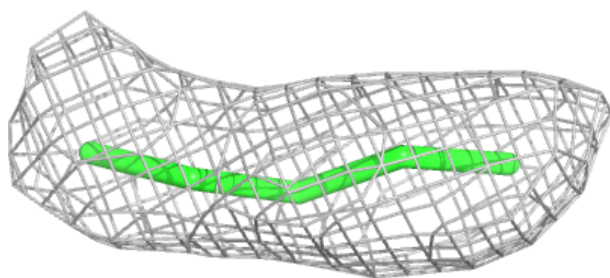
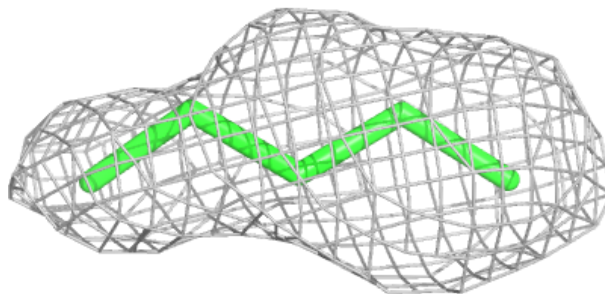
**Electron density around LFA B 314:**

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

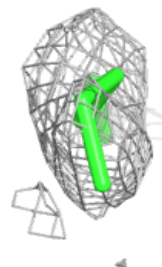
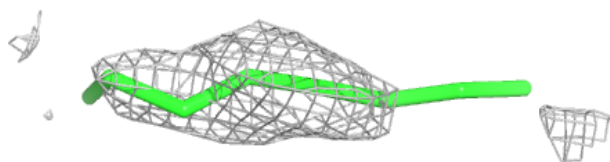
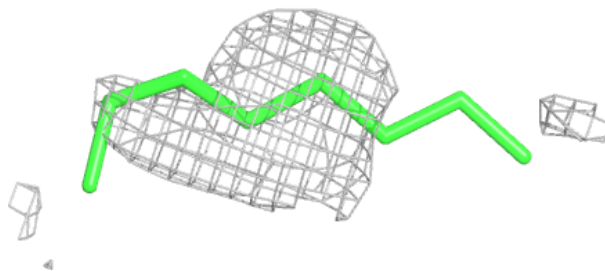


Electron density around LFA B 316:

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

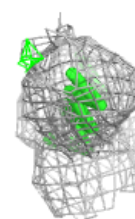
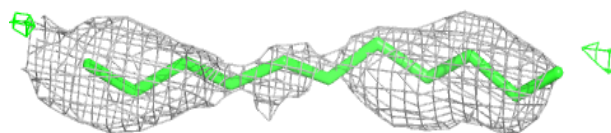
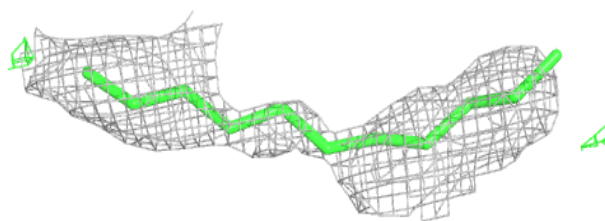
**Electron density around LFA A 814:**

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

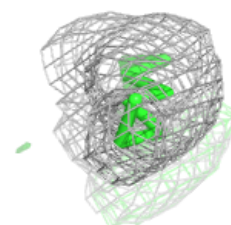
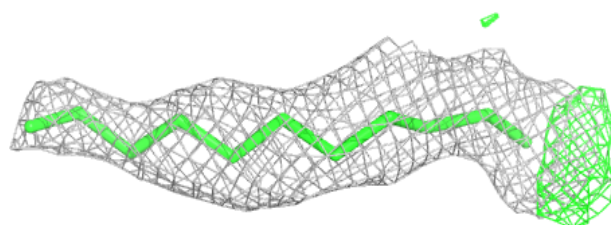
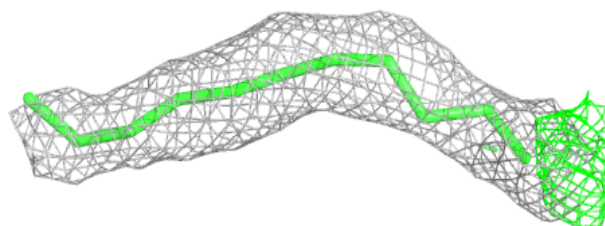


Electron density around LFA C 313:

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

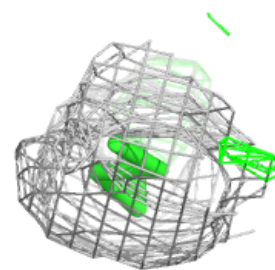
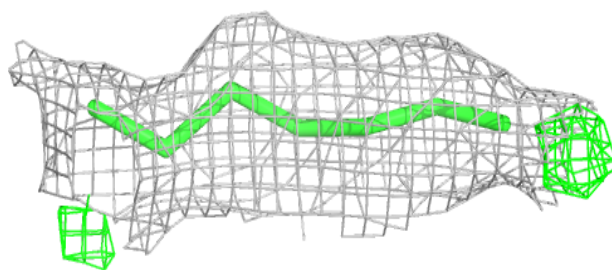
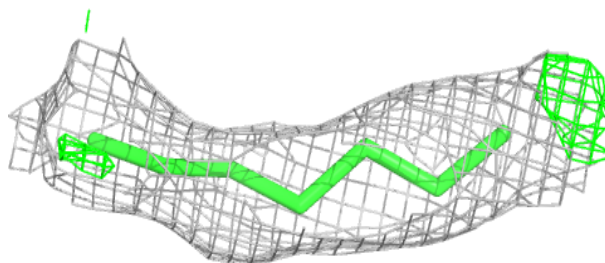
**Electron density around LFA A 808:**

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

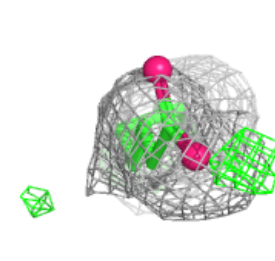
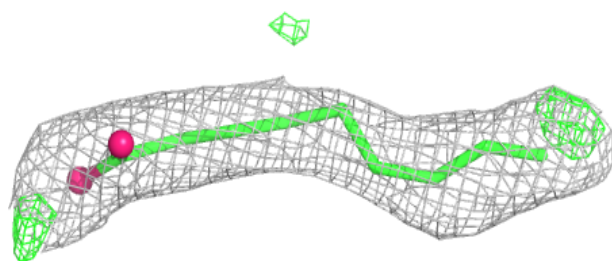
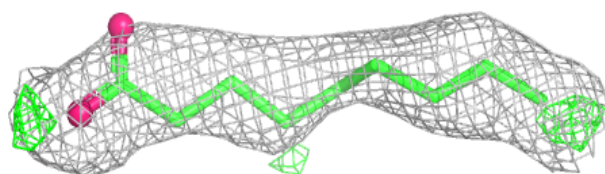


Electron density around LFA B 315:

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

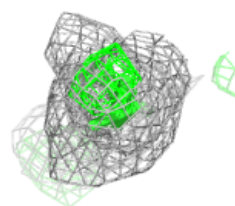
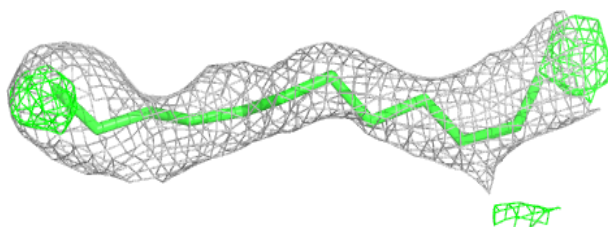
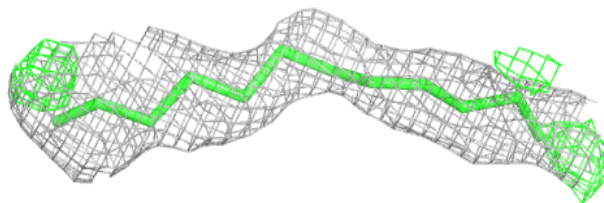
**Electron density around OLA A 805:**

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

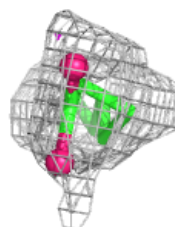
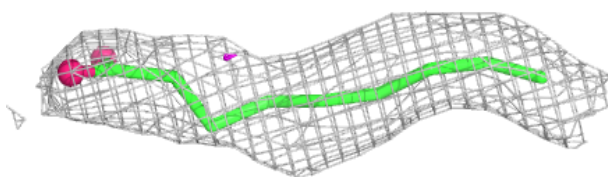
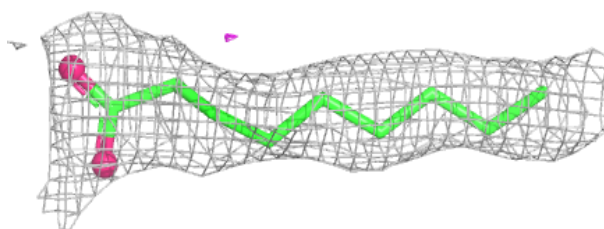


Electron density around LFA A 813:

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

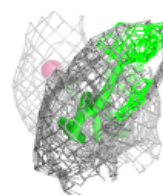
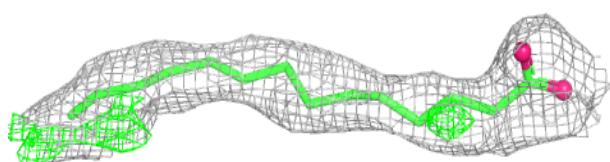
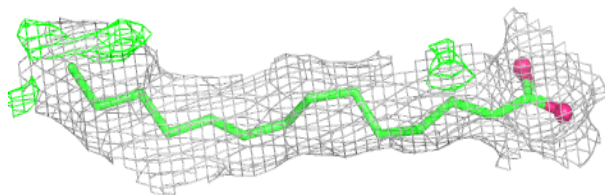
**Electron density around OLA B 308:**

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

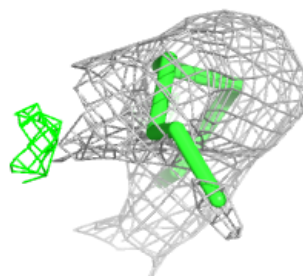
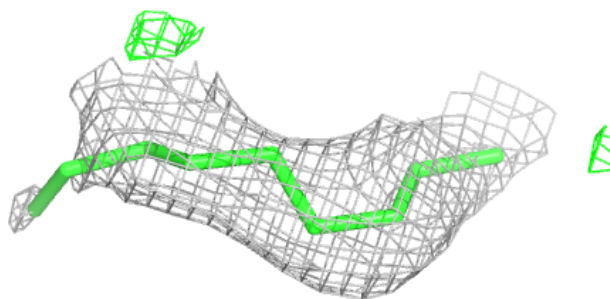
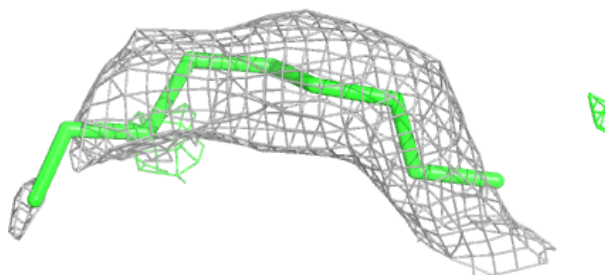


Electron density around OLA C 305:

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

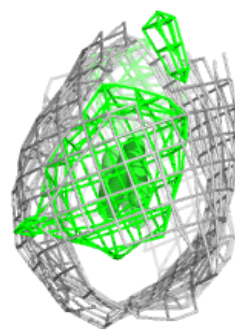
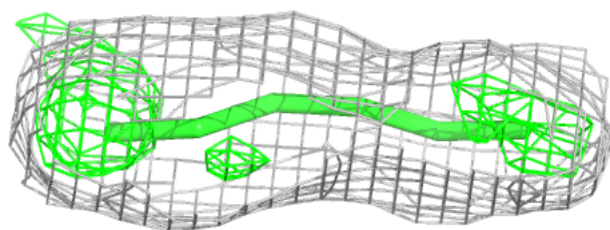
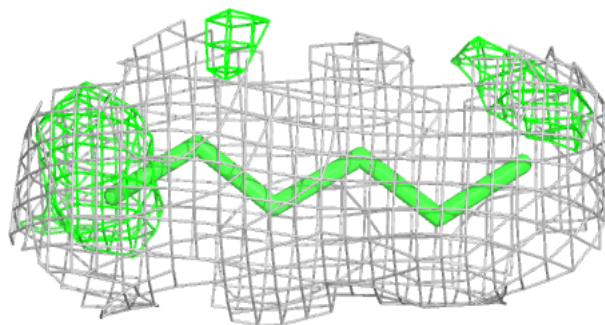
**Electron density around LFA C 311:**

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

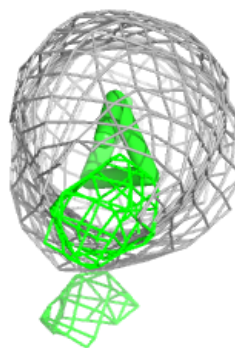
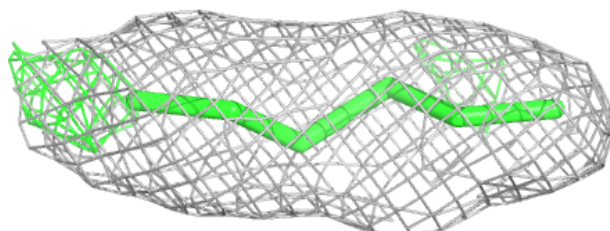
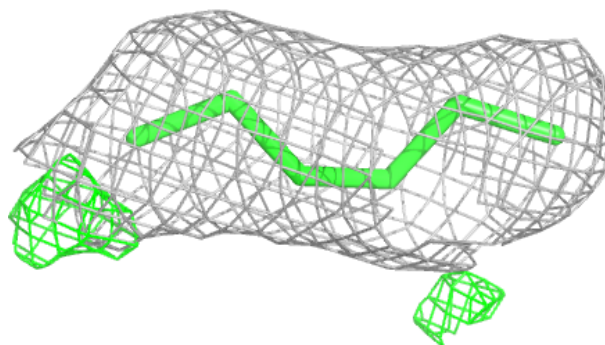


Electron density around LFA A 815:

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

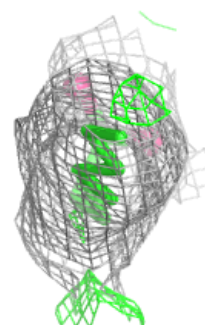
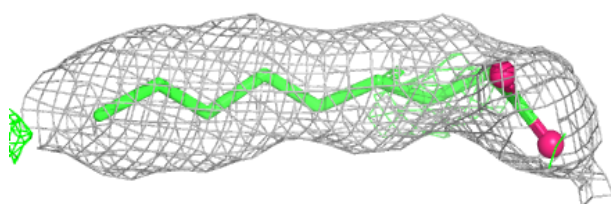
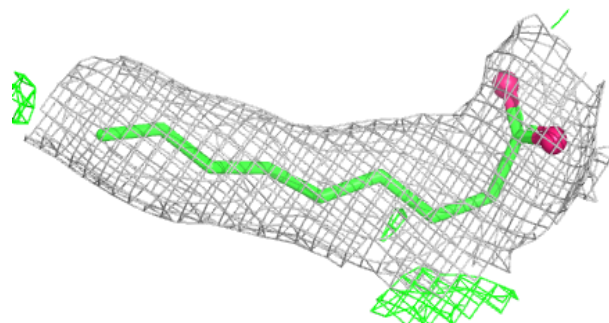
**Electron density around LFA C 317:**

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

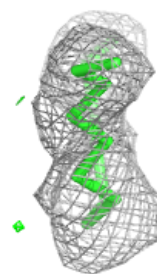
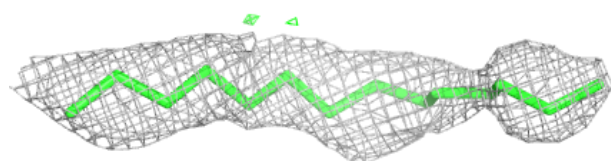
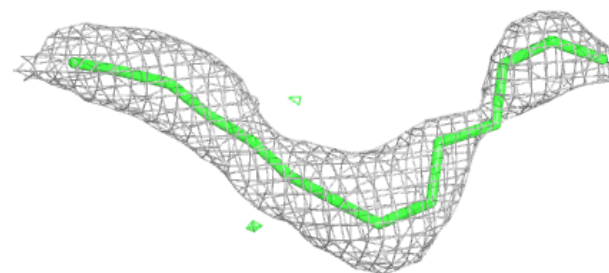


Electron density around OLA A 802:

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

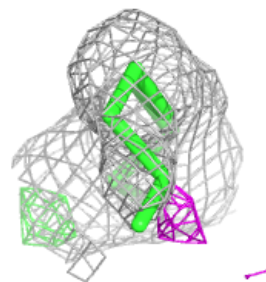
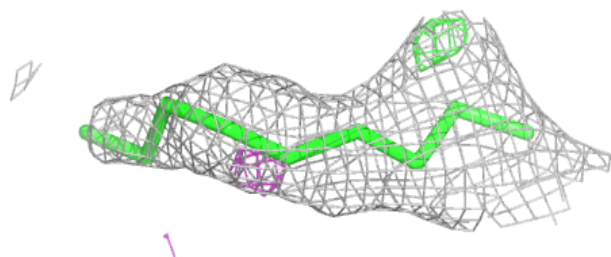
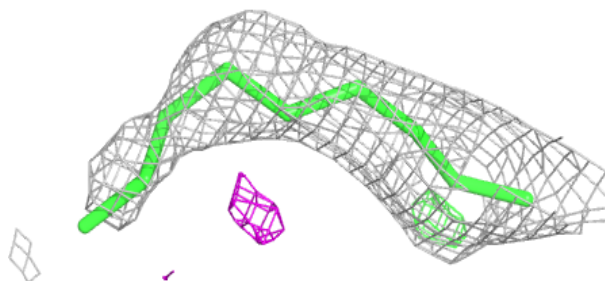
**Electron density around LFA B 311:**

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

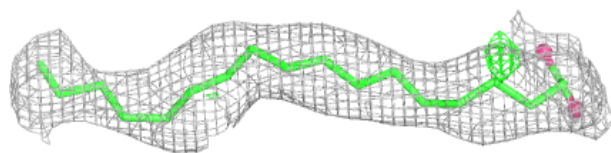
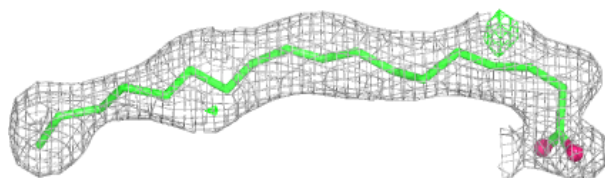


Electron density around LFA A 810:

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

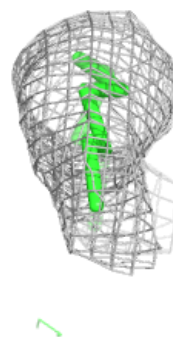
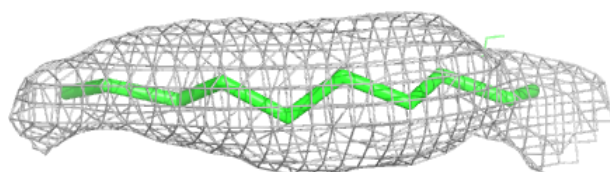
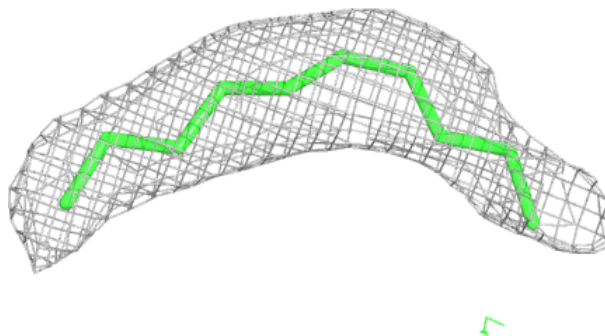
**Electron density around OLA A 803:**

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

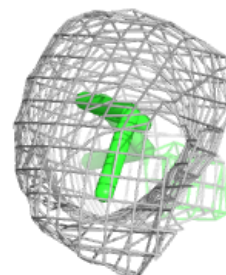
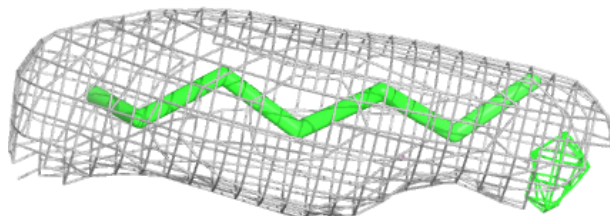
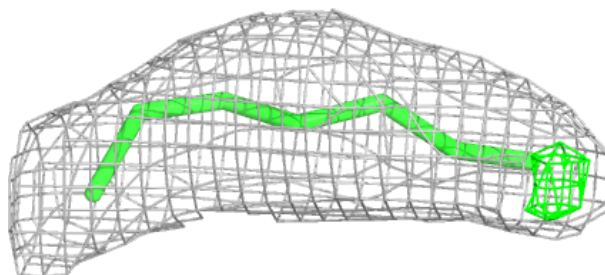


Electron density around LFA C 310:

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

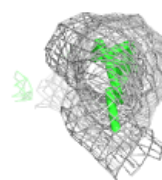
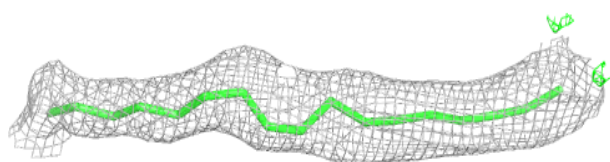
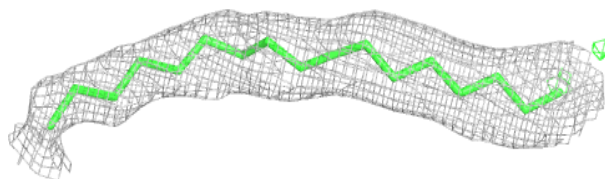
**Electron density around LFA B 302:**

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

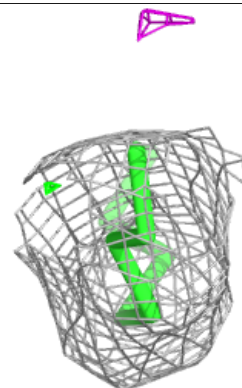
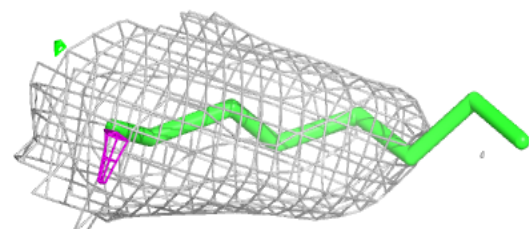
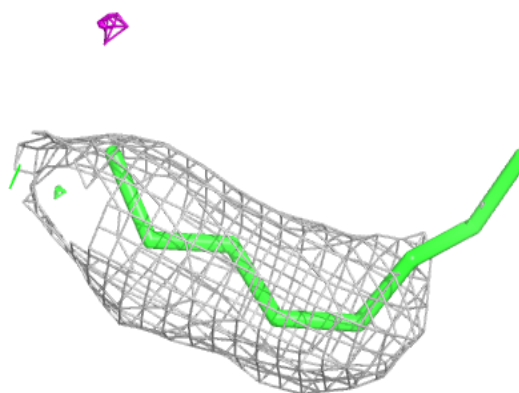


Electron density around LFA C 303:

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

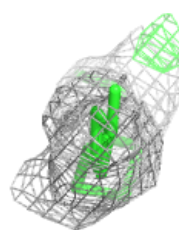
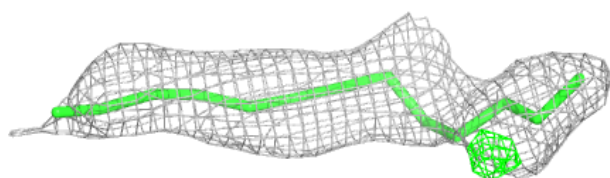
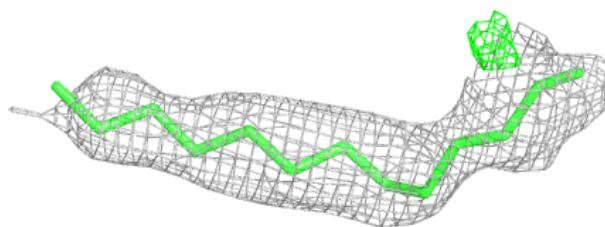
**Electron density around LFA B 310:**

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

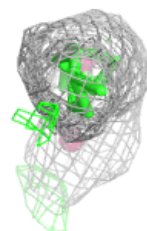
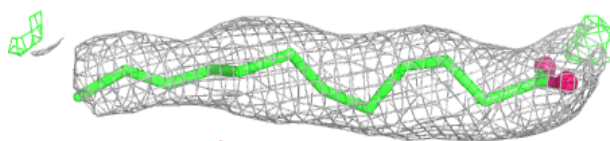
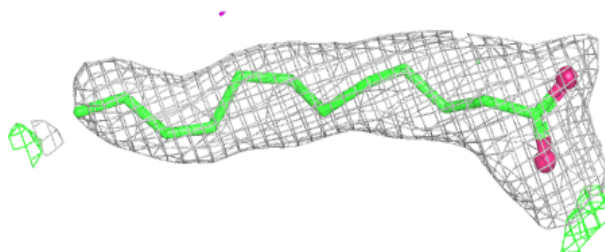


Electron density around LFA A 807:

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

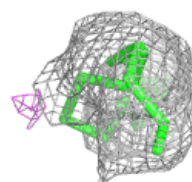
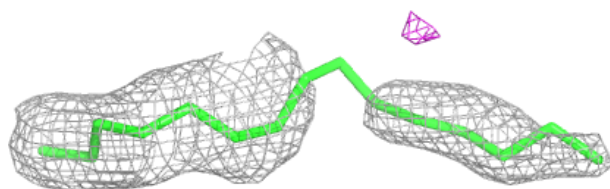
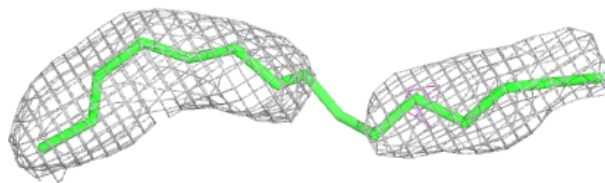
**Electron density around OLA B 306:**

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

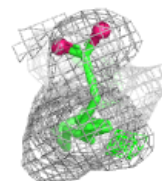
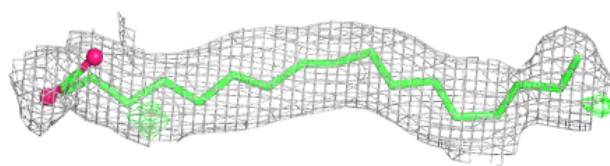
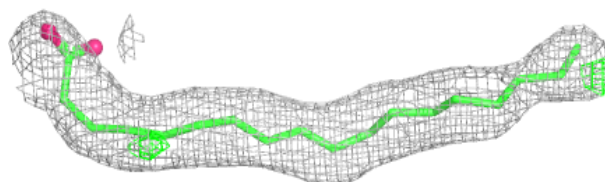


Electron density around LFA A 809:

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

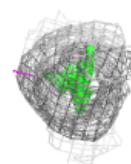
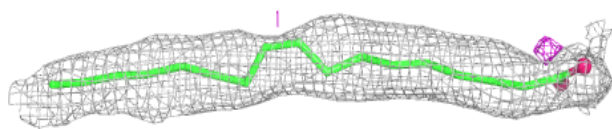
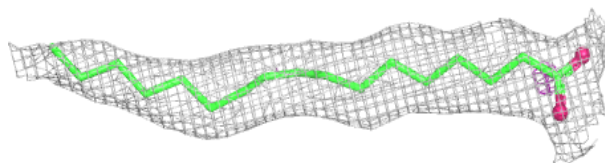
**Electron density around OLA C 301:**

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

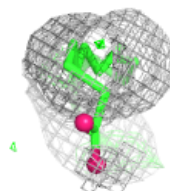
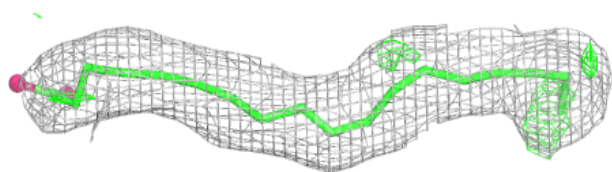
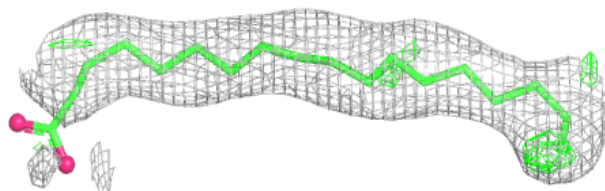


Electron density around OLA A 806:

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

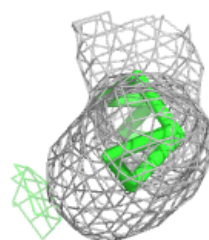
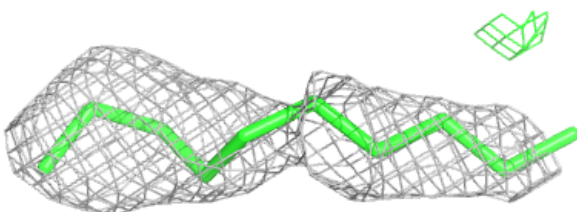
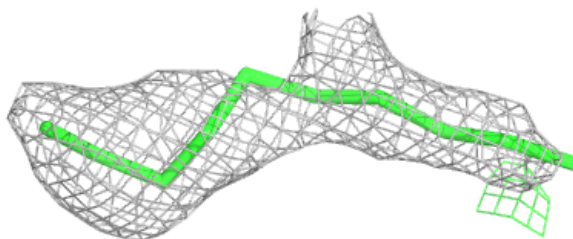
**Electron density around OLA B 301:**

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

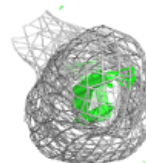
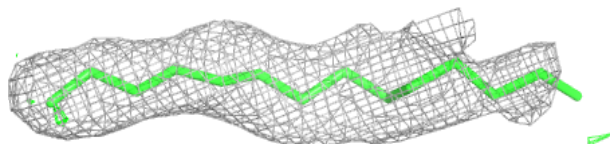
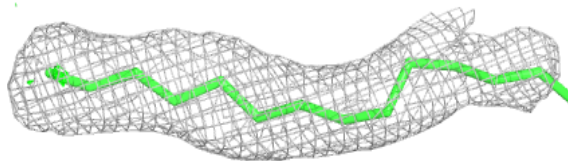


Electron density around LFA B 309:

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

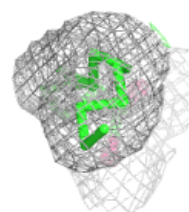
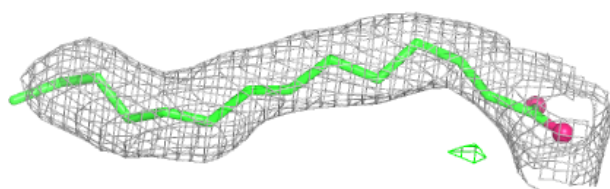
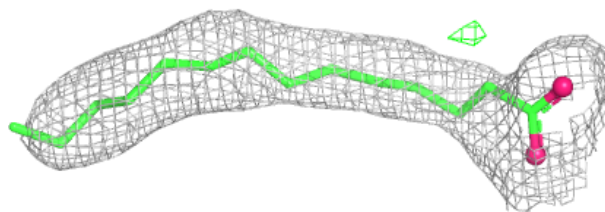
**Electron density around LFA B 317:**

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

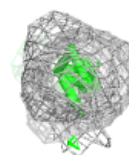
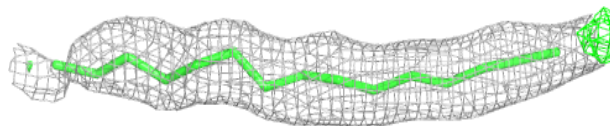
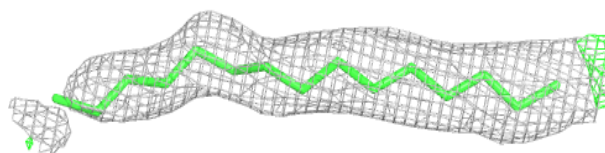


Electron density around OLA A 804:

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

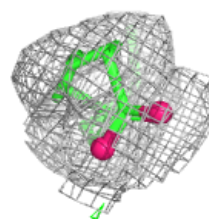
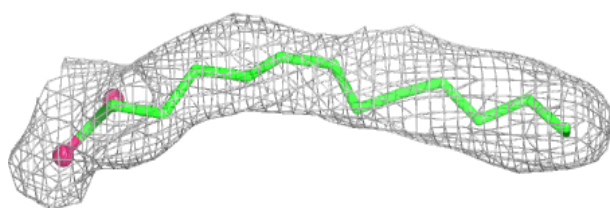
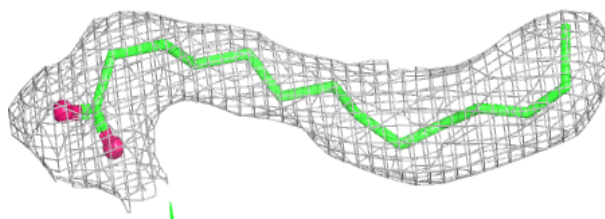
**Electron density around LFA B 303:**

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

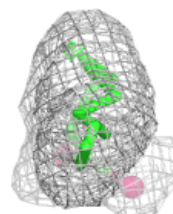
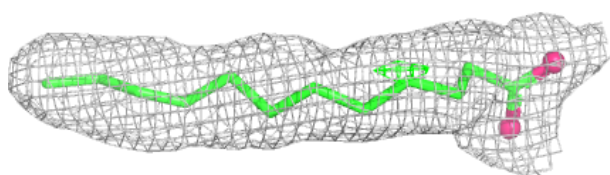
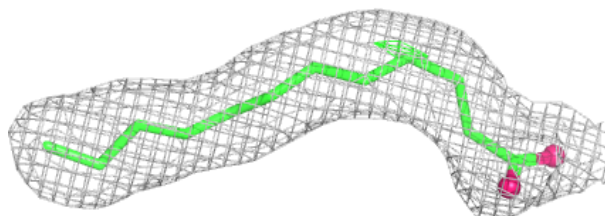


Electron density around OLA B 307:

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

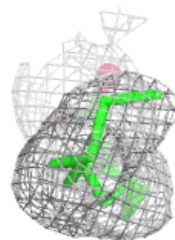
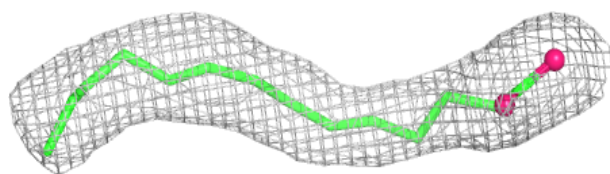
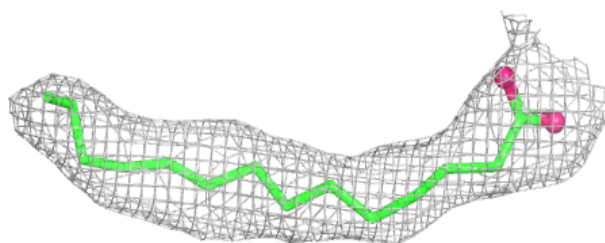
**Electron density around OLA C 304:**

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

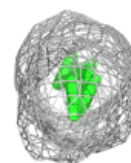
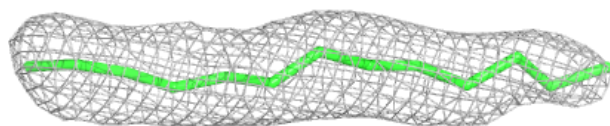
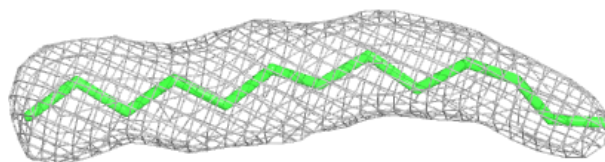


Electron density around OLA C 302:

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

**Electron density around LFA C 308:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.