Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2023 – 02:06 pm BST

PDB ID	:	7ZNE
Title	:	Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the ground state at pH 8.2 at room temperature, 7.5-ms-long snapshots
Authors	:	Kovalev, K.; Tsybrov, F.; Alekseev, A.; Bourenkov, G.; Gordeliy, V.
Deposited on	:	2022-04-20
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

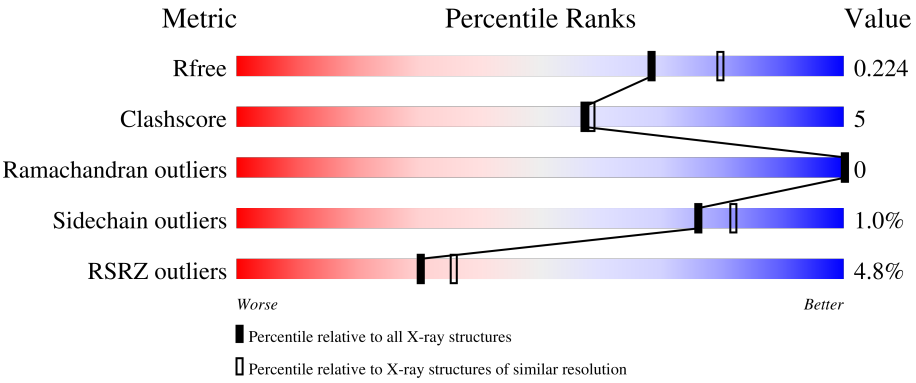
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 83% 13% .
1	B	229	5% 87% 9% .
1	C	229	5% 88% 9% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LFA	B	311	-	-	-	X
2	LFA	C	308	-	-	-	X
2	LFA	C	309	-	-	-	X
4	PO4	C	317	-	-	-	X

2 Entry composition (i)

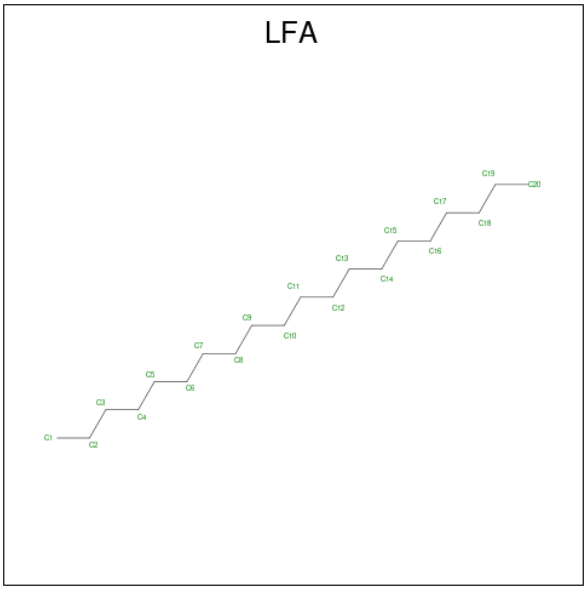
There are 5 unique types of molecules in this entry. The entry contains 5857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	222	Total	C	N	O	S	0	1	0
			1747	1191	261	289	6			
1	B	221	Total	C	N	O	S	0	2	0
			1746	1188	264	289	5			
1	C	223	Total	C	N	O	S	0	1	0
			1756	1196	264	290	6			

- Molecule 2 is EICOSANE (three-letter code: 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
			9	9		
2	A	1	Total	C	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	A	1	Total C 13 13	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 15 15	0	0
2	A	1	Total C 9 9	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 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	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	C	1	Total C 17 17	0	0
2	C	1	Total C 11 11	0	0

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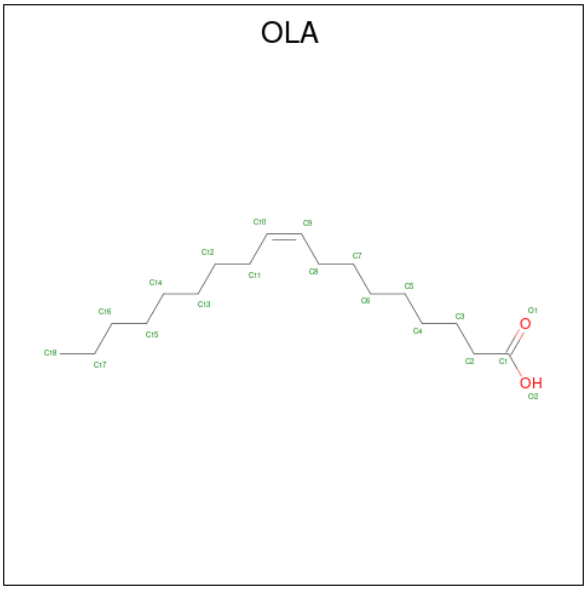
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 4 4	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 13 13	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 17 17	0	0

- Molecule 3 is OLEIC ACID (three-letter code: 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

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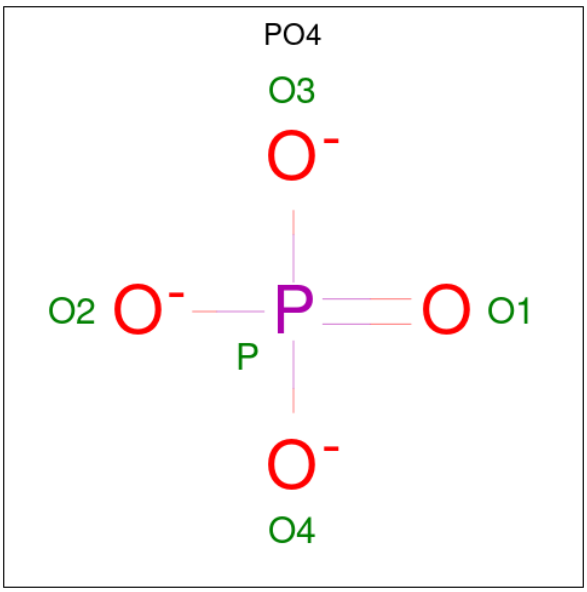
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 16 14 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 19 17 2	0	0
3	B	1	Total C O 20 18 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 16 14 2	0	0
3	B	1	Total C O 11 9 2	0	0
3	C	1	Total C O 14 12 2	0	0
3	C	1	Total C O 16 14 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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

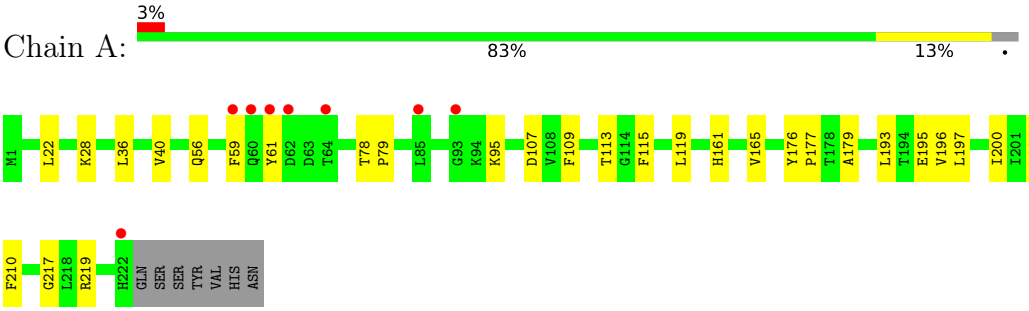
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 28 28	0	1
5	B	21	Total O 22 22	0	1
5	C	24	Total O 25 25	0	1

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.

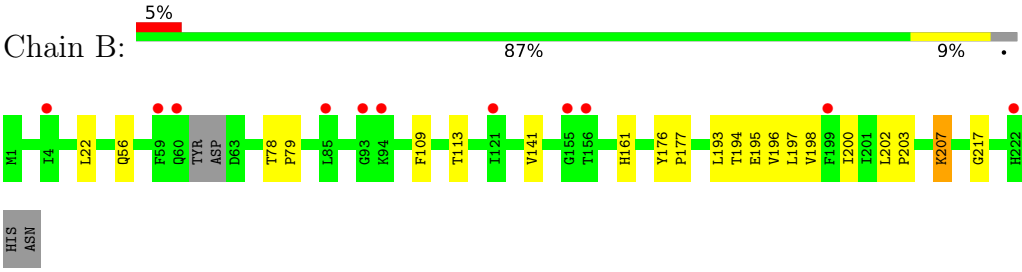
• Molecule 1: xenorhodopsin

Chain A:



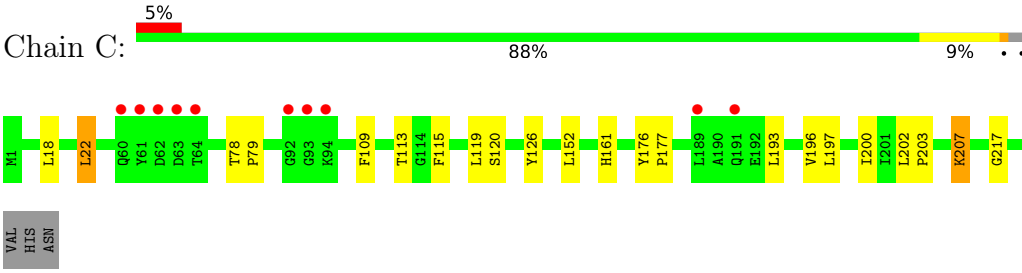
• Molecule 1: xenorhodopsin

Chain B:



• Molecule 1: xenorhodopsin

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.50Å 111.50Å 119.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.10) 100.0 (19.88-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.215 0.198 , 0.224	Depositor DCC
R_{free} test set	1728 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 97.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5857	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, LFA, PO4, FME, 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	0.63	0/1754	0.62	0/2399
1	B	0.63	0/1754	0.61	0/2395
1	C	0.63	0/1763	0.62	0/2411
All	All	0.63	0/5271	0.62	0/7205

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1747	0	1818	23	0
1	B	1746	0	1814	18	0
1	C	1756	0	1824	16	0
2	A	96	0	176	2	0
2	B	112	0	206	3	0
2	C	116	0	214	2	0
3	A	77	0	111	1	0
3	B	61	0	87	4	0
3	C	66	0	95	1	0
4	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	0	0	0
5	B	22	0	0	0	0
5	C	25	0	0	1	0
All	All	5857	0	6345	59	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 (59) 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)
2:C:306:LFA:H131	2:C:315:LFA:C12	1.93	0.96
1:B:207:LYR:H192	1:B:207:LYR:H9	1.75	0.68
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.76	0.68
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.77	0.66
1:C:193:LEU:O	1:C:197:LEU:HD23	1.95	0.66
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.78	0.66
1:B:198:VAL:HG22	2:B:309:LFA:H81	1.78	0.65
1:A:193:LEU:O	1:A:197:LEU:HD23	1.96	0.64
1:B:193:LEU:O	1:B:197:LEU:HD23	1.97	0.64
1:A:165:VAL:HG13	1:A:210:PHE:CE1	2.32	0.63
1:A:207:LYR:H192	1:A:207:LYR:H9	1.81	0.63
1:B:194:THR:HG21	3:B:308:OLA:H21	1.80	0.62
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.36	0.60
1:C:207:LYR:H183	1:C:207:LYR:H9	1.84	0.59
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.37	0.59
1:B:207:LYR:H192	1:B:207:LYR:C9	2.33	0.59
1:C:120:SER:O	5:C:401:HOH:O	2.17	0.59
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.38	0.58
1:C:207:LYR:H9	1:C:207:LYR:H192	1.85	0.58
1:B:195[A]:GLU:HB2	2:B:315:LFA:H11	1.85	0.57
1:A:207:LYR:H192	1:A:207:LYR:C9	2.35	0.56
2:C:306:LFA:C13	2:C:315:LFA:C12	2.77	0.56
1:A:56:GLN:HB3	3:A:804:OLA:H52	1.88	0.56
1:A:207:LYR:H9	1:A:207:LYR:H183	1.89	0.55
1:C:207:LYR:H192	1:C:207:LYR:C9	2.37	0.54
1:A:179:ALA:HA	2:A:815:LFA:H172	1.88	0.54
1:A:78:THR:N	1:A:79:PRO:HD2	2.26	0.51
1:B:207:LYR:H9	1:B:207:LYR:H183	1.92	0.51
1:C:78:THR:N	1:C:79:PRO:HD2	2.27	0.49
1:B:194:THR:HG21	3:B:308:OLA:C2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:VAL:O	1:C:200:ILE:HG12	2.13	0.49
1:A:195:GLU:HB2	2:A:815:LFA:C18	2.43	0.49
1:B:78:THR:N	1:B:79:PRO:HD2	2.27	0.48
1:A:28:LYS:HD2	1:A:219:ARG:NH1	2.28	0.47
1:B:141:VAL:HG22	3:B:306:OLA:H62	1.96	0.47
1:A:202:LEU:CB	1:A:203:PRO:HD3	2.44	0.47
1:A:95:LYS:N	1:A:95:LYS:HD2	2.29	0.47
1:B:195[B]:GLU:HB2	2:B:315:LFA:H11	1.96	0.46
1:A:196:VAL:O	1:A:200:ILE:HG12	2.17	0.45
1:C:126:TYR:CD1	3:C:303:OLA:H52	2.52	0.45
1:A:59:PHE:HE1	1:A:61:TYR:HB2	1.83	0.44
1:B:176:TYR:N	1:B:177:PRO:HD2	2.33	0.44
1:B:56:GLN:HG2	3:B:307:OLA:H31	2.00	0.43
1:B:196:VAL:O	1:B:200:ILE:HG12	2.17	0.43
1:C:109:PHE:O	1:C:113:THR:HG23	2.18	0.43
1:A:59:PHE:CE1	1:A:61:TYR:HB2	2.53	0.43
1:C:202:LEU:CB	1:C:203:PRO:HD3	2.46	0.43
1:A:165:VAL:CG1	1:A:210:PHE:CE1	3.02	0.43
1:C:22:LEU:HD12	1:C:22:LEU:HA	1.84	0.43
1:B:109:PHE:O	1:B:113:THR:HG23	2.19	0.42
1:C:115:PHE:CZ	1:C:119:LEU:HD11	2.54	0.42
1:B:202:LEU:CB	1:B:203:PRO:HD3	2.46	0.42
1:A:115:PHE:CZ	1:A:119:LEU:HD11	2.55	0.42
1:A:176:TYR:N	1:A:177:PRO:HD2	2.35	0.42
1:C:176:TYR:N	1:C:177:PRO:HD2	2.35	0.42
1:A:36:LEU:O	1:A:40:VAL:HG23	2.21	0.41
1:A:109:PHE:O	1:A:113:THR:HG23	2.20	0.41
1:A:78:THR:OG1	1:A:107:ASP:OD2	2.39	0.40
1:C:207:LYR:H10	1:C:207:LYR:H81	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/229 (96%)	218 (99%)	2 (1%)	0	100	100
1	B	218/229 (95%)	217 (100%)	1 (0%)	0	100	100
1	C	221/229 (96%)	219 (99%)	2 (1%)	0	100	100
All	All	659/687 (96%)	654 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/189 (93%)	175 (99%)	1 (1%)	86	90
1	B	176/189 (93%)	175 (99%)	1 (1%)	86	90
1	C	176/189 (93%)	173 (98%)	3 (2%)	60	67
All	All	528/567 (93%)	523 (99%)	5 (1%)	76	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	B	22	LEU
1	C	18	LEU
1	C	22	LEU
1	C	152	LEU

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

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

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Mol	Chain	Res	Type
1	B	191	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	C	207	1	27,29,30	1.18	3 (11%)	30,37,39	1.09	2 (6%)
1	FME	B	1	1	5,6,10	0.66	0	3,6,11	0.85	0
1	FME	C	1	1	8,9,10	0.40	0	7,9,11	0.63	0
1	FME	A	1	1	8,9,10	0.39	0	7,9,11	0.76	0
1	LYR	A	207	1	27,29,30	1.21	3 (11%)	30,37,39	1.12	2 (6%)
1	LYR	B	207	1	27,29,30	1.22	3 (11%)	30,37,39	1.08	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	C	207	1	-	1/22/40/42	0/1/1/1
1	FME	B	1	1	-	0/2/5/11	-
1	FME	C	1	1	-	1/7/9/11	-
1	FME	A	1	1	-	1/7/9/11	-
1	LYR	A	207	1	-	1/22/40/42	0/1/1/1
1	LYR	B	207	1	-	1/22/40/42	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	LYR	C7-C80	3.69	1.40	1.35
1	A	207	LYR	C7-C80	3.36	1.40	1.35
1	C	207	LYR	C7-C80	3.13	1.39	1.35
1	A	207	LYR	C9-C80	-2.67	1.40	1.45
1	C	207	LYR	C9-C80	-2.67	1.40	1.45
1	B	207	LYR	C9-C80	-2.66	1.40	1.45
1	A	207	LYR	C4-C3	-2.22	1.46	1.50
1	C	207	LYR	C4-C3	-2.02	1.46	1.50
1	B	207	LYR	C4-C3	-2.01	1.46	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	LYR	C8-C80-C7	-4.17	117.08	122.92
1	C	207	LYR	C8-C80-C7	-4.16	117.09	122.92
1	B	207	LYR	C8-C80-C7	-4.11	117.17	122.92
1	C	207	LYR	C8-C80-C9	2.47	121.97	118.08
1	B	207	LYR	C8-C80-C9	2.35	121.78	118.08
1	A	207	LYR	C8-C80-C9	2.33	121.75	118.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1	FME	CB-CG-SD-CE
1	B	207	LYR	CD-CE-NZ-C1
1	C	207	LYR	CD-CE-NZ-C1
1	A	1	FME	CA-CB-CG-SD
1	A	207	LYR	CD-CE-NZ-C1

There are no ring outliers.

3 monomers are involved in 10 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

48 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	312	-	4,4,19	0.15	0	3,3,18	0.23	0
2	LFA	A	810	-	7,7,19	0.11	0	6,6,18	0.09	0
2	LFA	C	313	-	5,5,19	0.11	0	4,4,18	0.10	0
3	OLA	A	804	-	15,15,19	0.58	0	15,15,19	0.53	0
2	LFA	B	316	-	13,13,19	0.09	0	12,12,18	0.07	0
2	LFA	A	815	-	8,8,19	0.09	0	7,7,18	0.11	0
2	LFA	C	312	-	12,12,19	0.09	0	11,11,18	0.08	0
2	LFA	B	303	-	14,14,19	0.09	0	13,13,18	0.08	0
2	LFA	B	313	-	13,13,19	0.09	0	12,12,18	0.12	0
3	OLA	C	305	-	15,15,19	0.60	0	15,15,19	0.53	0
2	LFA	A	814	-	14,14,19	0.10	0	13,13,18	0.06	0
3	OLA	B	307	-	15,15,19	0.60	0	15,15,19	0.53	0
2	LFA	C	301	-	16,16,19	0.10	0	15,15,18	0.07	0
2	LFA	A	808	-	5,5,19	0.12	0	4,4,18	0.10	0
2	LFA	C	314	-	9,9,19	0.10	0	8,8,18	0.08	0
2	LFA	B	302	-	6,6,19	0.10	0	5,5,18	0.13	0
2	LFA	C	308	-	7,7,19	0.11	0	6,6,18	0.07	0
2	LFA	B	311	-	6,6,19	0.13	0	5,5,18	0.08	0
2	LFA	A	811	-	5,5,19	0.12	0	4,4,18	0.08	0
3	OLA	A	802	-	10,10,19	0.68	0	10,10,19	0.63	0
2	LFA	B	310	-	6,6,19	0.11	0	5,5,18	0.09	0
2	LFA	C	316	-	16,16,19	0.09	0	15,15,18	0.08	0
3	OLA	B	301	-	19,19,19	0.50	0	19,19,19	0.49	0
2	LFA	C	315	-	8,8,19	0.10	0	7,7,18	0.07	0
2	LFA	B	309	-	8,8,19	0.10	0	7,7,18	0.11	0
2	LFA	C	311	-	8,8,19	0.10	0	7,7,18	0.09	0
3	OLA	B	308	-	10,10,19	0.68	0	10,10,19	0.64	0
2	LFA	B	304	-	8,8,19	0.10	0	7,7,18	0.07	0
3	OLA	A	803	-	19,19,19	0.52	0	19,19,19	0.47	0
2	LFA	A	807	-	8,8,19	0.10	0	7,7,18	0.07	0
3	OLA	A	806	-	18,18,19	0.54	0	18,18,19	0.47	0
2	LFA	A	812	-	12,12,19	0.07	0	11,11,18	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LFA	A	801	-	6,6,19	0.12	0	5,5,18	0.14	0
3	OLA	C	302	-	13,13,19	0.61	0	12,13,19	0.59	0
2	LFA	A	809	-	11,11,19	0.11	0	10,10,18	0.05	0
2	LFA	C	307	-	3,3,19	0.23	0	2,2,18	0.46	0
3	OLA	A	805	-	10,10,19	0.71	0	10,10,19	0.59	0
3	OLA	B	306	-	13,13,19	0.62	0	12,13,19	0.56	0
3	OLA	C	304	-	19,19,19	0.51	0	19,19,19	0.50	0
2	LFA	C	309	-	5,5,19	0.11	0	4,4,18	0.10	0
2	LFA	A	813	-	10,10,19	0.10	0	9,9,18	0.07	0
2	LFA	C	310	-	5,5,19	0.14	0	4,4,18	0.10	0
3	OLA	C	303	-	15,15,19	0.58	0	15,15,19	0.53	0
2	LFA	B	315	-	7,7,19	0.11	0	6,6,18	0.09	0
2	LFA	B	314	-	9,9,19	0.09	0	8,8,18	0.07	0
2	LFA	B	305	-	6,6,19	0.12	0	5,5,18	0.07	0
4	PO4	C	317	-	4,4,4	0.66	0	6,6,6	0.42	0
2	LFA	C	306	-	10,10,19	0.09	0	9,9,18	0.08	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	312	-	-	1/2/2/17	-
2	LFA	A	810	-	-	1/5/5/17	-
2	LFA	C	313	-	-	0/3/3/17	-
3	OLA	A	804	-	-	6/13/13/17	-
2	LFA	B	316	-	-	1/11/11/17	-
2	LFA	A	815	-	-	2/6/6/17	-
2	LFA	C	312	-	-	4/10/10/17	-
2	LFA	B	303	-	-	4/12/12/17	-
2	LFA	B	313	-	-	3/11/11/17	-
3	OLA	C	305	-	-	4/13/13/17	-
2	LFA	A	814	-	-	5/12/12/17	-
3	OLA	B	307	-	-	6/13/13/17	-
2	LFA	C	301	-	-	5/14/14/17	-
2	LFA	A	808	-	-	0/3/3/17	-
2	LFA	C	314	-	-	0/7/7/17	-
2	LFA	B	302	-	-	0/4/4/17	-
2	LFA	C	308	-	-	3/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	B	311	-	-	2/4/4/17	-
2	LFA	A	811	-	-	1/3/3/17	-
3	OLA	A	802	-	-	2/8/8/17	-
2	LFA	B	310	-	-	1/4/4/17	-
2	LFA	C	316	-	-	1/14/14/17	-
3	OLA	B	301	-	-	6/17/17/17	-
2	LFA	C	315	-	-	0/6/6/17	-
2	LFA	B	309	-	-	0/6/6/17	-
2	LFA	C	311	-	-	0/6/6/17	-
3	OLA	B	308	-	-	4/8/8/17	-
2	LFA	B	304	-	-	0/6/6/17	-
3	OLA	A	803	-	-	10/17/17/17	-
2	LFA	A	807	-	-	2/6/6/17	-
3	OLA	A	806	-	-	2/16/16/17	-
2	LFA	A	812	-	-	2/10/10/17	-
2	LFA	A	801	-	-	0/4/4/17	-
3	OLA	C	302	-	-	5/11/11/17	-
2	LFA	A	809	-	-	2/9/9/17	-
2	LFA	C	307	-	-	0/1/1/17	-
3	OLA	A	805	-	-	1/8/8/17	-
3	OLA	B	306	-	-	9/11/11/17	-
3	OLA	C	304	-	-	8/17/17/17	-
2	LFA	C	309	-	-	2/3/3/17	-
2	LFA	A	813	-	-	2/8/8/17	-
2	LFA	C	310	-	-	0/3/3/17	-
3	OLA	C	303	-	-	5/13/13/17	-
2	LFA	B	315	-	-	0/5/5/17	-
2	LFA	B	314	-	-	1/7/7/17	-
2	LFA	B	305	-	-	0/4/4/17	-
2	LFA	C	306	-	-	1/8/8/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	306	OLA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	C	302	OLA	C9-C10-C11-C12
3	B	307	OLA	C11-C10-C9-C8
3	B	308	OLA	C1-C2-C3-C4
2	B	313	LFA	C11-C10-C9-C8
3	B	306	OLA	C3-C4-C5-C6
3	C	303	OLA	C4-C5-C6-C7
3	C	302	OLA	C11-C10-C9-C8
3	A	803	OLA	C5-C6-C7-C8
2	C	301	LFA	C11-C10-C9-C8
3	A	805	OLA	C4-C5-C6-C7
3	A	803	OLA	C10-C11-C12-C13
2	A	807	LFA	C4-C5-C6-C7
2	B	303	LFA	C4-C5-C6-C7
2	B	303	LFA	C3-C4-C5-C6
3	A	803	OLA	C3-C4-C5-C6
2	B	311	LFA	C3-C4-C5-C6
2	A	814	LFA	C6-C7-C8-C9
3	A	803	OLA	C4-C5-C6-C7
2	C	316	LFA	C11-C10-C9-C8
2	B	303	LFA	C6-C7-C8-C9
2	B	310	LFA	C2-C3-C4-C5
3	A	806	OLA	C6-C7-C8-C9
3	A	804	OLA	C11-C10-C9-C8
2	A	813	LFA	C15-C16-C17-C18
3	B	307	OLA	C5-C6-C7-C8
2	B	316	LFA	C12-C13-C14-C15
2	C	301	LFA	C9-C10-C11-C12
2	C	308	LFA	C17-C18-C19-C20
3	A	803	OLA	C6-C7-C8-C9
3	B	307	OLA	C6-C7-C8-C9
3	B	301	OLA	C11-C12-C13-C14
3	B	306	OLA	C11-C10-C9-C8
2	A	809	LFA	C9-C10-C11-C12
2	A	807	LFA	C6-C7-C8-C9
2	C	308	LFA	C16-C17-C18-C19
3	B	306	OLA	C5-C6-C7-C8
3	C	302	OLA	C5-C6-C7-C8
3	C	303	OLA	C5-C6-C7-C8
3	C	303	OLA	C2-C3-C4-C5
2	A	814	LFA	C11-C12-C13-C14
2	A	812	LFA	C5-C6-C7-C8
3	B	307	OLA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	C	309	LFA	C4-C5-C6-C7
3	A	804	OLA	C4-C5-C6-C7
3	C	304	OLA	C5-C6-C7-C8
2	A	810	LFA	C3-C4-C5-C6
2	C	312	LFA	C9-C10-C11-C12
3	A	803	OLA	C14-C15-C16-C17
2	A	813	LFA	C10-C11-C12-C13
2	A	814	LFA	C2-C3-C4-C5
3	C	304	OLA	C11-C10-C9-C8
3	A	804	OLA	C5-C6-C7-C8
3	B	301	OLA	C6-C7-C8-C9
3	B	306	OLA	C1-C2-C3-C4
2	C	301	LFA	C10-C11-C12-C13
2	C	301	LFA	C5-C6-C7-C8
2	A	812	LFA	C7-C8-C9-C10
2	C	309	LFA	C3-C4-C5-C6
3	A	803	OLA	C7-C8-C9-C10
3	C	304	OLA	C7-C8-C9-C10
2	B	313	LFA	C7-C8-C9-C10
3	C	304	OLA	C1-C2-C3-C4
3	B	301	OLA	C15-C16-C17-C18
2	B	314	LFA	C4-C5-C6-C7
2	C	312	LFA	C6-C7-C8-C9
2	C	308	LFA	C13-C14-C15-C16
3	B	307	OLA	O2-C1-C2-C3
3	A	804	OLA	O2-C1-C2-C3
3	C	304	OLA	C2-C3-C4-C5
3	A	804	OLA	O1-C1-C2-C3
3	C	305	OLA	O1-C1-C2-C3
3	B	308	OLA	O2-C1-C2-C3
3	B	307	OLA	O1-C1-C2-C3
2	A	814	LFA	C9-C10-C11-C12
2	B	313	LFA	C3-C4-C5-C6
3	B	308	OLA	O1-C1-C2-C3
3	B	306	OLA	C4-C5-C6-C7
2	A	814	LFA	C10-C11-C12-C13
3	C	305	OLA	O2-C1-C2-C3
3	C	304	OLA	C10-C11-C12-C13
2	B	311	LFA	C2-C3-C4-C5
3	B	306	OLA	O1-C1-C2-C3
3	B	306	OLA	O2-C1-C2-C3
2	A	809	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	815	LFA	C13-C14-C15-C16
3	B	301	OLA	C12-C13-C14-C15
2	C	301	LFA	C13-C14-C15-C16
3	B	301	OLA	O2-C1-C2-C3
3	A	802	OLA	O2-C1-C2-C3
3	C	302	OLA	O2-C1-C2-C3
3	A	803	OLA	O2-C1-C2-C3
3	A	802	OLA	O1-C1-C2-C3
3	A	806	OLA	C9-C10-C11-C12
3	B	301	OLA	O1-C1-C2-C3
3	A	803	OLA	O1-C1-C2-C3
2	B	312	LFA	C16-C17-C18-C19
3	B	306	OLA	C7-C8-C9-C10
3	C	305	OLA	C7-C8-C9-C10
2	C	312	LFA	C2-C3-C4-C5
3	B	308	OLA	C2-C3-C4-C5
3	C	302	OLA	O1-C1-C2-C3
2	C	312	LFA	C11-C10-C9-C8
2	B	303	LFA	C11-C10-C9-C8
3	A	803	OLA	C13-C14-C15-C16
2	A	815	LFA	C11-C12-C13-C14
3	C	305	OLA	C3-C4-C5-C6
3	A	804	OLA	C7-C8-C9-C10
2	A	811	LFA	C2-C3-C4-C5
3	C	303	OLA	O2-C1-C2-C3
3	C	304	OLA	O2-C1-C2-C3
3	C	304	OLA	O1-C1-C2-C3
2	C	306	LFA	C10-C11-C12-C13
3	C	303	OLA	C7-C8-C9-C10

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	OLA	1	0
2	A	815	LFA	2	0
3	B	307	OLA	1	0
2	C	315	LFA	2	0
2	B	309	LFA	1	0
3	B	308	OLA	2	0
3	B	306	OLA	1	0
3	C	303	OLA	1	0

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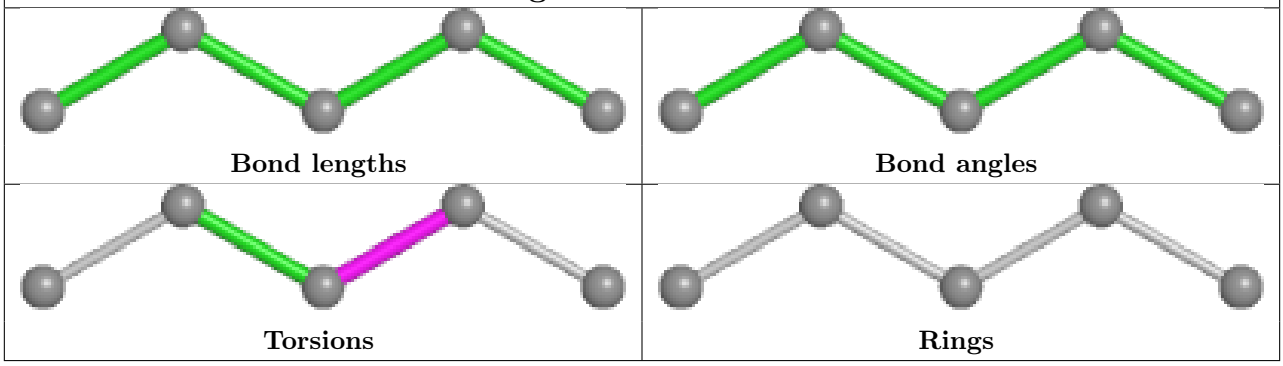
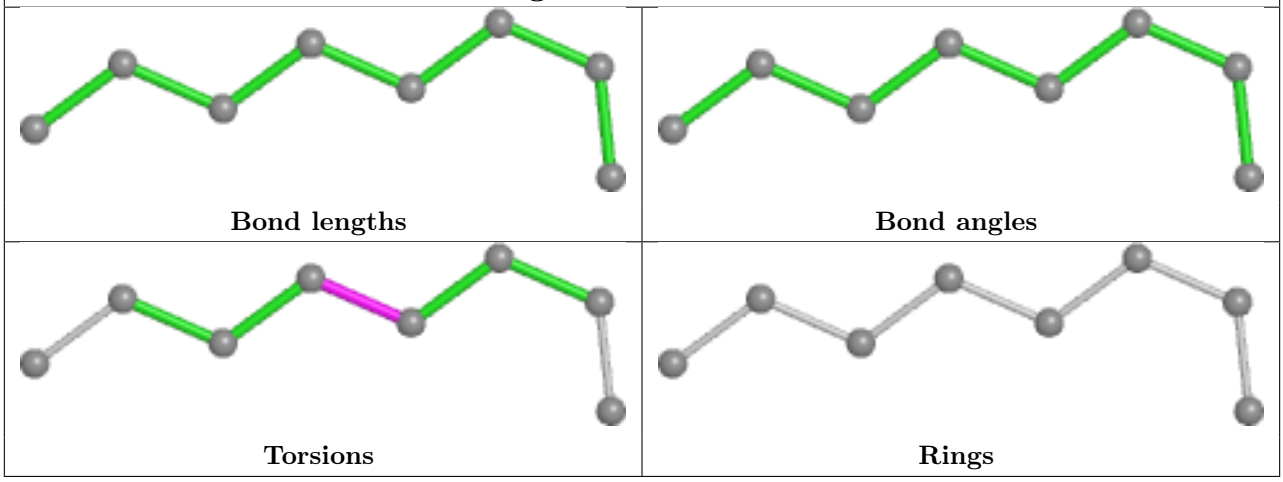
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	315	LFA	2	0
2	C	306	LFA	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

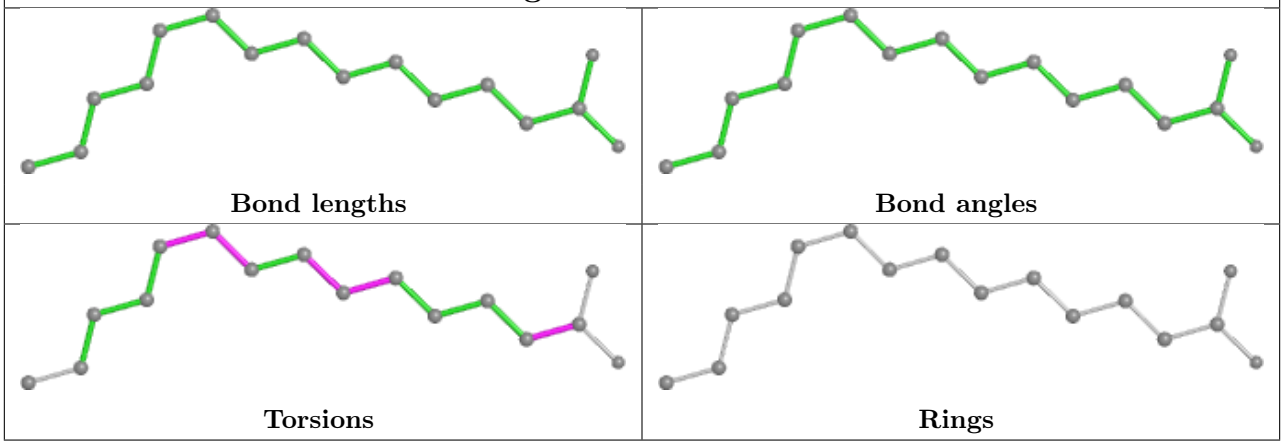
Ligand LFA B 312



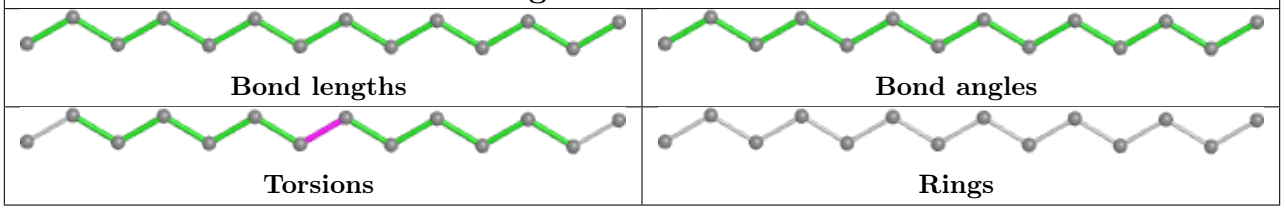
Ligand LFA A 810



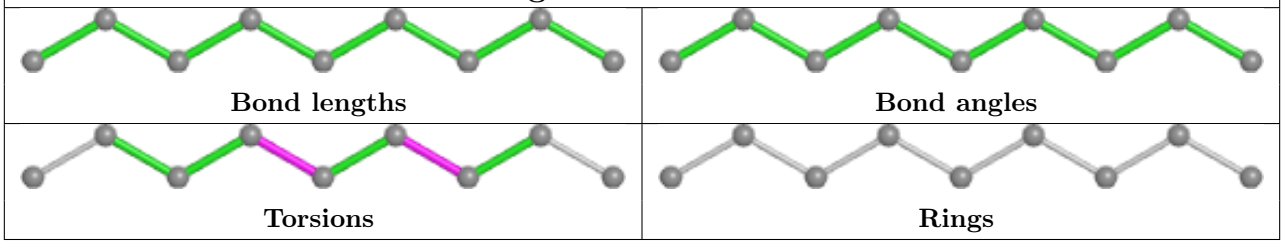
Ligand OLA A 804



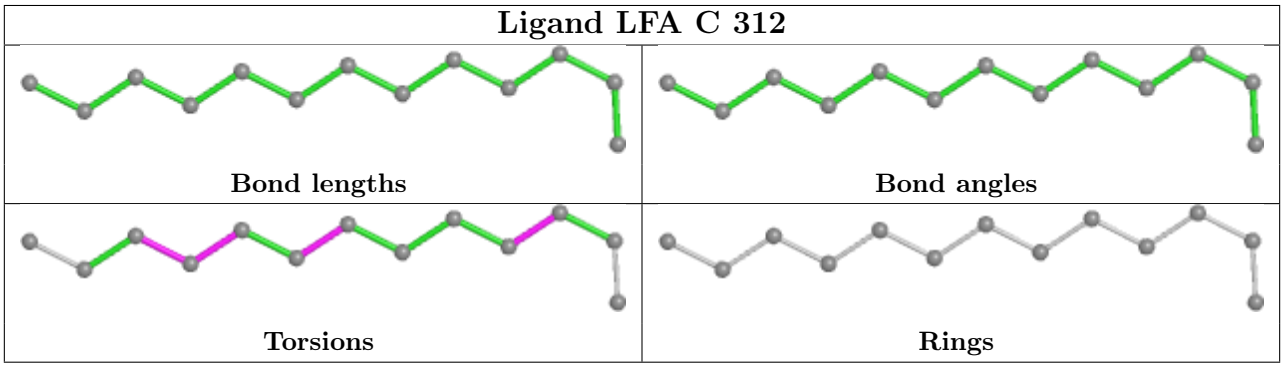
Ligand LFA B 316



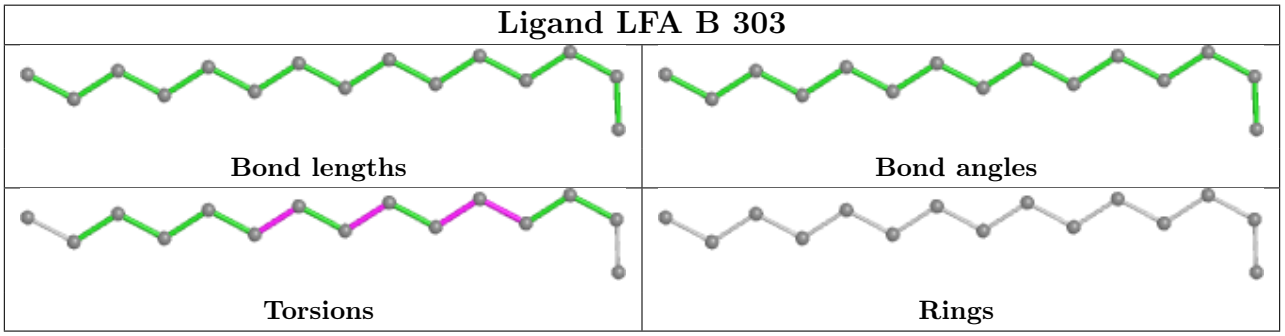
Ligand LFA A 815



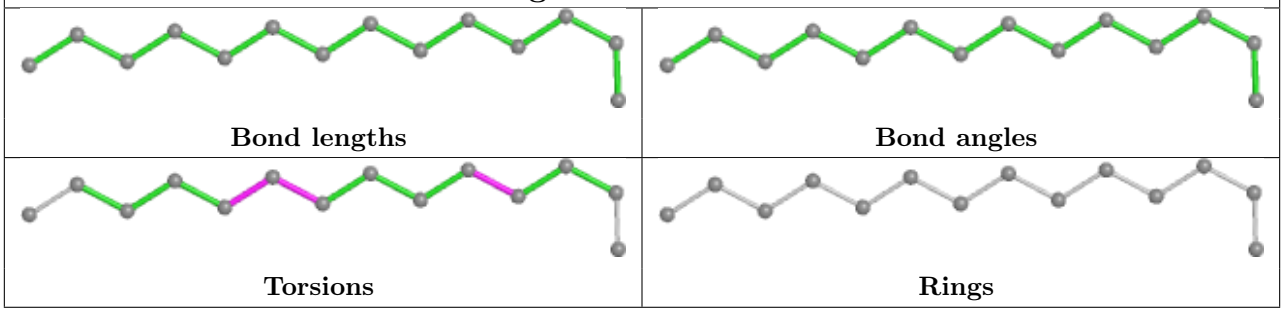
Ligand LFA C 312



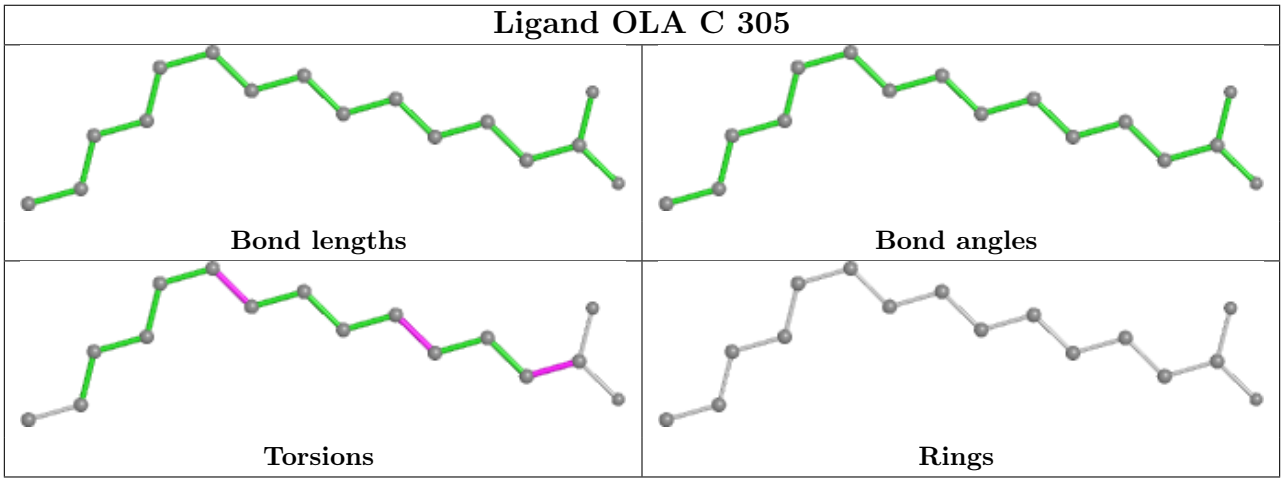
Ligand LFA B 303



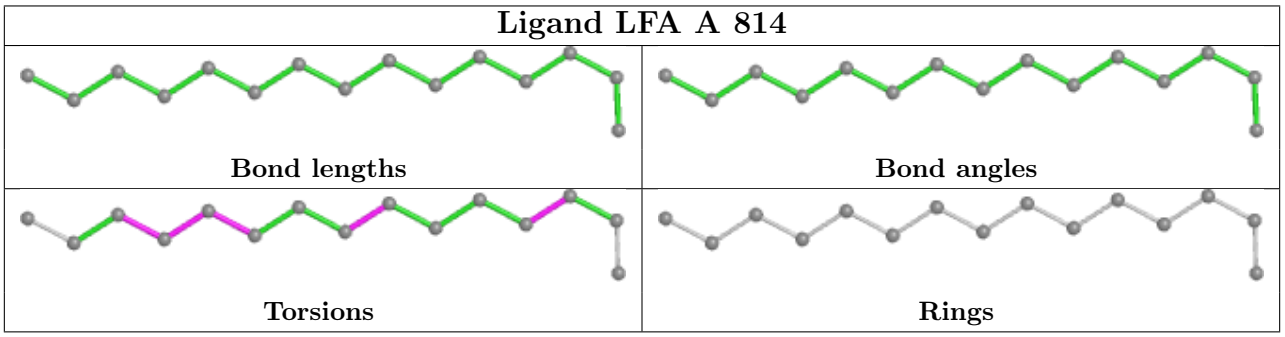
Ligand LFA B 313



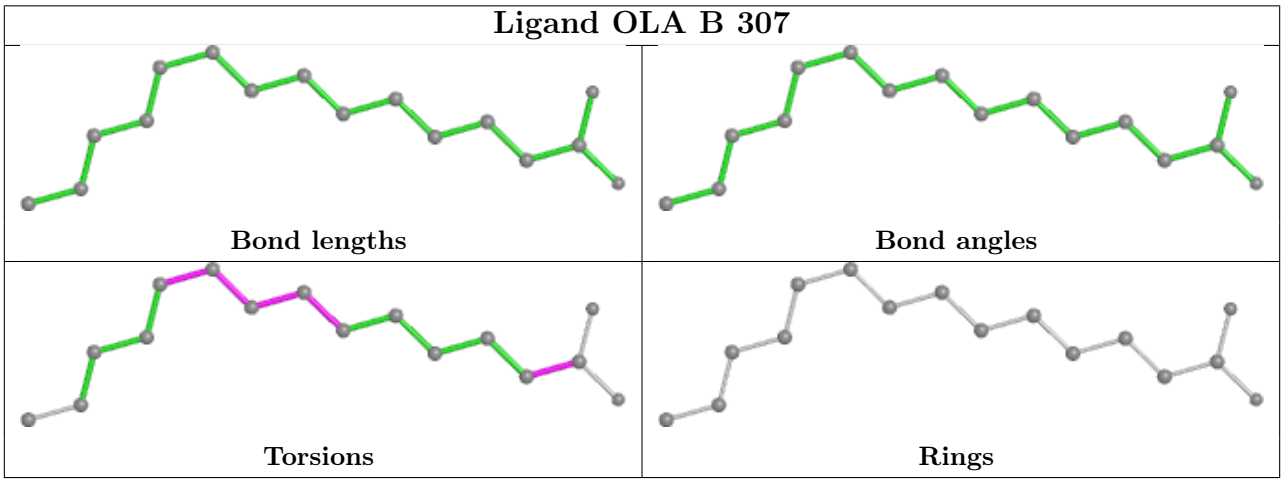
Ligand OLA C 305



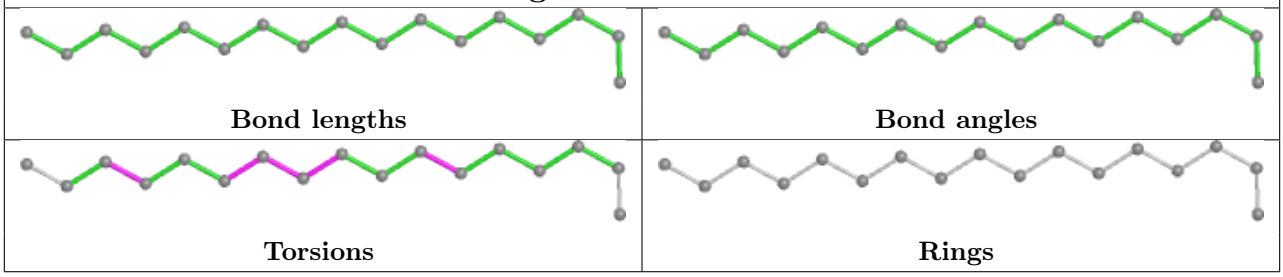
Ligand LFA A 814



Ligand OLA B 307



Ligand LFA C 301



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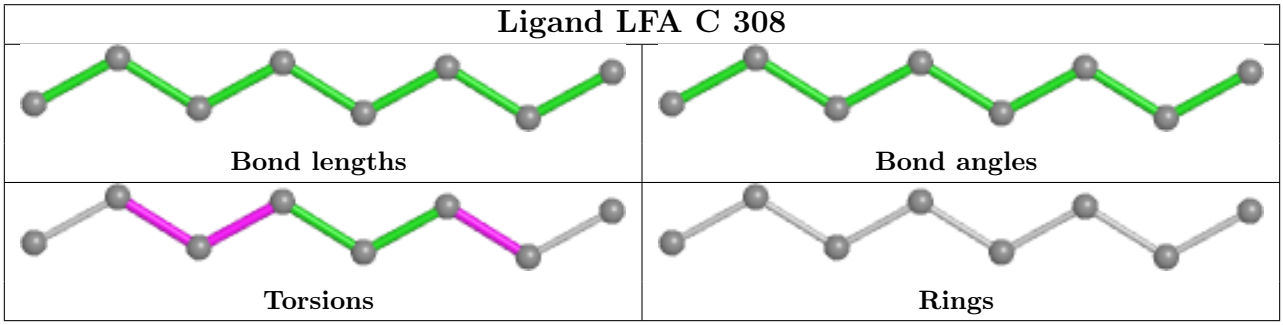

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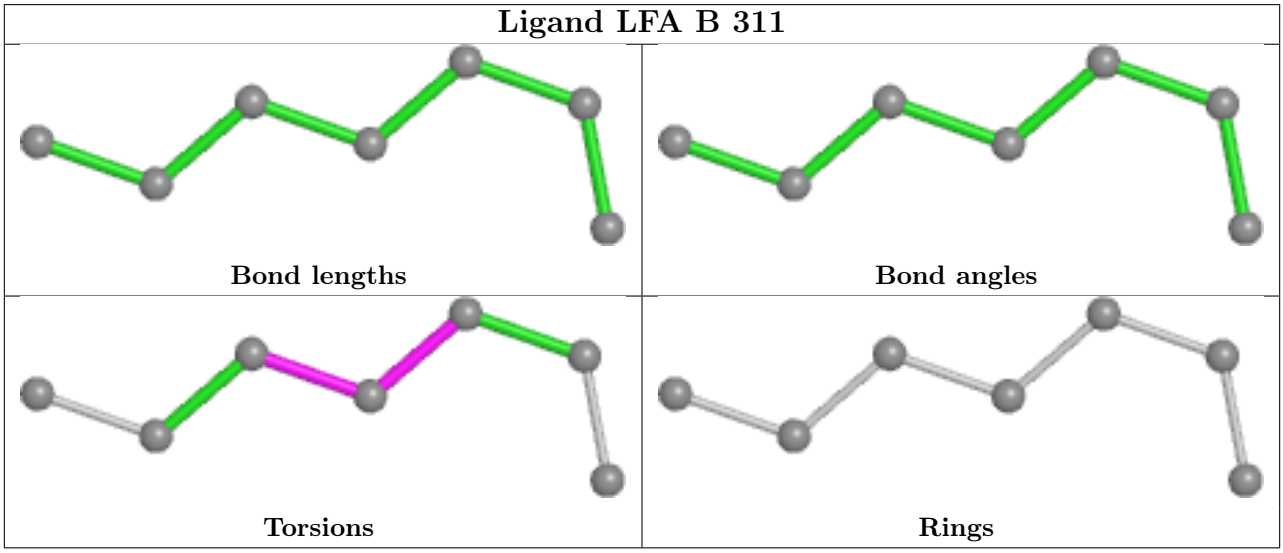

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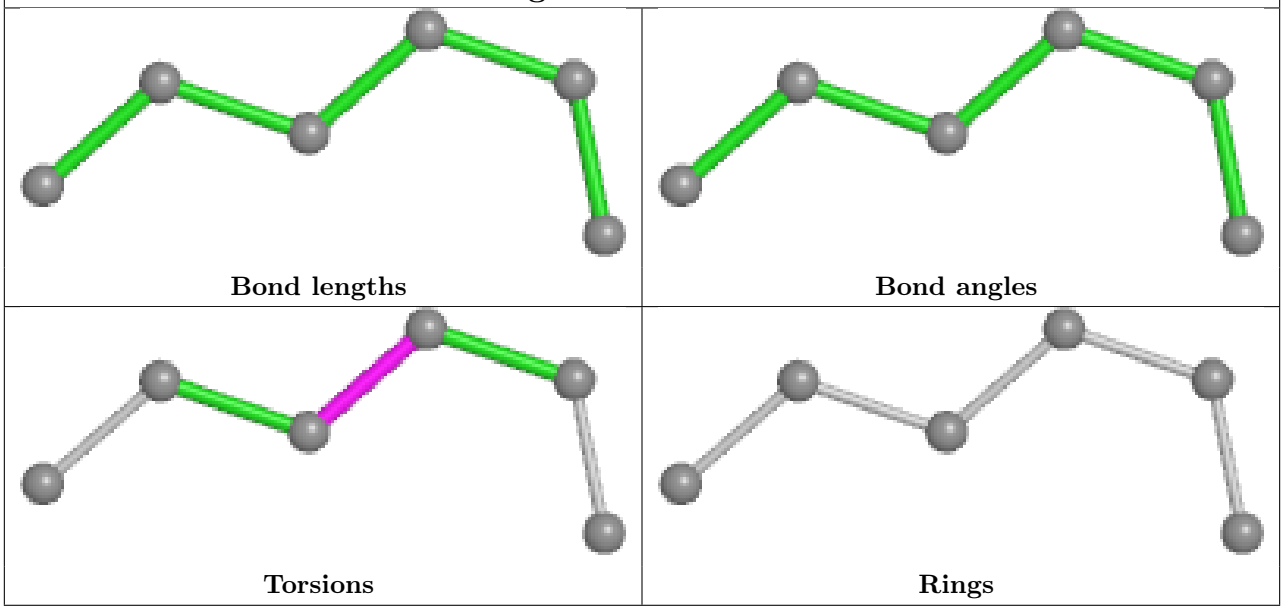

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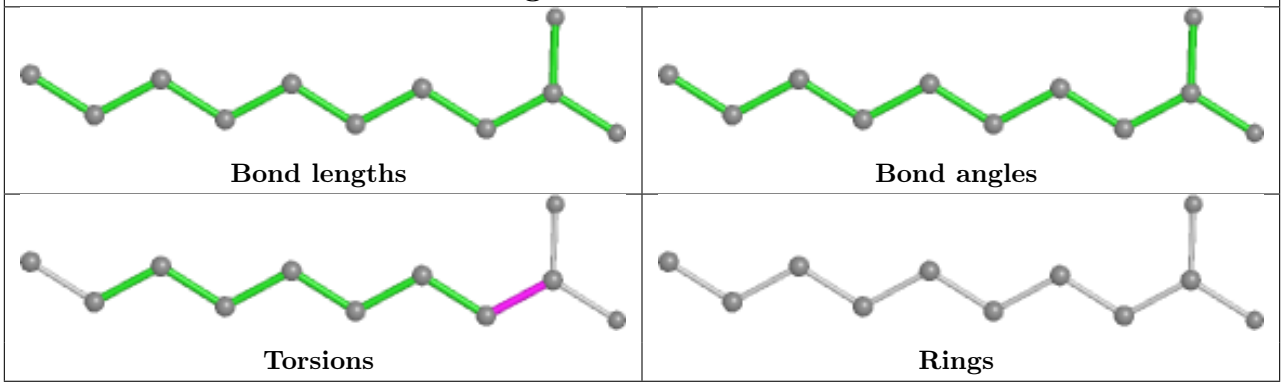

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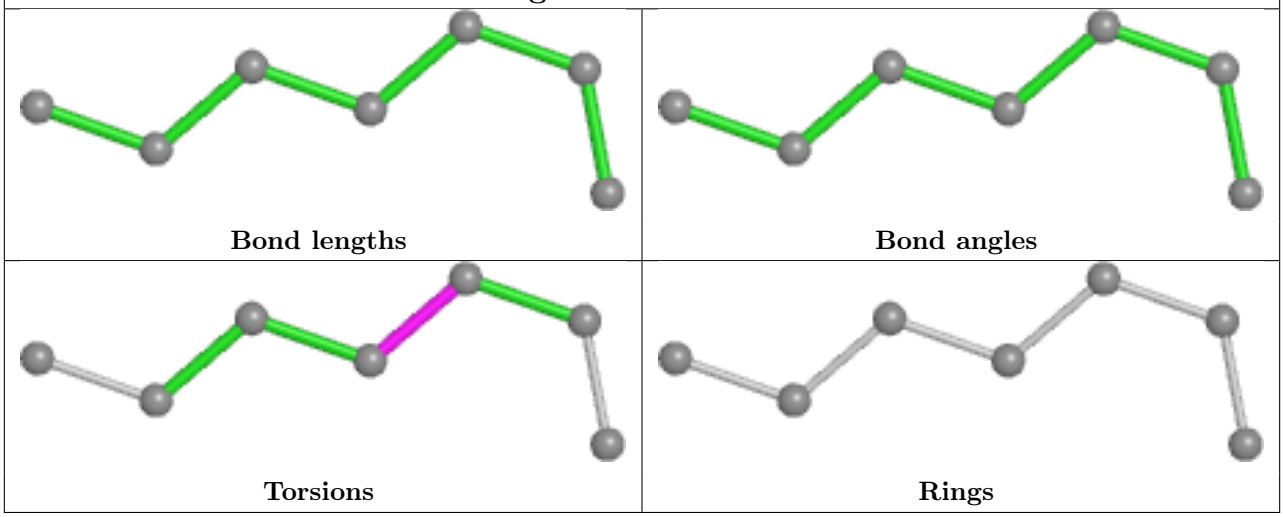

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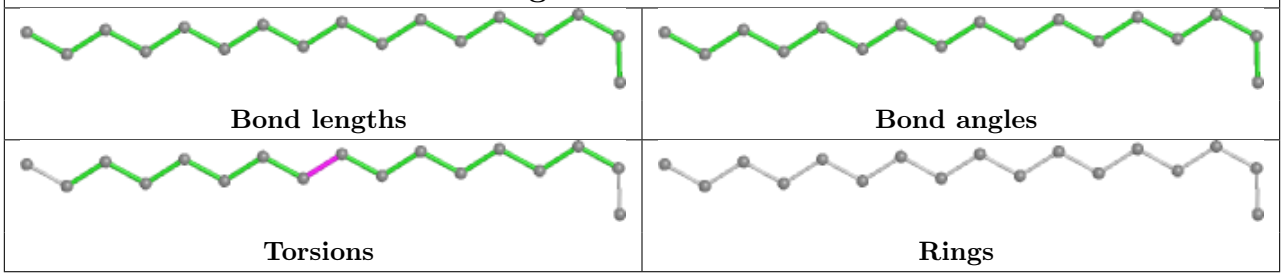

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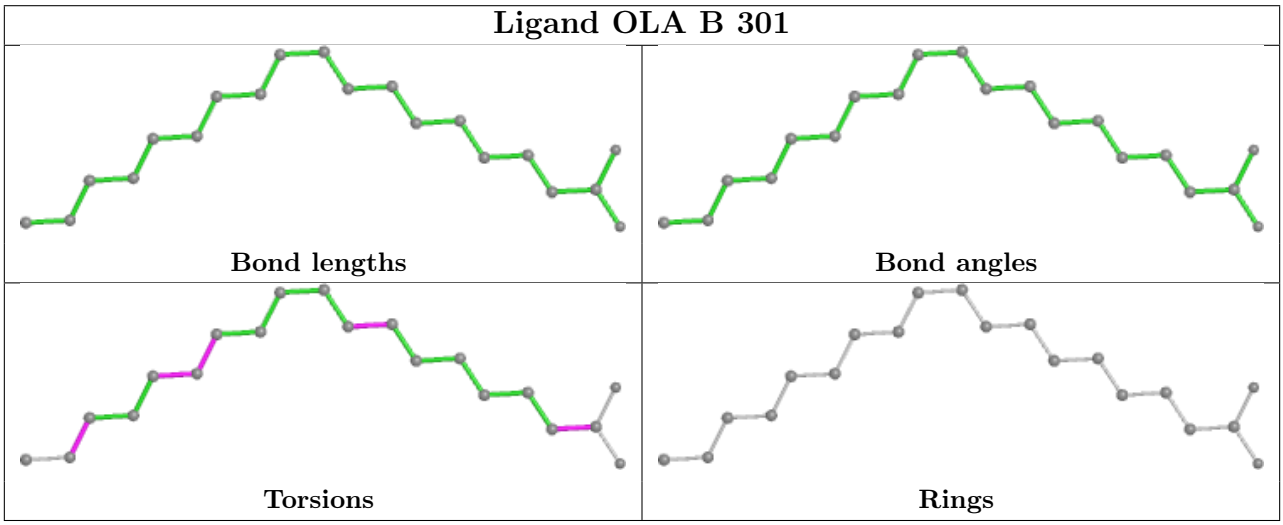
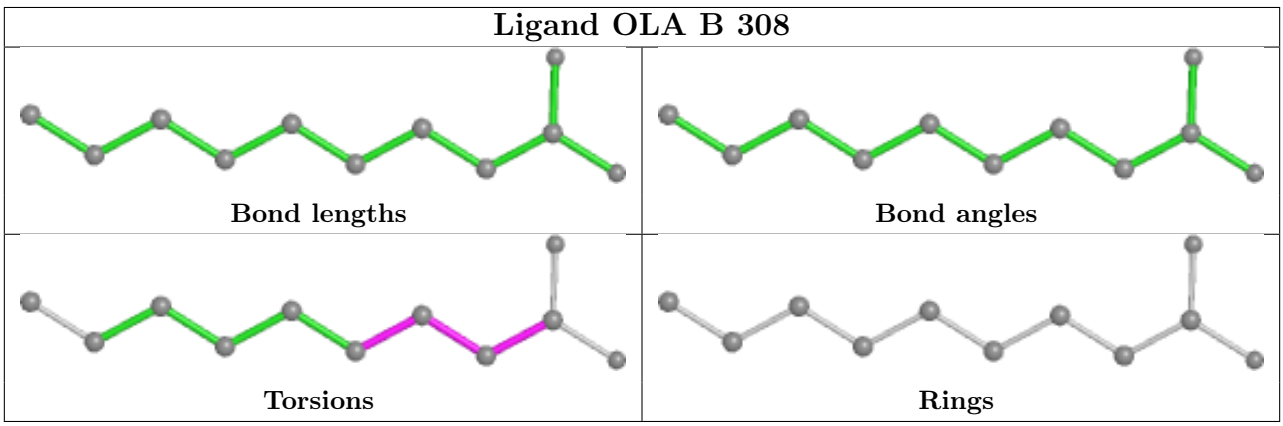
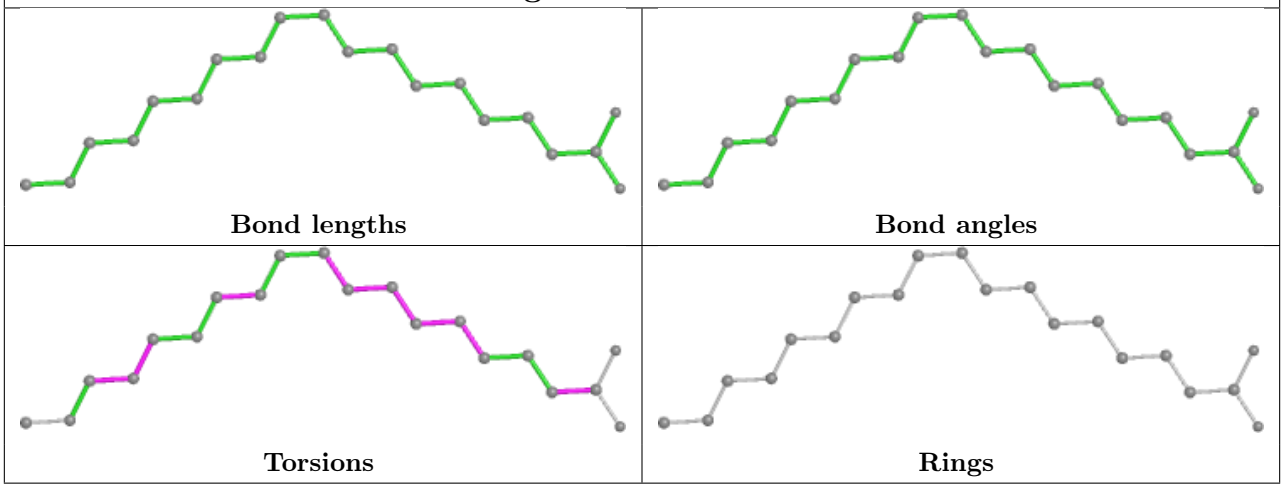


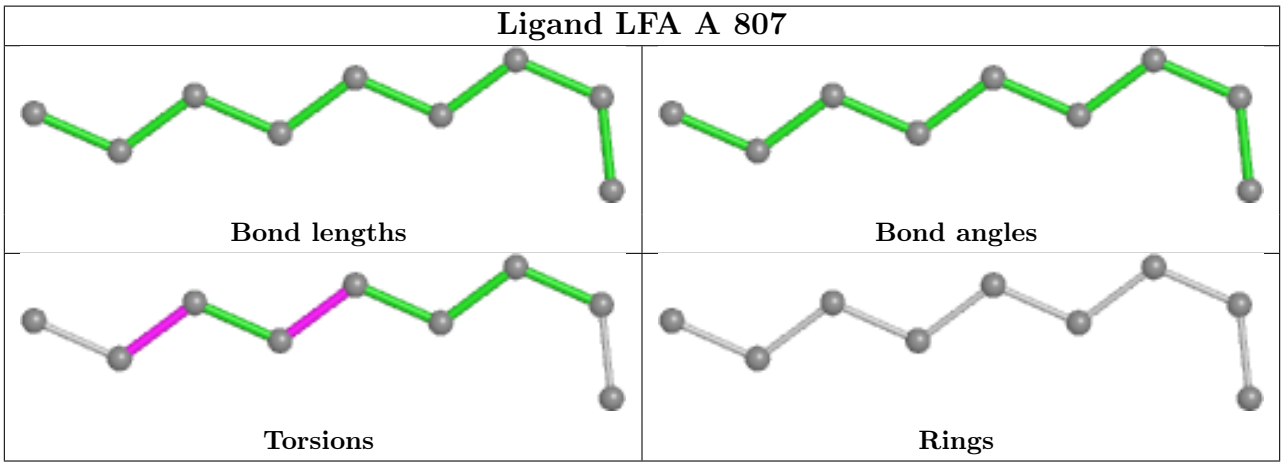
Ligand OLA B 308



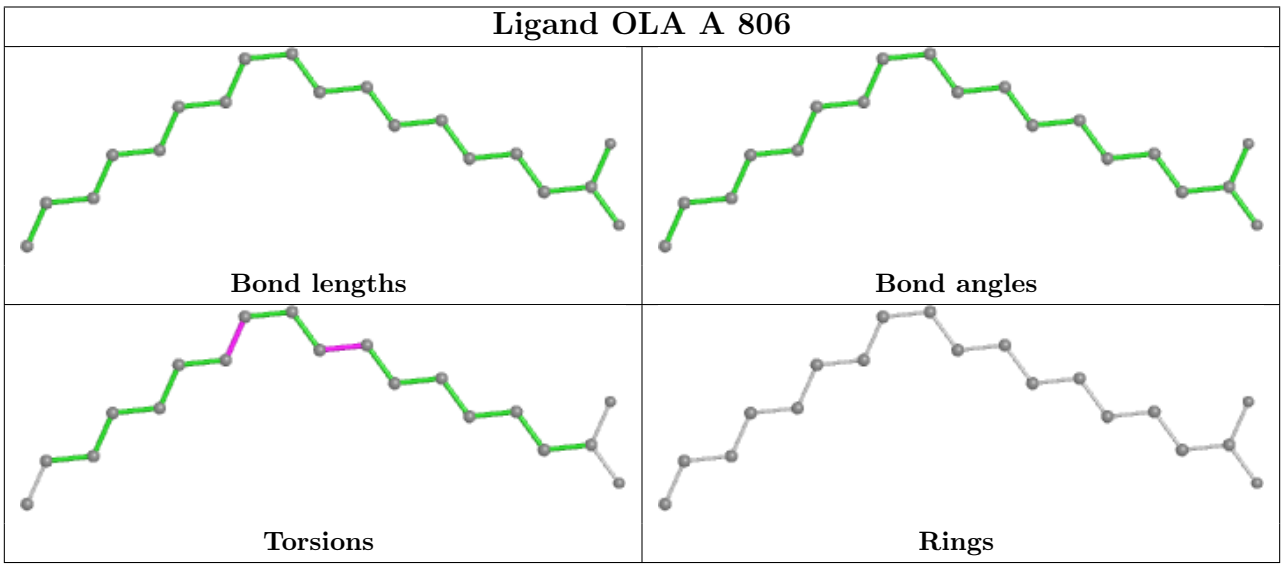
Ligand OLA A 803



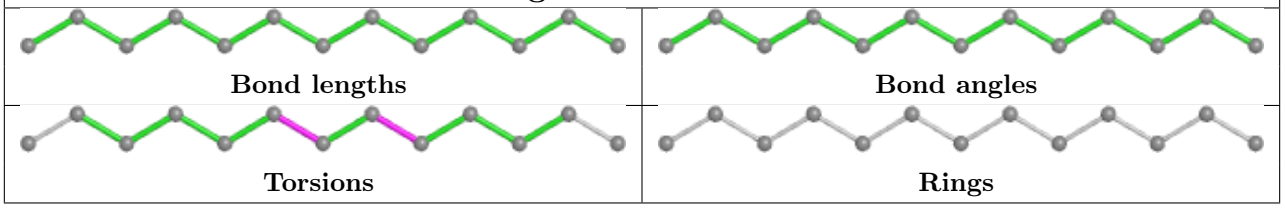
Ligand LFA A 807



Ligand OLA A 806

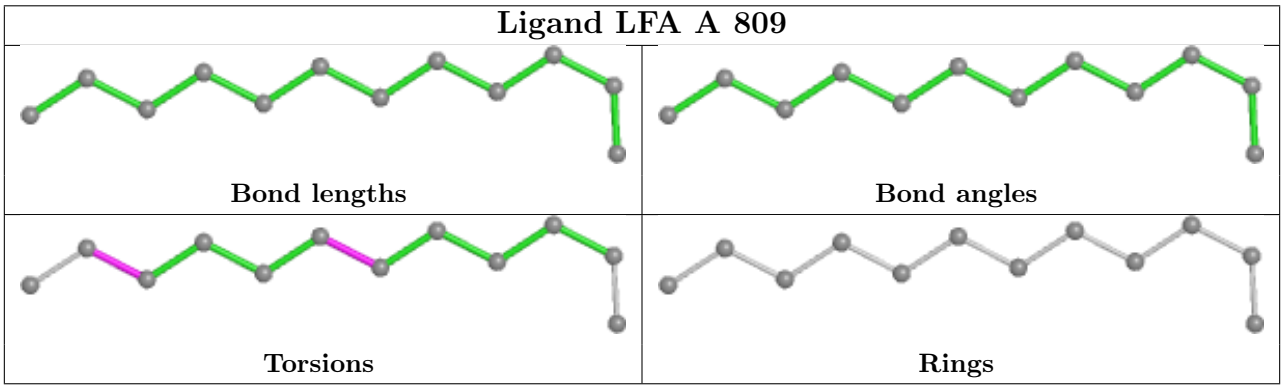


Ligand LFA A 812



Ligand OLA C 302

Ligand LFA A 809



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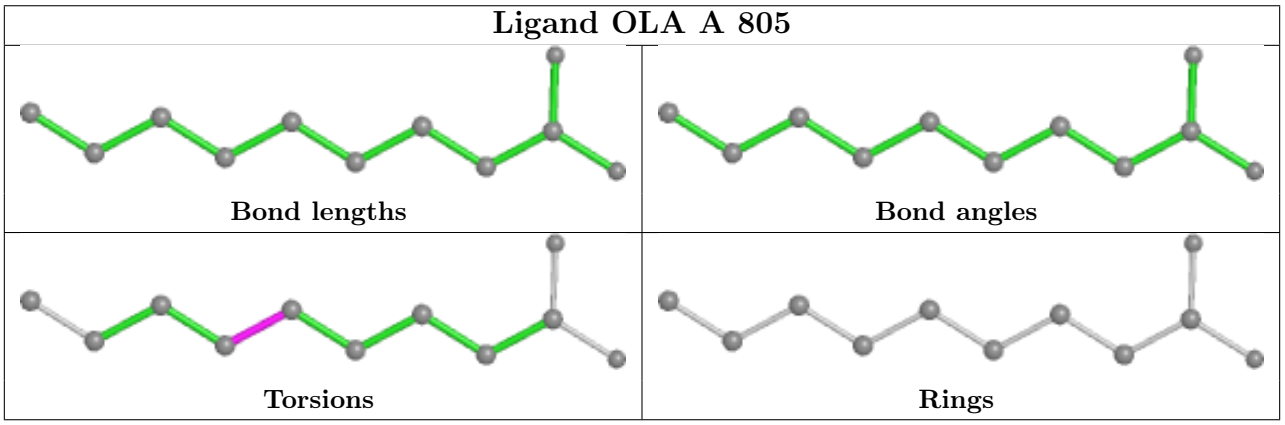

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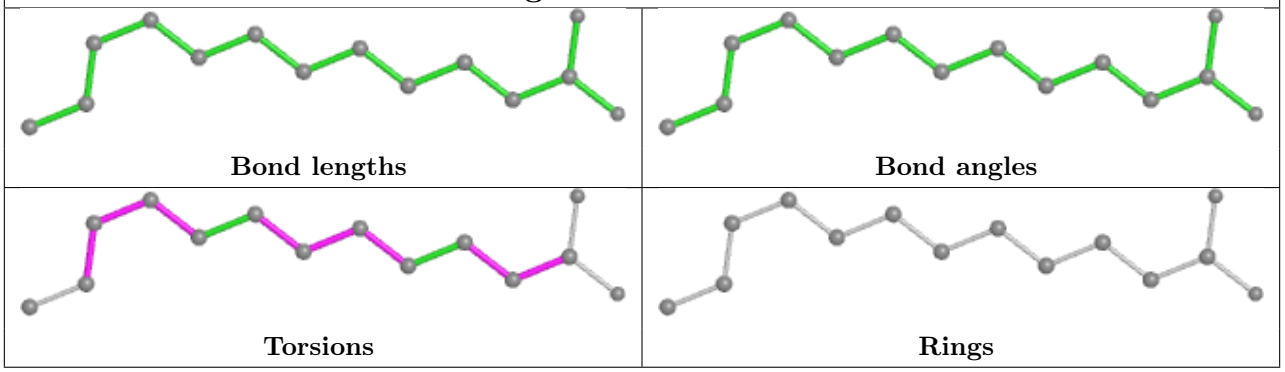

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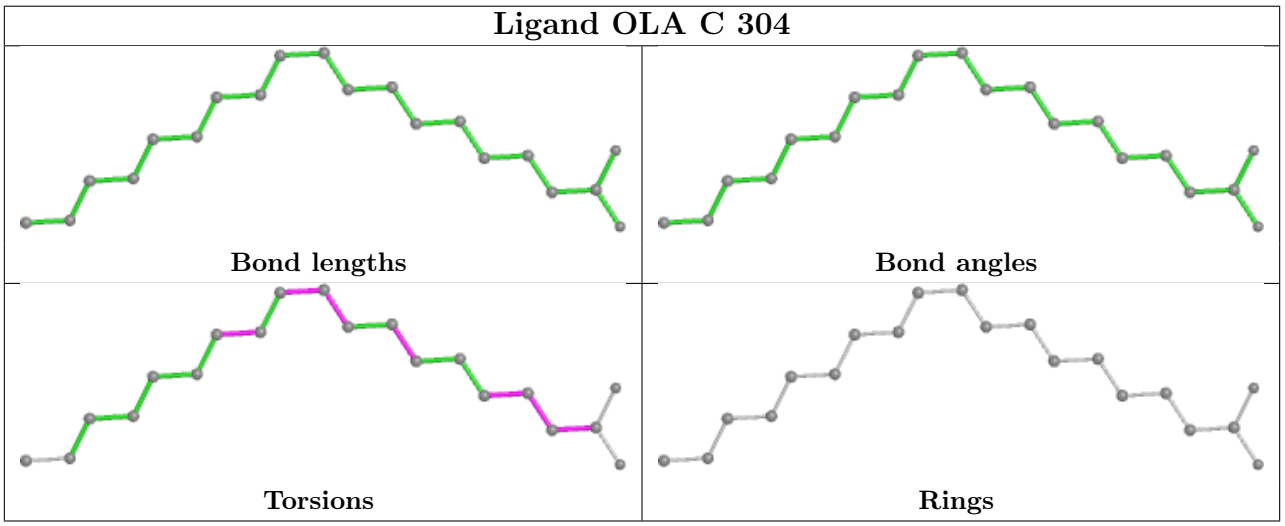
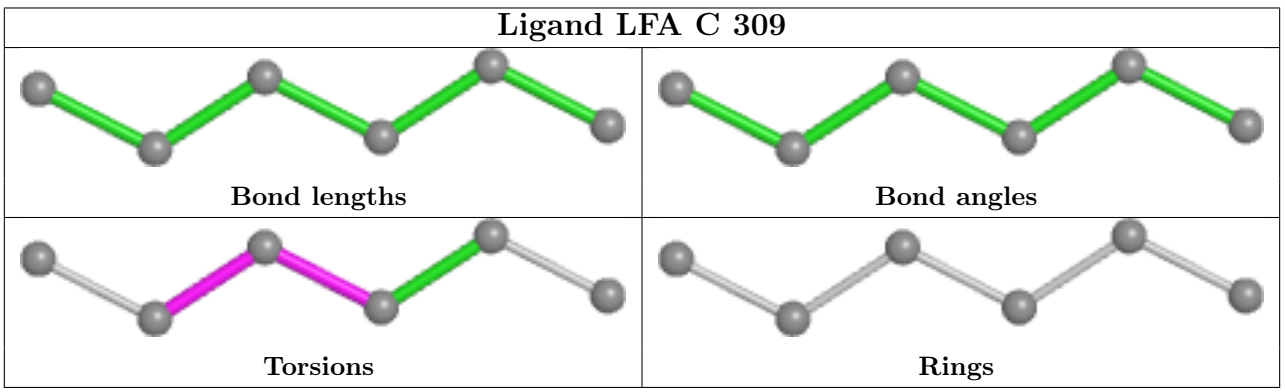
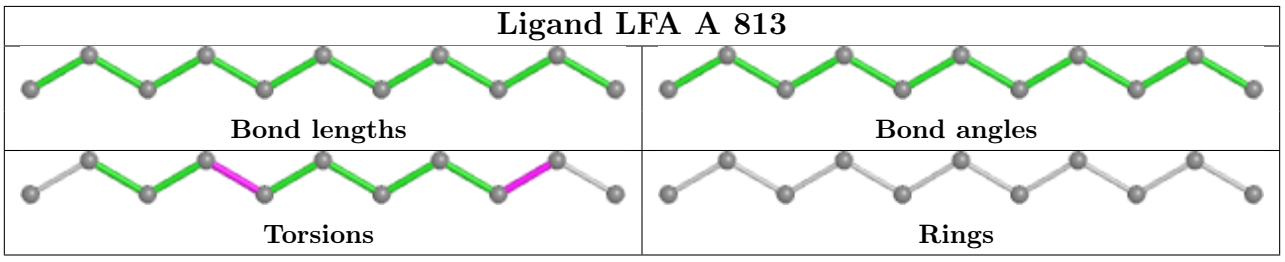
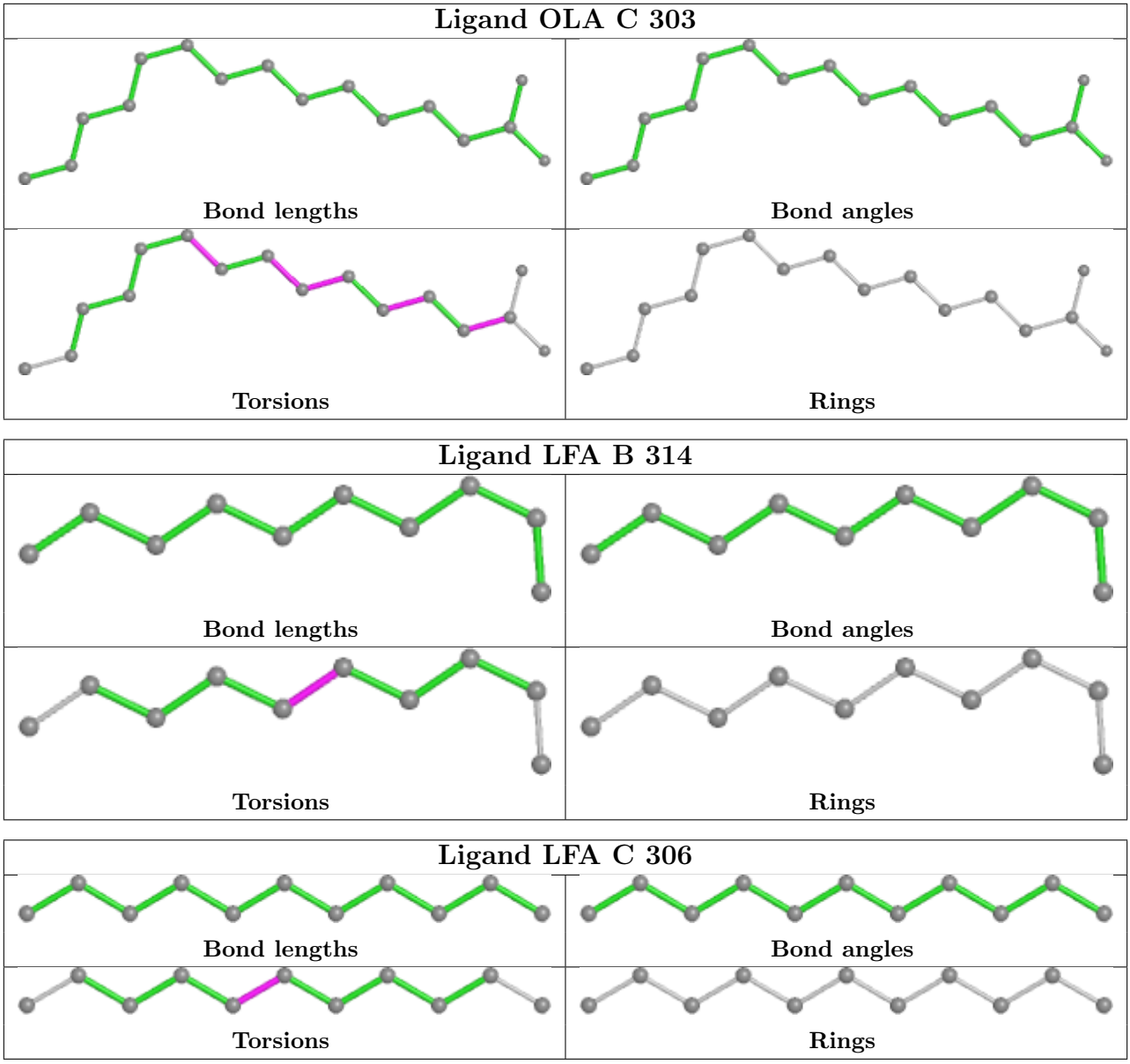


Ligand LFA C 309



Ligand LFA A 813





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	220/229 (96%)	-0.07	8 (3%)	42	49	41, 52, 75, 136	0
1	B	219/229 (95%)	0.05	12 (5%)	25	31	42, 55, 79, 124	0
1	C	221/229 (96%)	0.04	12 (5%)	25	31	42, 55, 81, 133	0
All	All	660/687 (96%)	0.01	32 (4%)	30	36	41, 54, 81, 136	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	TYR	7.1
1	C	61	TYR	5.7
1	A	62	ASP	5.0
1	C	223	GLN	4.9
1	B	222	HIS	4.6
1	C	64	THR	3.9
1	B	59	PHE	3.8
1	C	62	ASP	3.7
1	A	64	THR	3.7
1	B	223	GLN	3.6
1	B	60	GLN	3.5
1	A	60	GLN	3.4
1	B	85	LEU	3.2
1	C	60	GLN	3.2
1	C	189	LEU	3.2
1	A	59	PHE	3.1
1	C	222	HIS	3.0
1	B	93	GLY	2.8
1	B	199	PHE	2.7
1	C	93	GLY	2.5
1	B	156	THR	2.5
1	C	63	ASP	2.4
1	C	191	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	93	GLY	2.4
1	A	85	LEU	2.2
1	B	155	GLY	2.2
1	A	222	HIS	2.1
1	B	4	ILE	2.1
1	B	121	ILE	2.1
1	C	92	GLY	2.1
1	C	94	LYS	2.1
1	B	94	LYS	2.0

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, 95^{th} 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	A	1	10/11	0.84	0.27	70,82,126,131	0
1	FME	B	1	7/11	0.87	0.22	74,82,89,98	0
1	FME	C	1	10/11	0.90	0.29	68,78,125,134	0
1	LYR	C	207	29/30	0.91	0.19	39,47,55,75	0
1	LYR	B	207	29/30	0.92	0.15	40,45,57,65	0
1	LYR	A	207	29/30	0.93	0.19	38,46,55,67	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	B	311	7/20	0.30	0.41	85,95,109,110	0
2	LFA	B	305	7/20	0.31	0.30	87,89,106,108	0
2	LFA	A	810	8/20	0.38	0.34	92,105,127,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLA	B	307	16/20	0.52	0.29	68,86,115,120	0
3	OLA	C	303	16/20	0.53	0.30	83,102,123,129	0
3	OLA	A	803	20/20	0.54	0.22	71,81,100,108	0
3	OLA	B	301	20/20	0.54	0.24	55,76,100,113	0
3	OLA	C	304	20/20	0.54	0.21	61,77,97,111	0
3	OLA	A	802	11/20	0.57	0.16	75,82,108,110	0
2	LFA	C	308	8/20	0.61	0.47	104,110,117,118	0
2	LFA	C	315	9/20	0.62	0.36	98,110,113,117	0
2	LFA	A	809	12/20	0.63	0.25	80,100,107,115	0
2	LFA	A	811	6/20	0.64	0.23	83,96,99,101	0
2	LFA	C	313	6/20	0.65	0.17	72,84,93,94	0
2	LFA	A	807	9/20	0.65	0.33	96,100,115,123	0
2	LFA	B	314	10/20	0.67	0.26	76,102,107,111	0
2	LFA	A	814	15/20	0.68	0.20	84,97,113,123	0
3	OLA	A	806	19/20	0.70	0.19	65,80,109,113	0
3	OLA	B	308	11/20	0.70	0.16	83,89,98,108	0
2	LFA	A	808	6/20	0.71	0.36	72,78,84,90	0
2	LFA	C	309	6/20	0.71	0.43	96,101,105,108	0
2	LFA	B	316	14/20	0.71	0.21	72,86,98,100	0
2	LFA	C	316	17/20	0.73	0.25	79,85,96,100	0
2	LFA	B	313	14/20	0.73	0.31	65,76,109,115	0
2	LFA	C	301	17/20	0.73	0.22	63,78,97,104	0
2	LFA	B	303	15/20	0.74	0.18	60,70,86,88	0
2	LFA	A	815	9/20	0.74	0.25	74,81,95,97	0
2	LFA	C	306	11/20	0.75	0.24	111,119,127,127	0
2	LFA	B	312	5/20	0.76	0.15	81,82,87,95	0
3	OLA	A	805	11/20	0.76	0.18	79,86,107,107	0
4	PO4	C	317	5/5	0.76	0.47	126,128,142,149	0
3	OLA	C	302	14/20	0.79	0.33	63,84,123,129	0
2	LFA	C	314	10/20	0.79	0.14	89,94,101,102	0
2	LFA	B	309	9/20	0.80	0.13	93,108,113,117	0
3	OLA	C	305	16/20	0.80	0.14	64,73,93,109	0
3	OLA	B	306	14/20	0.80	0.22	74,95,117,117	0
3	OLA	A	804	16/20	0.81	0.16	71,85,113,119	0
2	LFA	A	801	7/20	0.82	0.28	74,77,82,83	0
2	LFA	A	813	11/20	0.82	0.15	82,87,92,94	0
2	LFA	A	812	13/20	0.83	0.23	86,95,112,113	0
2	LFA	B	310	7/20	0.84	0.10	73,87,98,99	0
2	LFA	C	311	9/20	0.86	0.20	70,76,81,88	0
2	LFA	C	307	4/20	0.87	0.16	83,84,85,87	0
2	LFA	C	312	13/20	0.88	0.20	61,73,90,92	0
2	LFA	B	304	9/20	0.89	0.22	69,78,88,89	0

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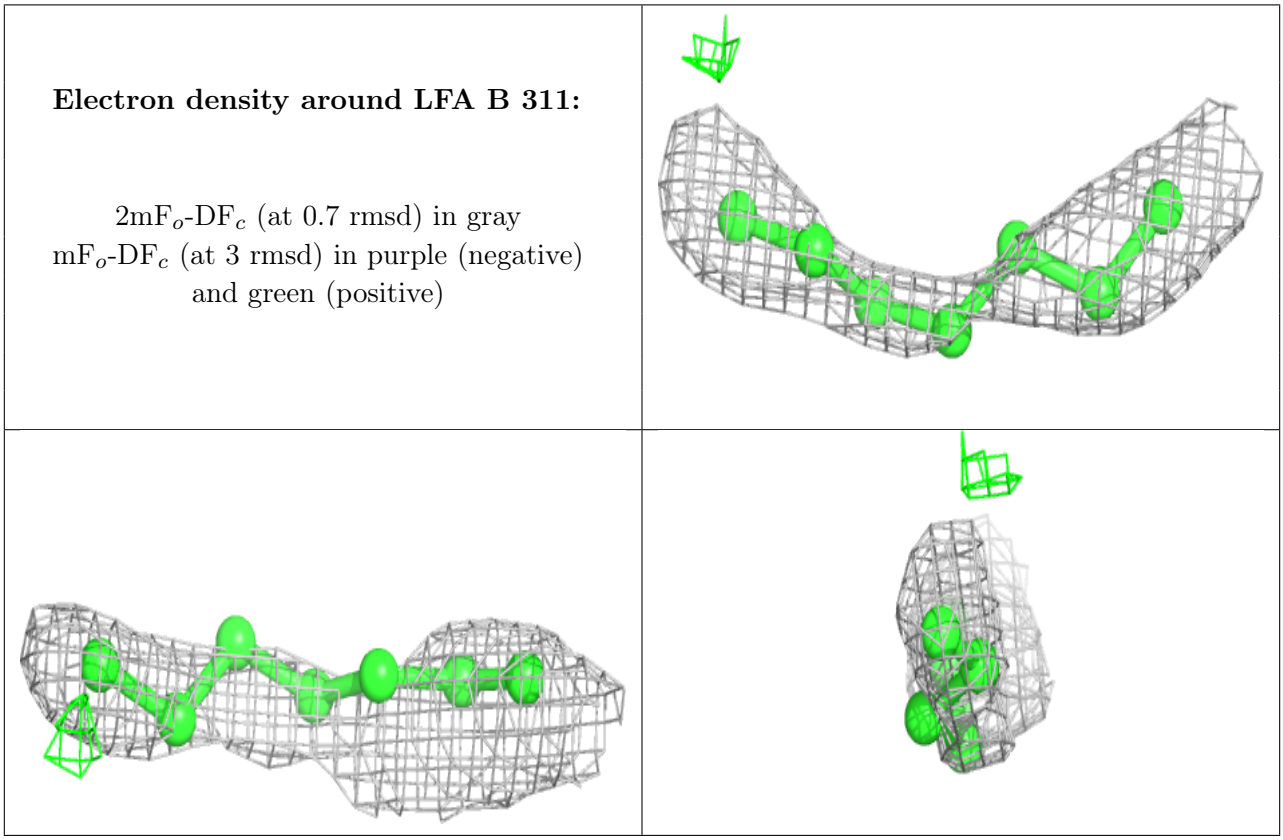
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	B	302	7/20	0.89	0.10	73,76,81,89	0
2	LFA	B	315	8/20	0.90	0.28	78,81,86,90	0
2	LFA	C	310	6/20	0.90	0.35	64,77,84,85	0

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.

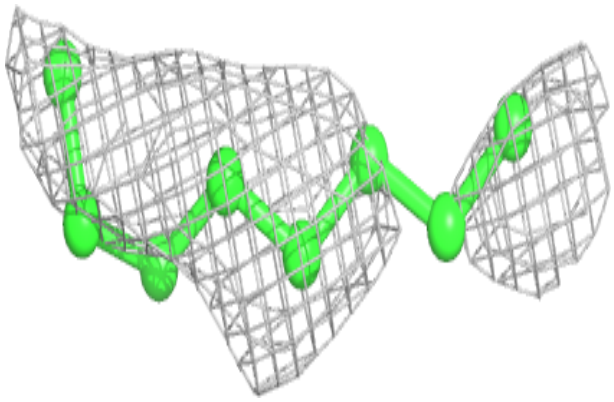
Electron density around LFA B 311:

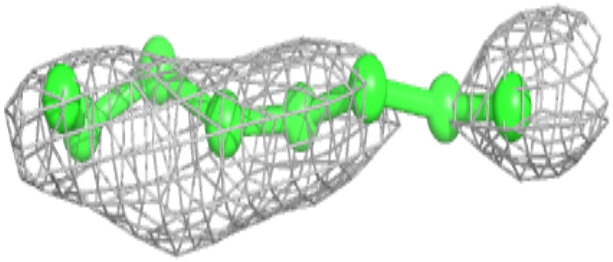
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

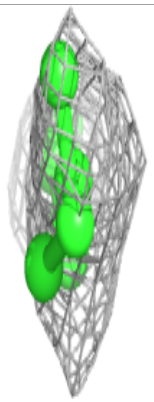


Electron density around LFA A 810:

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

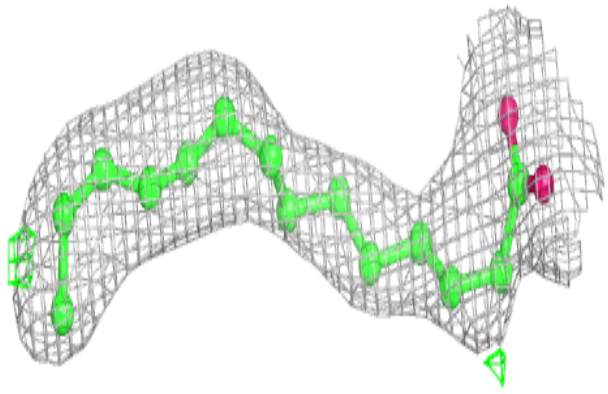


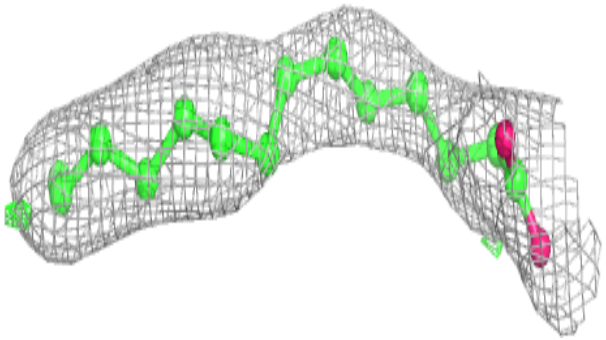


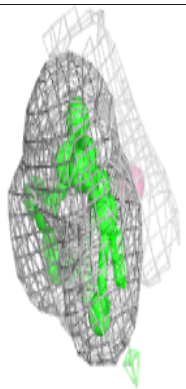


Electron density around OLA B 307:

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

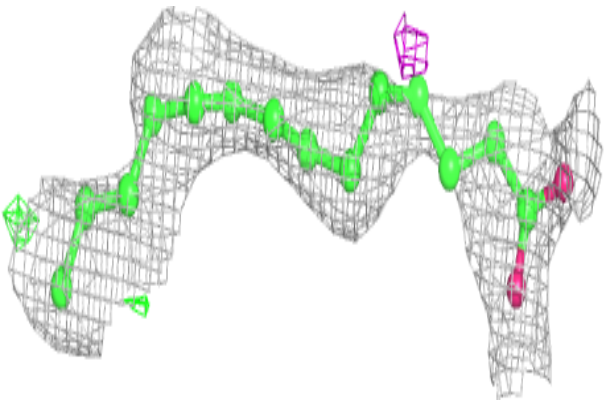


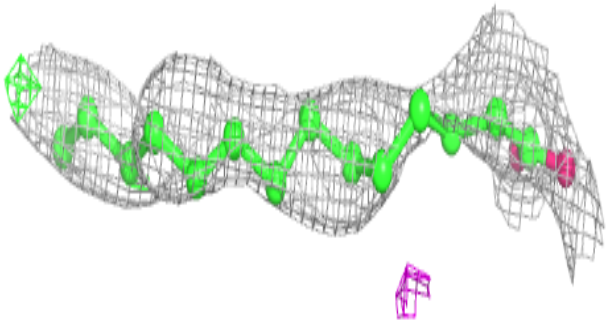


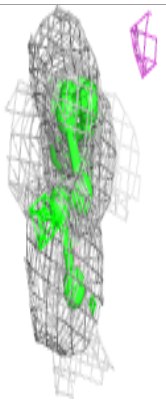


Electron density around OLA C 303:

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

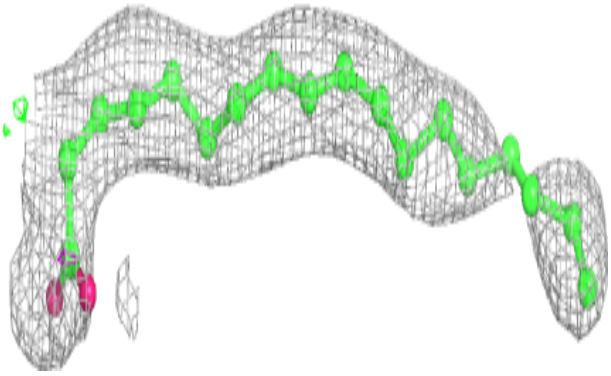


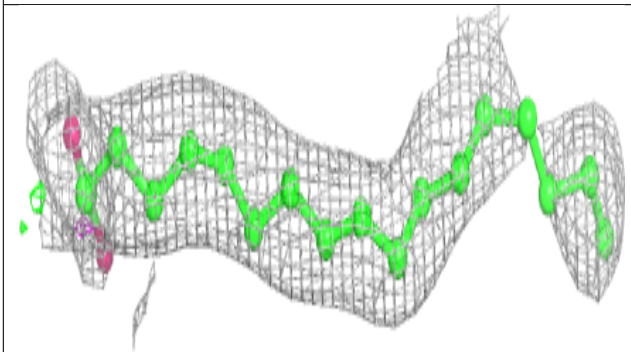


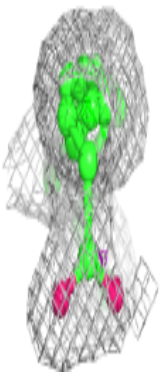


Electron density around OLA A 803:

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

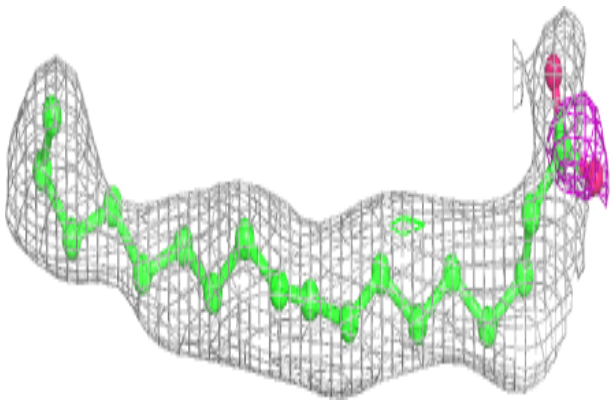


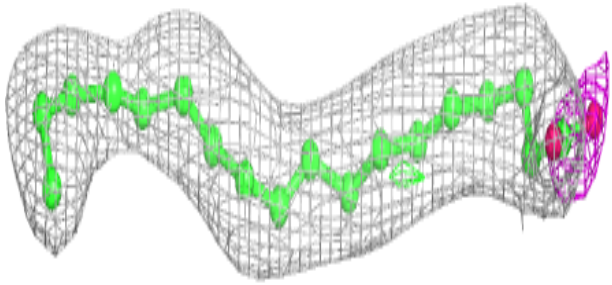


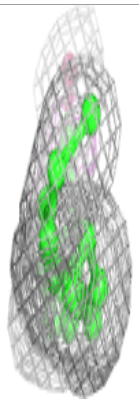


Electron density around OLA B 301:

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

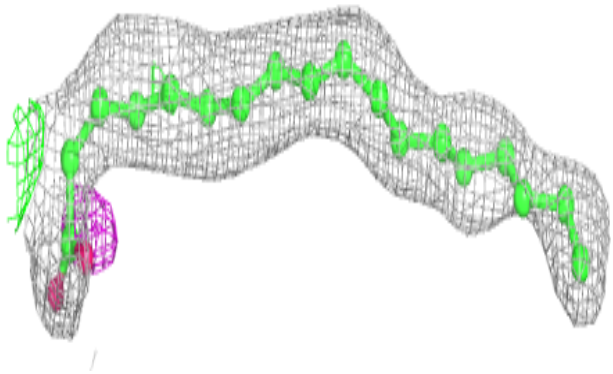


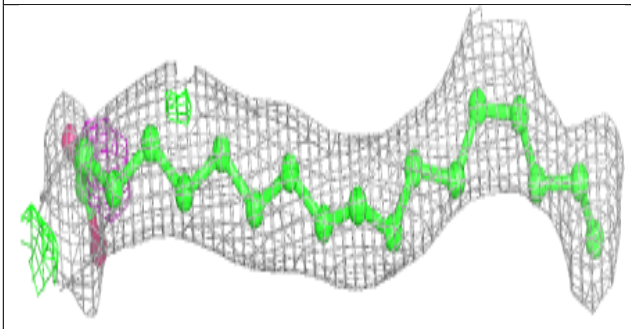


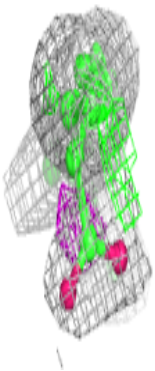


Electron density around OLA C 304:

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

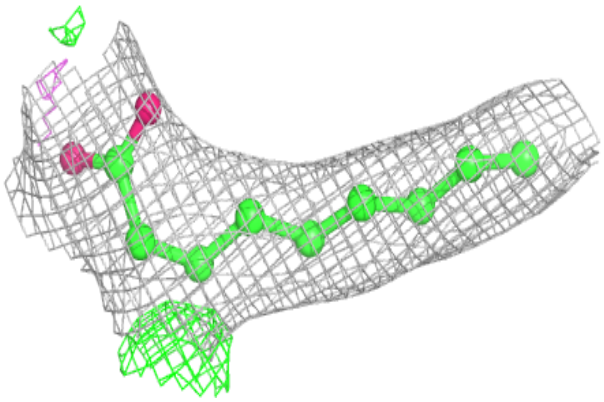


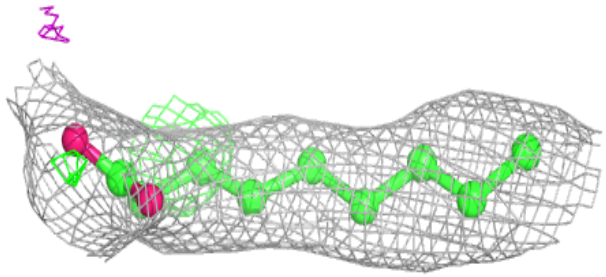


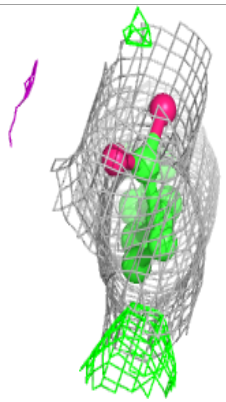


Electron density around OLA A 802:

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

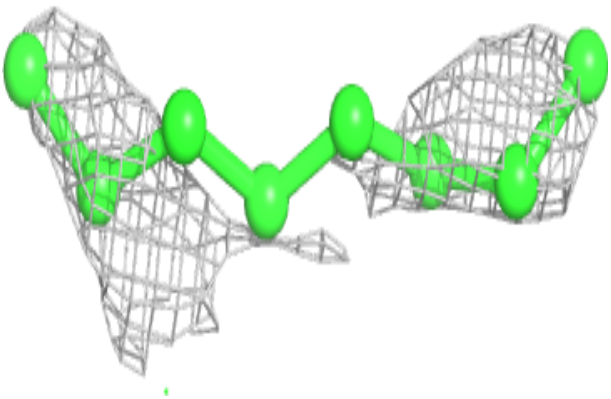


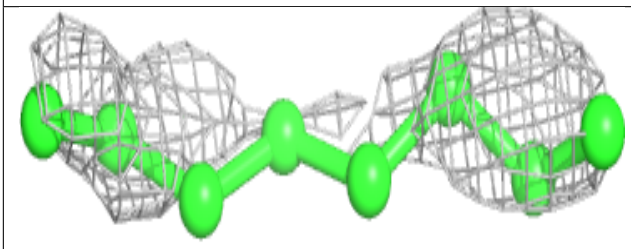




Electron density around LFA C 308:

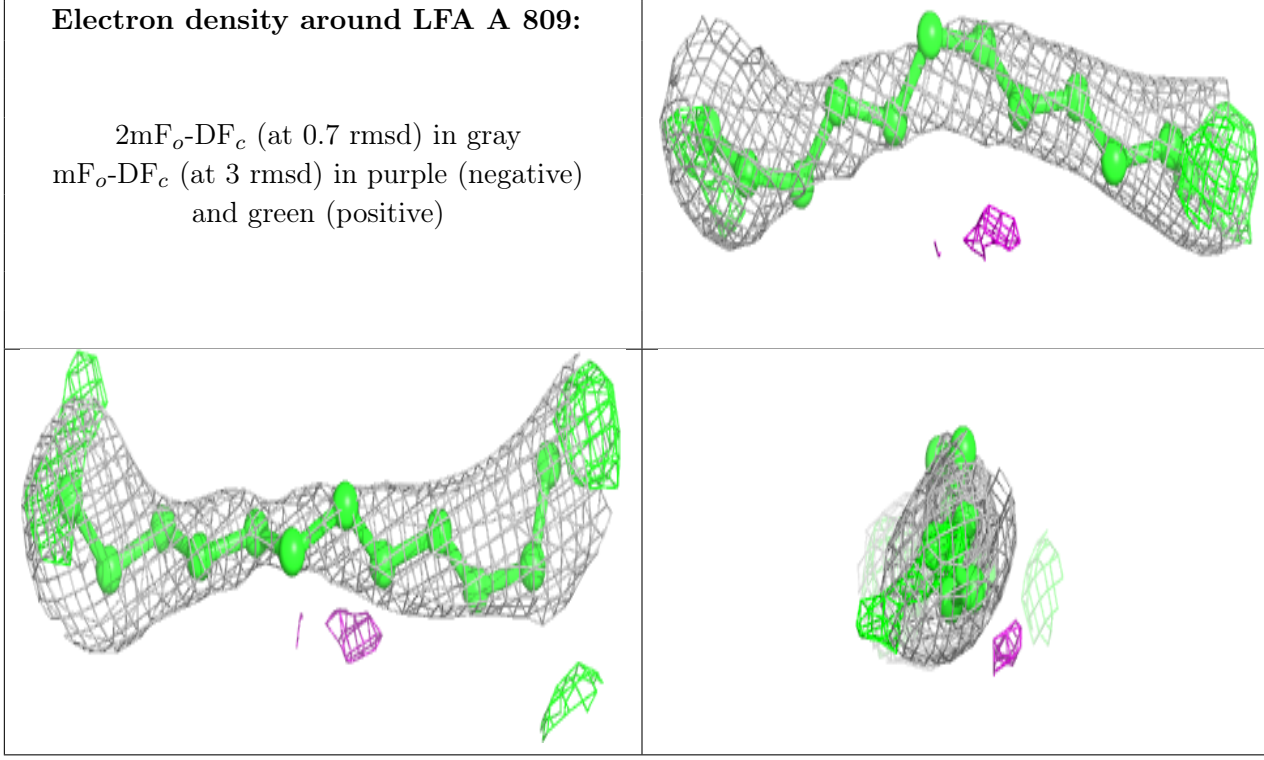
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





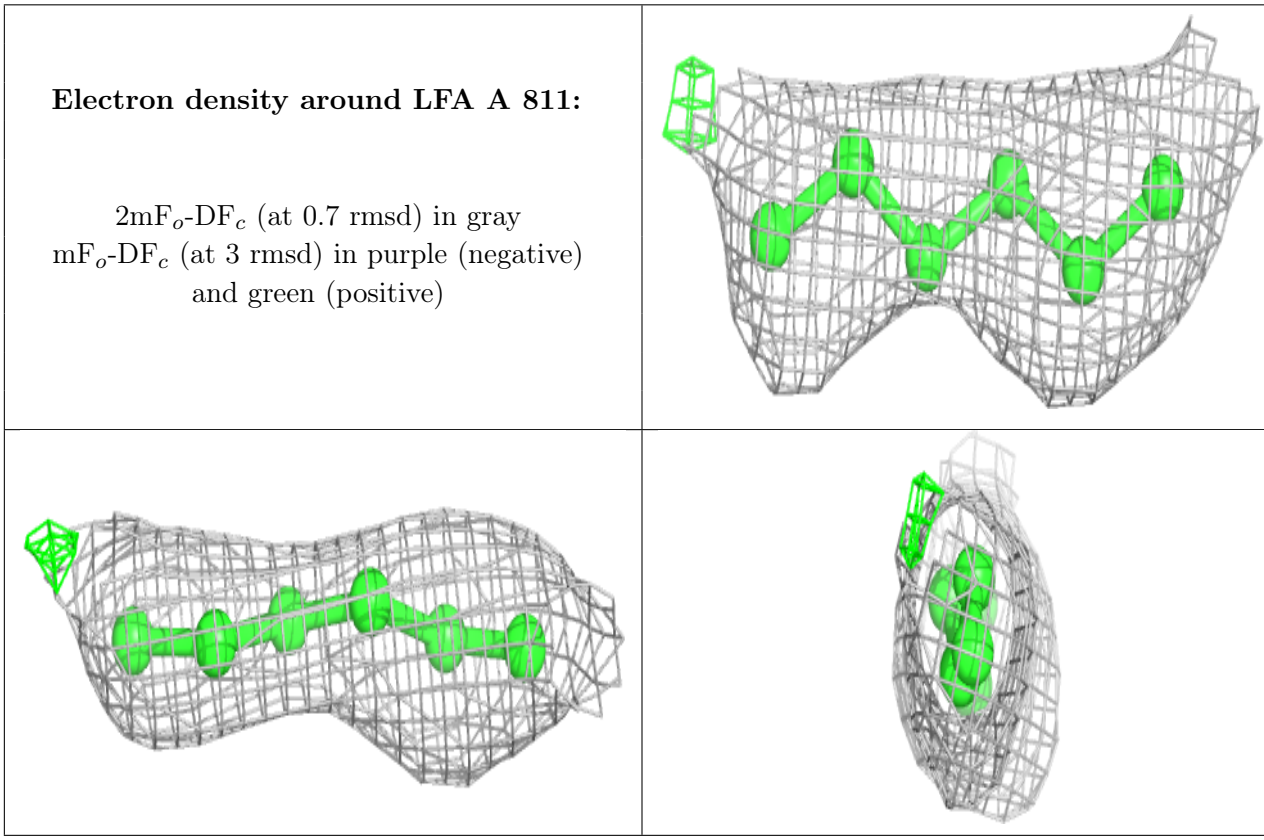
Electron density around LFA A 809:

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



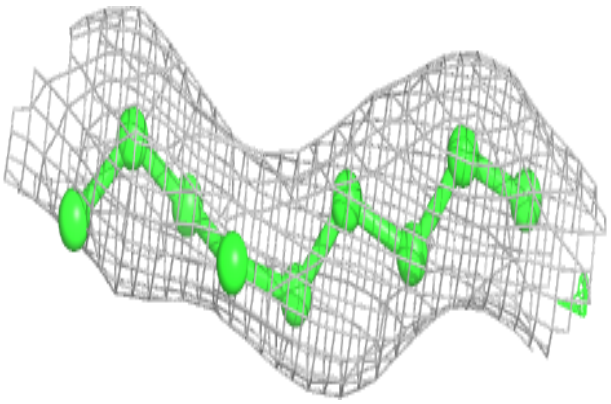
Electron density around LFA A 811:

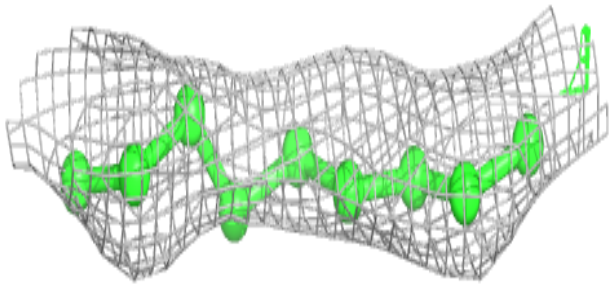
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

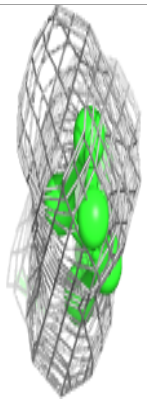


Electron density around LFA A 807:

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

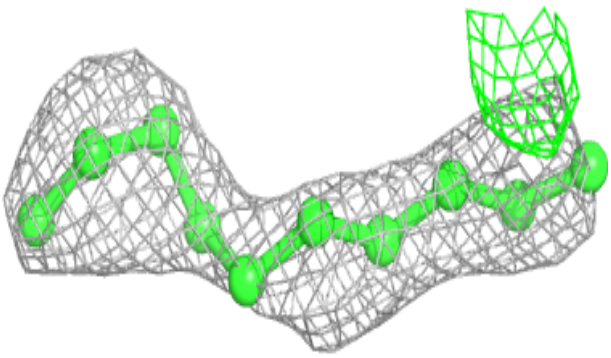


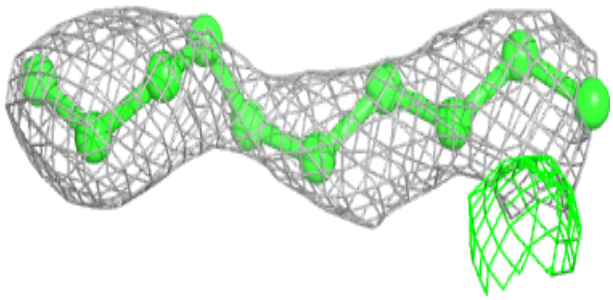


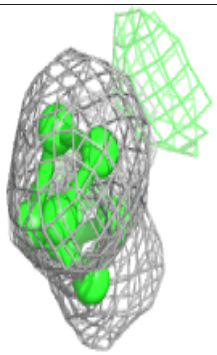


Electron density around LFA B 314:

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

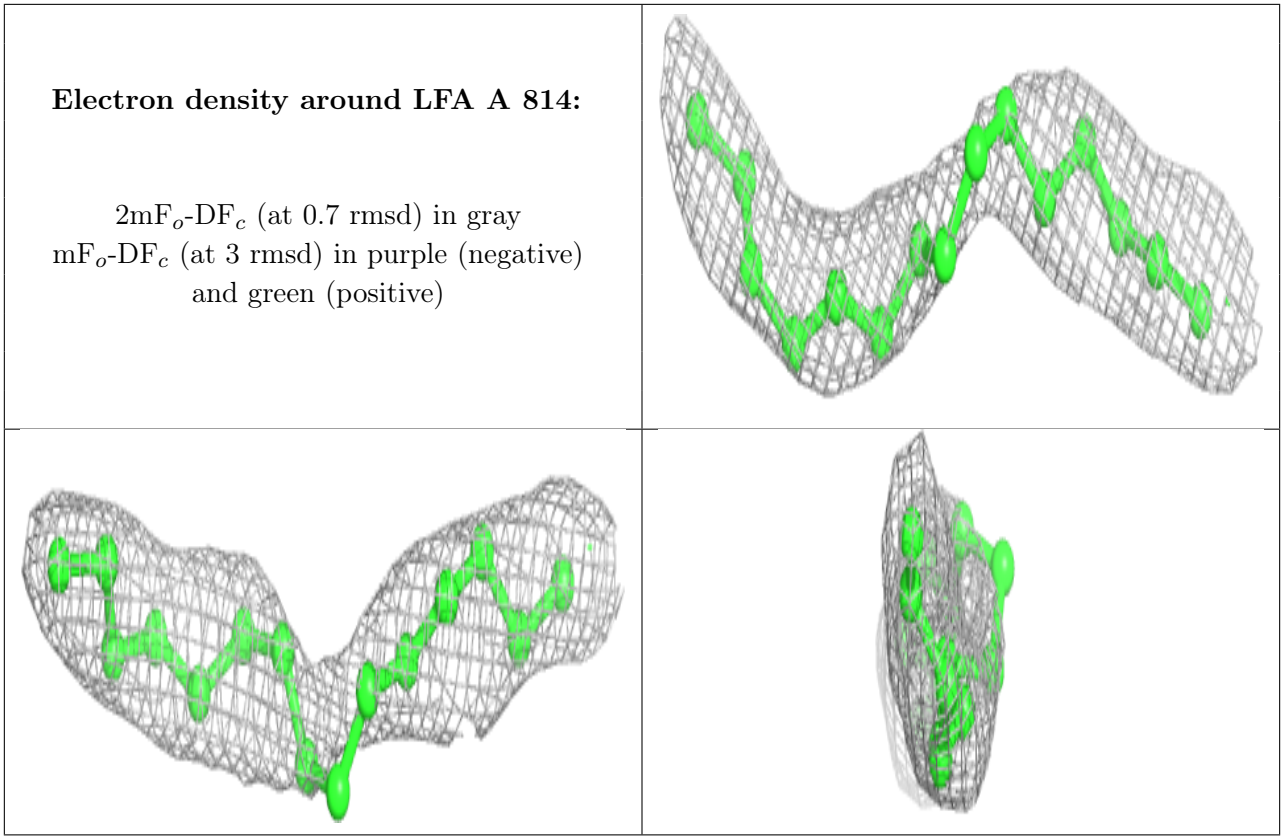






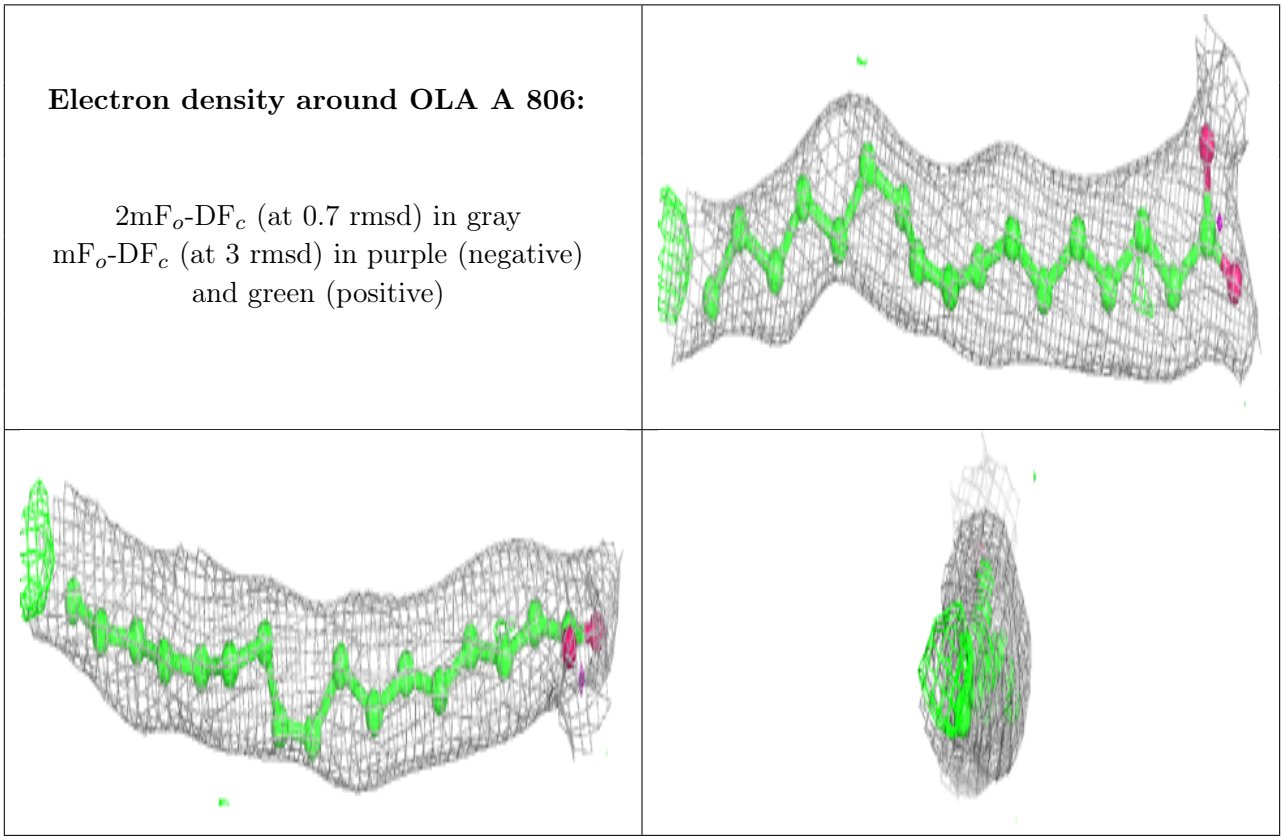
Electron density around LFA A 814:

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



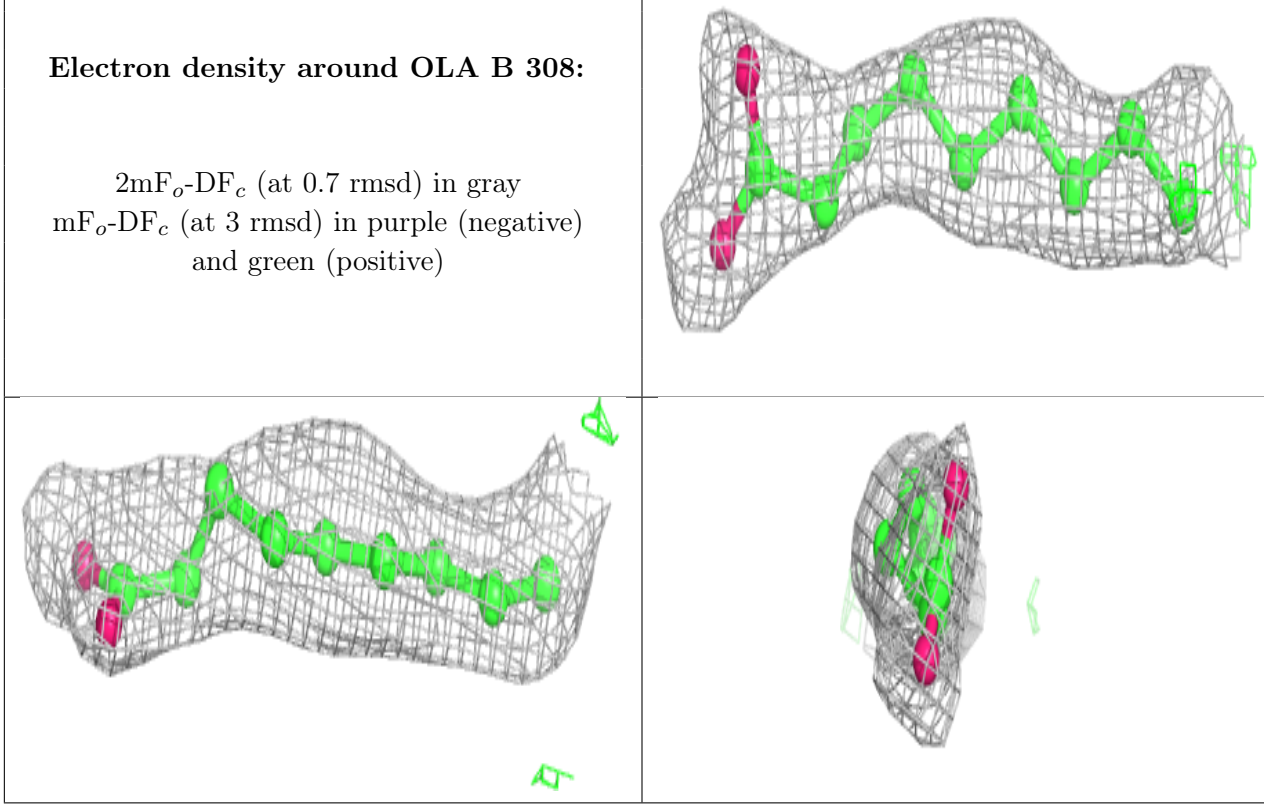
Electron density around OLA A 806:

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



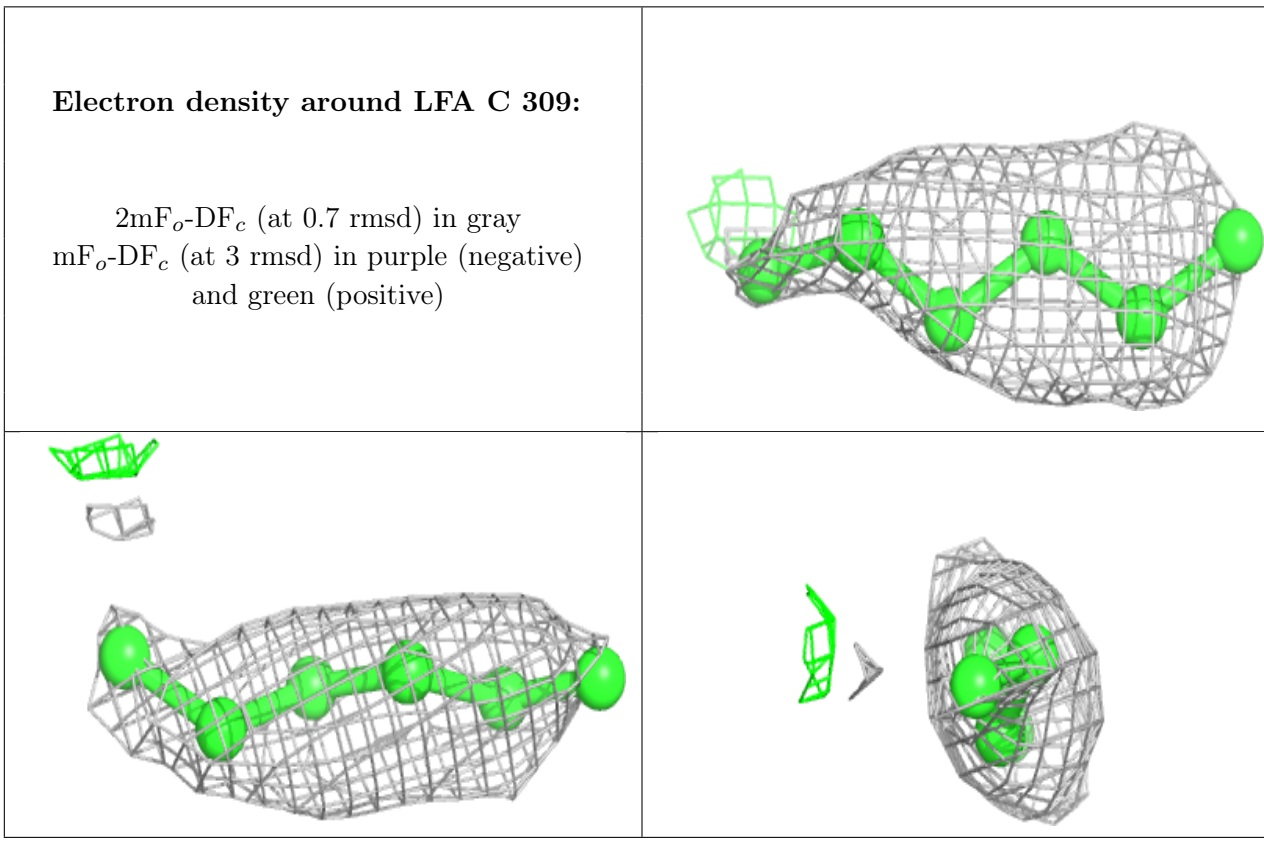
Electron density around OLA B 308:

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



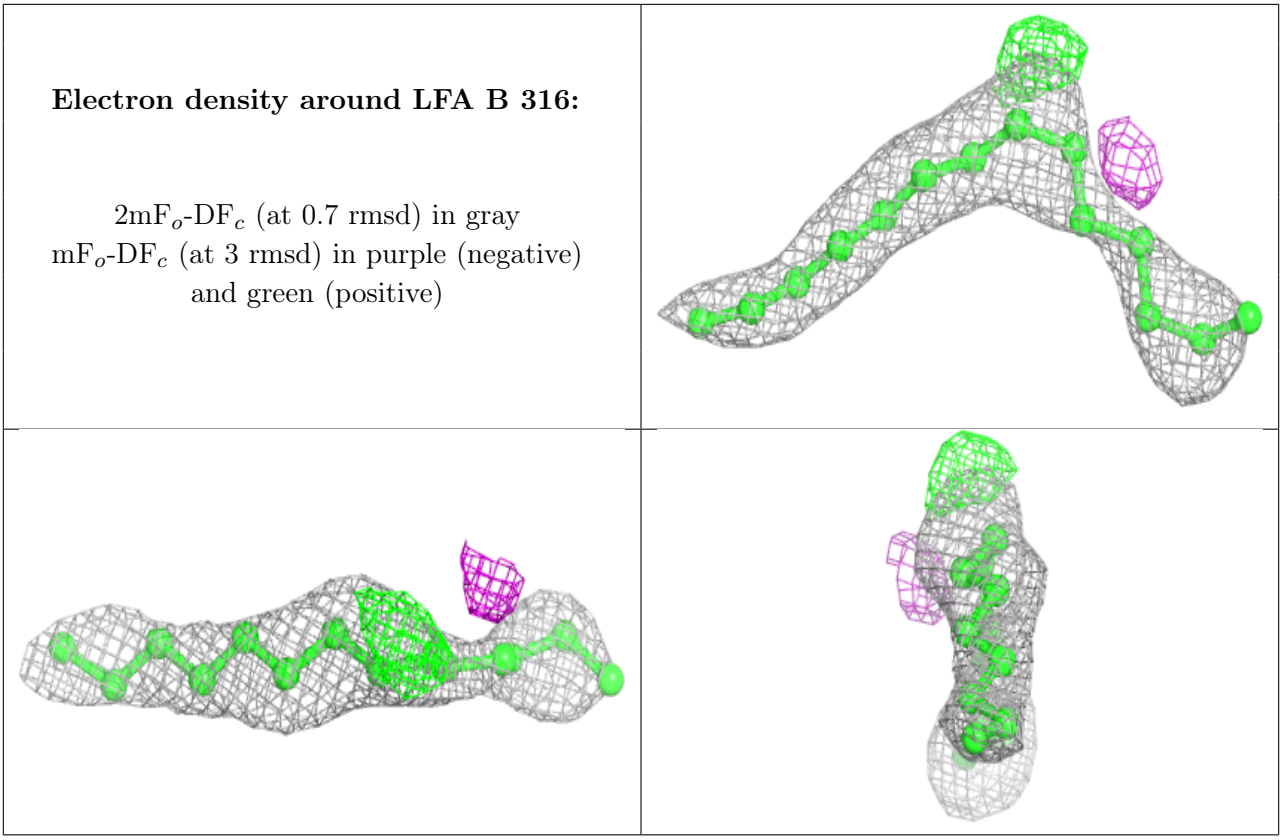
Electron density around LFA C 309:

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



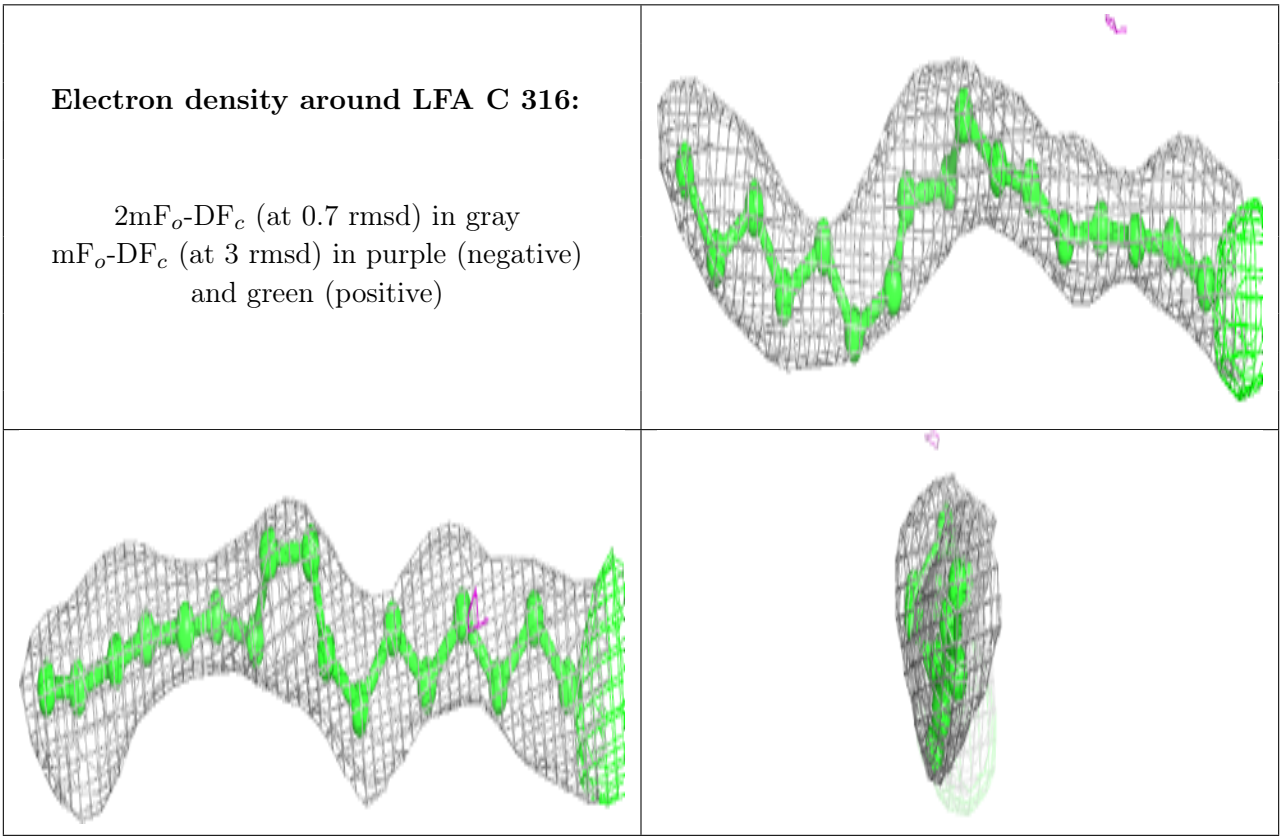
Electron density around LFA B 316:

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



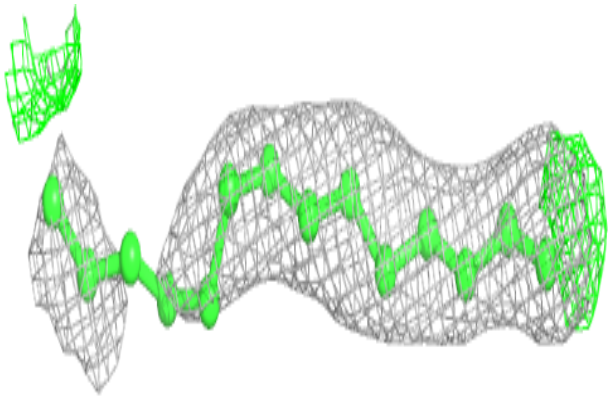
Electron density around LFA C 316:

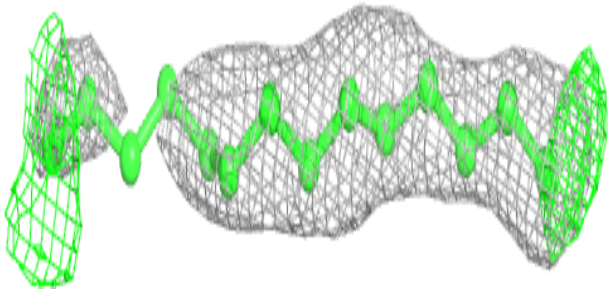
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

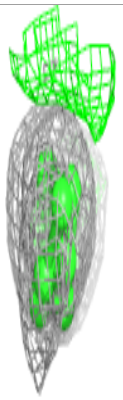


Electron density around LFA B 313:

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

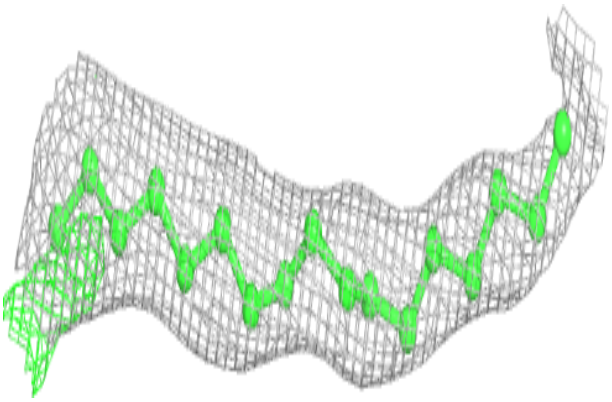


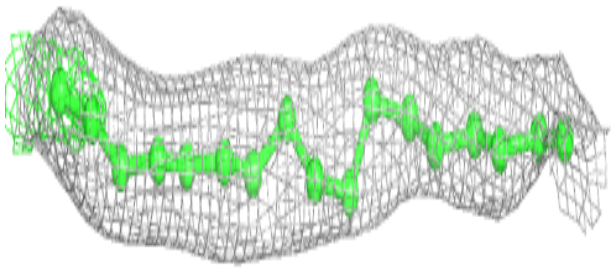


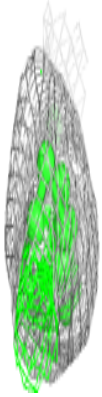


Electron density around LFA C 301:

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

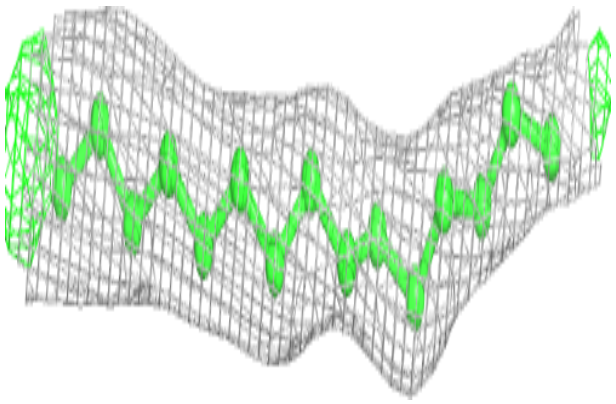


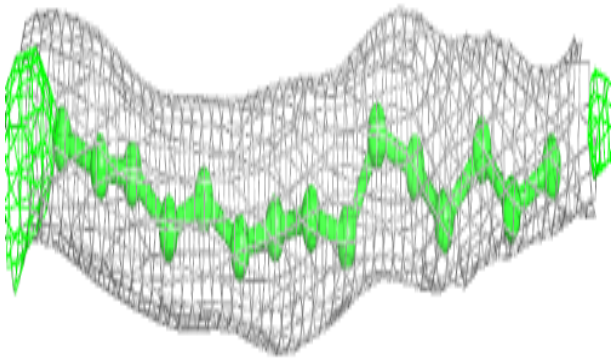


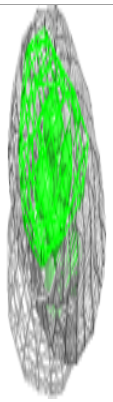


Electron density around LFA B 303:

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

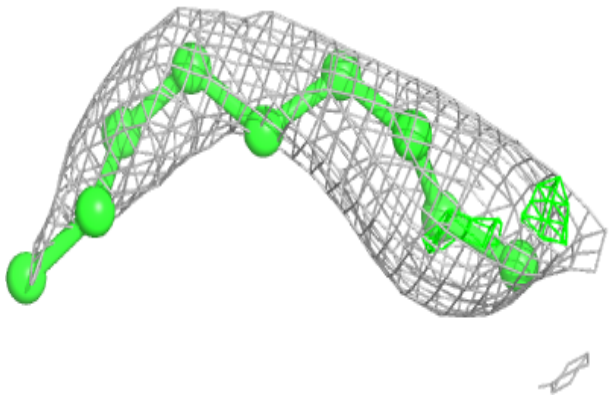


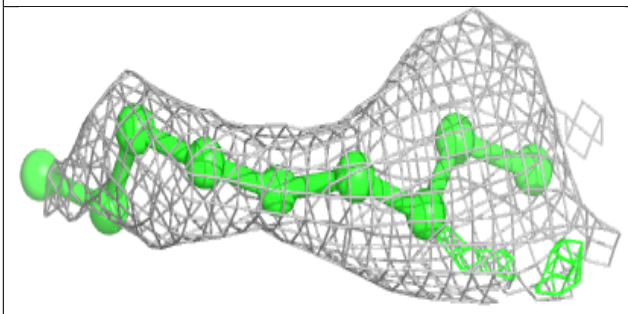


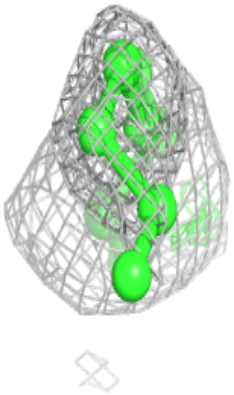


Electron density around LFA A 815:

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

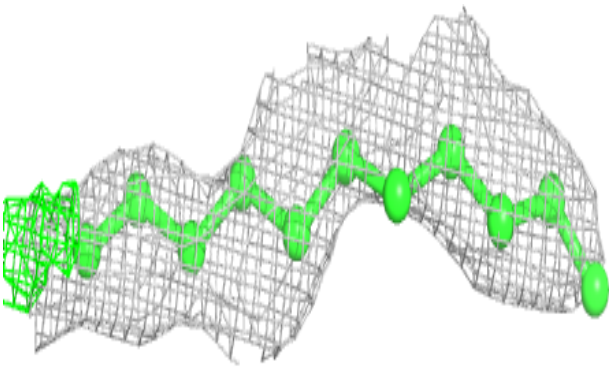


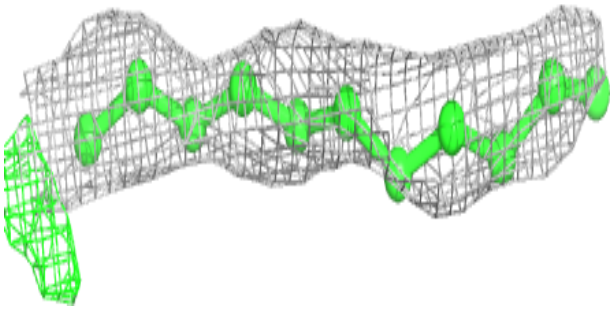


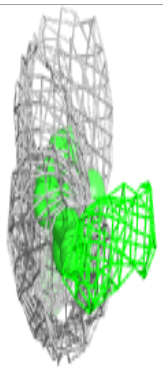


Electron density around LFA C 306:

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

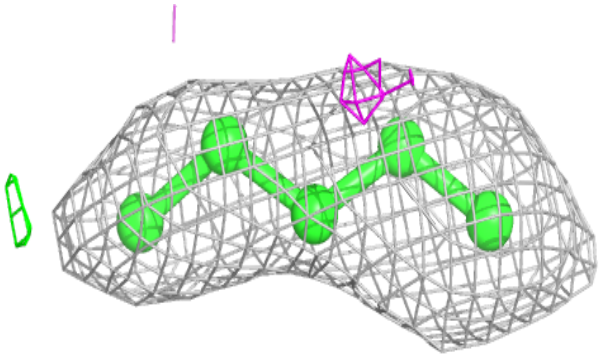


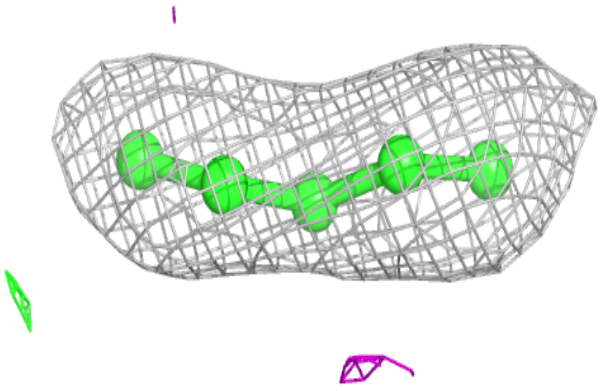


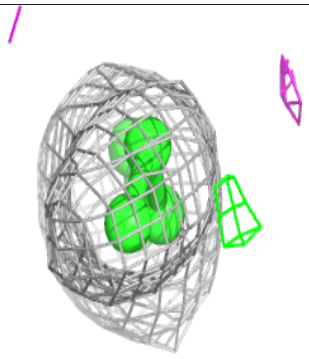


Electron density around LFA B 312:

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

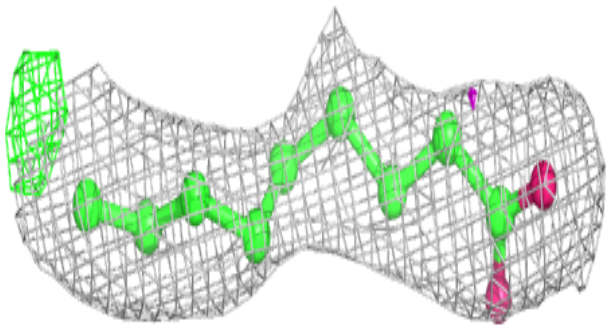


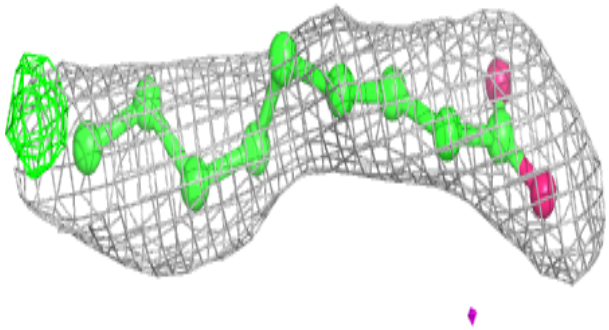


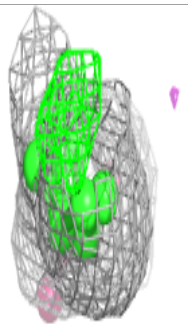


Electron density around OLA A 805:

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

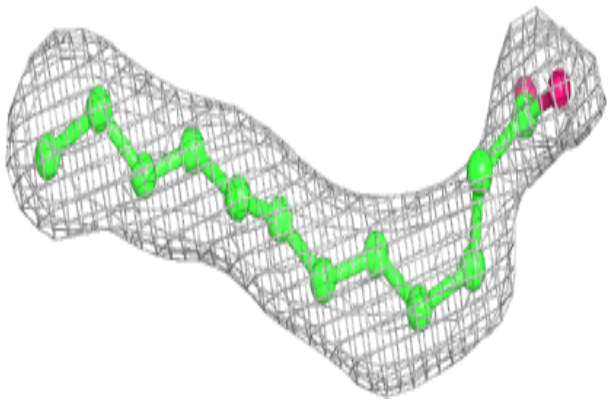


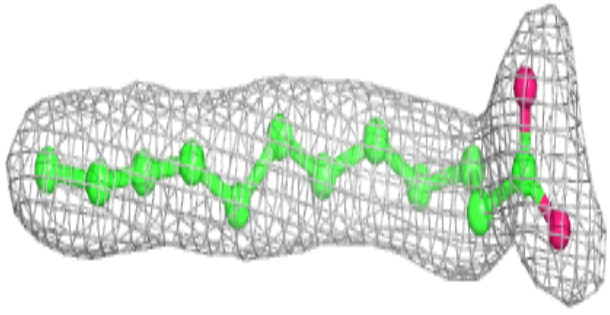


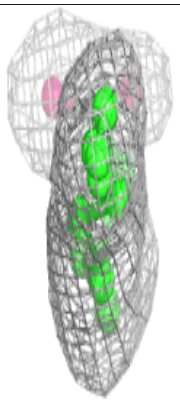


Electron density around OLA C 302:

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

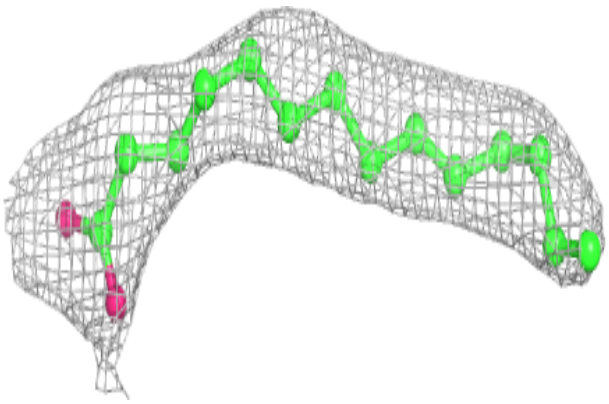


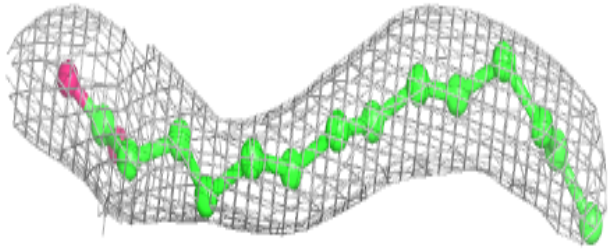


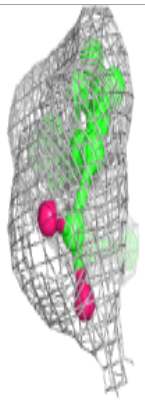


Electron density around OLA C 305:

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

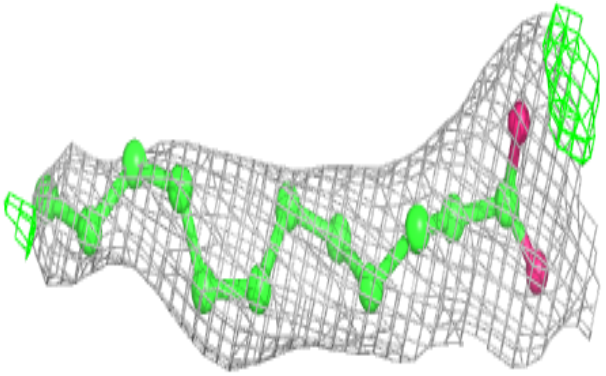


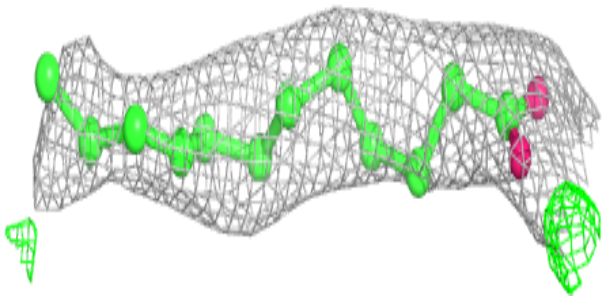


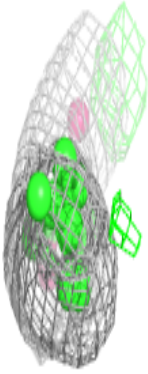


Electron density around OLA B 306:

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

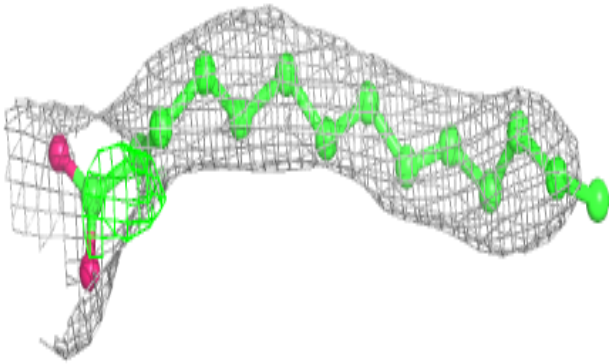


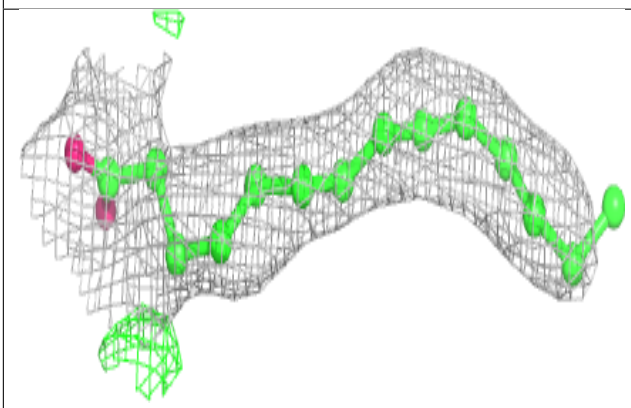


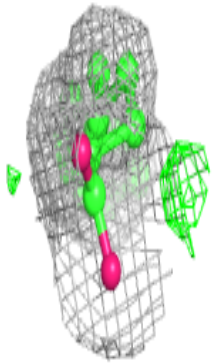


Electron density around OLA A 804:

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

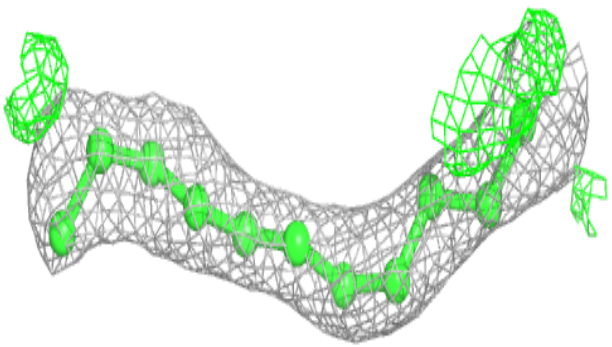


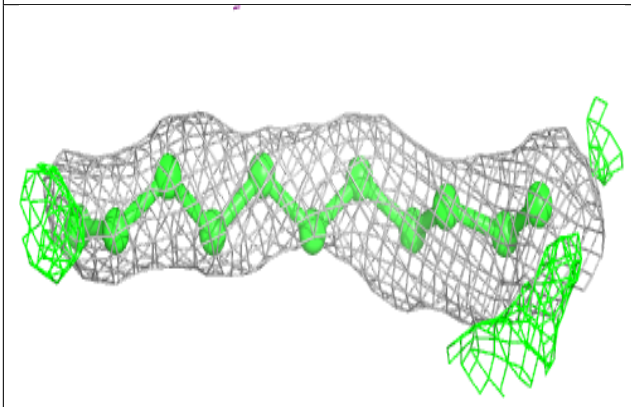


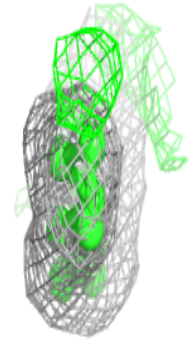


Electron density around LFA A 813:

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

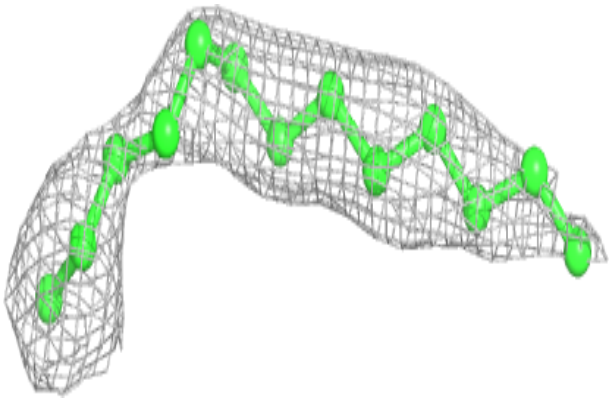


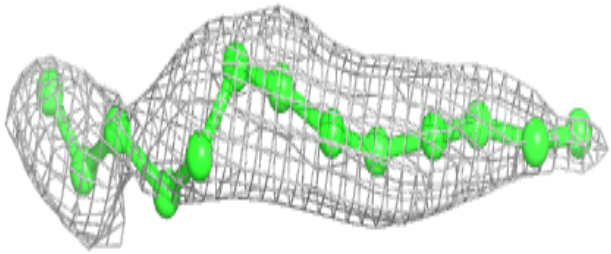


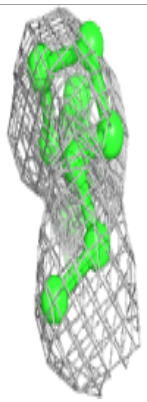


Electron density around LFA A 812:

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

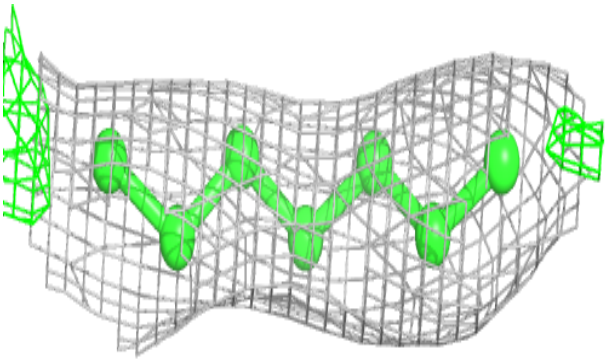


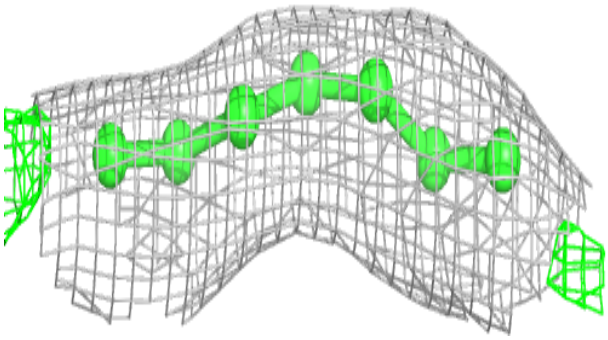


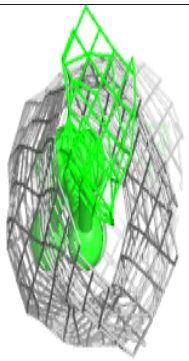


Electron density around LFA B 310:

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

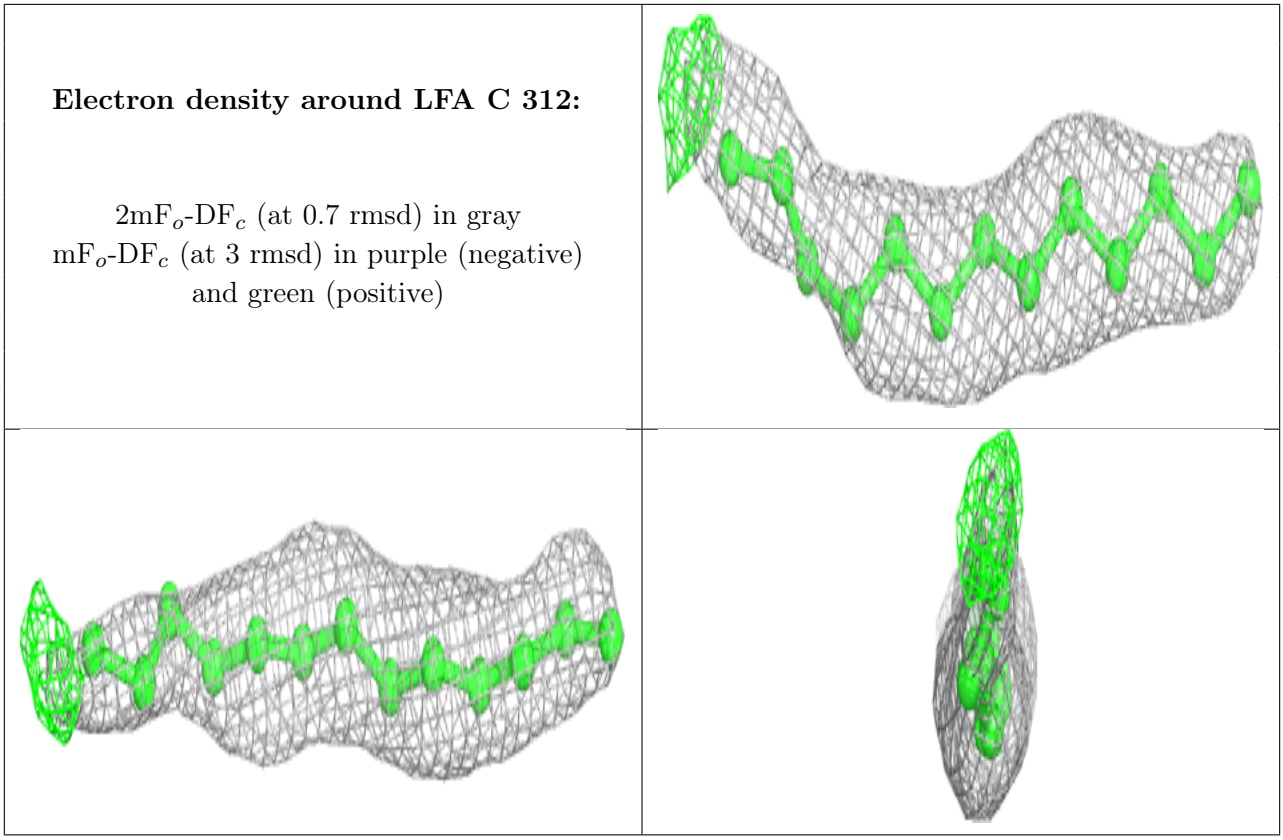






Electron density around LFA C 312:

$2mF_o$-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.