Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2024 – 04:17 pm GMT

PDB ID	:	6YC2
Title	:	Crystal structure of the light-driven sodium pump KR2 in the pentameric form at room temperature, pH 8.0
Authors	:	Kovalev, K.; Gushchin, I.; Gordeliy, V.
Deposited on	:	2020-03-18
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

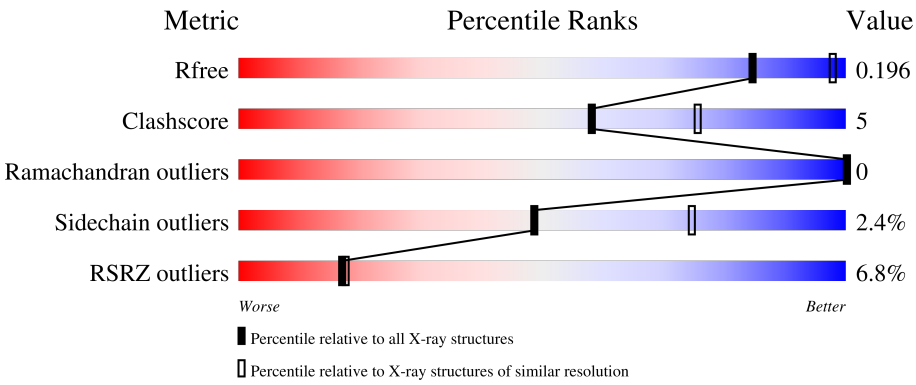
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	273	8% 87% 11% • •
1	B	273	7% 86% 11% • •
1	C	273	7% 87% 10% • •
1	D	273	6% 87% 11% •
1	E	273	5% 86% 11% • •

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
3	LFA	E	808	-	-	-	X
5	OLA	B	304	-	-	-	X
5	OLA	C	305	-	-	-	X
5	OLA	C	307	-	-	-	X
5	OLA	D	502	-	-	-	X
5	OLA	E	806	-	-	-	X
6	ALA	C	301	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11432 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.

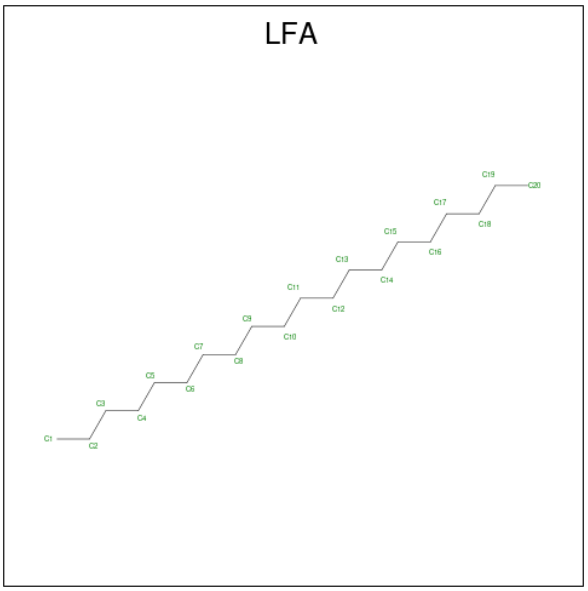
- Molecule 1 is a protein called Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	2166	1451	324	382	9	0	2	0
1	B	268	2168	1451	326	382	9	0	2	0
1	C	268	2166	1450	325	382	9	0	2	0
1	D	269	2172	1455	325	383	9	0	2	0
1	E	268	2167	1452	324	382	9	0	2	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 20	C 20	0	0
3	A	1	Total 13	C 13	0	0
3	A	1	Total 6	C 6	0	0
3	A	1	Total 5	C 5	0	0
3	B	1	Total 17	C 17	0	0
3	B	1	Total 13	C 13	0	0
3	B	1	Total 13	C 13	0	0
3	C	1	Total 17	C 17	0	0
3	C	1	Total 15	C 15	0	0
3	C	1	Total 4	C 4	0	0
3	C	1	Total 10	C 10	0	0
3	C	1	Total 12	C 12	0	0
3	D	1	Total 14	C 14	0	0
3	D	1	Total 16	C 16	0	0

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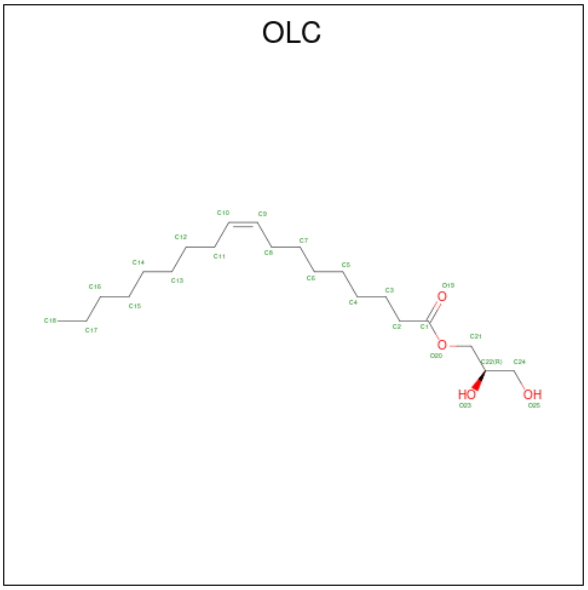
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C 10 10	0	0
3	D	1	Total C 5 5	0	0
3	E	1	Total C 9 9	0	0
3	E	1	Total C 5 5	0	0
3	E	1	Total C 17 17	0	0
3	E	1	Total C 13 13	0	0
3	E	1	Total C 18 18	0	0

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 5 2	0	0
4	B	1	Total C O 9 5 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	D	1	Total C O 6 4 2	0	0

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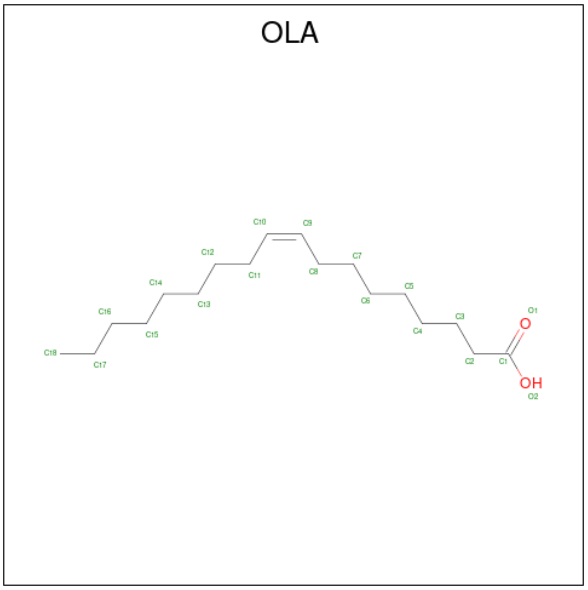
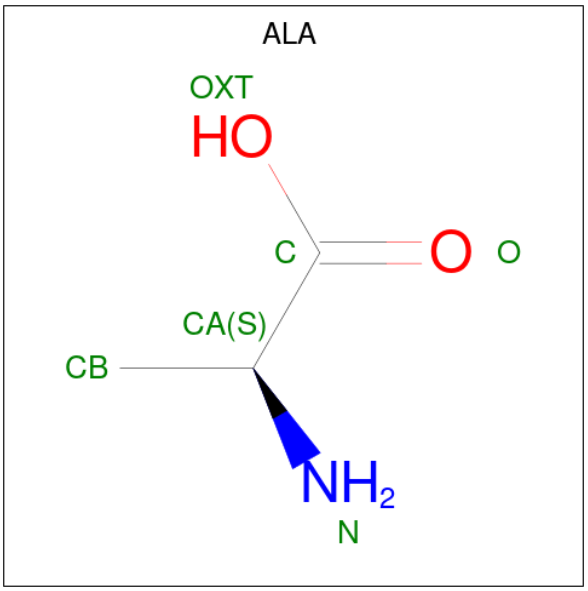
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	E	1	7	5	2	0	0

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	19	17	2	0	0
			Total	C	O		
5	C	1	20	18	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	D	1	18	16	2	0	0
			Total	C	O		
5	E	1	10	8	2	0	0

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	5	3	1	1	0	0

- Molecule 7 is water.

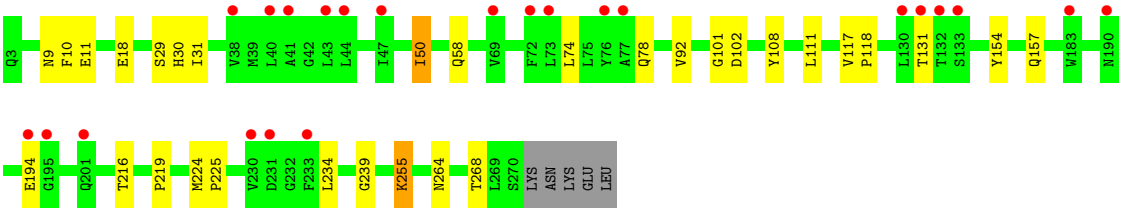
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	43	43	43	0	0
			Total	O		
7	B	37	37	37	0	0
			Total	O		
7	C	49	49	49	0	0
			Total	O		
7	D	52	52	52	0	0
			Total	O		
7	E	40	40	40	0	0

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.

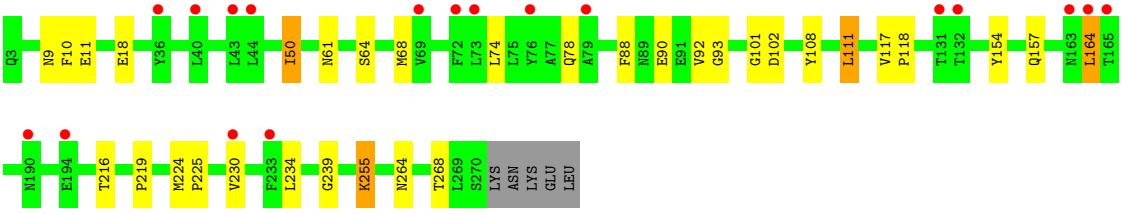
• Molecule 1: Sodium pumping rhodopsin

Chain A:



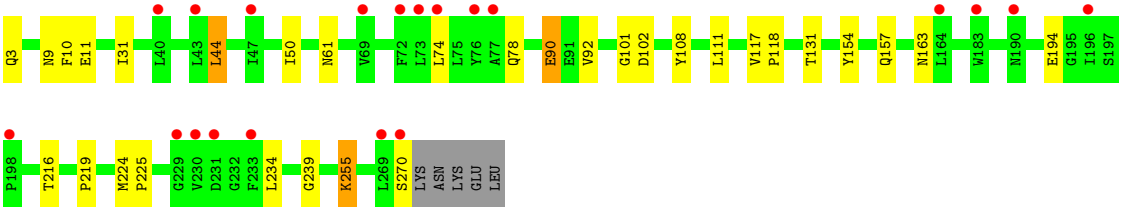
• Molecule 1: Sodium pumping rhodopsin

Chain B:



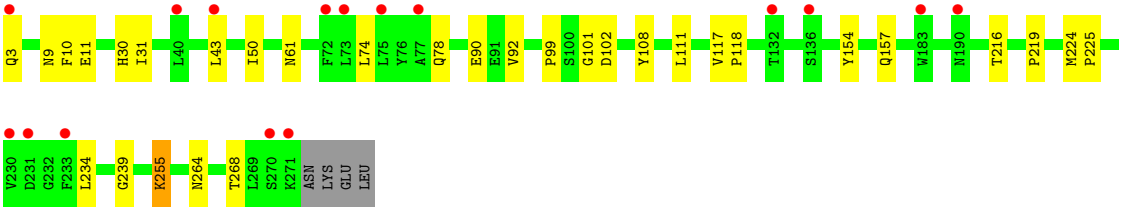
• Molecule 1: Sodium pumping rhodopsin

Chain C:



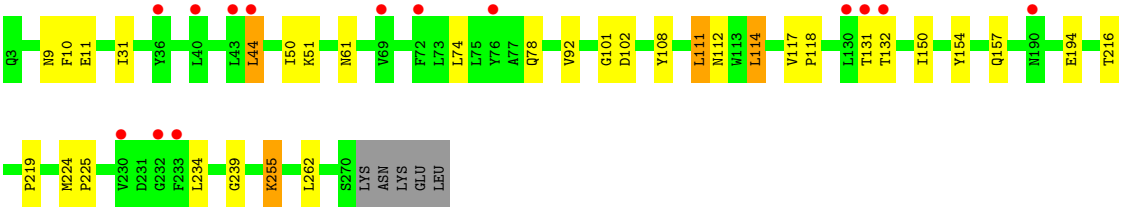
• Molecule 1: Sodium pumping rhodopsin

Chain D:



- Molecule 1: Sodium pumping rhodopsin

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	135.54Å 240.13Å 138.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 48.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.50) 100.0 (48.86-2.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.163 , 0.188 0.174 , 0.196	Depositor DCC
R_{free} test set	3769 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11432	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 5.31% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.64	0/2194	0.64	0/2984
1	B	0.64	0/2196	0.64	0/2986
1	C	0.64	0/2194	0.63	0/2984
1	D	0.64	0/2200	0.64	0/2992
1	E	0.64	0/2195	0.63	0/2985
All	All	0.64	0/10979	0.64	0/14931

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2166	0	2150	20	0
1	B	2168	0	2160	20	0
1	C	2166	0	2153	24	0
1	D	2172	0	2154	20	0
1	E	2167	0	2152	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	44	0	84	1	0
3	B	43	0	83	1	0
3	C	58	0	108	0	0
3	D	45	0	83	0	0
3	E	62	0	116	8	0
4	A	7	0	4	0	0
4	B	9	0	7	0	0
4	C	10	0	9	2	0
4	D	6	0	4	0	0
4	E	7	0	4	0	0
5	B	19	0	28	1	0
5	C	24	0	33	0	0
5	D	18	0	26	0	0
5	E	10	0	12	4	0
6	C	5	0	4	2	0
7	A	43	0	0	1	0
7	B	37	0	0	1	0
7	C	49	0	0	0	0
7	D	52	0	0	0	0
7	E	40	0	0	1	0
All	All	11432	0	11374	109	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 (109) 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:C:270:SER:C	6:C:301:ALA:N	2.04	1.11
3:E:801:LFA:C9	3:E:802:LFA:H12	1.99	0.92
1:C:255:LYR:H183	1:C:255:LYR:H9	1.58	0.85
1:A:255:LYR:H9	1:A:255:LYR:H183	1.58	0.84
3:E:801:LFA:H12	5:E:806:OLA:C8	2.08	0.84
1:B:255:LYR:H9	1:B:255:LYR:H183	1.58	0.83
1:E:255:LYR:H193	1:E:255:LYR:H9	1.60	0.81
3:A:304:LFA:C15	5:B:304:OLA:C17	2.61	0.78
1:C:90:GLU:HB3	1:D:3:GLN:HE21	1.53	0.73
1:D:255:LYR:H9	1:D:255:LYR:H182	1.73	0.70
1:A:18:GLU:OE1	7:A:401:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLU:OE1	7:B:401:HOH:O	2.12	0.66
1:C:163:ASN:HD22	4:C:306:OLC:H24A	1.60	0.66
1:D:255:LYR:H182	1:D:255:LYR:C9	2.27	0.63
1:C:163:ASN:HD22	4:C:306:OLC:C24	2.13	0.61
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.84	0.60
1:E:51:LYS:HE2	3:E:808:LFA:H172	1.84	0.60
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.86	0.58
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.84	0.58
1:B:255:LYR:H183	1:B:255:LYR:C9	2.32	0.56
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.85	0.56
1:A:255:LYR:H183	1:A:255:LYR:C9	2.33	0.56
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.88	0.56
1:A:50[A]:ILE:HD11	1:A:58:GLN:HB3	1.87	0.56
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.88	0.55
1:C:74:LEU:HD21	1:C:108:TYR:HB3	1.92	0.52
1:E:74:LEU:HD21	1:E:108:TYR:HB3	1.92	0.52
1:E:255:LYR:H193	1:E:255:LYR:C9	2.35	0.52
1:B:216:THR:O	1:B:219:PRO:HG2	2.11	0.50
1:D:216:THR:O	1:D:219:PRO:HG2	2.10	0.50
1:C:216:THR:O	1:C:219:PRO:HG2	2.12	0.50
1:A:234:LEU:O	1:A:239:GLY:HA3	2.12	0.50
1:E:111:LEU:O	1:E:114:LEU:HB2	2.11	0.50
1:D:255:LYR:H9	1:D:255:LYR:H193	1.94	0.49
1:B:74:LEU:HD21	1:B:108:TYR:HB3	1.94	0.49
1:C:234:LEU:O	1:C:239:GLY:HA3	2.13	0.49
1:E:234:LEU:O	1:E:239:GLY:HA3	2.13	0.49
1:D:74:LEU:HD21	1:D:108:TYR:HB3	1.95	0.48
1:A:216:THR:O	1:A:219:PRO:HG2	2.13	0.48
1:B:234:LEU:O	1:B:239:GLY:HA3	2.13	0.48
1:D:234:LEU:O	1:D:239:GLY:HA3	2.13	0.48
1:E:216:THR:O	1:E:219:PRO:HG2	2.14	0.48
1:C:255:LYR:H183	1:C:255:LYR:C9	2.32	0.48
1:B:264:ASN:O	1:B:268:THR:HG23	2.14	0.48
1:D:264:ASN:O	1:D:268:THR:HG23	2.14	0.48
1:A:74:LEU:HD21	1:A:108:TYR:HB3	1.96	0.47
1:D:78:GLN:HA	1:D:78:GLN:OE1	2.14	0.47
1:A:78:GLN:HA	1:A:78:GLN:OE1	2.15	0.47
1:D:101:GLY:O	1:D:102:ASP:HB2	2.15	0.47
1:E:78:GLN:HA	1:E:78:GLN:OE1	2.15	0.47
1:B:101:GLY:O	1:B:102:ASP:HB2	2.15	0.47
3:E:801:LFA:C9	3:E:802:LFA:C1	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLN:HA	1:C:78:GLN:OE1	2.14	0.47
1:A:264:ASN:O	1:A:268:THR:HG23	2.16	0.46
1:B:78:GLN:OE1	1:B:78:GLN:HA	2.15	0.46
3:E:801:LFA:H12	5:E:806:OLA:C7	2.45	0.46
1:C:101:GLY:O	1:C:102:ASP:HB2	2.16	0.46
1:C:154:TYR:O	1:C:157:GLN:HG3	2.15	0.46
1:D:154:TYR:O	1:D:157:GLN:HG3	2.16	0.46
1:A:30:HIS:HB3	1:B:111:LEU:HD22	1.99	0.45
1:C:50[B]:ILE:HD12	1:C:61:ASN:HB2	1.98	0.45
1:A:101:GLY:O	1:A:102:ASP:HB2	2.17	0.45
1:E:50[A]:ILE:HD12	1:E:61:ASN:HB2	1.97	0.44
1:E:154:TYR:O	1:E:157:GLN:HG3	2.17	0.44
3:E:802:LFA:H11	3:E:808:LFA:H11	2.00	0.44
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.83	0.44
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.84	0.44
3:E:801:LFA:C1	5:E:806:OLA:C8	2.90	0.44
1:A:29[B]:SER:HB3	1:B:108:TYR:HH	1.81	0.44
1:A:154:TYR:O	1:A:157:GLN:HG3	2.18	0.43
1:C:90:GLU:HG2	1:D:99:PRO:HG2	2.00	0.43
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.81	0.43
1:B:154:TYR:O	1:B:157:GLN:HG3	2.18	0.43
1:C:255:LYR:H10	1:C:255:LYR:H81	1.91	0.43
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.19	0.43
3:B:306:LFA:H111	3:B:306:LFA:H81	1.89	0.43
1:C:255:LYR:H6	1:C:255:LYR:H41	1.92	0.43
1:E:114:LEU:HD12	1:E:114:LEU:HA	1.85	0.43
3:E:801:LFA:H12	5:E:806:OLA:H71	2.01	0.43
1:D:224:MET:N	1:D:225:PRO:HD2	2.34	0.42
1:A:224:MET:N	1:A:225:PRO:HD2	2.34	0.42
1:C:131:THR:HG21	1:C:194:GLU:OE1	2.19	0.42
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.20	0.42
1:E:31:ILE:HD12	1:E:31:ILE:HA	1.92	0.42
1:E:101:GLY:O	1:E:102:ASP:HB2	2.19	0.42
1:A:131:THR:HG21	1:A:194:GLU:OE1	2.18	0.42
1:C:31:ILE:HD12	1:C:31:ILE:HA	1.90	0.42
1:C:224:MET:N	1:C:225:PRO:HD2	2.34	0.42
1:D:50[A]:ILE:HD12	1:D:61:ASN:HB2	2.01	0.42
1:E:224:MET:N	1:E:225:PRO:HD2	2.34	0.42
1:B:50[A]:ILE:HD12	1:B:61:ASN:HB2	2.01	0.42
1:B:224:MET:N	1:B:225:PRO:HD2	2.35	0.42
1:D:31:ILE:HD12	1:D:31:ILE:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:HIS:HB3	1:E:111:LEU:HD22	2.02	0.41
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.20	0.41
1:A:31:ILE:HD12	1:A:31:ILE:HA	1.93	0.41
1:A:255:LYR:H6	1:A:255:LYR:H41	1.93	0.41
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.20	0.41
1:E:131:THR:HG21	1:E:194:GLU:OE1	2.20	0.41
1:B:88:PHE:CZ	1:B:93:GLY:HA2	2.56	0.41
1:C:270:SER:C	6:C:301:ALA:CA	2.86	0.41
1:C:44:LEU:HD11	1:D:43:LEU:HD11	2.03	0.41
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.21	0.41
1:E:255:LYR:H10	1:E:255:LYR:H81	1.90	0.41
1:E:262:LEU:HD23	1:E:262:LEU:HA	1.93	0.41
1:D:255:LYR:H6	1:D:255:LYR:H41	1.92	0.40
1:A:30:HIS:CB	1:B:111:LEU:HD22	2.52	0.40
1:B:64:SER:O	1:B:68:MET:HG2	2.22	0.40
1:E:112:ASN:HB3	7:E:914:HOH:O	2.22	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	267/273 (98%)	262 (98%)	5 (2%)	0	100	100
1	B	267/273 (98%)	263 (98%)	4 (2%)	0	100	100
1	C	267/273 (98%)	262 (98%)	5 (2%)	0	100	100
1	D	268/273 (98%)	262 (98%)	6 (2%)	0	100	100
1	E	267/273 (98%)	262 (98%)	5 (2%)	0	100	100
All	All	1336/1365 (98%)	1311 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/233 (97%)	222 (98%)	5 (2%)	52	77
1	B	229/233 (98%)	221 (96%)	8 (4%)	36	62
1	C	228/233 (98%)	222 (97%)	6 (3%)	46	72
1	D	227/233 (97%)	223 (98%)	4 (2%)	59	81
1	E	227/233 (97%)	221 (97%)	6 (3%)	46	72
All	All	1138/1165 (98%)	1109 (98%)	29 (2%)	49	73

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	50[A]	ILE
1	A	50[B]	ILE
1	A	92	VAL
1	A	111	LEU
1	B	10	PHE
1	B	50[A]	ILE
1	B	50[B]	ILE
1	B	90	GLU
1	B	92	VAL
1	B	111	LEU
1	B	164	LEU
1	B	230	VAL
1	C	3	GLN
1	C	10	PHE
1	C	44	LEU
1	C	90	GLU
1	C	92	VAL
1	C	111	LEU
1	D	10	PHE
1	D	90	GLU
1	D	92	VAL
1	D	111	LEU

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Mol	Chain	Res	Type
1	E	10	PHE
1	E	44	LEU
1	E	92	VAL
1	E	111	LEU
1	E	114	LEU
1	E	132	THR

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

Mol	Chain	Res	Type
1	C	3	GLN
1	C	163	ASN
1	D	3	GLN
1	D	141	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)

5 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	255	1	27,29,30	1.25	2 (7%)	30,37,39	1.08	1 (3%)
1	LYR	B	255	1	27,29,30	1.28	2 (7%)	30,37,39	1.10	2 (6%)
1	LYR	E	255	1	27,29,30	1.26	2 (7%)	30,37,39	1.08	1 (3%)
1	LYR	C	255	1	27,29,30	1.25	2 (7%)	30,37,39	1.12	3 (10%)
1	LYR	D	255	1	27,29,30	1.24	2 (7%)	30,37,39	1.13	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	255	1	-	3/22/40/42	0/1/1/1
1	LYR	B	255	1	-	3/22/40/42	0/1/1/1
1	LYR	E	255	1	-	3/22/40/42	0/1/1/1
1	LYR	C	255	1	-	4/22/40/42	0/1/1/1
1	LYR	D	255	1	-	4/22/40/42	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	LYR	C7-C80	4.37	1.41	1.35
1	E	255	LYR	C7-C80	4.09	1.41	1.35
1	A	255	LYR	C7-C80	4.07	1.41	1.35
1	C	255	LYR	C7-C80	3.99	1.41	1.35
1	D	255	LYR	C7-C80	3.99	1.41	1.35
1	E	255	LYR	C9-C80	-2.61	1.40	1.45
1	A	255	LYR	C9-C80	-2.57	1.40	1.45
1	C	255	LYR	C9-C80	-2.57	1.40	1.45
1	B	255	LYR	C9-C80	-2.51	1.40	1.45
1	D	255	LYR	C9-C80	-2.42	1.40	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	255	LYR	C8-C80-C7	-4.12	117.15	122.92
1	C	255	LYR	C8-C80-C7	-4.11	117.17	122.92
1	B	255	LYR	C8-C80-C7	-3.96	117.37	122.92
1	A	255	LYR	C8-C80-C7	-3.96	117.38	122.92
1	E	255	LYR	C8-C80-C7	-3.91	117.44	122.92
1	C	255	LYR	C9-C80-C7	2.06	122.10	118.94
1	D	255	LYR	C9-C80-C7	2.04	122.07	118.94
1	C	255	LYR	C16-C17-C11	2.02	113.58	110.48
1	B	255	LYR	C9-C80-C7	2.02	122.03	118.94

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	255	LYR	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	E	255	LYR	CE-CD-CG-CB
1	B	255	LYR	CE-CD-CG-CB
1	D	255	LYR	CE-CD-CG-CB
1	A	255	LYR	NZ-C1-C2-C3
1	B	255	LYR	NZ-C1-C2-C3
1	C	255	LYR	NZ-C1-C2-C3
1	D	255	LYR	NZ-C1-C2-C3
1	E	255	LYR	NZ-C1-C2-C3
1	C	255	LYR	CE-CD-CG-CB
1	A	255	LYR	CD-CE-NZ-C1
1	C	255	LYR	CD-CE-NZ-C1
1	D	255	LYR	CD-CE-NZ-C1
1	B	255	LYR	CD-CE-NZ-C1
1	E	255	LYR	CD-CE-NZ-C1
1	C	255	LYR	C2-C1-NZ-CE
1	D	255	LYR	C2-C1-NZ-CE

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	255	LYR	3	0
1	B	255	LYR	2	0
1	E	255	LYR	3	0
1	C	255	LYR	4	0
1	D	255	LYR	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 5 are monoatomic - leaving 32 for Mogul analysis.

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	$\#\|Z\| > 2$
3	LFA	A	302	-	19,19,19	0.08	0	18,18,18	0.04	0
3	LFA	D	501	-	13,13,19	0.11	0	12,12,18	0.06	0
3	LFA	E	805	-	12,12,19	0.10	0	11,11,18	0.08	0
3	LFA	A	304	-	5,5,19	0.13	0	4,4,18	0.09	0
3	LFA	A	306	-	4,4,19	0.14	0	3,3,18	0.23	0
3	LFA	E	802	-	4,4,19	0.16	0	3,3,18	0.26	0
5	OLA	C	305	-	19,19,19	0.52	0	19,19,19	0.50	0
3	LFA	C	304	-	14,14,19	0.09	0	13,13,18	0.05	0
5	OLA	B	304	-	18,18,19	0.52	0	18,18,19	0.50	0
4	OLC	D	506	-	5,5,24	2.07	1 (20%)	5,5,25	1.31	1 (20%)
3	LFA	E	808	-	17,17,19	0.08	0	16,16,18	0.05	0
3	LFA	B	302	-	16,16,19	0.11	0	15,15,18	0.11	0
3	LFA	E	804	-	16,16,19	0.09	0	15,15,18	0.06	0
4	OLC	E	807	-	6,6,24	1.81	1 (16%)	6,6,25	1.44	1 (16%)
3	LFA	E	801	-	8,8,19	0.10	0	7,7,18	0.08	0
3	LFA	B	303	-	12,12,19	0.11	0	11,11,18	0.07	0
5	OLA	C	307	-	3,3,19	0.90	0	3,3,19	0.74	0
3	LFA	C	309	-	9,9,19	0.12	0	8,8,18	0.08	0
5	OLA	E	806	-	9,9,19	0.71	0	9,9,19	0.68	0
3	LFA	B	306	-	12,12,19	0.12	0	11,11,18	0.10	0
3	LFA	A	303	-	12,12,19	0.09	0	11,11,18	0.06	0
3	LFA	C	303	-	16,16,19	0.08	0	15,15,18	0.07	0
3	LFA	D	505	-	9,9,19	0.13	0	8,8,18	0.07	0
3	LFA	D	504	-	15,15,19	0.09	0	14,14,18	0.06	0
4	OLC	C	306	-	9,9,24	1.50	1 (11%)	10,10,25	1.46	2 (20%)
3	LFA	C	310	-	11,11,19	0.11	0	10,10,18	0.08	0
6	ALA	C	301	-	3,4,5	0.61	0	2,4,6	0.65	0
5	OLA	D	502	-	17,17,19	0.54	0	17,17,19	0.50	0
3	LFA	D	507	-	4,4,19	0.13	0	3,3,18	0.23	0
4	OLC	A	305	-	6,6,24	1.84	1 (16%)	6,6,25	1.36	1 (16%)
4	OLC	B	305	-	8,8,24	1.04	1 (12%)	9,9,25	1.04	1 (11%)
3	LFA	C	308	-	3,3,19	0.24	0	2,2,18	0.43	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
3	LFA	A	302	-	-	11/17/17/17	-
3	LFA	D	501	-	-	6/11/11/17	-
3	LFA	E	805	-	-	8/10/10/17	-
3	LFA	A	304	-	-	1/3/3/17	-
3	LFA	A	306	-	-	1/2/2/17	-
3	LFA	E	802	-	-	1/2/2/17	-
5	OLA	C	305	-	-	13/17/17/17	-
3	LFA	C	304	-	-	8/12/12/17	-
5	OLA	B	304	-	-	8/16/16/17	-
4	OLC	D	506	-	-	1/3/3/24	-
3	LFA	E	808	-	-	8/15/15/17	-
3	LFA	B	302	-	-	10/14/14/17	-
3	LFA	E	804	-	-	6/14/14/17	-
4	OLC	E	807	-	-	2/5/5/24	-
3	LFA	E	801	-	-	2/6/6/17	-
3	LFA	B	303	-	-	7/10/10/17	-
3	LFA	C	309	-	-	4/7/7/17	-
5	OLA	E	806	-	-	3/7/7/17	-
3	LFA	B	306	-	-	7/10/10/17	-
3	LFA	A	303	-	-	5/10/10/17	-
3	LFA	C	303	-	-	8/14/14/17	-
3	LFA	D	505	-	-	3/7/7/17	-
3	LFA	D	504	-	-	9/13/13/17	-
4	OLC	C	306	-	-	6/9/9/24	-
3	LFA	C	310	-	-	6/9/9/17	-
6	ALA	C	301	-	-	0/0/2/4	-
5	OLA	D	502	-	-	6/15/15/17	-
3	LFA	D	507	-	-	2/2/2/17	-
4	OLC	A	305	-	-	2/5/5/24	-
4	OLC	B	305	-	-	6/7/7/24	-
3	LFA	C	308	-	-	0/1/1/17	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	506	OLC	O20-C1	4.55	1.46	1.30
4	A	305	OLC	O20-C1	4.36	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	306	OLC	O20-C1	4.34	1.46	1.33
4	E	807	OLC	O20-C1	4.29	1.46	1.33
4	B	305	OLC	O20-C1	2.65	1.46	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	306	OLC	O20-C1-C2	3.73	121.16	111.38
4	E	807	OLC	O20-C1-C2	2.28	121.26	112.23
4	C	306	OLC	O20-C1-O19	-2.22	117.98	123.59
4	B	305	OLC	O20-C1-C2	2.17	121.85	112.38
4	A	305	OLC	O20-C1-C2	2.09	120.51	112.23
4	D	506	OLC	O20-C1-O19	-2.02	118.26	123.30

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	305	OLC	C21-C22-C24-O25
4	B	305	OLC	O20-C21-C22-O23
4	C	306	OLC	O20-C21-C22-C24
4	C	306	OLC	O20-C21-C22-O23
4	A	305	OLC	C2-C1-O20-C21
3	B	302	LFA	C5-C6-C7-C8
4	C	306	OLC	C2-C1-O20-C21
3	B	306	LFA	C11-C10-C9-C8
4	C	306	OLC	O19-C1-O20-C21
5	C	305	OLA	C1-C2-C3-C4
4	A	305	OLC	O19-C1-O20-C21
3	B	303	LFA	C3-C4-C5-C6
3	C	303	LFA	C4-C5-C6-C7
3	D	505	LFA	C3-C4-C5-C6
3	E	804	LFA	C4-C5-C6-C7
5	B	304	OLA	C13-C14-C15-C16
4	B	305	OLC	O20-C21-C22-C24
3	A	303	LFA	C9-C10-C11-C12
3	D	504	LFA	C7-C8-C9-C10
3	B	302	LFA	C3-C4-C5-C6
3	C	303	LFA	C11-C12-C13-C14
5	C	305	OLA	C11-C10-C9-C8
3	A	302	LFA	C2-C3-C4-C5
3	A	302	LFA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	E	801	LFA	C4-C5-C6-C7
5	B	304	OLA	C3-C4-C5-C6
3	C	303	LFA	C7-C8-C9-C10
3	C	304	LFA	C6-C7-C8-C9
5	C	305	OLA	C13-C14-C15-C16
3	D	504	LFA	C3-C4-C5-C6
3	B	306	LFA	C6-C7-C8-C9
3	B	306	LFA	C7-C8-C9-C10
3	D	501	LFA	C4-C5-C6-C7
3	B	302	LFA	C7-C8-C9-C10
4	C	306	OLC	C21-C22-C24-O25
3	B	302	LFA	C6-C7-C8-C9
3	B	303	LFA	C6-C7-C8-C9
5	C	305	OLA	C6-C7-C8-C9
3	B	302	LFA	C11-C12-C13-C14
3	E	805	LFA	C10-C11-C12-C13
5	C	305	OLA	C3-C4-C5-C6
3	C	304	LFA	C11-C10-C9-C8
3	C	310	LFA	C12-C13-C14-C15
3	E	805	LFA	C12-C13-C14-C15
3	E	804	LFA	C7-C8-C9-C10
3	A	302	LFA	C14-C15-C16-C17
3	E	804	LFA	C2-C3-C4-C5
3	C	304	LFA	C11-C12-C13-C14
3	D	504	LFA	C4-C5-C6-C7
3	E	805	LFA	C14-C15-C16-C17
3	A	303	LFA	C2-C3-C4-C5
5	D	502	OLA	C5-C6-C7-C8
4	B	305	OLC	O23-C22-C24-O25
3	E	805	LFA	C13-C14-C15-C16
4	D	506	OLC	C1-C2-C3-C4
3	A	302	LFA	C11-C10-C9-C8
3	E	808	LFA	C4-C5-C6-C7
3	A	302	LFA	C3-C4-C5-C6
3	D	504	LFA	C11-C12-C13-C14
3	E	804	LFA	C11-C12-C13-C14
5	B	304	OLA	C5-C6-C7-C8
3	D	501	LFA	C2-C3-C4-C5
3	E	808	LFA	C2-C3-C4-C5
3	E	805	LFA	C9-C10-C11-C12
3	E	808	LFA	C11-C10-C9-C8
5	C	305	OLA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	C	309	LFA	C5-C6-C7-C8
3	A	302	LFA	C7-C8-C9-C10
3	C	304	LFA	C10-C11-C12-C13
4	B	305	OLC	C2-C1-O20-C21
3	B	303	LFA	C7-C8-C9-C10
5	B	304	OLA	C12-C13-C14-C15
3	D	504	LFA	C12-C13-C14-C15
3	C	304	LFA	C2-C3-C4-C5
3	D	505	LFA	C2-C3-C4-C5
3	C	309	LFA	C4-C5-C6-C7
3	D	501	LFA	C3-C4-C5-C6
5	D	502	OLA	C12-C13-C14-C15
3	A	302	LFA	C12-C13-C14-C15
5	D	502	OLA	C2-C3-C4-C5
3	D	505	LFA	C1-C2-C3-C4
3	E	808	LFA	C15-C16-C17-C18
3	D	504	LFA	C13-C14-C15-C16
3	B	302	LFA	C11-C10-C9-C8
3	E	804	LFA	C6-C7-C8-C9
3	C	309	LFA	C1-C2-C3-C4
3	B	303	LFA	C1-C2-C3-C4
3	A	303	LFA	C5-C6-C7-C8
5	D	502	OLA	C13-C14-C15-C16
5	C	305	OLA	C10-C11-C12-C13
3	C	310	LFA	C5-C6-C7-C8
3	B	306	LFA	C3-C4-C5-C6
3	C	309	LFA	C2-C3-C4-C5
3	B	306	LFA	C5-C6-C7-C8
5	C	305	OLA	C2-C3-C4-C5
3	C	303	LFA	C10-C11-C12-C13
3	C	304	LFA	C12-C13-C14-C15
5	E	806	OLA	C3-C4-C5-C6
3	B	302	LFA	C14-C15-C16-C17
3	D	501	LFA	C1-C2-C3-C4
5	C	305	OLA	C12-C13-C14-C15
3	C	304	LFA	C5-C6-C7-C8
3	B	303	LFA	C9-C10-C11-C12
3	B	306	LFA	C10-C11-C12-C13
3	E	805	LFA	C11-C12-C13-C14
3	B	302	LFA	C13-C14-C15-C16
3	E	808	LFA	C7-C8-C9-C10
5	D	502	OLA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	C	303	LFA	C3-C4-C5-C6
3	C	310	LFA	C11-C12-C13-C14
3	E	808	LFA	C10-C11-C12-C13
3	B	303	LFA	C4-C5-C6-C7
5	B	304	OLA	C6-C7-C8-C9
5	C	305	OLA	C15-C16-C17-C18
3	A	302	LFA	C13-C14-C15-C16
3	D	504	LFA	C10-C11-C12-C13
5	B	304	OLA	C10-C11-C12-C13
3	B	302	LFA	C1-C2-C3-C4
3	A	302	LFA	C11-C12-C13-C14
3	C	310	LFA	C9-C10-C11-C12
3	B	306	LFA	C4-C5-C6-C7
4	B	305	OLC	O19-C1-O20-C21
5	C	305	OLA	C11-C12-C13-C14
3	E	802	LFA	C1-C2-C3-C4
3	E	808	LFA	C13-C14-C15-C16
5	C	305	OLA	C7-C8-C9-C10
3	C	303	LFA	C1-C2-C3-C4
3	E	805	LFA	C11-C10-C9-C8
3	B	302	LFA	C12-C13-C14-C15
3	A	304	LFA	C16-C17-C18-C19
3	C	310	LFA	C10-C11-C12-C13
3	C	310	LFA	C6-C7-C8-C9
3	A	306	LFA	C2-C3-C4-C5
3	D	504	LFA	C11-C10-C9-C8
3	A	303	LFA	C7-C8-C9-C10
3	D	504	LFA	C6-C7-C8-C9
3	E	804	LFA	C14-C15-C16-C17
5	C	305	OLA	C9-C10-C11-C12
3	A	302	LFA	C6-C7-C8-C9
3	D	501	LFA	C6-C7-C8-C9
3	C	303	LFA	C14-C15-C16-C17
5	E	806	OLA	O2-C1-C2-C3
3	B	303	LFA	C2-C3-C4-C5
3	D	507	LFA	C3-C4-C5-C6
3	C	303	LFA	C6-C7-C8-C9
3	E	801	LFA	C2-C3-C4-C5
3	E	805	LFA	C6-C7-C8-C9
5	E	806	OLA	O1-C1-C2-C3
4	E	807	OLC	O20-C1-C2-C3
5	B	304	OLA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	B	304	OLA	C9-C10-C11-C12
4	C	306	OLC	O23-C22-C24-O25
4	E	807	OLC	O19-C1-C2-C3
5	D	502	OLA	C11-C12-C13-C14
3	E	808	LFA	C6-C7-C8-C9
3	D	501	LFA	C11-C12-C13-C14
3	C	304	LFA	C1-C2-C3-C4
3	A	303	LFA	C1-C2-C3-C4
3	A	302	LFA	C15-C16-C17-C18
3	D	507	LFA	C2-C3-C4-C5

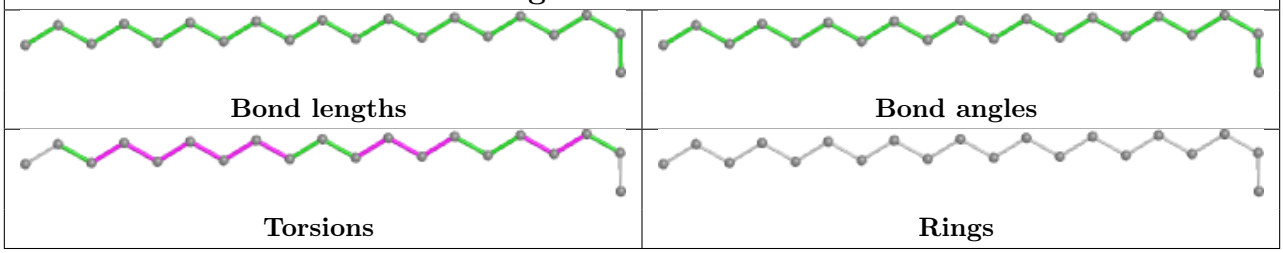
There are no ring outliers.

9 monomers are involved in 14 short contacts:

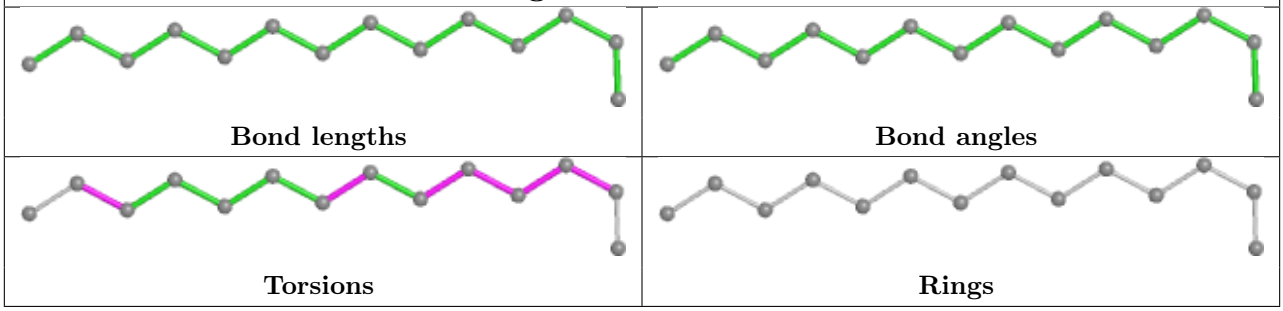
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	LFA	1	0
3	E	802	LFA	3	0
5	B	304	OLA	1	0
3	E	808	LFA	2	0
3	E	801	LFA	6	0
5	E	806	OLA	4	0
3	B	306	LFA	1	0
4	C	306	OLC	2	0
6	C	301	ALA	2	0

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.

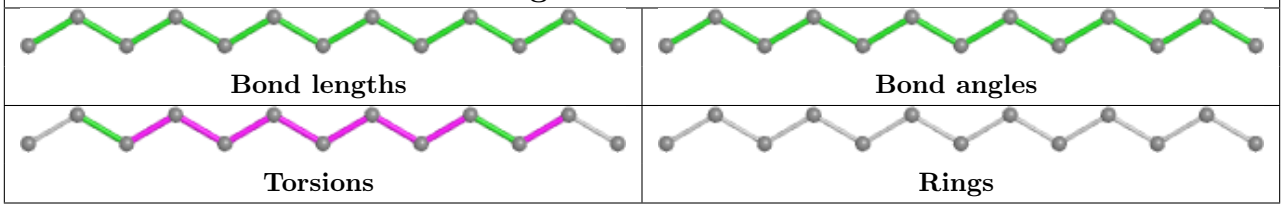
Ligand LFA A 302



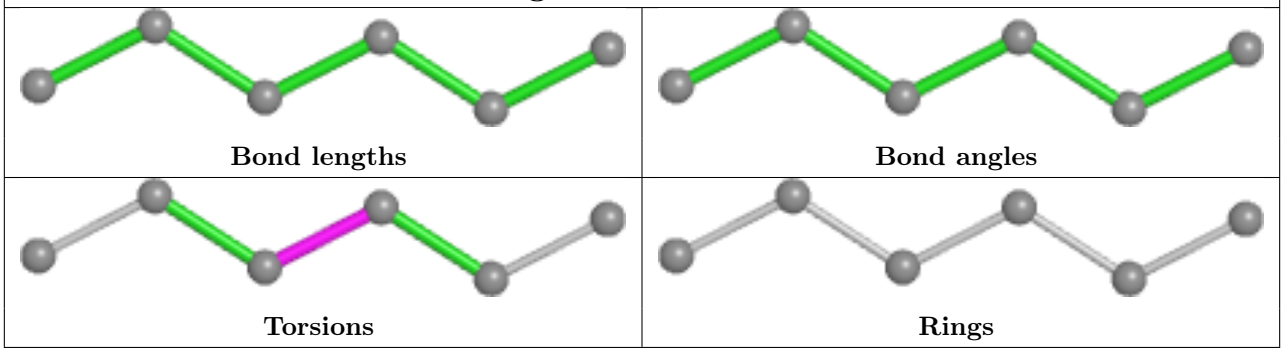
Ligand LFA D 501



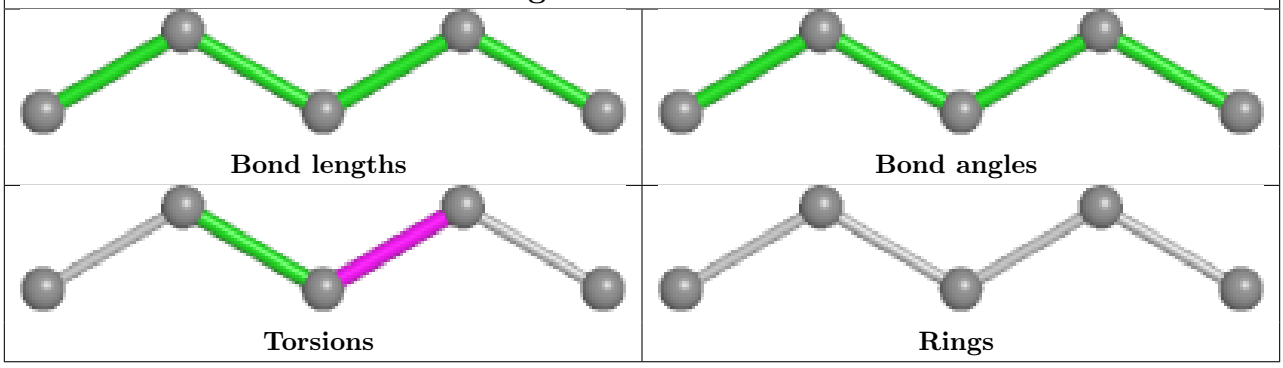
Ligand LFA E 805



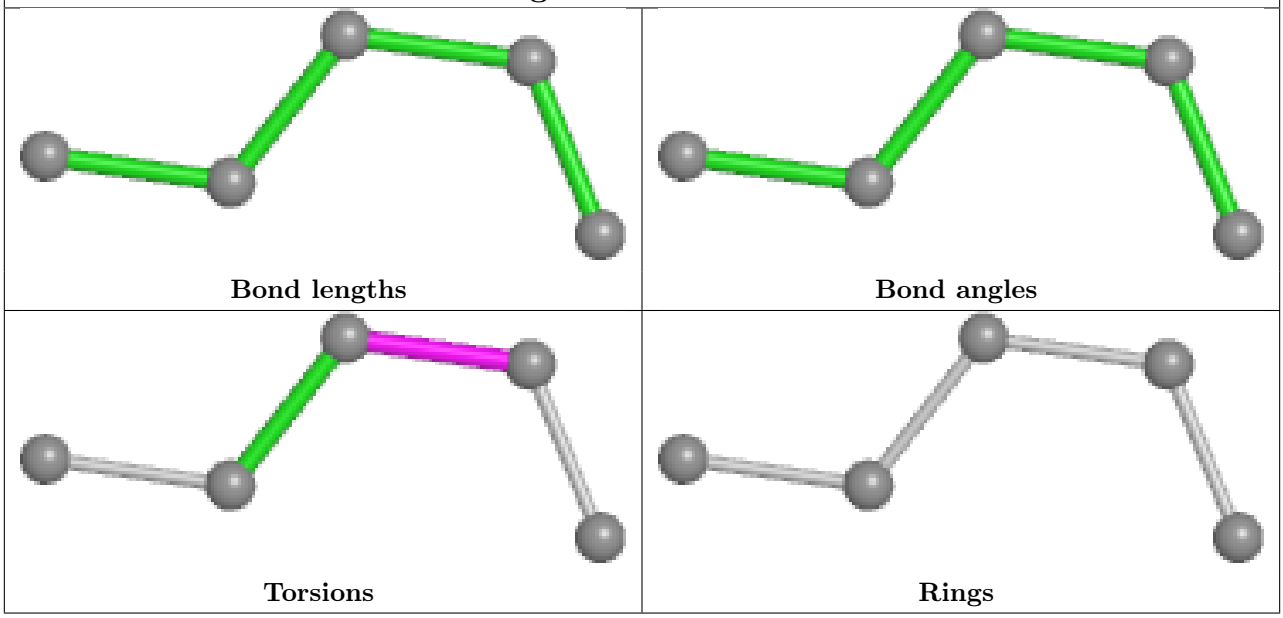
Ligand LFA A 304



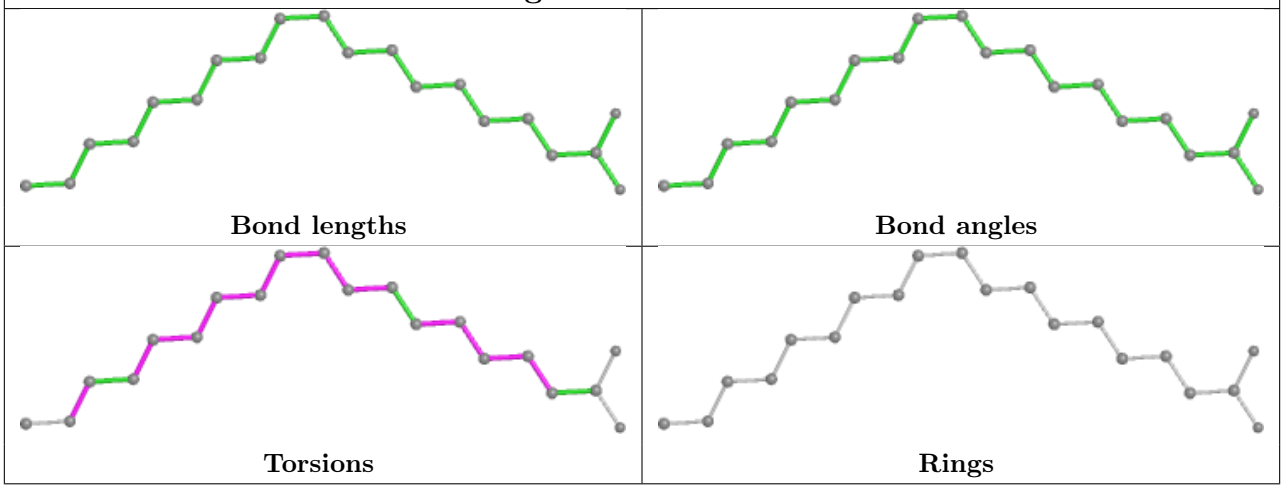
Ligand LFA A 306



Ligand LFA E 802



Ligand OLA C 305



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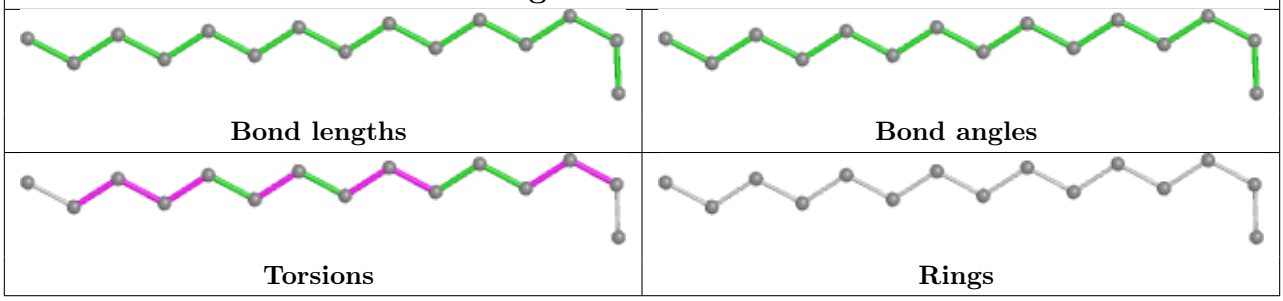
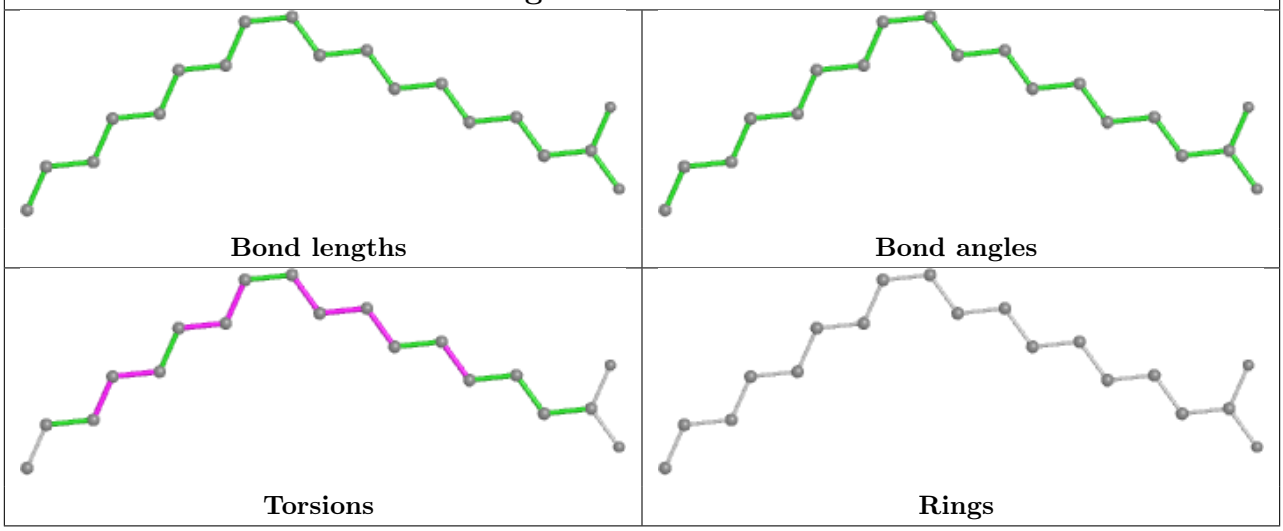
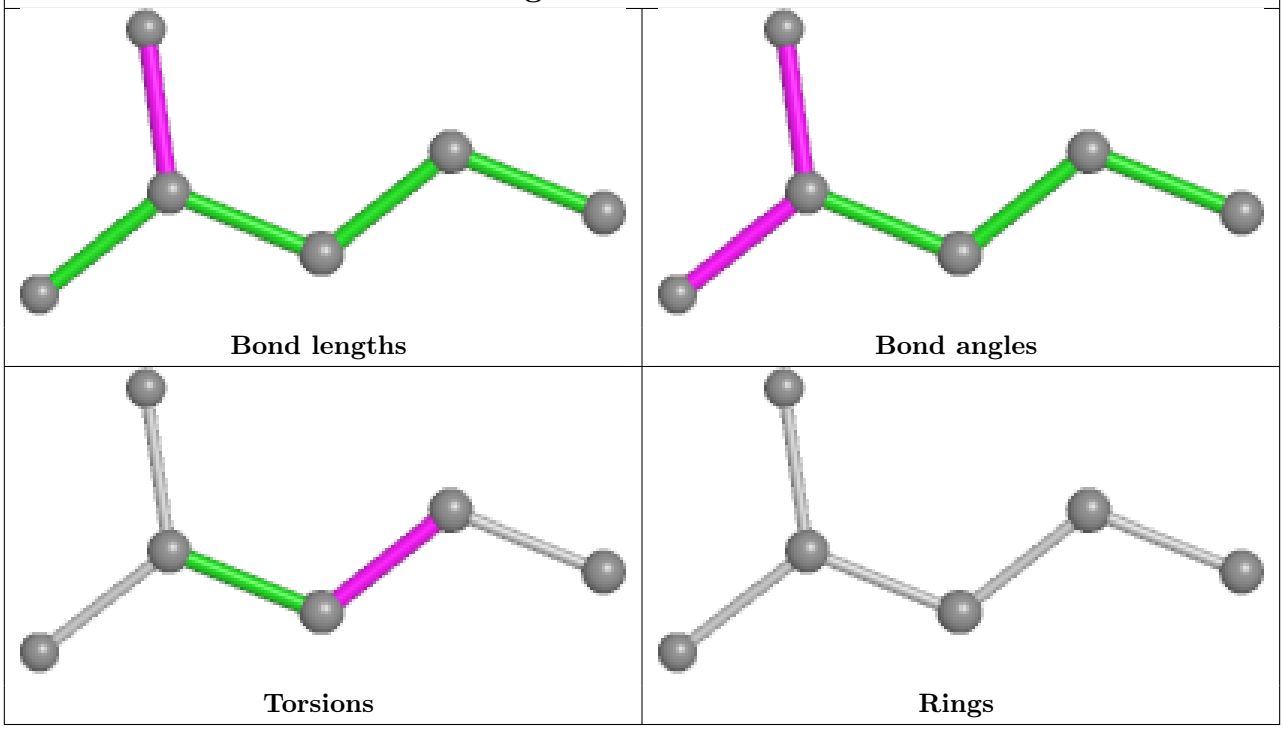


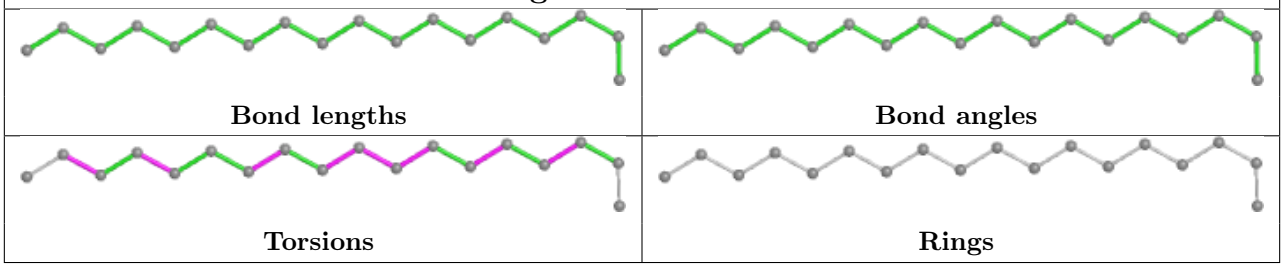
Ligand OLA B 304



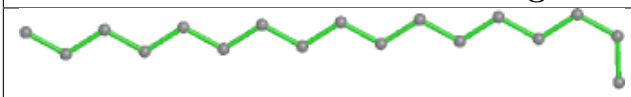
Ligand OLC D 506



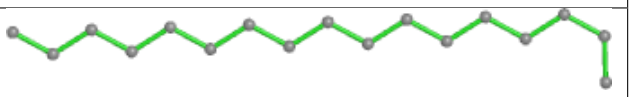
Ligand LFA E 808



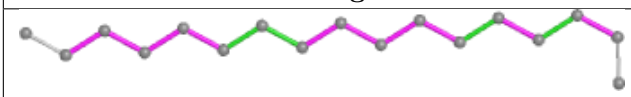
Ligand LFA B 302



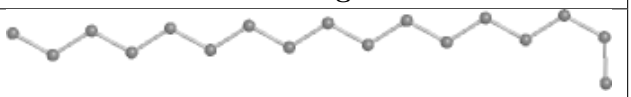
Bond lengths



Bond angles

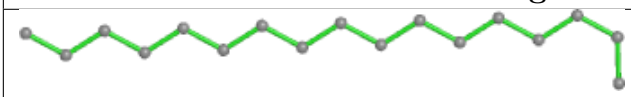


Torsions

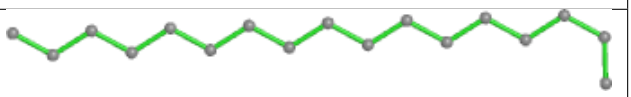


Rings

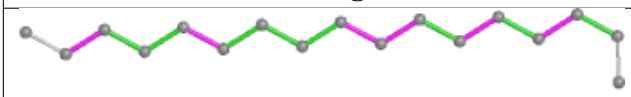
Ligand LFA E 804



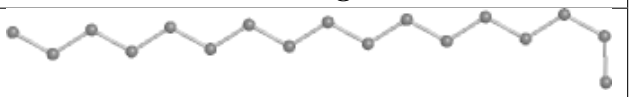
Bond lengths



Bond angles

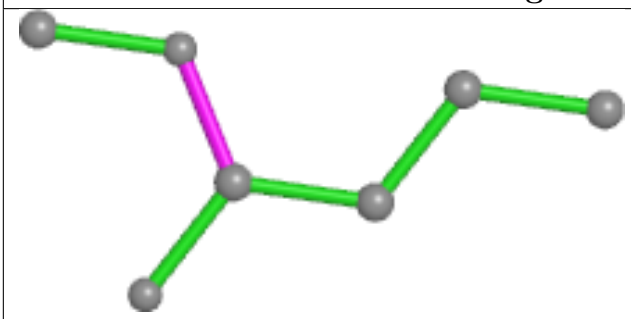


Torsions

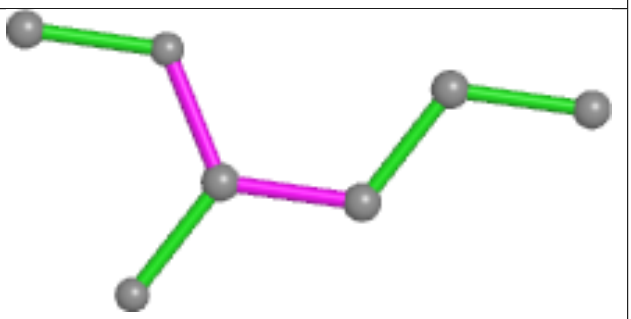


Rings

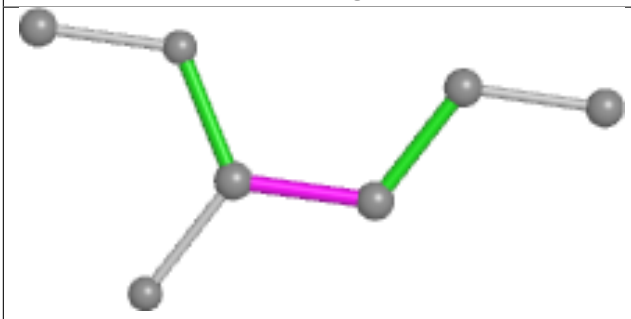
Ligand OLC E 807



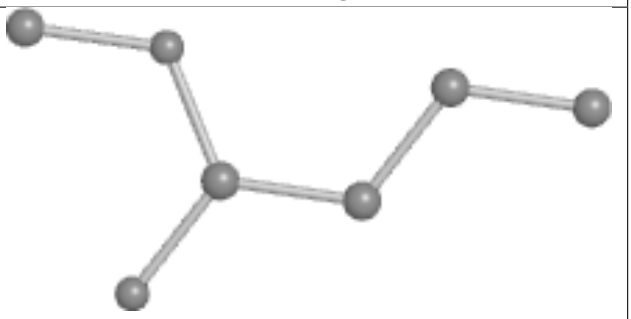
Bond lengths



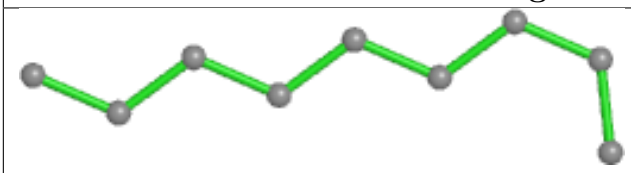
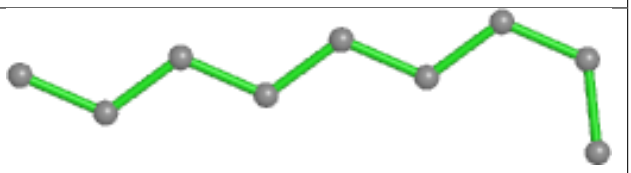
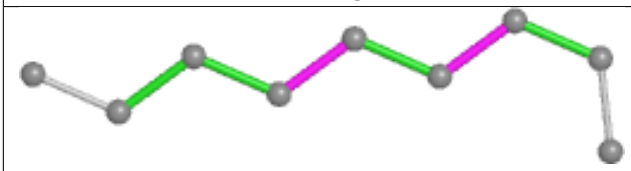
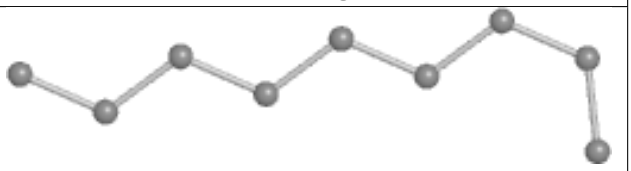
Bond angles

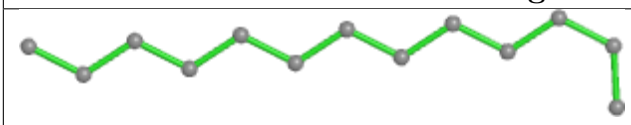
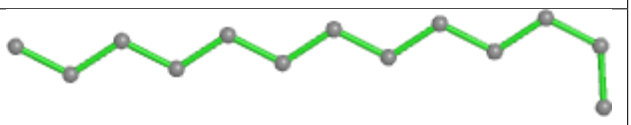
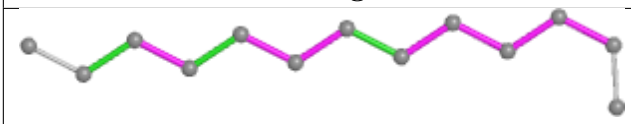
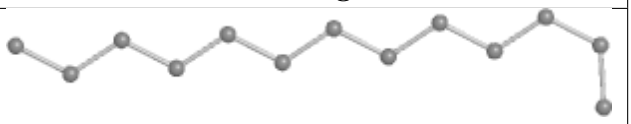


Torsions

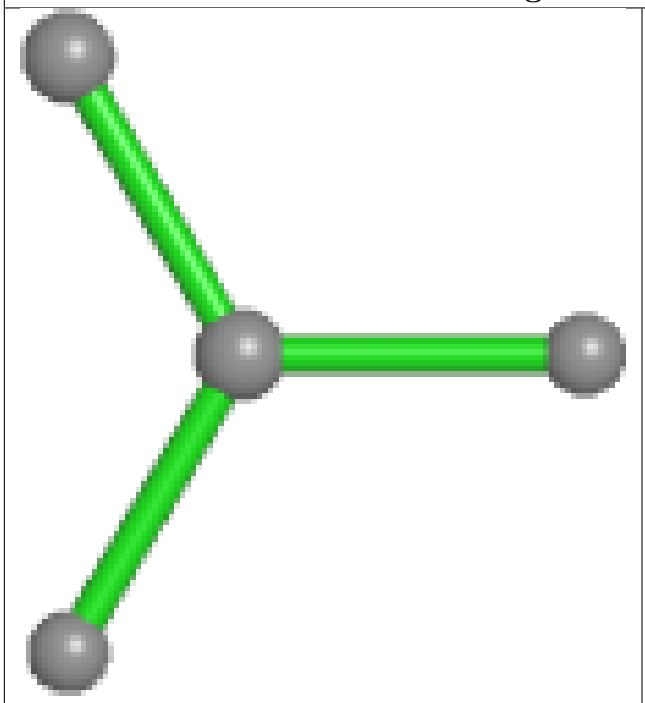


Rings

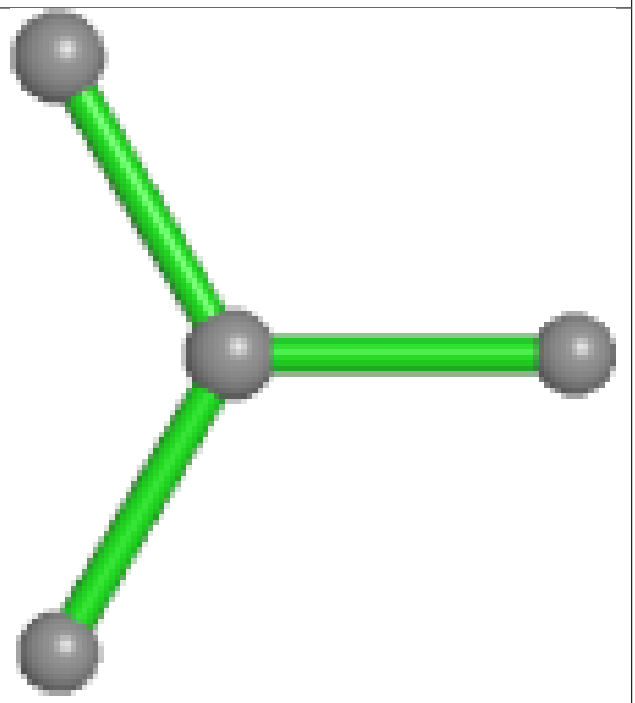
Ligand LFA E 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LFA B 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

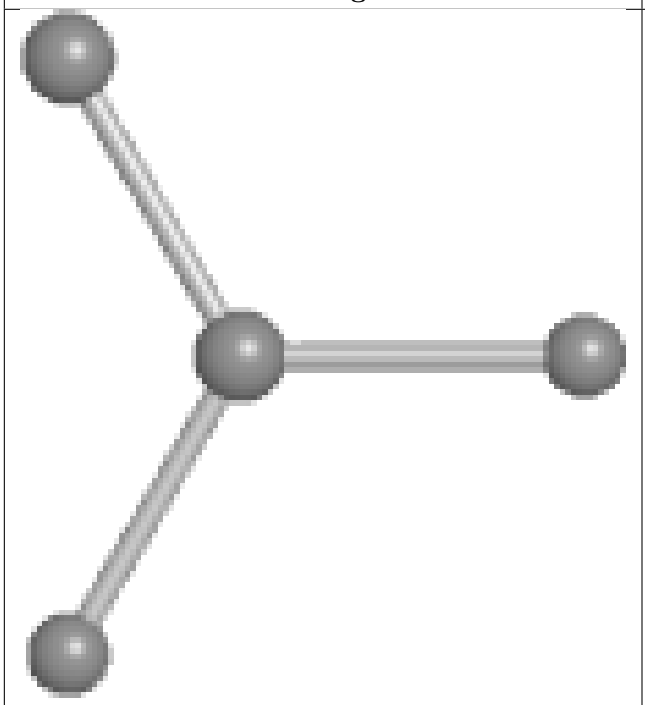
Ligand OLA C 307



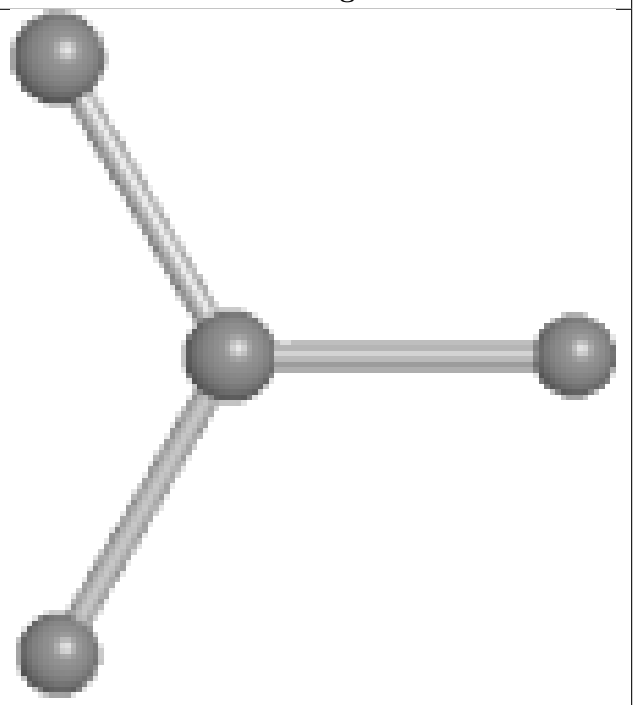
Bond lengths



Bond angles

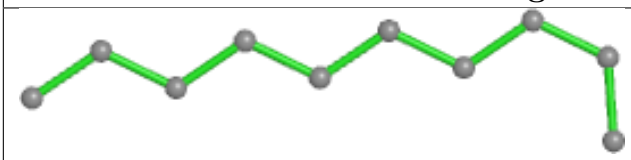


Torsions

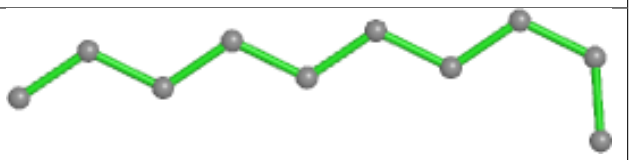


Rings

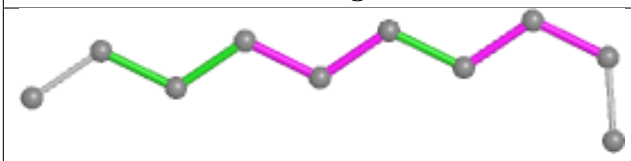
Ligand LFA C 309



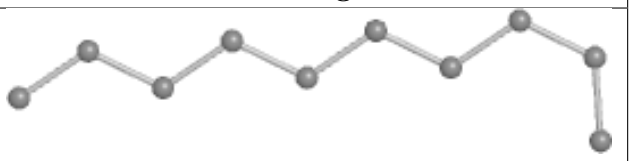
Bond lengths



Bond angles

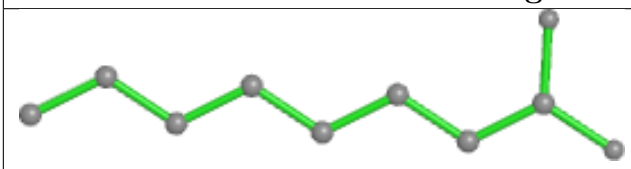


Torsions



Rings

Ligand OLA E 806



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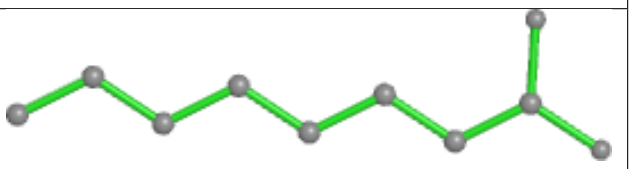
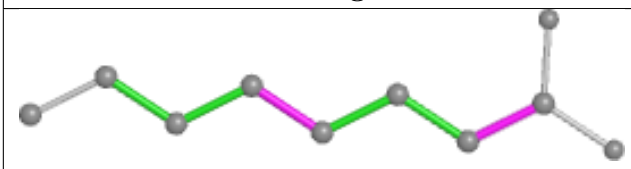
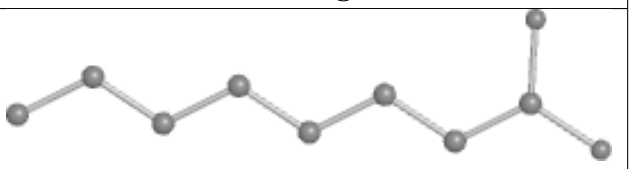


Bond angles

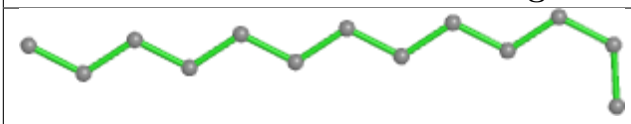


Torsions

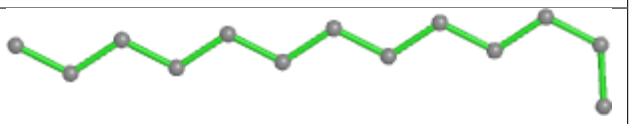


Rings

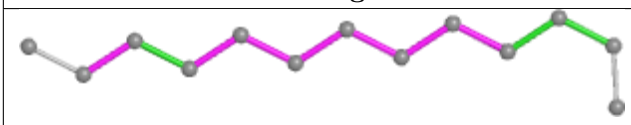
Ligand LFA B 306



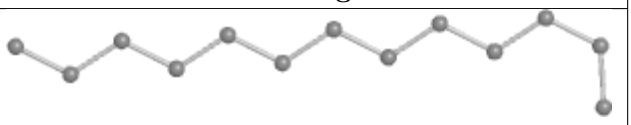
Bond lengths



Bond angles

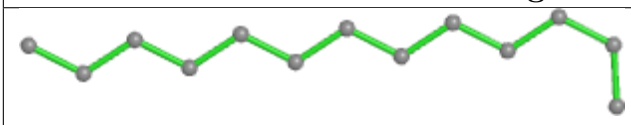


Torsions

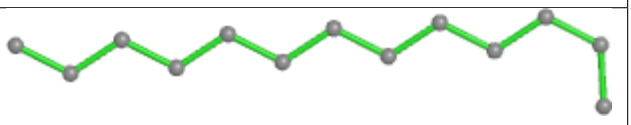


Rings

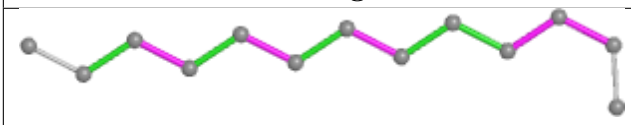
Ligand LFA A 303



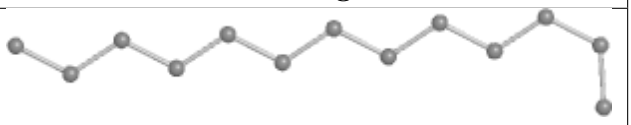
Bond lengths



Bond angles

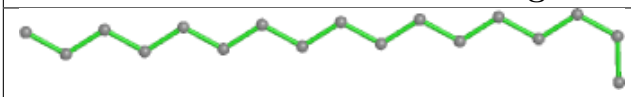


Torsions

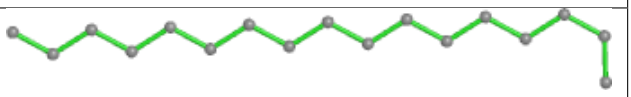


Rings

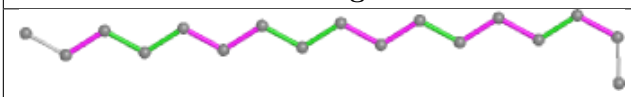
Ligand LFA C 303



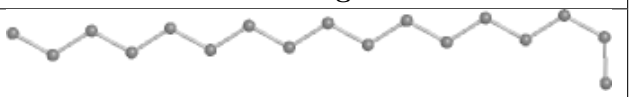
Bond lengths



Bond angles

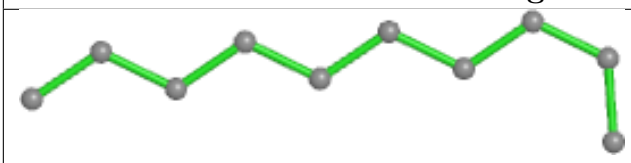


Torsions

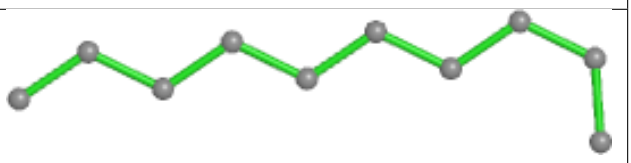


Rings

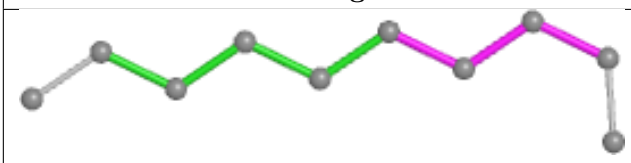
Ligand LFA D 505



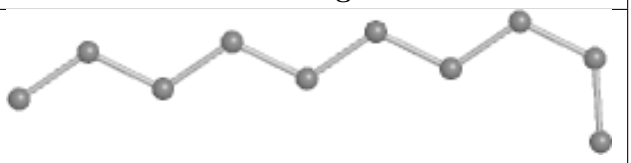
Bond lengths



Bond angles

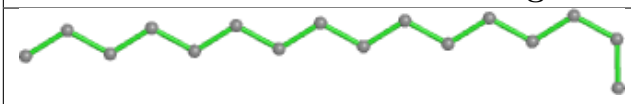


Torsions

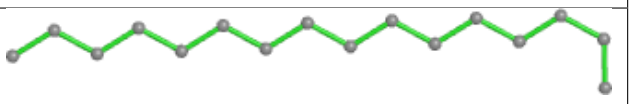


Rings

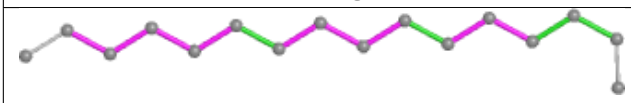
Ligand LFA D 504



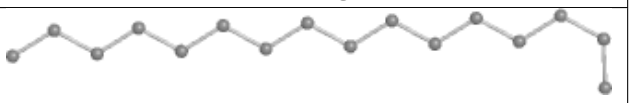
Bond lengths



Bond angles

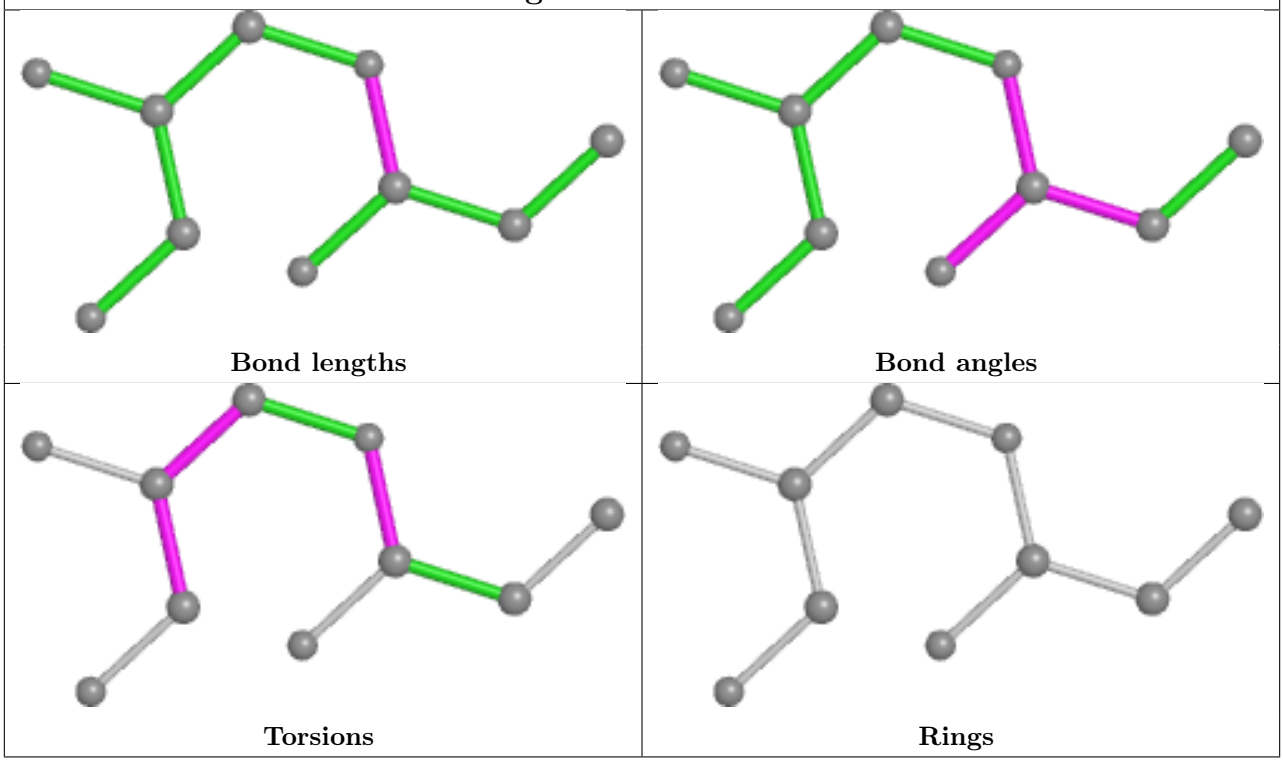


Torsions

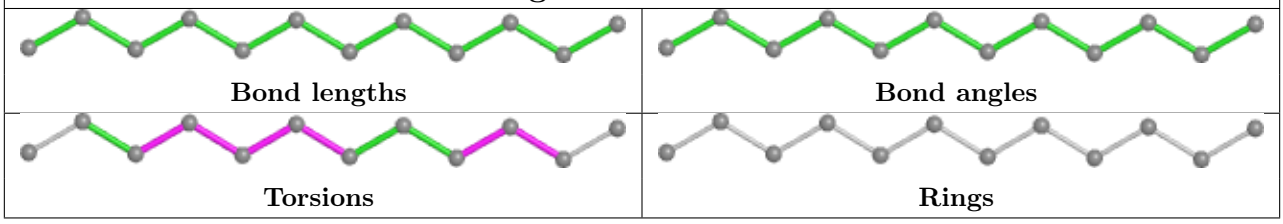


Rings

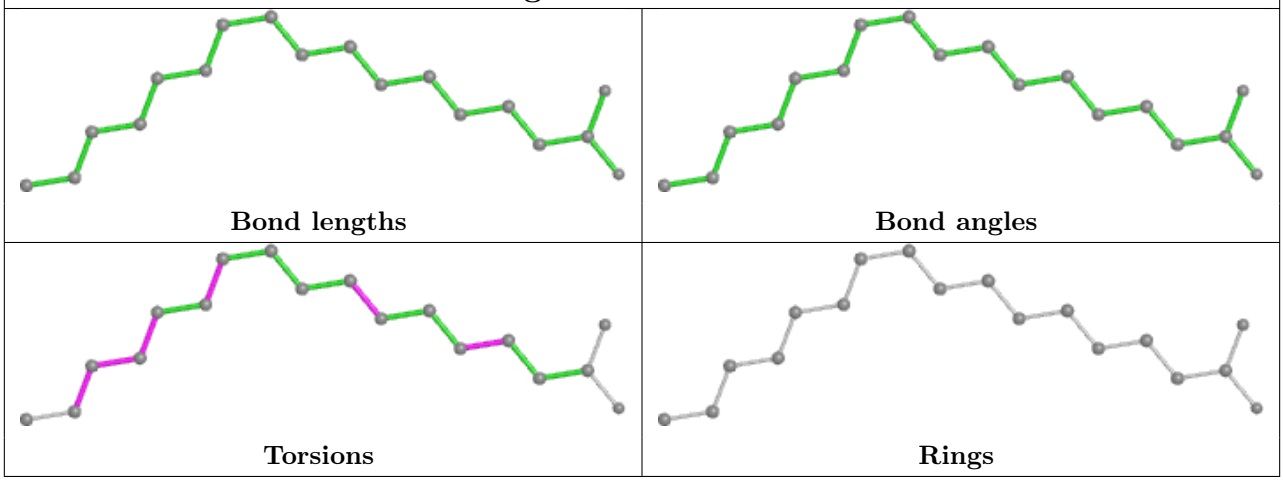
Ligand OLC C 306



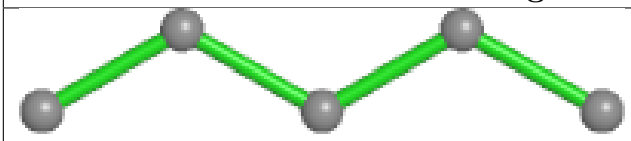
Ligand LFA C 310



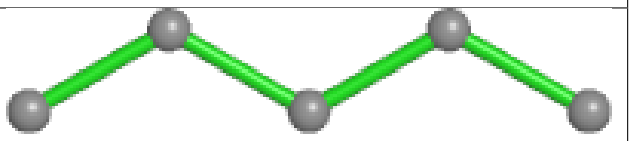
Ligand OLA D 502



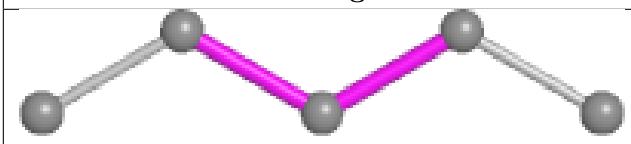
Ligand LFA D 507



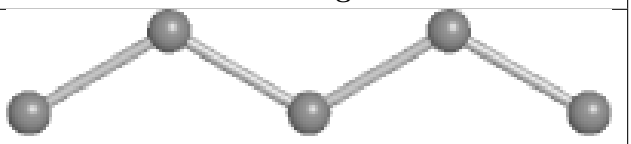
Bond lengths



Bond angles

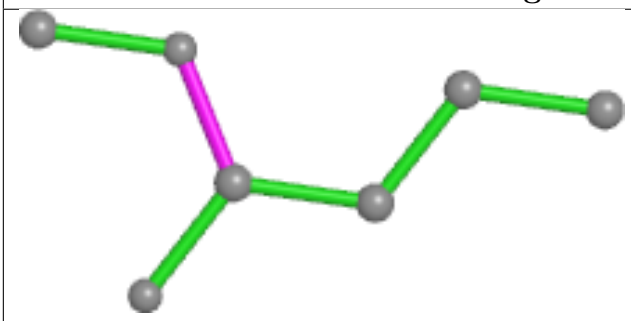


Torsions

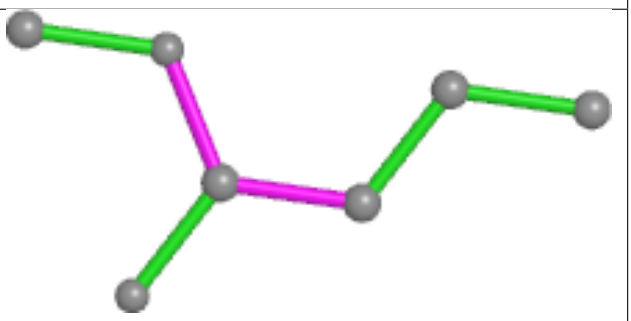


Rings

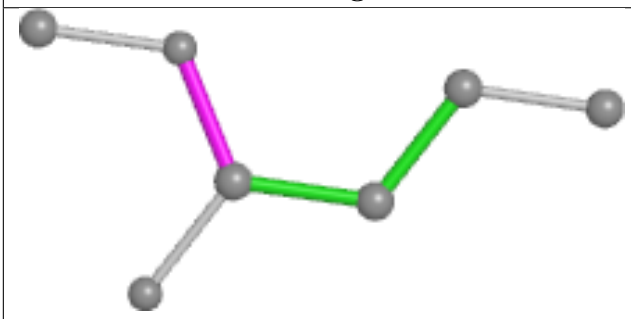
Ligand OLC A 305



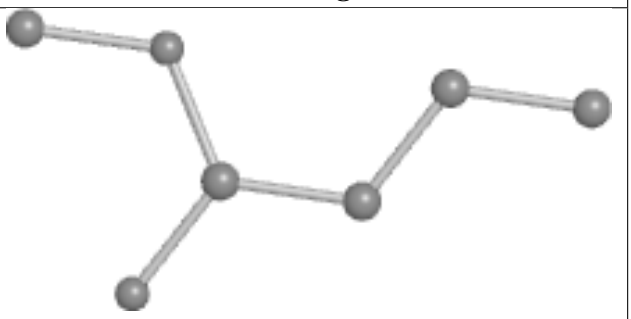
Bond lengths



Bond angles

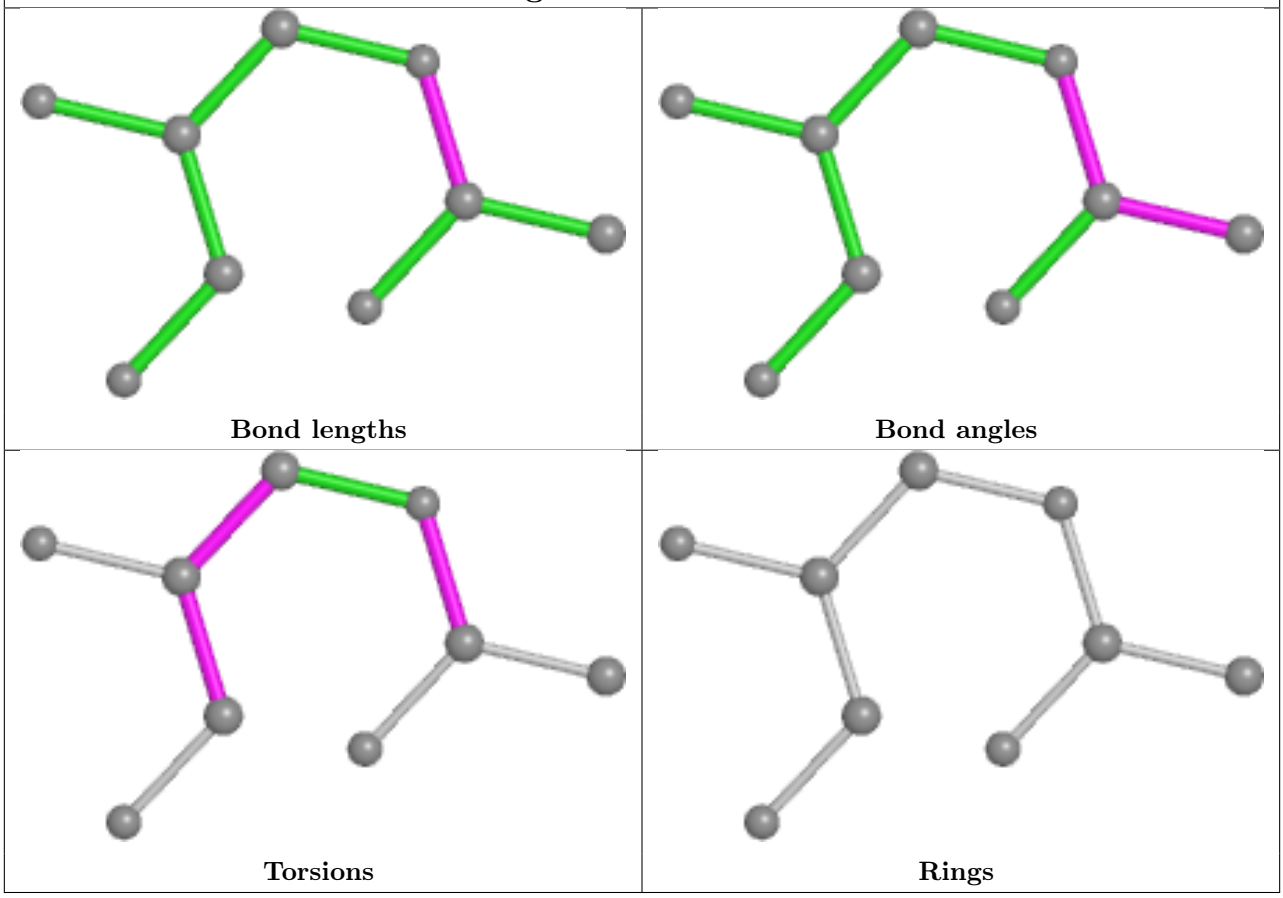


Torsions



Rings

Ligand OLC B 305



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	267/273 (97%)	0.32	23 (8%)	10	10	38, 50, 78, 108	0
1	B	267/273 (97%)	0.24	18 (6%)	17	18	38, 48, 73, 112	0
1	C	267/273 (97%)	0.20	20 (7%)	14	14	37, 49, 73, 110	0
1	D	268/273 (98%)	0.11	16 (5%)	21	22	36, 48, 70, 110	0
1	E	267/273 (97%)	0.13	14 (5%)	27	29	36, 48, 71, 104	0
All	All	1336/1365 (97%)	0.20	91 (6%)	17	17	36, 49, 74, 112	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	PHE	6.0
1	A	132	THR	5.5
1	E	230	VAL	4.5
1	D	230	VAL	4.1
1	C	230	VAL	4.1
1	A	133	SER	4.1
1	A	230	VAL	4.0
1	A	130	LEU	3.9
1	A	195	GLY	3.9
1	B	40	LEU	3.9
1	B	233	PHE	3.8
1	A	131	THR	3.6
1	B	230	VAL	3.6
1	B	76	TYR	3.4
1	D	3	GLN	3.3
1	A	43	LEU	3.3
1	E	76	TYR	3.3
1	A	40	LEU	3.3
1	E	232	GLY	3.2
1	C	73	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	233	PHE	3.2
1	B	164	LEU	3.2
1	B	190	ASN	3.1
1	D	190	ASN	3.1
1	E	132	THR	3.1
1	C	270	SER	3.1
1	B	72	PHE	3.0
1	A	76	TYR	3.0
1	C	196	ILE	3.0
1	C	183	TRP	3.0
1	C	190	ASN	2.9
1	E	40	LEU	2.9
1	A	69	VAL	2.9
1	C	72	PHE	2.9
1	C	76	TYR	2.8
1	A	72	PHE	2.8
1	B	43	LEU	2.8
1	D	270	SER	2.8
1	C	69	VAL	2.8
1	B	165	THR	2.7
1	D	73	LEU	2.7
1	A	231	ASP	2.7
1	C	231	ASP	2.7
1	D	132	THR	2.6
1	D	271	LYS	2.6
1	B	44	LEU	2.6
1	A	233	PHE	2.6
1	B	163	ASN	2.6
1	C	43	LEU	2.6
1	C	77	ALA	2.5
1	B	36	TYR	2.5
1	A	73	LEU	2.5
1	C	229	GLY	2.5
1	D	183	TRP	2.5
1	D	40	LEU	2.5
1	A	194	GLU	2.5
1	E	130	LEU	2.4
1	A	44	LEU	2.4
1	C	40	LEU	2.4
1	D	43	LEU	2.4
1	E	43	LEU	2.4
1	C	198	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	233	PHE	2.4
1	A	41	ALA	2.3
1	A	183	TRP	2.3
1	D	72	PHE	2.3
1	A	190	ASN	2.3
1	C	164	LEU	2.3
1	E	69	VAL	2.3
1	D	136	SER	2.3
1	B	132	THR	2.3
1	B	79	ALA	2.2
1	E	72	PHE	2.2
1	B	73	LEU	2.2
1	E	190	ASN	2.2
1	A	201	GLN	2.2
1	D	231	ASP	2.1
1	B	131	THR	2.1
1	C	74	LEU	2.1
1	B	69	VAL	2.1
1	E	131	THR	2.1
1	C	269	LEU	2.1
1	E	36	TYR	2.0
1	B	194	GLU	2.0
1	A	77	ALA	2.0
1	A	38	VAL	2.0
1	A	47	ILE	2.0
1	C	47	ILE	2.0
1	D	75	LEU	2.0
1	E	44	LEU	2.0
1	D	77	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LYR	A	255	29/30	0.94	0.16	40,49,61,64	0
1	LYR	B	255	29/30	0.94	0.17	38,44,53,59	0
1	LYR	C	255	29/30	0.94	0.15	38,45,50,51	0
1	LYR	D	255	29/30	0.95	0.16	36,45,53,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LYR	E	255	29/30	0.95	0.15	35,48,55,62	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, 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
5	OLA	B	304	19/20	0.65	0.84	78,94,101,102	0
5	OLA	C	305	20/20	0.65	0.80	83,95,111,113	0
6	ALA	C	301	5/6	0.65	0.44	100,101,105,112	0
4	OLC	D	506	6/25	0.68	0.34	78,81,86,89	0
5	OLA	D	502	18/20	0.68	0.74	68,89,104,105	0
5	OLA	E	806	10/20	0.68	0.52	66,97,111,111	0
3	LFA	E	808	18/20	0.68	0.83	75,91,101,102	0
3	LFA	C	310	12/20	0.72	0.36	68,92,103,104	0
4	OLC	A	305	7/25	0.73	0.21	66,83,91,93	0
5	OLA	C	307	4/20	0.76	0.79	74,83,86,89	0
3	LFA	D	507	5/20	0.77	0.17	74,77,81,88	0
4	OLC	B	305	9/25	0.78	0.34	77,95,110,120	0
3	LFA	D	505	10/20	0.80	0.22	68,80,89,96	0
3	LFA	B	306	13/20	0.80	0.24	73,88,97,100	0
4	OLC	E	807	7/25	0.80	0.26	67,76,88,91	0
3	LFA	B	303	13/20	0.82	0.33	71,81,89,94	0
3	LFA	E	805	13/20	0.84	0.32	73,81,100,102	0
3	LFA	C	309	10/20	0.85	0.19	70,81,92,95	0
3	LFA	D	501	14/20	0.85	0.20	77,83,99,103	0
4	OLC	C	306	10/25	0.86	0.32	71,85,101,101	0
3	LFA	A	303	13/20	0.86	0.33	74,86,90,91	0
3	LFA	E	801	9/20	0.86	0.96	79,89,102,105	0
3	LFA	C	304	15/20	0.87	0.30	73,88,101,103	0
3	LFA	A	302	20/20	0.88	0.42	62,73,101,103	0
3	LFA	A	306	5/20	0.89	0.14	66,73,81,81	0
2	NA	C	302	1/1	0.89	0.09	44,44,44,44	0
3	LFA	C	308	4/20	0.89	0.13	76,78,80,85	0

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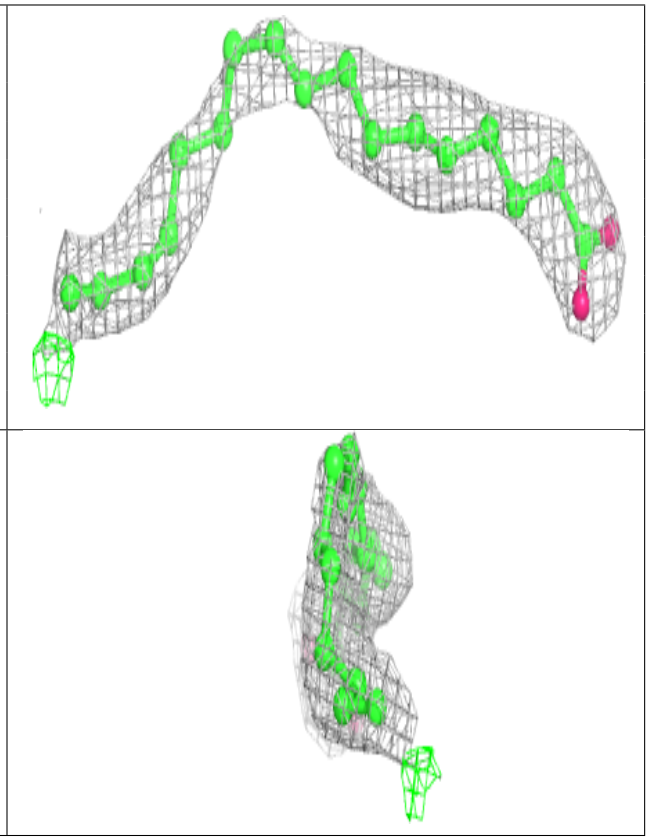
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFA	D	504	16/20	0.89	0.39	59,64,71,72	0
3	LFA	E	802	5/20	0.91	1.44	74,74,81,94	0
3	LFA	B	302	17/20	0.91	0.36	55,62,75,76	0
3	LFA	C	303	17/20	0.92	0.35	54,65,77,80	0
2	NA	A	301	1/1	0.93	0.09	44,44,44,44	0
3	LFA	E	804	17/20	0.94	0.36	62,67,80,82	0
3	LFA	A	304	6/20	0.95	1.25	73,77,87,88	0
2	NA	D	503	1/1	0.95	0.06	40,40,40,40	0
2	NA	B	301	1/1	0.98	0.10	39,39,39,39	0
2	NA	E	803	1/1	0.98	0.07	41,41,41,41	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.

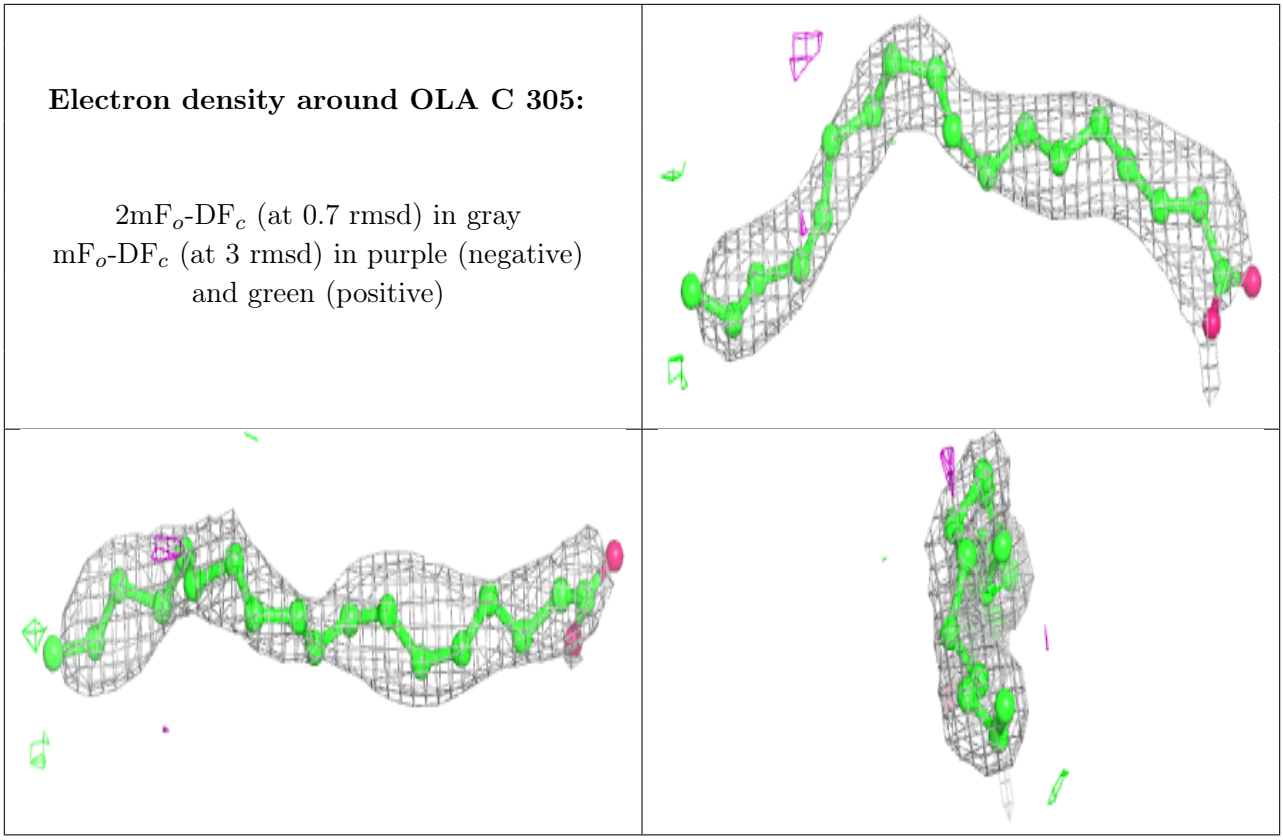
Electron density around OLA B 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



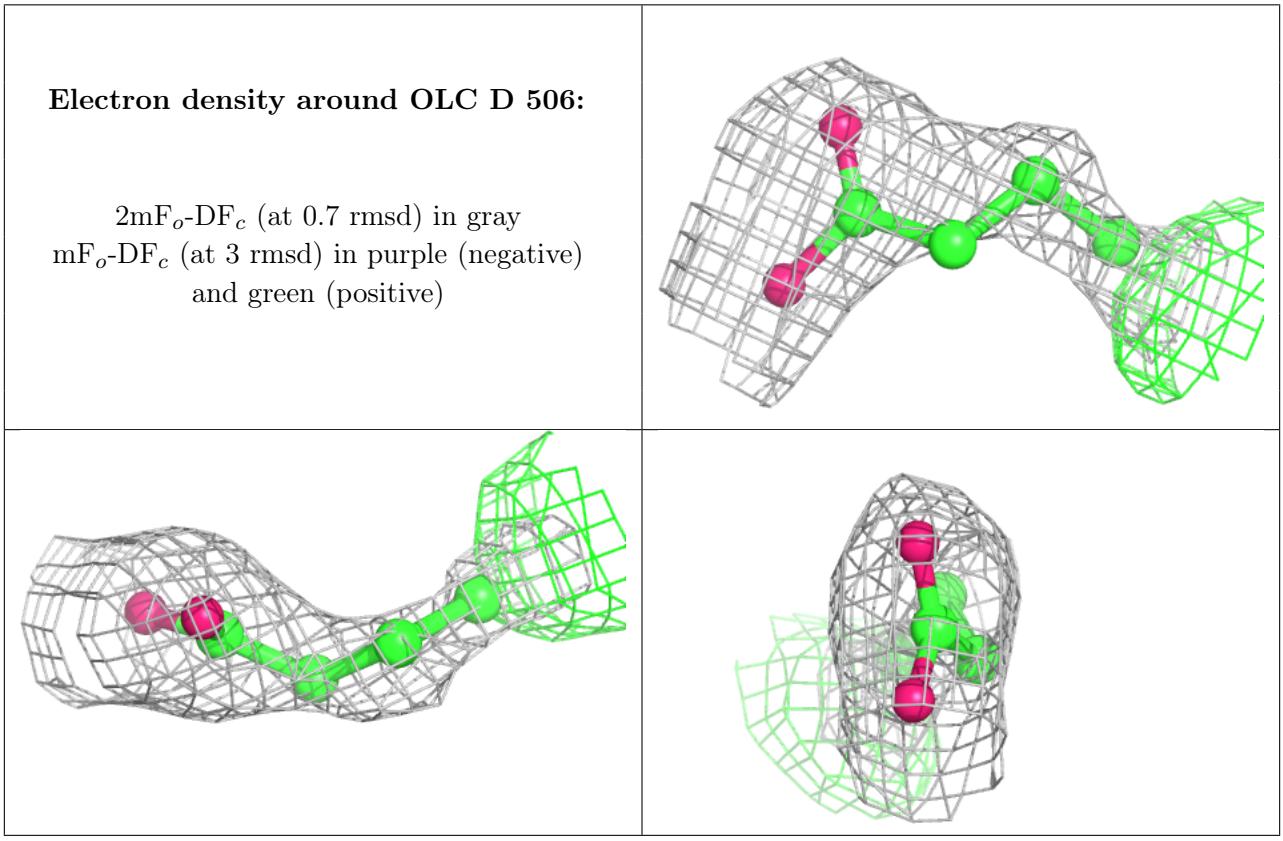
Electron density around OLA C 305:

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



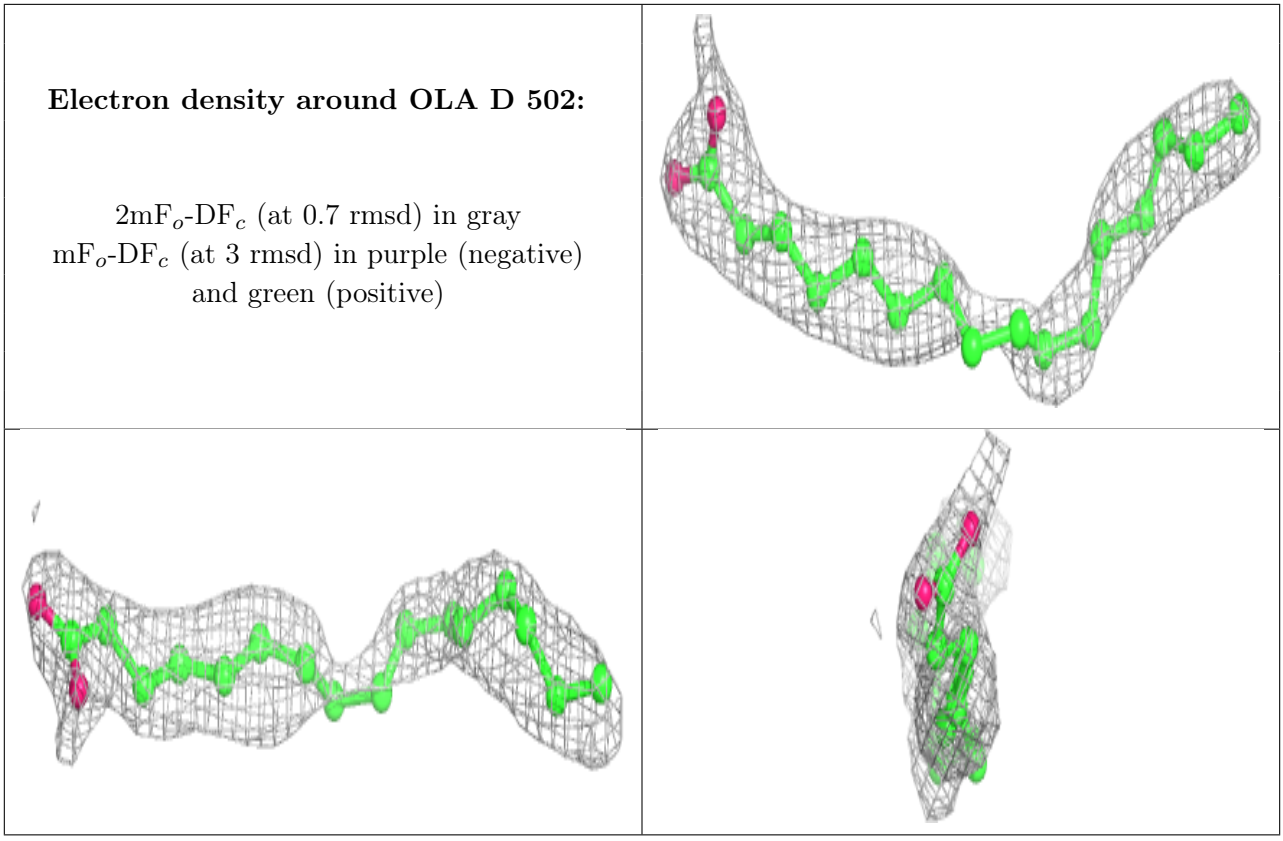
Electron density around OLC D 506:

$2mF_o$-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 D 502:

$2mF_o$-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 E 806:

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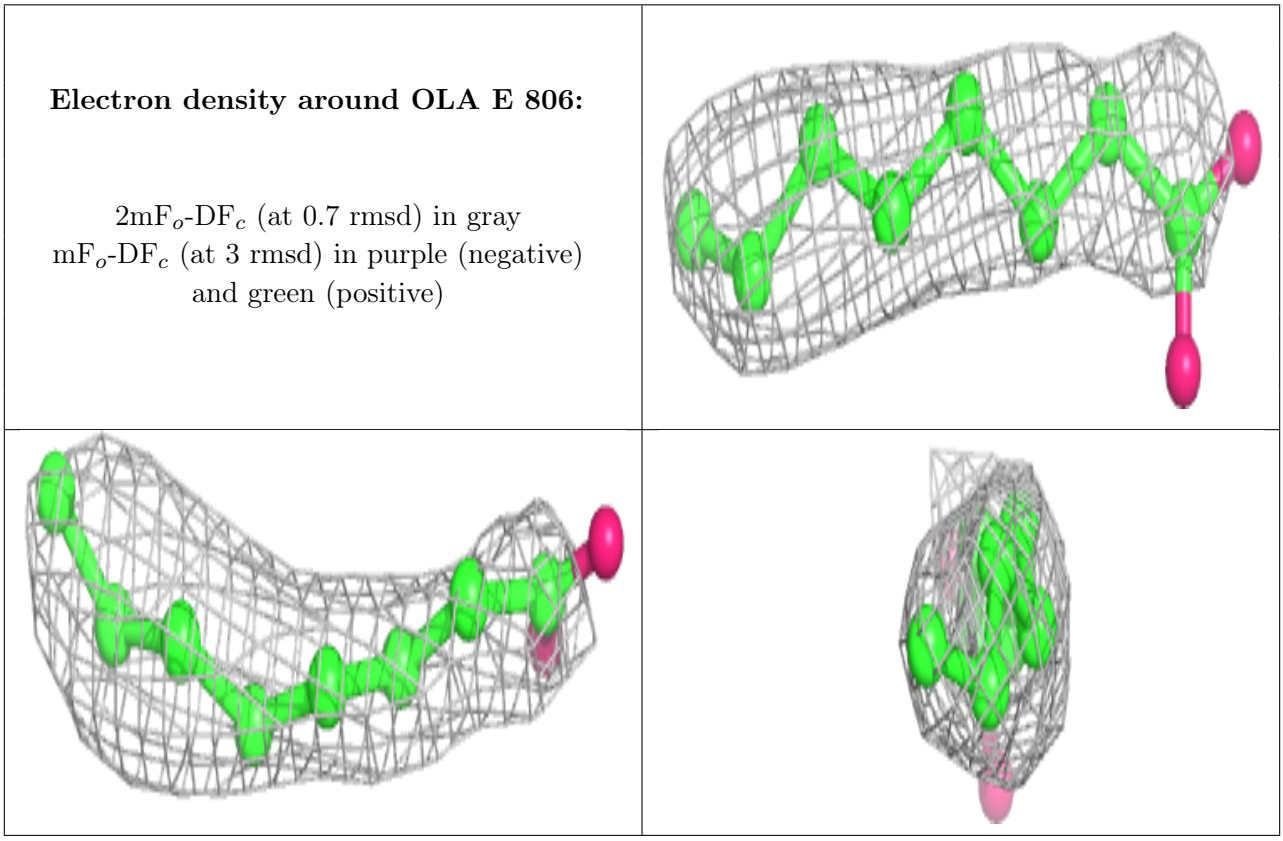
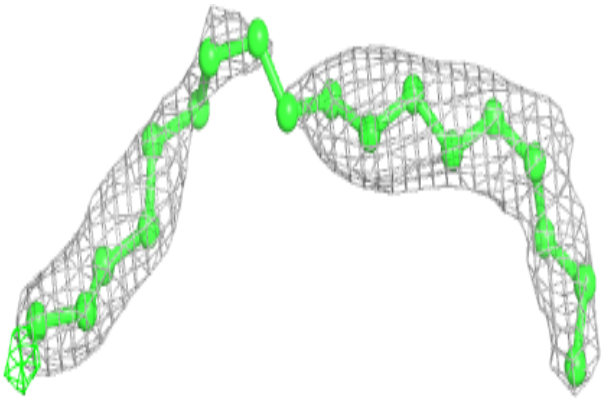
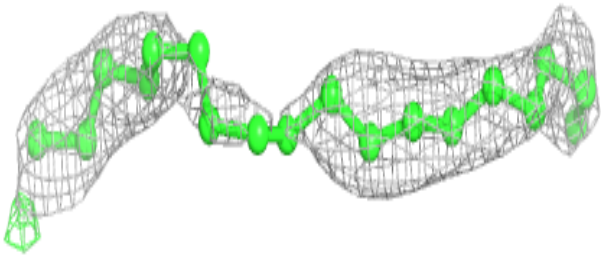
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

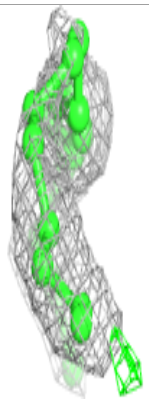


Electron density around LFA E 808:

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

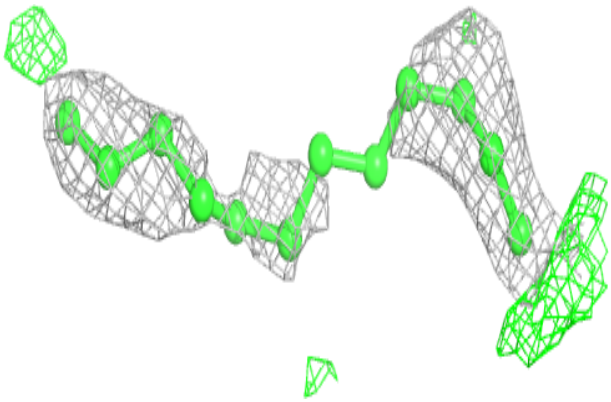


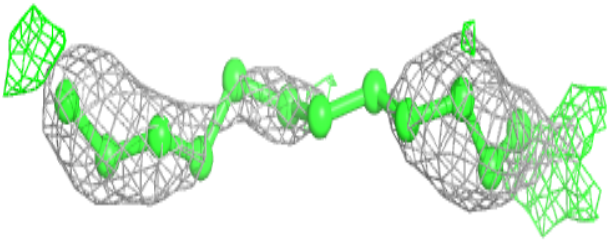


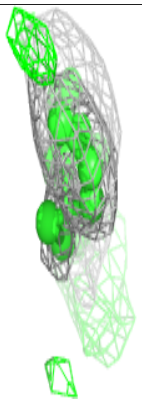


Electron density around LFA C 310:

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

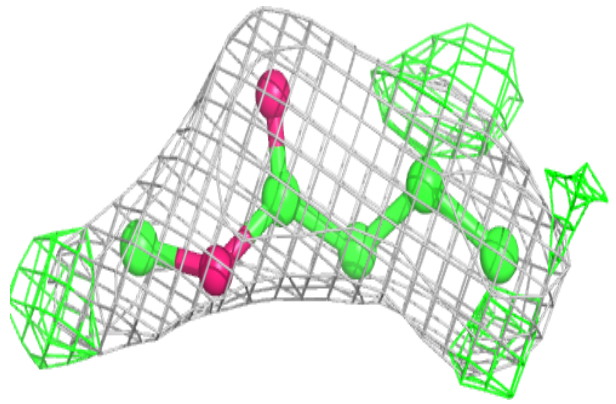


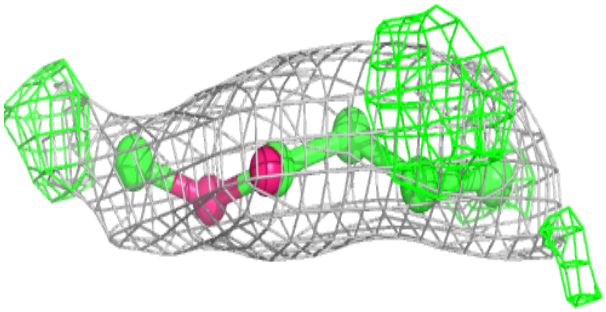


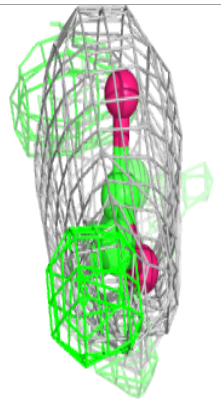


Electron density around OLC A 305:

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

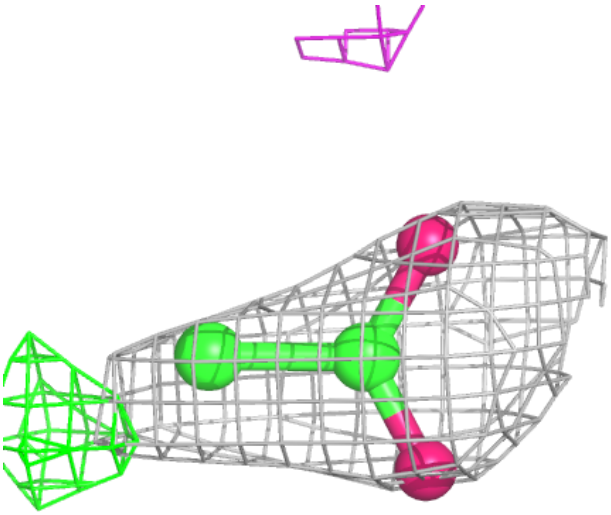


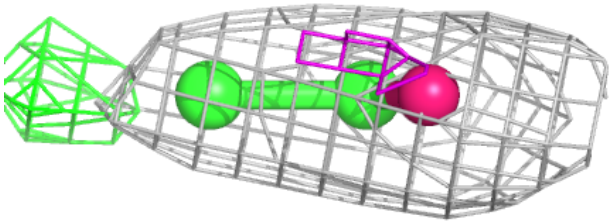


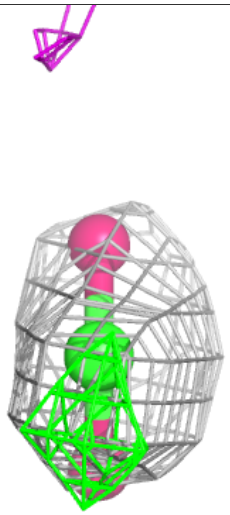


Electron density around OLA C 307:

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

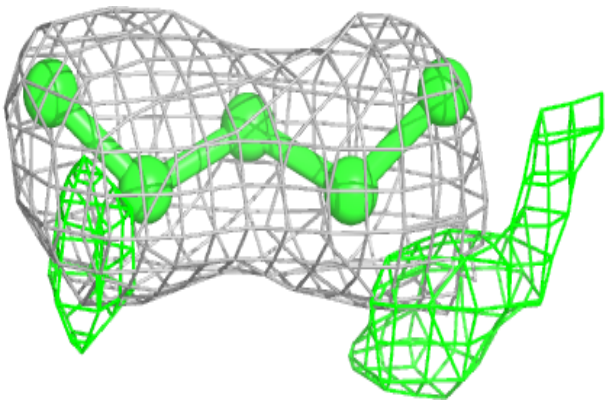


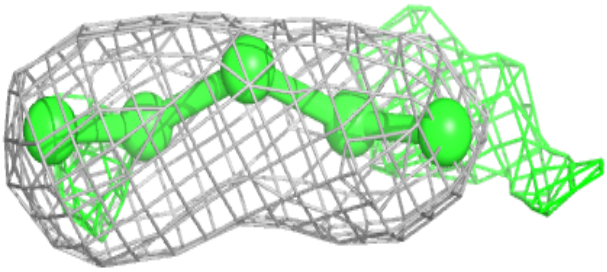


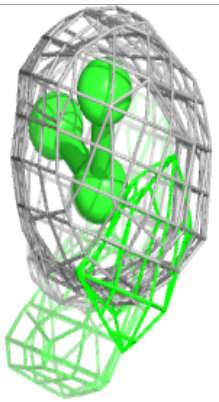


Electron density around LFA D 507:

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

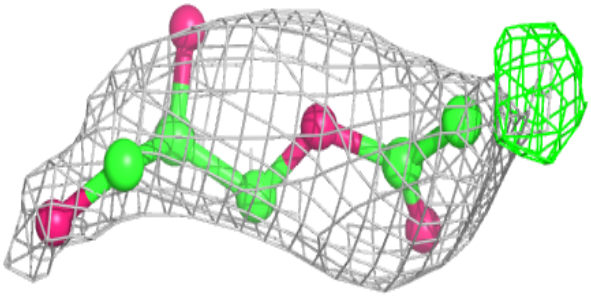


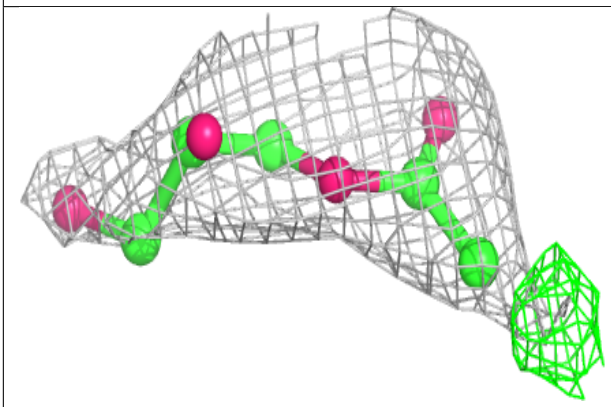


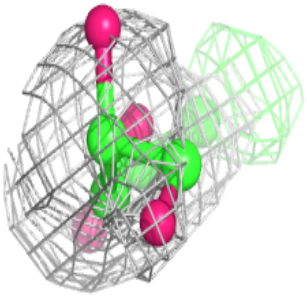


Electron density around OLC B 305:

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

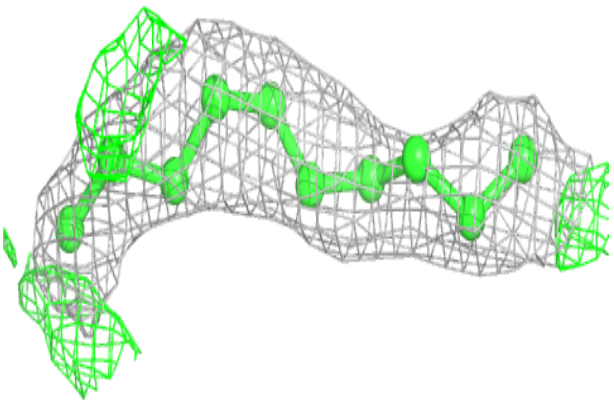


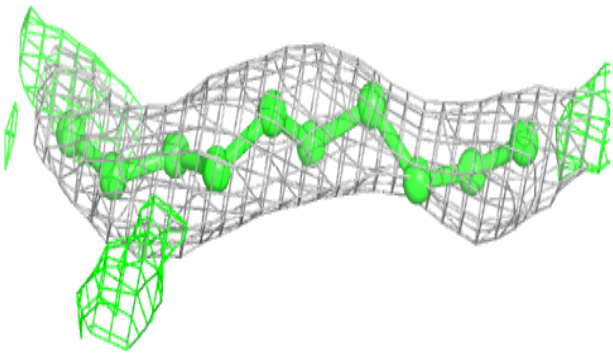


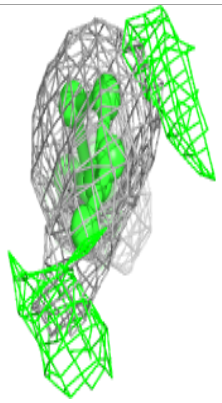


Electron density around LFA D 505:

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

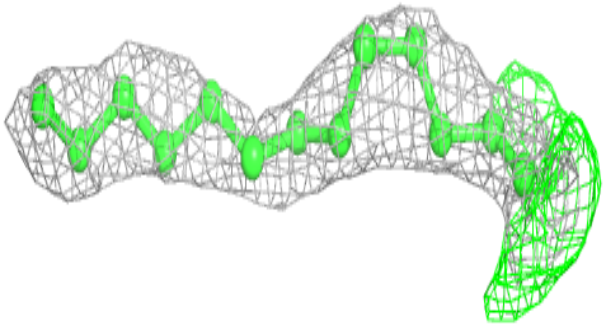


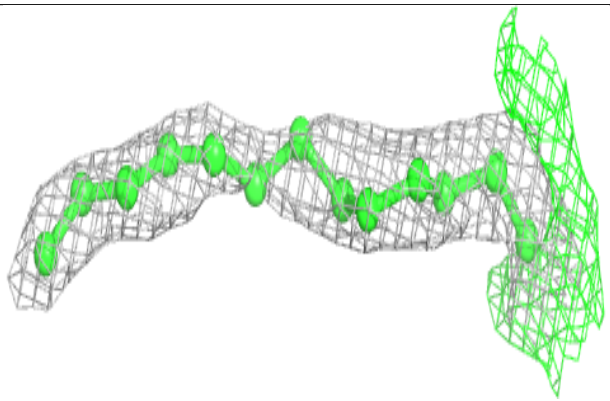


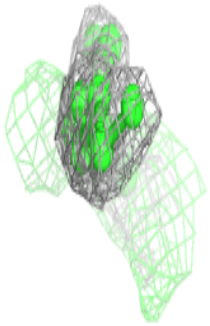


Electron density around LFA B 306:

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

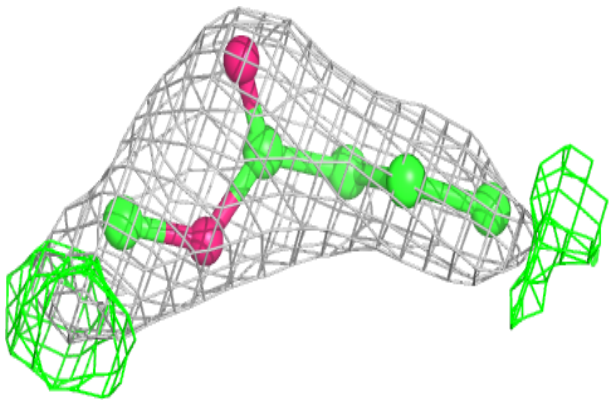


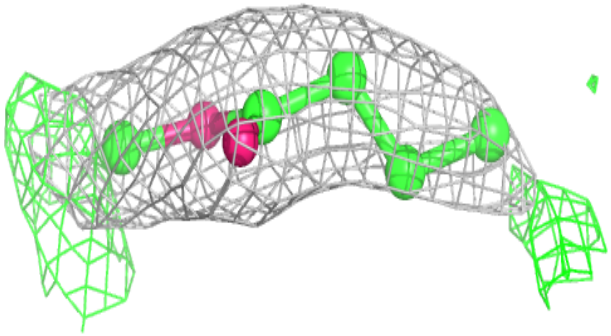


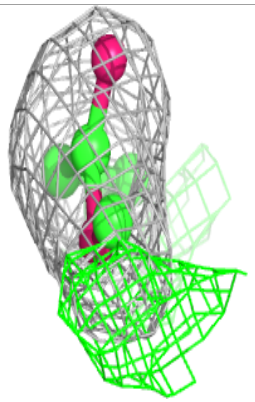


Electron density around OLC E 807:

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

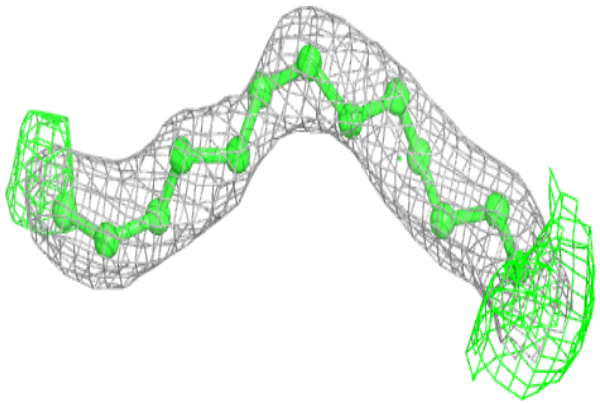


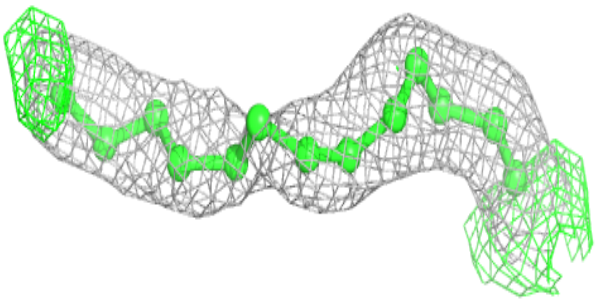


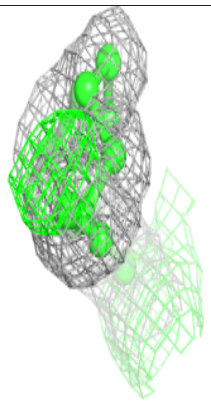


Electron density around LFA B 303:

$2mF_o$-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 E 805:

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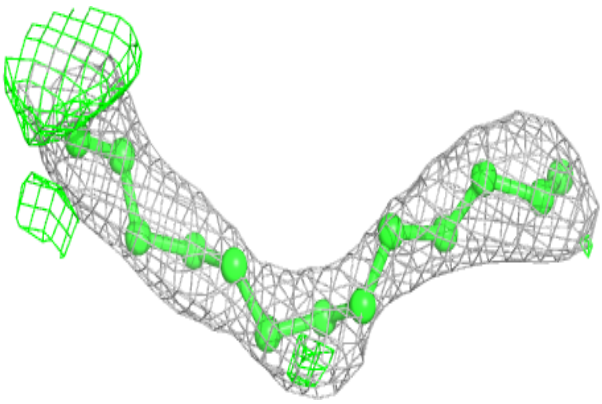
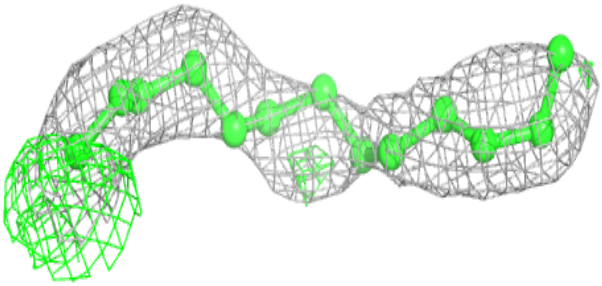
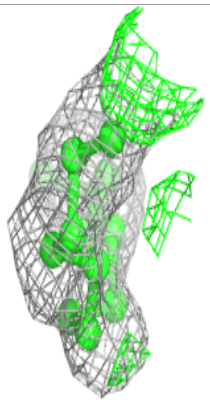
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

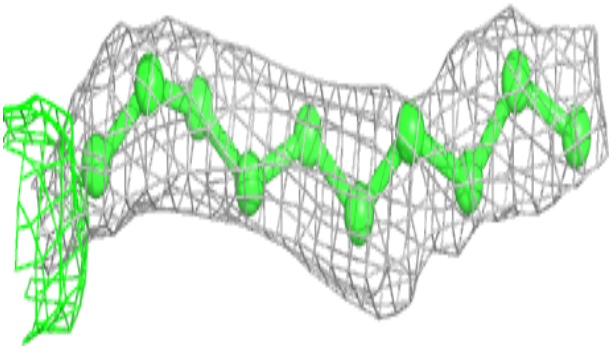


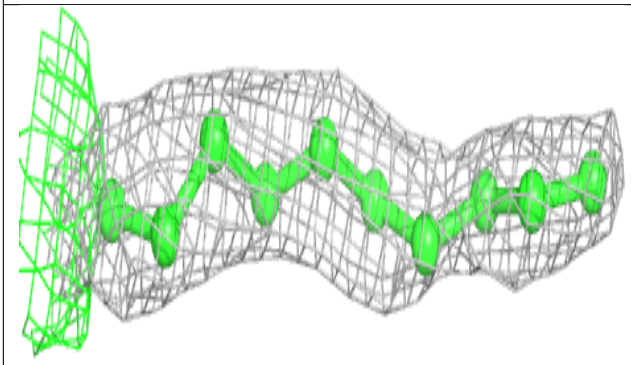


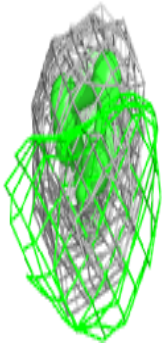


Electron density around LFA C 309:

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

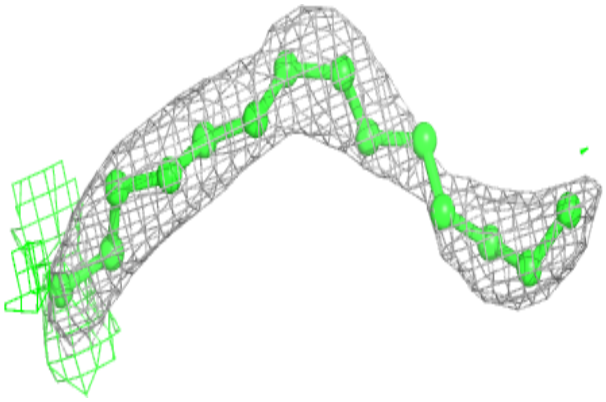


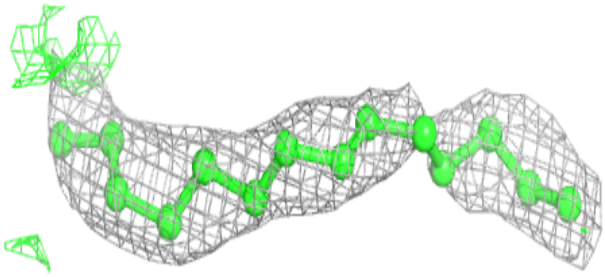


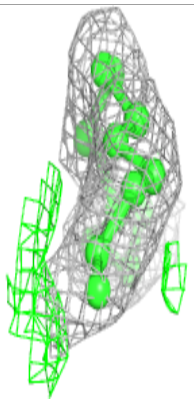


Electron density around LFA D 501:

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

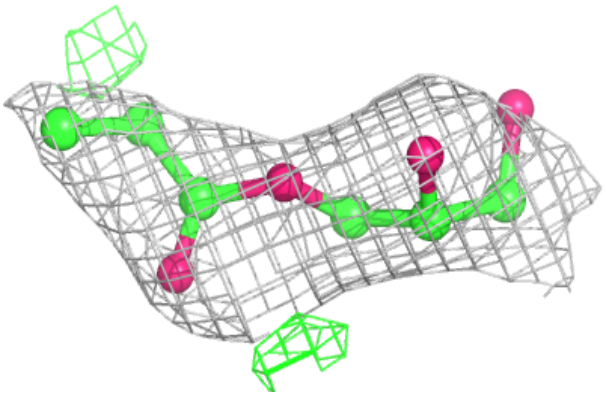


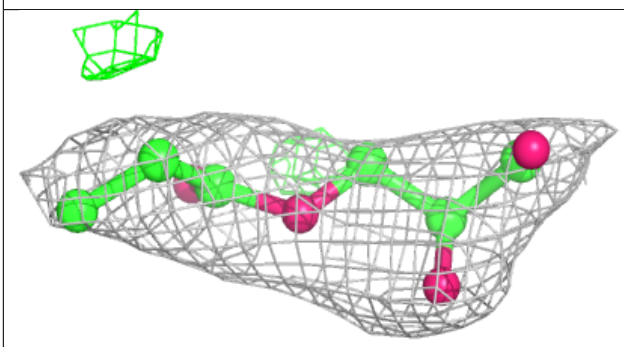


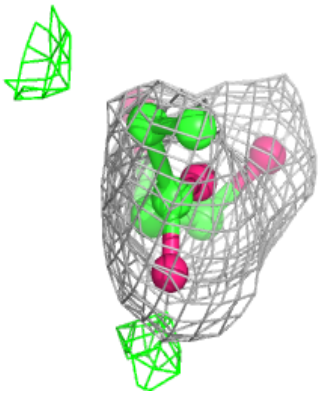


Electron density around OLC C 306:

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

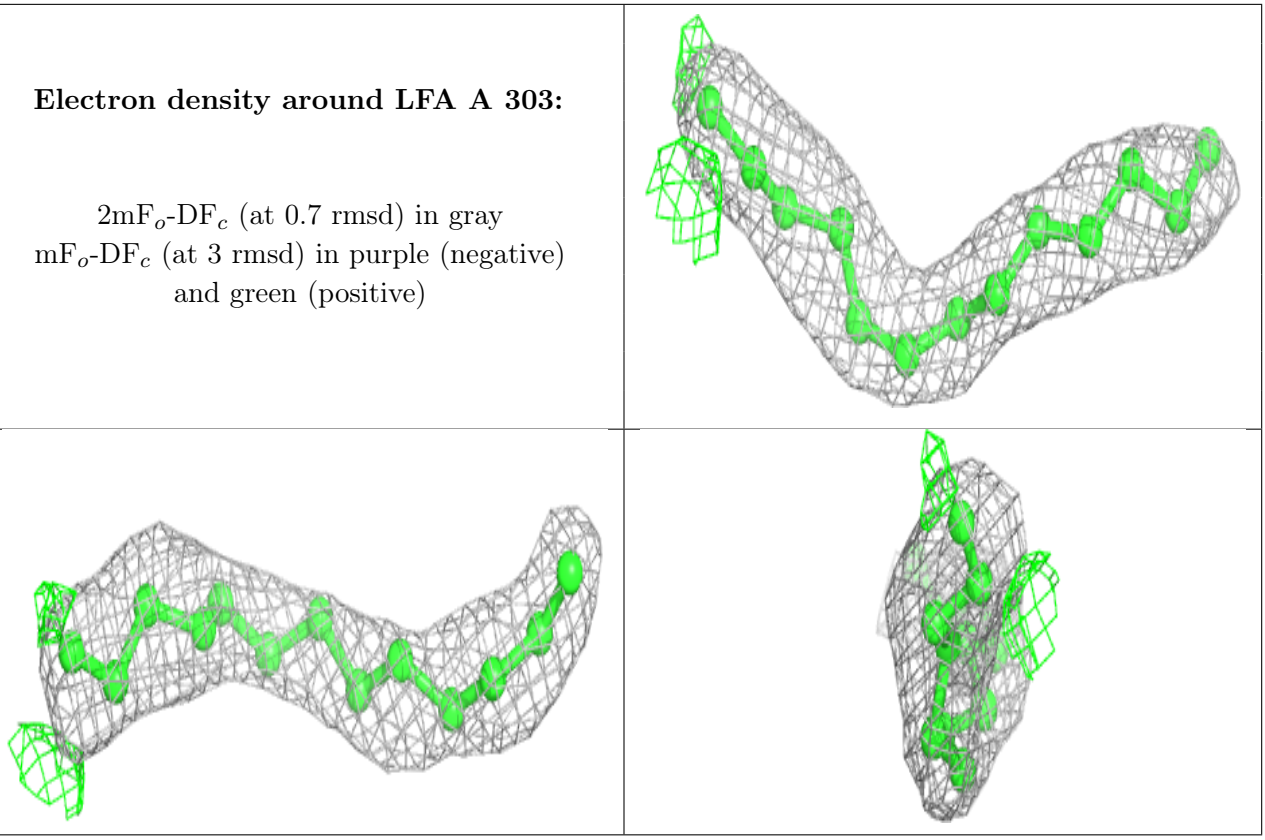






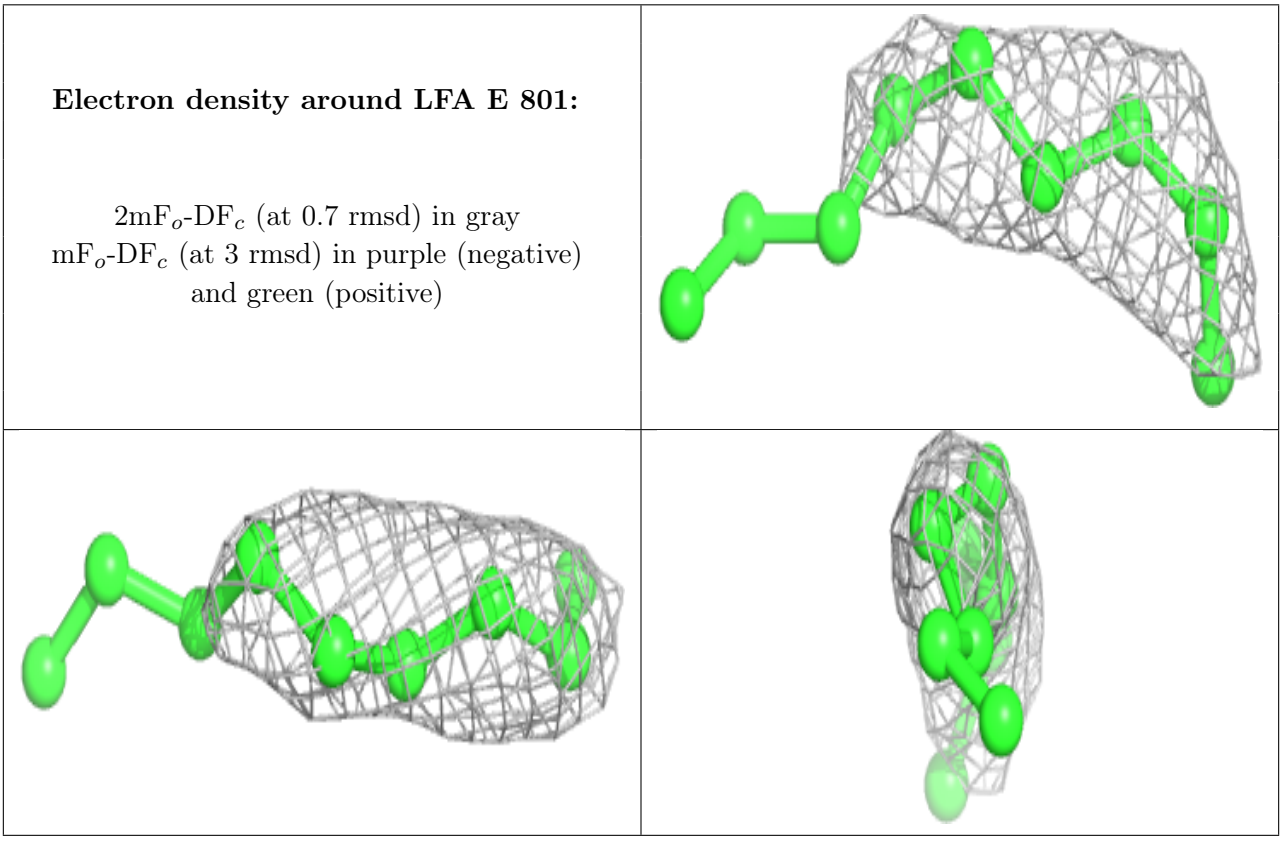
Electron density around LFA A 303:

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



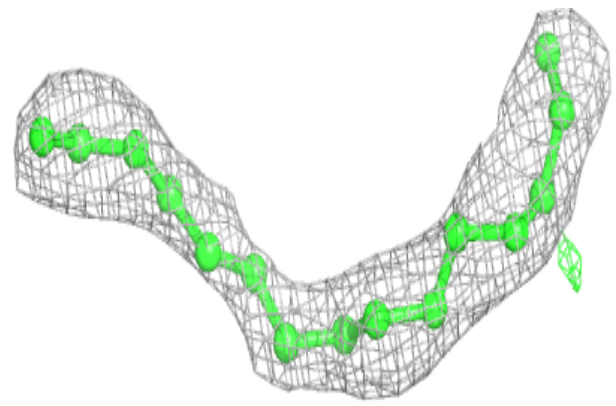
Electron density around LFA E 801:

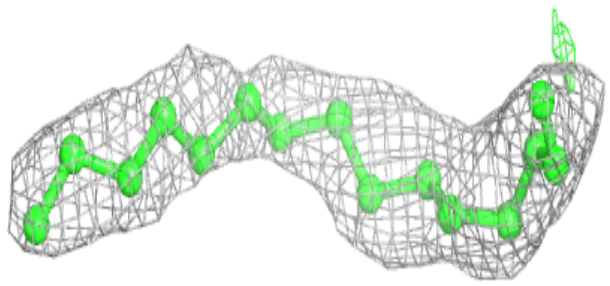
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

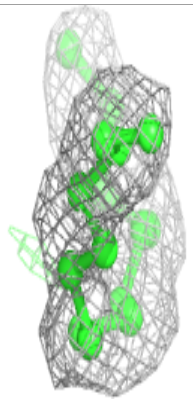


Electron density around LFA C 304:

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

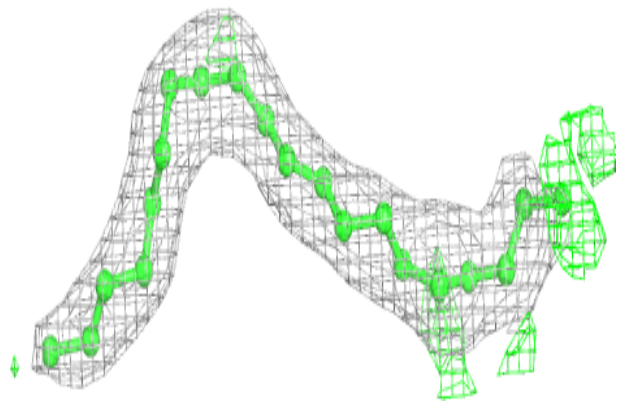


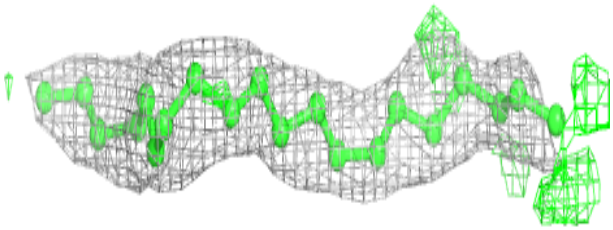


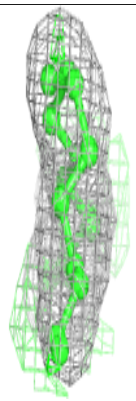


Electron density around LFA A 302:

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

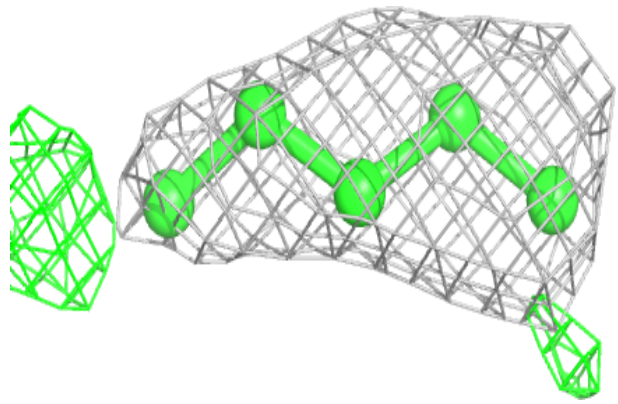


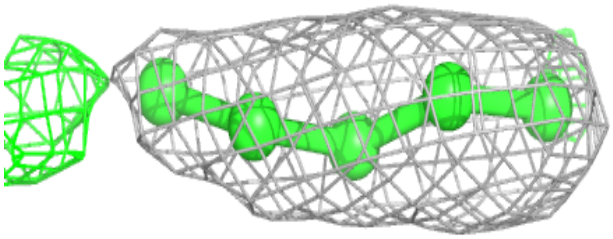


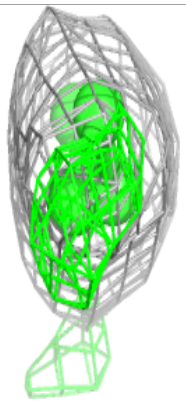


Electron density around LFA A 306:

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

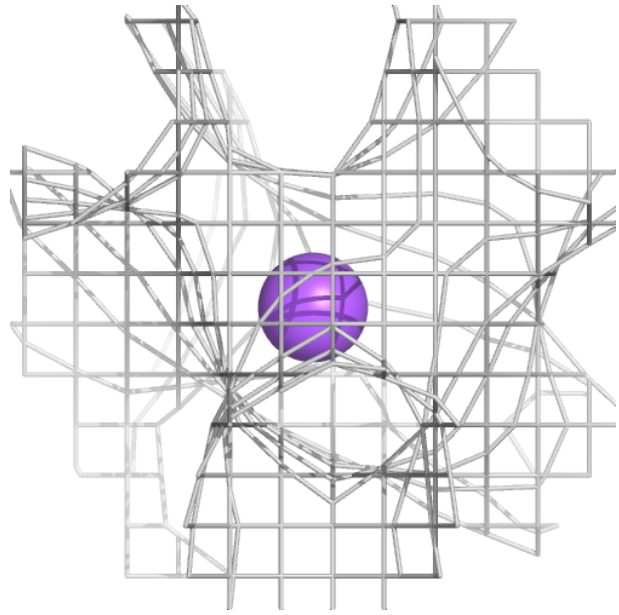


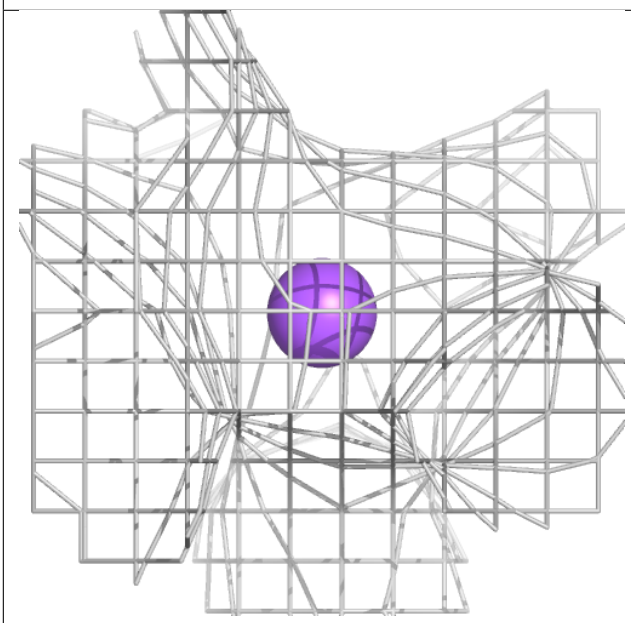


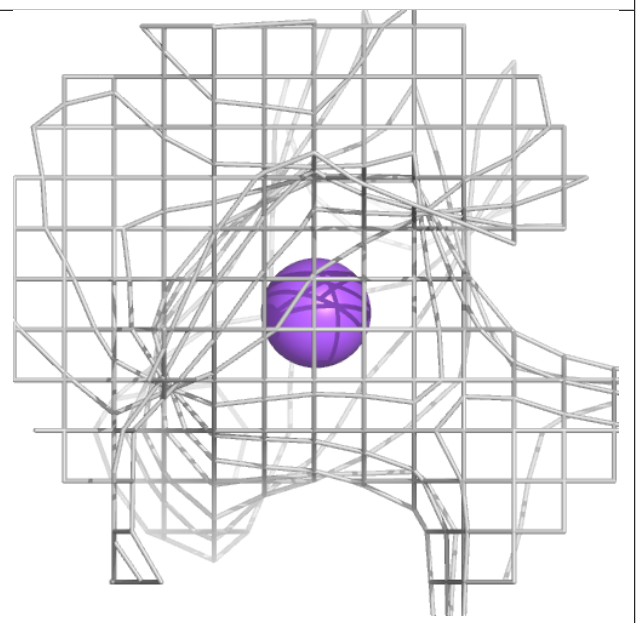


Electron density around NA C 302:

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

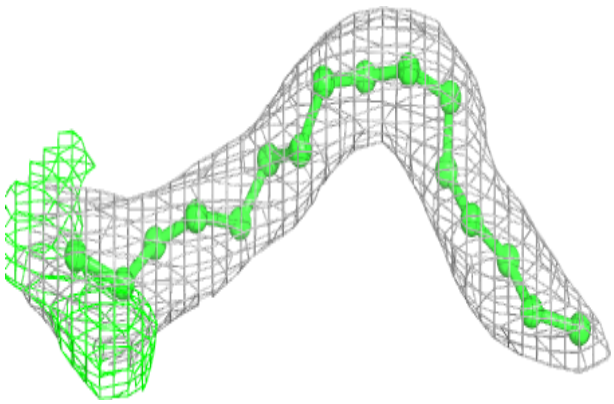


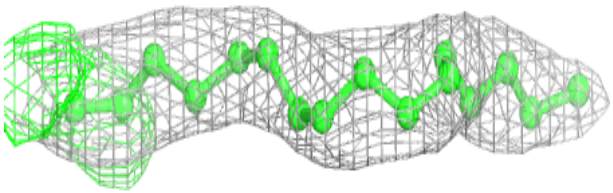


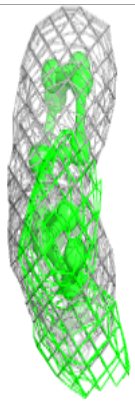


Electron density around LFA D 504:

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

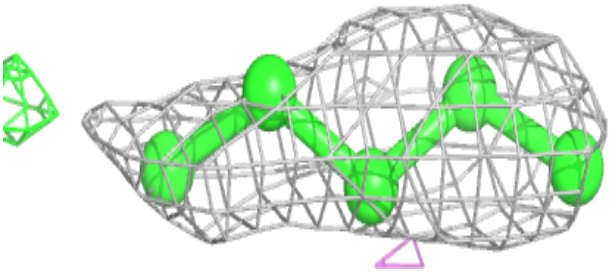


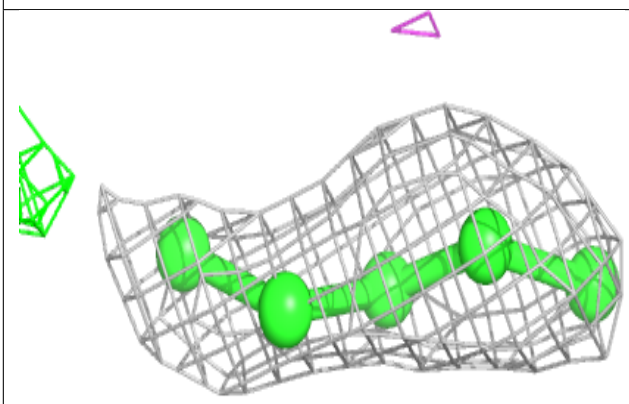


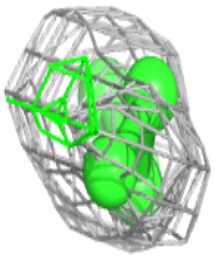


Electron density around LFA E 802:

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

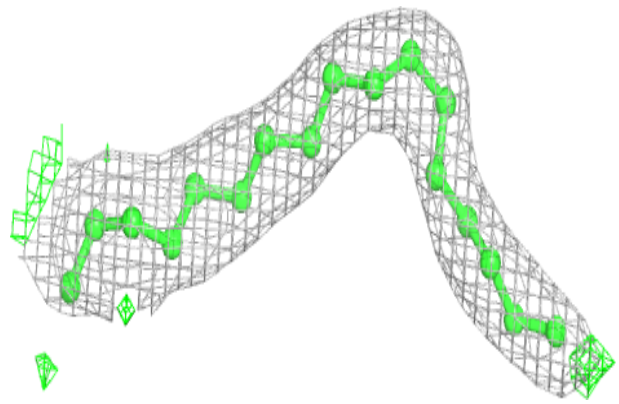


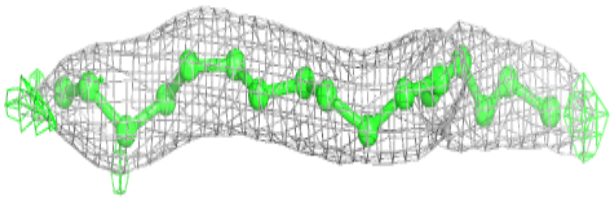


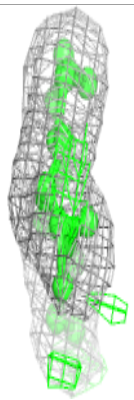


Electron density around LFA B 302:

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

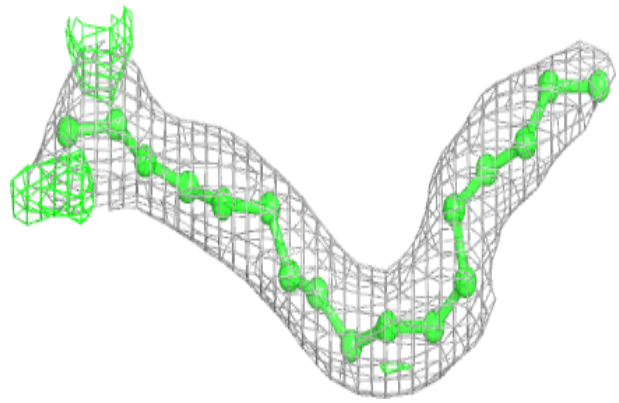


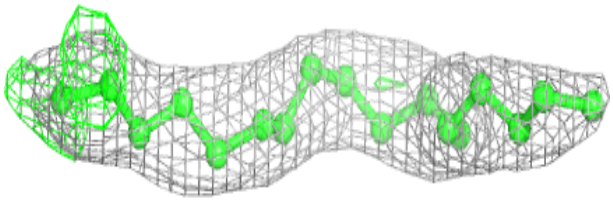


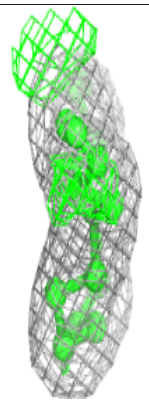


Electron density around LFA C 303:

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

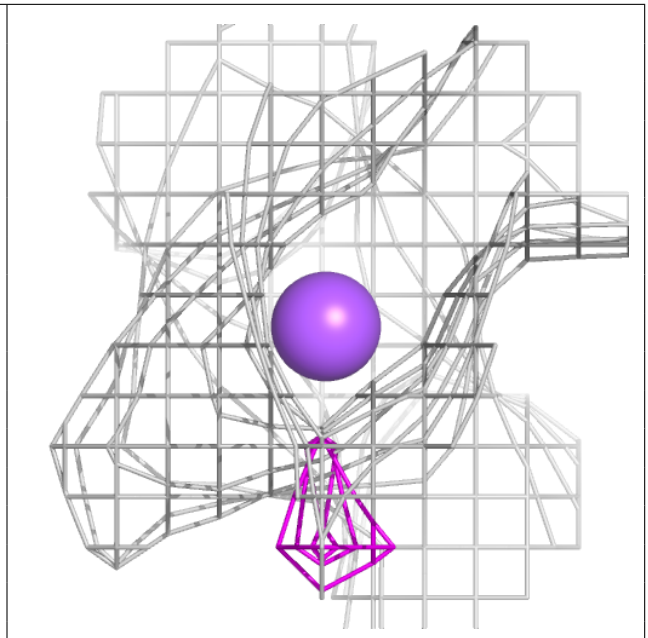


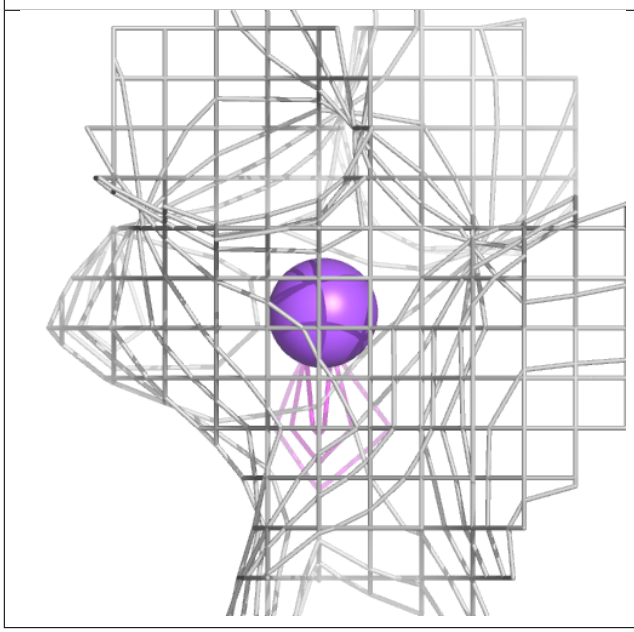


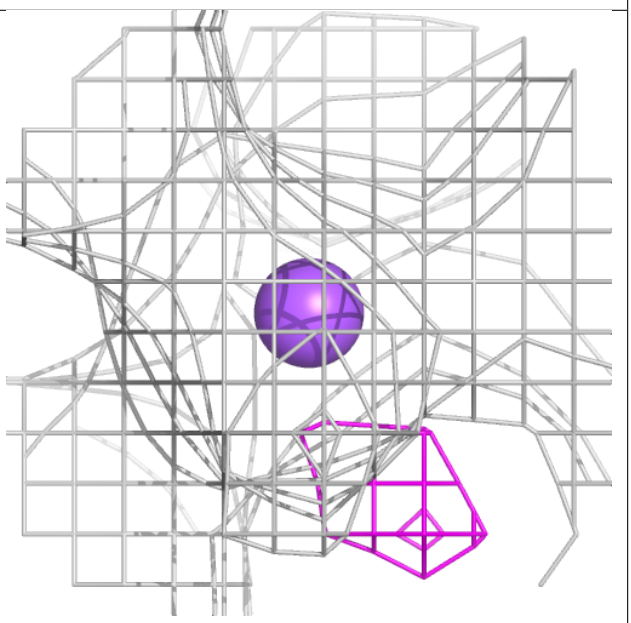


Electron density around NA A 301:

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

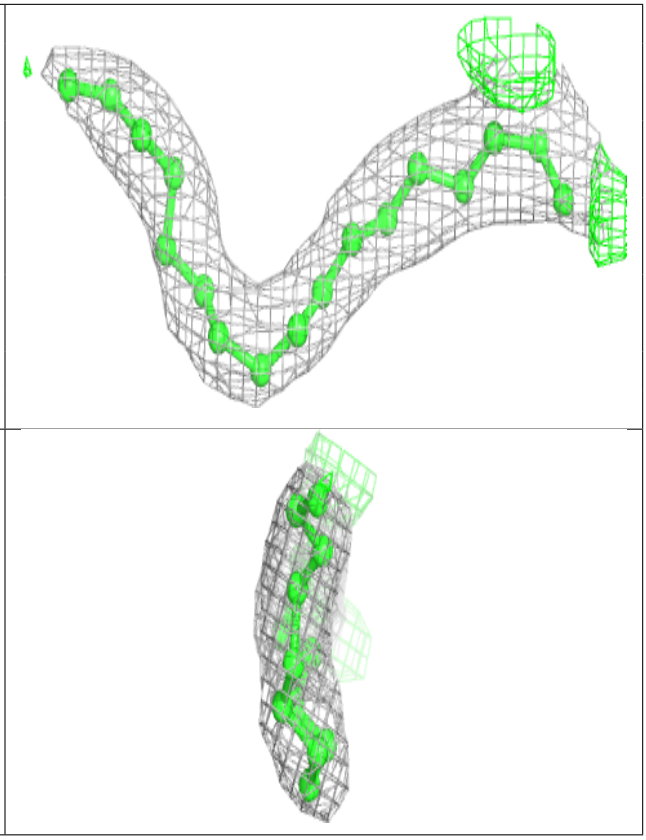






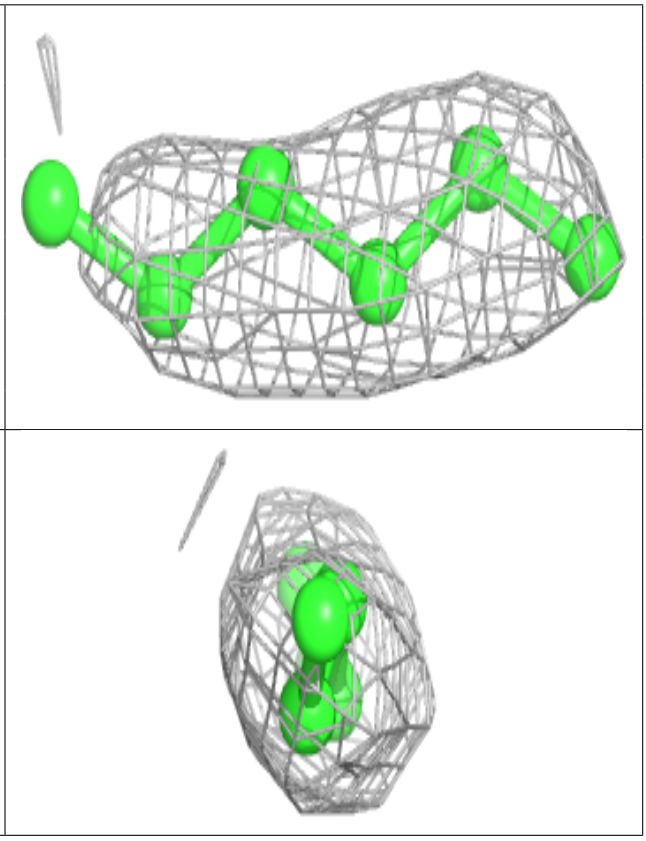
Electron density around LFA E 804:

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



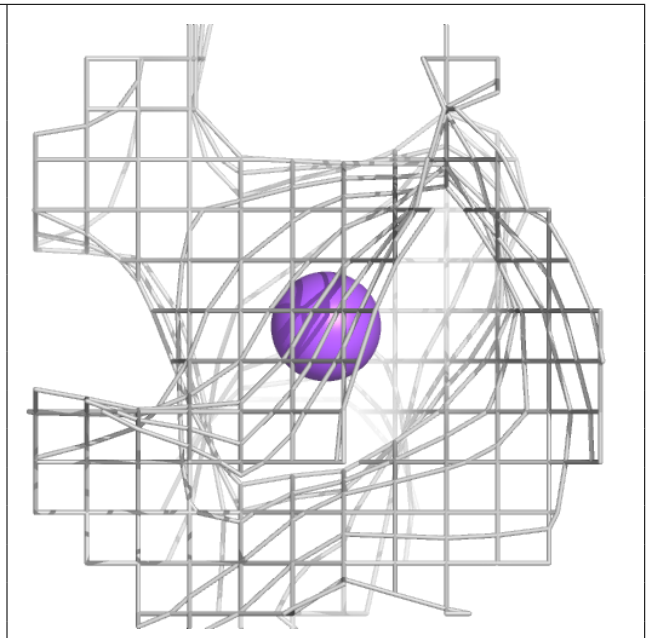
Electron density around LFA A 304:

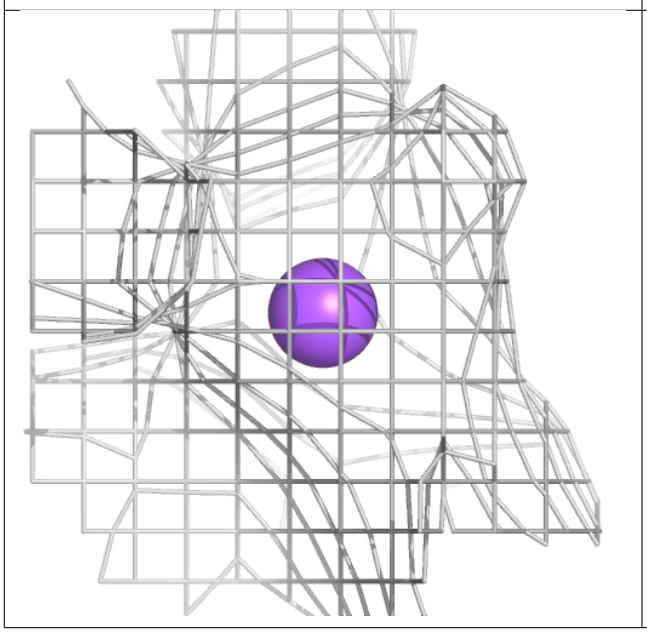
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

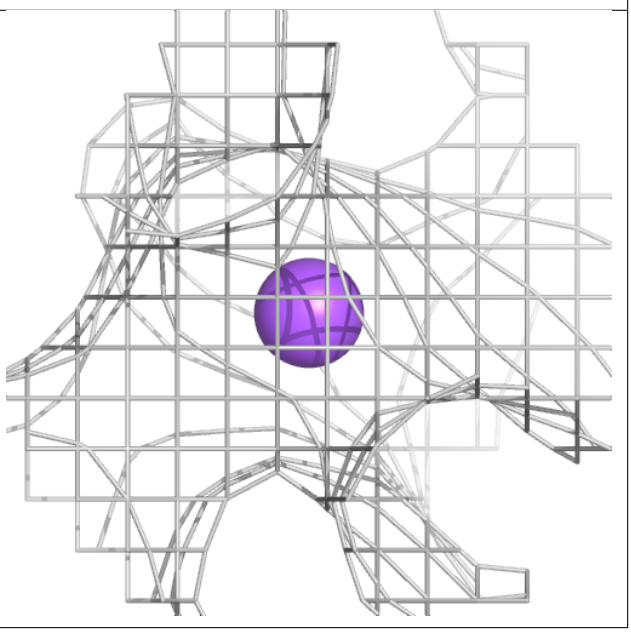


Electron density around NA D 503:

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

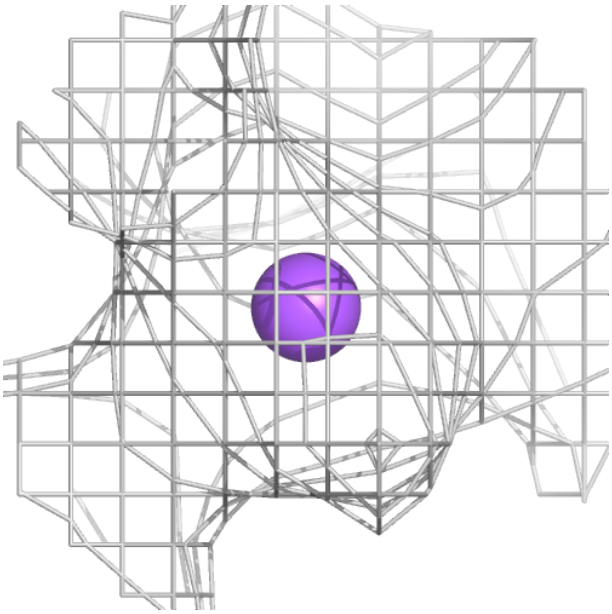


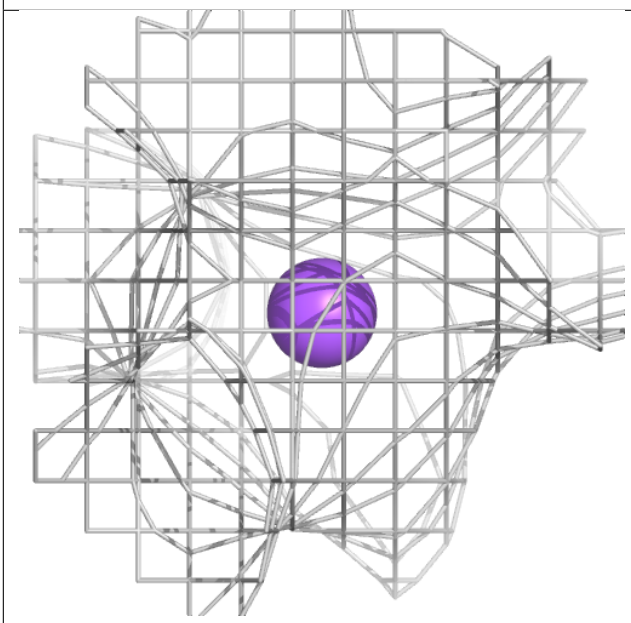


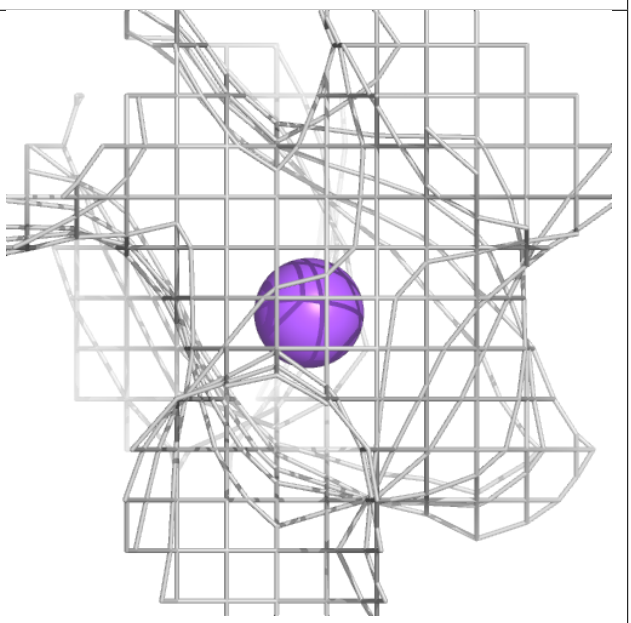


Electron density around NA B 301:

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

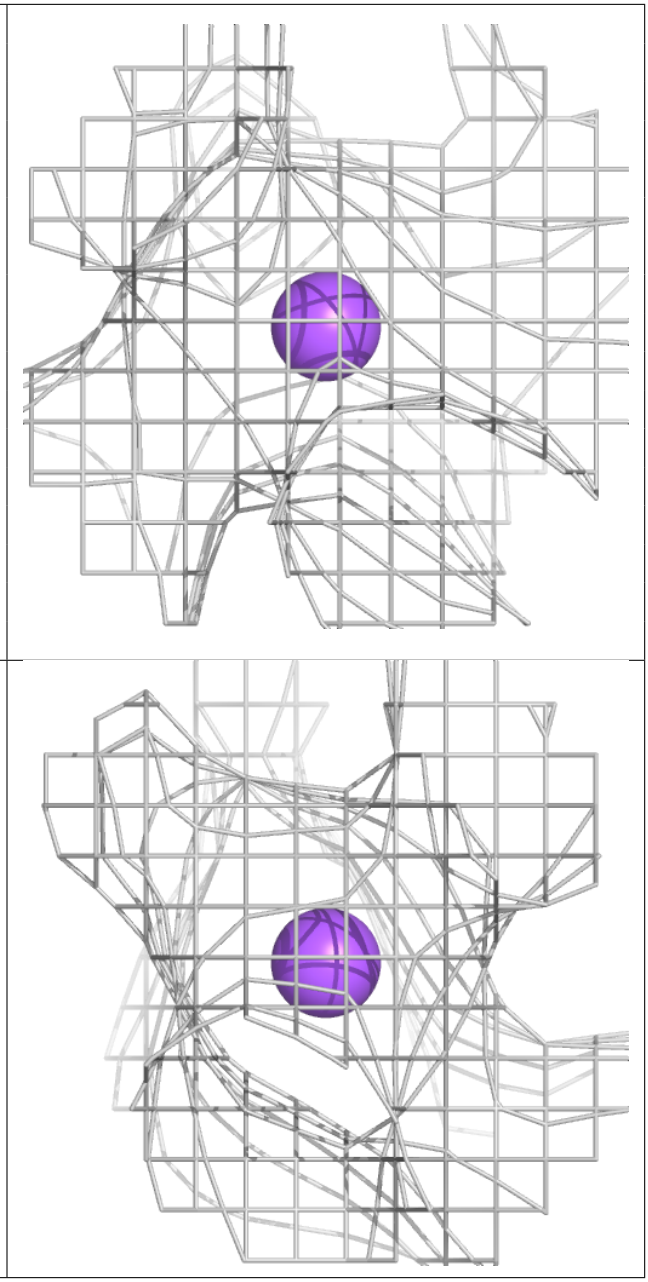






Electron density around NA E 803:

$2mF_o$-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.