wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 04:34 PM EDT

PDB ID	:	5LWE
Title	:	Crystal structure of the human CC chemokine receptor type 9 (CCR9) in complex with vercirnon
Authors	:	Oswald, C.; Rappas, M.; Kean, J.; Dore, A.S.; Errey, J.C.; Bennett, K.; Deflorian, F.; Christopher, J.A.; Jazayeri, A.; Mason, J.S.; Congreve, M.; Cooke, R.M.; Marshall, F.H.
Deposited on	:	2016-09-16
Resolution	:	2.80 Å(reported)

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

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

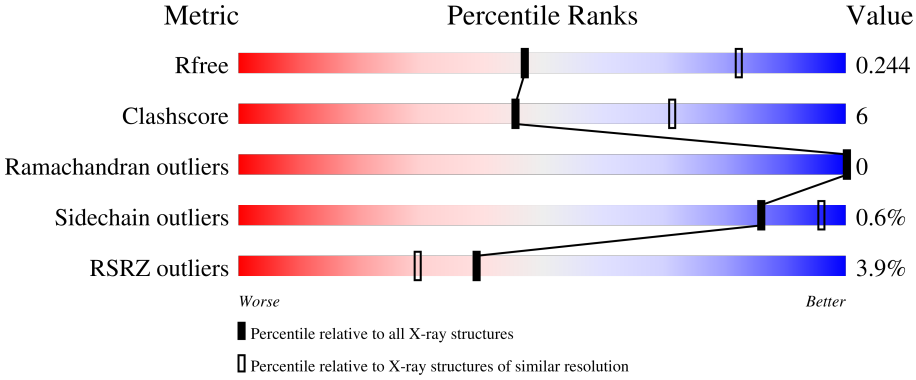
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	331	5% 73% 9% • 17%
1	B	331	2% 79% 7% 14%

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	OLA	A	404	-	-	X	-
3	OLA	A	412	-	-	-	X
3	OLA	B	411	-	-	-	X
3	OLA	B	414	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5054 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 C-C chemokine receptor type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2196	1469	352	351	24	0	2	0
1	B	285	2270	1513	364	369	24	0	1	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ALA	SER	conflict	UNP P51686
A	34	GLU	THR	conflict	UNP P51686
A	77	ALA	THR	conflict	UNP P51686
A	79	ALA	VAL	conflict	UNP P51686
A	82	ALA	MET	conflict	UNP P51686
A	141	CYS	SER	conflict	UNP P51686
A	216	ALA	THR	conflict	UNP P51686
A	255	ALA	VAL	conflict	UNP P51686
A	294	ALA	ASN	conflict	UNP P51686
A	304	ALA	THR	conflict	UNP P51686
A	337	ALA	CYS	conflict	UNP P51686
A	342	ALA	-	expression tag	UNP P51686
A	343	ALA	-	expression tag	UNP P51686
A	344	HIS	-	expression tag	UNP P51686
A	345	HIS	-	expression tag	UNP P51686
A	346	HIS	-	expression tag	UNP P51686
A	347	HIS	-	expression tag	UNP P51686
A	348	HIS	-	expression tag	UNP P51686
A	349	HIS	-	expression tag	UNP P51686
A	350	HIS	-	expression tag	UNP P51686
A	351	HIS	-	expression tag	UNP P51686
A	352	HIS	-	expression tag	UNP P51686
A	353	HIS	-	expression tag	UNP P51686
B	23	ALA	SER	conflict	UNP P51686
B	34	GLU	THR	conflict	UNP P51686

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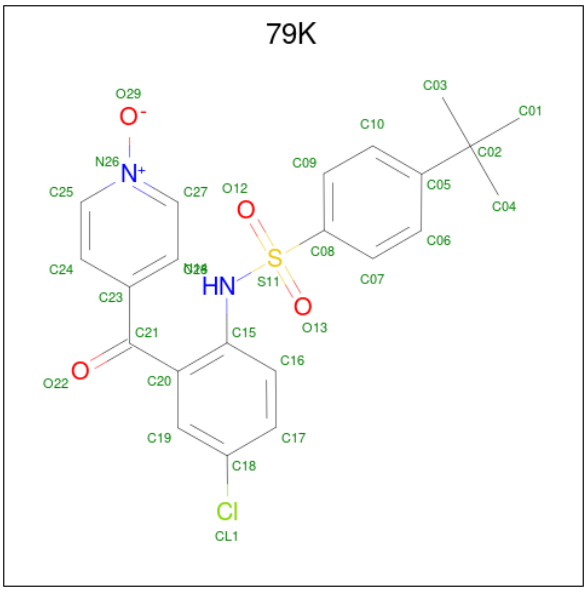
Chain	Residue	Modelled	Actual	Comment	Reference
B	77	ALA	THR	conflict	UNP P51686
B	79	ALA	VAL	conflict	UNP P51686
B	82	ALA	MET	conflict	UNP P51686
B	141	CYS	SER	conflict	UNP P51686
B	216	ALA	THR	conflict	UNP P51686
B	255	ALA	VAL	conflict	UNP P51686
B	294	ALA	ASN	conflict	UNP P51686
B	304	ALA	THR	conflict	UNP P51686
B	337	ALA	CYS	conflict	UNP P51686
B	342	ALA	-	expression tag	UNP P51686
B	343	ALA	-	expression tag	UNP P51686
B	344	HIS	-	expression tag	UNP P51686
B	345	HIS	-	expression tag	UNP P51686
B	346	HIS	-	expression tag	UNP P51686
B	347	HIS	-	expression tag	UNP P51686
B	348	HIS	-	expression tag	UNP P51686
B	349	HIS	-	expression tag	UNP P51686
B	350	HIS	-	expression tag	UNP P51686
B	351	HIS	-	expression tag	UNP P51686
B	352	HIS	-	expression tag	UNP P51686
B	353	HIS	-	expression tag	UNP P51686

- Molecule 2 is Vercirnon (three-letter code: 79K) (formula: $C_{22}H_{21}ClN_2O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	A	1	30	22	1	2	4	1	0	0

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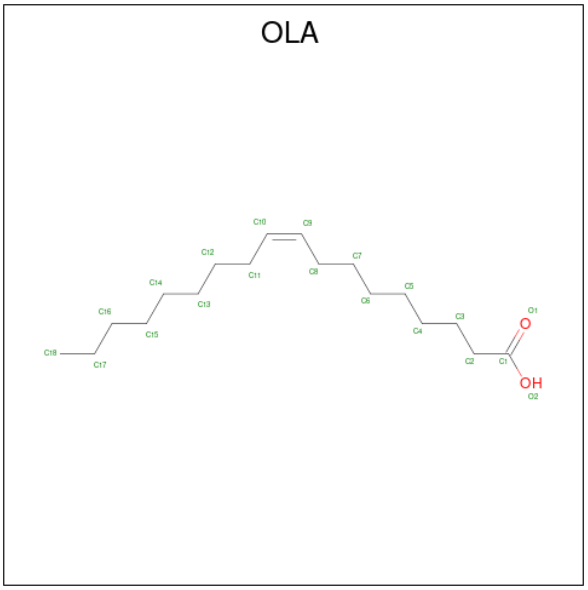
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
2	B	1	30	22	1	2	4	1	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	20	18	2	0	0
			Total	C	O		
3	A	1	18	16	2	0	0
			Total	C	O		
3	A	1	19	17	2	0	0
			Total	C	O		
3	A	1	11	9	2	0	0
			Total	C	O		
3	A	1	11	9	2	0	0
			Total	C	O		
3	A	1	11	9	2	0	0
			Total	C	O		
3	A	1	14	12	2	0	0
			Total	C	O		
3	A	1	8	6	2	0	0
			Total	C	O		
3	A	1	19	17	2	0	0
			Total	C	O		
3	A	1	9	7	2	0	0

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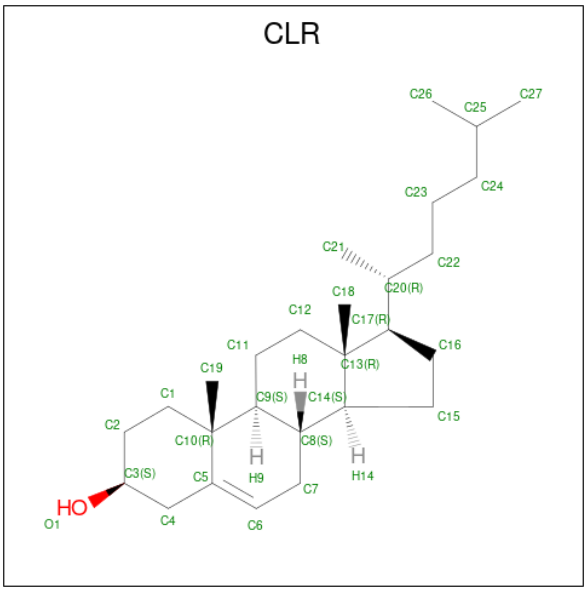
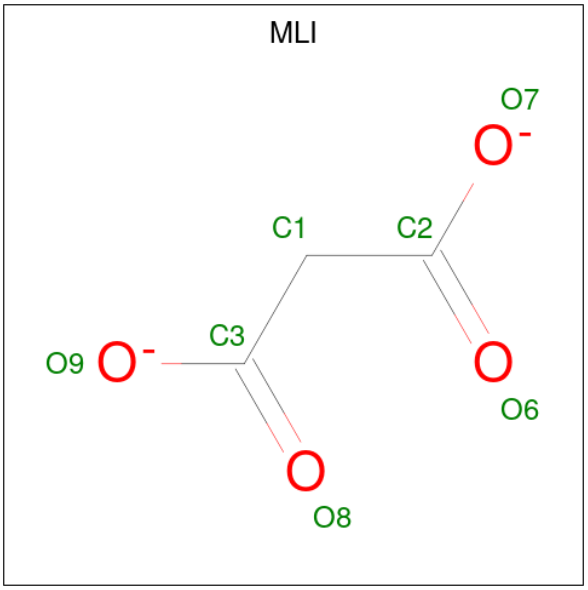
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	13	11	2	0	0
			Total	C	O		
3	A	1	20	18	2	0	0
			Total	C	O		
3	A	1	10	8	2	0	0
			Total	C	O		
3	A	1	12	10	2	0	0
			Total	C	O		
3	A	1	17	15	2	0	0
			Total	C	O		
3	B	1	20	18	2	0	0
			Total	C	O		
3	B	1	20	18	2	0	0
			Total	C	O		
3	B	1	20	18	2	0	0
			Total	C	O		
3	B	1	16	14	2	0	0
			Total	C	O		
3	B	1	15	13	2	0	0
			Total	C	O		
3	B	1	18	16	2	0	0
			Total	C	O		
3	B	1	13	11	2	0	0
			Total	C	O		
3	B	1	18	16	2	0	0
			Total	C	O		
3	B	1	12	10	2	0	0
			Total	C	O		
3	B	1	16	14	2	0	0
			Total	C	O		
3	B	1	19	17	2	0	0
			Total	C	O		
3	B	1	15	13	2	0	0
			Total	C	O		
3	B	1	20	18	2	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	28	27	1	0	0

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	7	3	4	0	0
5	B	1	7	3	4	0	0

- Molecule 6 is water.

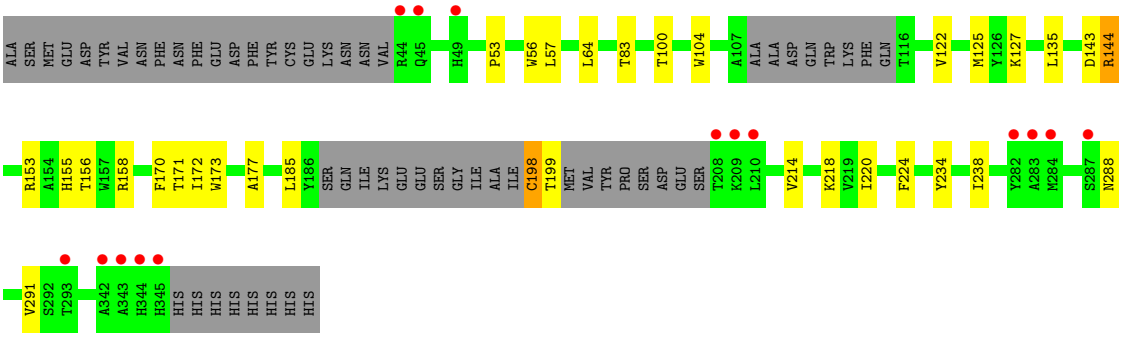
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	23	23	23	0	0
			Total	O		
6	B	29	29	29	0	0

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.

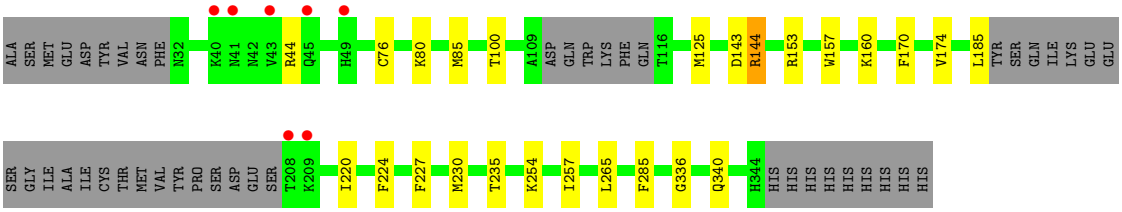
• Molecule 1: C-C chemokine receptor type 9

Chain A:



• Molecule 1: C-C chemokine receptor type 9

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.57Å 66.20Å 68.42Å 74.02° 64.72° 62.29°	Depositor
Resolution (Å)	19.97 – 2.80 51.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.97-2.80) 98.9 (51.86-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.215 , 0.243 0.219 , 0.244	Depositor DCC
R_{free} test set	1135 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 78.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5054	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.11% 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, CLR, MLI, 79K

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	0.26	0/2254	0.37	0/3061
1	B	0.25	0/2327	0.37	0/3161
All	All	0.25	0/4581	0.37	0/6222

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	2196	0	2311	26	0
1	B	2270	0	2367	19	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
3	A	212	0	293	24	0
3	B	222	0	327	16	0
4	A	28	0	46	0	0
5	A	7	0	2	0	0
5	B	7	0	2	1	0
6	A	23	0	0	0	0
6	B	29	0	0	0	0
All	All	5054	0	5348	66	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 6.

The worst 5 of 66 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:410:OLA:H21	3:A:416:OLA:H21	1.54	0.89
3:B:404:OLA:H31	3:B:405:OLA:H72	1.63	0.79
3:B:408:OLA:H52	3:B:409:OLA:H62	1.73	0.70
1:B:254:LYS:HG3	3:B:403:OLA:H42	1.80	0.63
3:A:408:OLA:H32	3:A:413:OLA:H32	1.80	0.63

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	269/331 (81%)	268 (100%)	1 (0%)	0	100	100
1	B	280/331 (85%)	277 (99%)	3 (1%)	0	100	100
All	All	549/662 (83%)	545 (99%)	4 (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	240/289 (83%)	238 (99%)	2 (1%)	81 94
1	B	247/289 (86%)	246 (100%)	1 (0%)	91 97
All	All	487/578 (84%)	484 (99%)	3 (1%)	86 96

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

Mol	Chain	Res	Type
1	A	144	ARG
1	A	198	CYS
1	B	144	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	123	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

33 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	$\#\|Z\| > 2$
3	OLA	B	406	-	14,14,19	0.53	0	14,14,19	0.99	2 (14%)
3	OLA	A	404	-	18,18,19	0.67	0	18,18,19	0.79	2 (11%)
3	OLA	A	409	-	7,7,19	0.91	0	7,7,19	1.20	1 (14%)
3	OLA	B	413	-	14,14,19	0.54	0	14,14,19	0.98	2 (14%)
3	OLA	A	410	3	18,18,19	0.67	0	18,18,19	0.77	1 (5%)
3	OLA	A	412	-	12,12,19	0.76	0	12,12,19	0.96	1 (8%)
3	OLA	B	404	-	19,19,19	0.67	0	19,19,19	0.76	1 (5%)
3	OLA	B	412	3	18,18,19	0.67	0	18,18,19	0.78	1 (5%)
3	OLA	A	416	-	16,16,19	0.69	0	16,16,19	0.83	1 (6%)
3	OLA	A	405	-	10,10,19	0.54	0	10,10,19	1.17	2 (20%)
3	OLA	A	406	-	10,10,19	0.54	0	10,10,19	1.15	2 (20%)
2	79K	A	401	-	32,32,32	2.63	14 (43%)	48,48,48	2.44	15 (31%)
3	OLA	B	408	-	12,12,19	0.76	0	12,12,19	0.97	1 (8%)
3	OLA	B	405	-	15,15,19	0.70	0	15,15,19	0.86	1 (6%)
3	OLA	B	411	-	15,15,19	0.54	0	15,15,19	0.95	2 (13%)
3	OLA	A	403	-	17,17,19	0.68	0	17,17,19	0.80	1 (5%)
3	OLA	A	414	-	9,9,19	0.80	0	9,9,19	1.06	1 (11%)
3	OLA	A	413	-	19,19,19	0.67	0	19,19,19	0.76	1 (5%)
3	OLA	A	407	-	10,10,19	0.77	0	10,10,19	1.02	1 (10%)
3	OLA	B	407	-	17,17,19	0.54	0	17,17,19	0.90	2 (11%)
3	OLA	B	403	-	19,19,19	0.66	0	19,19,19	0.75	1 (5%)
3	OLA	A	402	-	19,19,19	0.66	0	19,19,19	0.75	1 (5%)
3	OLA	B	410	-	11,11,19	0.81	0	11,11,19	1.01	1 (9%)
5	MLI	A	418	-	6,6,6	1.31	0	7,7,7	1.27	0
4	CLR	A	417	-	31,31,31	0.64	0	48,48,48	0.98	0
3	OLA	B	402	-	19,19,19	0.67	0	19,19,19	0.76	1 (5%)
3	OLA	A	415	-	11,11,19	0.82	0	11,11,19	1.01	1 (9%)
5	MLI	B	415	-	6,6,6	1.31	0	7,7,7	1.29	0
3	OLA	B	414	-	19,19,19	0.66	0	19,19,19	0.75	1 (5%)
3	OLA	A	408	-	13,13,19	0.75	0	12,13,19	0.95	1 (8%)
2	79K	B	401	-	32,32,32	2.68	14 (43%)	48,48,48	2.45	15 (31%)
3	OLA	A	411	-	8,8,19	0.59	0	8,8,19	1.26	2 (25%)
3	OLA	B	409	-	17,17,19	0.68	0	17,17,19	0.80	1 (5%)

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	OLA	B	406	-	-	7/12/12/17	-
3	OLA	A	404	-	-	5/16/16/17	-
3	OLA	A	409	-	-	0/5/5/17	-
3	OLA	B	413	-	-	8/12/12/17	-
3	OLA	A	410	3	-	10/16/16/17	-
3	OLA	A	412	-	-	3/10/10/17	-
3	OLA	B	404	-	-	6/17/17/17	-
3	OLA	B	412	3	-	8/16/16/17	-
3	OLA	A	416	-	-	4/14/14/17	-
3	OLA	A	405	-	-	4/8/8/17	-
3	OLA	A	406	-	-	5/8/8/17	-
2	79K	A	401	-	-	0/25/25/25	0/3/3/3
3	OLA	B	408	-	-	3/10/10/17	-
3	OLA	B	405	-	-	6/13/13/17	-
3	OLA	B	411	-	-	6/13/13/17	-
3	OLA	A	403	-	-	7/15/15/17	-
3	OLA	A	414	-	-	6/7/7/17	-
3	OLA	A	413	-	-	8/17/17/17	-
3	OLA	A	407	-	-	3/8/8/17	-
3	OLA	B	407	-	-	8/15/15/17	-
3	OLA	B	403	-	-	9/17/17/17	-
3	OLA	A	402	-	-	7/17/17/17	-
3	OLA	B	410	-	-	7/9/9/17	-
5	MLI	A	418	-	-	2/4/4/4	-
4	CLR	A	417	-	-	1/10/68/68	0/4/4/4
3	OLA	B	402	-	-	8/17/17/17	-
3	OLA	A	415	-	-	9/9/9/17	-
5	MLI	B	415	-	-	2/4/4/4	-
3	OLA	B	414	-	-	7/17/17/17	-
3	OLA	A	408	-	-	6/11/11/17	-
2	79K	B	401	-	-	0/25/25/25	0/3/3/3
3	OLA	A	411	-	-	5/6/6/17	-
3	OLA	B	409	-	-	9/15/15/17	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	79K	C08-S11	8.28	1.89	1.76
2	A	401	79K	C08-S11	7.71	1.88	1.76
2	B	401	79K	S11-N14	6.48	1.74	1.63
2	A	401	79K	S11-N14	6.38	1.74	1.63
2	A	401	79K	O29-N26	-4.96	1.17	1.36

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	79K	C09-C08-C07	-5.82	112.32	120.44
2	A	401	79K	C28-C23-C24	-5.69	110.48	118.59
2	B	401	79K	C28-C23-C24	-5.67	110.50	118.59
2	A	401	79K	C09-C08-C07	-5.65	112.56	120.44
2	B	401	79K	O13-S11-O12	-5.02	113.38	119.55

There are no chirality outliers.

5 of 179 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	408	OLA	C9-C10-C11-C12
3	A	406	OLA	C3-C4-C5-C6
3	A	413	OLA	C11-C12-C13-C14
3	A	413	OLA	C4-C5-C6-C7
3	B	409	OLA	C12-C13-C14-C15

There are no ring outliers.

18 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	OLA	9	0
3	A	410	OLA	2	0
3	A	412	OLA	1	0
3	B	404	OLA	4	0
3	A	416	OLA	1	0
3	A	405	OLA	1	0
3	B	408	OLA	5	0
3	B	405	OLA	3	0
3	B	411	OLA	1	0
3	A	403	OLA	8	0
3	A	413	OLA	6	0

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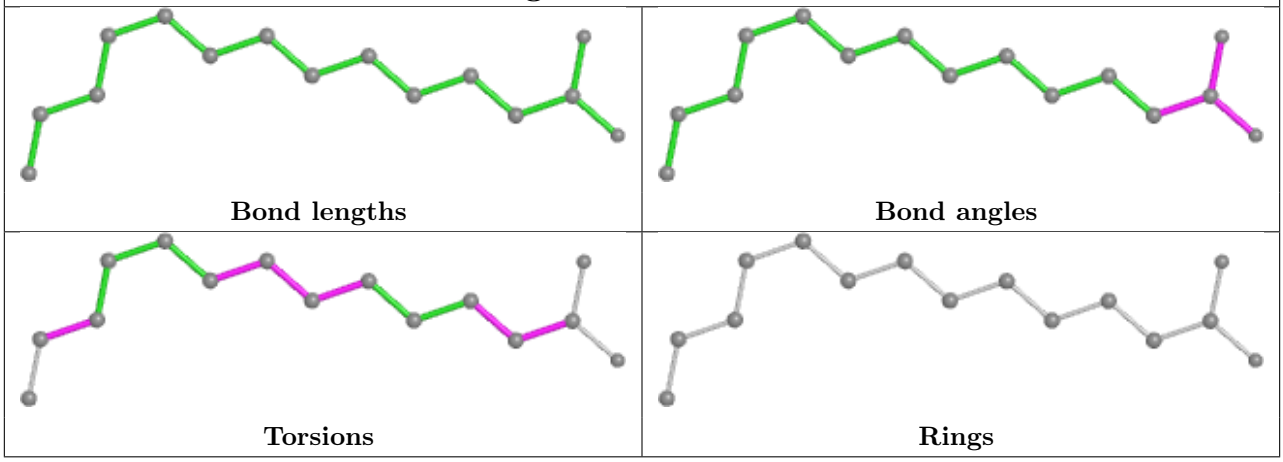
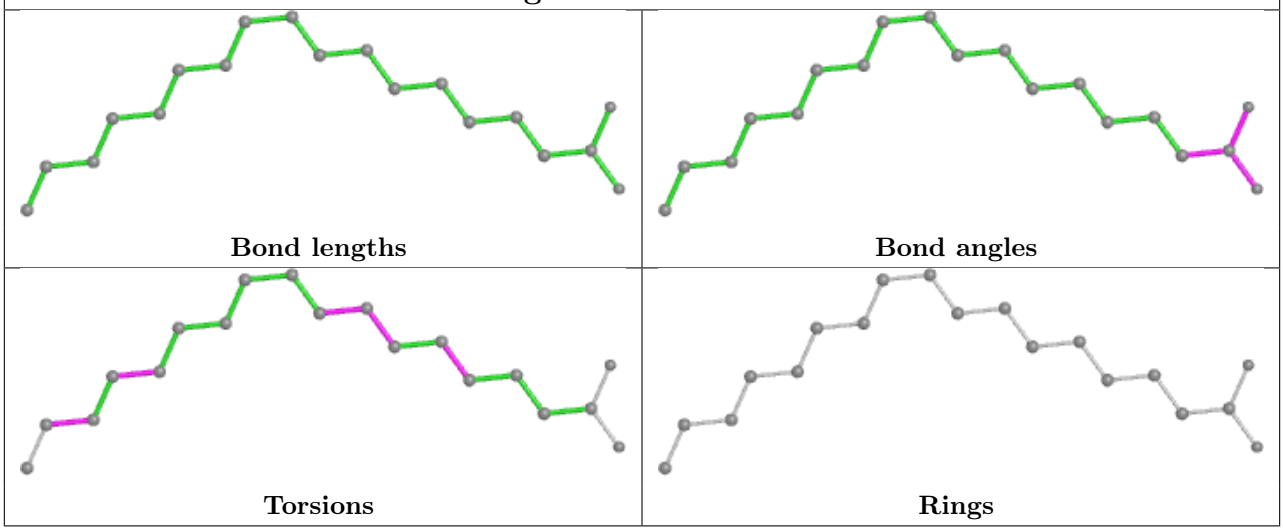
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	407	OLA	3	0
3	B	407	OLA	1	0
3	B	403	OLA	2	0
5	B	415	MLI	1	0
3	B	414	OLA	1	0
3	A	408	OLA	2	0
3	B	409	OLA	6	0

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 OLA B 406



Ligand OLA A 404



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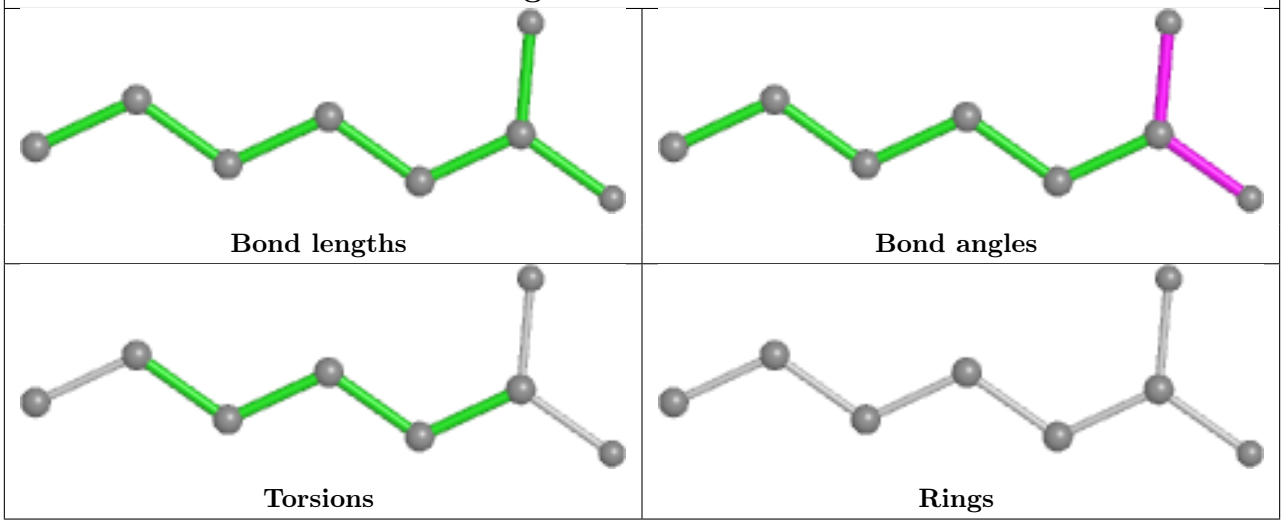

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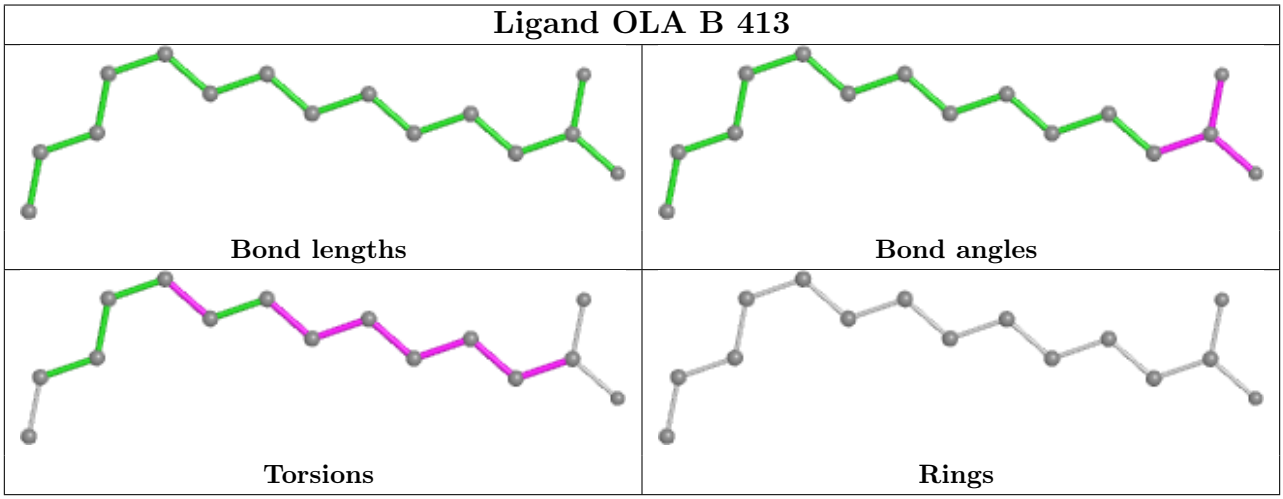

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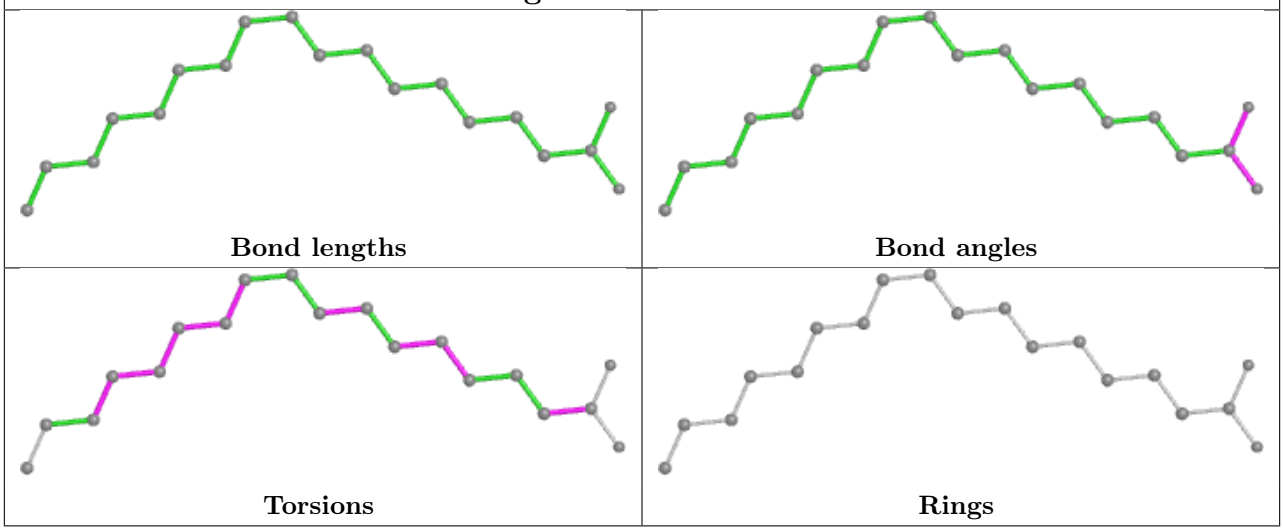

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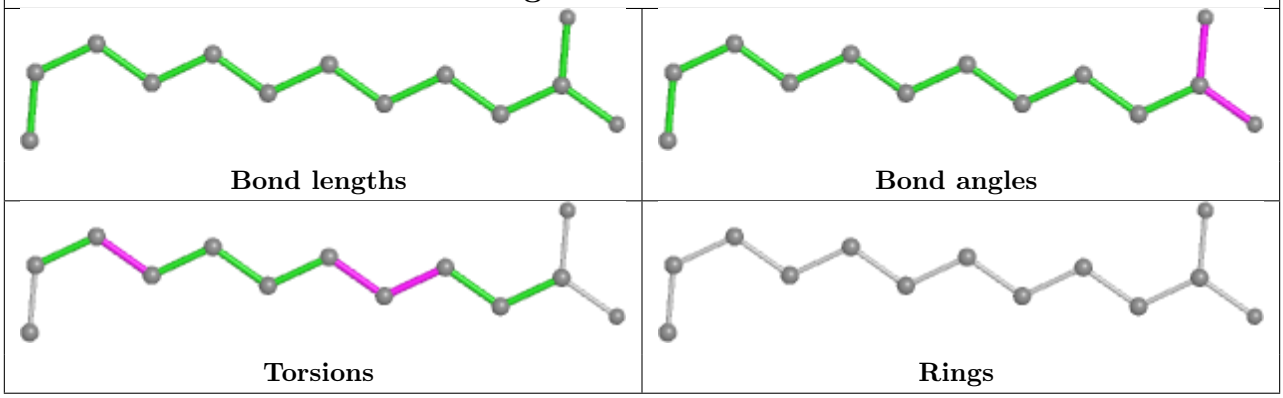

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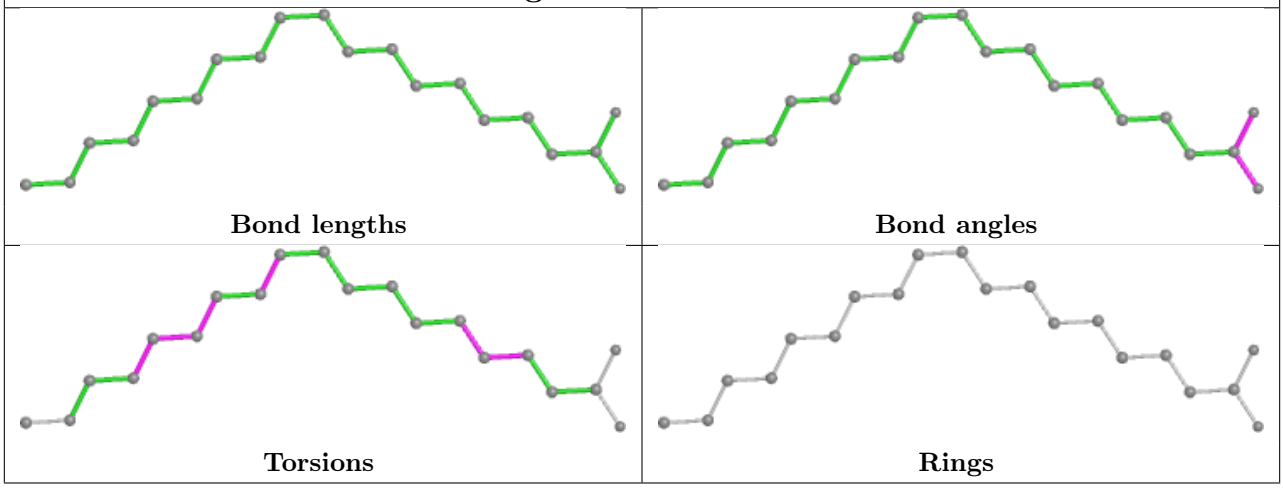

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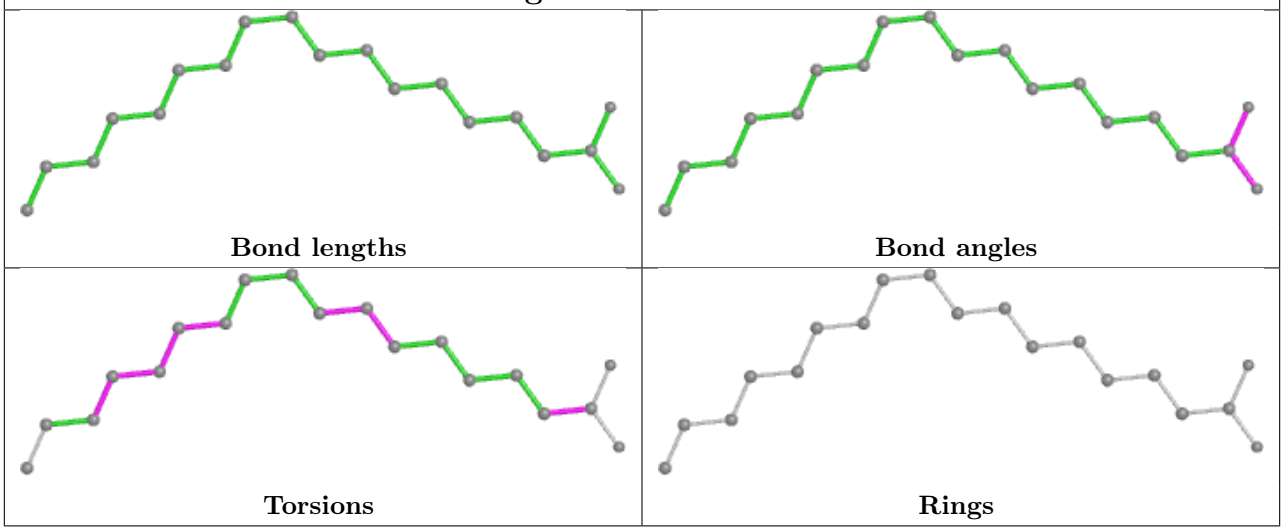

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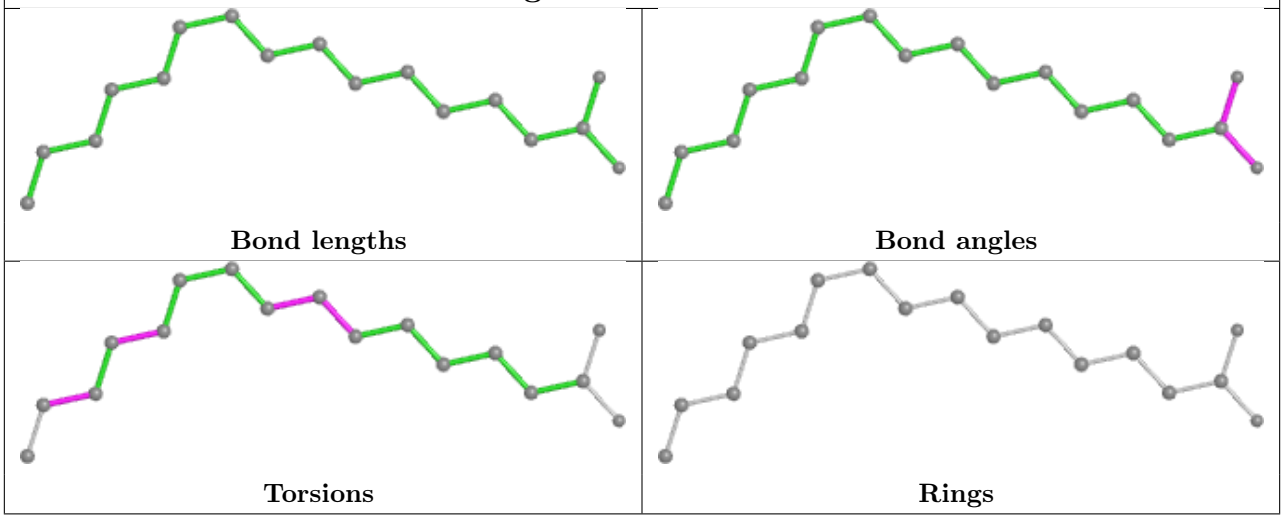

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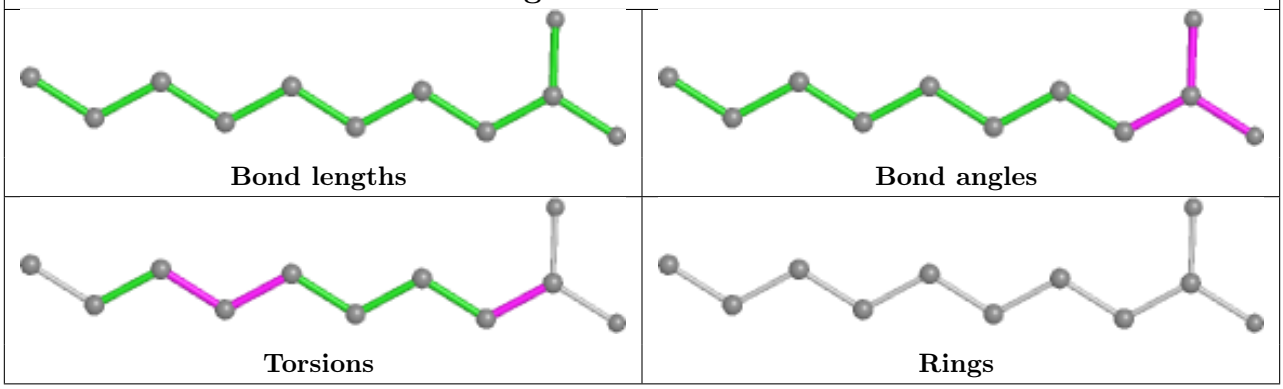

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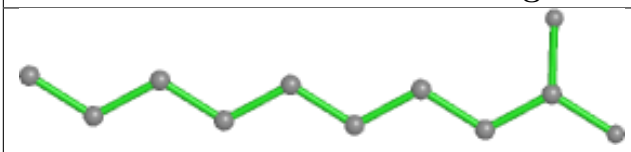
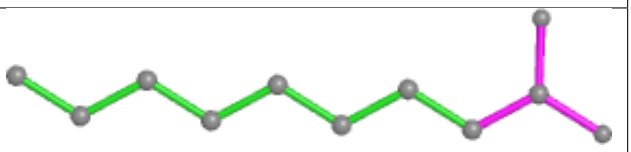
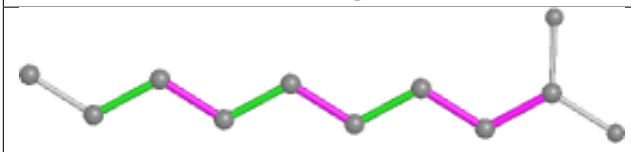


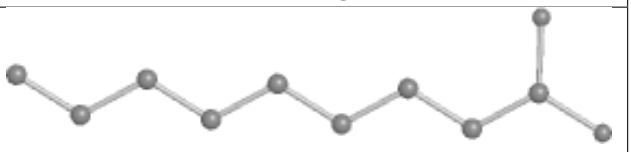
Bond lengths



Bond angles

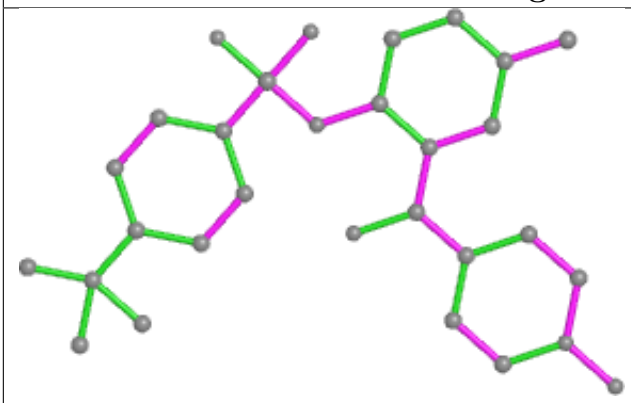


Torsions



Rings

Ligand 79K A 401



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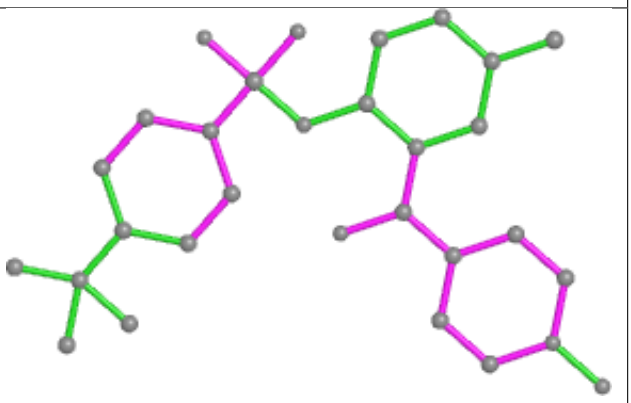

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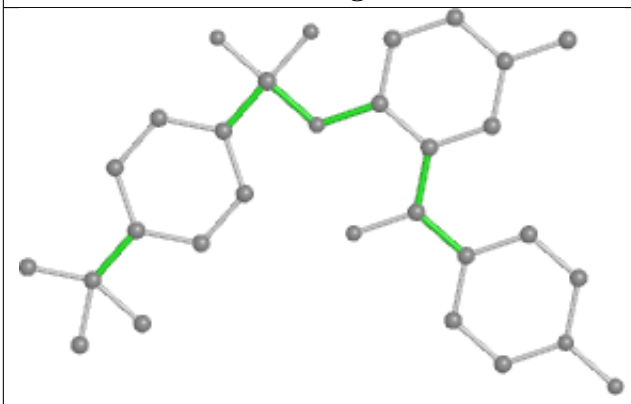

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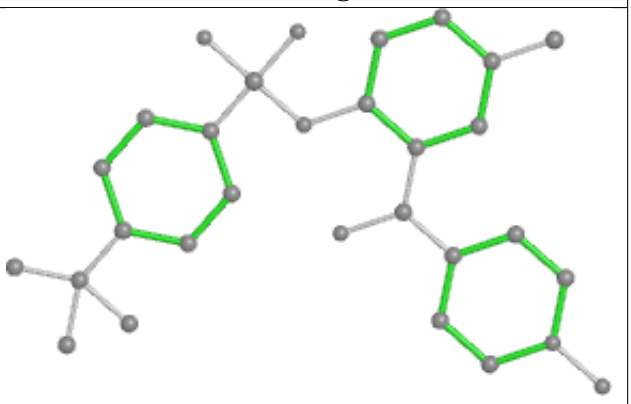
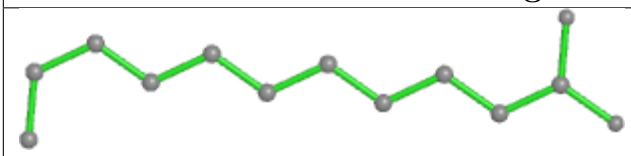


Rings

Ligand OLA B 408



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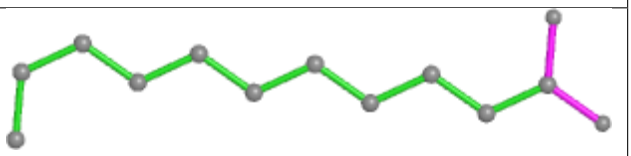

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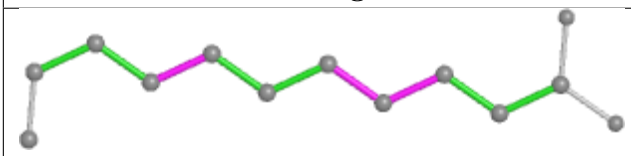

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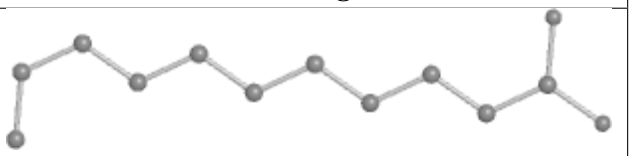

Rings

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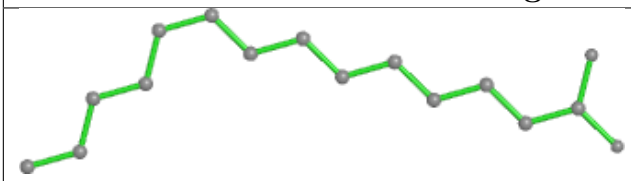

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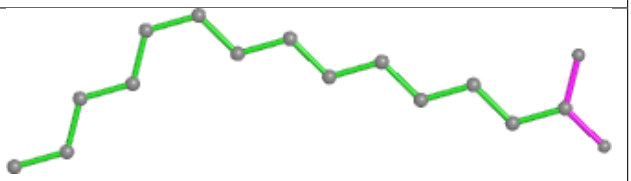

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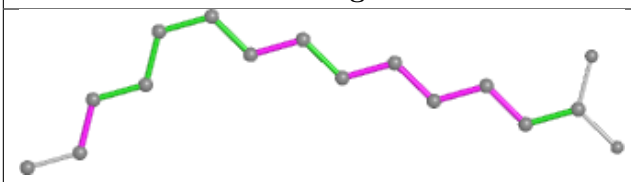

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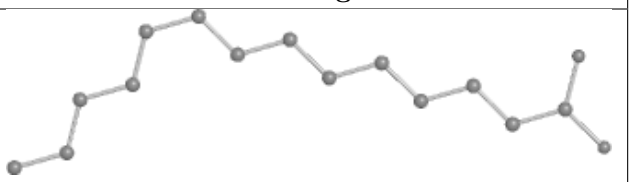

Rings

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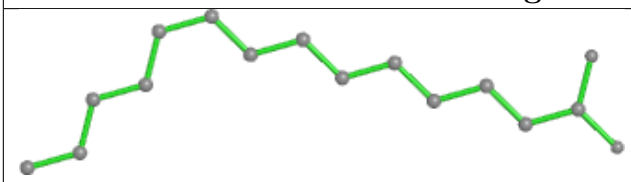

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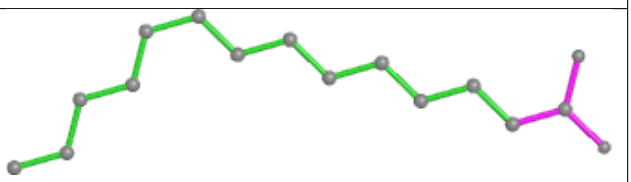

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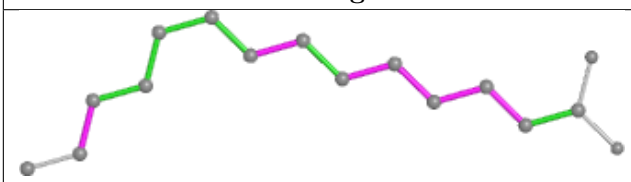

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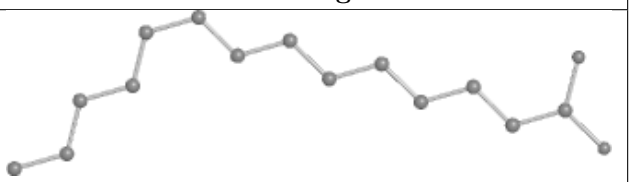
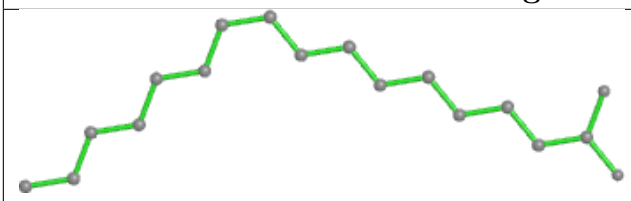


Rings

Ligand OLA A 403



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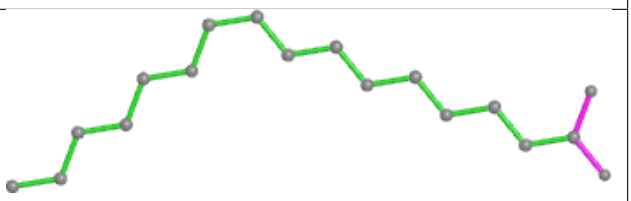
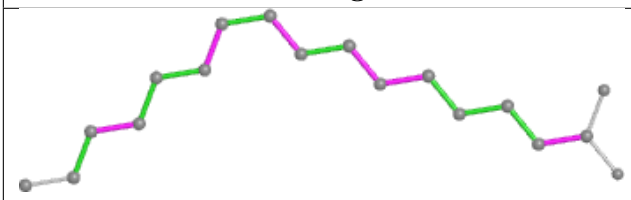


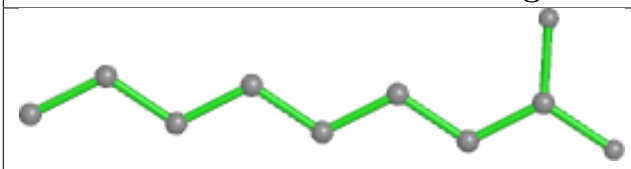
Bond angles



Torsions

Rings

Ligand OLA A 414



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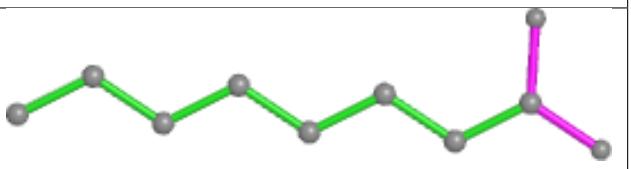
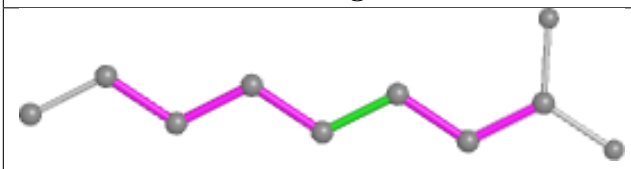
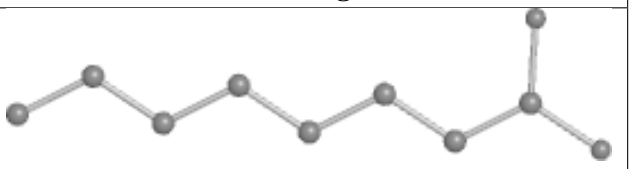


Bond angles



Torsions



Rings

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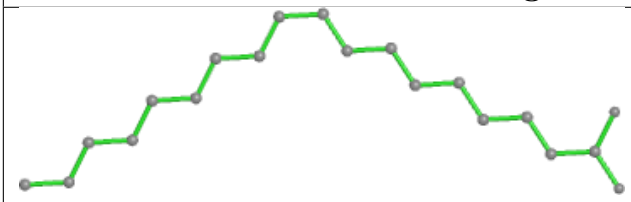

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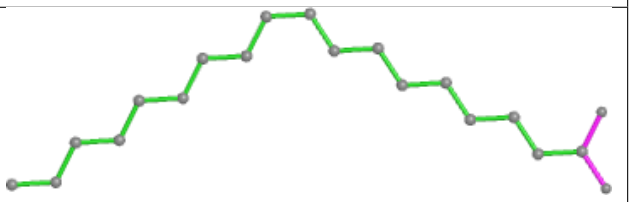
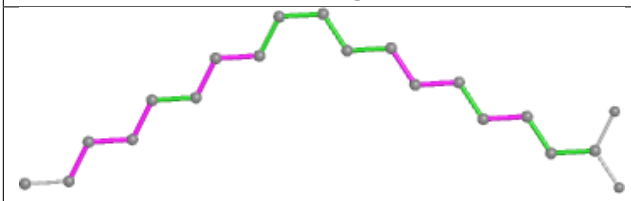
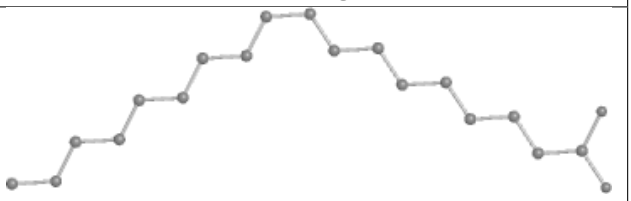


Bond angles

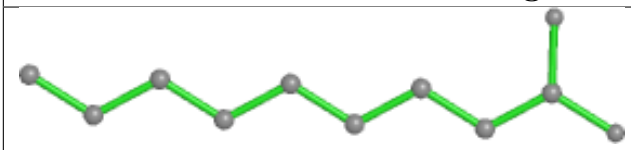


Torsions

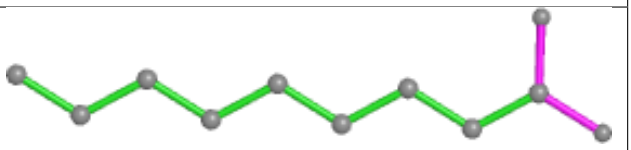


Rings

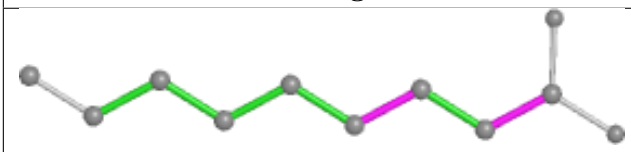
Ligand OLA A 407



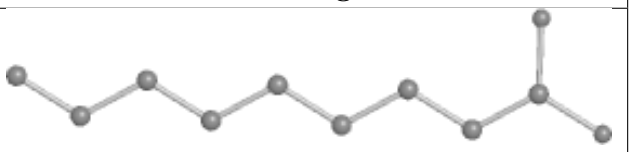
Bond lengths



Bond angles

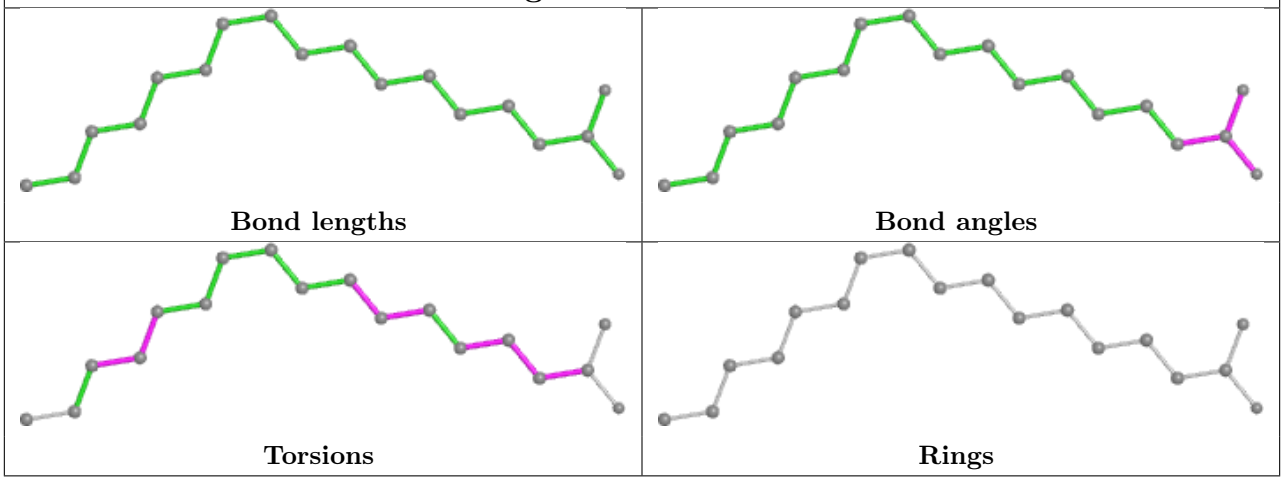


Torsions

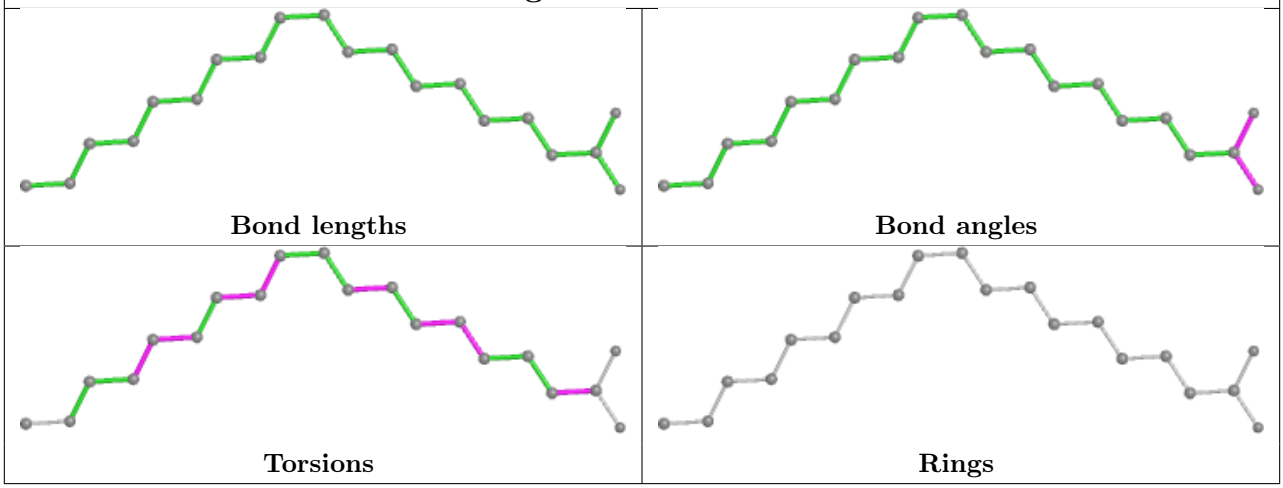


Rings

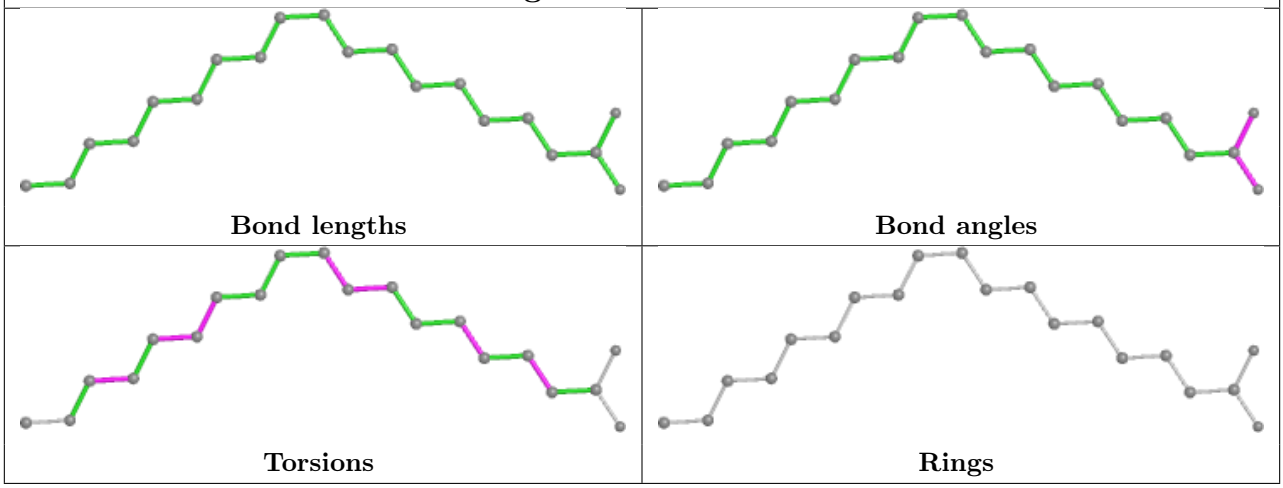
Ligand OLA B 407



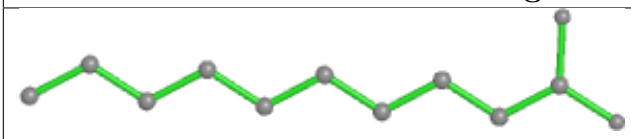
Ligand OLA B 403



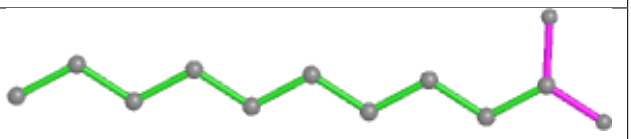
Ligand OLA A 402



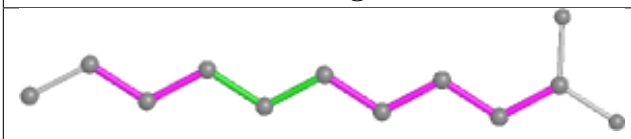
Ligand OLA B 410



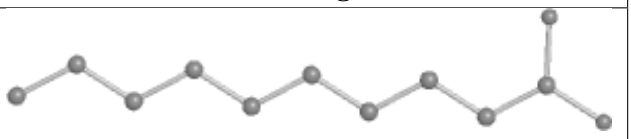
Bond lengths



Bond angles

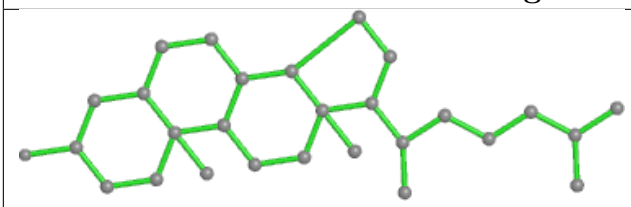


Torsions

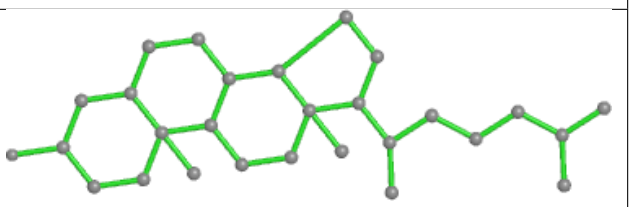


Rings

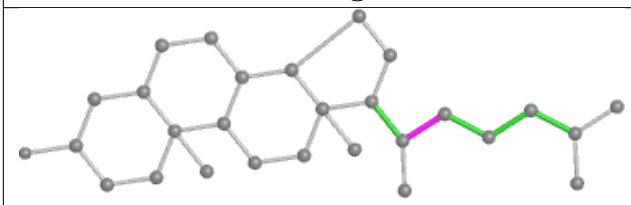
Ligand CLR A 417



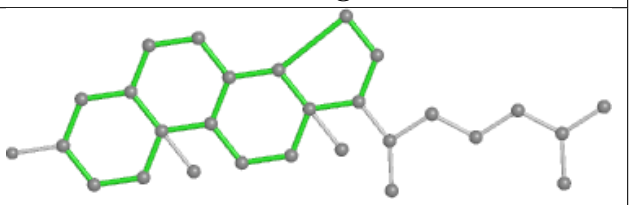
Bond lengths



Bond angles

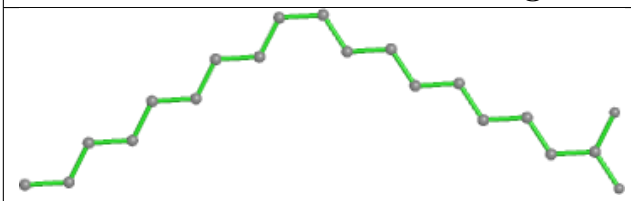


Torsions

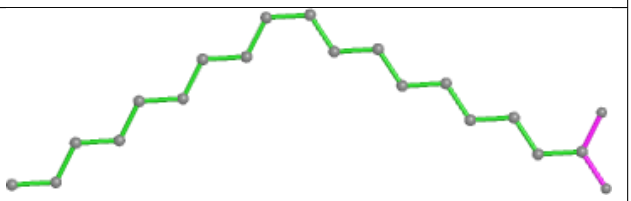


Rings

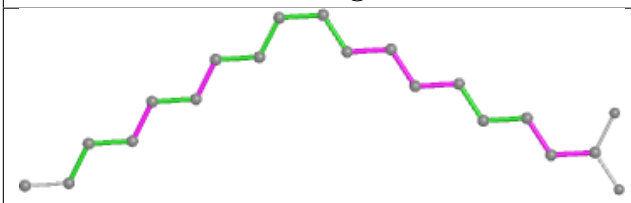
Ligand OLA B 402



Bond lengths



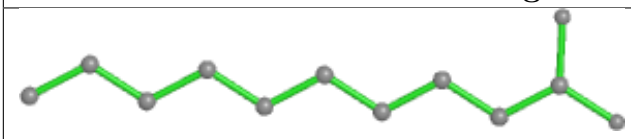
Bond angles



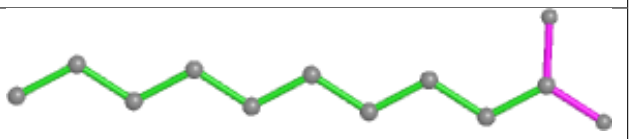
Torsions

Rings

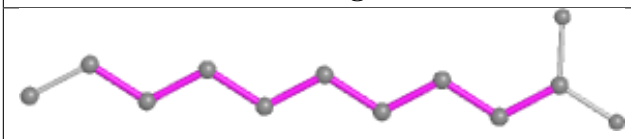
Ligand OLA A 415



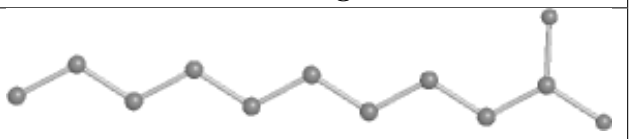
Bond lengths



Bond angles

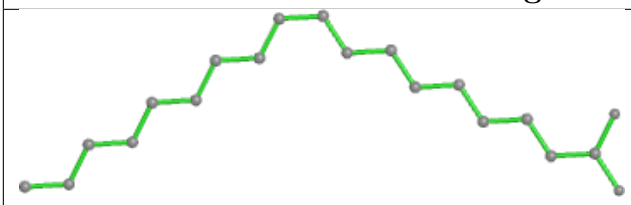


Torsions

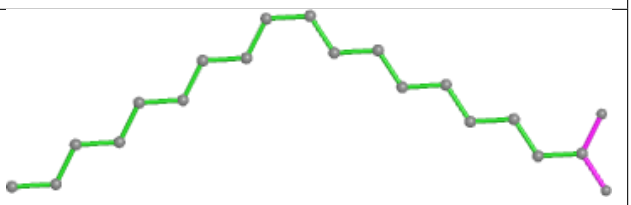


Rings

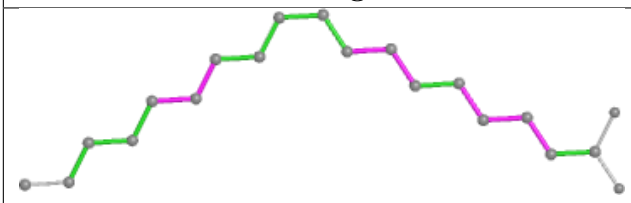
Ligand OLA B 414



Bond lengths



Bond angles



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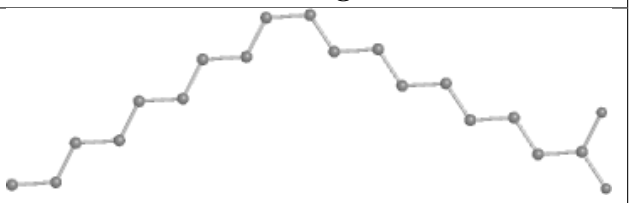
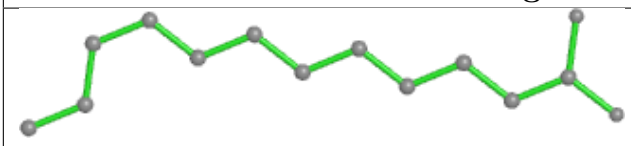


Rings

Ligand OLA A 408



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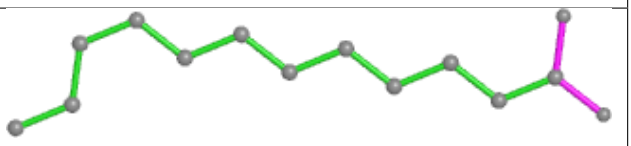
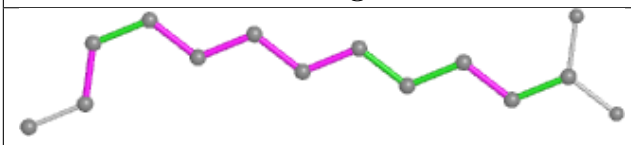
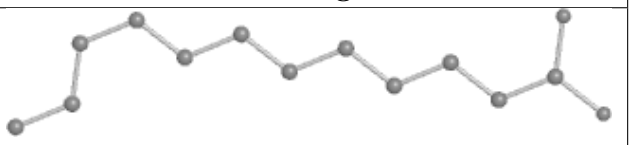


Bond angles

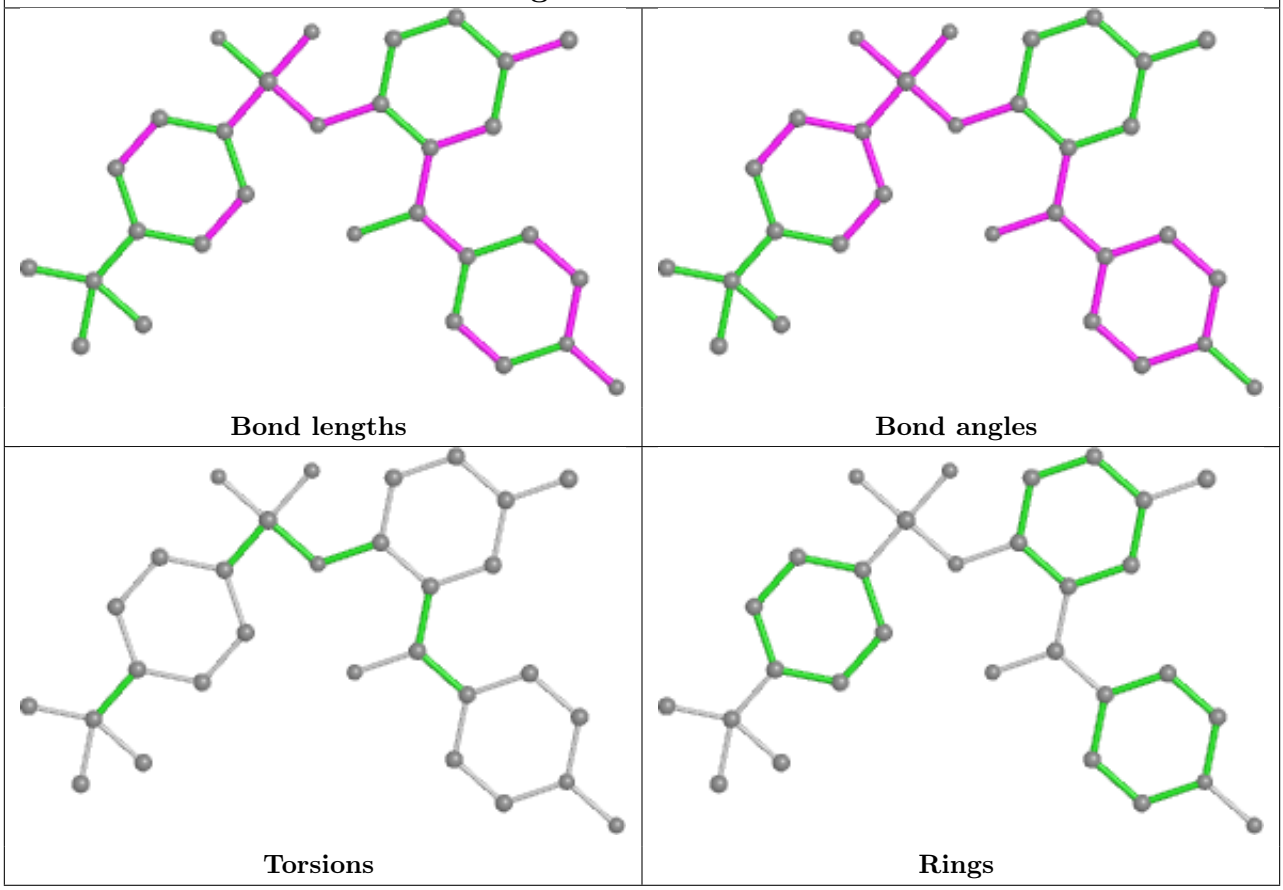


Torsions

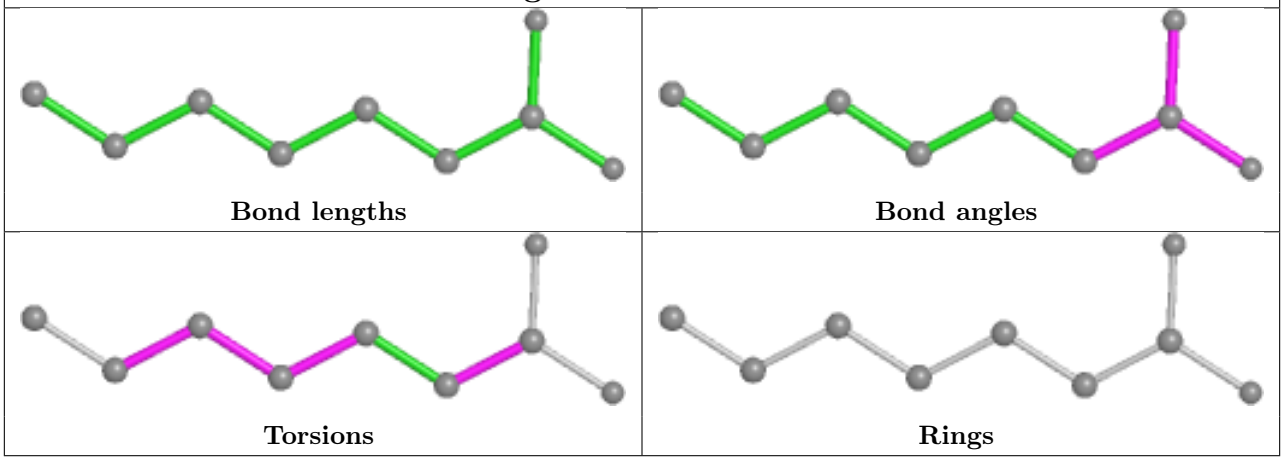


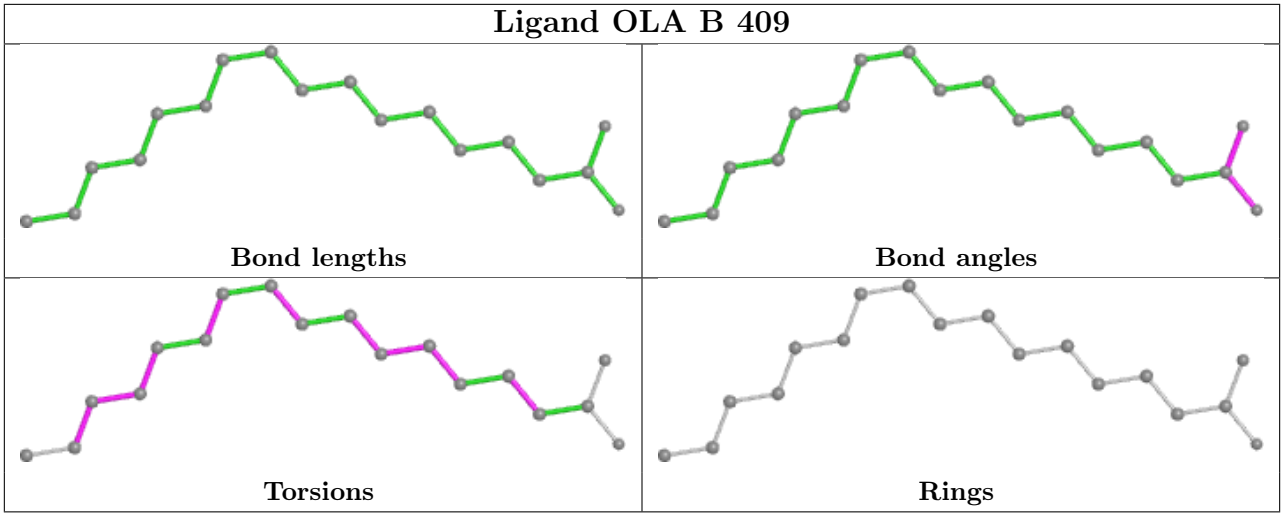
Rings

Ligand 79K B 401



Ligand OLA A 411





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	275/331 (83%)	-0.14	15 (5%)	25	16	24, 59, 151, 209	0
1	B	285/331 (86%)	-0.27	7 (2%)	57	47	26, 51, 137, 177	0
All	All	560/662 (84%)	-0.20	22 (3%)	39	29	24, 54, 144, 209	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	343	ALA	5.7
1	A	45	GLN	4.8
1	B	208	THR	4.1
1	A	284	MET	3.9
1	A	49	HIS	3.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

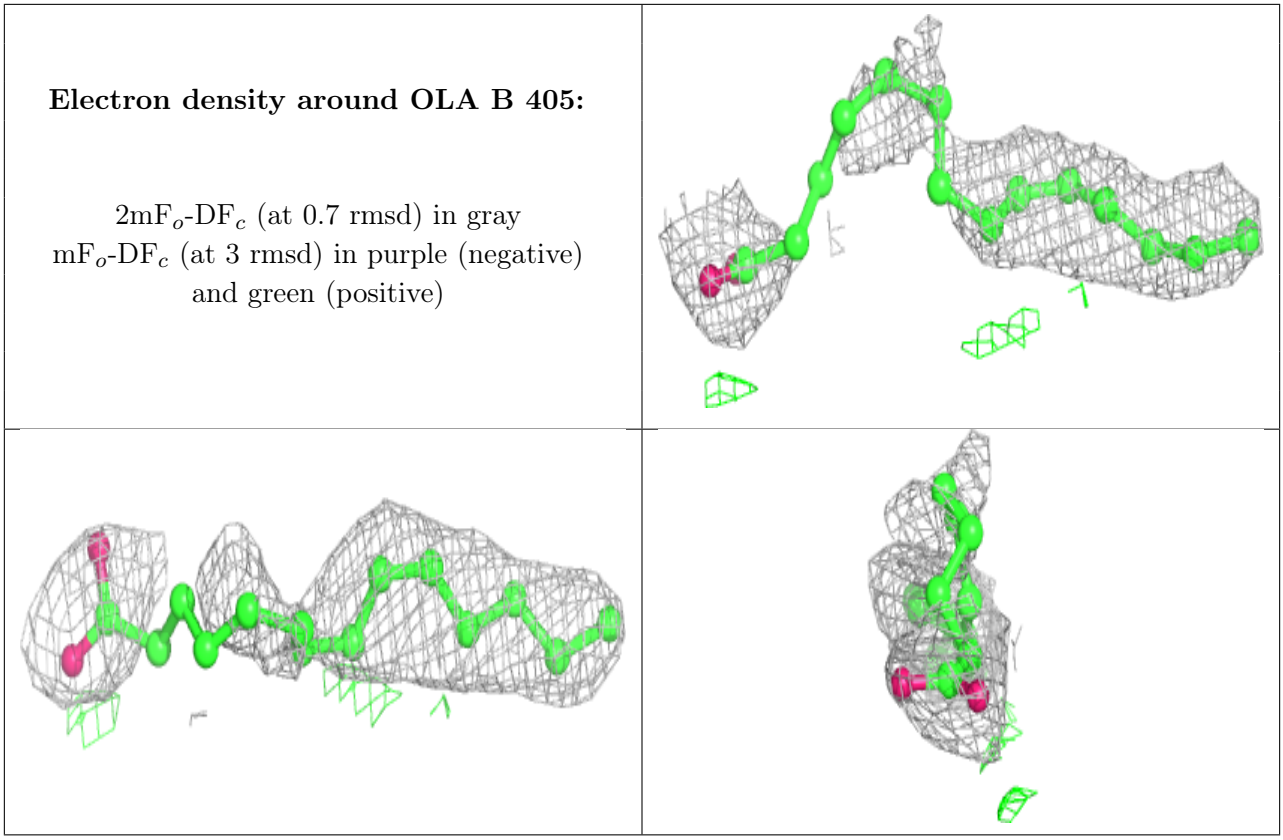
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLA	B	405	16/20	0.63	0.30	79,92,103,104	0
3	OLA	B	411	16/20	0.64	0.44	83,85,89,90	0
3	OLA	B	414	20/20	0.69	0.46	88,94,107,108	0
3	OLA	B	413	15/20	0.71	0.22	78,85,98,98	0
3	OLA	A	413	20/20	0.72	0.20	81,85,93,94	0
3	OLA	B	409	18/20	0.75	0.20	81,83,91,91	0
3	OLA	B	404	20/20	0.76	0.21	75,78,85,86	0
3	OLA	B	408	13/20	0.77	0.18	92,95,103,104	0
3	OLA	A	415	12/20	0.78	0.26	71,72,76,79	0
3	OLA	B	402	20/20	0.78	0.18	70,79,81,81	0
3	OLA	A	403	18/20	0.78	0.33	82,87,95,97	0
3	OLA	A	408	14/20	0.79	0.15	68,74,80,81	0
3	OLA	A	410	19/20	0.79	0.28	61,68,89,90	0
4	CLR	A	417	28/28	0.79	0.29	95,97,99,99	0
3	OLA	A	412	13/20	0.80	0.41	71,78,82,83	0
3	OLA	A	416	17/20	0.81	0.37	77,79,81,81	0
3	OLA	A	406	11/20	0.81	0.17	74,74,76,77	0
3	OLA	A	404	19/20	0.82	0.23	80,86,95,95	0
3	OLA	B	403	20/20	0.82	0.22	58,62,82,83	0
3	OLA	A	411	9/20	0.82	0.22	75,77,79,80	0
3	OLA	B	410	12/20	0.82	0.25	67,71,81,82	0
3	OLA	B	412	19/20	0.83	0.29	63,75,91,91	0
3	OLA	B	406	15/20	0.84	0.25	63,69,77,78	0
3	OLA	B	407	18/20	0.84	0.27	74,79,82,83	0
3	OLA	A	402	20/20	0.85	0.19	62,71,76,76	0
3	OLA	A	405	11/20	0.85	0.25	72,76,80,80	0
3	OLA	A	407	11/20	0.88	0.25	65,67,77,78	0
3	OLA	A	414	10/20	0.88	0.20	66,66,70,71	0
5	MLI	A	418	7/7	0.88	0.17	90,91,92,92	0
3	OLA	A	409	8/20	0.90	0.26	76,81,82,83	0
5	MLI	B	415	7/7	0.92	0.16	74,75,75,77	0
2	79K	B	401	30/30	0.95	0.16	30,40,54,60	0
2	79K	A	401	30/30	0.96	0.17	34,40,52,60	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.

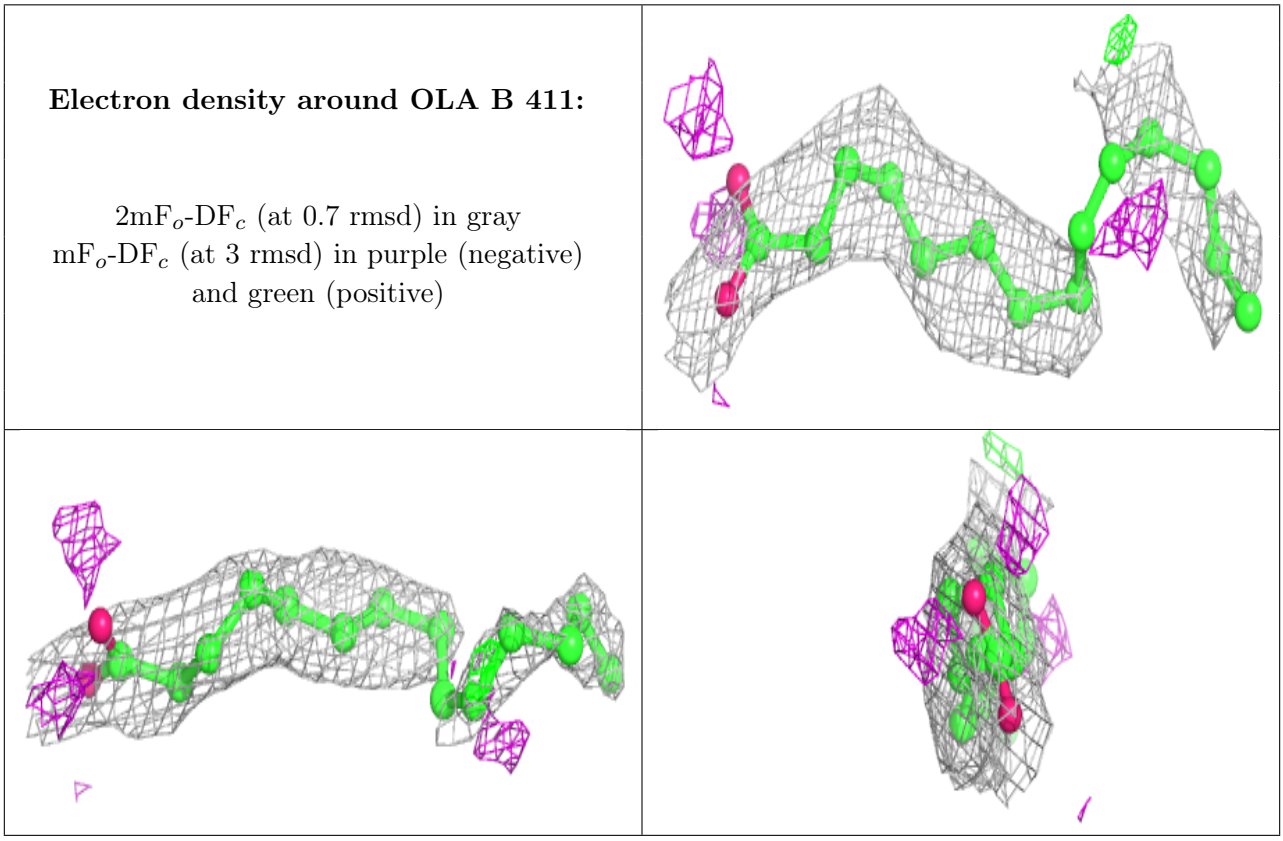
Electron density around OLA B 405:

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



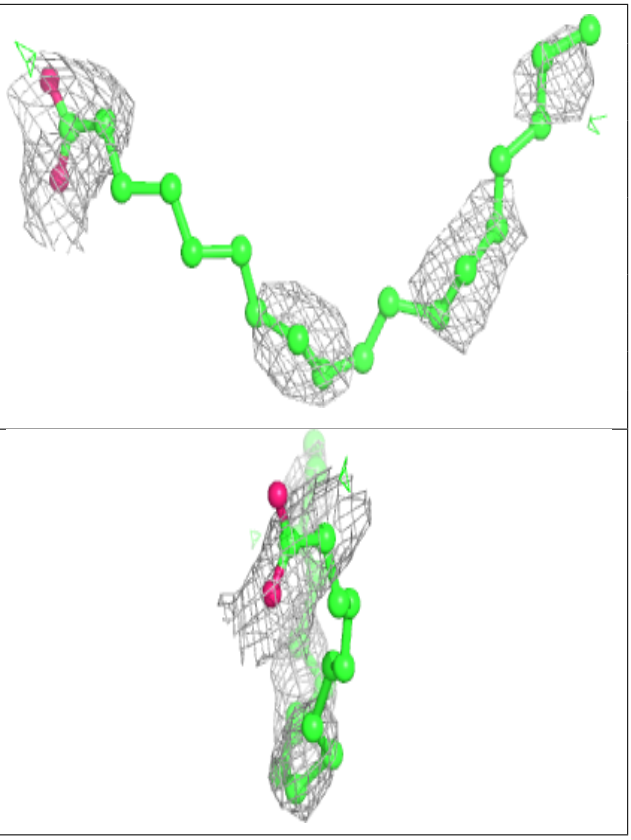
Electron density around OLA B 411:

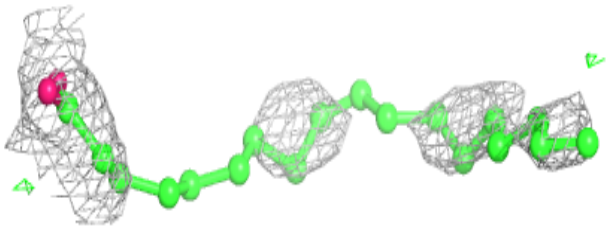
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLA B 414:

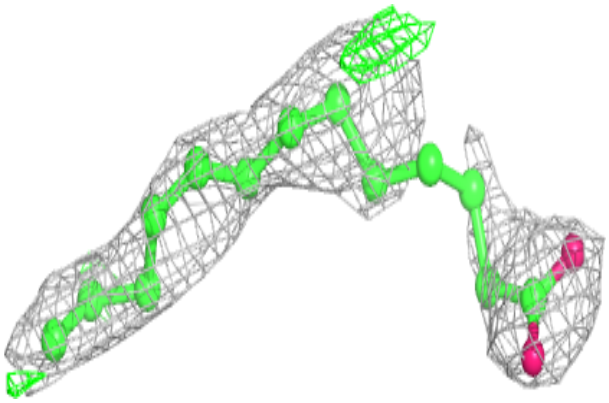
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

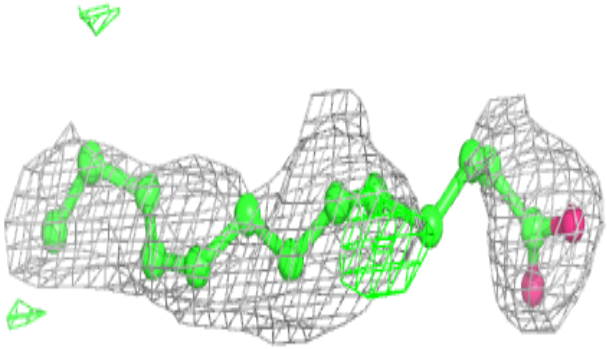


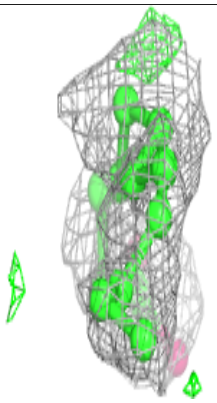


Electron density around OLA B 413:

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

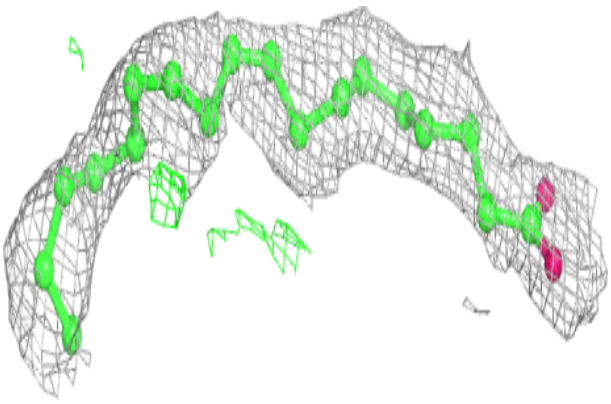


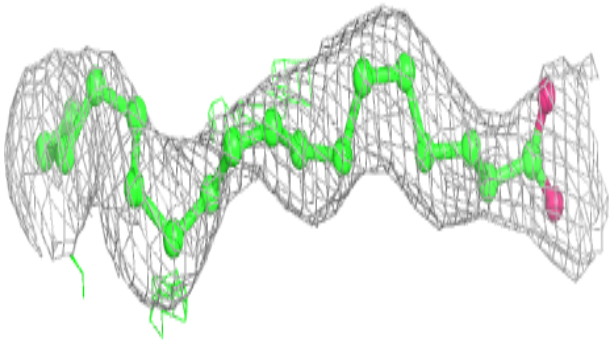


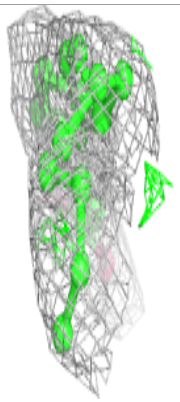


Electron density around OLA A 413:

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

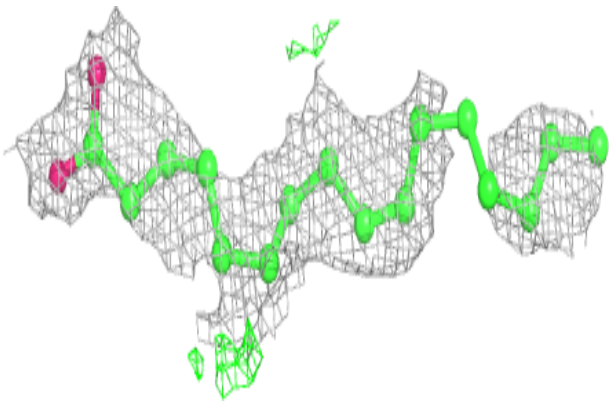


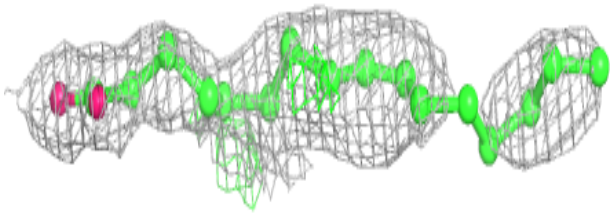


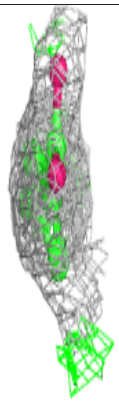


Electron density around OLA B 409:

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

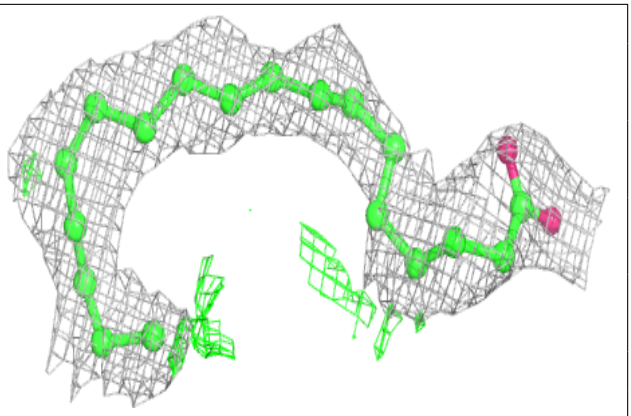


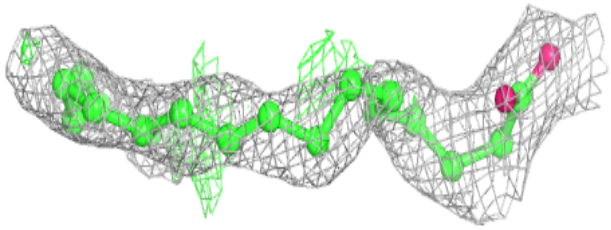


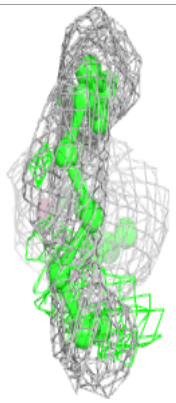


Electron density around OLA B 404:

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

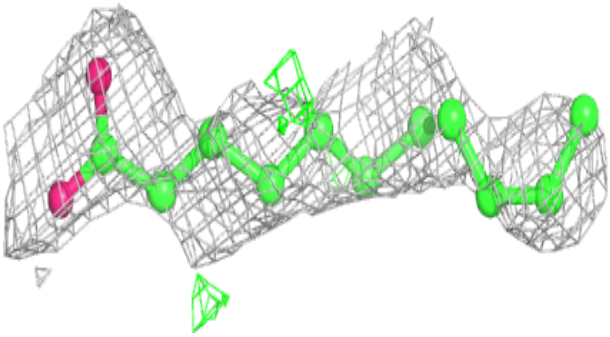


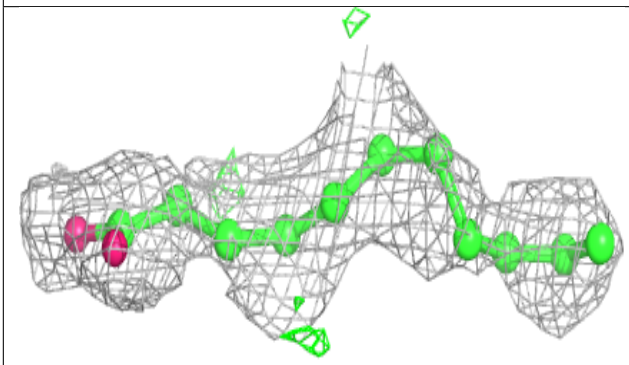


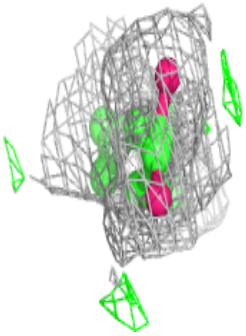


Electron density around OLA B 408:

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

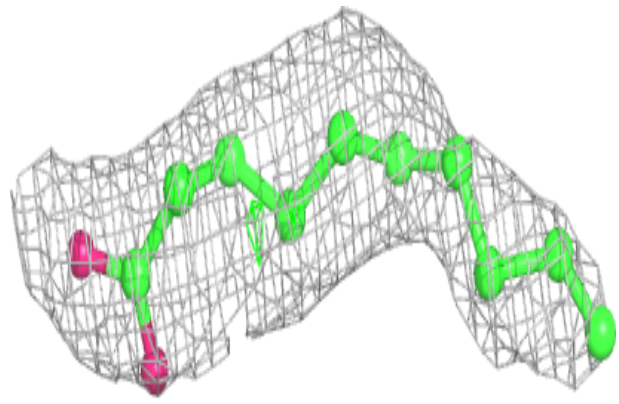


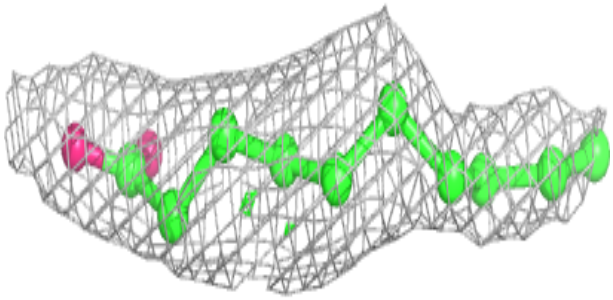


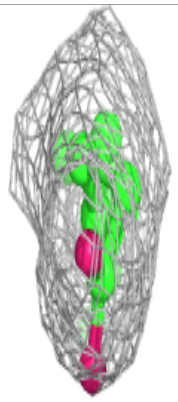


Electron density around OLA A 415:

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

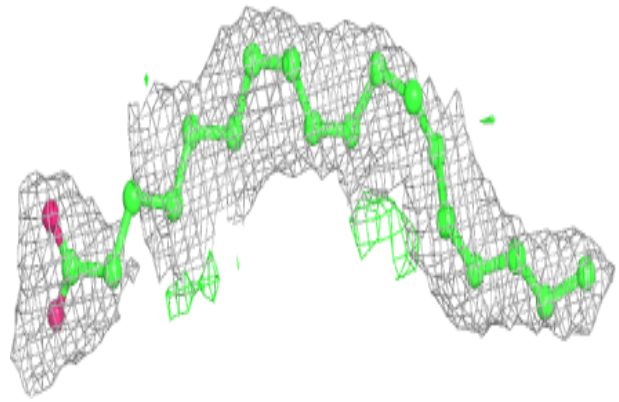


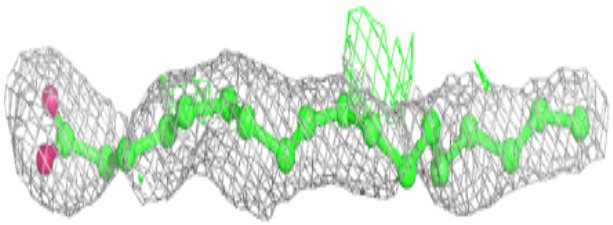


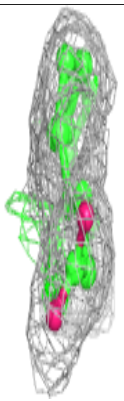


Electron density around OLA B 402:

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

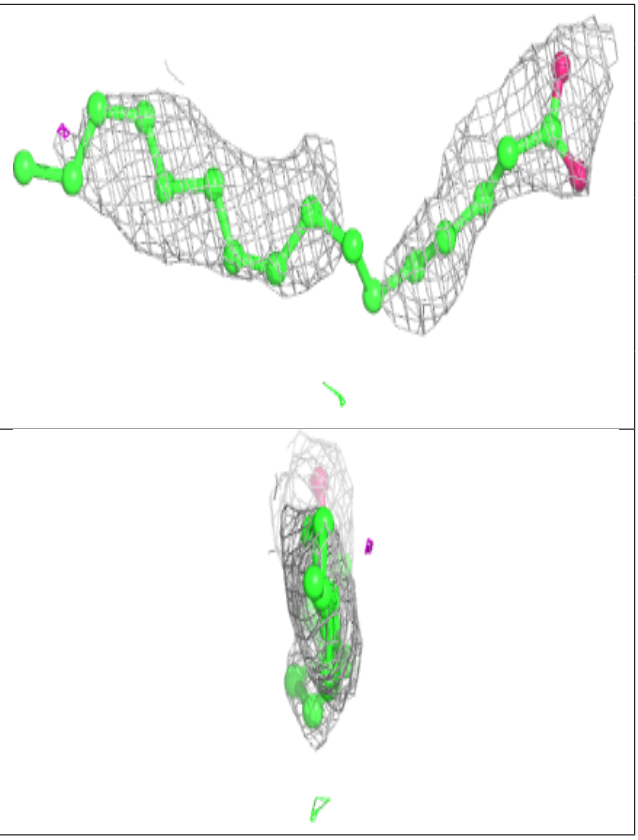






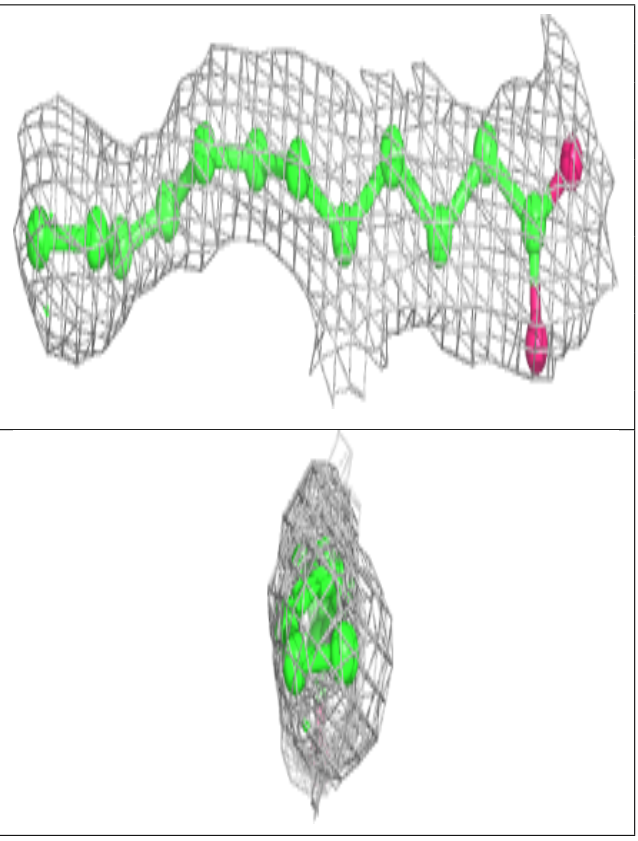
Electron density around OLA A 403:

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



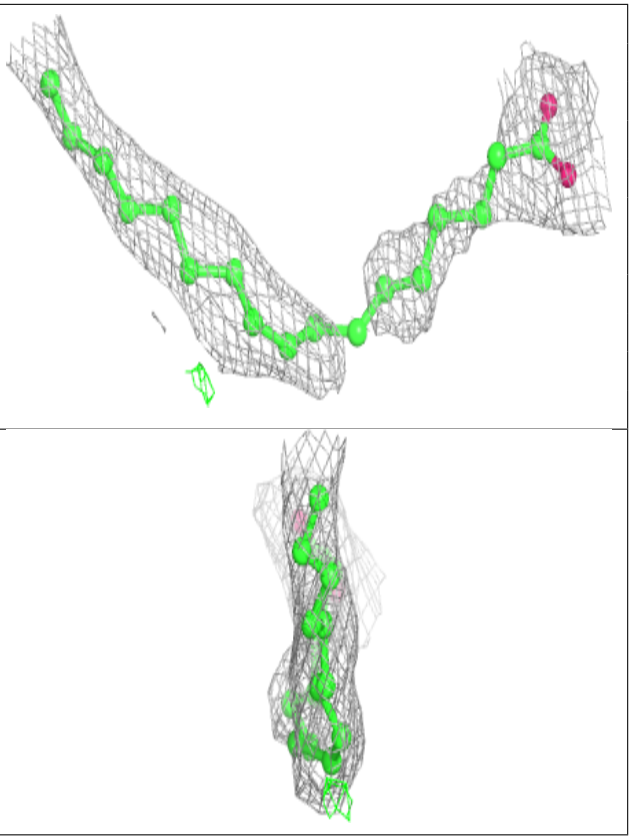
Electron density around OLA A 408:

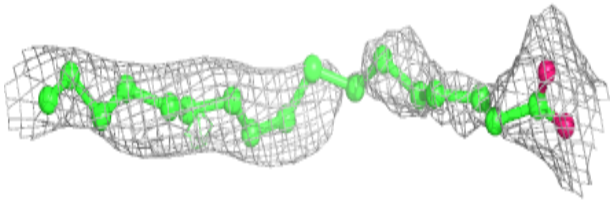
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLA A 410:

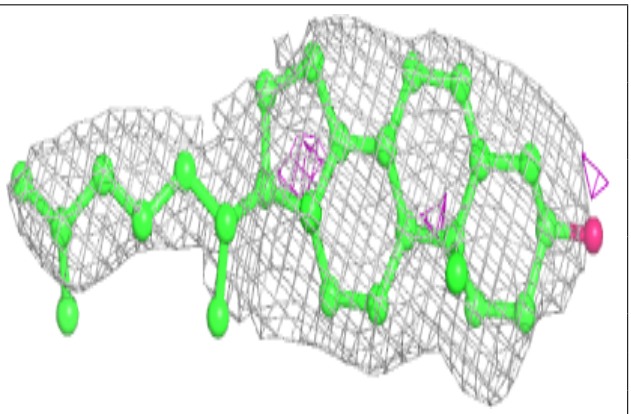
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

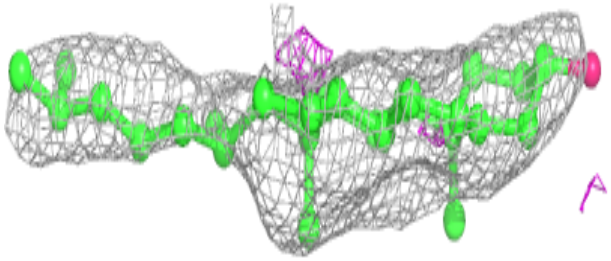


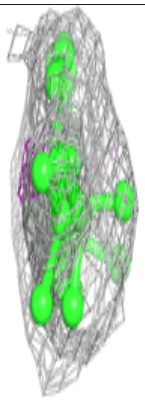


Electron density around CLR A 417:

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

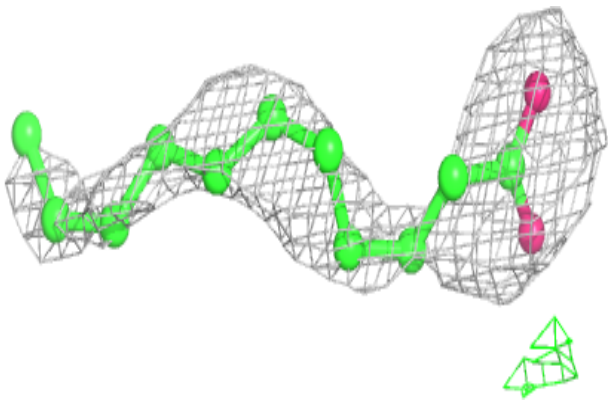


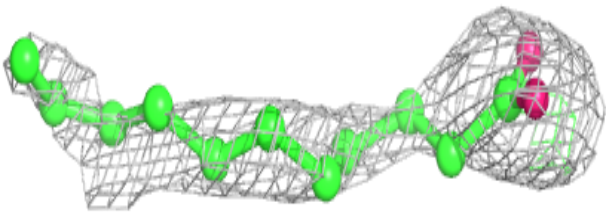


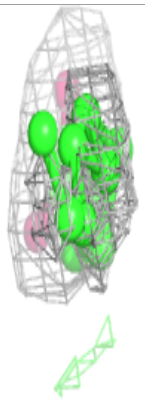


Electron density around OLA A 412:

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

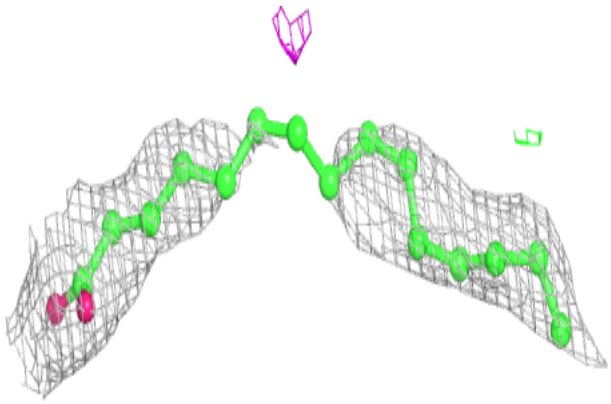


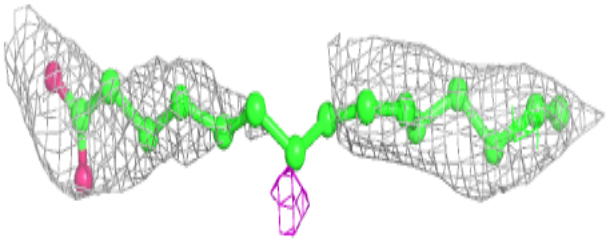


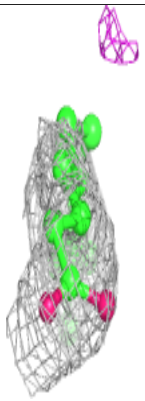


Electron density around OLA A 416:

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

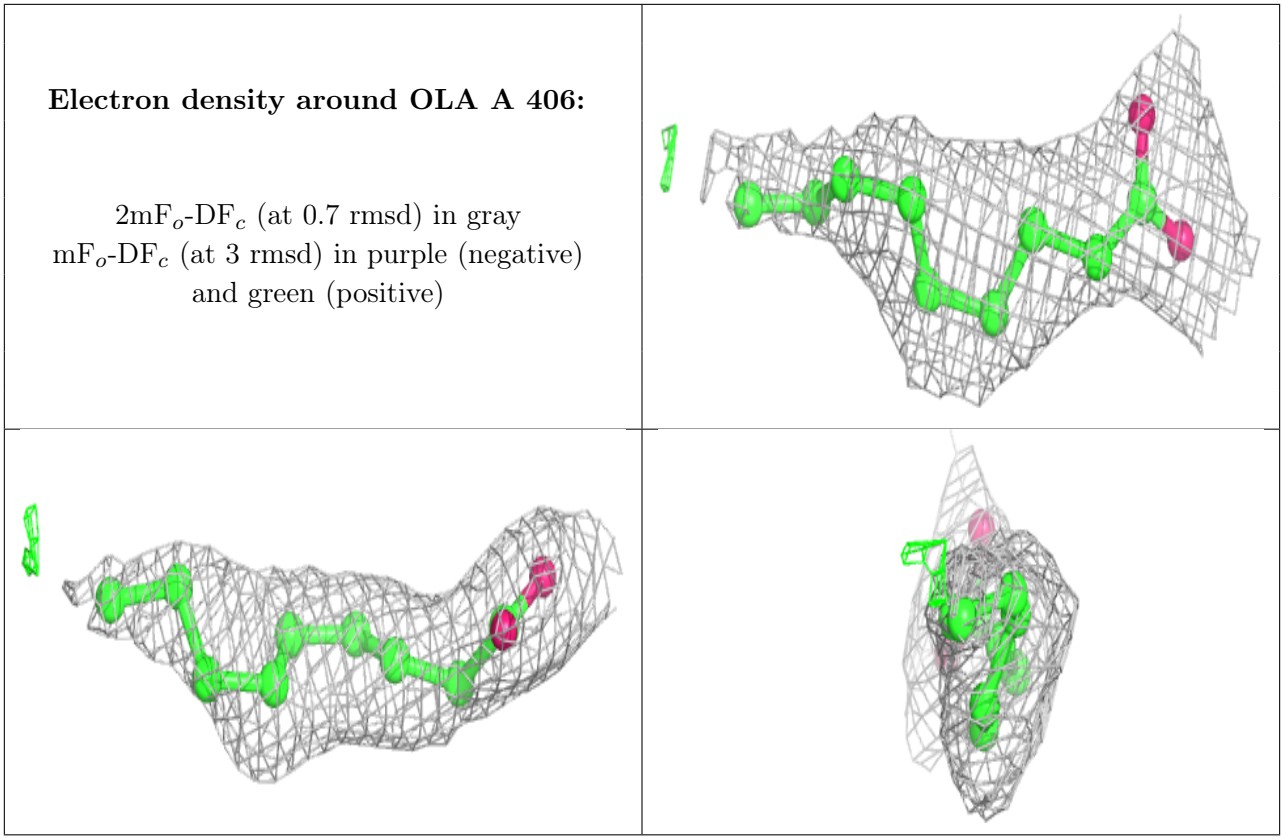






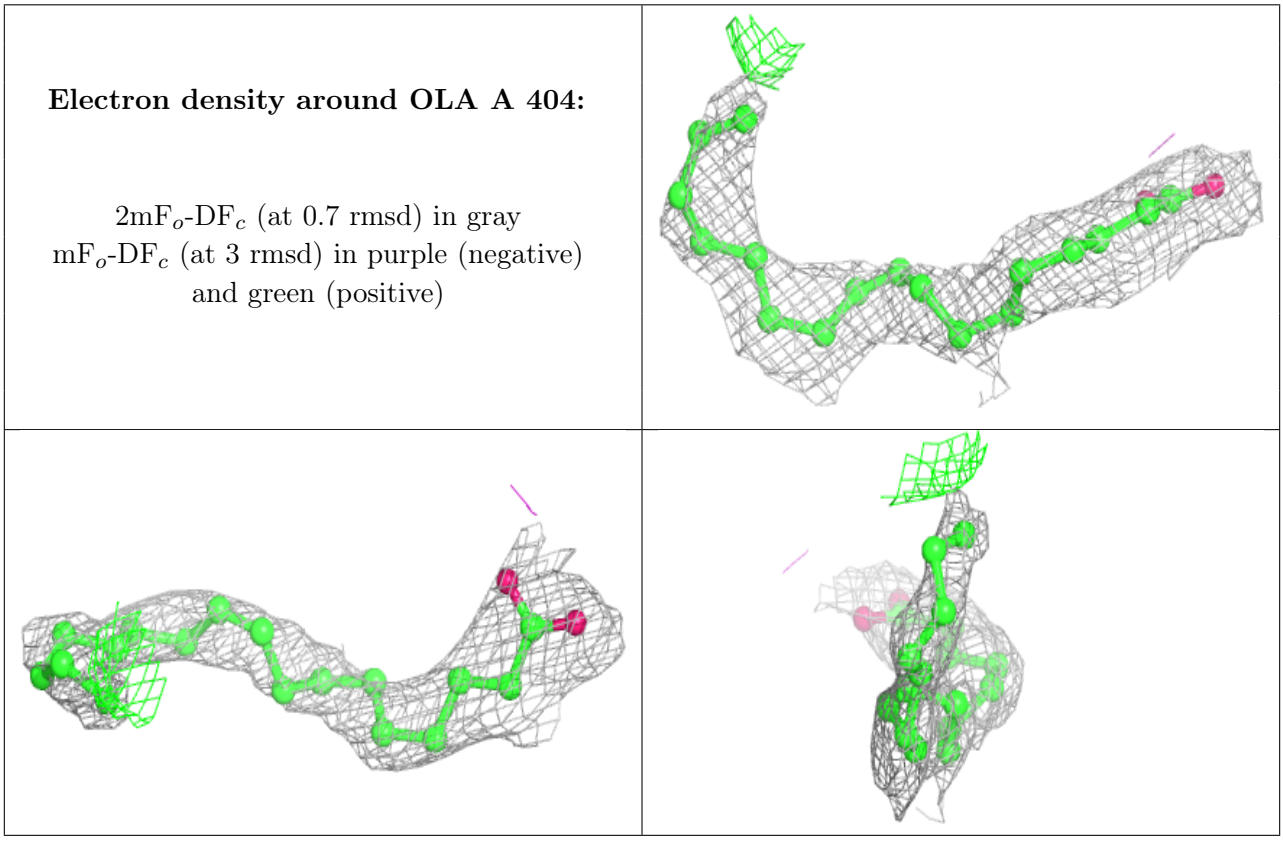
Electron density around OLA A 406:

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



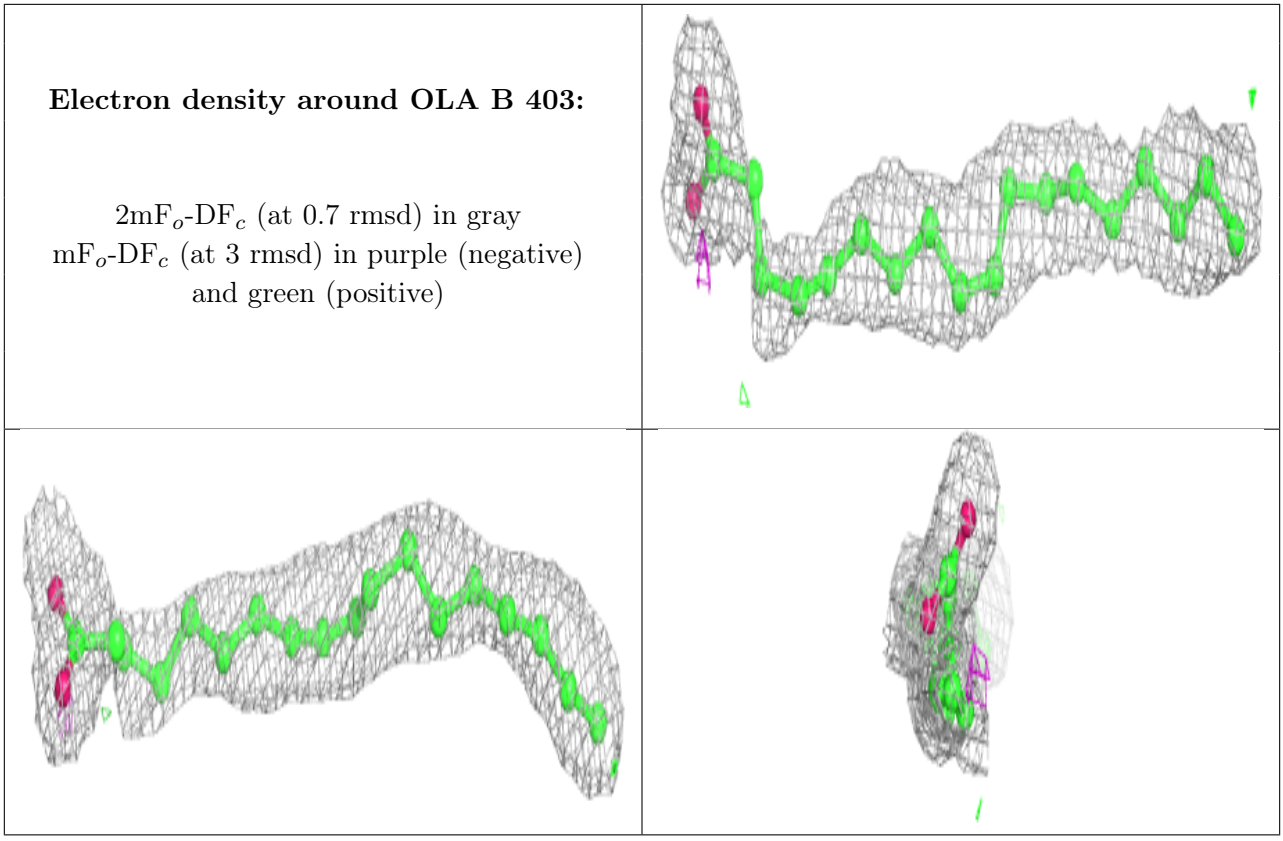
Electron density around OLA A 404:

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



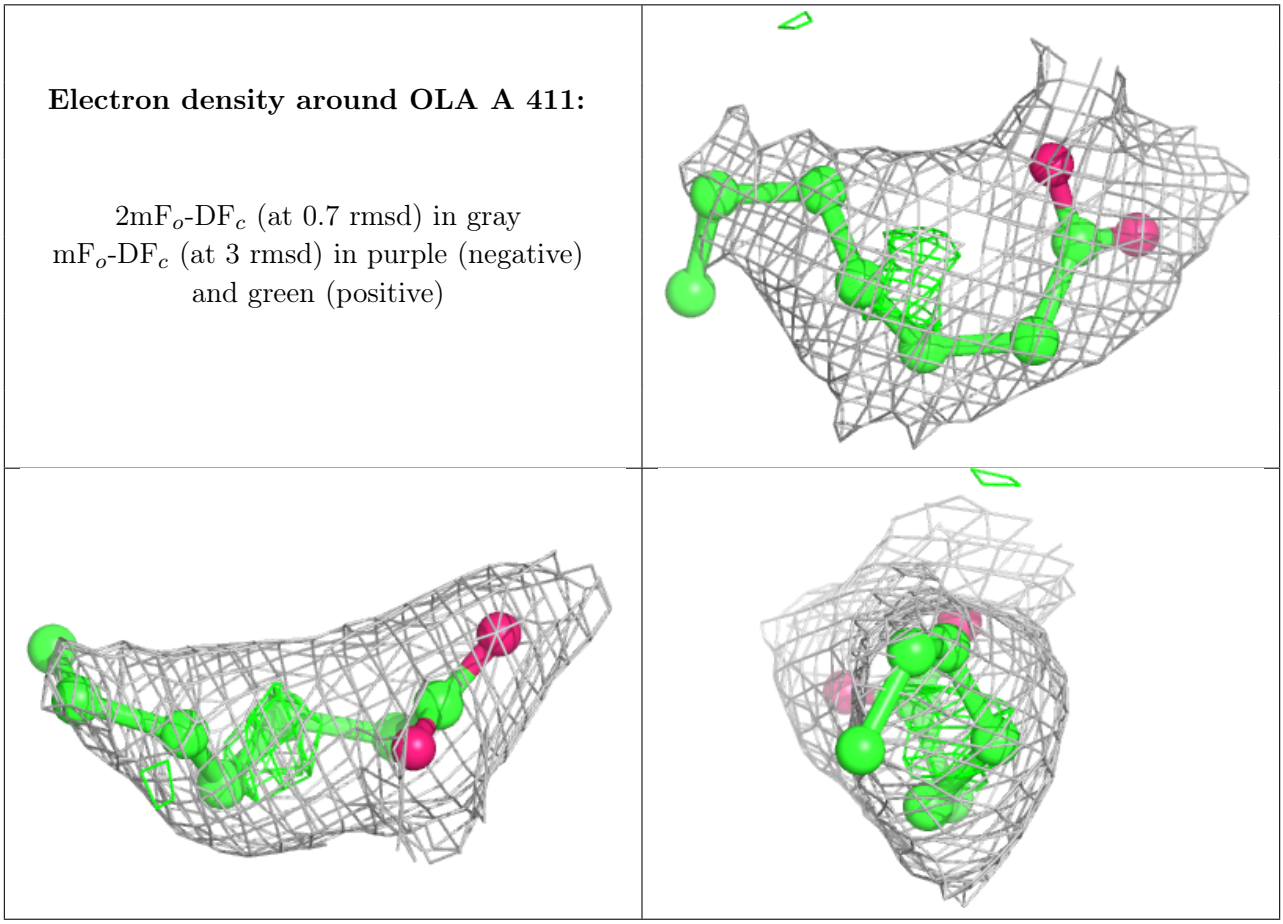
Electron density around OLA B 403:

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



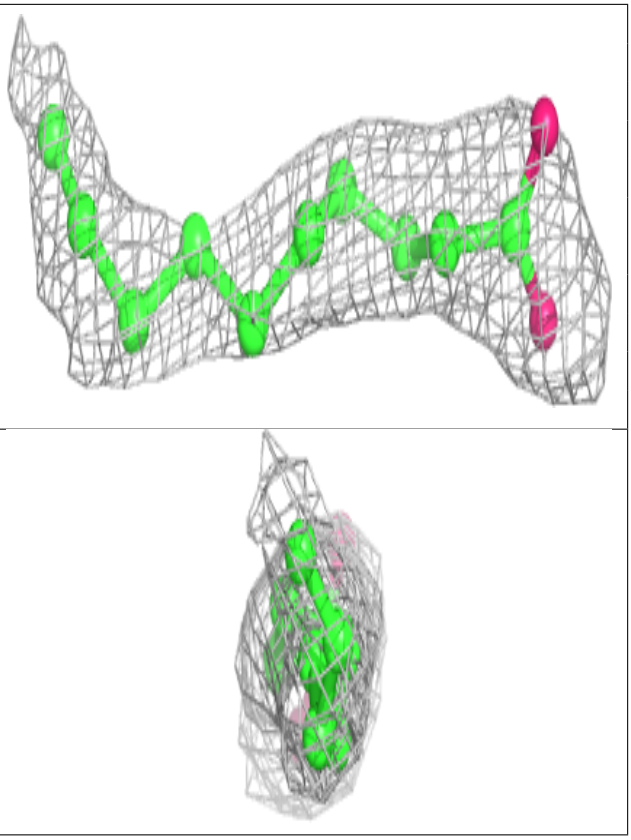
Electron density around OLA A 411:

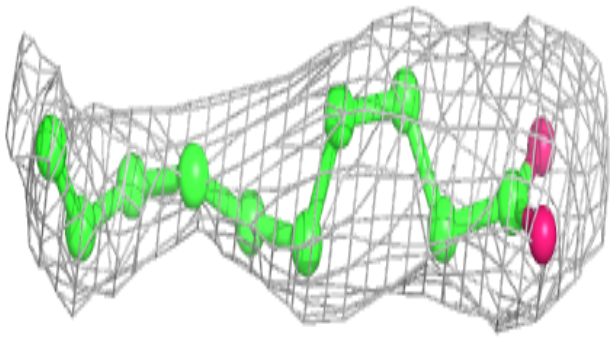
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLA B 410:

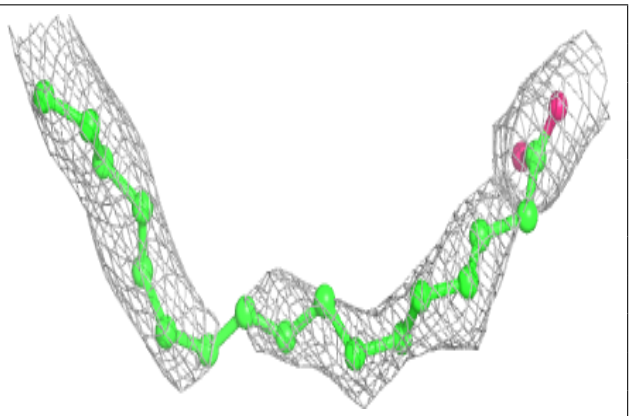
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

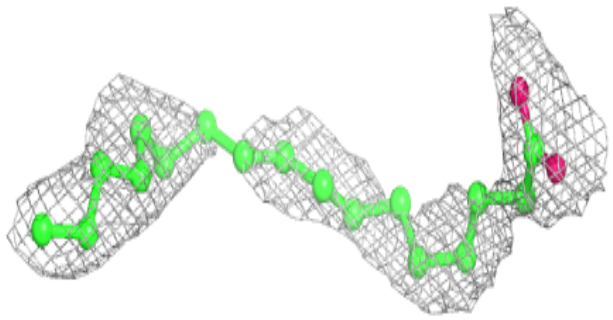


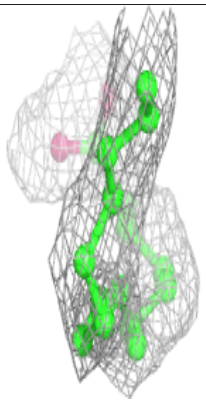


Electron density around OLA B 412:

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

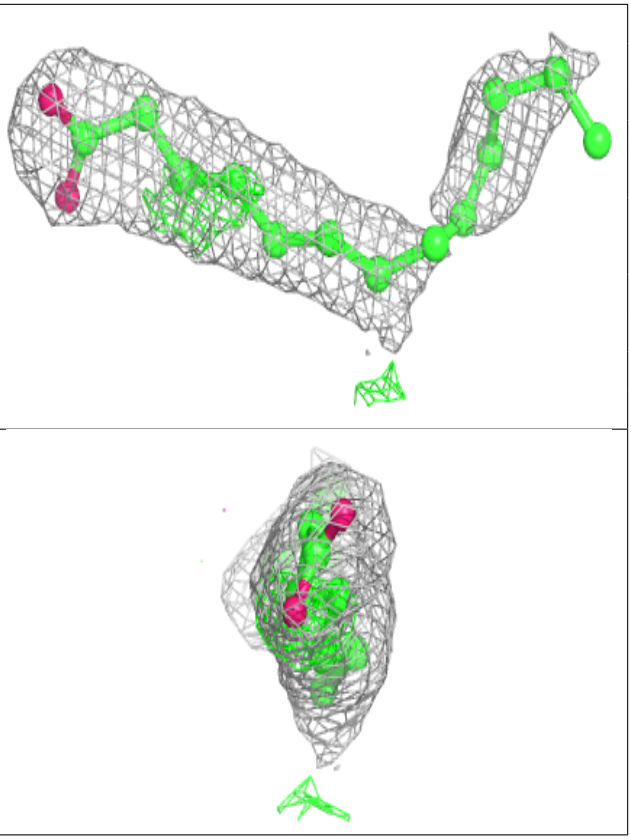


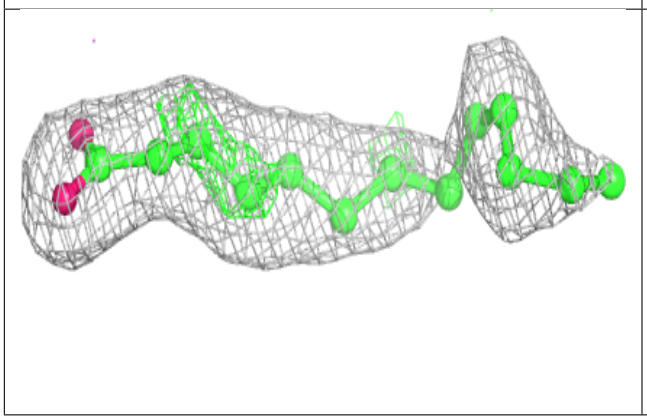




Electron density around OLA B 406:

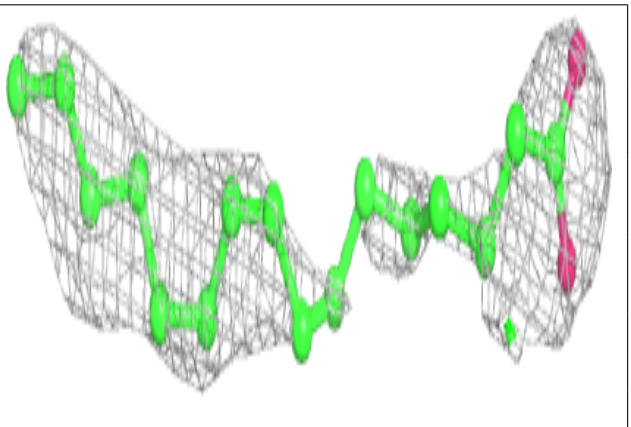
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

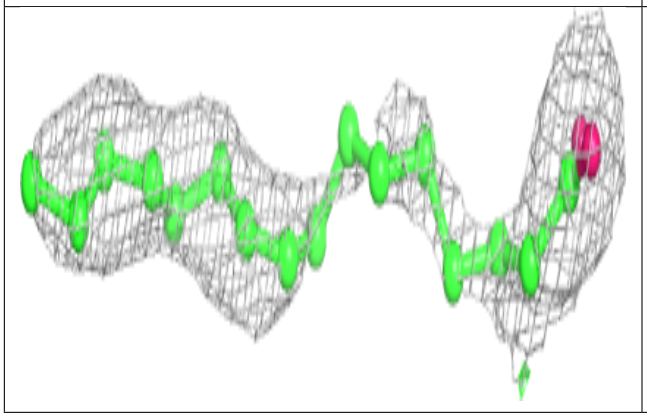


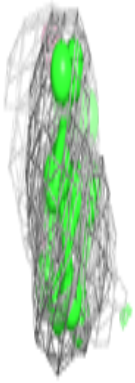


Electron density around OLA B 407:

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

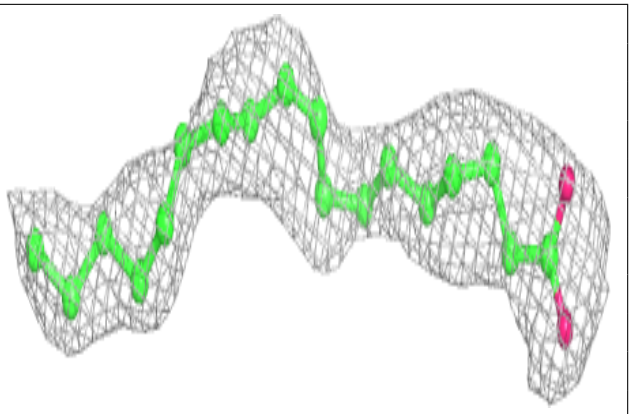


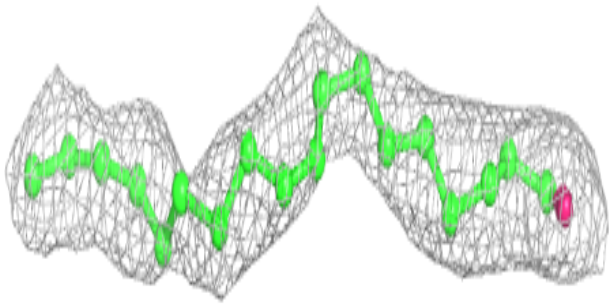


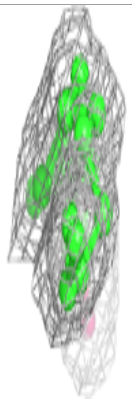


Electron density around OLA A 402:

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

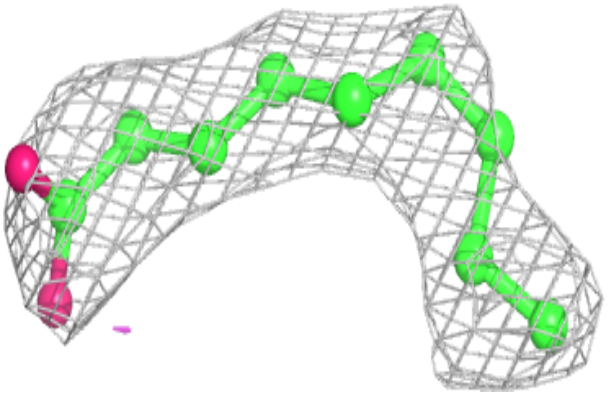


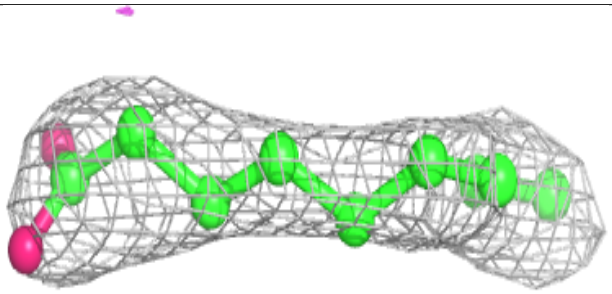


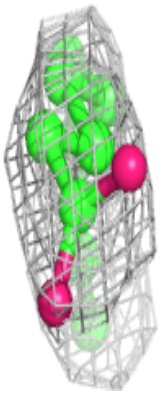


Electron density around OLA A 405:

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

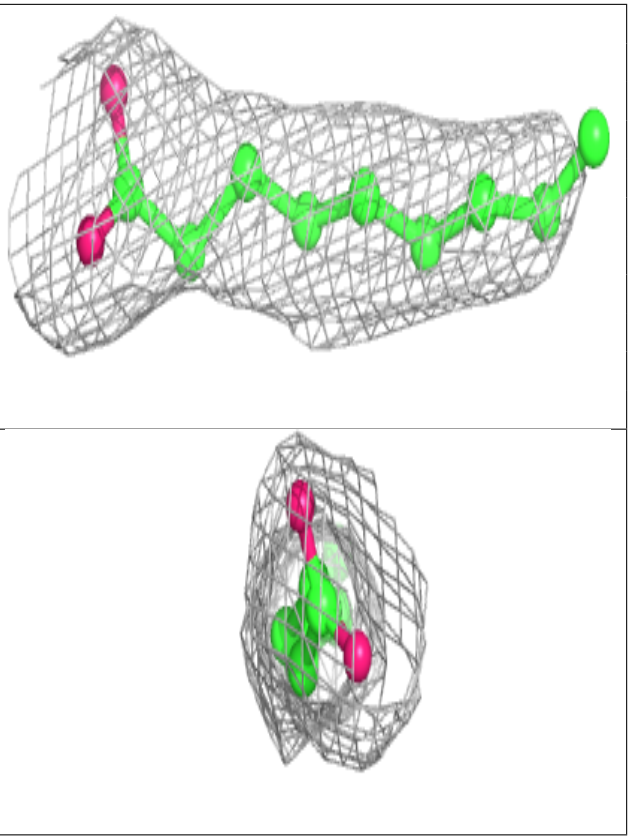






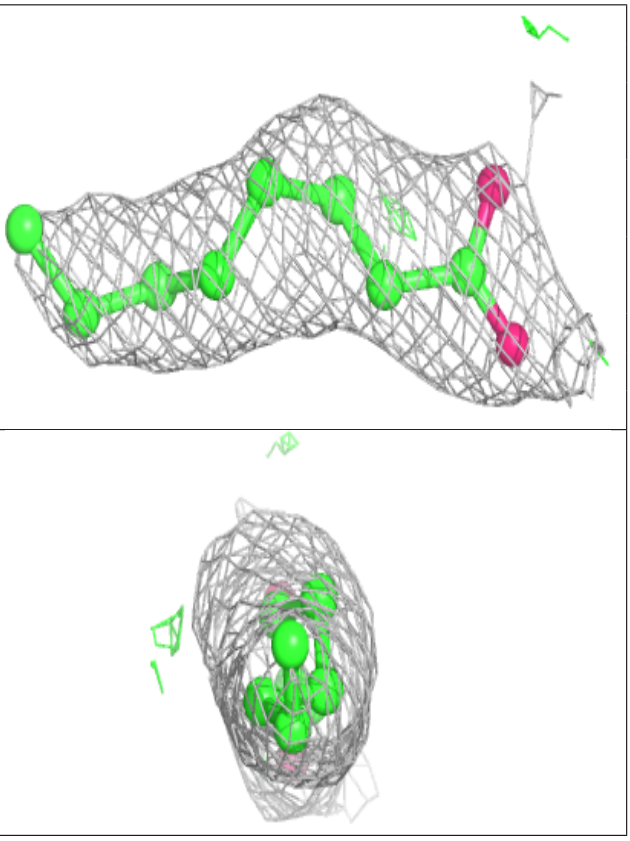
Electron density around OLA A 407:

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



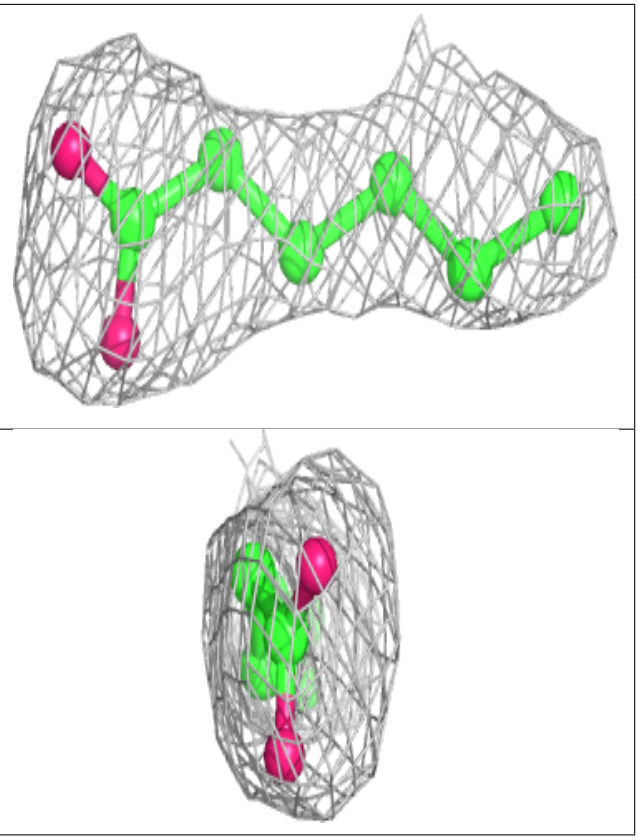
Electron density around OLA A 414:

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



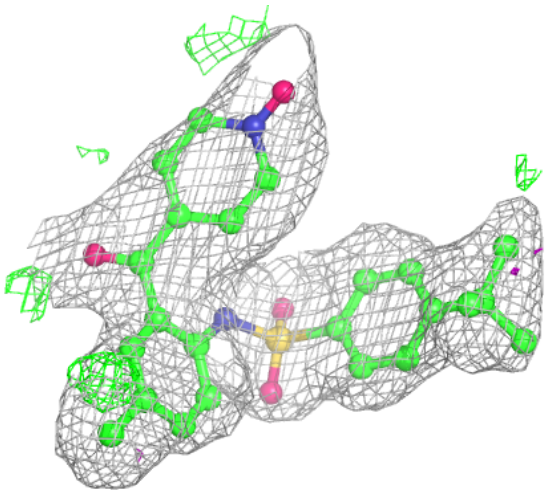
Electron density around OLA A 409:

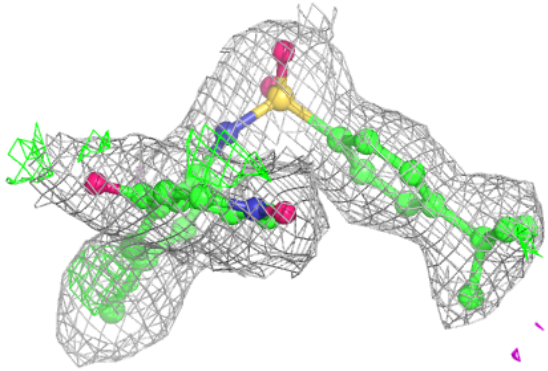
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

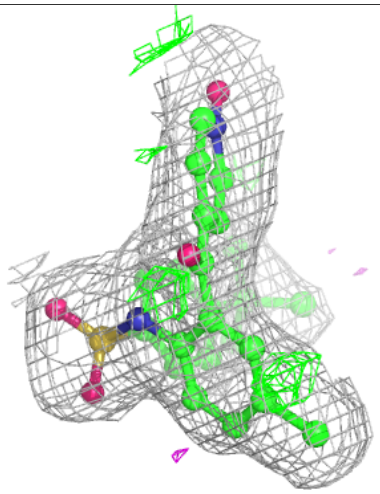


Electron density around 79K B 401:

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

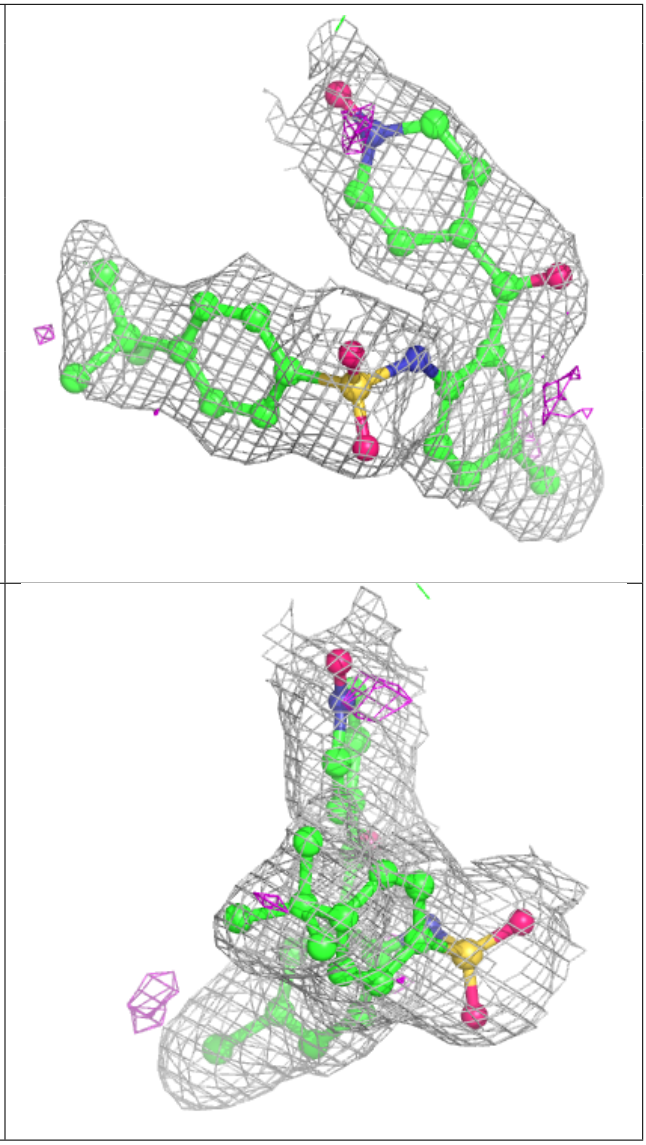






Electron density around 79K A 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.