Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 01:15 AM EDT

PDB ID	:	5O9H
Title	:	Crystal structure of thermostabilised human C5a anaphylatoxin chemotactic receptor 1 (C5aR) in complex with NDT9513727
Authors	:	Robertson, N.; Rappas, M.; Dore, A.S.; Brown, J.; Bottegoni, G.; Koglin, M.; Cansfield, J.; Jazayeri, A.; Cooke, R.M.; Marshall, F.H.
Deposited on	:	2017-06-19
Resolution	:	2.70 Å(reported)

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

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

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

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

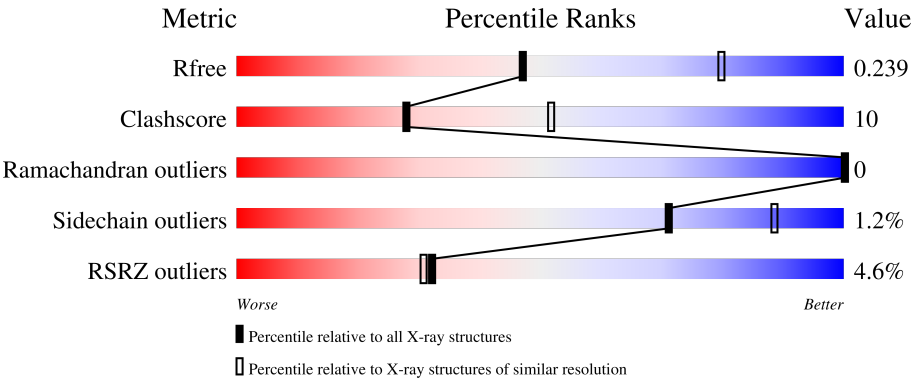
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	317	3% 74% 19% 7%
1	B	317	5% 79% 14% 7%

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	TLA	A	402	X	X	-	-
3	TLA	A	403	X	X	-	-
3	TLA	B	402	X	X	-	-
4	OLA	A	408	-	-	-	X
4	OLA	B	419	-	-	X	-
5	CIT	B	420	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5349 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 C5a anaphylatoxin chemotactic receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2324	1555	380	377	12			
1	B	295	Total	C	N	O	S	0	0	0
			2338	1562	383	381	12			

There are 50 discrepancies between the modelled and reference sequences:

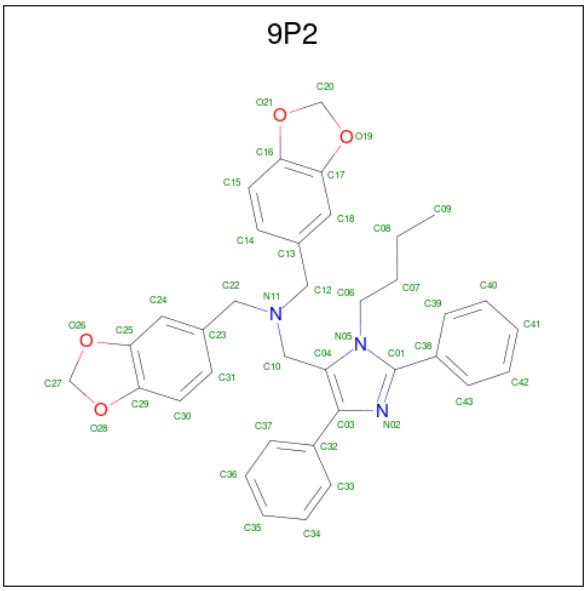
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP P21730
A	85	ALA	SER	engineered mutation	UNP P21730
A	91	ALA	ILE	engineered mutation	UNP P21730
A	142	ALA	ILE	engineered mutation	UNP P21730
A	146	ARG	ASN	engineered mutation	UNP P21730
A	156	LEU	ALA	engineered mutation	UNP P21730
A	172	ALA	PHE	engineered mutation	UNP P21730
A	232	ALA	ARG	engineered mutation	UNP P21730
A	234	GLU	ALA	engineered mutation	UNP P21730
A	311	GLU	LEU	engineered mutation	UNP P21730
A	317	GLU	SER	engineered mutation	UNP P21730
A	321	GLU	ASN	engineered mutation	UNP P21730
A	334	ALA	-	expression tag	UNP P21730
A	335	ALA	-	expression tag	UNP P21730
A	336	ALA	-	expression tag	UNP P21730
A	337	HIS	-	expression tag	UNP P21730
A	338	HIS	-	expression tag	UNP P21730
A	339	HIS	-	expression tag	UNP P21730
A	340	HIS	-	expression tag	UNP P21730
A	341	HIS	-	expression tag	UNP P21730
A	342	HIS	-	expression tag	UNP P21730
A	343	HIS	-	expression tag	UNP P21730
A	344	HIS	-	expression tag	UNP P21730
A	345	HIS	-	expression tag	UNP P21730
A	346	HIS	-	expression tag	UNP P21730

Continued on next page...

Continued from previous page...

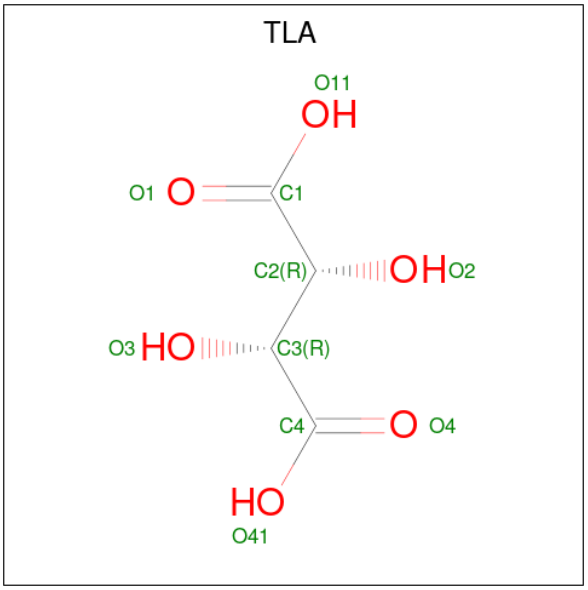
Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	initiating methionine	UNP P21730
B	85	ALA	SER	engineered mutation	UNP P21730
B	91	ALA	ILE	engineered mutation	UNP P21730
B	142	ALA	ILE	engineered mutation	UNP P21730
B	146	ARG	ASN	engineered mutation	UNP P21730
B	156	LEU	ALA	engineered mutation	UNP P21730
B	172	ALA	PHE	engineered mutation	UNP P21730
B	232	ALA	ARG	engineered mutation	UNP P21730
B	234	GLU	ALA	engineered mutation	UNP P21730
B	311	GLU	LEU	engineered mutation	UNP P21730
B	317	GLU	SER	engineered mutation	UNP P21730
B	321	GLU	ASN	engineered mutation	UNP P21730
B	334	ALA	-	expression tag	UNP P21730
B	335	ALA	-	expression tag	UNP P21730
B	336	ALA	-	expression tag	UNP P21730
B	337	HIS	-	expression tag	UNP P21730
B	338	HIS	-	expression tag	UNP P21730
B	339	HIS	-	expression tag	UNP P21730
B	340	HIS	-	expression tag	UNP P21730
B	341	HIS	-	expression tag	UNP P21730
B	342	HIS	-	expression tag	UNP P21730
B	343	HIS	-	expression tag	UNP P21730
B	344	HIS	-	expression tag	UNP P21730
B	345	HIS	-	expression tag	UNP P21730
B	346	HIS	-	expression tag	UNP P21730

- Molecule 2 is 1-(1,3-benzodioxol-5-yl)- {N}-(1,3-benzodioxol-5-ylmethyl)- {N}-[(3-butyl-2,5-diphenyl-imidazol-4-yl)methyl]methanamine (three-letter code: 9P2) (formula: $C_{36}H_{35}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	36	3	4		
2	B	1	Total	C	N	O	0	0
			43	36	3	4		

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



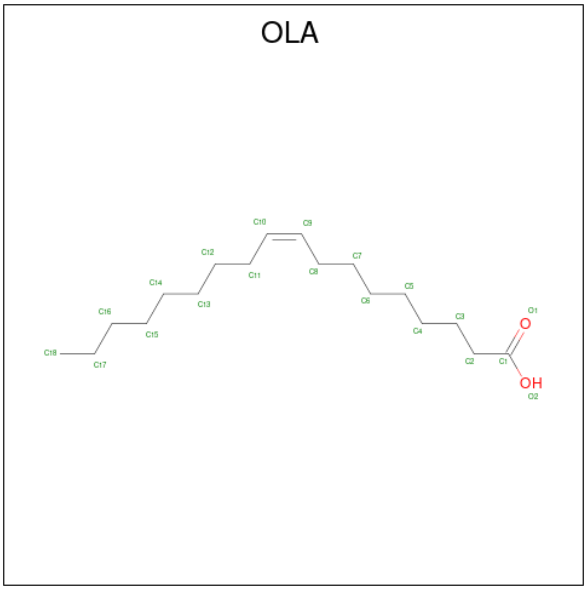
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	A	1	Total	C	O	0	0
			10	4	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 10 4 6	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 17 15 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C 15 15	0	0
4	A	1	Total C O 14 12 2	0	0
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C O 18 16 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C 13 13	0	0

Continued on next page...

Continued from previous page...

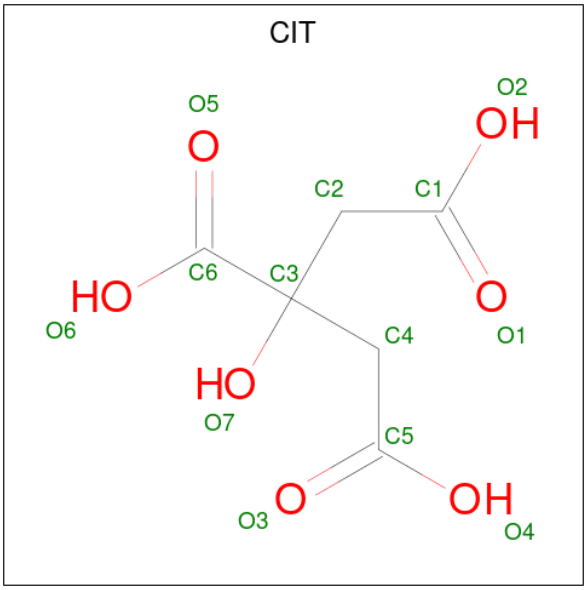
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C 15 15	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 11 9 2	0	0
4	B	1	Total C O 13 11 2	0	0
4	B	1	Total C O 10 8 2	0	0
4	B	1	Total C O 15 13 2	0	0
4	B	1	Total C O 14 12 2	0	0
4	B	1	Total C O 13 11 2	0	0
4	B	1	Total C O 7 5 2	0	0
4	B	1	Total C O 16 14 2	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 14 12 2	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 14 12 2	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 16 14 2	0	0
4	B	1	Total C O 15 13 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 14 14	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 13 6 7	0	0

- Molecule 6 is water.

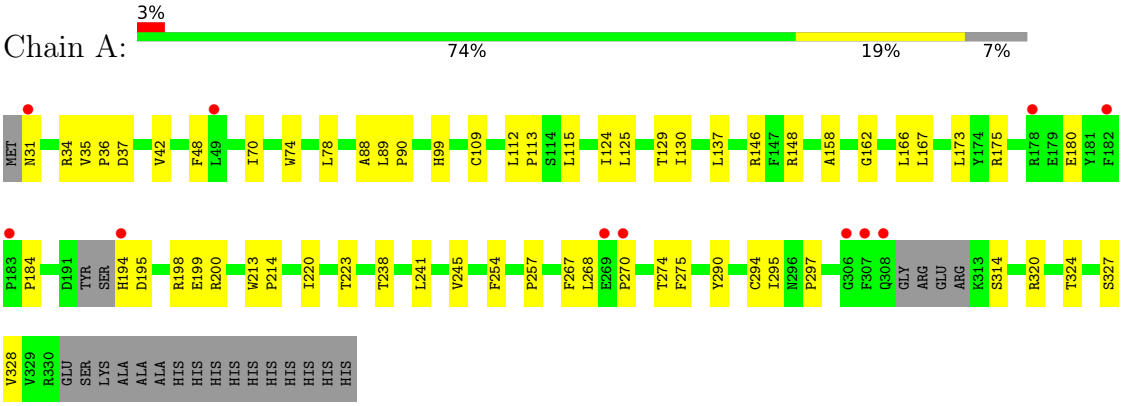
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	39	Total O 39 39	0	0
6	B	32	Total O 32 32	0	0

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.

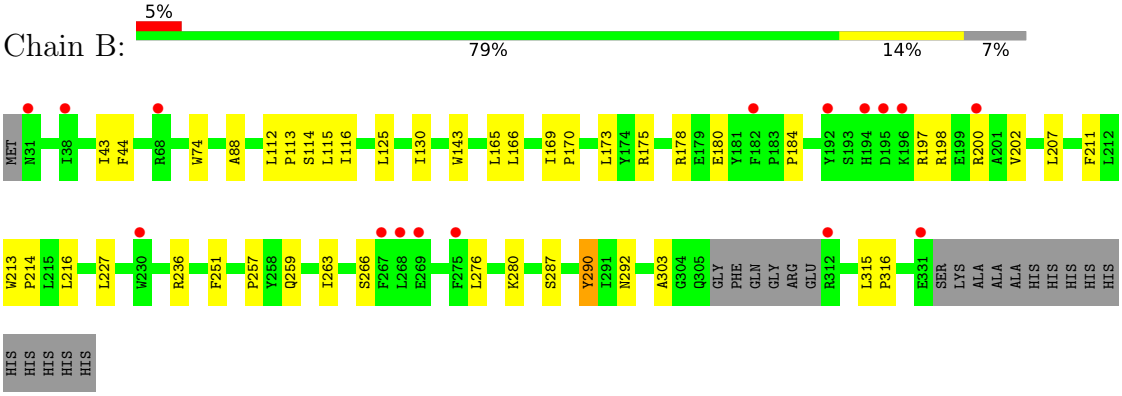
• Molecule 1: C5a anaphylatoxin chemotactic receptor 1

Chain A:



• Molecule 1: C5a anaphylatoxin chemotactic receptor 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.09Å 51.10Å 118.94Å 90.00° 106.73° 90.00°	Depositor
Resolution (Å)	19.89 – 2.70 34.59 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.89-2.70) 99.2 (34.59-2.70)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.238 0.211 , 0.239	Depositor DCC
R_{free} test set	1357 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 74.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5349	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TLA, CIT, OLA, 9P2

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	0.27	0/2384	0.44	0/3257
1	B	0.26	0/2399	0.44	0/3279
All	All	0.27	0/4783	0.44	0/6536

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2324	0	2442	46	0
1	B	2338	0	2456	33	1
2	A	43	0	0	0	0
2	B	43	0	0	1	0
3	A	20	0	4	2	1
3	B	10	0	2	0	0
4	A	237	0	361	28	0
4	B	250	0	362	32	0
5	B	13	0	5	0	0
6	A	39	0	0	1	0
6	B	32	0	0	1	0
All	All	5349	0	5632	108	1

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 10.

All (108) 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:A:166:LEU:HG	4:B:419:OLA:H10	1.55	0.87
4:A:405:OLA:H71	4:A:406:OLA:H52	1.59	0.85
4:B:410:OLA:H10	4:B:417:OLA:H41	1.61	0.83
1:B:251:PHE:HA	1:B:292:ASN:HD21	1.45	0.81
1:A:162:GLY:HA3	4:A:416:OLA:H152	1.66	0.79
4:A:405:OLA:H52	4:A:406:OLA:H51	1.64	0.78
4:A:412:OLA:H10	4:A:417:OLA:H162	1.71	0.72
1:A:70:ILE:HB	1:A:148:ARG:HH21	1.56	0.69
4:A:405:OLA:H182	4:A:406:OLA:H131	1.74	0.68
1:B:114:SER:OG	1:B:175:ARG:NH2	2.28	0.66
1:A:70:ILE:N	3:A:402:TLA:O4	2.26	0.65
1:B:88:ALA:HB2	1:B:115:LEU:HD12	1.78	0.65
4:A:416:OLA:H9	4:B:406:OLA:H42	1.79	0.65
4:A:405:OLA:H71	4:A:406:OLA:C5	2.27	0.64
1:A:31:ASN:O	1:A:99:HIS:NE2	2.29	0.64
1:A:173:LEU:HD13	1:B:198:ARG:HG2	1.81	0.63
1:A:137:LEU:HD21	1:A:148:ARG:HH11	1.65	0.61
1:A:254:PHE:HE2	1:A:295:ILE:HD12	1.66	0.60
1:A:295:ILE:HD11	4:A:413:OLA:H141	1.82	0.60
1:B:303:ALA:HB2	4:B:416:OLA:H21	1.83	0.60
1:A:146:ARG:HH21	1:B:143:TRP:HE1	1.51	0.59
1:A:167:LEU:HD23	4:B:419:OLA:H142	1.84	0.58
1:A:158:ALA:HB1	4:A:416:OLA:H112	1.85	0.57
1:A:166:LEU:CG	4:B:419:OLA:H10	2.32	0.57
1:B:170:PRO:HD3	4:B:419:OLA:H152	1.87	0.56
1:B:211:PHE:HB2	1:B:259:GLN:HE21	1.71	0.55
1:A:320:ARG:O	1:A:324:THR:OG1	2.18	0.55
1:B:178:ARG:NH1	1:B:180:GLU:OE2	2.40	0.54
4:B:410:OLA:C10	4:B:417:OLA:H41	2.33	0.54
1:A:88:ALA:HB2	1:A:115:LEU:HD12	1.90	0.54
1:A:245:VAL:HG13	4:A:417:OLA:H181	1.89	0.53
1:A:137:LEU:HD11	1:A:148:ARG:NH1	2.23	0.53
1:B:276:LEU:HG	1:B:280:LYS:HE2	1.91	0.53
1:B:180:GLU:O	1:B:184:PRO:HA	2.11	0.51
4:B:415:OLA:H162	4:B:416:OLA:H161	1.93	0.51
1:A:220:ILE:HG12	4:A:411:OLA:H141	1.92	0.50
4:B:415:OLA:C16	4:B:416:OLA:H161	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:403:OLA:H72	4:B:403:OLA:H31	1.92	0.50
1:B:216:LEU:HD13	4:B:412:OLA:H172	1.95	0.49
1:B:170:PRO:HD3	4:B:419:OLA:H132	1.95	0.49
4:B:409:OLA:H42	4:B:409:OLA:H81	1.94	0.48
1:A:254:PHE:CE2	1:A:295:ILE:HD12	2.45	0.48
1:B:165:LEU:O	1:B:169:ILE:HG13	2.14	0.48
1:A:194:HIS:CG	1:A:195:ASP:H	2.32	0.48
1:B:169:ILE:HA	4:B:409:OLA:H9	1.96	0.48
4:B:411:OLA:H72	4:B:411:OLA:C11	2.44	0.47
1:A:148:ARG:NH1	1:A:327:SER:HB2	2.29	0.47
4:A:406:OLA:H61	4:B:405:OLA:H22	1.95	0.47
4:A:405:OLA:H122	4:A:406:OLA:H171	1.96	0.47
1:B:74:TRP:CG	1:B:130:ILE:HG12	2.48	0.47
1:A:48:PHE:HB2	1:A:89:LEU:HD23	1.96	0.47
1:A:213:TRP:HB3	1:A:214:PRO:HD3	1.97	0.46
1:A:270:PRO:HA	1:A:275:PHE:CD1	2.50	0.46
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.97	0.46
4:A:410:OLA:H9	4:A:410:OLA:H61	1.67	0.46
4:A:405:OLA:H122	4:A:406:OLA:C17	2.45	0.46
1:B:112:LEU:HB2	1:B:113:PRO:HD3	1.96	0.46
1:A:328:VAL:N	3:A:402:TLA:O3	2.46	0.46
4:A:413:OLA:H10	4:A:413:OLA:H131	1.77	0.46
4:A:416:OLA:H9	4:B:406:OLA:H62	1.98	0.45
4:B:409:OLA:H111	4:B:409:OLA:H82	1.69	0.45
1:A:173:LEU:HD22	1:B:197:ARG:HD3	1.98	0.45
4:A:405:OLA:H82	4:A:405:OLA:H112	1.77	0.45
1:B:227:LEU:HD23	4:B:413:OLA:H21	1.98	0.45
1:B:166:LEU:O	4:B:419:OLA:H131	2.18	0.45
4:B:410:OLA:H9	4:B:417:OLA:C2	2.47	0.45
1:B:213:TRP:CZ3	4:B:406:OLA:H71	2.53	0.44
1:B:251:PHE:HA	1:B:292:ASN:ND2	2.23	0.44
1:A:109:CYS:O	1:A:175:ARG:HG2	2.17	0.44
4:A:408:OLA:H111	4:A:408:OLA:H82	1.76	0.44
1:A:238:THR:HG23	1:A:241:LEU:H	1.83	0.44
1:A:42:VAL:HG22	4:A:409:OLA:H10	2.00	0.43
1:A:167:LEU:HD23	4:B:419:OLA:C14	2.49	0.43
1:A:194:HIS:CE1	1:A:199:GLU:HB2	2.53	0.43
1:B:125:LEU:HD21	2:B:401:9P2:C15	2.47	0.43
4:B:410:OLA:H82	4:B:410:OLA:H111	1.71	0.43
1:B:202:VAL:HG22	4:B:419:OLA:H72	1.99	0.43
1:A:74:TRP:CG	1:A:130:ILE:HG12	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:CD2	4:B:419:OLA:H142	2.48	0.43
4:A:404:OLA:H52	4:A:404:OLA:H82	1.25	0.43
4:A:413:OLA:H111	4:A:413:OLA:H82	1.65	0.43
1:B:200:ARG:HG2	1:B:266:SER:HB3	1.99	0.43
4:B:405:OLA:H112	4:B:405:OLA:H82	1.80	0.43
1:A:257:PRO:HG2	6:A:504:HOH:O	2.18	0.42
1:B:315:LEU:HB3	1:B:316:PRO:HD3	2.01	0.42
1:A:223:THR:HA	4:A:412:OLA:H71	2.00	0.42
4:B:416:OLA:H10	4:B:416:OLA:H132	1.68	0.42
1:B:116:ILE:HD12	1:B:290:TYR:CD2	2.54	0.42
1:B:170:PRO:HG3	4:B:419:OLA:H111	2.01	0.42
1:A:200:ARG:HE	1:A:267:PHE:HA	1.85	0.41
1:A:90:PRO:HB3	4:A:408:OLA:H112	2.02	0.41
1:A:198:ARG:NH1	1:B:173:LEU:O	2.54	0.41
1:A:124:ILE:HD12	1:A:124:ILE:HA	1.90	0.41
1:A:294:CYS:O	1:A:297:PRO:HD2	2.19	0.41
1:B:43:ILE:HB	1:B:287:SER:OG	2.20	0.41
1:B:257:PRO:HG2	6:B:504:HOH:O	2.20	0.41
1:A:35:VAL:HB	1:A:36:PRO:HD3	2.02	0.41
1:A:34:ARG:HB3	1:A:36:PRO:HD2	2.01	0.41
1:A:268:LEU:HD13	1:A:274:THR:HG23	2.03	0.41
4:A:409:OLA:H111	4:A:409:OLA:H82	1.82	0.41
4:A:416:OLA:H142	4:B:406:OLA:C12	2.50	0.41
1:A:180:GLU:O	1:A:184:PRO:HA	2.21	0.41
1:B:213:TRP:HB3	1:B:214:PRO:HD3	2.02	0.41
1:B:207:LEU:HD22	1:B:263:ILE:HD13	2.03	0.40
4:A:417:OLA:H171	4:A:417:OLA:H142	1.67	0.40
4:A:410:OLA:H82	4:A:410:OLA:H111	1.74	0.40
1:A:125:LEU:O	1:A:129:THR:HG23	2.21	0.40
4:B:418:OLA:H81	4:B:418:OLA:H111	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:NH1	3:A:403:TLA:O11[2_856]	2.19	0.01

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	288/317 (91%)	284 (99%)	4 (1%)	0	100	100
1	B	291/317 (92%)	287 (99%)	4 (1%)	0	100	100
All	All	579/634 (91%)	571 (99%)	8 (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	252/271 (93%)	248 (98%)	4 (2%)	62	85
1	B	254/271 (94%)	252 (99%)	2 (1%)	81	93
All	All	506/542 (93%)	500 (99%)	6 (1%)	71	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	78	LEU
1	A	290	TYR
1	A	314	SER
1	B	44	PHE
1	B	290	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	B	292	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

38 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	$\#\|Z\| > 2$
4	OLA	B	403	-	12,12,19	0.60	0	12,12,19	1.14	0
4	OLA	A	410	-	9,9,19	0.27	0	8,8,19	0.64	0
4	OLA	B	416	-	19,19,19	0.52	0	19,19,19	0.94	0
4	OLA	A	406	-	14,14,19	0.28	0	13,13,19	0.72	0
4	OLA	B	411	-	13,13,19	0.59	0	12,13,19	1.09	0
4	OLA	B	415	-	19,19,19	0.51	0	19,19,19	1.03	0
4	OLA	A	415	-	14,14,19	0.30	0	13,13,19	0.73	0
4	OLA	B	418	-	14,14,19	0.56	0	14,14,19	1.04	0
4	OLA	A	418	-	10,10,19	0.65	0	10,10,19	1.19	1 (10%)
4	OLA	A	404	-	16,16,19	0.52	0	16,16,19	1.03	0
4	OLA	A	405	-	19,19,19	0.51	0	19,19,19	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OLA	B	408	-	6,6,19	0.78	0	6,6,19	1.34	1 (16%)
2	9P2	A	401	-	45,49,49	2.76	12 (26%)	59,68,68	1.20	5 (8%)
4	OLA	B	419	-	13,13,19	0.28	0	12,12,19	0.76	0
4	OLA	B	404	-	9,9,19	0.68	0	9,9,19	1.20	0
4	OLA	A	416	-	19,19,19	0.51	0	19,19,19	0.97	0
4	OLA	A	414	-	15,15,19	0.55	0	15,15,19	1.07	0
2	9P2	B	401	-	45,49,49	2.71	12 (26%)	59,68,68	1.20	7 (11%)
4	OLA	B	406	-	13,13,19	0.59	0	12,13,19	1.16	1 (8%)
4	OLA	B	414	-	8,8,19	0.31	0	7,7,19	0.74	0
4	OLA	B	417	-	15,15,19	0.54	0	15,15,19	1.04	0
4	OLA	A	417	-	19,19,19	0.50	0	19,19,19	1.02	0
5	CIT	B	420	-	12,12,12	1.32	1 (8%)	17,17,17	1.47	2 (11%)
4	OLA	A	411	-	17,17,19	0.52	0	17,17,19	1.06	1 (5%)
4	OLA	B	413	-	13,13,19	0.59	0	12,13,19	1.13	0
4	OLA	A	412	-	19,19,19	0.50	0	19,19,19	1.07	1 (5%)
4	OLA	A	413	-	12,12,19	0.29	0	11,11,19	0.70	0
3	TLA	A	403	-	9,9,9	1.14	0	12,12,12	3.55	8 (66%)
4	OLA	B	405	-	14,14,19	0.56	0	14,14,19	1.10	1 (7%)
4	OLA	A	409	-	11,11,19	0.31	0	10,10,19	0.69	0
3	TLA	B	402	-	9,9,9	1.11	0	12,12,12	3.60	8 (66%)
4	OLA	B	410	-	19,19,19	0.51	0	19,19,19	1.00	0
3	TLA	A	402	-	9,9,9	1.08	0	12,12,12	3.68	8 (66%)
4	OLA	B	412	-	19,19,19	0.52	0	19,19,19	0.97	0
4	OLA	B	407	-	12,12,19	0.59	0	12,12,19	1.21	1 (8%)
4	OLA	A	408	-	15,15,19	0.54	0	15,15,19	1.06	0
4	OLA	B	409	-	15,15,19	0.54	0	15,15,19	1.01	1 (6%)
4	OLA	A	407	-	13,13,19	0.60	0	12,13,19	1.11	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
4	OLA	B	403	-	-	7/10/10/17	-
4	OLA	A	410	-	-	0/7/7/17	-
4	OLA	B	416	-	-	5/17/17/17	-
4	OLA	A	406	-	-	7/12/12/17	-
4	OLA	B	411	-	-	6/11/11/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	B	415	-	-	5/17/17/17	-
4	OLA	A	415	-	-	5/12/12/17	-
4	OLA	B	418	-	-	7/12/12/17	-
4	OLA	A	418	-	-	1/8/8/17	-
4	OLA	A	404	-	-	9/14/14/17	-
4	OLA	A	405	-	-	8/17/17/17	-
4	OLA	B	408	-	-	0/4/4/17	-
2	9P2	A	401	-	-	7/23/36/36	0/7/7/7
4	OLA	B	419	-	-	5/11/11/17	-
4	OLA	B	404	-	-	1/7/7/17	-
4	OLA	A	416	-	-	10/17/17/17	-
4	OLA	A	414	-	-	3/13/13/17	-
2	9P2	B	401	-	-	7/23/36/36	0/7/7/7
4	OLA	B	406	-	-	4/11/11/17	-
4	OLA	B	414	-	-	2/6/6/17	-
4	OLA	B	417	-	-	6/13/13/17	-
4	OLA	A	417	-	-	10/17/17/17	-
5	CIT	B	420	-	-	11/16/16/16	-
4	OLA	A	411	-	-	7/15/15/17	-
4	OLA	B	413	-	-	6/11/11/17	-
4	OLA	A	412	-	-	4/17/17/17	-
4	OLA	A	413	-	-	4/10/10/17	-
3	TLA	A	403	-	2/2/4/4	6/12/12/12	-
4	OLA	B	405	-	-	3/12/12/17	-
4	OLA	A	409	-	-	2/9/9/17	-
3	TLA	B	402	-	2/2/4/4	8/12/12/12	-
4	OLA	B	410	-	-	9/17/17/17	-
3	TLA	A	402	-	2/2/4/4	8/12/12/12	-
4	OLA	B	412	-	-	9/17/17/17	-
4	OLA	B	407	-	-	4/10/10/17	-
4	OLA	A	408	-	-	7/13/13/17	-
4	OLA	B	409	-	-	5/13/13/17	-
4	OLA	A	407	-	-	1/11/11/17	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	9P2	C32-C03	-10.61	1.37	1.49
2	B	401	9P2	C32-C03	-10.19	1.37	1.49
2	A	401	9P2	C24-C25	6.48	1.50	1.38
2	B	401	9P2	C24-C25	6.38	1.50	1.38
2	B	401	9P2	C18-C17	5.96	1.49	1.38
2	A	401	9P2	C18-C17	5.87	1.49	1.38
2	A	401	9P2	C14-C15	5.07	1.48	1.38
2	B	401	9P2	C14-C15	5.00	1.47	1.38
2	A	401	9P2	O19-C17	4.41	1.44	1.38
2	B	401	9P2	O19-C17	4.30	1.44	1.38
2	A	401	9P2	O21-C16	4.10	1.44	1.38
2	B	401	9P2	C01-N02	4.05	1.41	1.35
2	A	401	9P2	C01-N02	3.93	1.41	1.35
2	B	401	9P2	O21-C16	3.92	1.44	1.38
2	A	401	9P2	C22-C23	3.42	1.57	1.51
2	B	401	9P2	C22-C23	3.34	1.57	1.51
2	B	401	9P2	C31-C23	2.95	1.45	1.38
2	A	401	9P2	O28-C27	-2.93	1.37	1.43
2	A	401	9P2	C31-C23	2.89	1.45	1.38
2	B	401	9P2	O28-C27	-2.80	1.37	1.43
5	B	420	CIT	C3-C6	-2.76	1.50	1.53
2	B	401	9P2	C31-C30	2.72	1.43	1.38
2	A	401	9P2	C31-C30	2.71	1.43	1.38
2	B	401	9P2	C30-C29	2.14	1.44	1.39
2	A	401	9P2	C30-C29	2.07	1.43	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	TLA	O3-C3-C2	6.15	122.45	110.23
3	A	402	TLA	O2-C2-C3	6.06	122.26	110.23
3	A	403	TLA	O2-C2-C3	5.57	121.29	110.23
3	B	402	TLA	C3-C2-C1	5.55	122.26	109.87
3	A	402	TLA	O3-C3-C2	5.51	121.17	110.23
3	A	403	TLA	O3-C3-C2	5.42	121.00	110.23
3	A	403	TLA	C2-C3-C4	4.95	120.93	109.87
3	A	403	TLA	C3-C2-C1	4.80	120.58	109.87
3	A	402	TLA	C3-C2-C1	4.68	120.31	109.87
3	B	402	TLA	O2-C2-C3	4.67	119.50	110.23
3	A	402	TLA	C2-C3-C4	4.28	119.44	109.87
3	B	402	TLA	C2-C3-C4	4.25	119.36	109.87
3	A	402	TLA	O3-C3-C4	4.15	119.37	110.66
5	B	420	CIT	O6-C6-C3	3.73	119.53	113.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	TLA	O2-C2-C1	3.61	118.23	110.66
3	B	402	TLA	O3-C3-C4	3.57	118.15	110.66
3	A	403	TLA	O2-C2-C1	3.56	118.12	110.66
3	A	403	TLA	O3-C3-C4	3.53	118.06	110.66
3	A	402	TLA	O41-C4-C3	3.50	122.73	113.27
2	A	401	9P2	C13-C12-N11	-3.49	106.35	113.12
3	A	402	TLA	O2-C2-C1	3.21	117.40	110.66
2	B	401	9P2	O26-C25-C24	3.10	132.00	127.85
2	A	401	9P2	O26-C25-C24	3.09	131.99	127.85
2	B	401	9P2	C13-C12-N11	-3.05	107.21	113.12
2	B	401	9P2	O19-C17-C18	3.01	131.87	127.85
2	A	401	9P2	N02-C01-N05	-2.88	107.87	115.11
2	B	401	9P2	N02-C01-N05	-2.86	107.92	115.11
2	B	401	9P2	C04-C10-N11	-2.79	106.41	113.06
2	A	401	9P2	C23-C22-N11	-2.77	107.75	113.12
2	A	401	9P2	O19-C17-C18	2.72	131.49	127.85
5	B	420	CIT	O5-C6-C3	-2.70	118.43	122.25
3	B	402	TLA	O41-C4-C3	2.69	120.55	113.27
3	B	402	TLA	O11-C1-C2	2.62	120.34	113.27
3	A	402	TLA	O11-C1-C2	2.56	120.19	113.27
3	A	403	TLA	O41-C4-C3	2.54	120.13	113.27
4	A	412	OLA	C3-C2-C1	-2.24	108.83	114.47
3	A	403	TLA	O11-C1-C2	2.20	119.23	113.27
4	B	405	OLA	C3-C2-C1	-2.16	109.03	114.47
2	B	401	9P2	C23-C22-N11	-2.15	108.95	113.12
4	A	411	OLA	C3-C2-C1	-2.07	109.24	114.47
4	B	407	OLA	C3-C2-C1	-2.05	109.30	114.47
4	B	408	OLA	C3-C2-C1	-2.05	109.31	114.47
2	B	401	9P2	O28-C29-C30	2.02	131.49	127.81
4	B	409	OLA	C3-C2-C1	-2.01	109.39	114.47
4	B	406	OLA	C3-C2-C1	-2.01	109.40	114.47
4	A	418	OLA	C3-C2-C1	-2.00	109.43	114.47

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	402	TLA	C3
3	A	402	TLA	C2
3	A	403	TLA	C3
3	A	403	TLA	C2
3	B	402	TLA	C3
3	B	402	TLA	C2

All (209) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	9P2	N02-C03-C32-C37
3	A	402	TLA	C1-C2-C3-C4
3	A	402	TLA	O2-C2-C3-O3
3	A	403	TLA	O11-C1-C2-O2
3	A	403	TLA	C1-C2-C3-C4
3	B	402	TLA	O2-C2-C3-O3
4	A	407	OLA	C9-C10-C11-C12
4	B	413	OLA	C9-C10-C11-C12
5	B	420	CIT	O7-C3-C6-O5
5	B	420	CIT	O7-C3-C6-O6
5	B	420	CIT	C4-C3-C6-O5
5	B	420	CIT	C4-C3-C6-O6
3	A	403	TLA	O2-C2-C3-O3
3	B	402	TLA	C1-C2-C3-C4
3	A	402	TLA	O3-C3-C4-O4
3	A	403	TLA	O1-C1-C2-O2
3	B	402	TLA	O3-C3-C4-O4
3	B	402	TLA	O3-C3-C4-O41
3	A	402	TLA	O11-C1-C2-C3
3	A	403	TLA	C2-C3-C4-O4
3	A	403	TLA	C2-C3-C4-O41
3	B	402	TLA	O1-C1-C2-C3
3	B	402	TLA	O11-C1-C2-C3
4	A	404	OLA	C5-C6-C7-C8
3	A	402	TLA	O3-C3-C4-O41
4	B	411	OLA	C1-C2-C3-C4
2	B	401	9P2	N05-C06-C07-C08
4	A	408	OLA	C1-C2-C3-C4
4	B	403	OLA	C1-C2-C3-C4
4	B	406	OLA	C1-C2-C3-C4
4	B	413	OLA	C1-C2-C3-C4
3	A	402	TLA	O1-C1-C2-C3
4	A	414	OLA	C6-C7-C8-C9
4	B	416	OLA	C14-C15-C16-C17
4	A	405	OLA	C13-C14-C15-C16
4	A	416	OLA	C14-C15-C16-C17
4	A	417	OLA	C4-C5-C6-C7
4	A	417	OLA	C11-C12-C13-C14
4	A	417	OLA	C6-C7-C8-C9
4	B	410	OLA	C10-C11-C12-C13
4	A	404	OLA	C3-C4-C5-C6
4	A	406	OLA	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	416	OLA	C13-C14-C15-C16
2	A	401	9P2	C23-C22-N11-C12
4	A	416	OLA	C2-C3-C4-C5
4	A	416	OLA	C4-C5-C6-C7
4	A	408	OLA	C5-C6-C7-C8
4	B	412	OLA	C14-C15-C16-C17
4	B	419	OLA	C13-C14-C15-C16
4	A	415	OLA	C3-C4-C5-C6
4	A	416	OLA	C12-C13-C14-C15
4	B	409	OLA	C4-C5-C6-C7
4	A	404	OLA	C4-C5-C6-C7
4	A	405	OLA	C11-C12-C13-C14
4	A	418	OLA	C2-C3-C4-C5
4	B	417	OLA	C10-C11-C12-C13
4	A	405	OLA	C1-C2-C3-C4
2	A	401	9P2	C23-C22-N11-C10
4	B	403	OLA	C3-C4-C5-C6
4	A	416	OLA	C10-C11-C12-C13
4	B	411	OLA	C3-C4-C5-C6
2	A	401	9P2	N02-C03-C32-C33
4	A	405	OLA	C14-C15-C16-C17
5	B	420	CIT	C1-C2-C3-C6
4	B	403	OLA	C5-C6-C7-C8
4	A	406	OLA	C10-C11-C12-C13
4	A	415	OLA	C10-C11-C12-C13
4	B	405	OLA	C6-C7-C8-C9
2	B	401	9P2	C13-C12-N11-C22
4	A	405	OLA	C5-C6-C7-C8
2	B	401	9P2	C13-C12-N11-C10
4	B	411	OLA	C4-C5-C6-C7
4	A	412	OLA	C12-C13-C14-C15
4	B	410	OLA	C5-C6-C7-C8
4	A	408	OLA	C6-C7-C8-C9
4	A	411	OLA	C6-C7-C8-C9
4	B	416	OLA	C10-C11-C12-C13
4	B	418	OLA	C6-C7-C8-C9
4	B	410	OLA	C13-C14-C15-C16
4	B	411	OLA	C5-C6-C7-C8
4	A	412	OLA	C5-C6-C7-C8
4	A	416	OLA	C5-C6-C7-C8
4	B	413	OLA	C5-C6-C7-C8
4	A	411	OLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	414	OLA	C10-C11-C12-C13
4	A	405	OLA	C10-C11-C12-C13
4	B	412	OLA	C6-C7-C8-C9
4	B	412	OLA	C1-C2-C3-C4
5	B	420	CIT	C1-C2-C3-O7
5	B	420	CIT	C1-C2-C3-C4
4	B	413	OLA	C6-C7-C8-C9
4	A	409	OLA	C11-C12-C13-C14
3	A	402	TLA	C2-C3-C4-O4
2	B	401	9P2	N02-C03-C32-C37
4	B	415	OLA	C15-C16-C17-C18
4	B	409	OLA	C11-C12-C13-C14
4	B	412	OLA	C13-C14-C15-C16
4	B	407	OLA	C3-C4-C5-C6
5	B	420	CIT	C2-C3-C6-O5
5	B	420	CIT	C2-C3-C6-O6
4	A	416	OLA	C3-C4-C5-C6
4	A	408	OLA	C11-C12-C13-C14
4	B	410	OLA	C1-C2-C3-C4
4	B	418	OLA	C4-C5-C6-C7
3	A	402	TLA	C2-C3-C4-O41
4	A	415	OLA	C12-C13-C14-C15
2	A	401	9P2	C13-C12-N11-C22
4	B	412	OLA	C12-C13-C14-C15
4	B	407	OLA	C5-C6-C7-C8
4	B	410	OLA	C11-C12-C13-C14
4	A	417	OLA	C15-C16-C17-C18
4	A	415	OLA	C5-C6-C7-C8
5	B	420	CIT	C6-C3-C4-C5
4	B	415	OLA	C5-C6-C7-C8
4	A	404	OLA	C6-C7-C8-C9
4	A	406	OLA	C6-C7-C8-C9
4	A	406	OLA	C5-C6-C7-C8
2	A	401	9P2	C13-C12-N11-C10
4	B	418	OLA	C2-C3-C4-C5
4	B	403	OLA	C4-C5-C6-C7
4	A	413	OLA	C5-C6-C7-C8
4	A	417	OLA	C12-C13-C14-C15
4	A	412	OLA	C10-C11-C12-C13
4	A	416	OLA	C6-C7-C8-C9
4	A	404	OLA	C12-C13-C14-C15
4	B	419	OLA	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	404	OLA	C1-C2-C3-C4
4	B	414	OLA	C12-C13-C14-C15
4	A	411	OLA	C4-C5-C6-C7
4	A	413	OLA	C6-C7-C8-C9
4	A	417	OLA	C10-C11-C12-C13
4	A	413	OLA	C4-C5-C6-C7
2	B	401	9P2	N02-C03-C32-C33
4	B	405	OLA	C3-C4-C5-C6
4	A	408	OLA	C4-C5-C6-C7
4	B	417	OLA	C11-C12-C13-C14
4	A	406	OLA	C4-C5-C6-C7
4	B	406	OLA	C5-C6-C7-C8
4	A	405	OLA	C3-C4-C5-C6
4	B	417	OLA	C3-C4-C5-C6
4	B	415	OLA	C13-C14-C15-C16
4	A	404	OLA	C11-C12-C13-C14
4	B	412	OLA	C11-C12-C13-C14
4	B	411	OLA	C7-C8-C9-C10
4	B	411	OLA	C2-C3-C4-C5
4	B	418	OLA	O1-C1-C2-C3
4	B	410	OLA	C12-C13-C14-C15
4	B	419	OLA	C12-C13-C14-C15
4	A	413	OLA	C11-C12-C13-C14
4	B	405	OLA	C10-C11-C12-C13
4	A	404	OLA	C2-C3-C4-C5
4	B	410	OLA	O1-C1-C2-C3
4	A	406	OLA	C9-C10-C11-C12
4	B	407	OLA	C2-C3-C4-C5
4	A	414	OLA	C10-C11-C12-C13
4	B	415	OLA	C10-C11-C12-C13
4	B	410	OLA	O2-C1-C2-C3
3	B	402	TLA	C2-C3-C4-O41
4	B	417	OLA	C4-C5-C6-C7
4	B	413	OLA	C2-C3-C4-C5
4	B	418	OLA	O2-C1-C2-C3
4	A	414	OLA	C7-C8-C9-C10
4	A	406	OLA	C11-C12-C13-C14
4	B	412	OLA	C15-C16-C17-C18
4	B	416	OLA	O2-C1-C2-C3
4	A	411	OLA	C12-C13-C14-C15
3	B	402	TLA	C2-C3-C4-O4
4	B	409	OLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	412	OLA	C9-C10-C11-C12
4	B	416	OLA	O1-C1-C2-C3
4	B	407	OLA	C4-C5-C6-C7
4	A	411	OLA	C10-C11-C12-C13
4	A	417	OLA	O1-C1-C2-C3
4	A	404	OLA	C7-C8-C9-C10
4	A	416	OLA	C9-C10-C11-C12
4	A	417	OLA	C9-C10-C11-C12
4	B	403	OLA	C7-C8-C9-C10
4	B	418	OLA	C7-C8-C9-C10
4	A	412	OLA	C15-C16-C17-C18
4	A	408	OLA	C10-C11-C12-C13
4	B	403	OLA	O1-C1-C2-C3
2	B	401	9P2	N02-C01-C38-C43
4	A	409	OLA	C7-C8-C9-C10
4	A	411	OLA	C9-C10-C11-C12
4	A	415	OLA	C7-C8-C9-C10
4	B	406	OLA	C7-C8-C9-C10
4	B	416	OLA	C7-C8-C9-C10
4	B	417	OLA	C9-C10-C11-C12
4	B	415	OLA	C3-C4-C5-C6
4	B	404	OLA	C5-C6-C7-C8
4	A	417	OLA	O2-C1-C2-C3
4	B	403	OLA	O2-C1-C2-C3
4	A	405	OLA	C12-C13-C14-C15
5	B	420	CIT	O7-C3-C4-C5
4	B	406	OLA	C3-C4-C5-C6
4	B	410	OLA	C4-C5-C6-C7
4	A	417	OLA	C14-C15-C16-C17
2	B	401	9P2	N02-C01-C38-C39
4	B	419	OLA	C6-C7-C8-C9
4	B	412	OLA	C3-C4-C5-C6
4	B	418	OLA	C1-C2-C3-C4
4	B	417	OLA	C7-C8-C9-C10
4	A	408	OLA	C3-C4-C5-C6
2	A	401	9P2	N05-C04-C10-N11
4	B	409	OLA	O1-C1-C2-C3
4	B	419	OLA	C11-C12-C13-C14
4	B	413	OLA	C7-C8-C9-C10
4	A	411	OLA	C2-C3-C4-C5
4	B	409	OLA	O2-C1-C2-C3

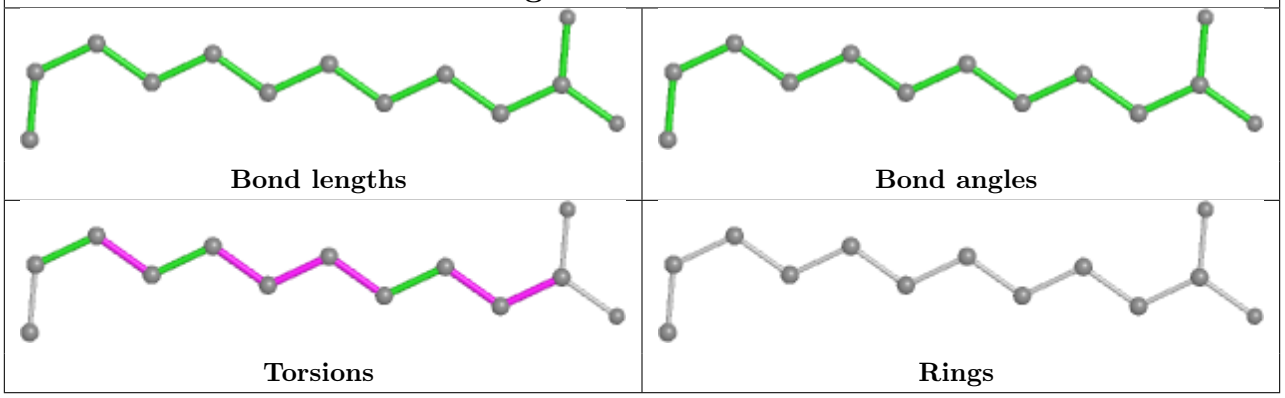
There are no ring outliers.

27 monomers are involved in 60 short contacts:

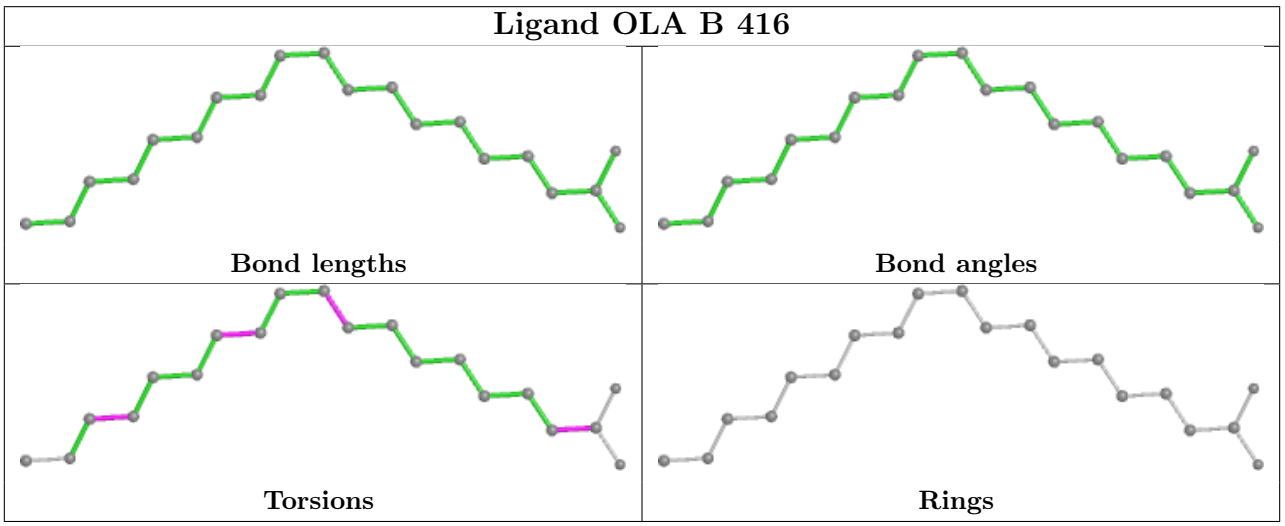
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	OLA	1	0
4	A	410	OLA	2	0
4	B	416	OLA	4	0
4	A	406	OLA	7	0
4	B	411	OLA	1	0
4	B	415	OLA	2	0
4	B	418	OLA	1	0
4	A	404	OLA	1	0
4	A	405	OLA	7	0
4	B	419	OLA	10	0
4	A	416	OLA	5	0
2	B	401	9P2	1	0
4	B	406	OLA	4	0
4	B	417	OLA	3	0
4	A	417	OLA	3	0
4	A	411	OLA	1	0
4	B	413	OLA	1	0
4	A	412	OLA	2	0
4	A	413	OLA	3	0
3	A	403	TLA	0	1
4	B	405	OLA	2	0
4	A	409	OLA	2	0
4	B	410	OLA	4	0
3	A	402	TLA	2	0
4	B	412	OLA	1	0
4	A	408	OLA	2	0
4	B	409	OLA	3	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.

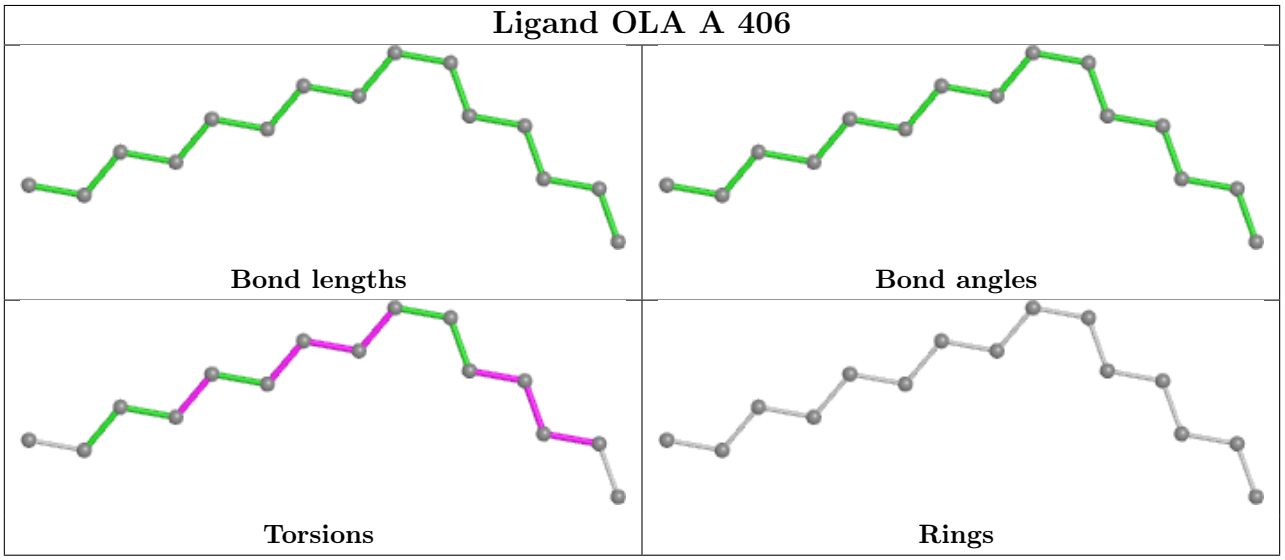
Ligand OLA B 403



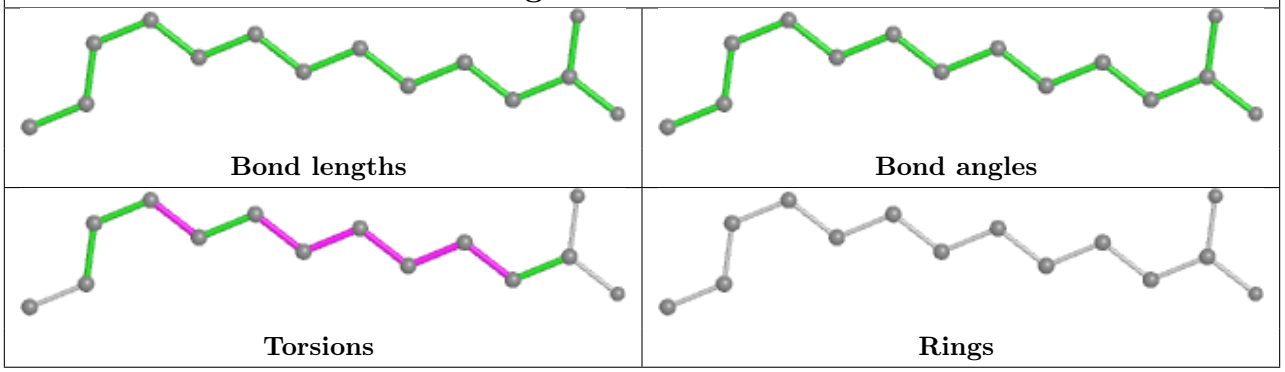
Ligand OLA B 416



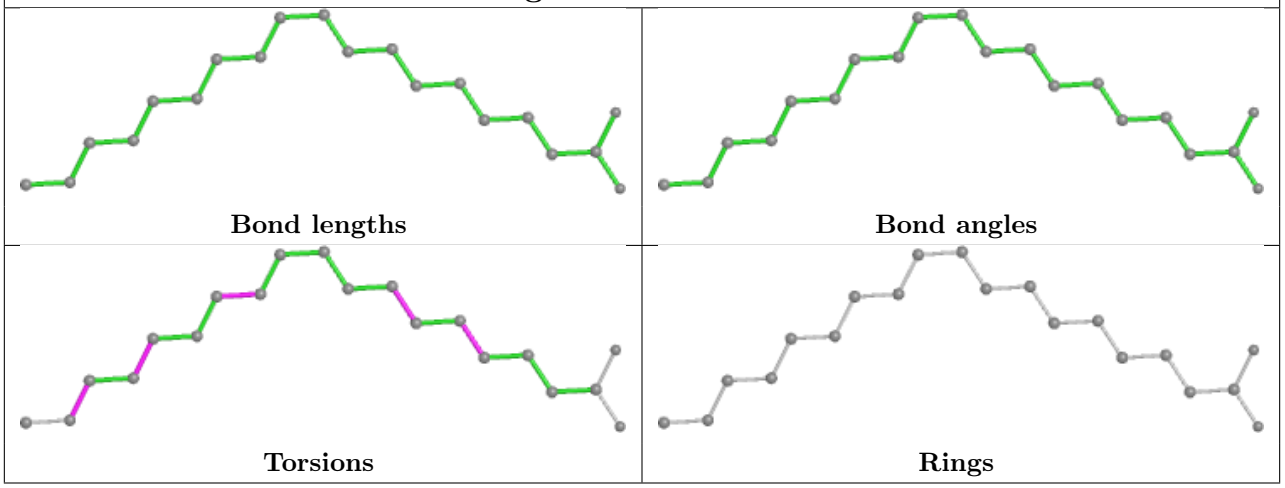
Ligand OLA A 406



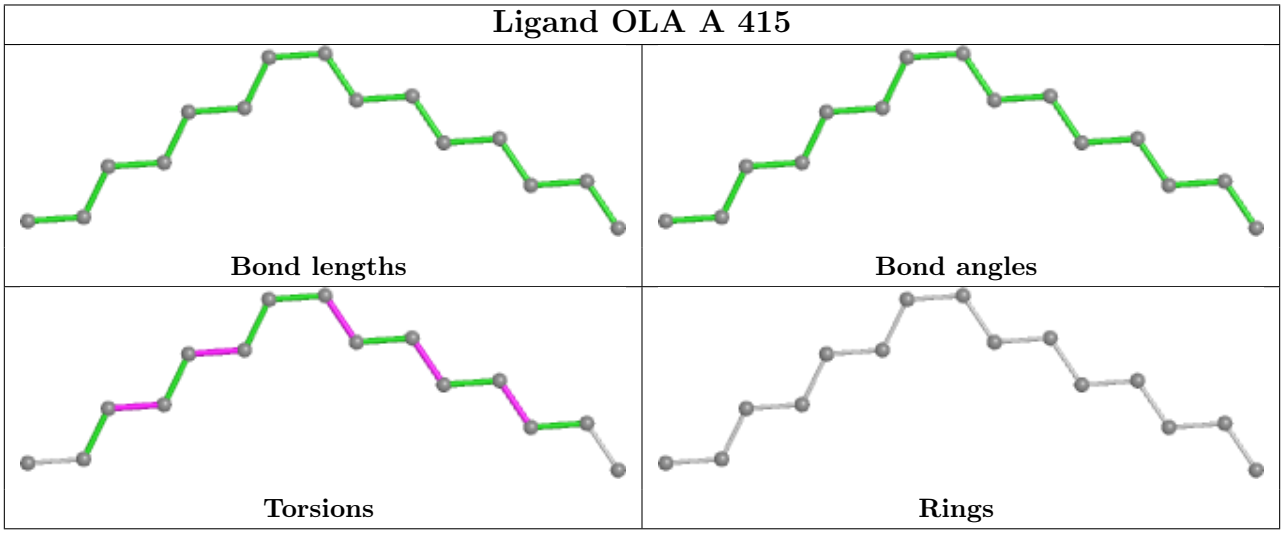
Ligand OLA B 411



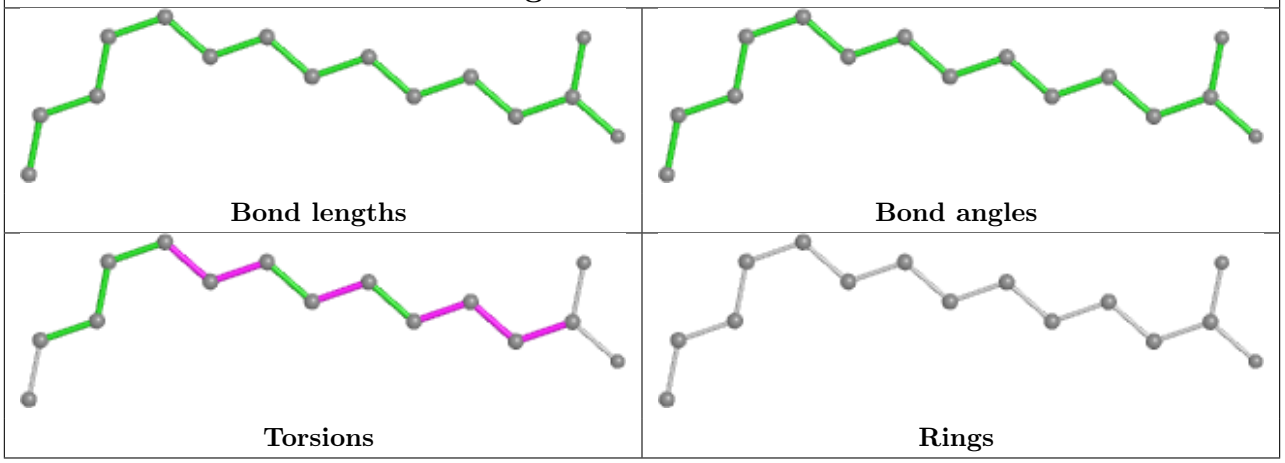
Ligand OLA B 415



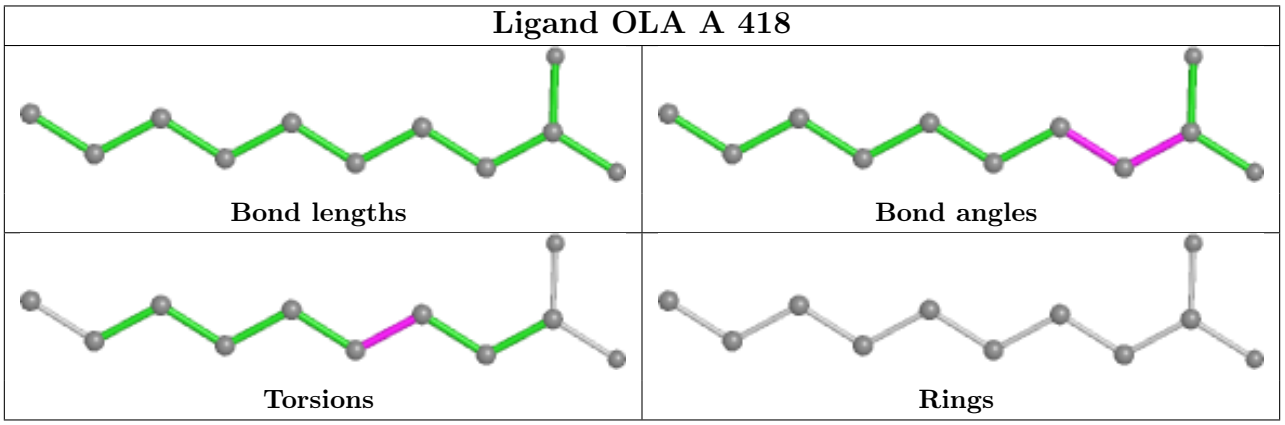
Ligand OLA A 415



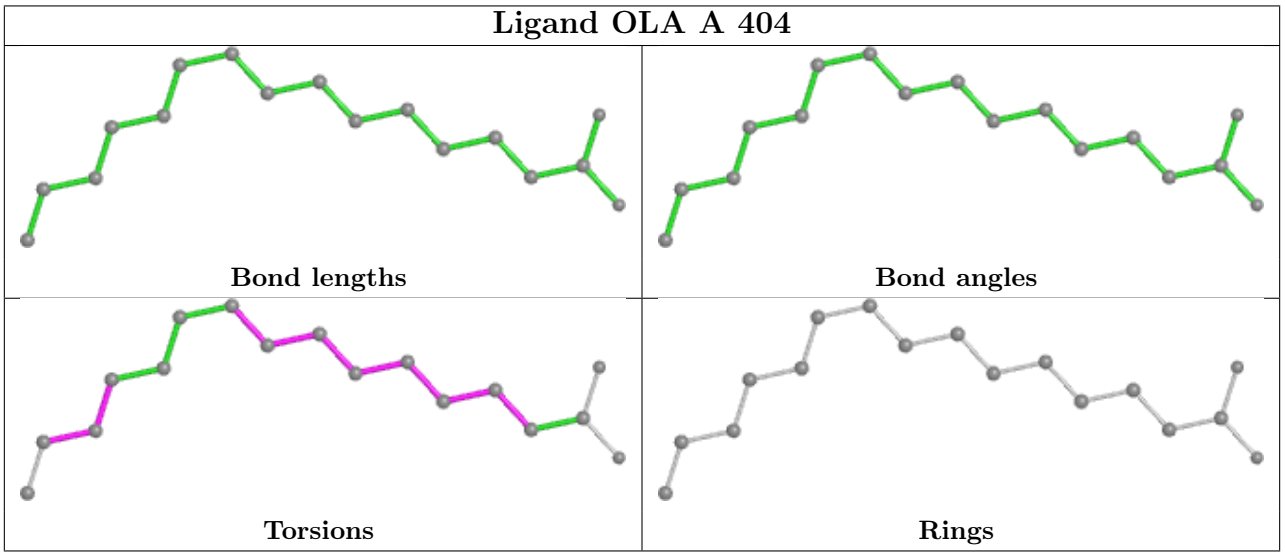
Ligand OLA B 418



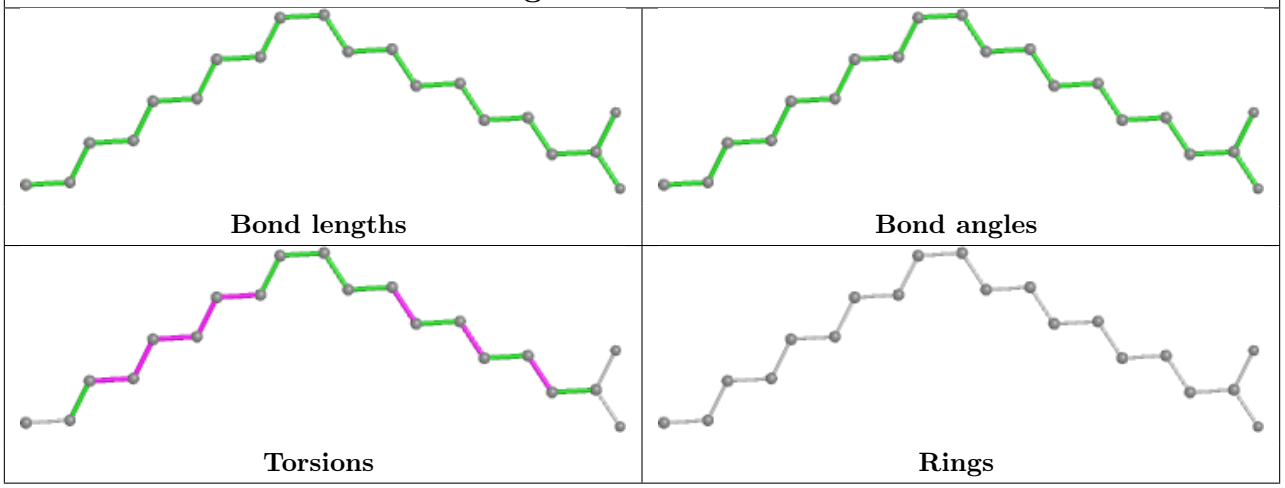
Ligand OLA A 418



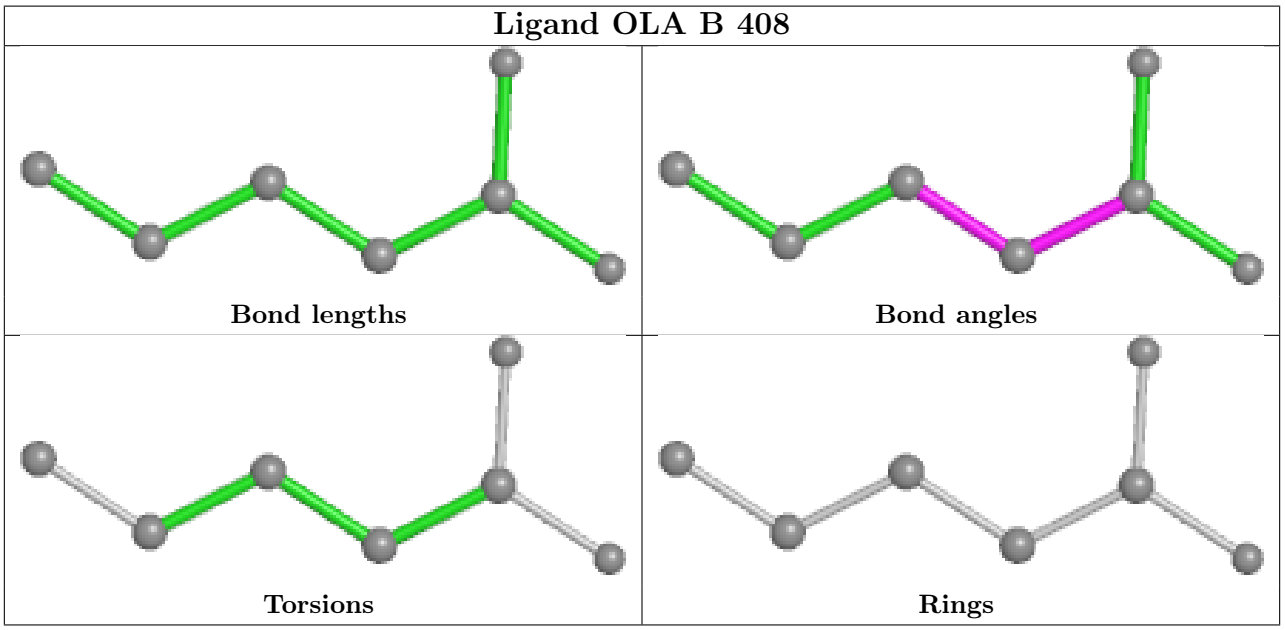
Ligand OLA A 404



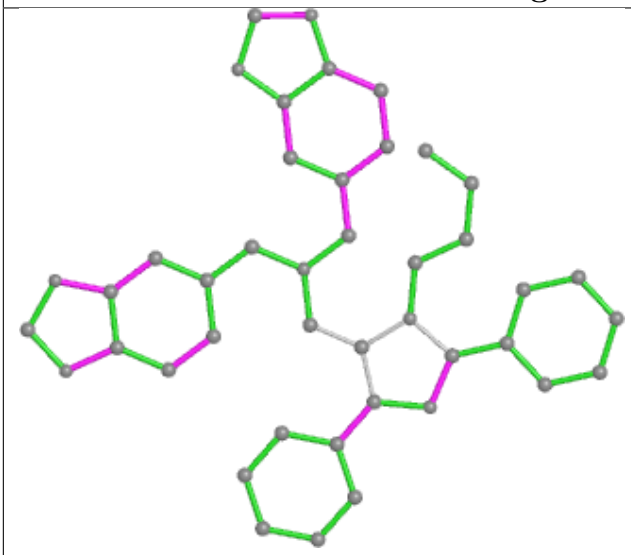
Ligand OLA A 405



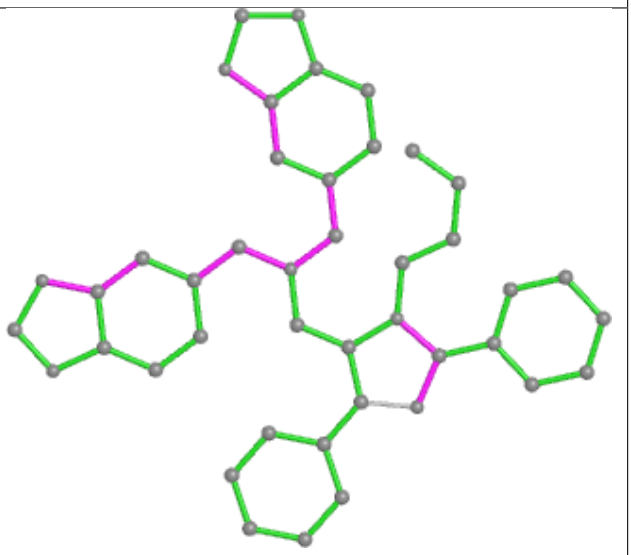
Ligand OLA B 408



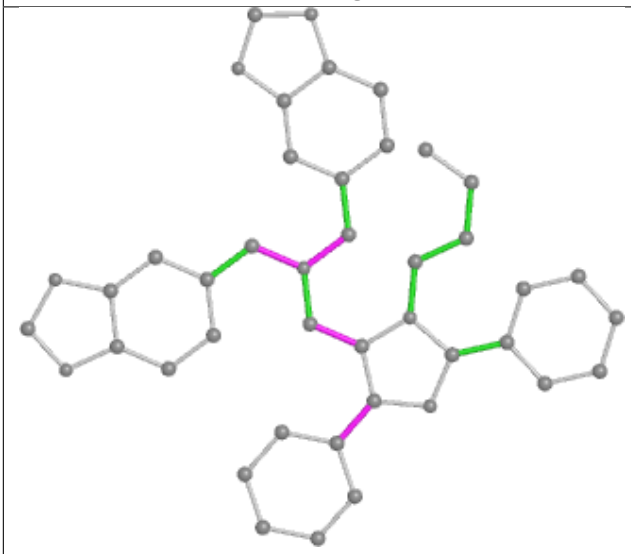
Ligand 9P2 A 401



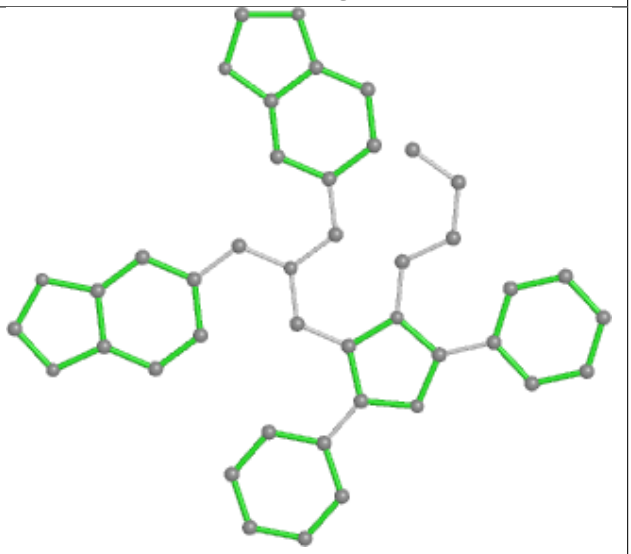
Bond lengths



Bond angles

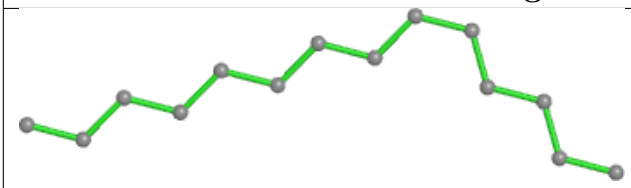


Torsions

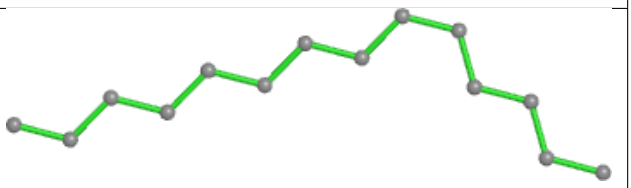


Rings

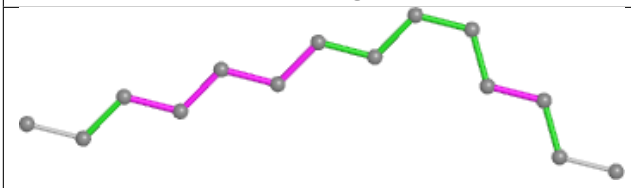
Ligand OLA B 419



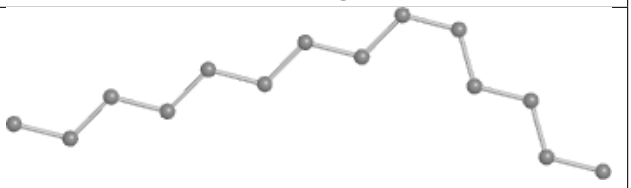
Bond lengths



Bond angles

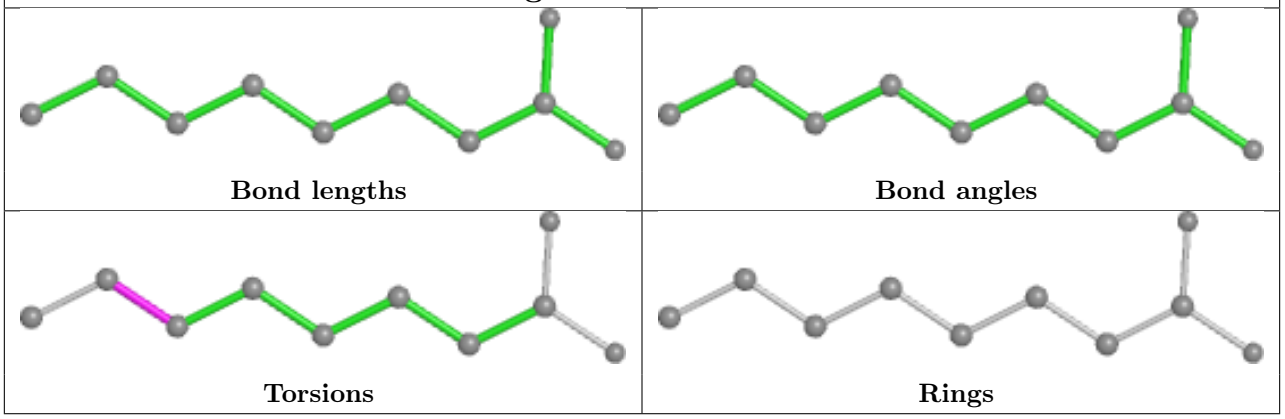


Torsions

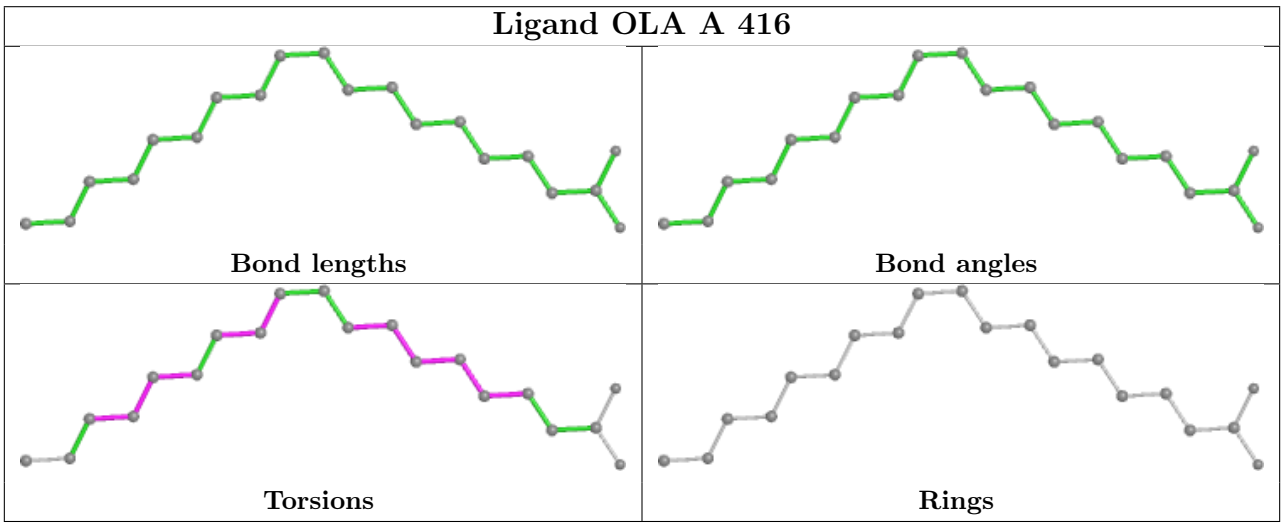


Rings

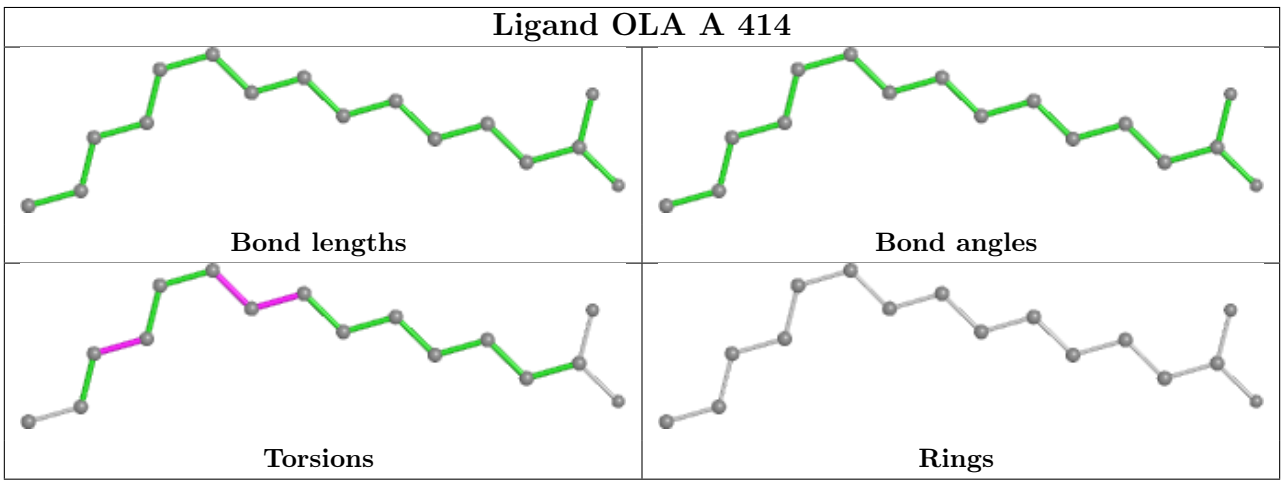
Ligand OLA B 404



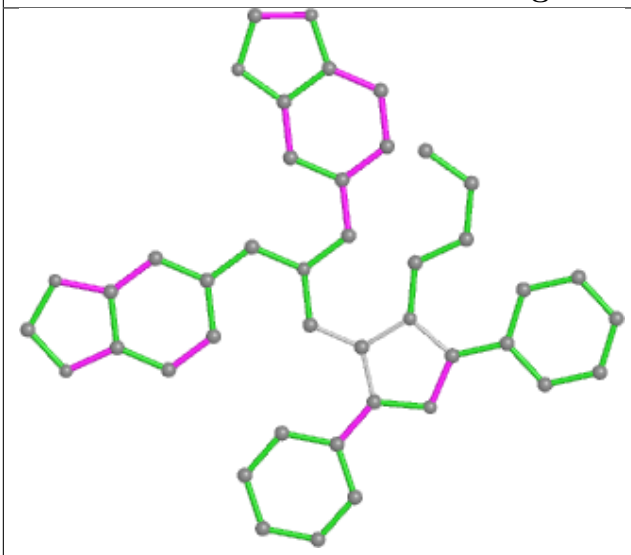
Ligand OLA A 416



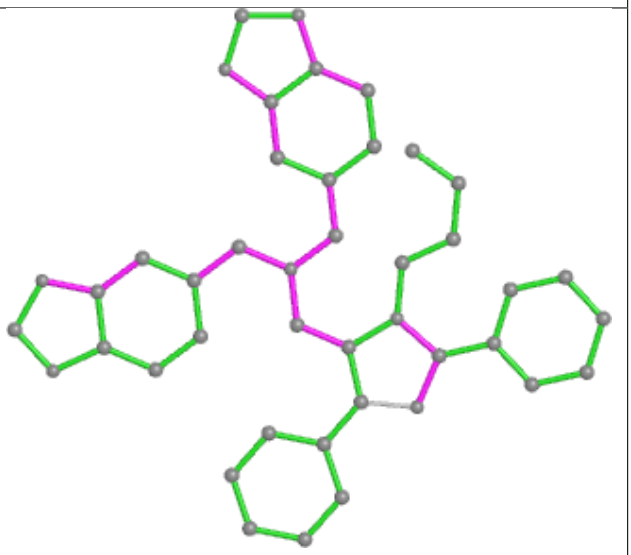
Ligand OLA A 414



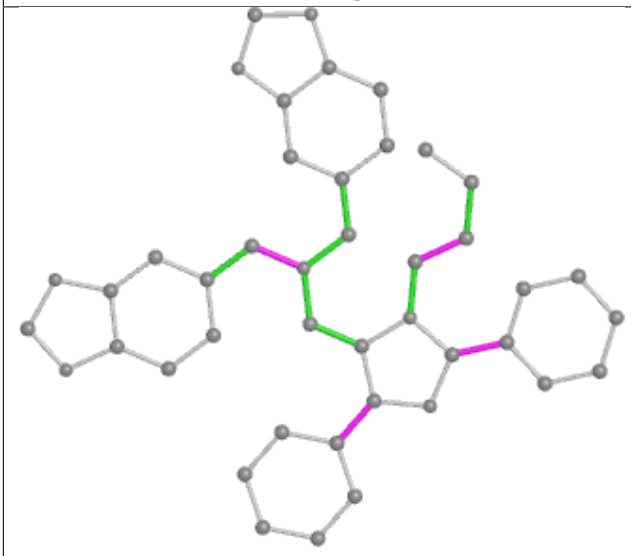
Ligand 9P2 B 401



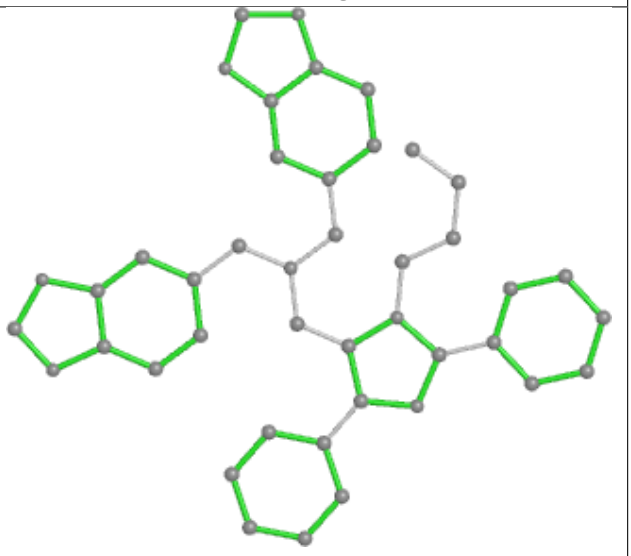
Bond lengths



Bond angles

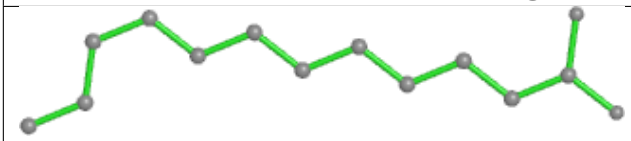


Torsions

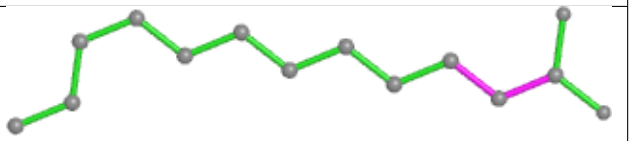


Rings

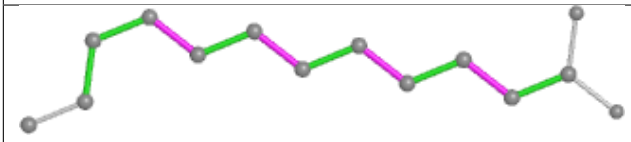
Ligand OLA B 406



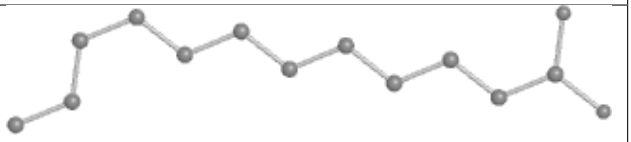
Bond lengths



Bond angles

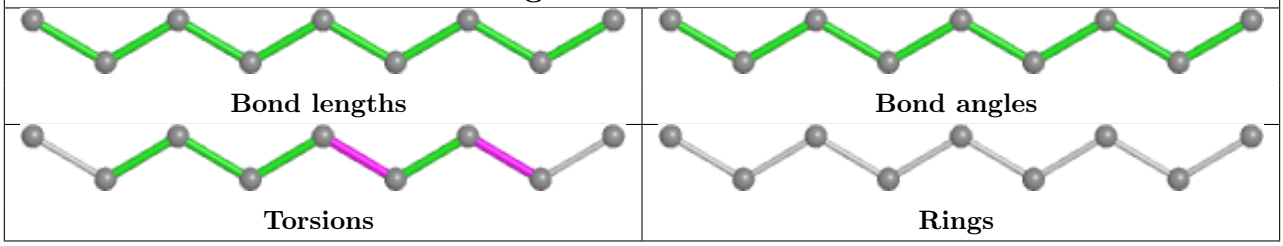


Torsions

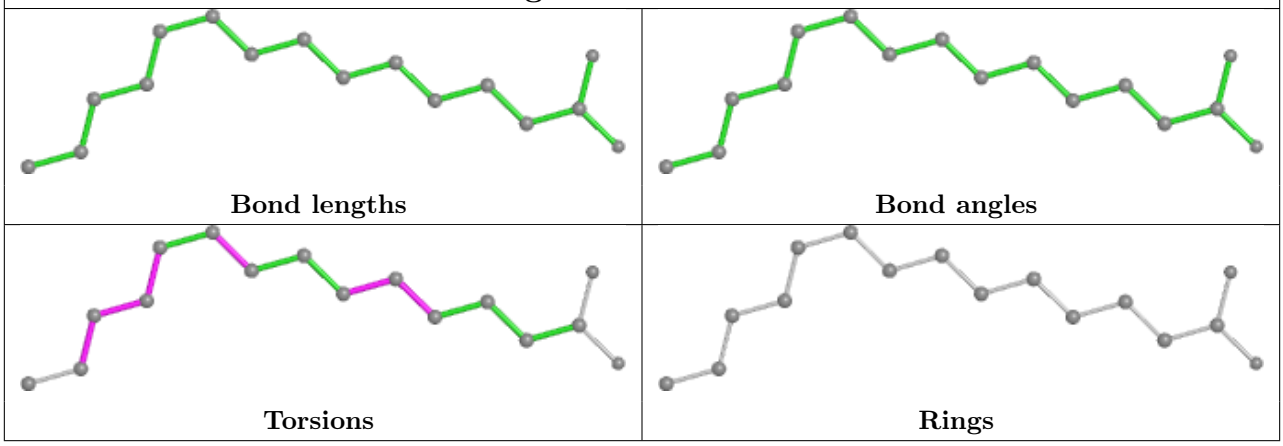


Rings

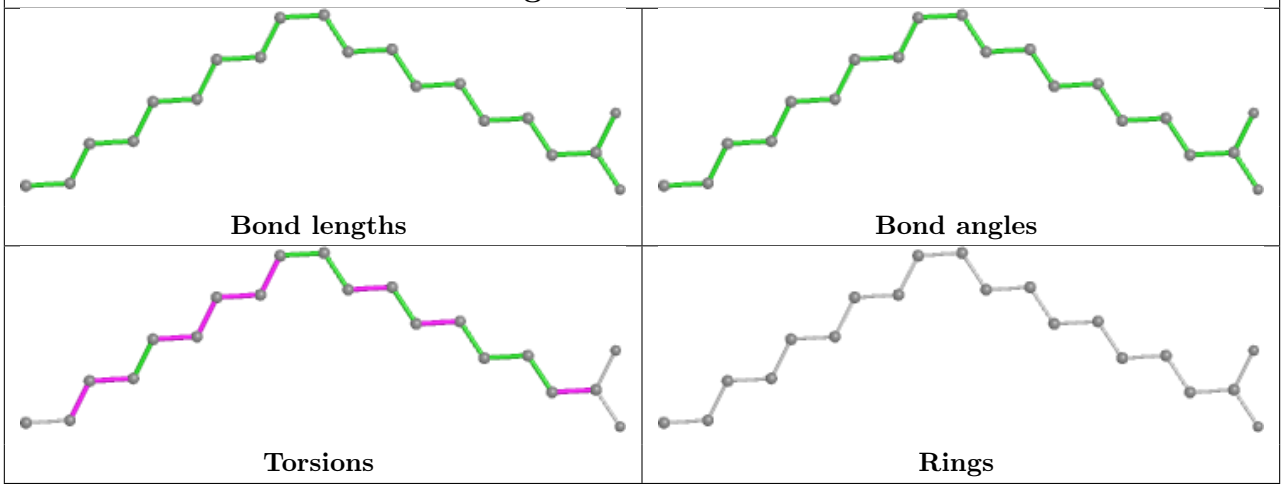
Ligand OLA B 414



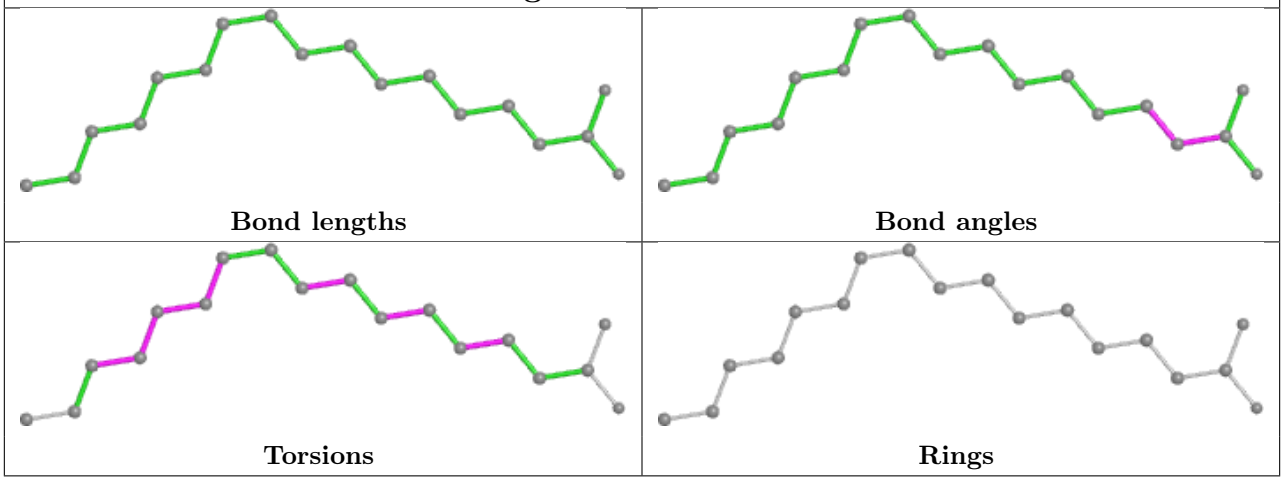
Ligand OLA B 417



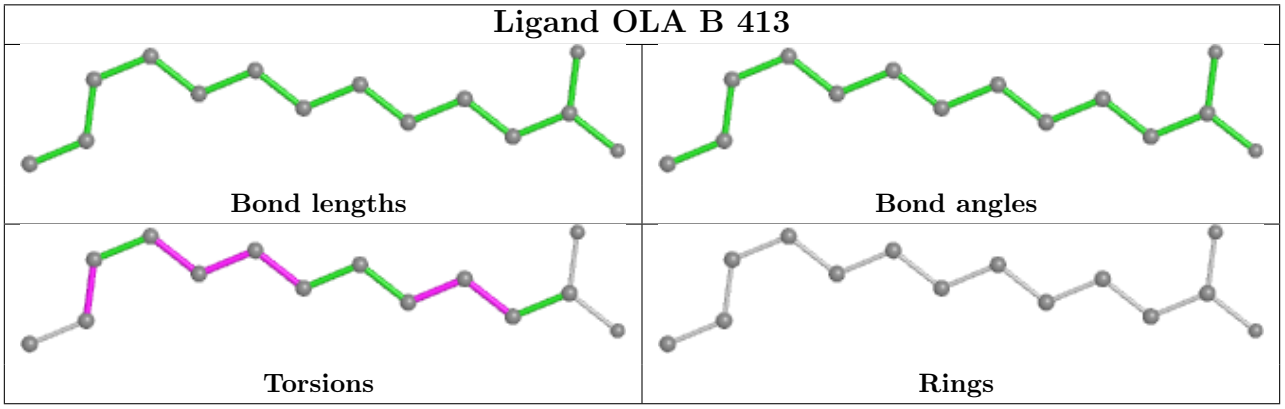
Ligand OLA A 417



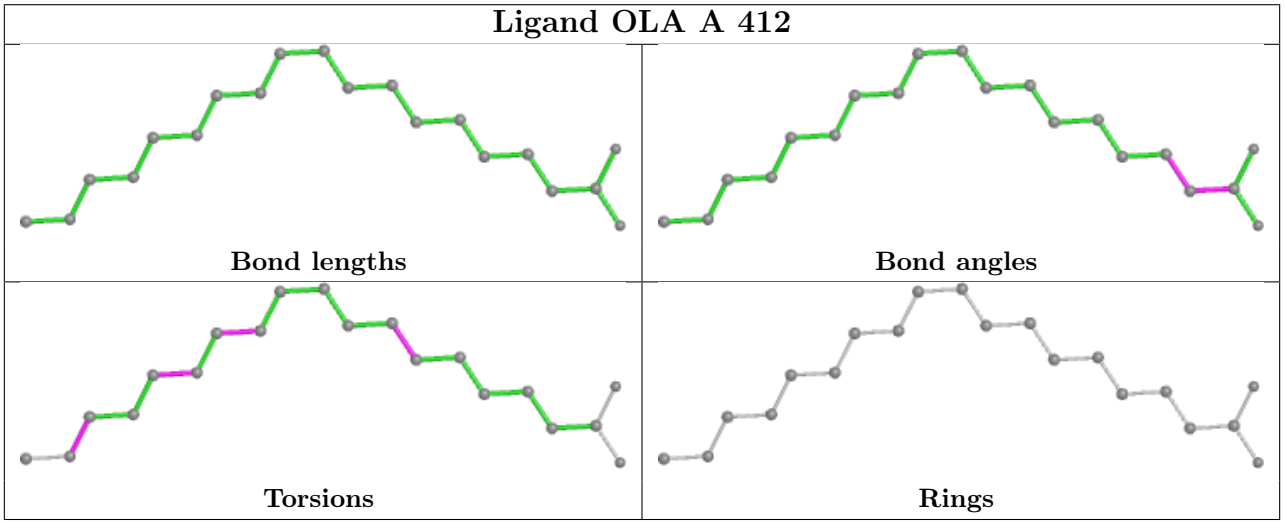
Ligand OLA A 411



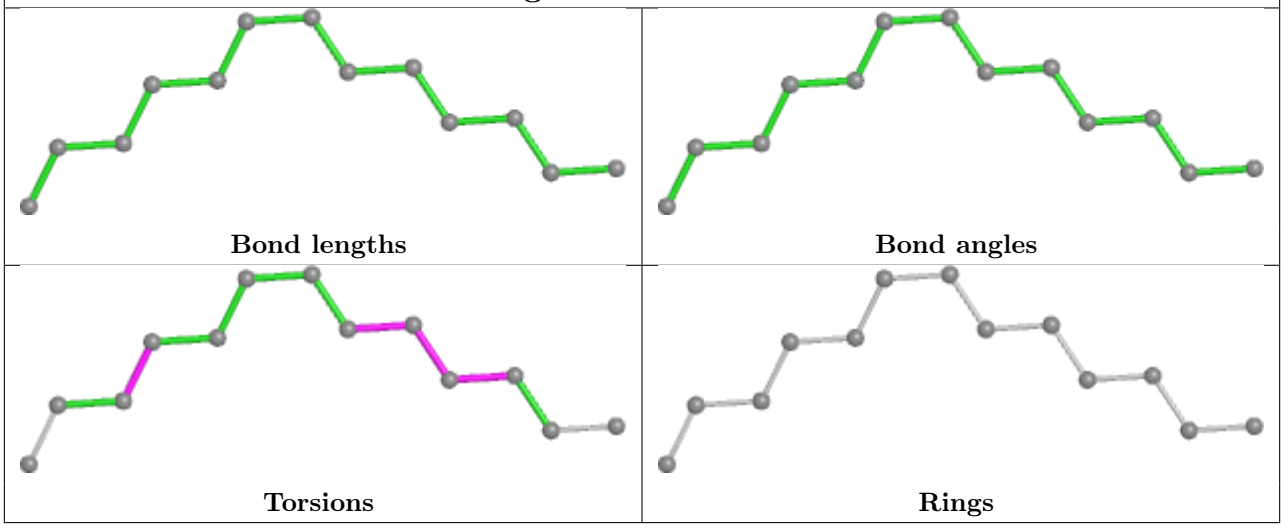
Ligand OLA B 413



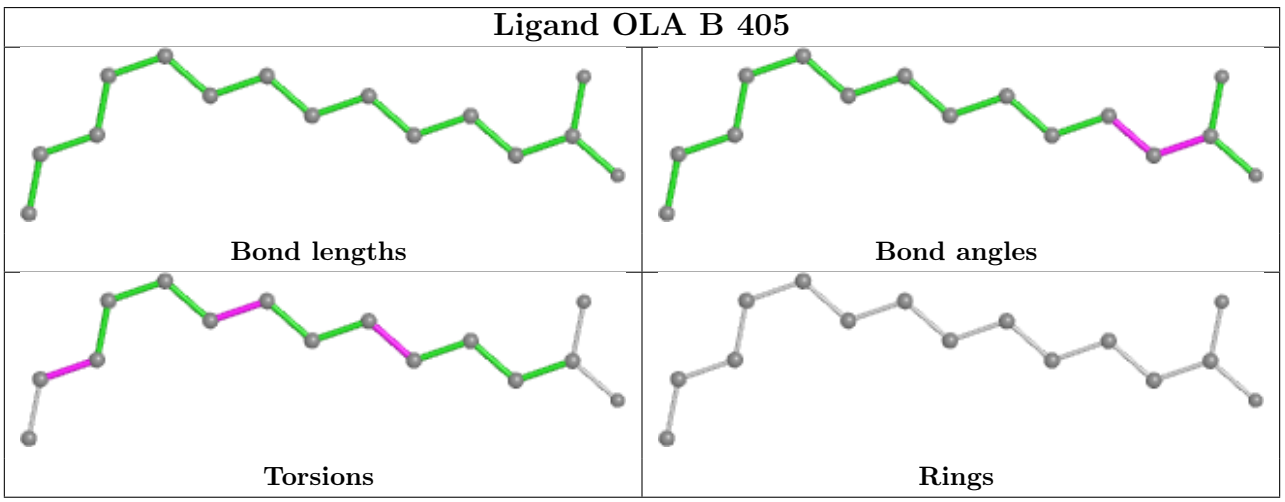
Ligand OLA A 412



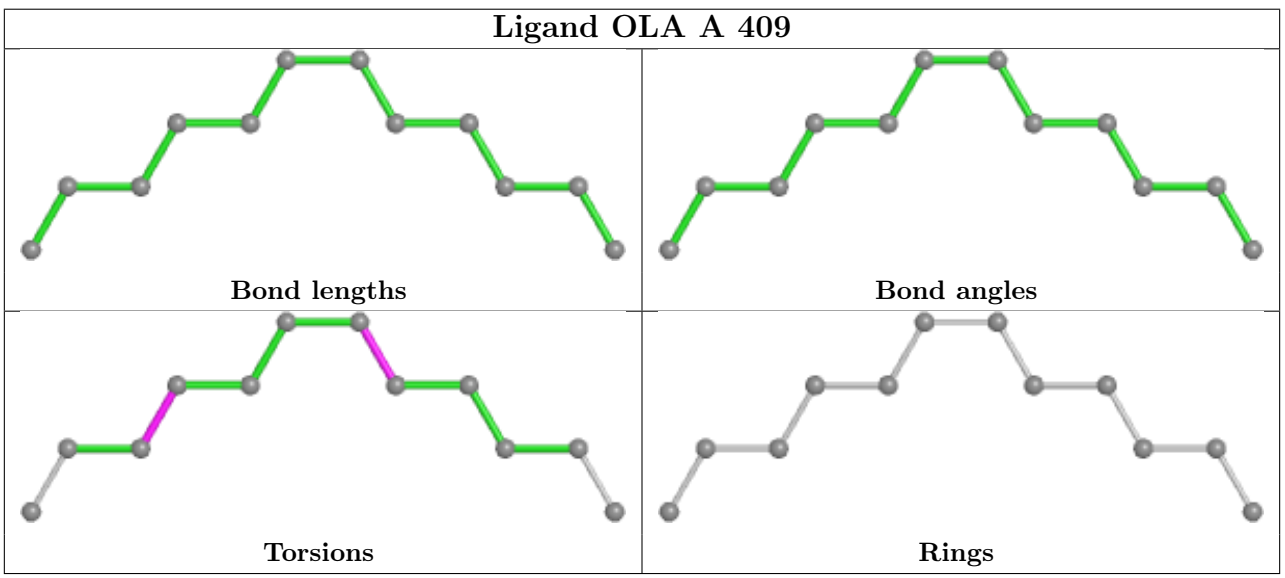
Ligand OLA A 413



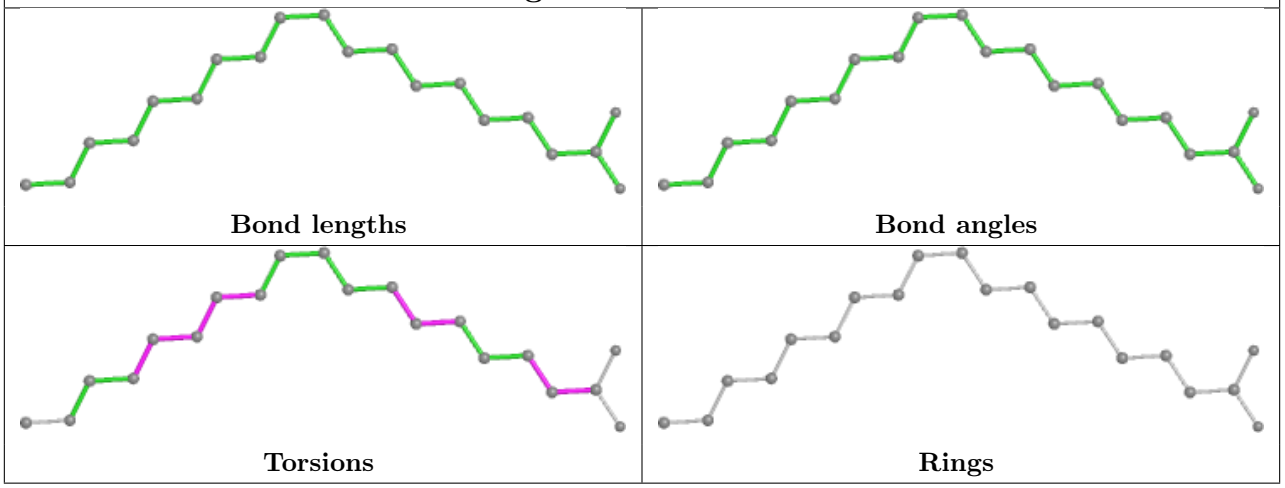
Ligand OLA B 405



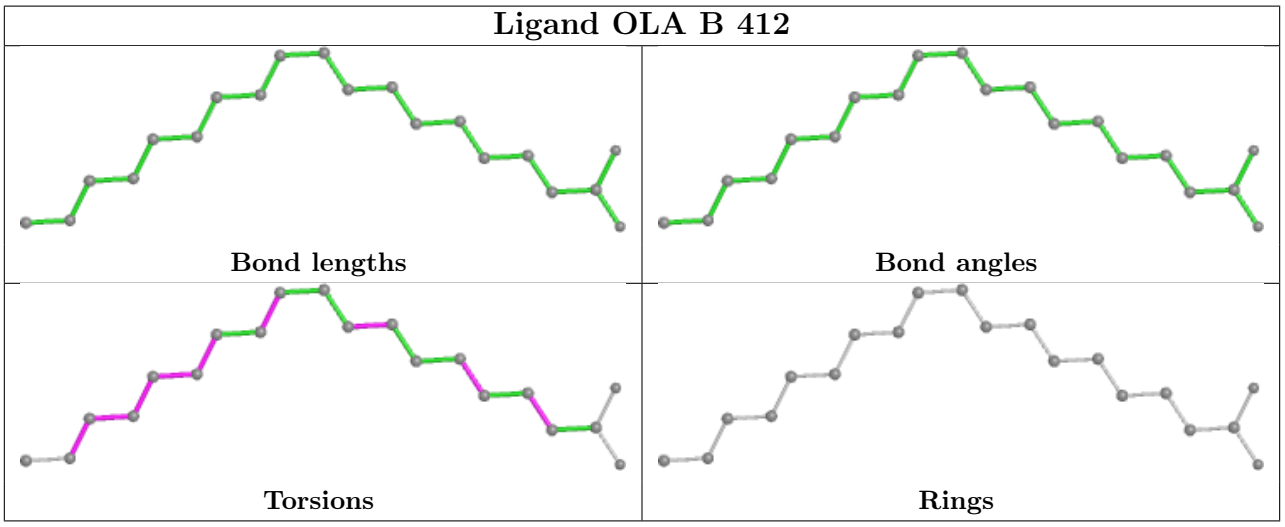
Ligand OLA A 409



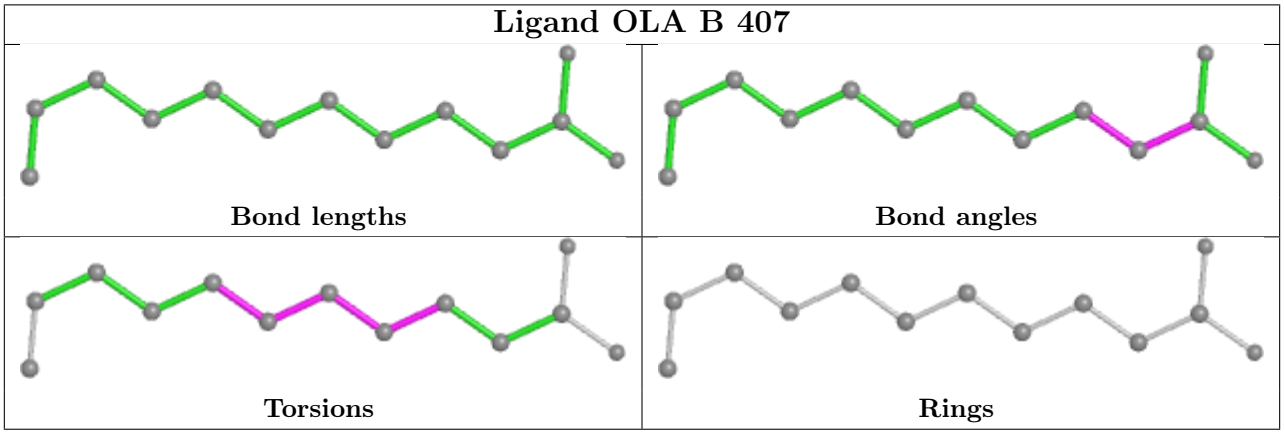
Ligand OLA B 410

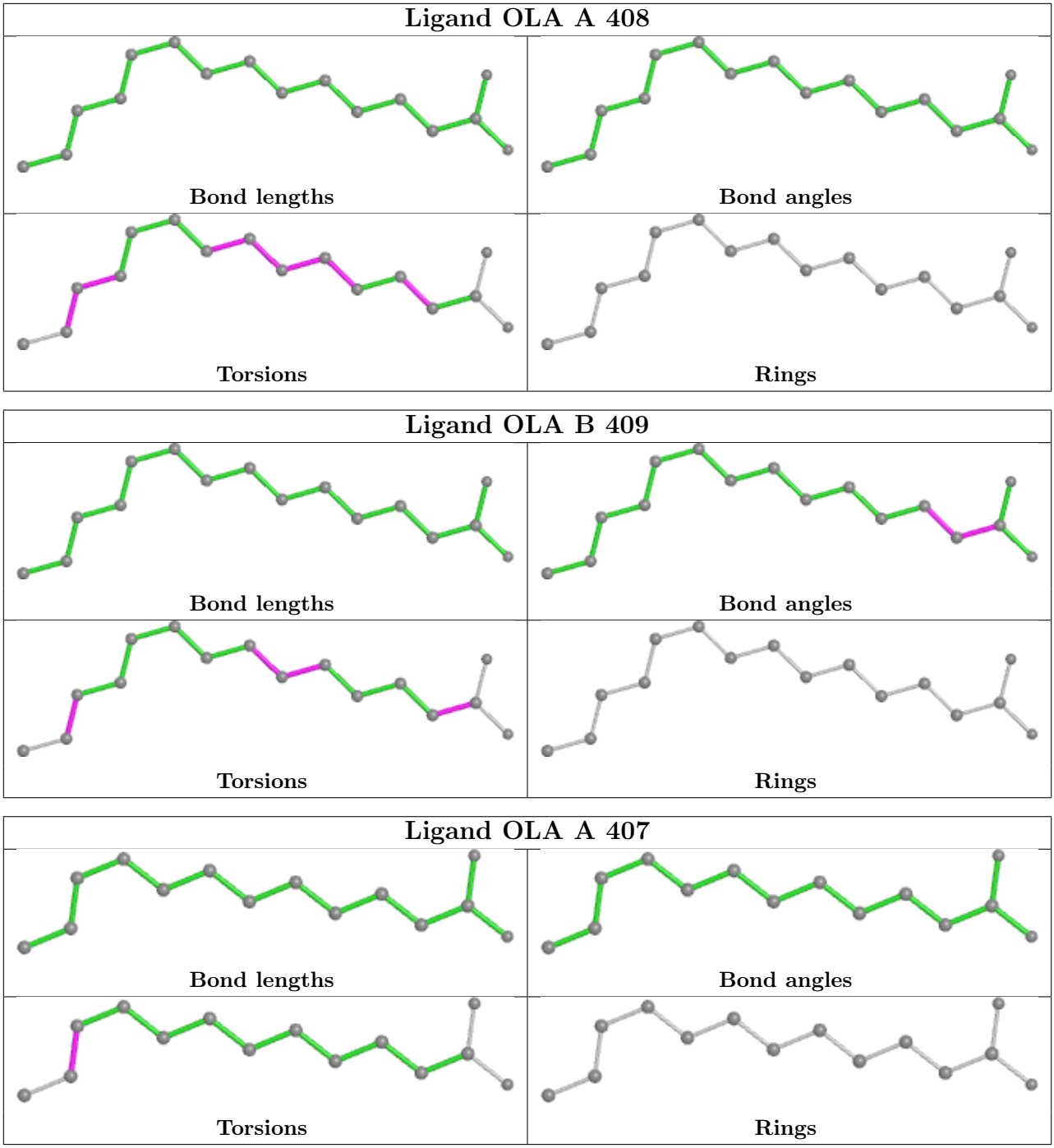


Ligand OLA B 412



Ligand OLA B 407





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	294/317 (92%)	0.02	11 (3%)	41	41	19, 41, 83, 108	0
1	B	295/317 (93%)	-0.03	16 (5%)	25	24	15, 39, 82, 125	0
All	All	589/634 (92%)	-0.01	27 (4%)	32	31	15, 40, 83, 125	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	ASN	6.3
1	A	182	PHE	6.0
1	B	195	ASP	5.2
1	B	196	LYS	4.8
1	B	194	HIS	4.4
1	A	31	ASN	4.4
1	B	267	PHE	4.4
1	B	331	GLU	4.3
1	B	192	TYR	4.2
1	B	312	ARG	4.1
1	A	308	GLN	4.1
1	A	183	PRO	3.4
1	A	194	HIS	3.3
1	B	268	LEU	3.1
1	A	270	PRO	3.0
1	B	182	PHE	3.0
1	B	230	TRP	2.9
1	B	269	GLU	2.9
1	B	200	ARG	2.8
1	B	38	ILE	2.6
1	A	269	GLU	2.6
1	A	307	PHE	2.5
1	B	68	ARG	2.4
1	A	306	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	49	LEU	2.2
1	B	275	PHE	2.2
1	A	178	ARG	2.2

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CIT	B	420	13/13	0.69	0.47	82,92,102,118	0
4	OLA	B	412	20/20	0.76	0.36	38,63,93,98	0
4	OLA	B	411	14/20	0.77	0.34	63,73,89,91	0
4	OLA	A	405	20/20	0.77	0.28	40,55,77,81	0
4	OLA	B	418	15/20	0.77	0.37	40,58,87,94	0
4	OLA	B	403	13/20	0.77	0.27	41,55,65,70	0
4	OLA	A	408	16/20	0.78	0.45	58,71,77,82	0
3	TLA	A	403	10/10	0.78	0.32	43,71,85,101	0
4	OLA	A	409	12/20	0.80	0.36	55,63,77,80	0
4	OLA	B	406	14/20	0.80	0.41	42,58,82,84	0
4	OLA	A	411	18/20	0.80	0.51	51,59,67,71	0
4	OLA	B	404	10/20	0.81	0.27	33,41,68,79	0
4	OLA	B	413	14/20	0.81	0.47	39,51,64,82	0
4	OLA	A	410	10/20	0.82	0.22	46,62,68,73	0
4	OLA	A	412	20/20	0.82	0.46	38,57,78,81	0
4	OLA	B	416	20/20	0.82	0.28	40,60,79,82	0
4	OLA	A	416	20/20	0.82	0.30	19,45,71,86	0
4	OLA	A	418	11/20	0.82	0.41	52,65,92,99	0
4	OLA	B	415	20/20	0.83	0.30	33,57,73,74	0
4	OLA	A	407	14/20	0.83	0.26	44,61,73,76	0

Continued on next page...

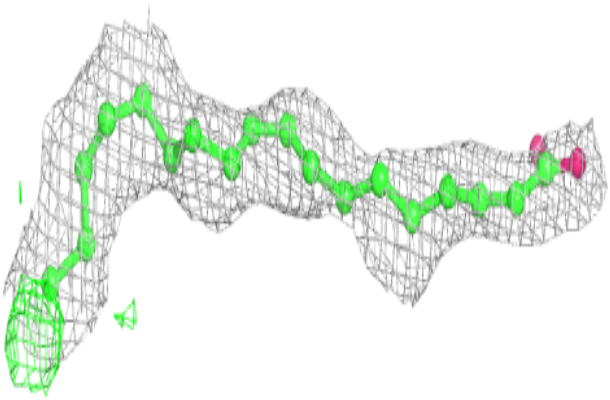
Continued from previous page...

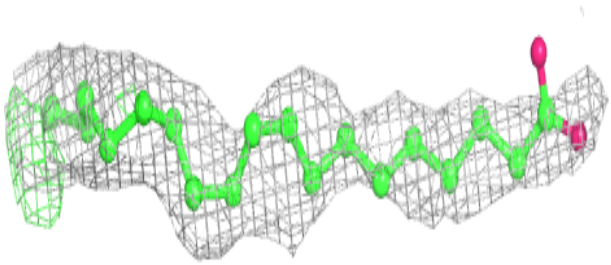
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLA	B	409	16/20	0.83	0.31	38,59,97,103	0
4	OLA	B	410	20/20	0.83	0.24	37,62,77,80	0
3	TLA	A	402	10/10	0.84	0.25	38,59,71,87	0
4	OLA	A	417	20/20	0.84	0.26	37,56,95,95	0
4	OLA	A	415	15/20	0.84	0.31	36,52,69,71	0
4	OLA	B	405	15/20	0.85	0.24	40,57,78,85	0
4	OLA	A	406	15/20	0.86	0.28	33,57,72,76	0
4	OLA	B	414	9/20	0.86	0.27	46,52,58,64	0
4	OLA	B	417	16/20	0.87	0.25	45,60,74,80	0
4	OLA	B	407	13/20	0.88	0.25	32,37,62,64	0
4	OLA	B	419	14/20	0.89	0.21	32,46,61,65	0
4	OLA	A	414	16/20	0.89	0.28	37,56,67,74	0
4	OLA	B	408	7/20	0.90	0.16	27,32,47,52	0
4	OLA	A	413	13/20	0.91	0.19	38,47,55,62	0
3	TLA	B	402	10/10	0.91	0.24	40,59,68,81	0
4	OLA	A	404	17/20	0.91	0.22	25,44,64,69	0
2	9P2	A	401	43/43	0.95	0.18	18,26,43,51	0
2	9P2	B	401	43/43	0.96	0.17	17,27,37,41	0

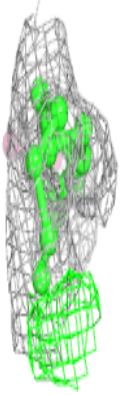
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA B 412:

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

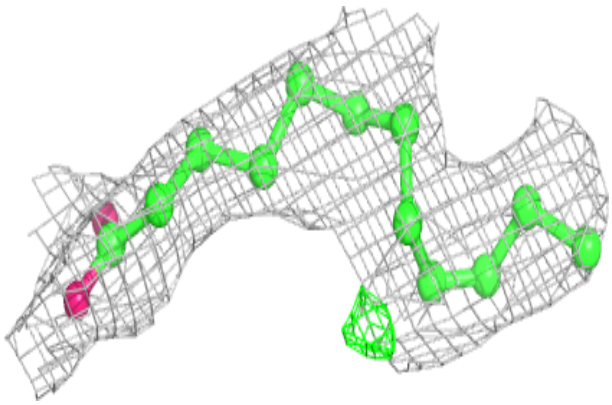


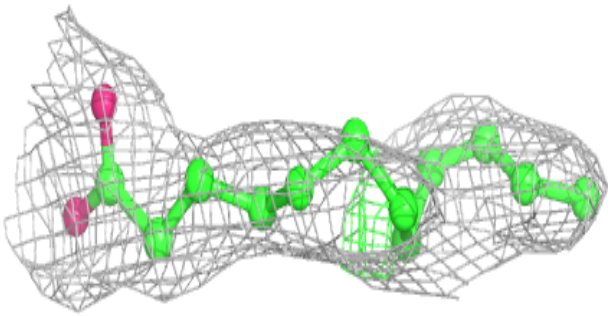


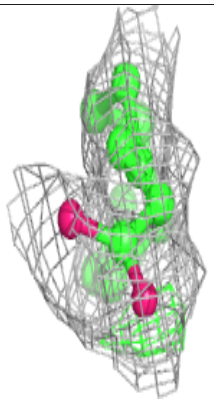


Electron density around OLA B 411:

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

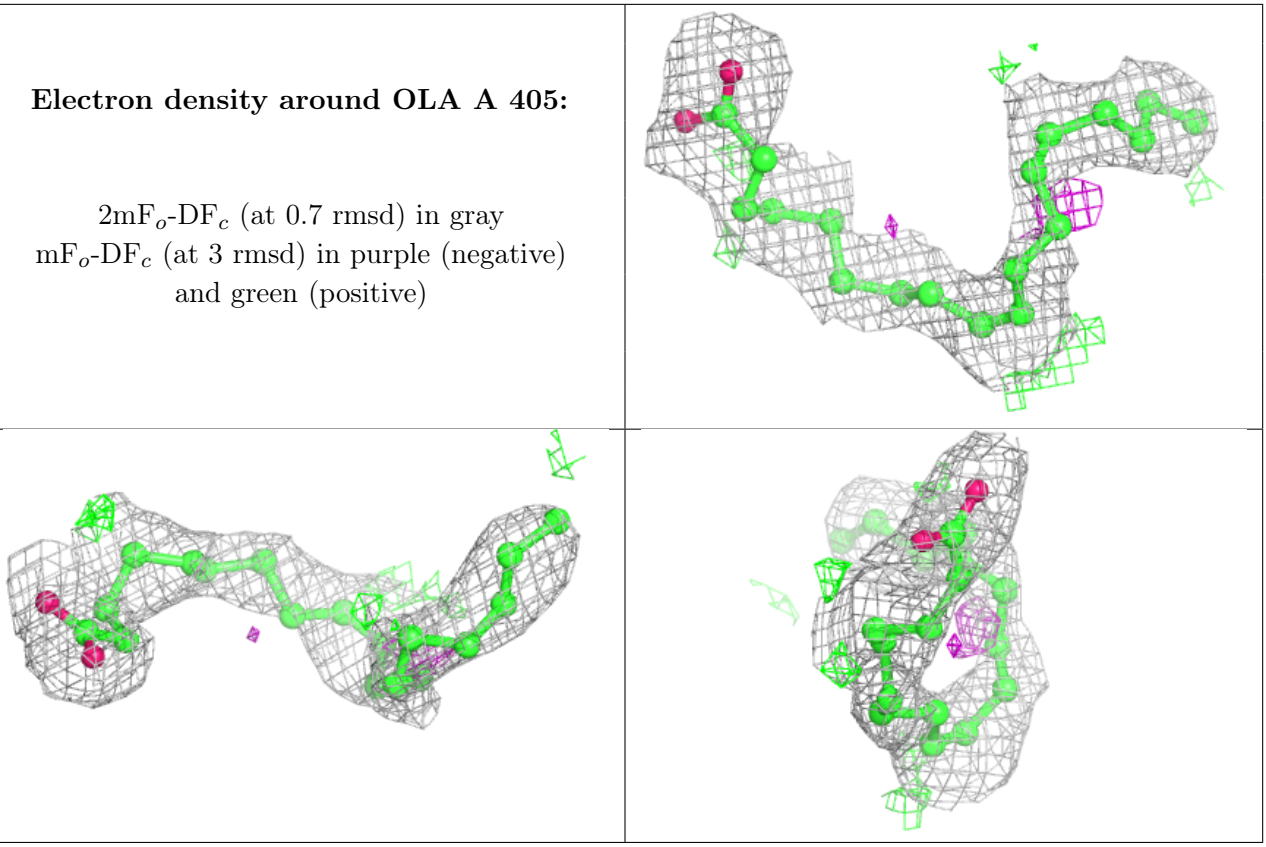






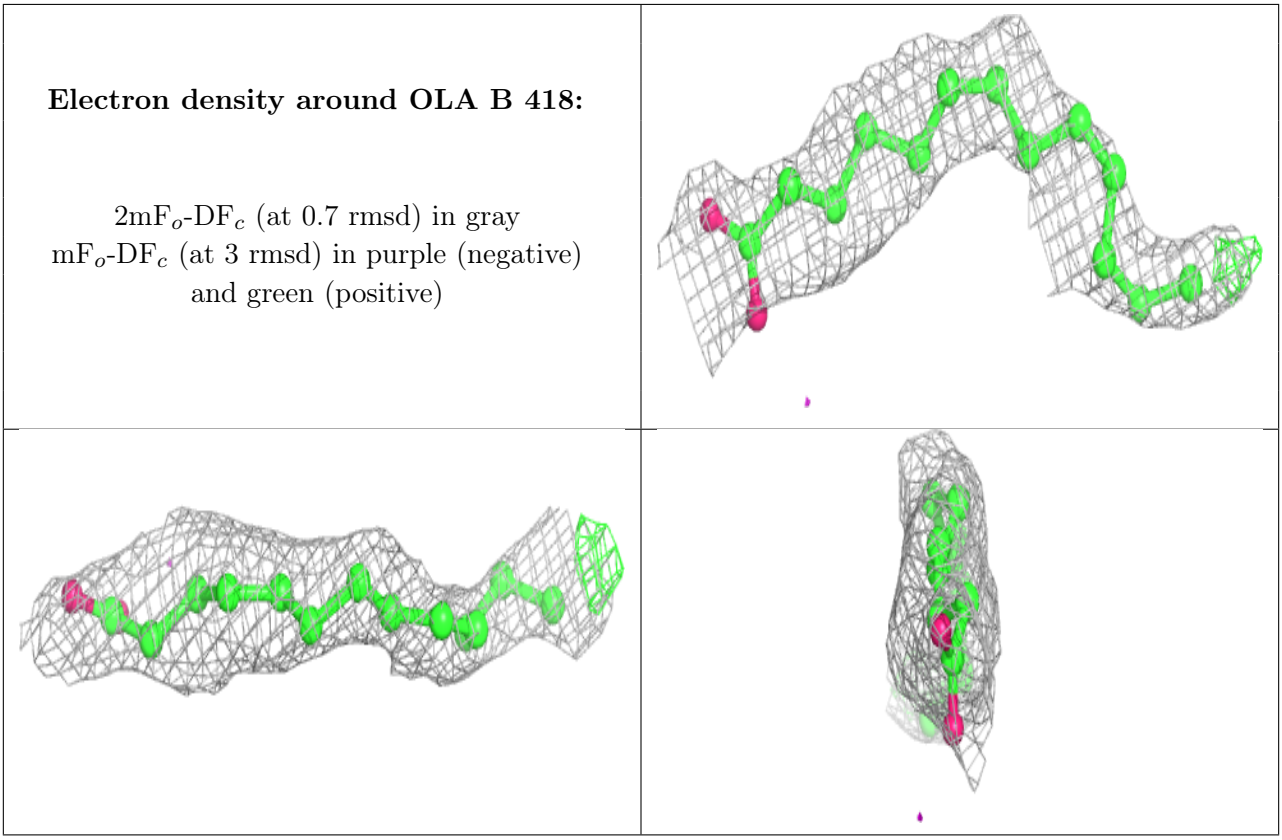
Electron density around OLA A 405:

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



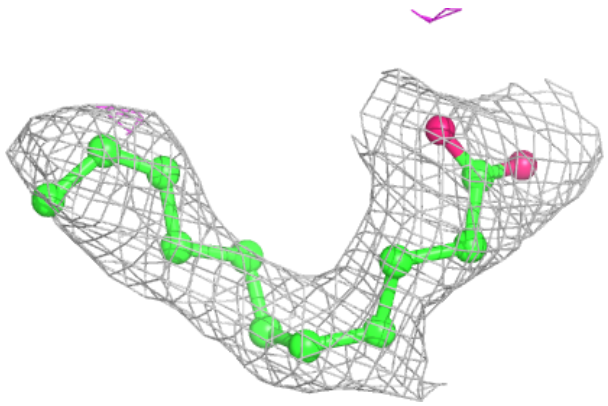
Electron density around OLA B 418:

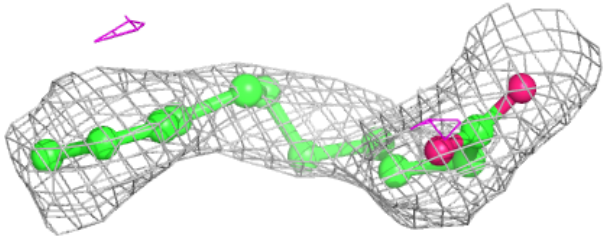
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

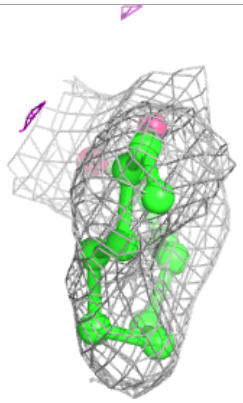


Electron density around OLA B 403:

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

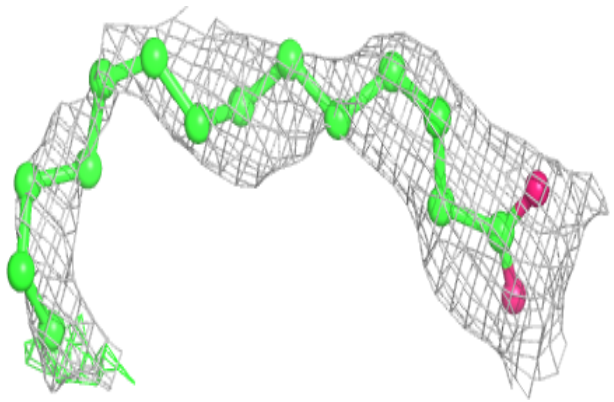


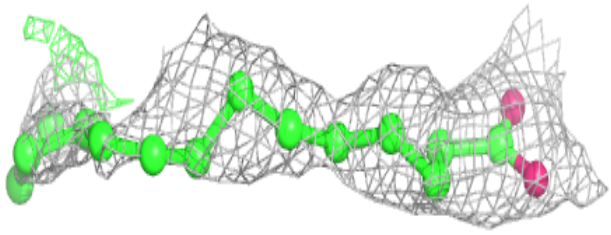


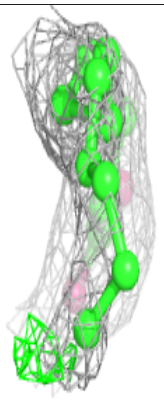


Electron density around OLA A 408:

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

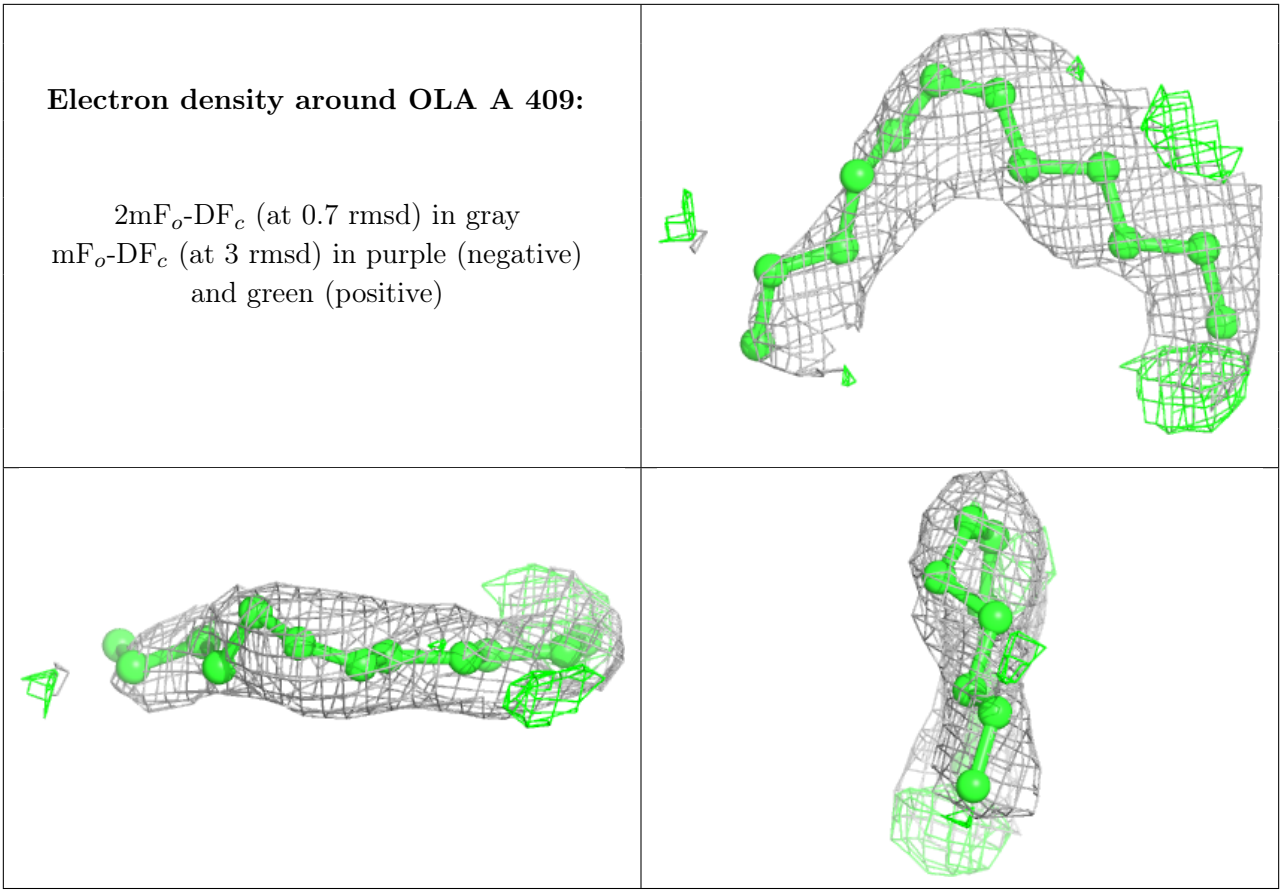






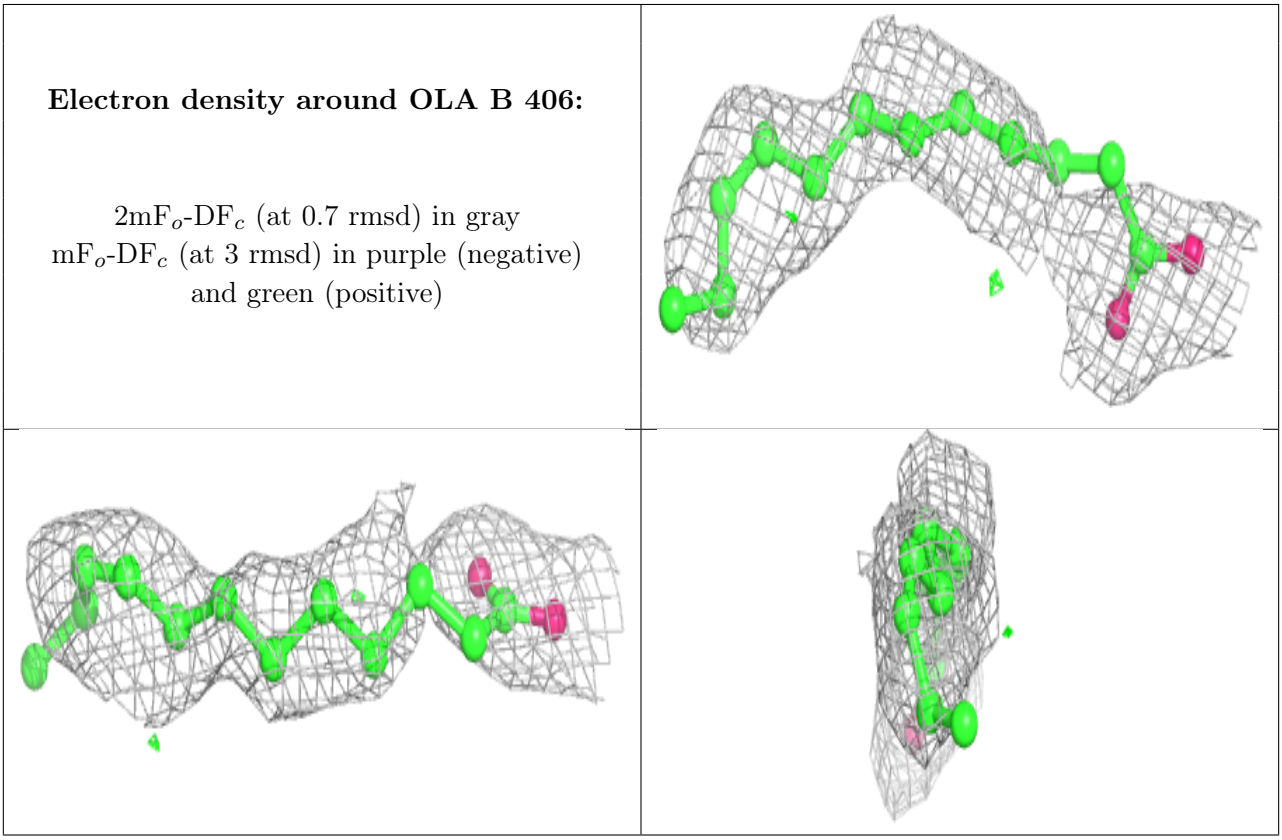
Electron density around OLA A 409:

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



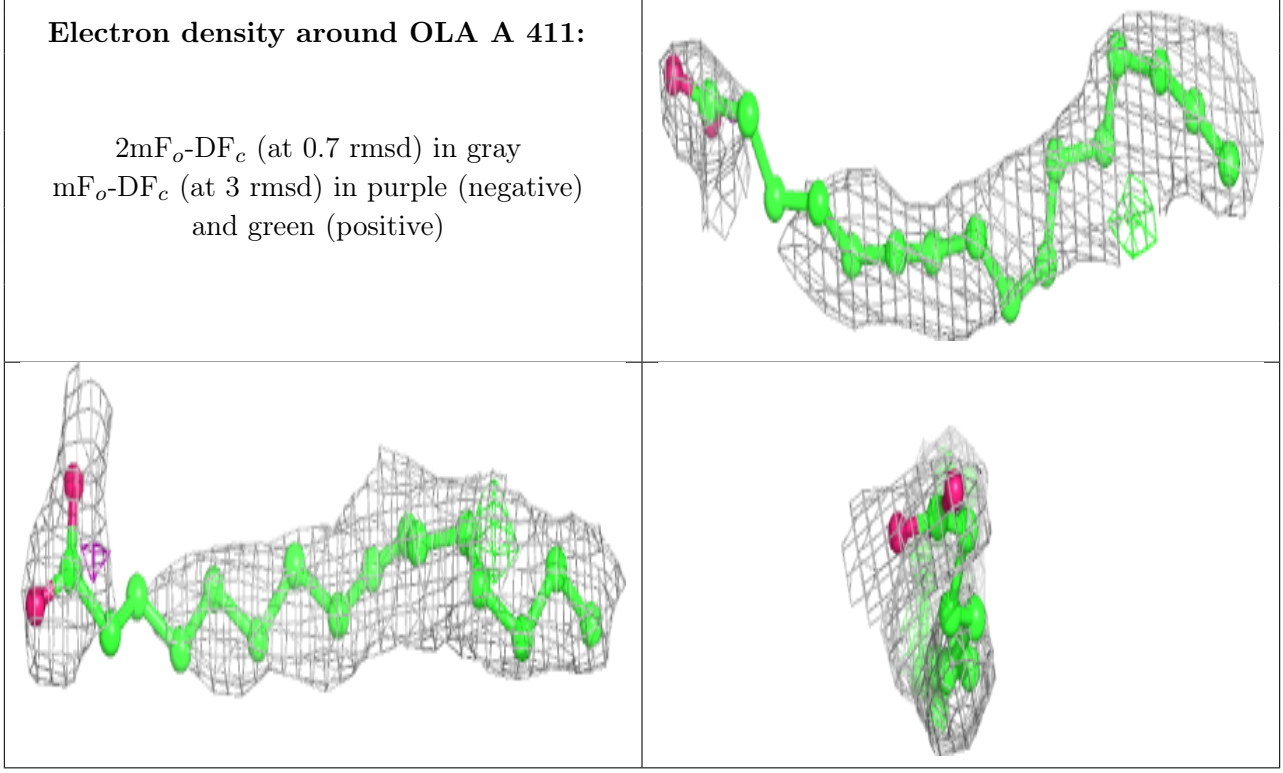
Electron density around OLA B 406:

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



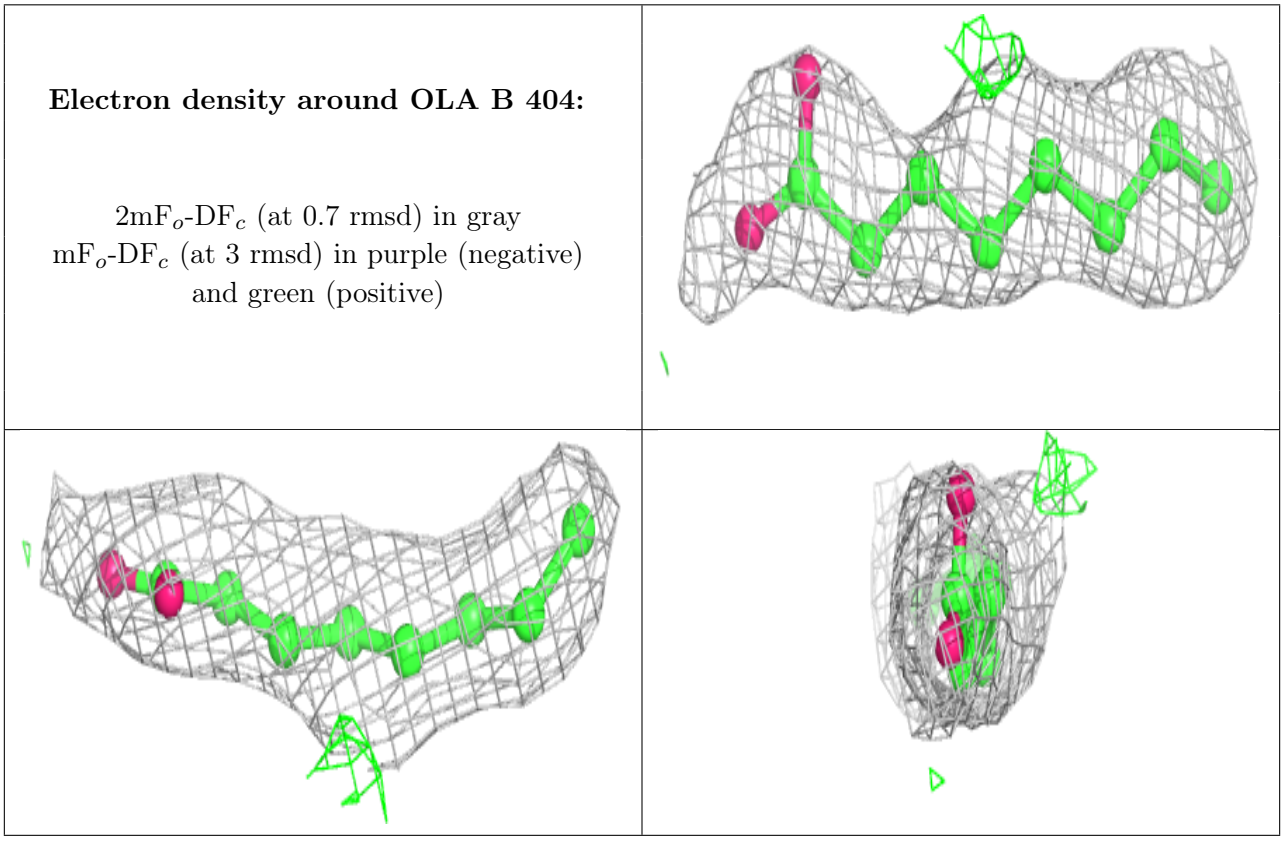
Electron density around OLA A 411:

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



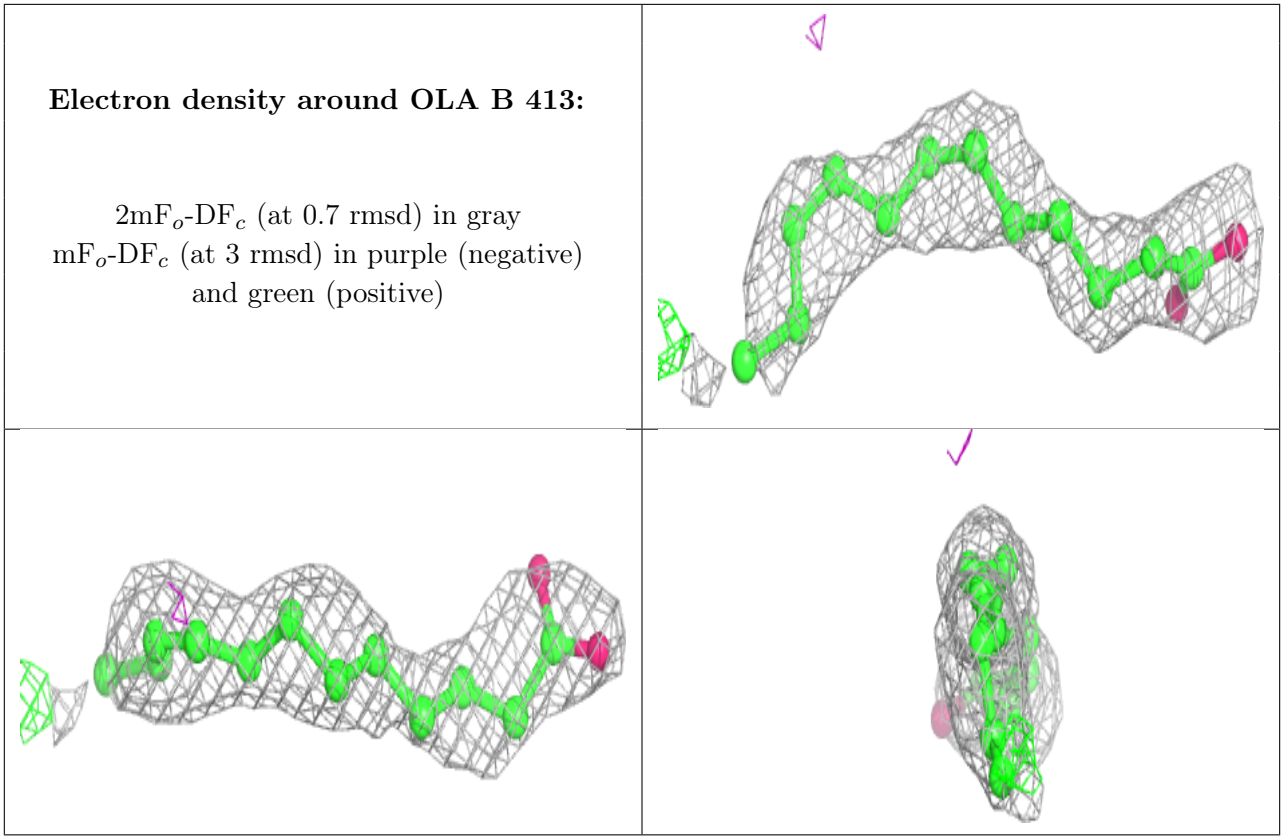
Electron density around OLA B 404:

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



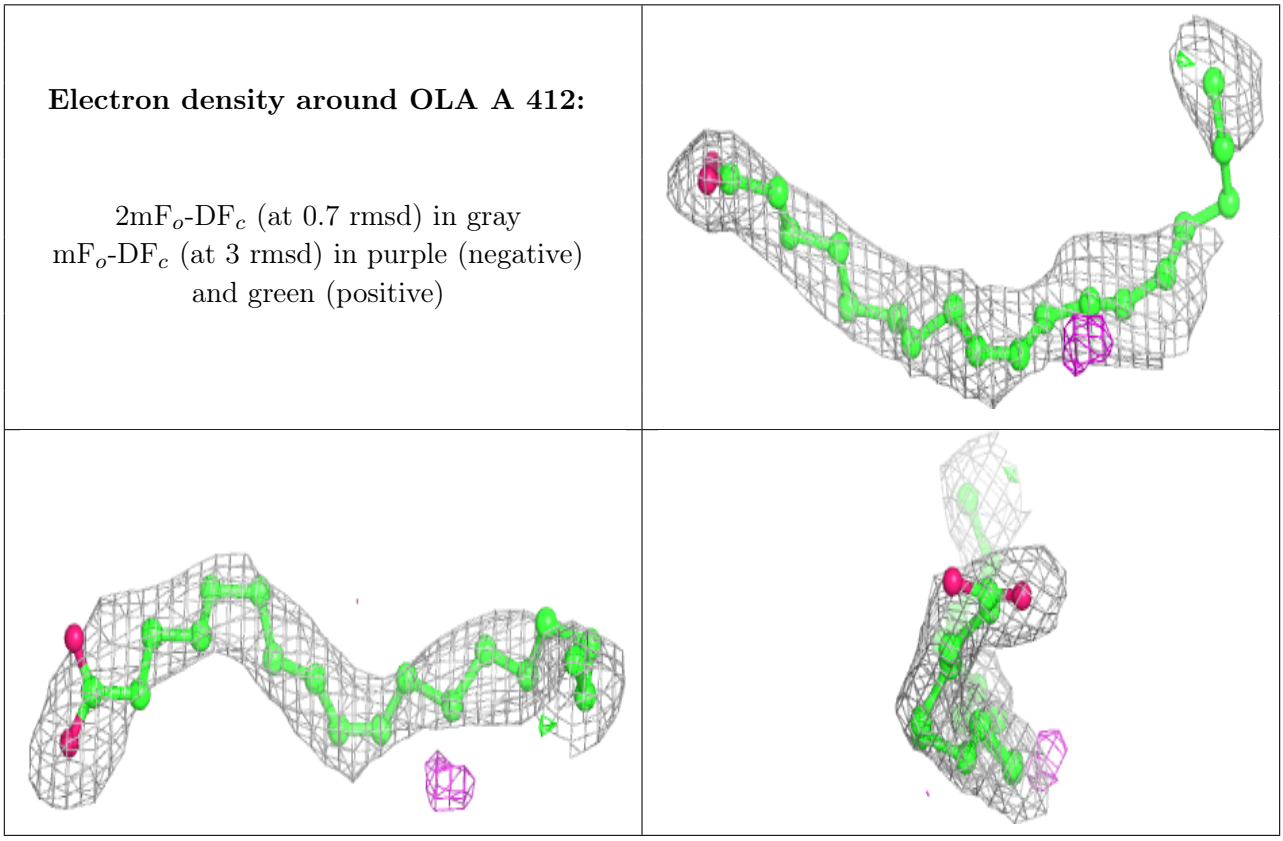
Electron density around OLA B 413:

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



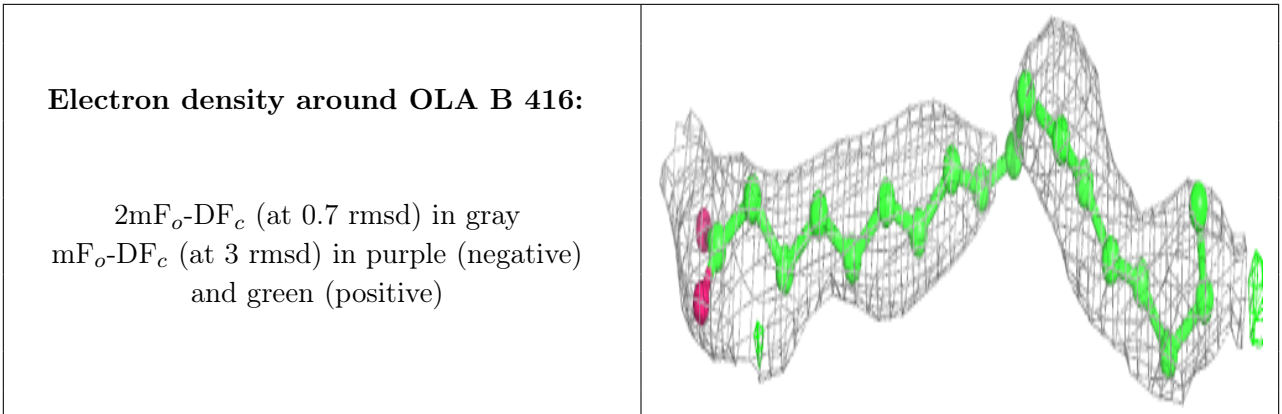
Electron density around OLA A 412:

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



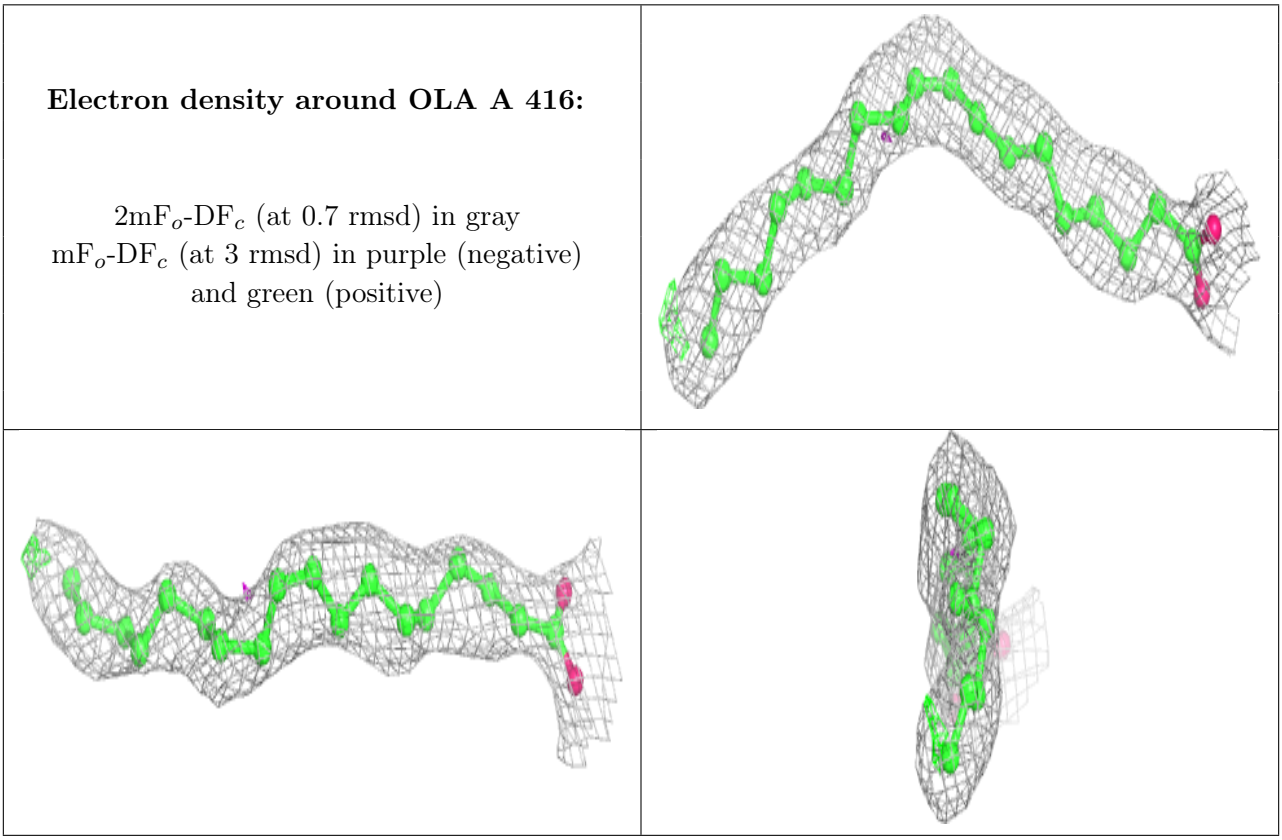
Electron density around OLA B 416:

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



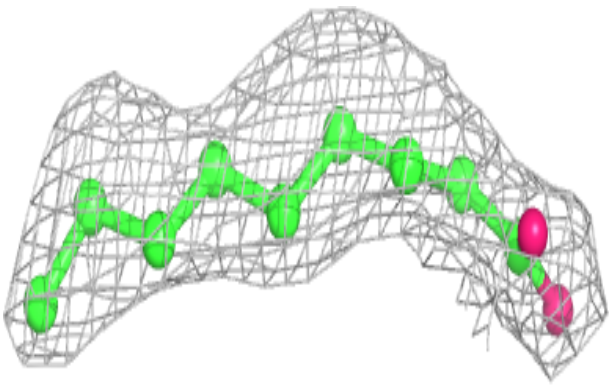
Electron density around OLA A 416:

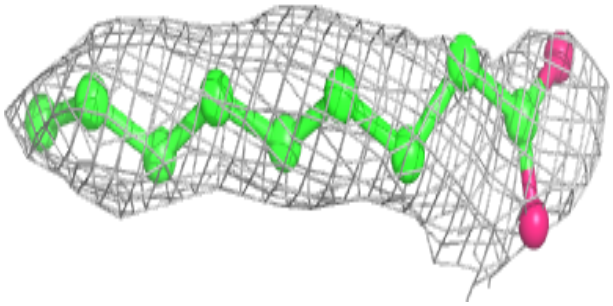
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

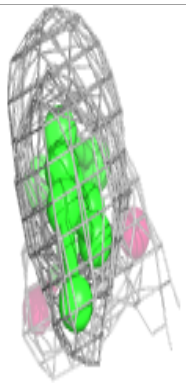


Electron density around OLA A 418:

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

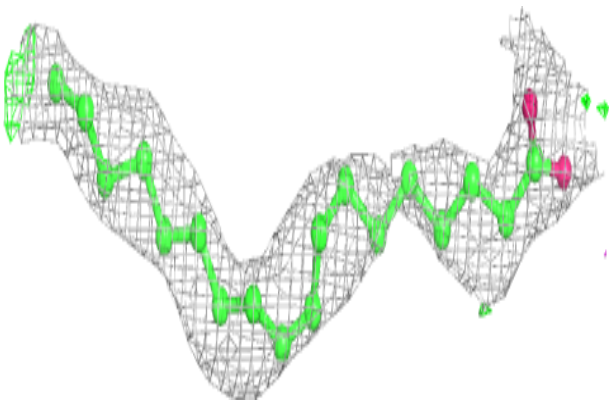


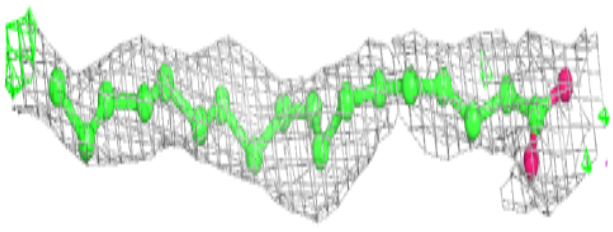


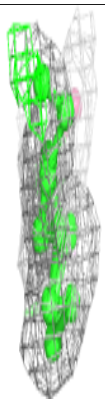


Electron density around OLA B 415:

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

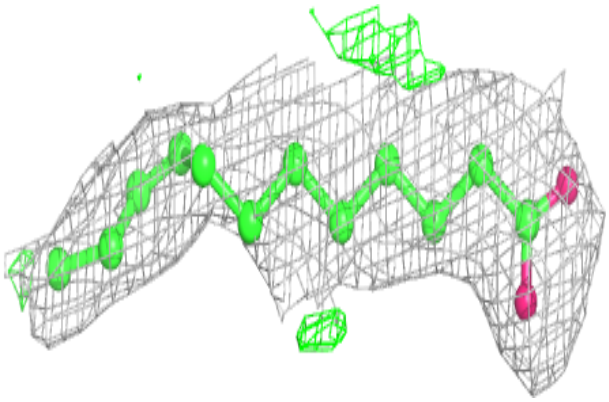


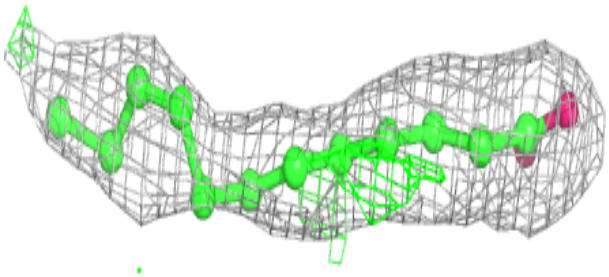


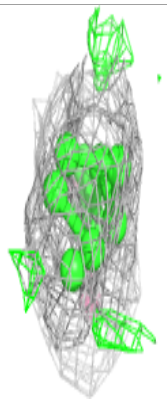


Electron density around OLA A 407:

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

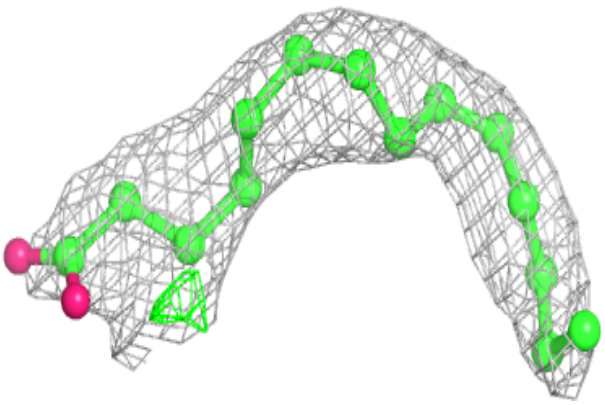


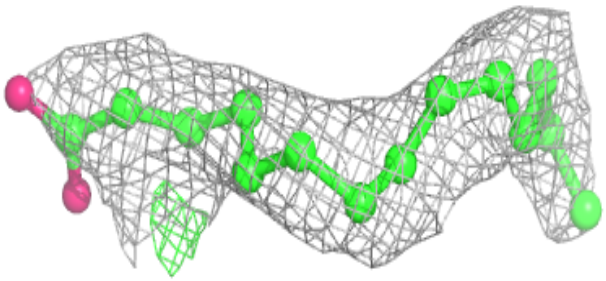


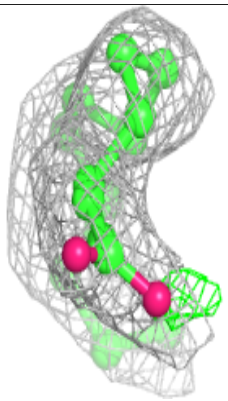


Electron density around OLA B 409:

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

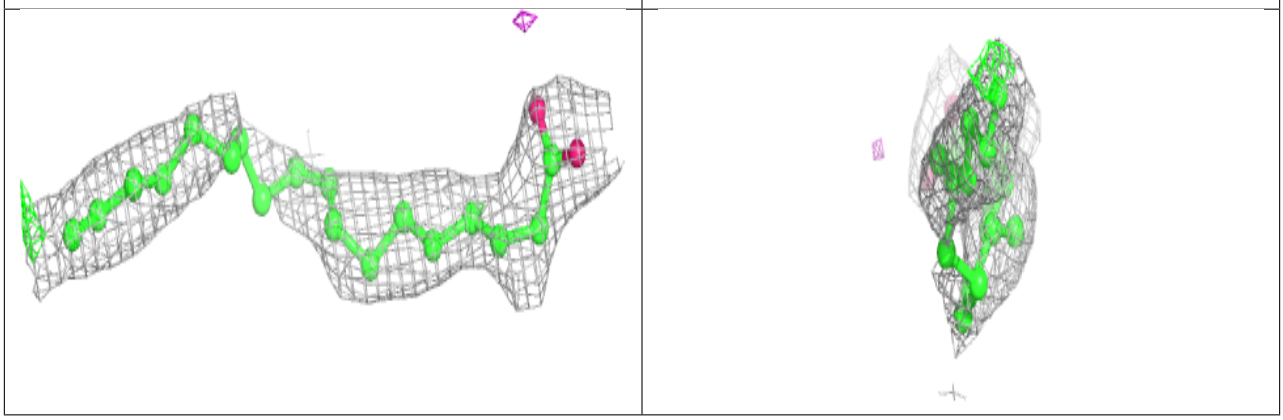






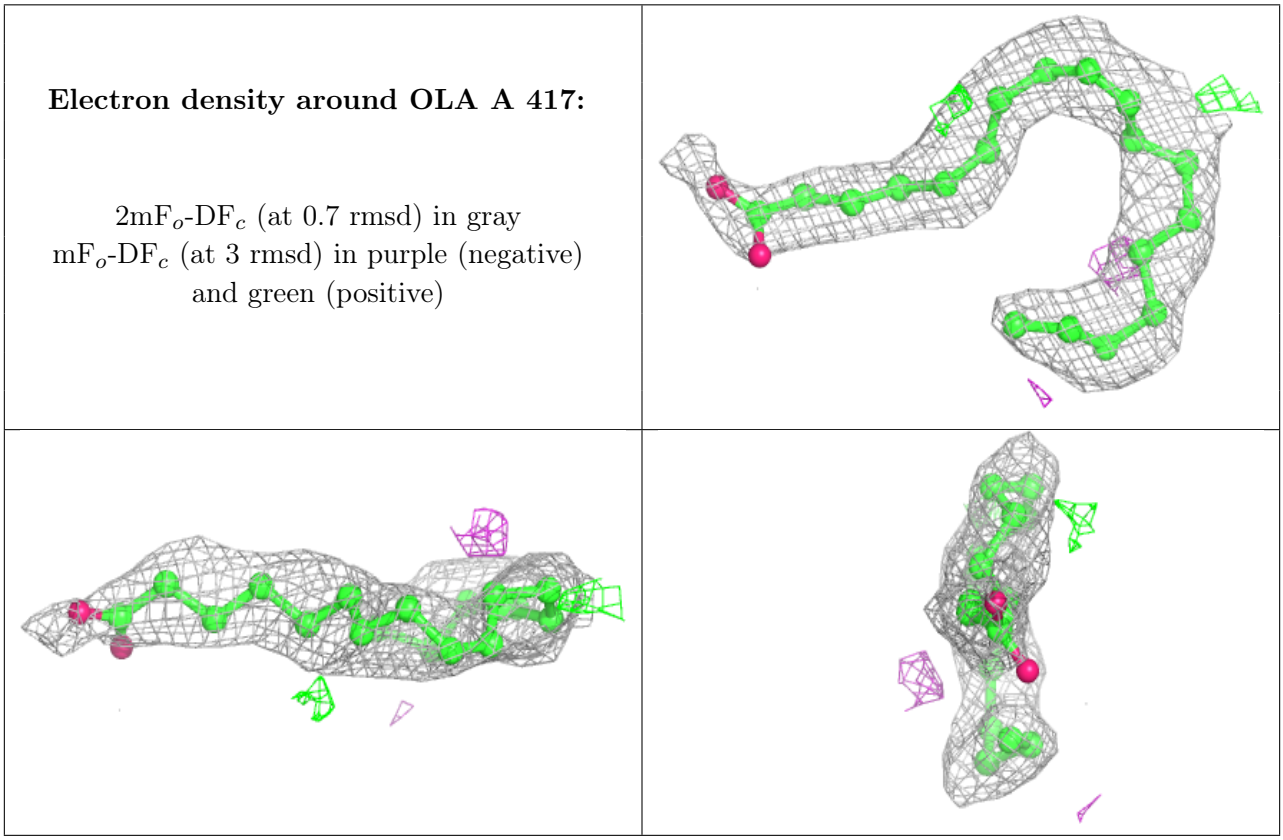
Electron density around OLA B 410:

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



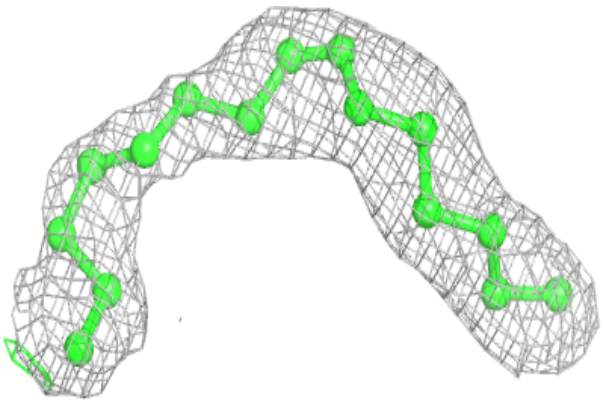
Electron density around OLA A 417:

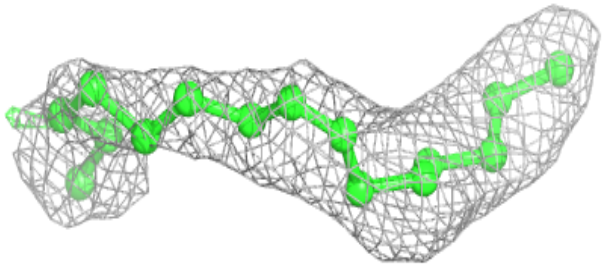
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

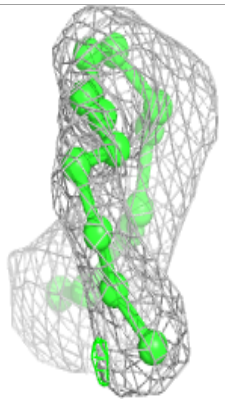


Electron density around OLA A 415:

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

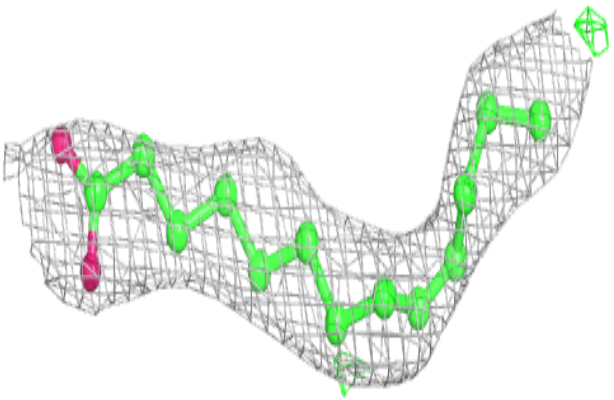


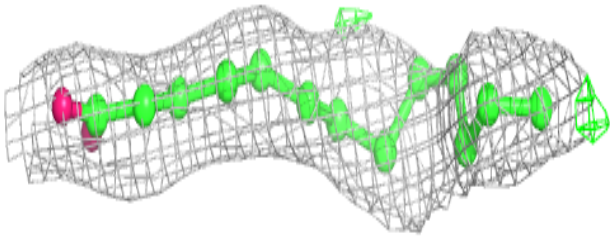


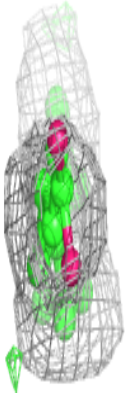


Electron density around OLA B 405:

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

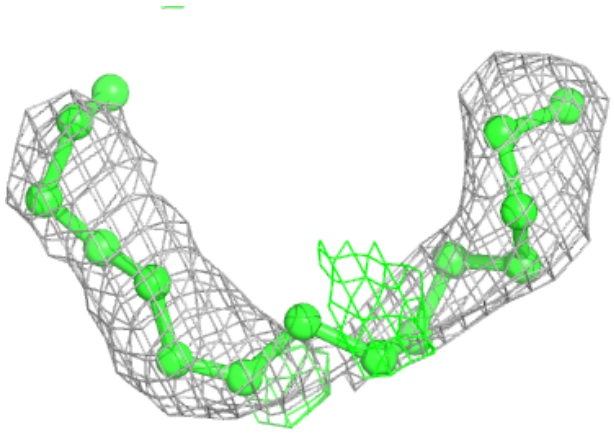


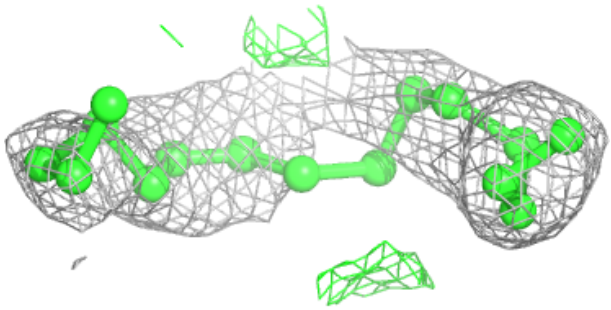


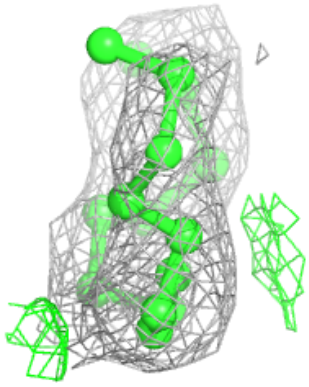


Electron density around OLA A 406:

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

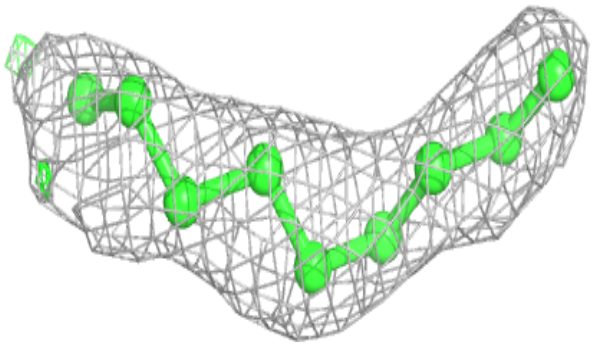


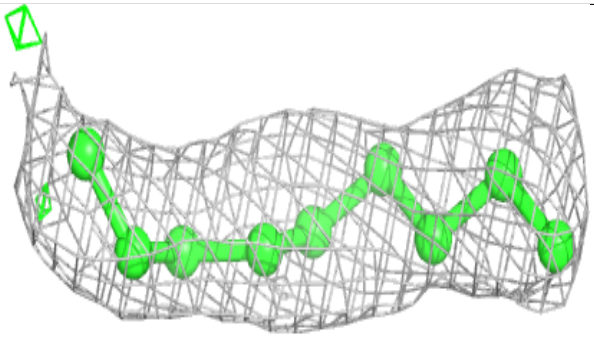


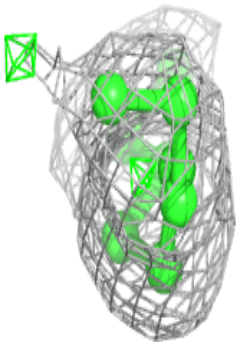


Electron density around OLA B 414:

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

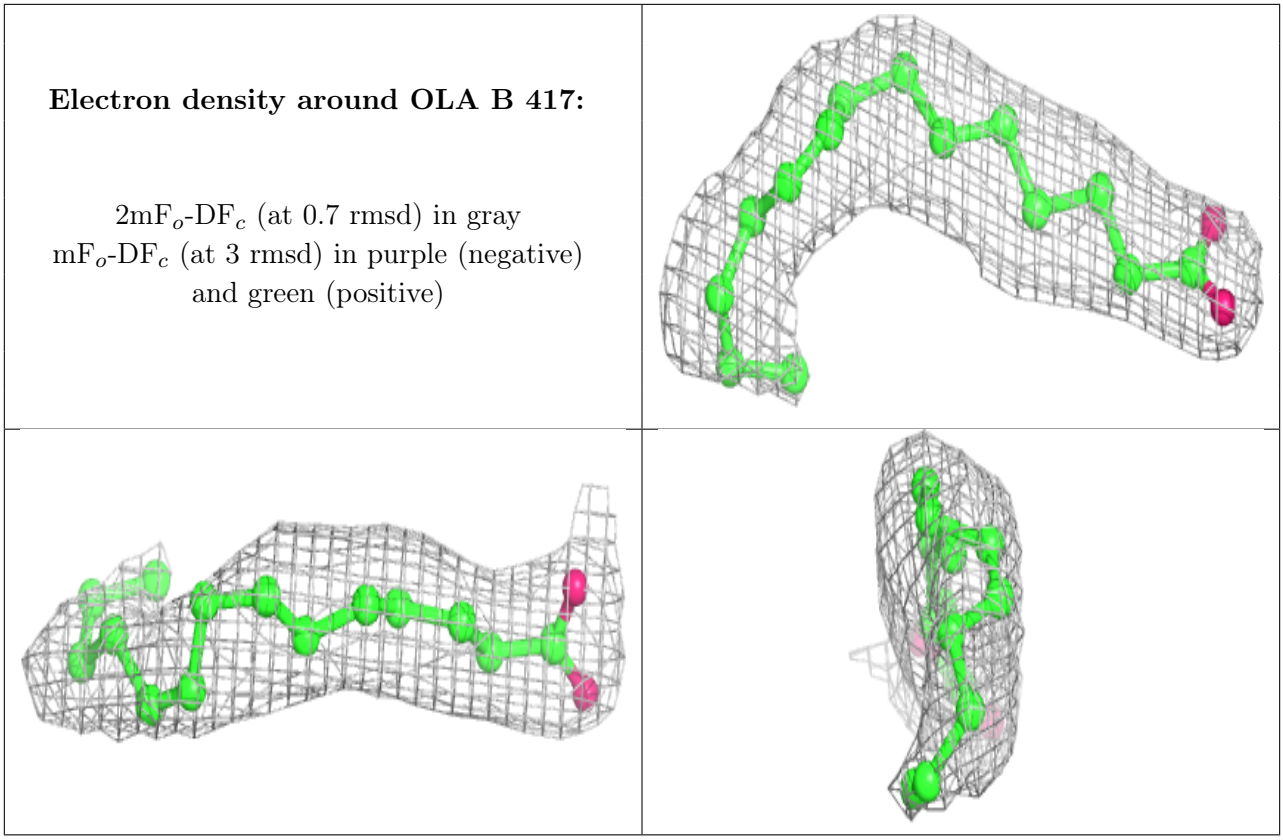






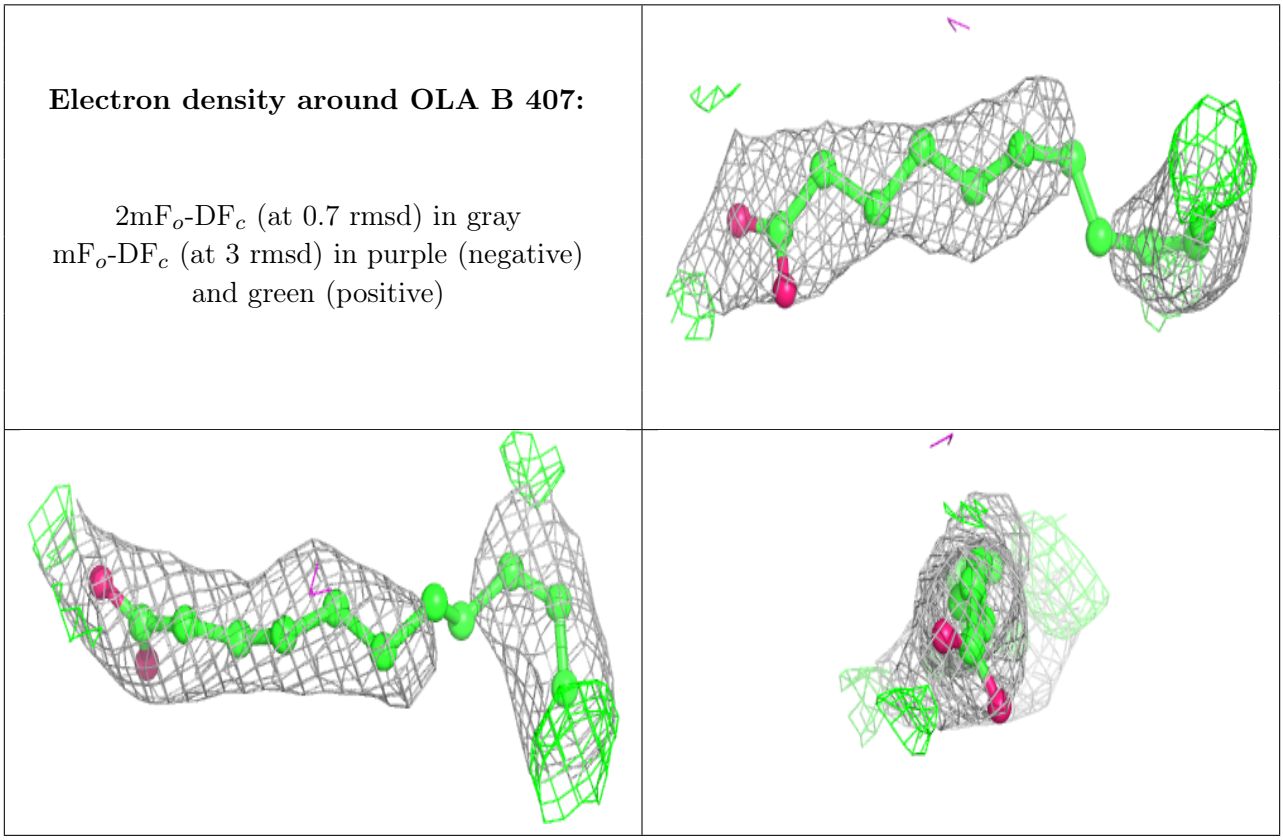
Electron density around OLA B 417:

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



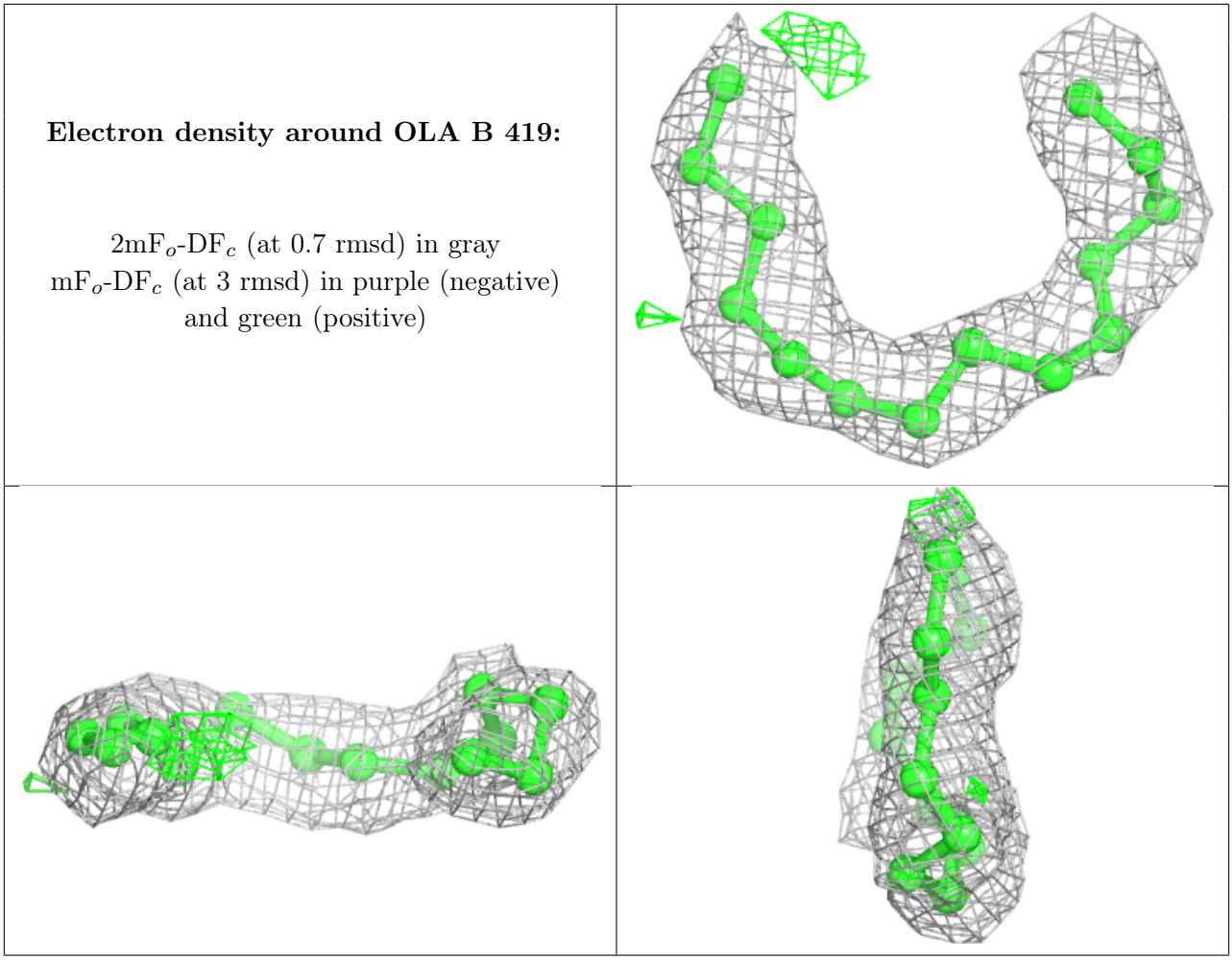
Electron density around OLA B 407:

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



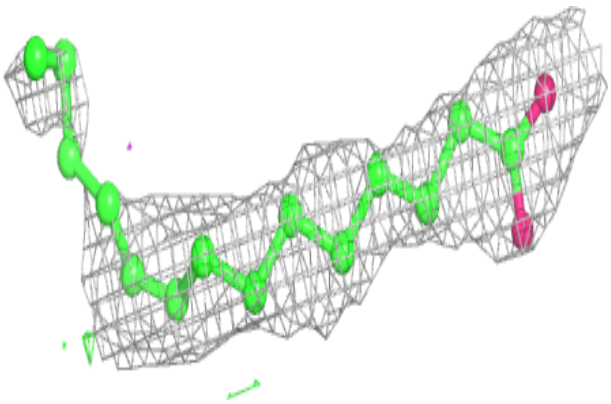
Electron density around OLA B 419:

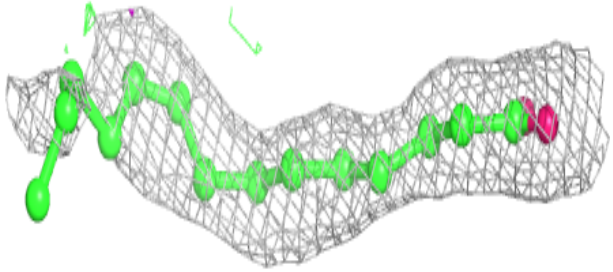
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

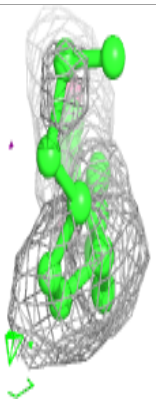


Electron density around OLA A 414:

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

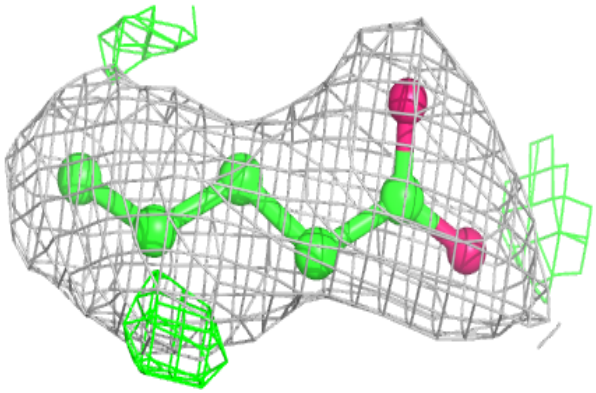


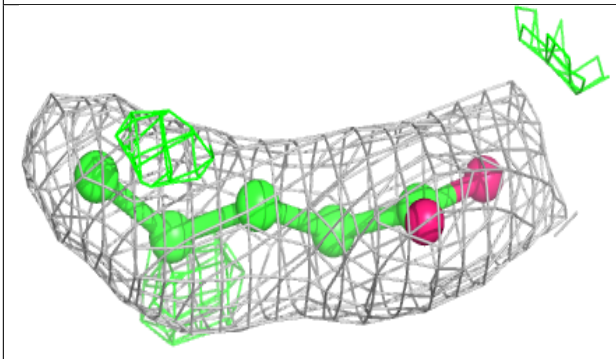


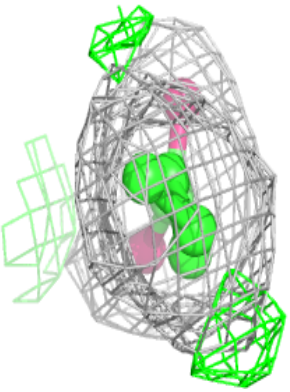


Electron density around OLA B 408:

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

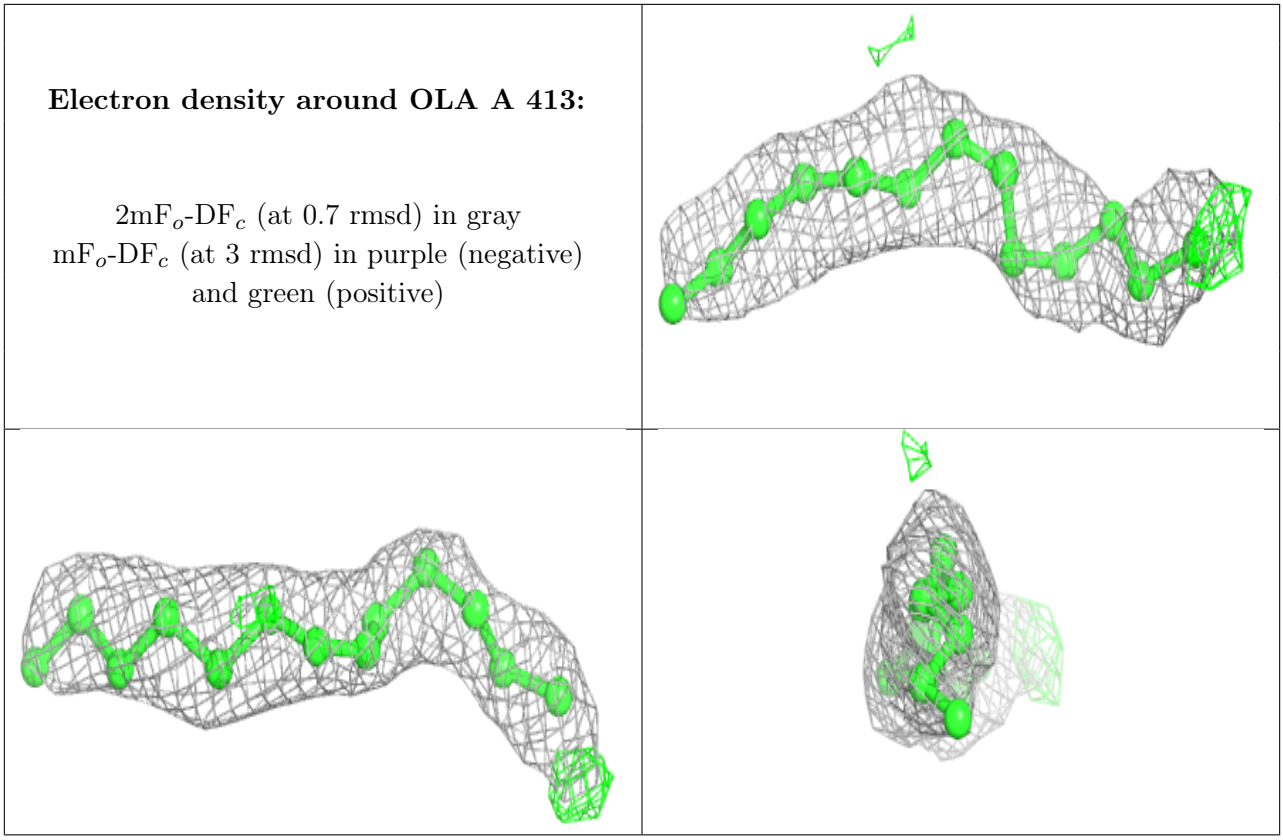






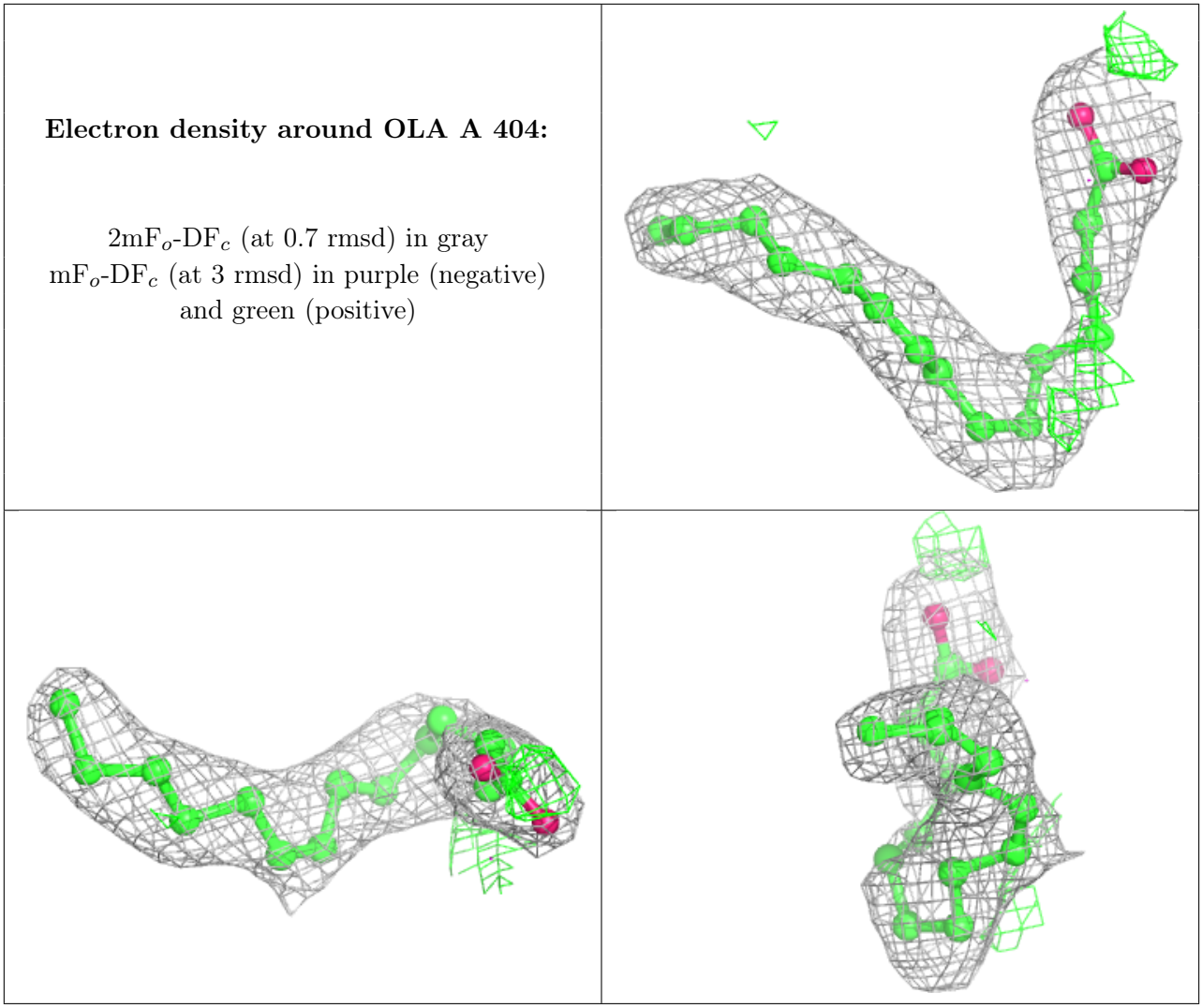
Electron density around OLA A 413:

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



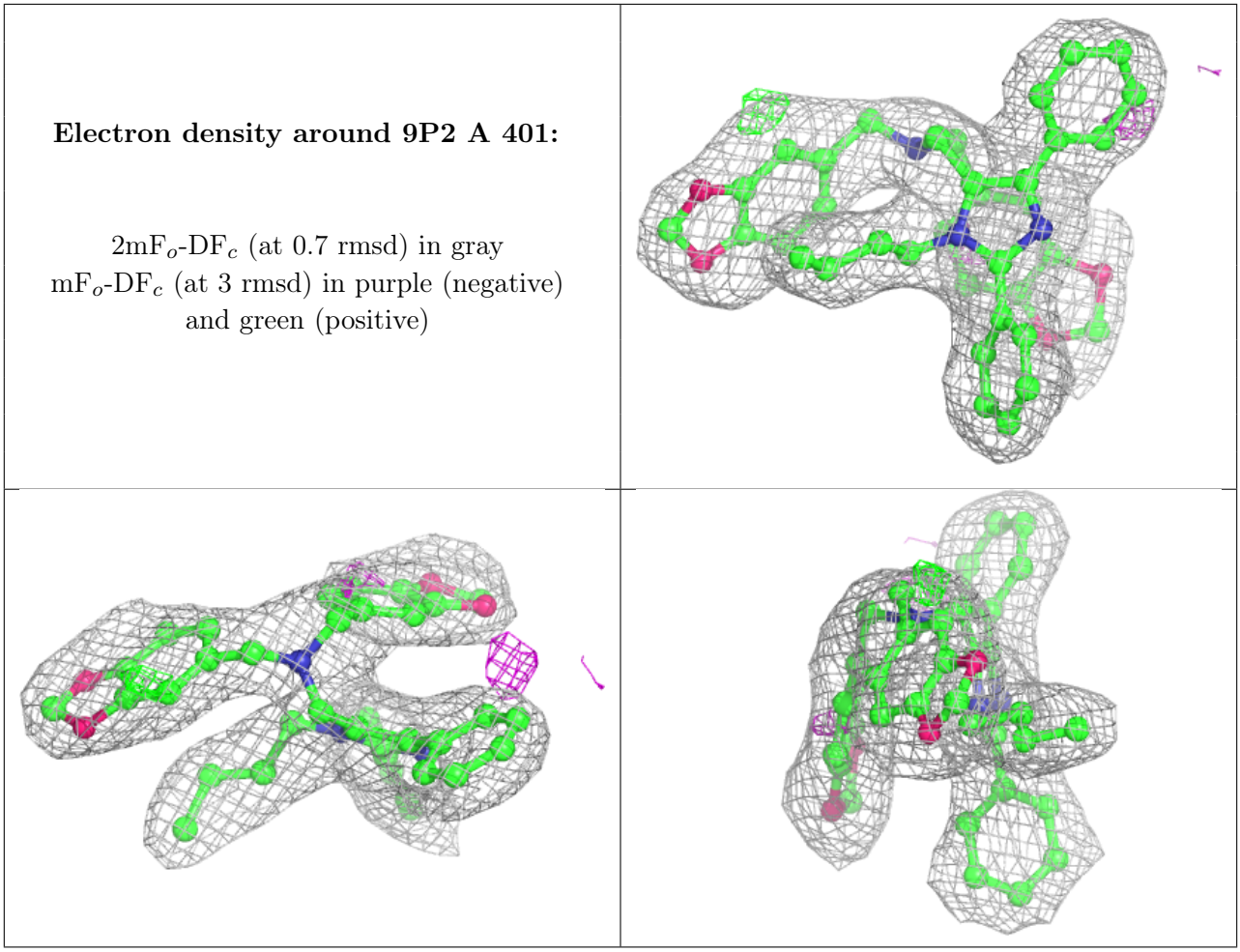
Electron density around OLA A 404:

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



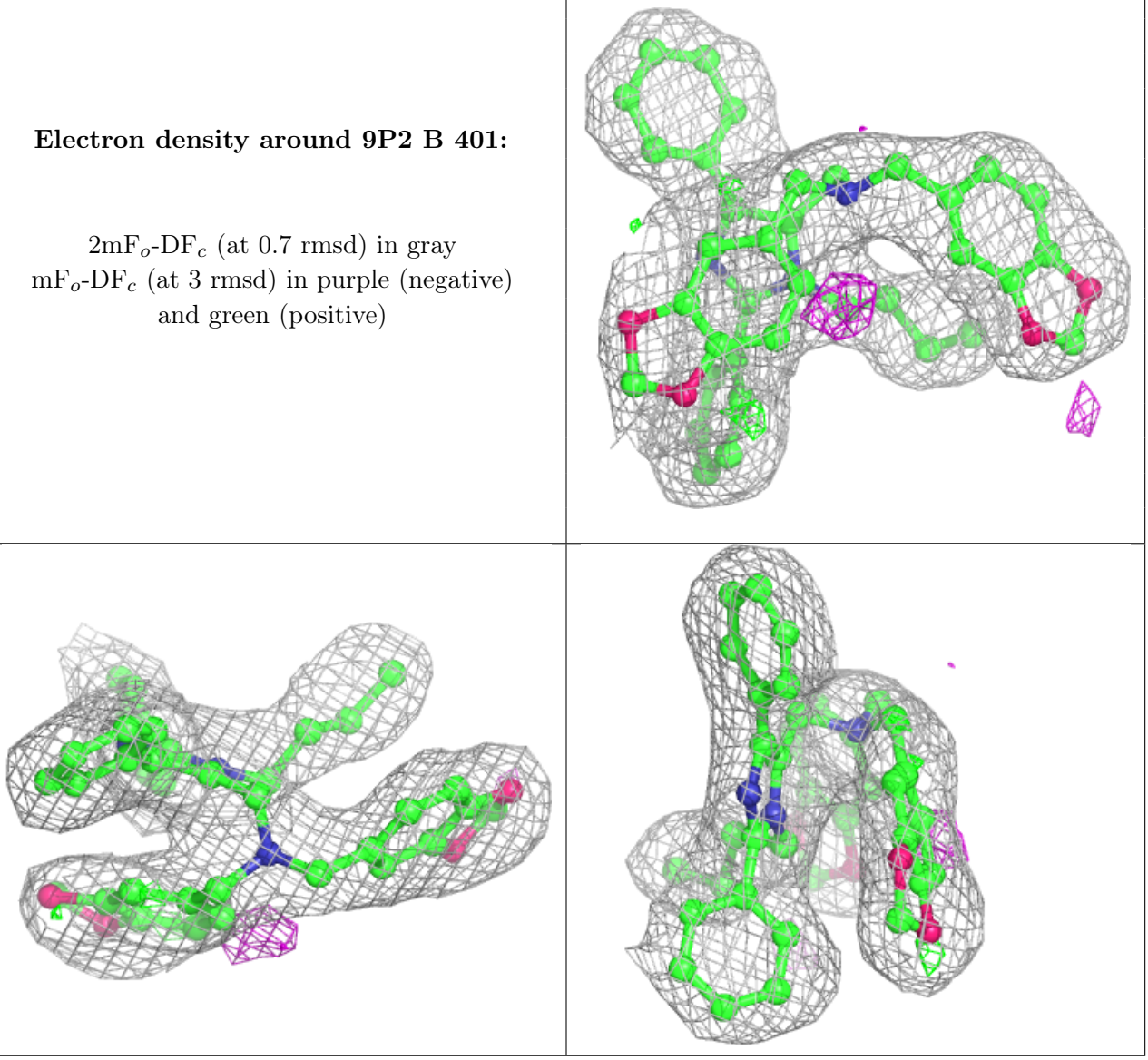
Electron density around 9P2 A 401:

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



Electron density around 9P2 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)



6.5 Other polymers

There are no such residues in this entry.