wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 03:32 pm BST

PDB ID	:	6LI0
Title	:	Crystal structure of GPR52 in complex with agonist c17
Authors	:	Luo, Z.P.; Lin, X.; Xu, F.; Han, G.W.
Deposited on	:	2019-12-10
Resolution	:	2.20 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 following versions of software and data (see references (i)) were used in the production of this report:

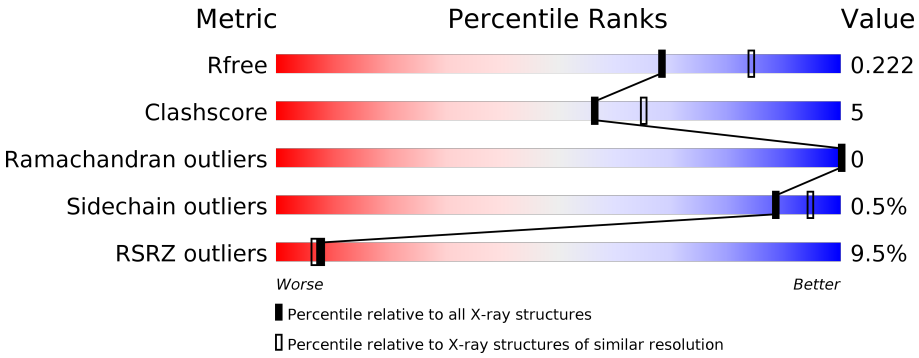
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	468	9% 85% 10% 6%

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
4	OLC	A	1418	-	-	-	X
4	OLC	A	1421	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3910 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 Chimera of G-protein coupled receptor 52 and Flavodoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	1	0
			3479	2270	556	628	25			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	expression tag	UNP Q9Y2T5
A	130	TRP	ALA	engineered mutation	UNP Q9Y2T5
A	1002	ALA	-	linker	UNP Q9Y2T5
A	1098	TRP	TYR	engineered mutation	UNP P00323
A	264	LEU	ALA	engineered mutation	UNP Q9Y2T5
A	278	GLN	TRP	engineered mutation	UNP Q9Y2T5
A	314	PRO	CYS	engineered mutation	UNP Q9Y2T5
A	318	ALA	SER	engineered mutation	UNP Q9Y2T5
A	321	ASP	ASN	engineered mutation	UNP Q9Y2T5
A	323	THR	VAL	engineered mutation	UNP Q9Y2T5
A	341	GLU	-	expression tag	UNP Q9Y2T5
A	342	PHE	-	expression tag	UNP Q9Y2T5
A	343	LEU	-	expression tag	UNP Q9Y2T5
A	344	GLU	-	expression tag	UNP Q9Y2T5
A	345	VAL	-	expression tag	UNP Q9Y2T5
A	346	LEU	-	expression tag	UNP Q9Y2T5
A	347	PHE	-	expression tag	UNP Q9Y2T5
A	348	GLN	-	expression tag	UNP Q9Y2T5
A	349	GLY	-	expression tag	UNP Q9Y2T5
A	350	PRO	-	expression tag	UNP Q9Y2T5
A	351	HIS	-	expression tag	UNP Q9Y2T5
A	352	HIS	-	expression tag	UNP Q9Y2T5
A	353	HIS	-	expression tag	UNP Q9Y2T5
A	354	HIS	-	expression tag	UNP Q9Y2T5
A	355	HIS	-	expression tag	UNP Q9Y2T5
A	356	HIS	-	expression tag	UNP Q9Y2T5
A	357	HIS	-	expression tag	UNP Q9Y2T5

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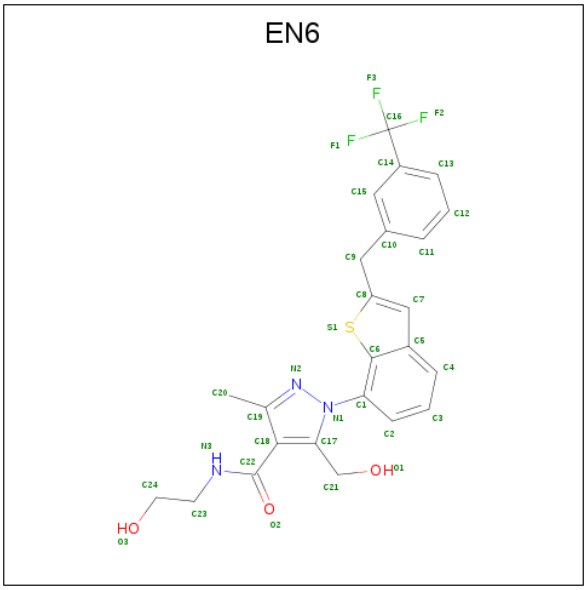
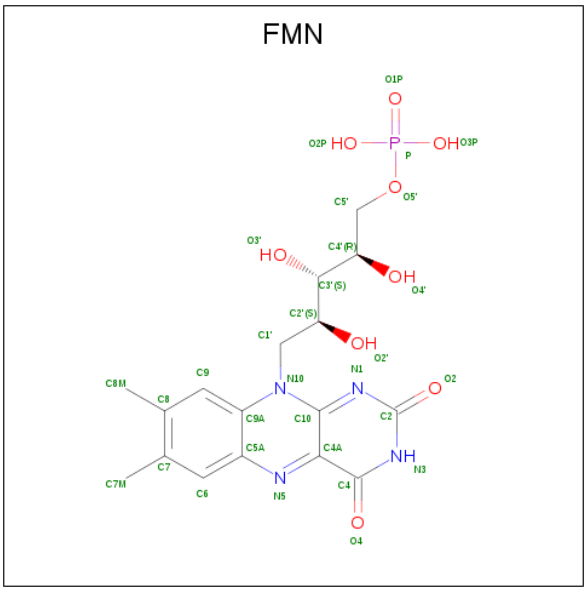
Chain	Residue	Modelled	Actual	Comment	Reference
A	358	HIS	-	expression tag	UNP Q9Y2T5
A	359	HIS	-	expression tag	UNP Q9Y2T5
A	360	HIS	-	expression tag	UNP Q9Y2T5

- Molecule 2 is N-(2-hydroxyethyl)-5-(hydroxymethyl)-3-methyl-1-[2-[[3-(trifluoromethyl)phenyl]methyl]-1-benzothiophen-7-yl]pyrazole-4-carboxamide (three-letter code: EN6) (formula: $C_{24}H_{22}F_3N_3O_3S$) (labeled as "Ligand of Interest" by author).



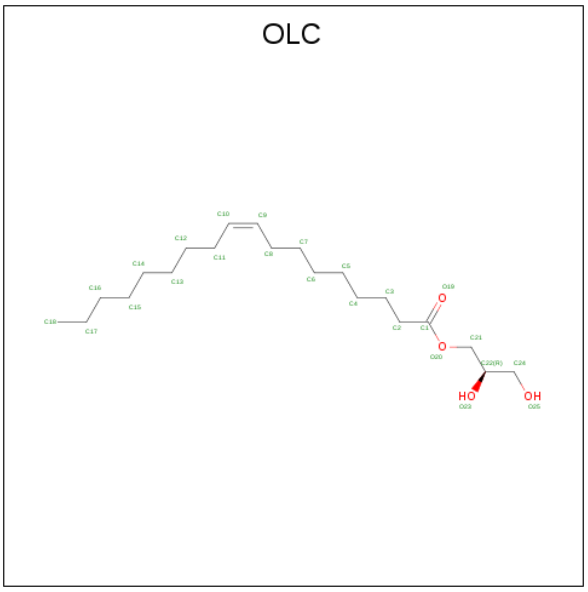
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			34	24	3	3	3	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			25	21	4			
4	A	1	Total	C	O		0	0
			25	21	4			

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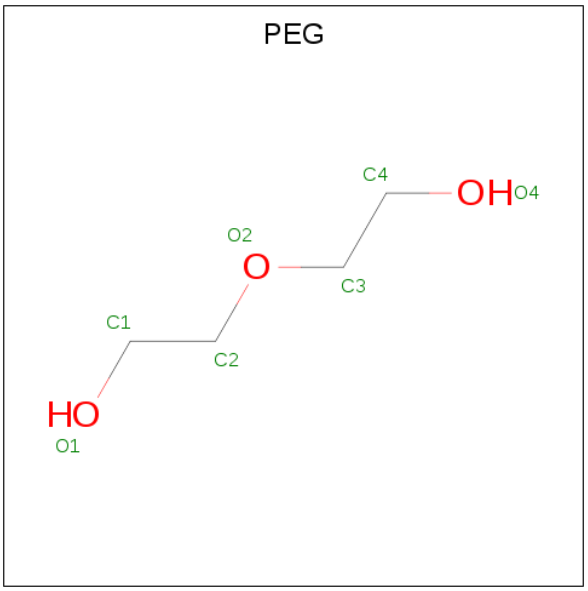
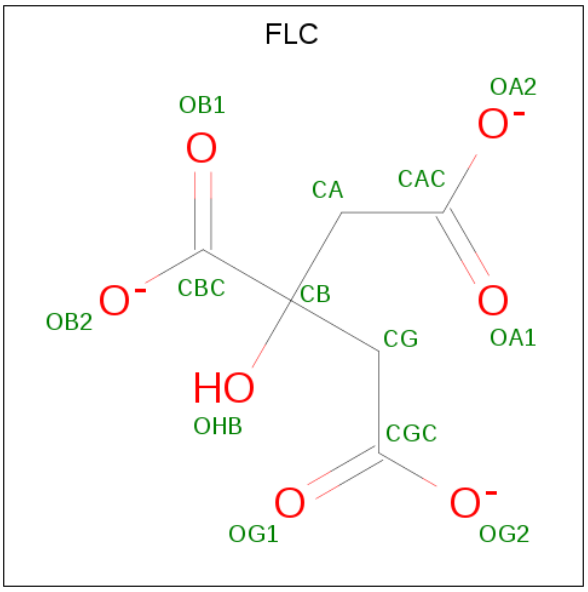
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 15 11 4	0	0
4	A	1	Total C O 16 12 4	0	0
4	A	1	Total C O 16 12 4	0	0
4	A	1	Total C O 12 8 4	0	0
4	A	1	Total C O 13 9 4	0	0
4	A	1	Total C O 23 19 4	0	0
4	A	1	Total C O 11 7 4	0	0
4	A	1	Total C O 9 5 4	0	0
4	A	1	Total C O 15 11 4	0	0
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 18 14 4	0	0
4	A	1	Total C O 16 12 4	0	0
4	A	1	Total C O 9 5 4	0	0
4	A	1	Total C O 9 5 4	0	0
4	A	1	Total C O 25 21 4	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

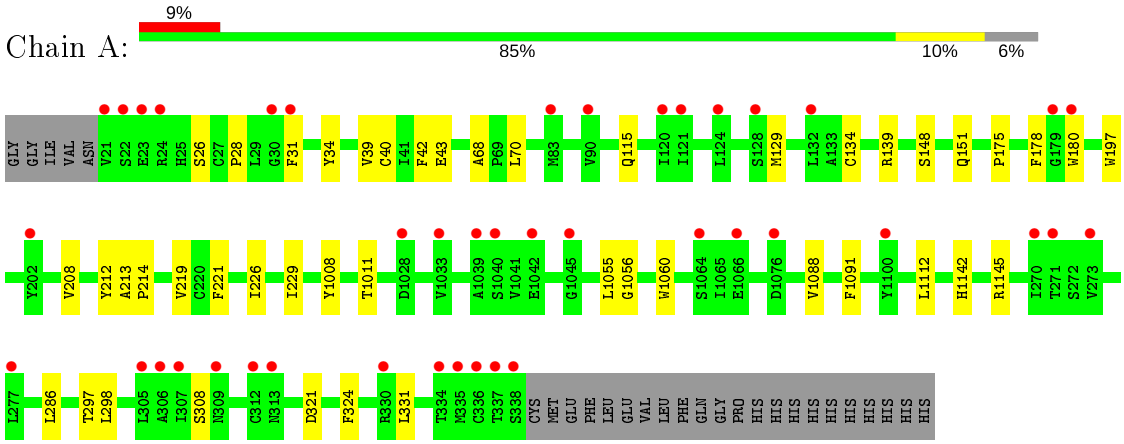
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	30	Total O 30 30	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Chimera of G-protein coupled receptor 52 and Flavodoxin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.97Å 88.36Å 156.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.89 – 2.20 41.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.89-2.20) 99.4 (41.89-2.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.194 , 0.220 0.199 , 0.222	Depositor DCC
R_{free} test set	2108 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	57.0	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3910	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: FMN, FLC, OLC, PEG, EN6

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	0.78	0/3573	0.82	0/4870

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	3479	0	3412	35	0
2	A	34	0	0	0	0
3	A	31	0	19	1	0
4	A	267	0	346	16	0
5	A	56	0	80	1	0
6	A	13	0	5	1	0
7	A	30	0	0	0	0
All	All	3910	0	3862	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 39 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:68:ALA:H	1:A:331:LEU:HD11	1.52	0.75
1:A:68:ALA:N	1:A:331:LEU:HD11	2.10	0.66
1:A:208:VAL:HG21	1:A:286:LEU:HD21	1.79	0.64
4:A:1411:OLC:H24A	4:A:1411:OLC:H2A	1.81	0.61
1:A:31:PHE:HB2	4:A:1417:OLC:H5A	1.82	0.61

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	440/468 (94%)	429 (98%)	11 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	379/404 (94%)	377 (100%)	2 (0%)	88 94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	70	LEU

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

Mol	Chain	Res	Type
1	A	151	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

28 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	OLC	A	1421	-	24,24,24	1.00	1 (4%)	25,25,25	0.91	2 (8%)
4	OLC	A	1412	-	10,10,24	1.86	1 (10%)	11,11,25	1.79	2 (18%)
4	OLC	A	1405	-	14,14,24	1.40	1 (7%)	15,15,25	1.11	1 (6%)
6	FLC	A	1414	-	3,12,12	0.78	0	3,17,17	2.54	2 (66%)
3	FMN	A	1402	-	31,33,33	2.29	7 (22%)	40,50,50	2.64	10 (25%)
4	OLC	A	1407	-	15,15,24	1.40	1 (6%)	16,16,25	1.04	2 (12%)
4	OLC	A	1409	-	12,12,24	1.30	1 (8%)	13,13,25	1.01	1 (7%)
4	OLC	A	1411	-	22,22,24	1.11	1 (4%)	23,23,25	1.27	1 (4%)
5	PEG	A	1424	-	6,6,6	0.37	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	A	1427	-	6,6,6	0.26	0	5,5,5	0.10	0
4	OLC	A	1413	-	8,8,24	1.13	1 (12%)	9,9,25	1.54	2 (22%)
4	OLC	A	1419	-	8,8,24	0.97	1 (12%)	9,9,25	1.15	1 (11%)
4	OLC	A	1404	-	24,24,24	1.12	1 (4%)	25,25,25	1.00	1 (4%)
5	PEG	A	1425	-	6,6,6	0.22	0	5,5,5	0.15	0
5	PEG	A	1422	-	6,6,6	0.23	0	5,5,5	0.34	0
2	EN6	A	1401	-	32,37,37	0.74	2 (6%)	35,54,54	0.78	1 (2%)
4	OLC	A	1420	-	8,8,24	1.17	1 (12%)	9,9,25	1.56	2 (22%)
5	PEG	A	1426	-	6,6,6	0.54	0	5,5,5	0.20	0
4	OLC	A	1416	-	9,9,24	1.85	1 (11%)	10,10,25	1.70	2 (20%)
5	PEG	A	1428	-	6,6,6	0.25	0	5,5,5	0.17	0
4	OLC	A	1408	-	11,11,24	1.60	1 (9%)	12,12,25	1.07	1 (8%)
4	OLC	A	1415	-	14,14,24	1.38	1 (7%)	15,15,25	1.10	2 (13%)
4	OLC	A	1403	-	24,24,24	1.08	2 (8%)	25,25,25	0.98	2 (8%)
5	PEG	A	1410	-	6,6,6	0.23	0	5,5,5	0.23	0
4	OLC	A	1406	-	15,15,24	1.16	1 (6%)	16,16,25	0.90	1 (6%)
5	PEG	A	1423	-	6,6,6	0.16	0	5,5,5	0.14	0
4	OLC	A	1418	-	15,15,24	1.11	1 (6%)	16,16,25	1.04	2 (12%)
4	OLC	A	1417	-	17,17,24	1.19	1 (5%)	18,18,25	1.02	2 (11%)

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	OLC	A	1421	-	-	11/24/24/24	-
4	OLC	A	1412	-	-	5/10/10/24	-
4	OLC	A	1405	-	-	6/14/14/24	-
6	FLC	A	1414	-	-	3/6/16/16	-
3	FMN	A	1402	-	-	1/18/18/18	0/3/3/3
4	OLC	A	1407	-	-	7/15/15/24	-
4	OLC	A	1409	-	-	5/12/12/24	-
4	OLC	A	1411	-	-	14/22/22/24	-
5	PEG	A	1424	-	-	3/4/4/4	-
5	PEG	A	1427	-	-	3/4/4/4	-
4	OLC	A	1413	-	-	2/7/7/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLC	A	1419	-	-	5/7/7/24	-
4	OLC	A	1404	-	-	12/24/24/24	-
5	PEG	A	1425	-	-	1/4/4/4	-
5	PEG	A	1422	-	-	3/4/4/4	-
2	EN6	A	1401	-	-	0/16/24/24	0/4/4/4
4	OLC	A	1420	-	-	2/7/7/24	-
5	PEG	A	1426	-	-	3/4/4/4	-
4	OLC	A	1416	-	-	3/9/9/24	-
5	PEG	A	1428	-	-	4/4/4/4	-
4	OLC	A	1408	-	-	3/11/11/24	-
4	OLC	A	1415	-	-	7/14/14/24	-
4	OLC	A	1403	-	-	14/24/24/24	-
5	PEG	A	1410	-	-	3/4/4/4	-
4	OLC	A	1406	-	-	5/15/15/24	-
5	PEG	A	1423	-	-	2/4/4/4	-
4	OLC	A	1418	-	-	7/15/15/24	-
4	OLC	A	1417	-	-	8/17/17/24	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	FMN	C4A-C10	8.60	1.47	1.38
4	A	1412	OLC	O20-C1	5.35	1.49	1.33
4	A	1416	OLC	O20-C1	5.34	1.49	1.33
4	A	1408	OLC	O20-C1	5.14	1.48	1.33
4	A	1404	OLC	O20-C1	5.07	1.48	1.33

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1402	FMN	C4-N3-C2	10.02	123.60	115.14
3	A	1402	FMN	C4-C4A-C10	-7.18	115.20	119.95
3	A	1402	FMN	C1'-N10-C9A	5.53	122.64	118.29
4	A	1416	OLC	O20-C1-C2	4.68	123.66	111.38
4	A	1412	OLC	O20-C1-C2	4.43	125.80	111.91

There are no chirality outliers.

5 of 142 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1412	OLC	O20-C21-C22-C24
4	A	1405	OLC	C21-C22-C24-O25
4	A	1405	OLC	O20-C21-C22-O23
6	A	1414	FLC	CAC-CA-CB-CBC
4	A	1419	OLC	C21-C22-C24-O25

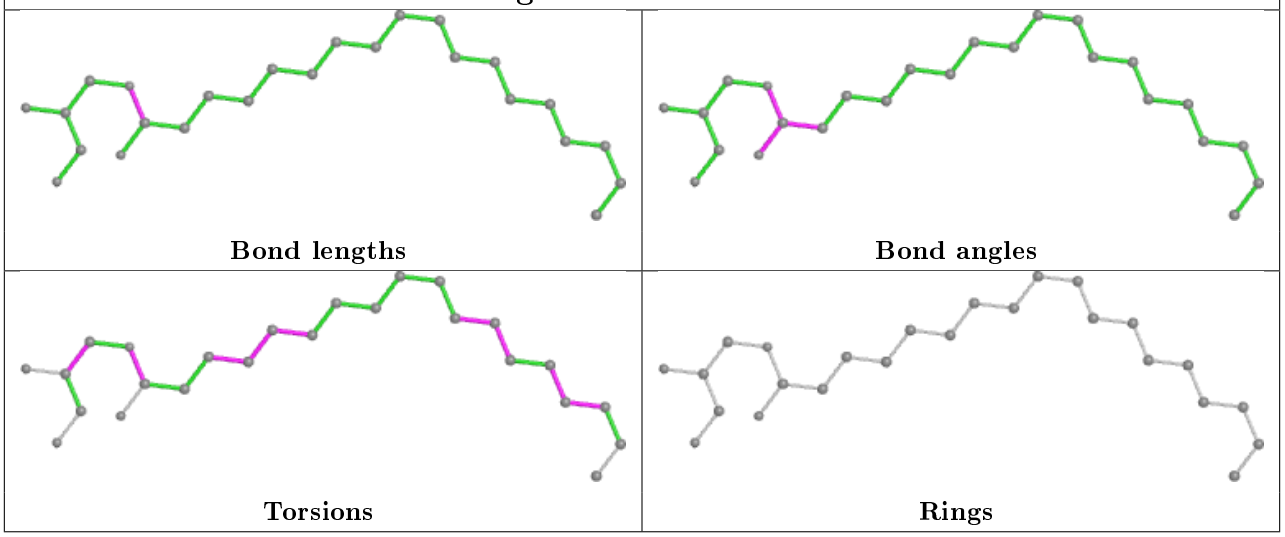
There are no ring outliers.

12 monomers are involved in 19 short contacts:

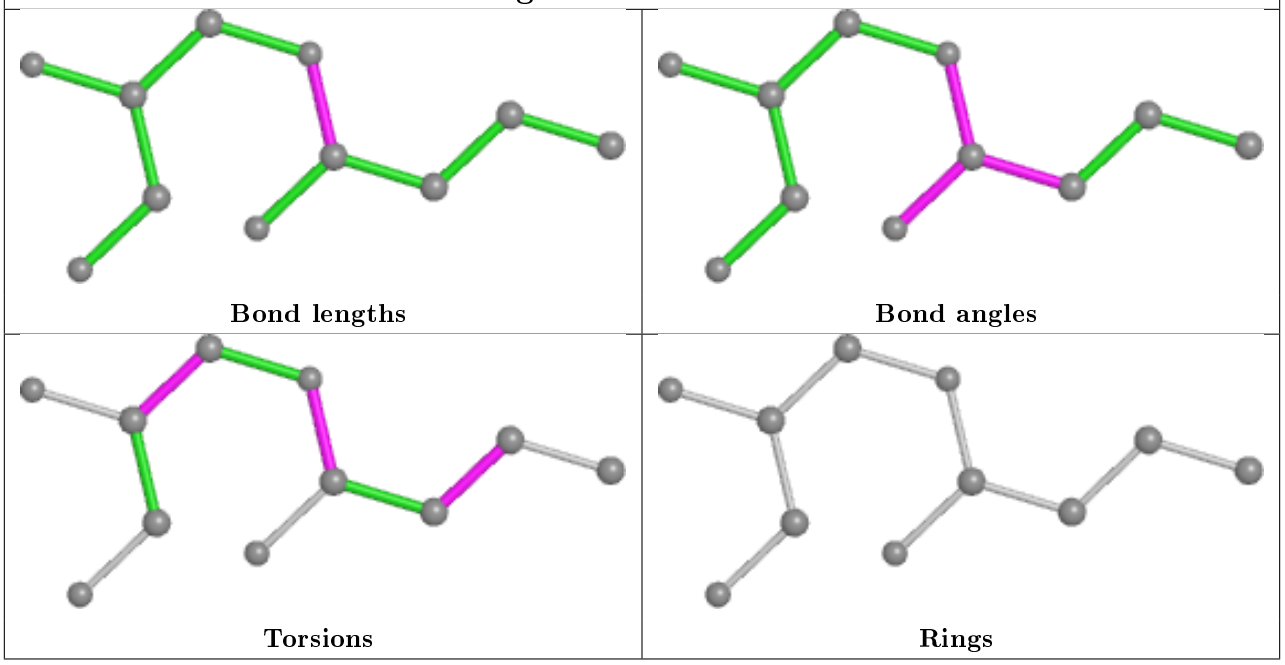
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1421	OLC	2	0
4	A	1412	OLC	1	0
6	A	1414	FLC	1	0
3	A	1402	FMN	1	0
4	A	1409	OLC	1	0
4	A	1411	OLC	2	0
4	A	1408	OLC	1	0
4	A	1415	OLC	1	0
5	A	1410	PEG	1	0
4	A	1406	OLC	2	0
4	A	1418	OLC	3	0
4	A	1417	OLC	3	0

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.

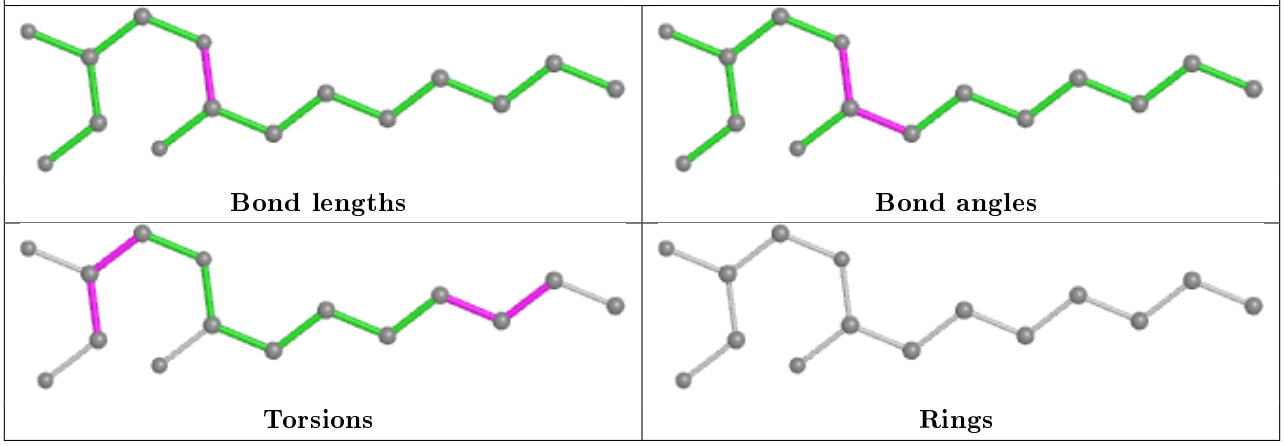
Ligand OLC A 1421



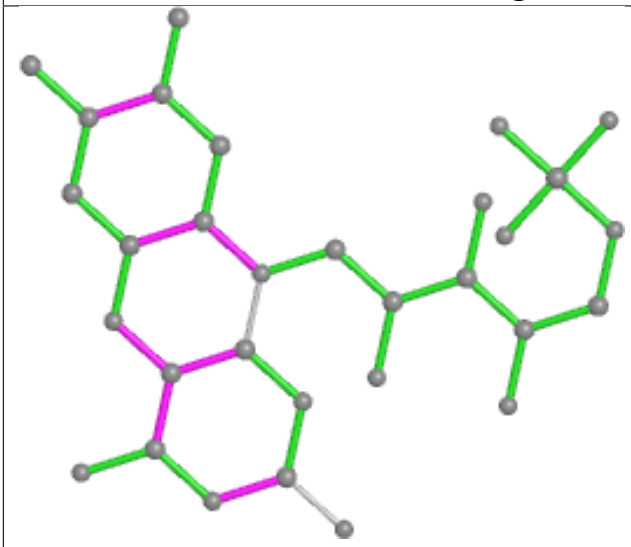
Ligand OLC A 1412



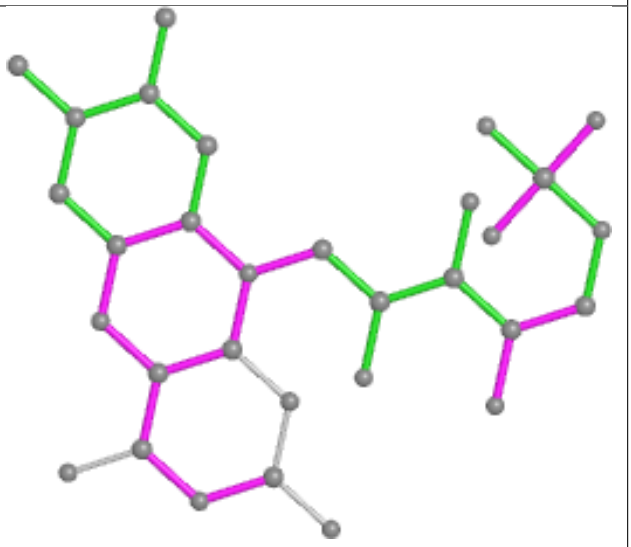
Ligand OLC A 1405



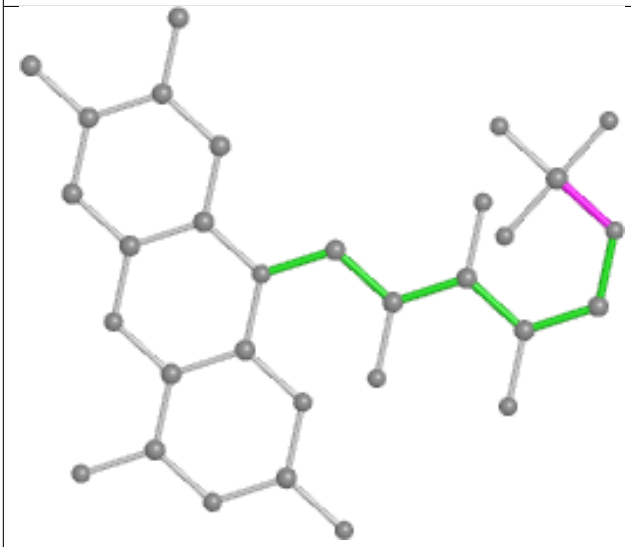
Ligand FMN A 1402



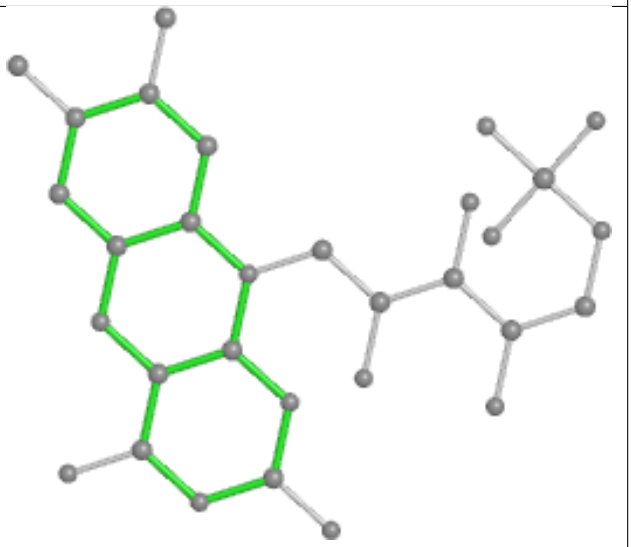
Bond lengths



Bond angles

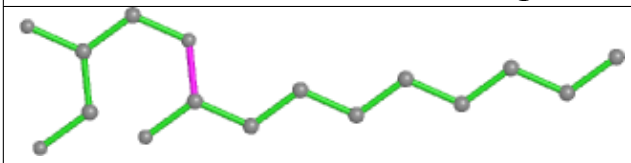


Torsions

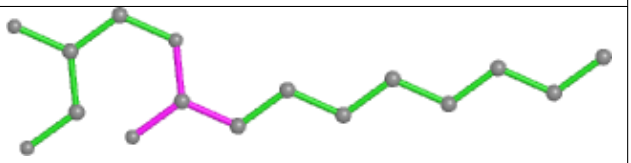


Rings

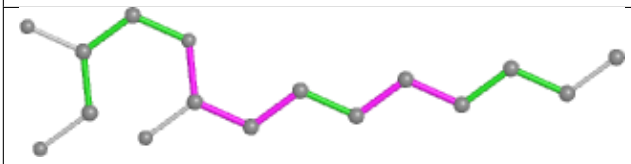
Ligand OLC A 1407



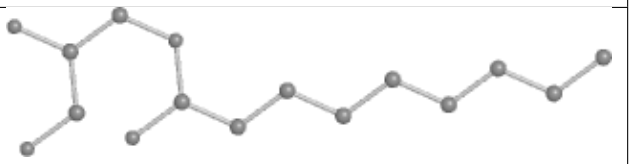
Bond lengths



Bond angles

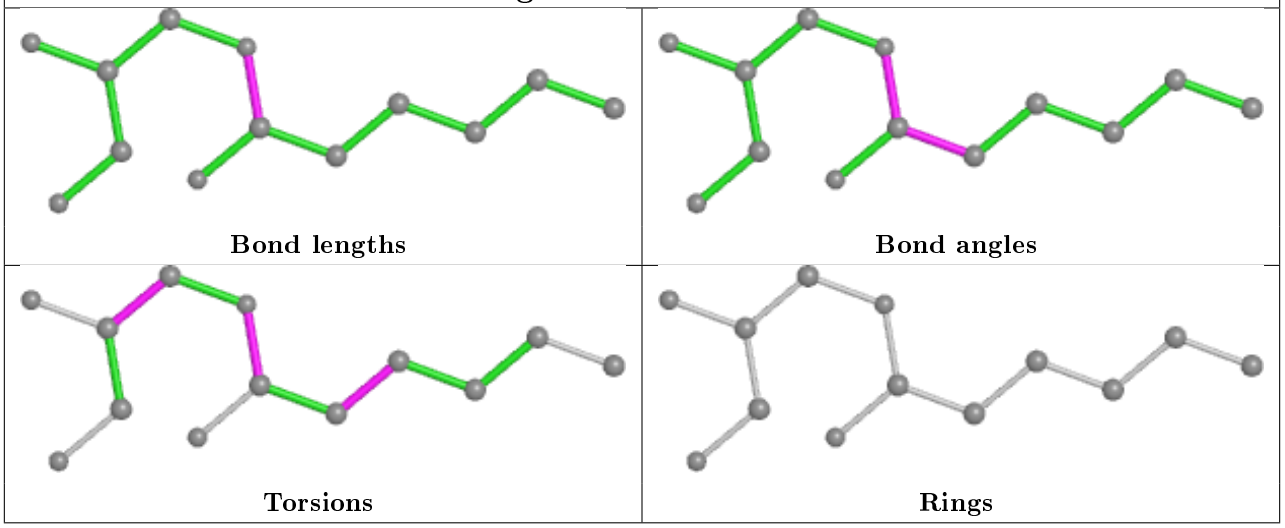


Torsions

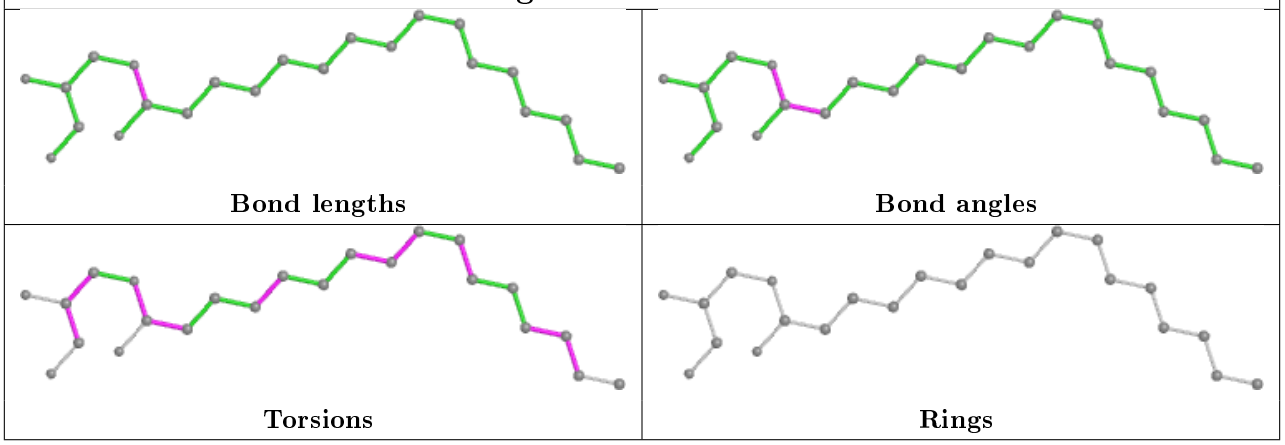


Rings

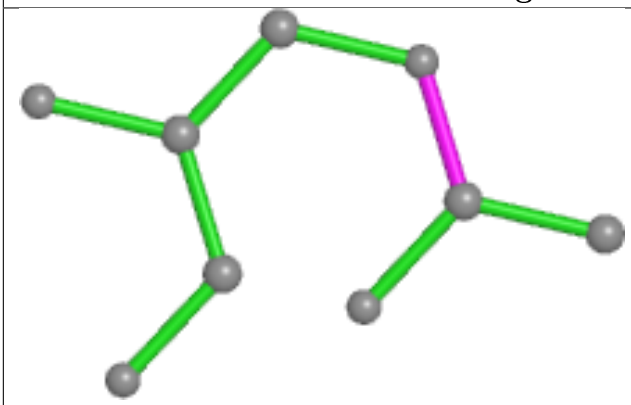
Ligand OLC A 1409



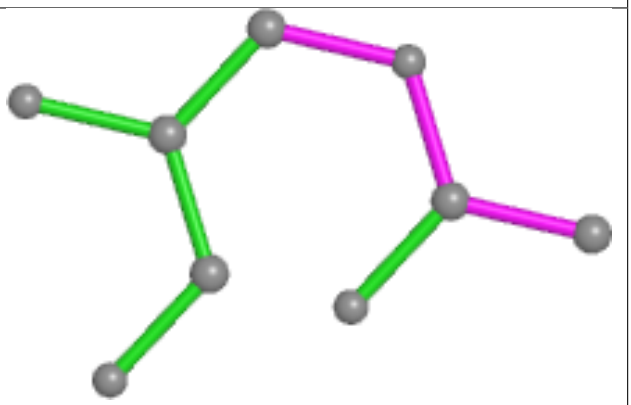
Ligand OLC A 1411



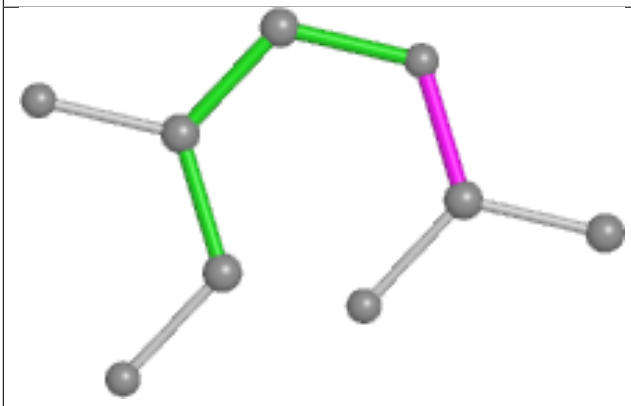
Ligand OLC A 1413



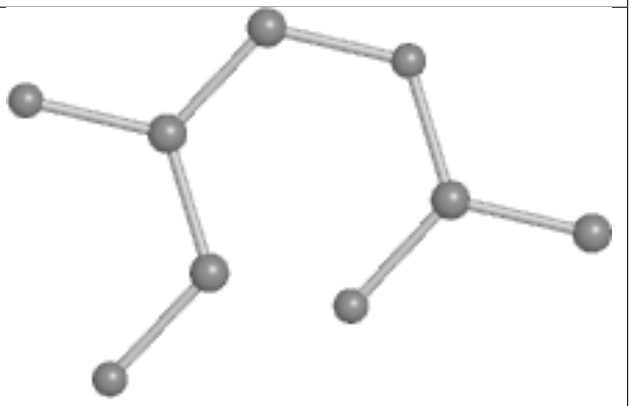
Bond lengths



Bond angles

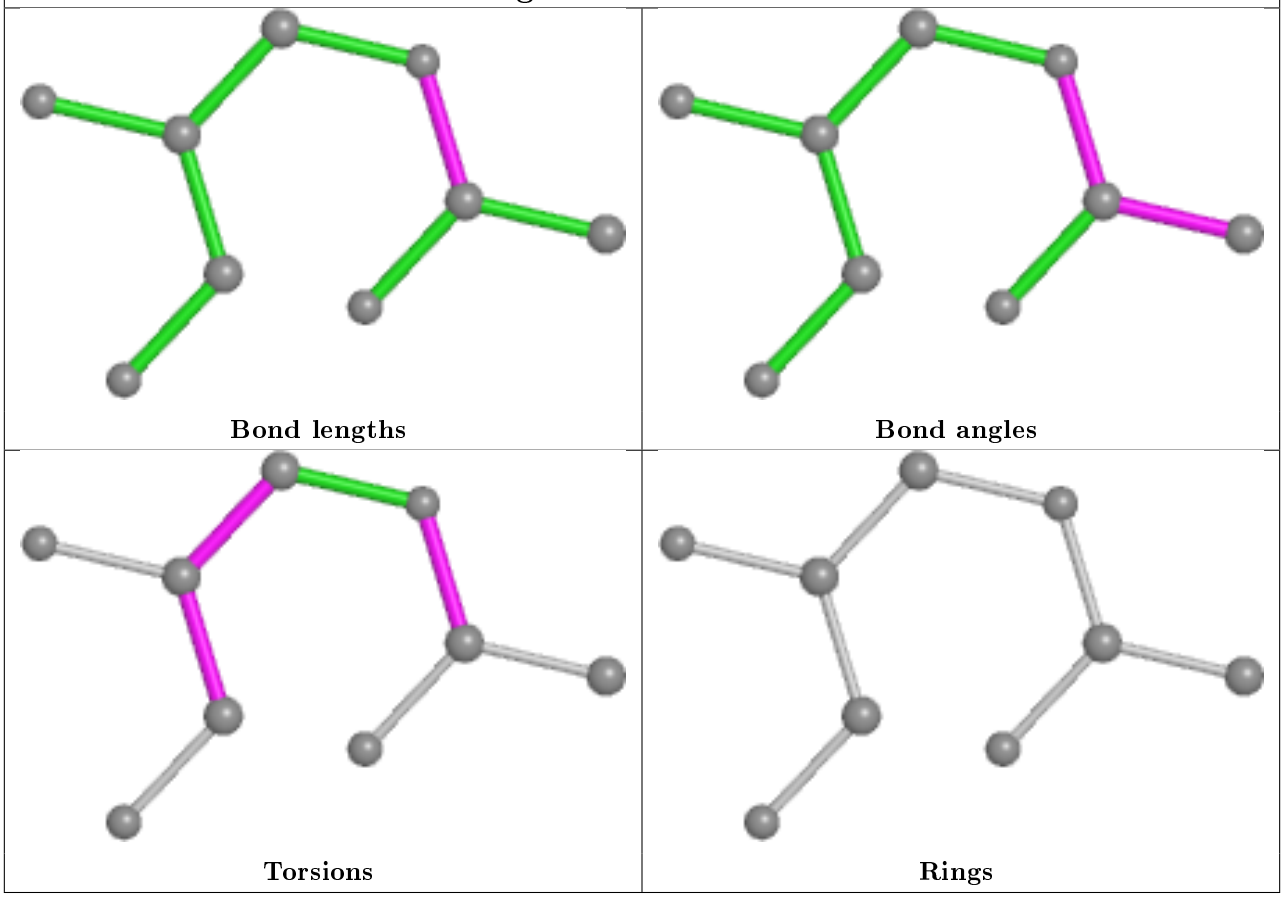


Torsions

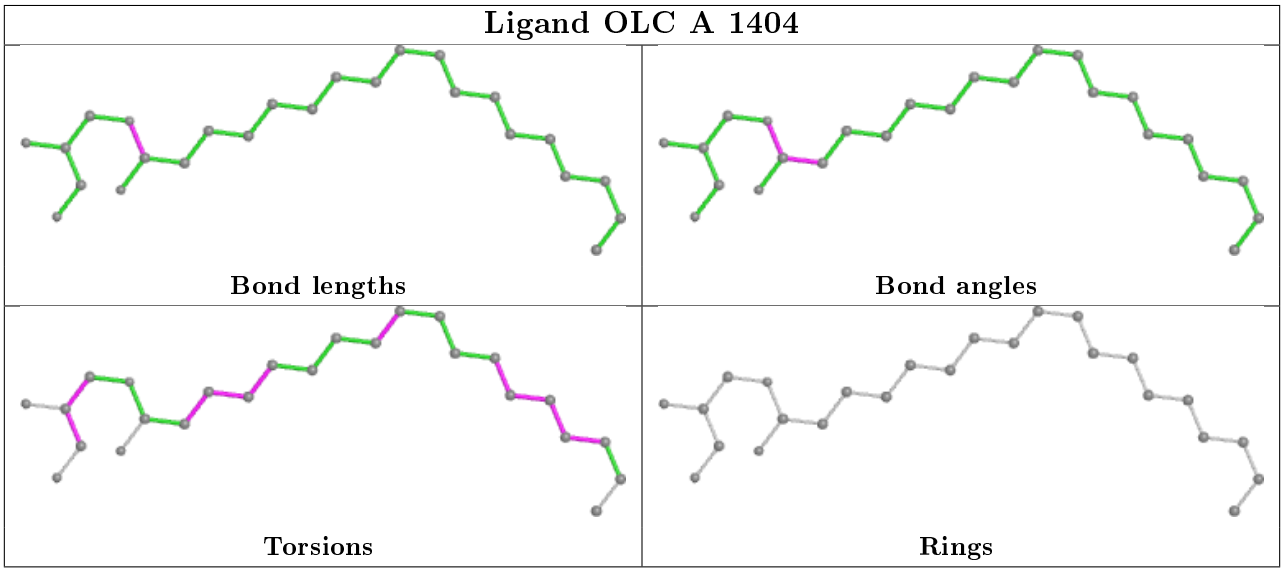


Rings

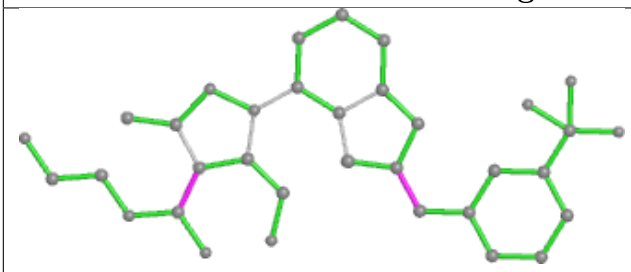
Ligand OLC A 1419



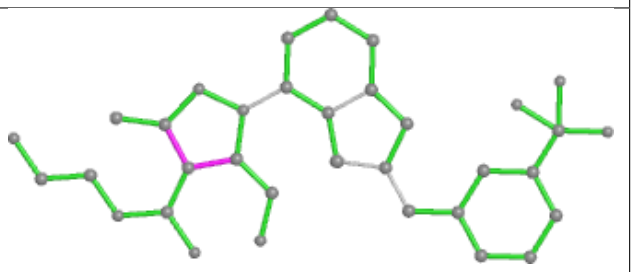
Ligand OLC A 1404



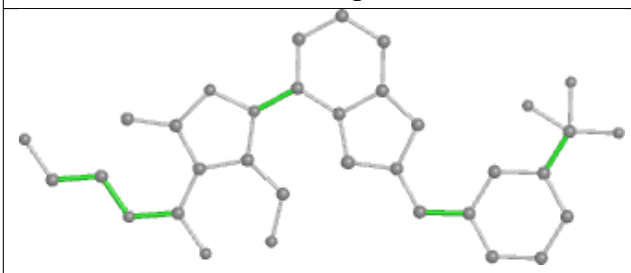
Ligand EN6 A 1401



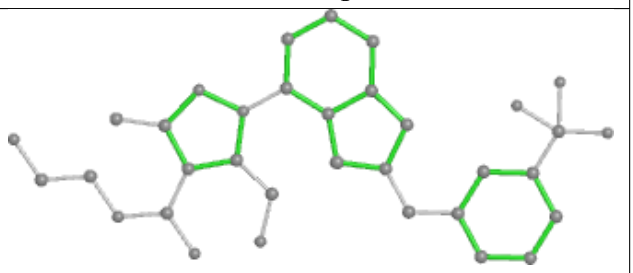
Bond lengths



Bond angles

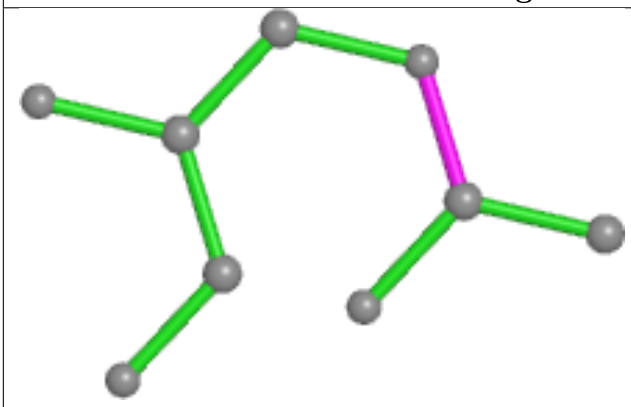


Torsions

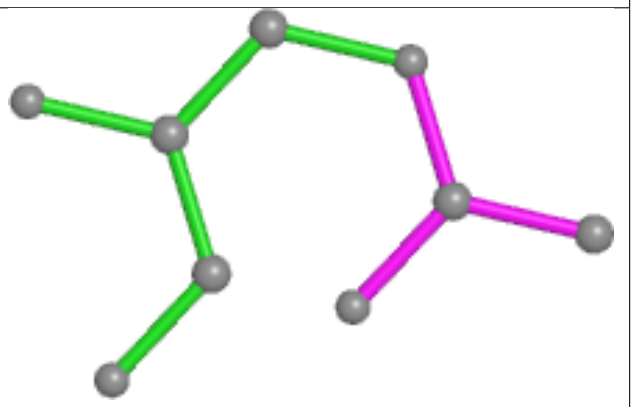


Rings

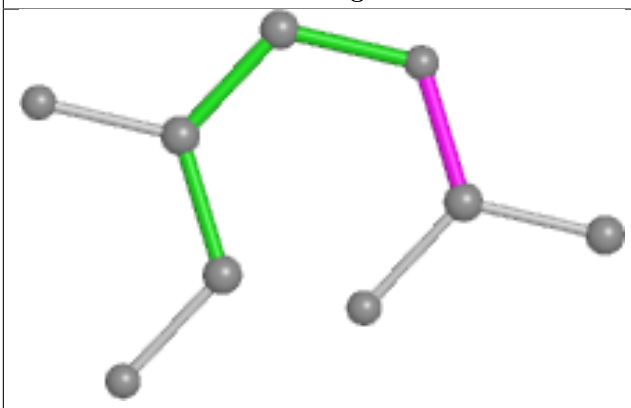
Ligand OLC A 1420



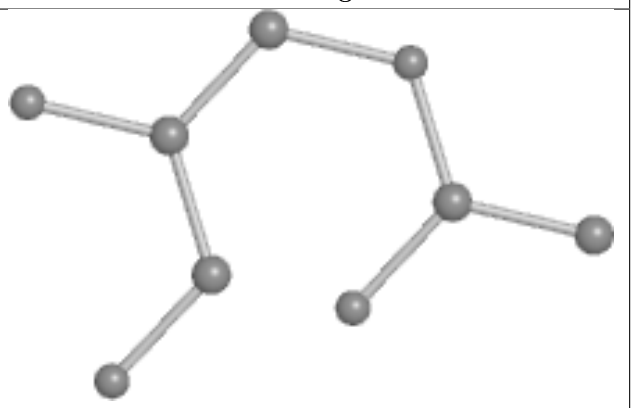
Bond lengths



Bond angles

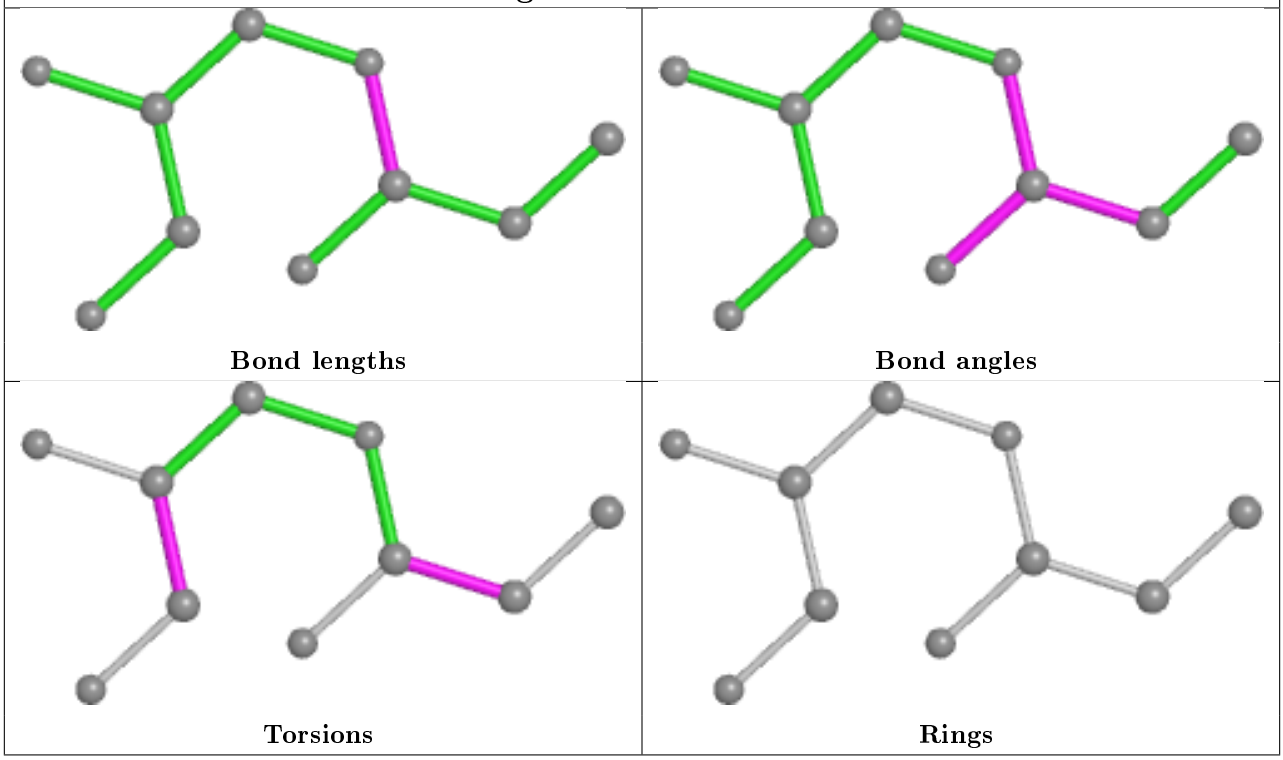


Torsions

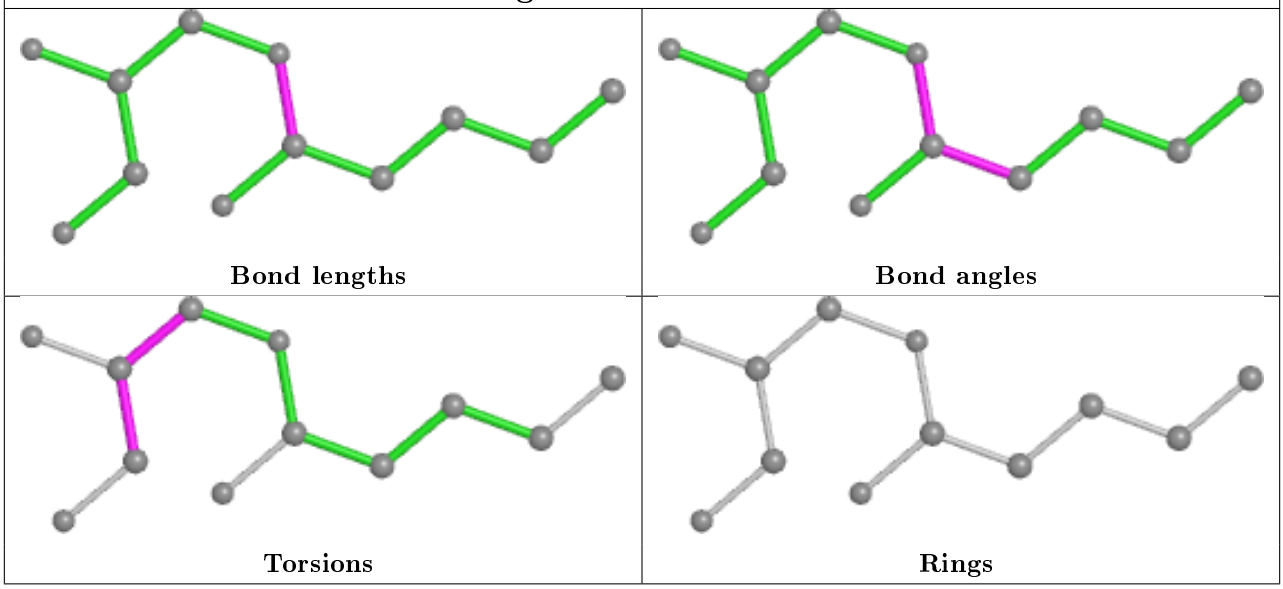


Rings

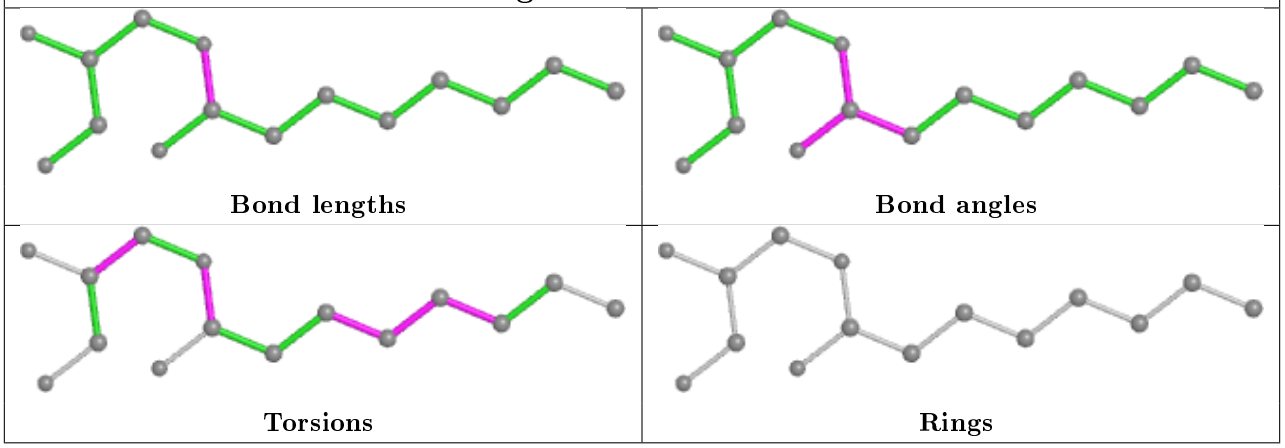
Ligand OLC A 1416



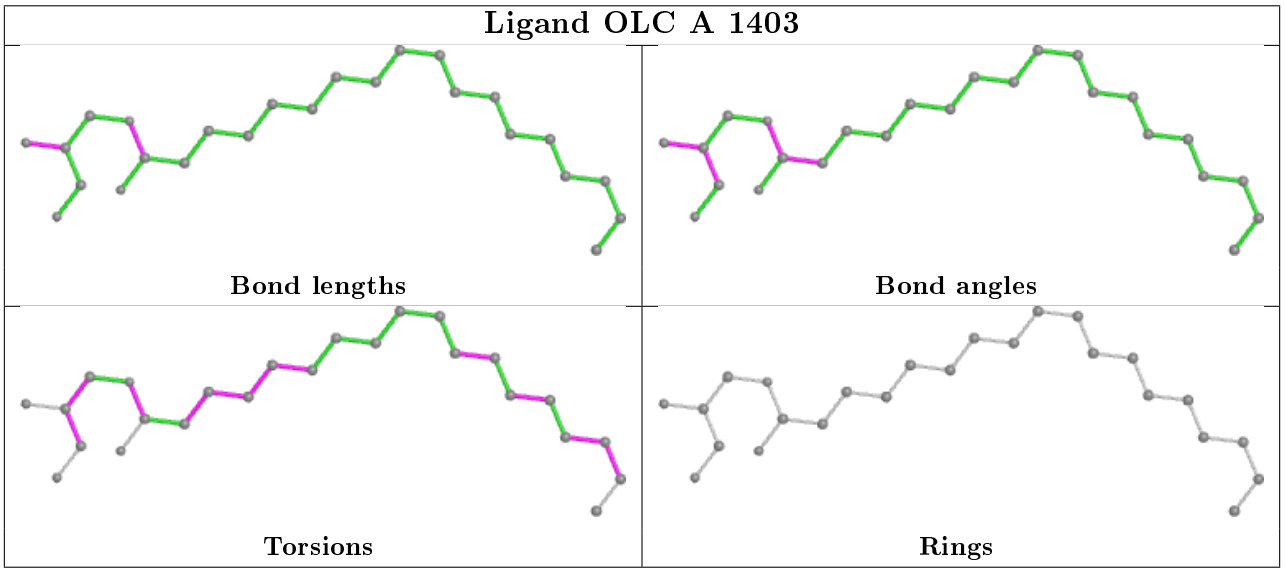
Ligand OLC A 1408



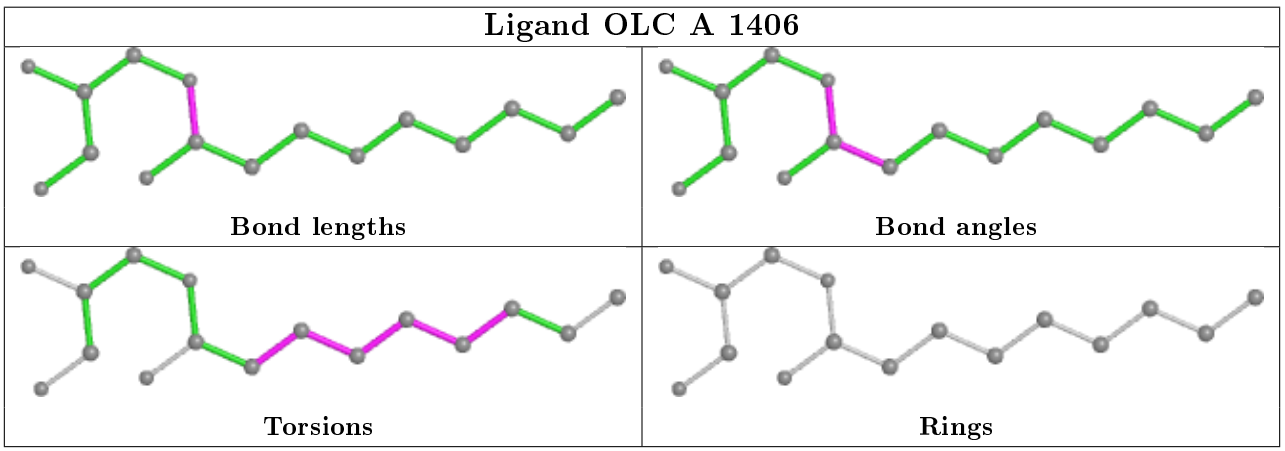
Ligand OLC A 1415

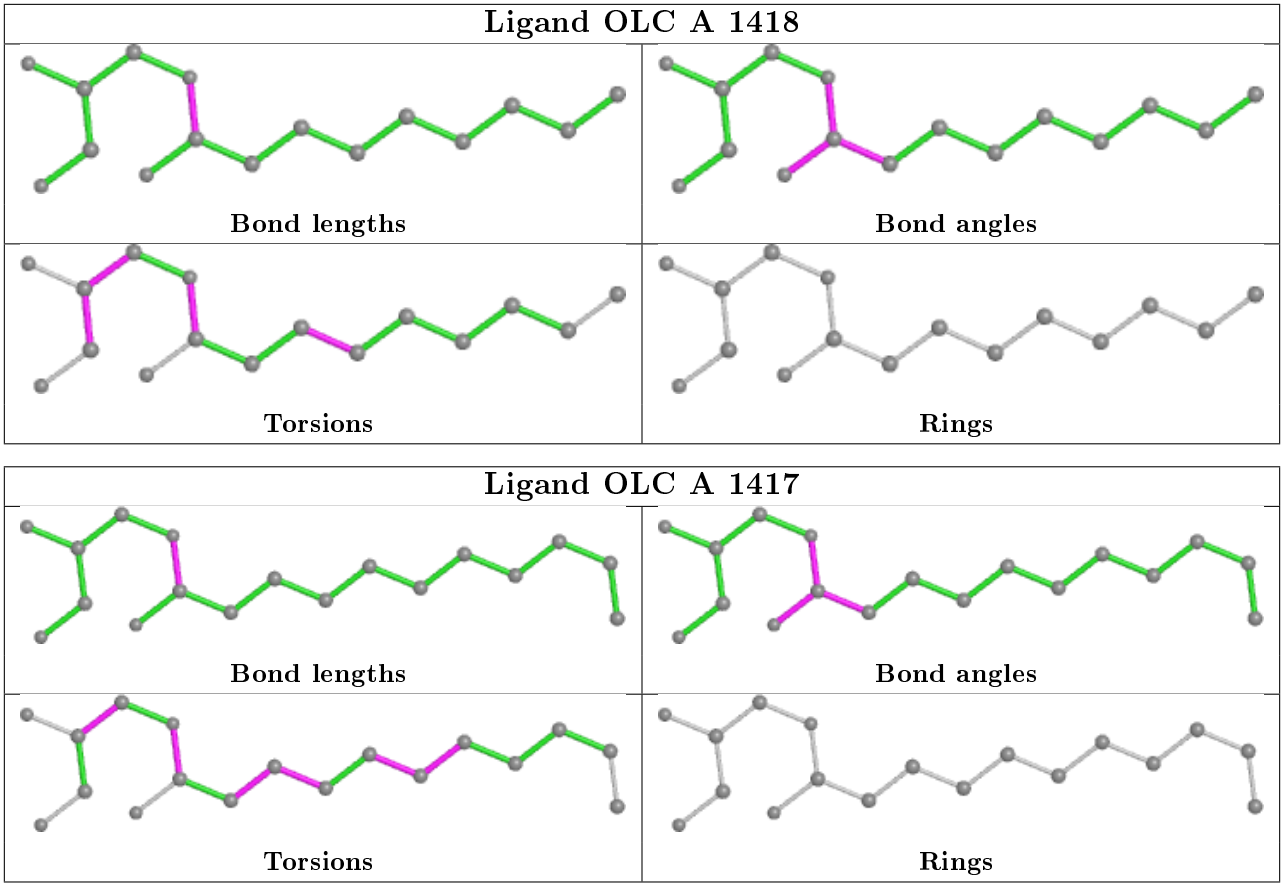


Ligand OLC A 1403



Ligand OLC A 1406





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	441/468 (94%)	0.26	42 (9%)	8	7	59, 76, 113, 173	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	VAL	5.0
1	A	23	GLU	4.7
1	A	334	THR	4.6
1	A	31	PHE	4.5
1	A	335	MET	4.5

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
4	OLC	A	1421	25/25	0.50	0.41	78,108,134,136	0
5	PEG	A	1423	7/7	0.51	0.30	112,120,133,138	0

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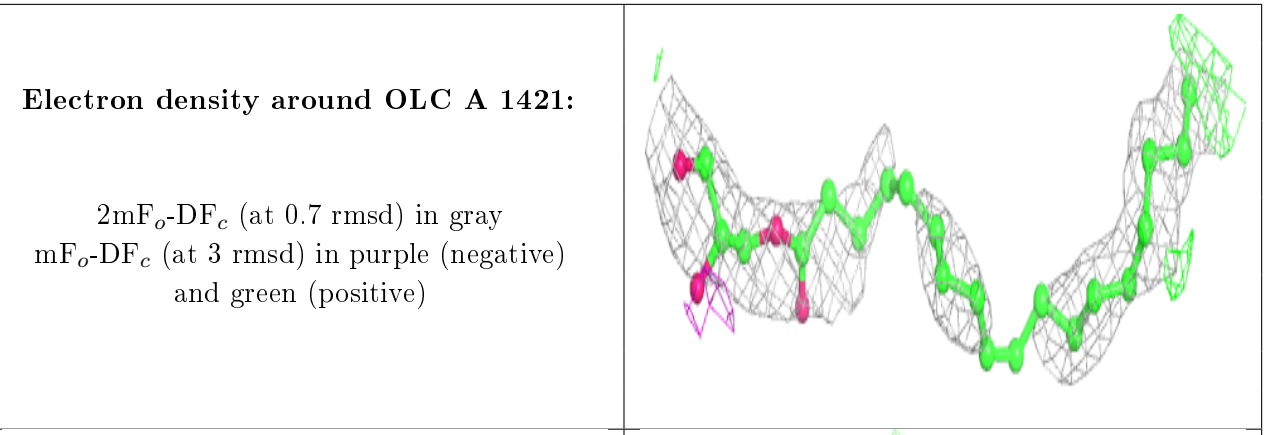
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLC	A	1409	13/25	0.65	0.36	100,121,144,147	0
4	OLC	A	1417	18/25	0.65	0.31	93,110,159,165	0
5	PEG	A	1425	7/7	0.70	0.36	128,134,160,162	0
4	OLC	A	1407	16/25	0.74	0.29	76,127,186,198	0
5	PEG	A	1410	7/7	0.75	0.39	101,126,146,152	0
5	PEG	A	1422	7/7	0.76	0.30	118,129,139,140	0
5	PEG	A	1424	7/7	0.77	0.20	106,115,130,131	0
4	OLC	A	1418	16/25	0.77	0.42	98,117,168,170	0
5	PEG	A	1428	7/7	0.77	0.30	109,113,123,146	0
4	OLC	A	1419	9/25	0.79	0.34	107,117,132,134	0
4	OLC	A	1406	16/25	0.81	0.20	104,121,160,163	0
4	OLC	A	1415	15/25	0.81	0.34	76,110,152,173	0
4	OLC	A	1416	10/25	0.82	0.24	92,103,118,129	0
5	PEG	A	1426	7/7	0.82	0.20	85,98,107,115	0
6	FLC	A	1414	13/13	0.83	0.23	63,78,97,109	13
4	OLC	A	1403	25/25	0.85	0.29	75,92,141,155	0
4	OLC	A	1412	11/25	0.85	0.22	87,96,111,118	0
4	OLC	A	1411	23/25	0.85	0.24	66,96,139,149	0
5	PEG	A	1427	7/7	0.87	0.25	85,103,120,128	0
4	OLC	A	1413	9/25	0.88	0.25	97,106,120,133	0
4	OLC	A	1420	9/25	0.89	0.49	84,111,147,172	0
4	OLC	A	1405	15/25	0.90	0.42	77,95,130,152	0
4	OLC	A	1408	12/25	0.92	0.13	94,106,120,122	0
4	OLC	A	1404	25/25	0.94	0.45	70,92,147,179	0
2	EN6	A	1401	34/34	0.95	0.10	56,68,80,87	0
3	FMN	A	1402	31/31	0.98	0.09	60,71,79,88	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.

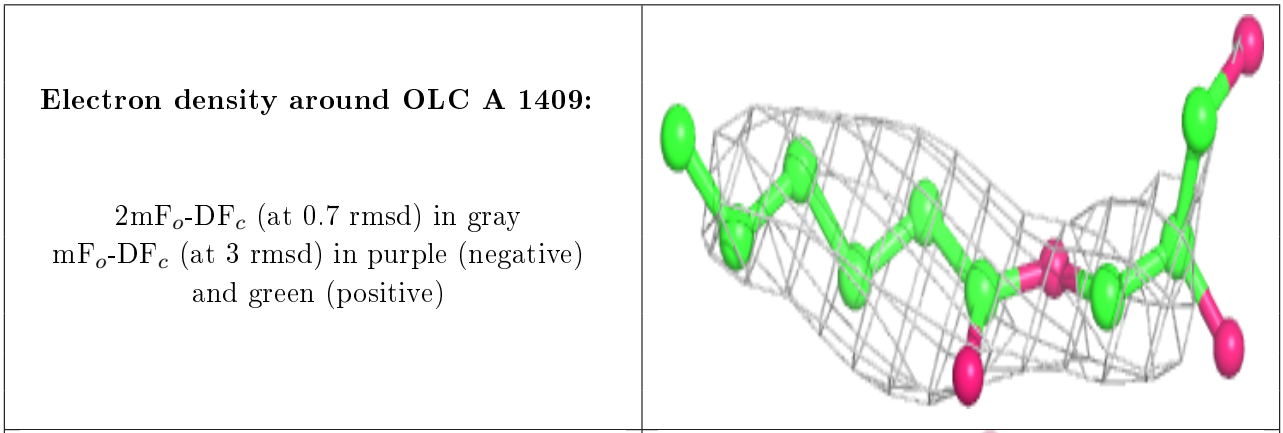
Electron density around OLC A 1421:

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



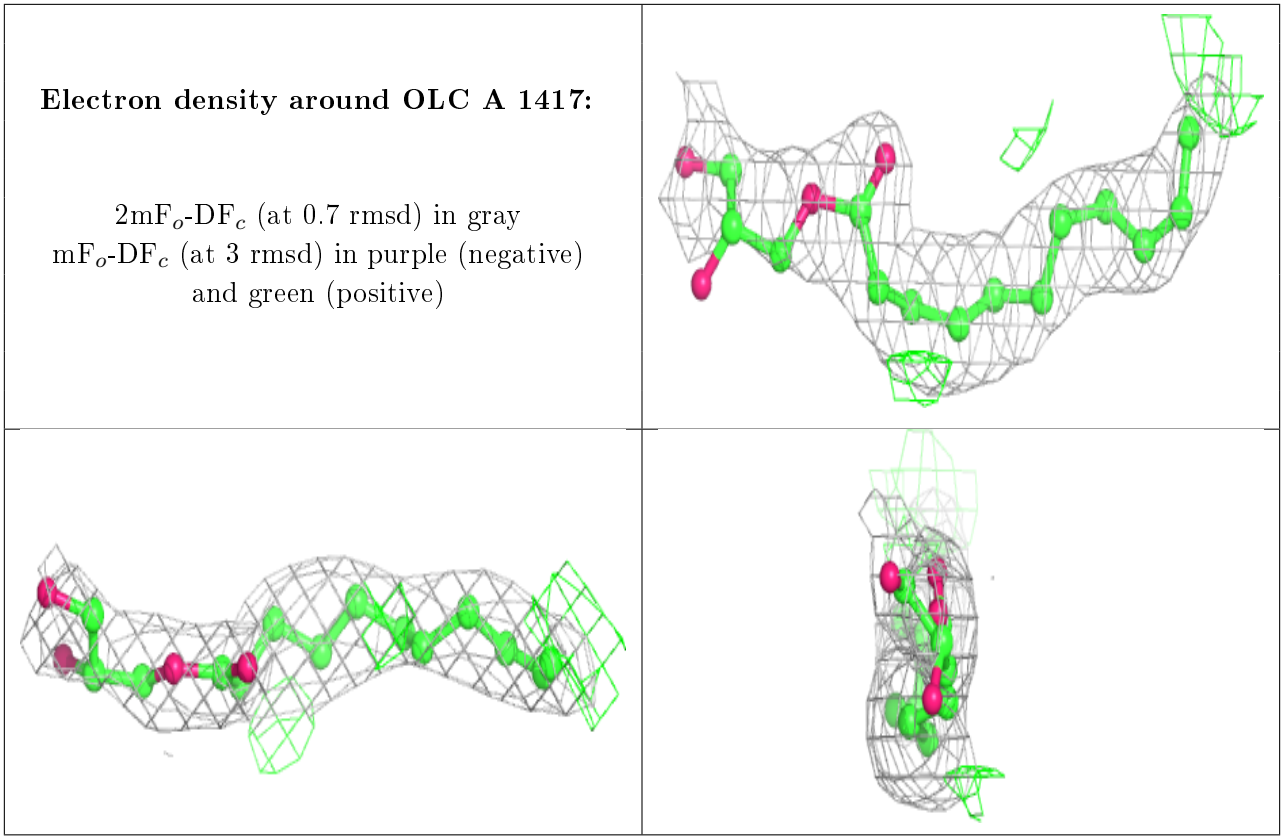
Electron density around OLC A 1409:

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



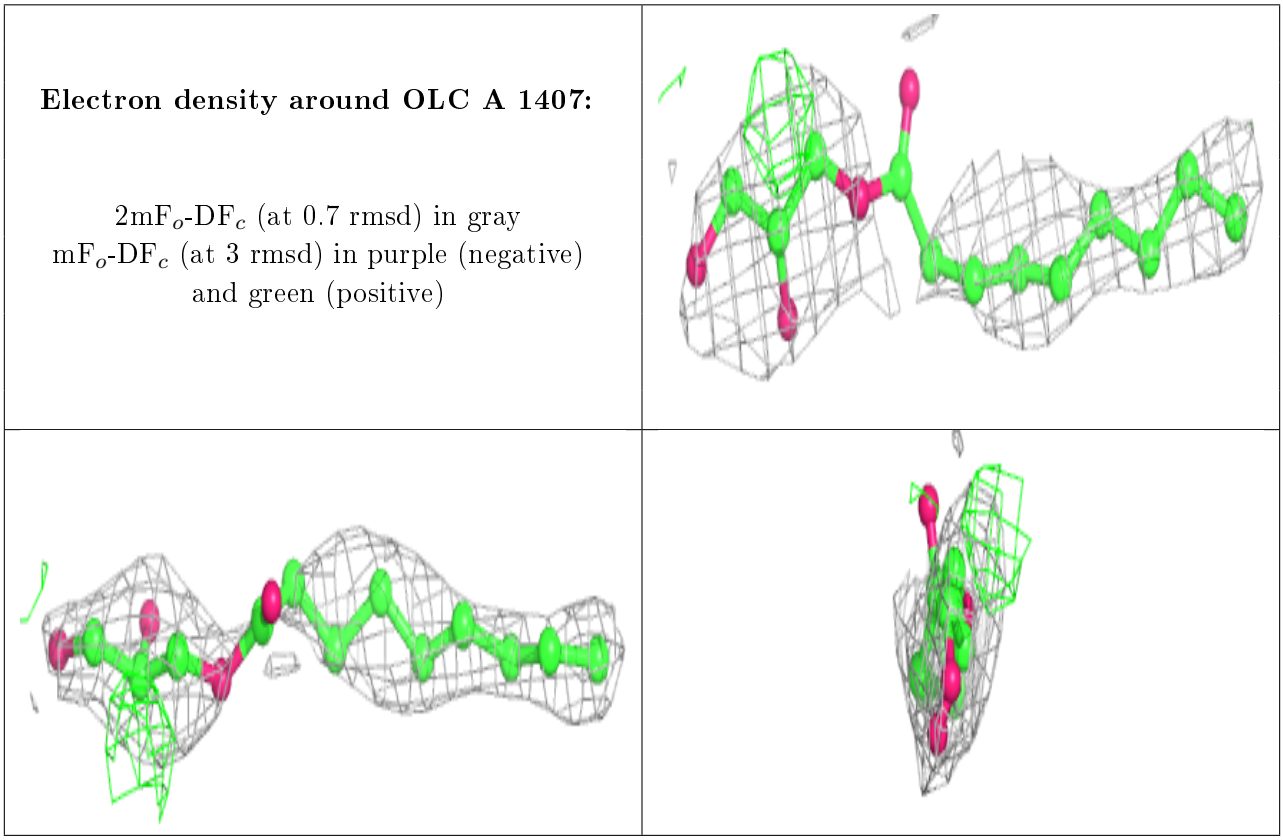
Electron density around OLC A 1417:

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



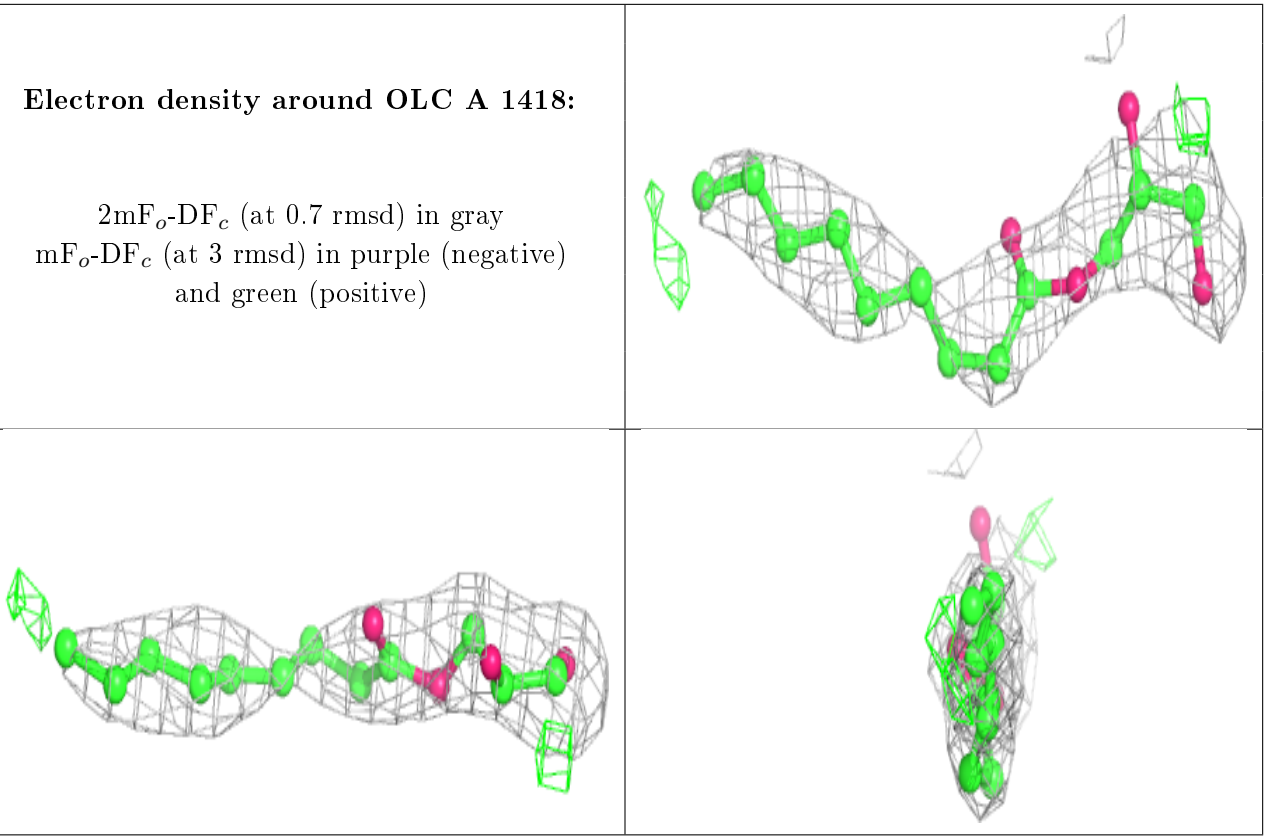
Electron density around OLC A 1407:

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



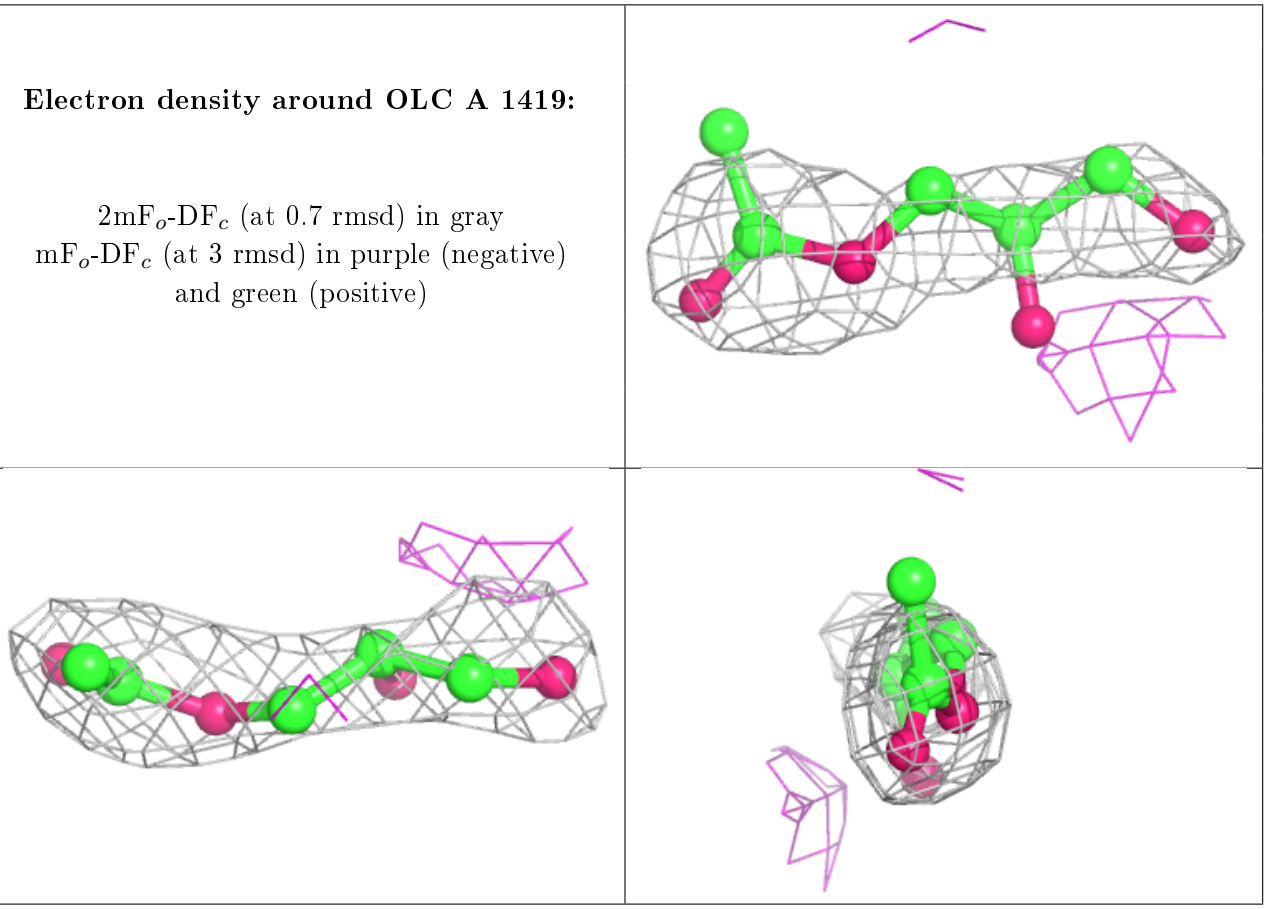
Electron density around OLC A 1418:

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



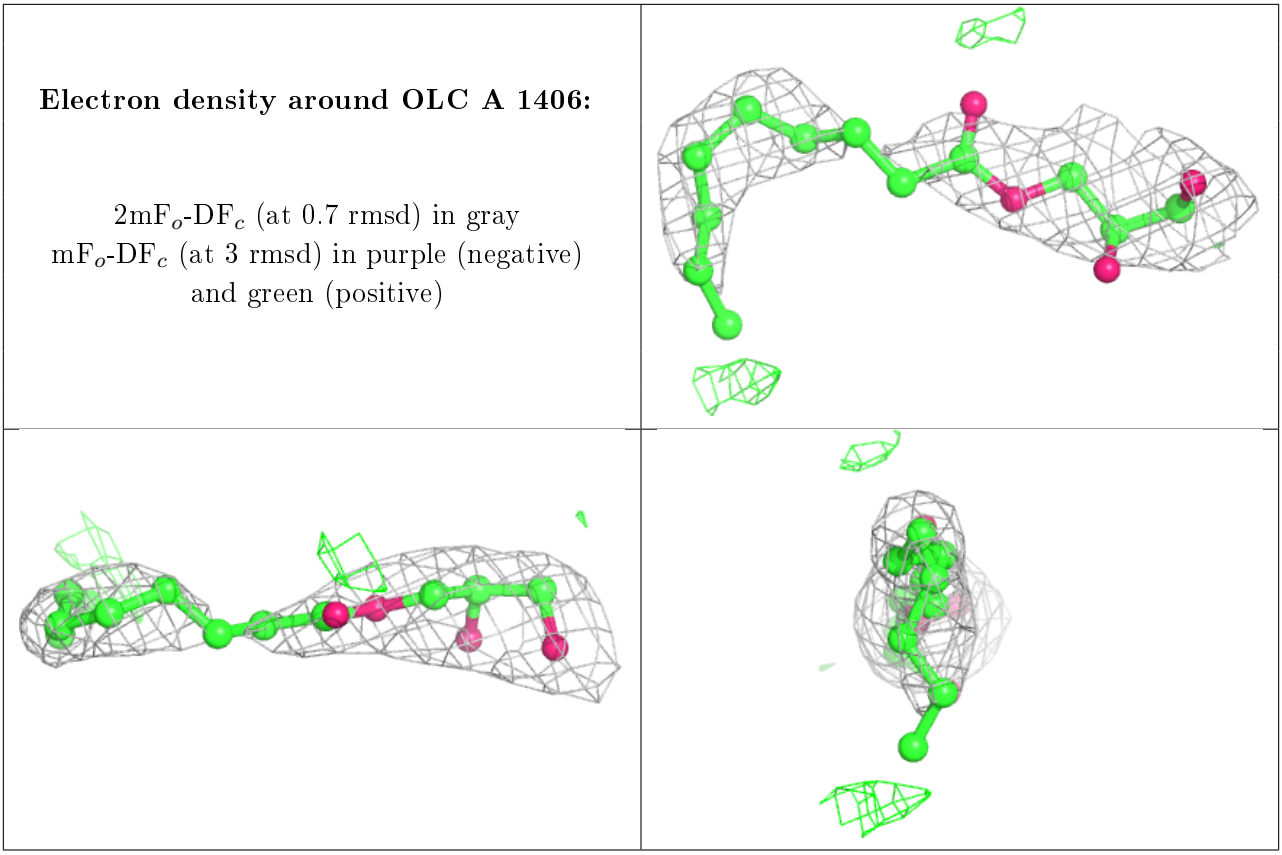
Electron density around OLC A 1419:

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



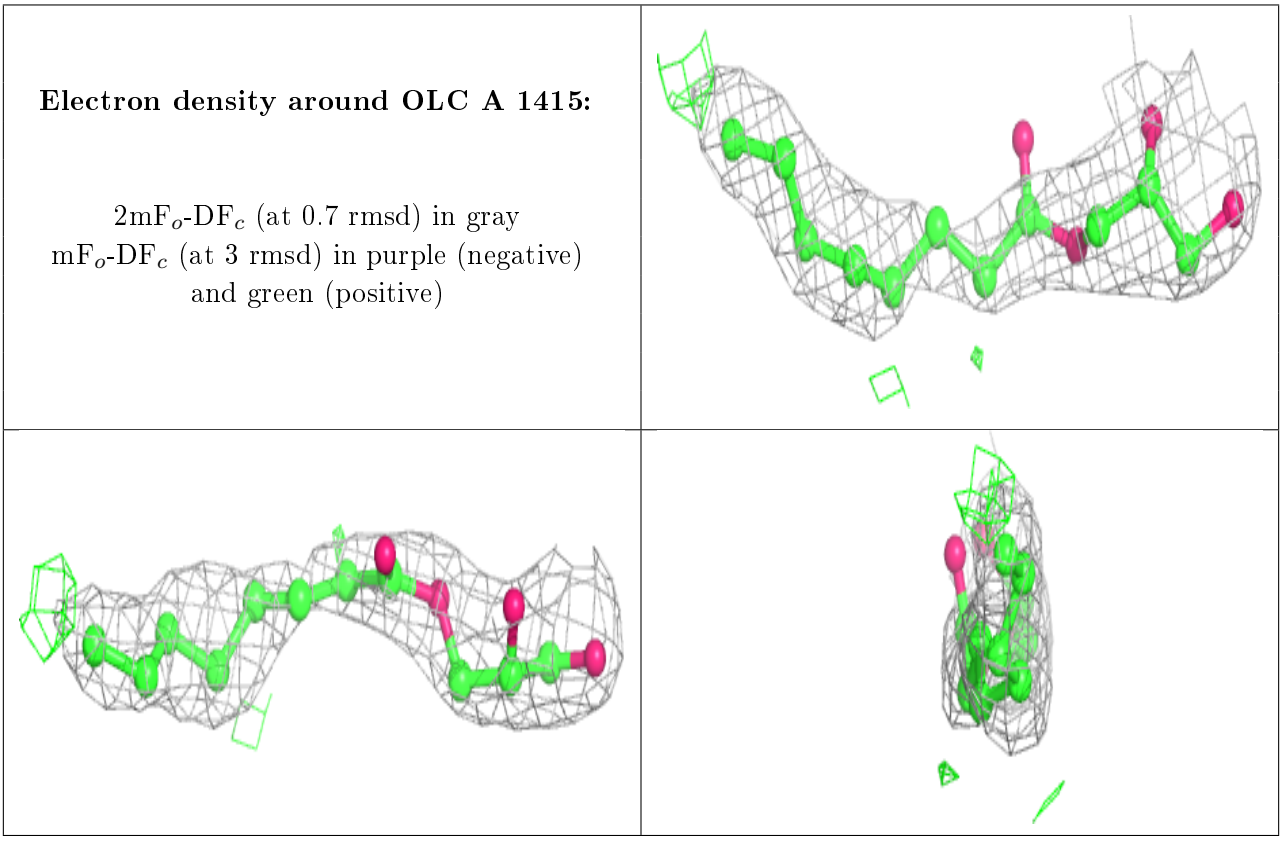
Electron density around OLC A 1406:

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



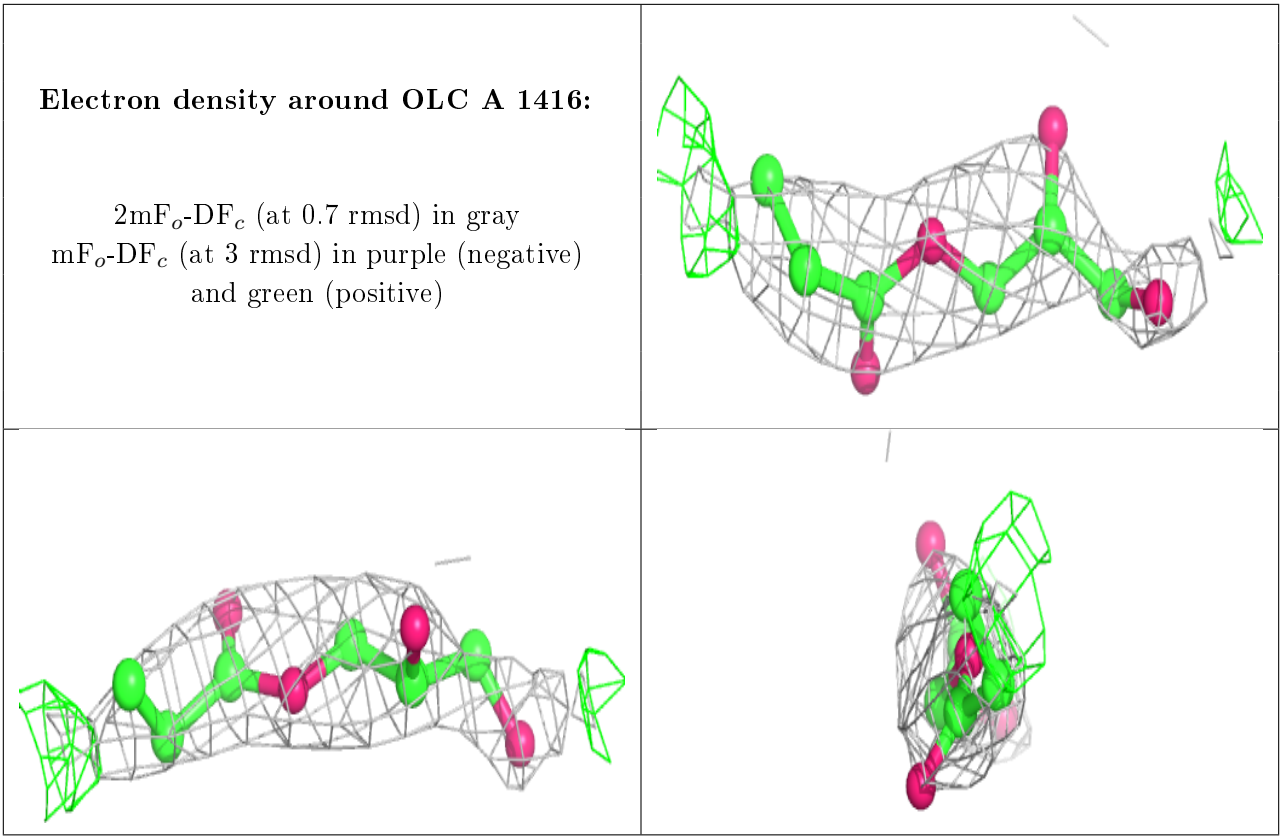
Electron density around OLC A 1415:

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



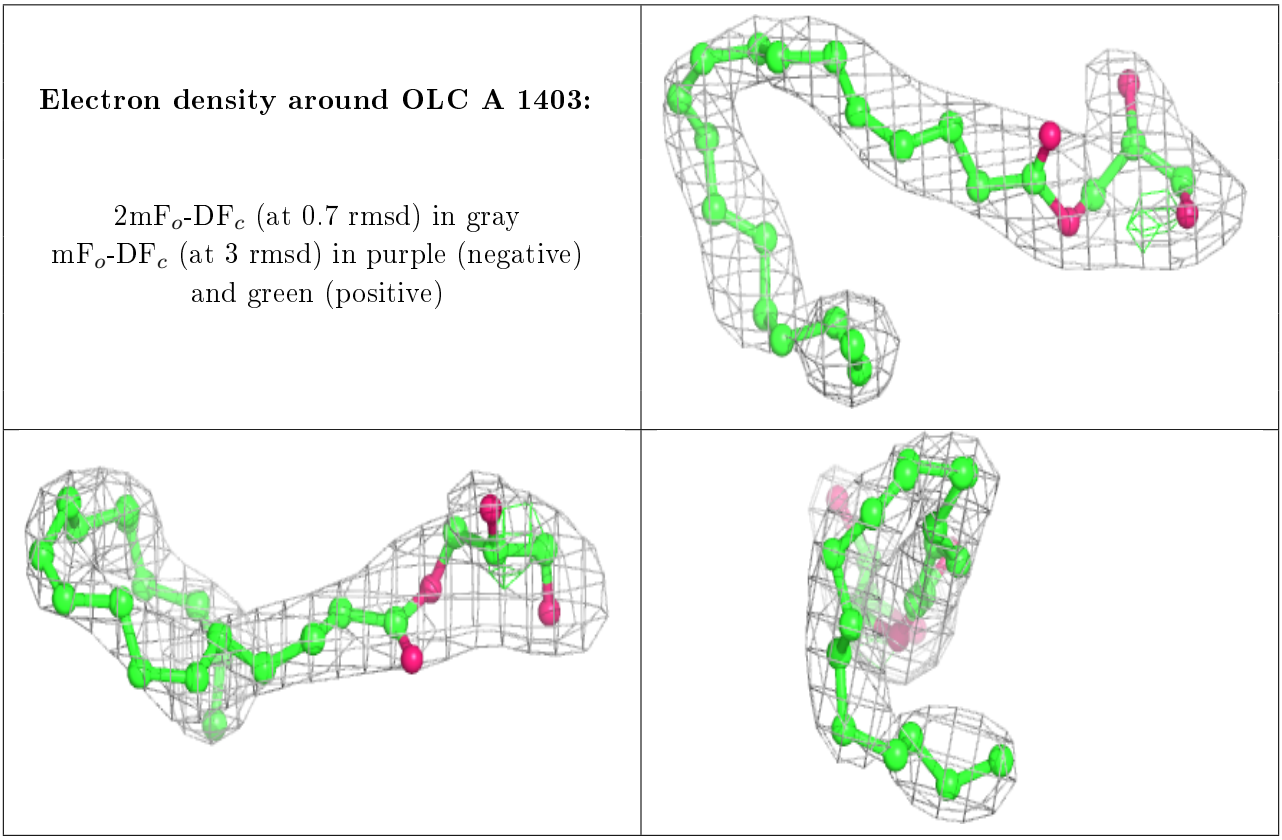
Electron density around OLC A 1416:

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



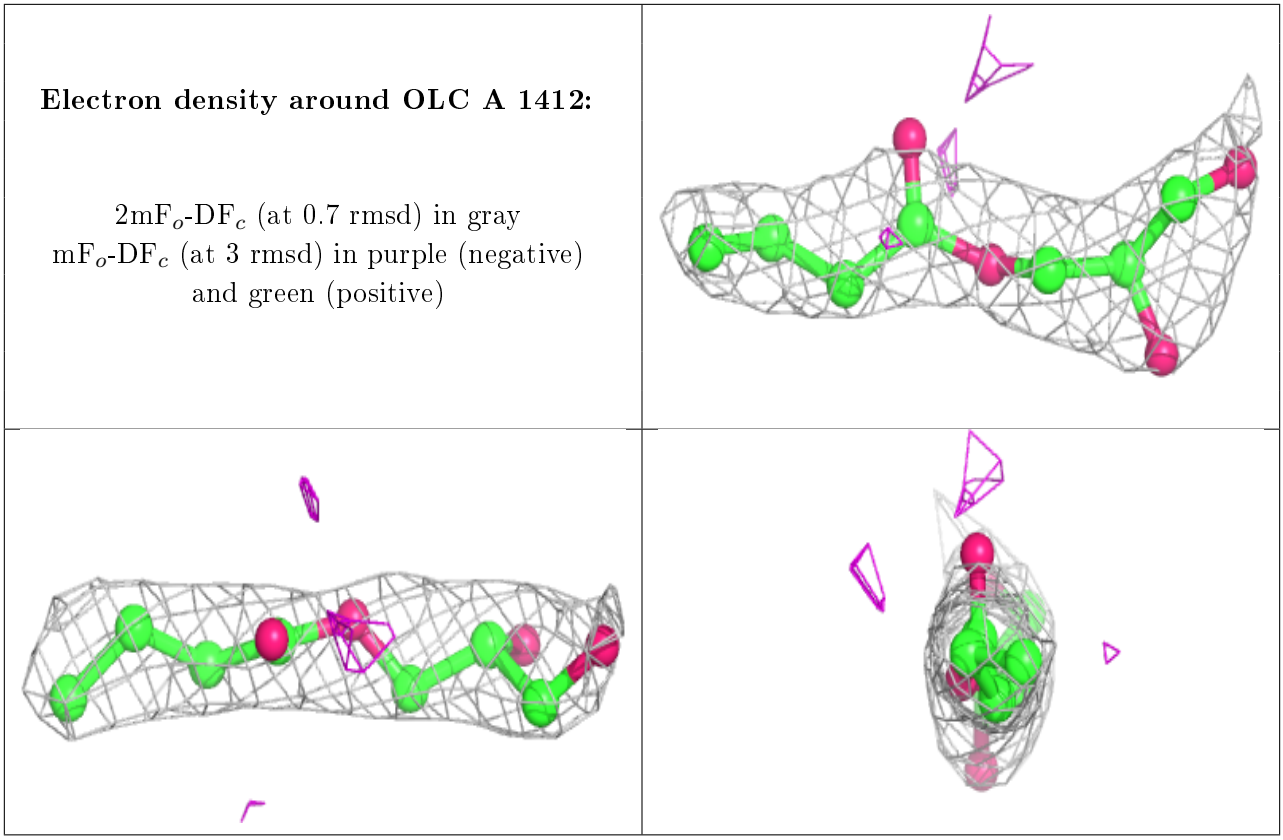
Electron density around OLC A 1403:

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



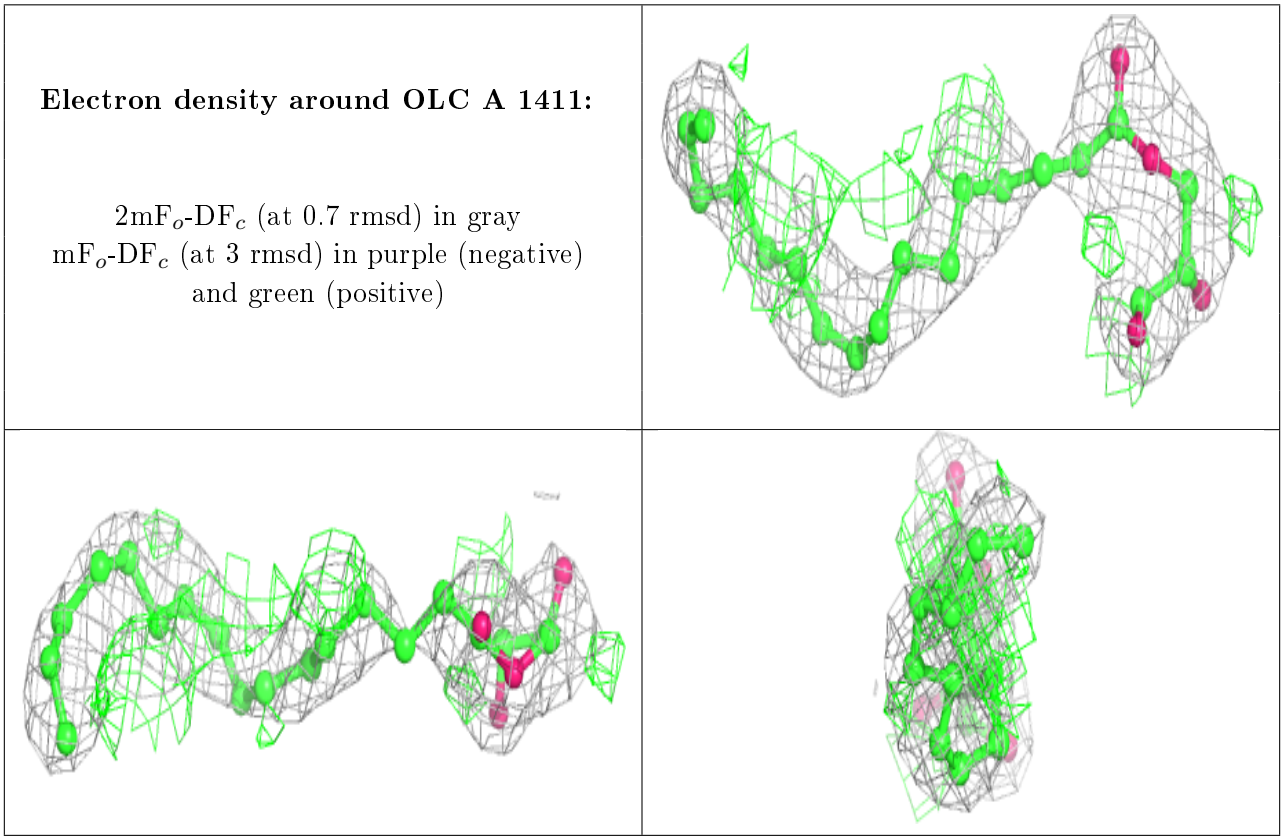
Electron density around OLC A 1412:

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



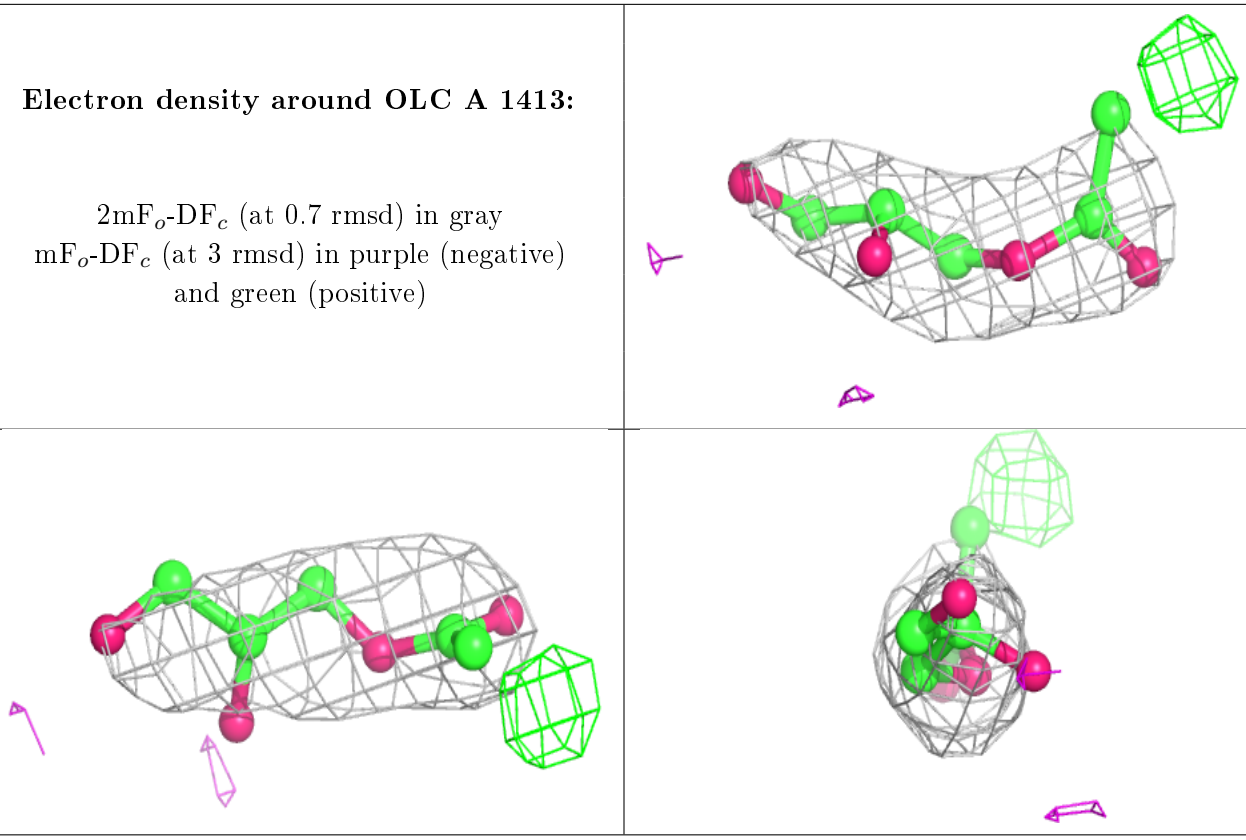
Electron density around OLC A 1411:

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



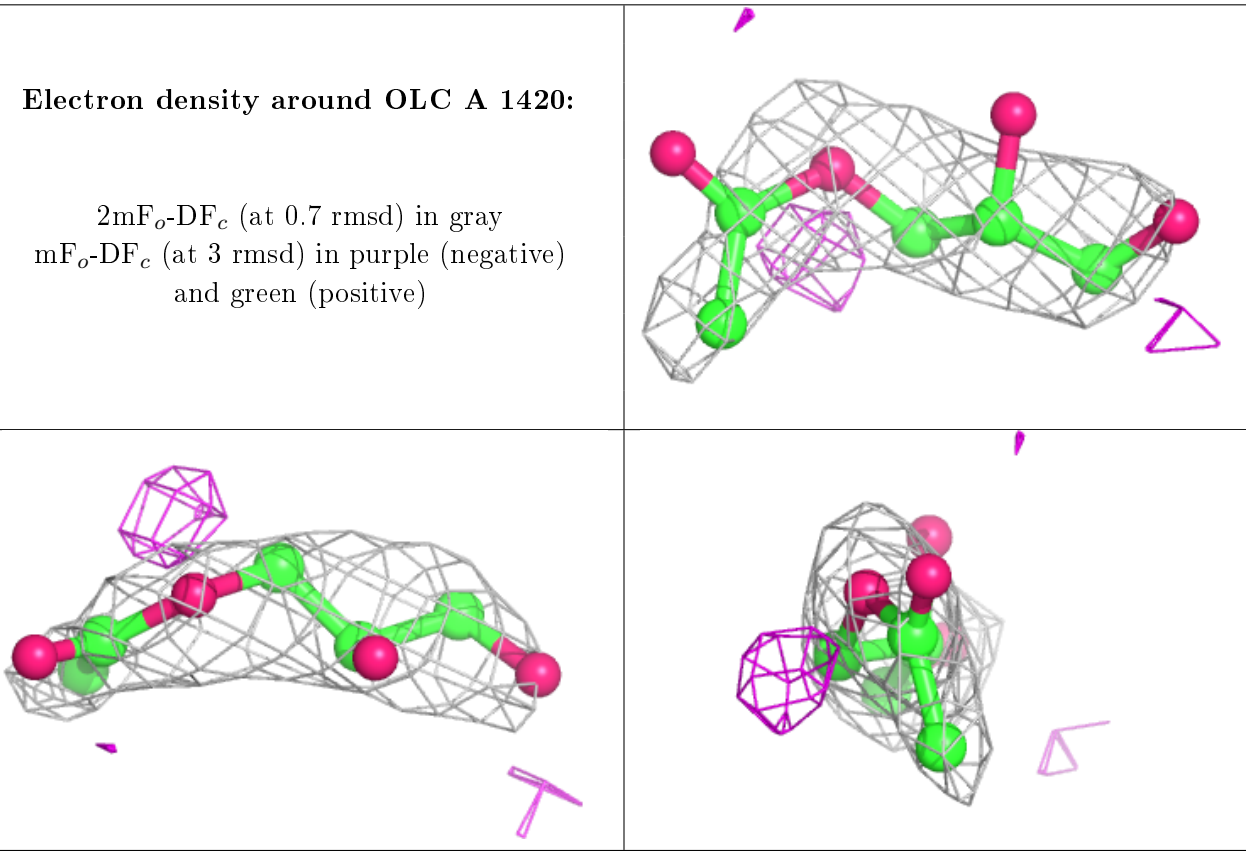
Electron density around OLC A 1413:

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



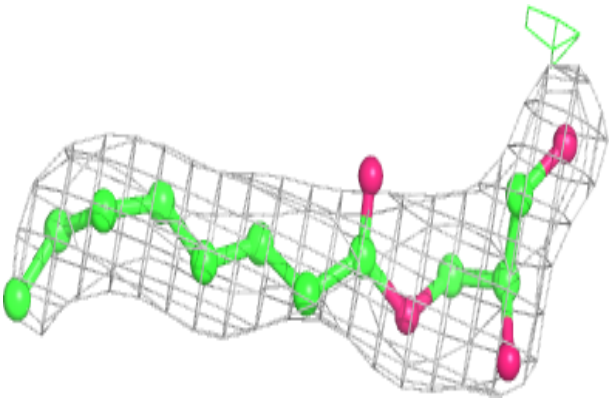
Electron density around OLC A 1420:

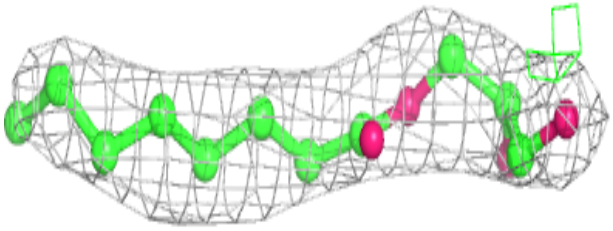
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

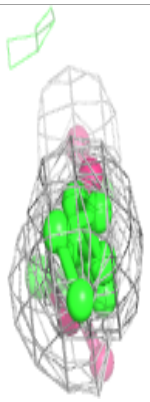


Electron density around OLC A 1405:

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

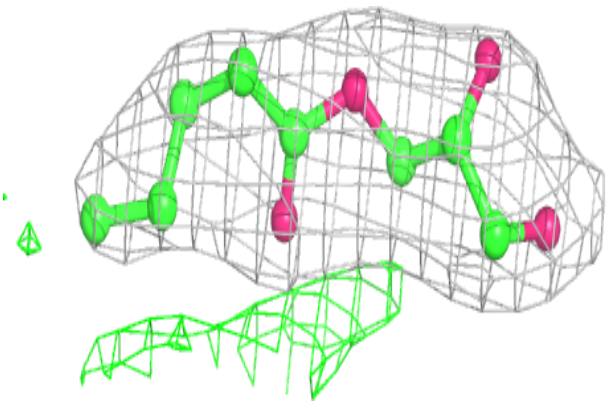


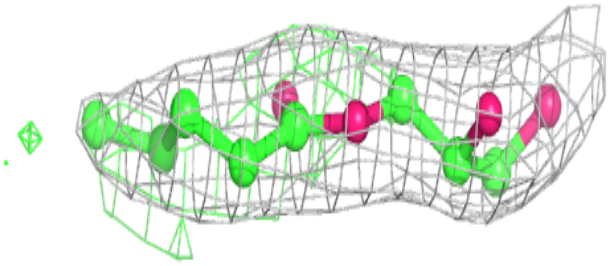


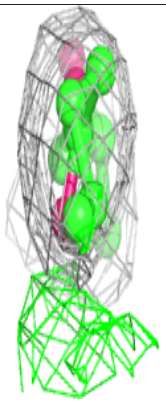


Electron density around OLC A 1408:

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

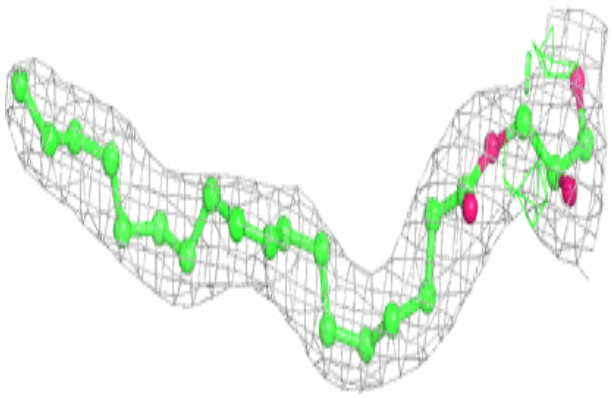


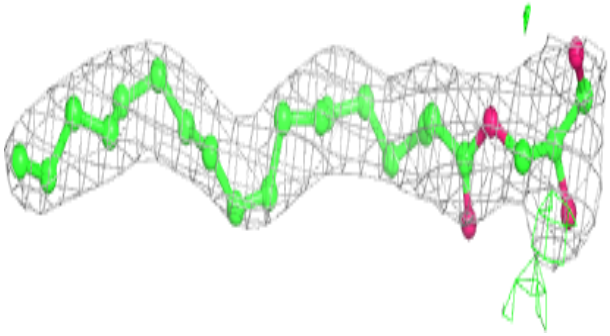


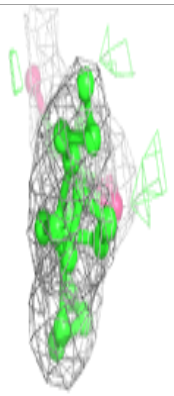


Electron density around OLC A 1404:

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

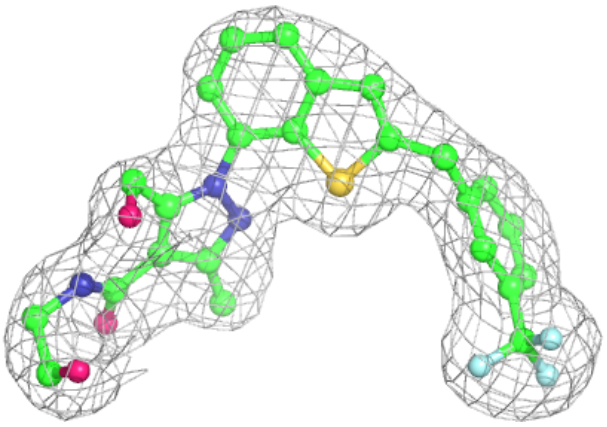


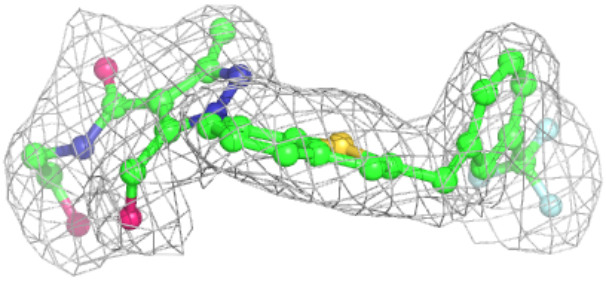


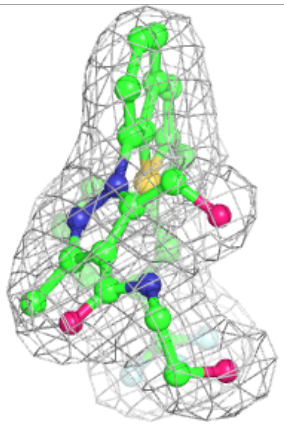


Electron density around EN6 A 1401:

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

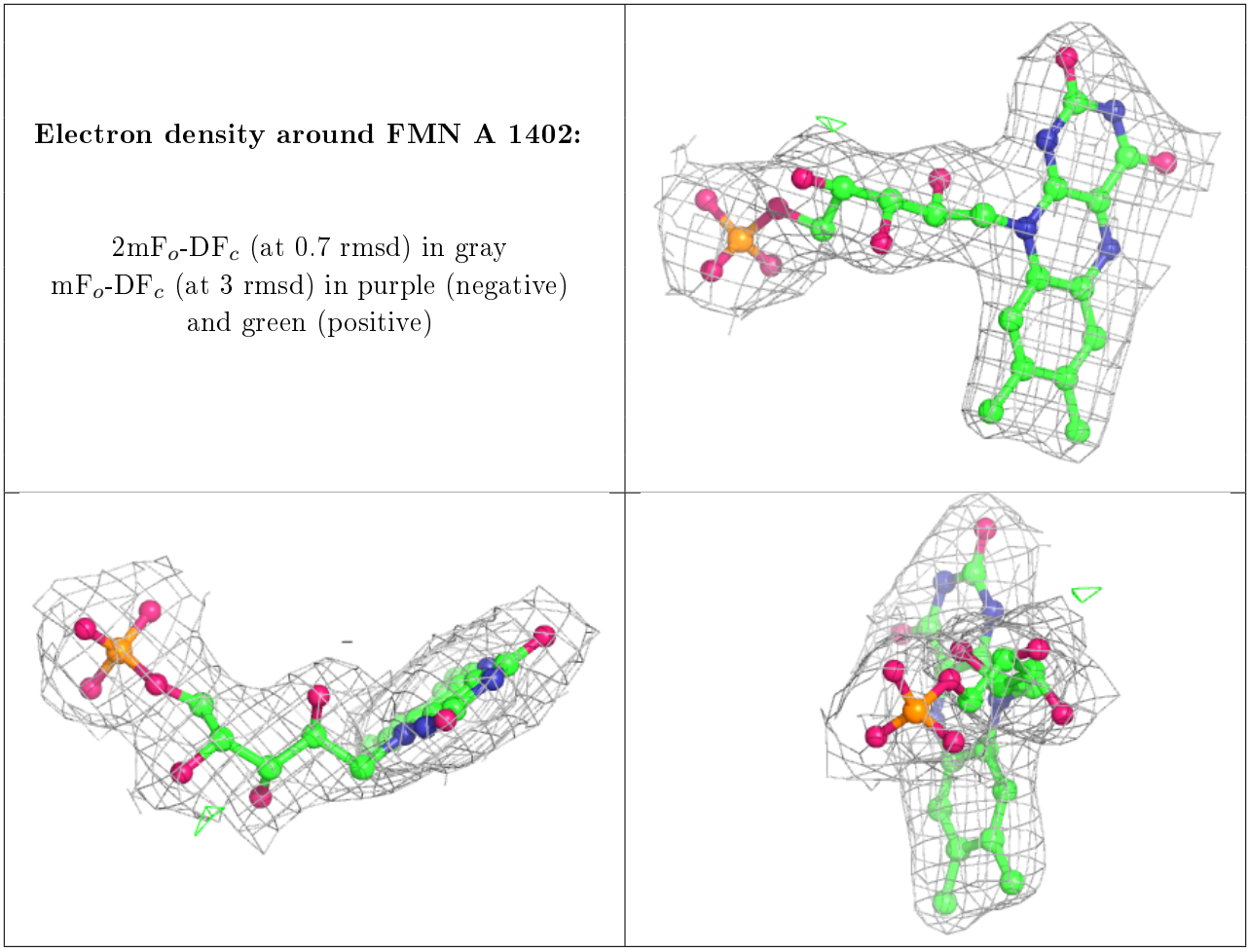






Electron density around FMN A 1402:

$2mF_o$-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.