wwPDB X-ray Structure Validation Summary Report (i)

Apr 23, 2024 – 02:09 PM EDT

PDB ID	:	6O9F
Title	:	The structure of Thermomyces Lanuginosa lipase in complex with 1,3 diacyl-glycerol in a monoclinic crystal form
Authors	:	McPherson, A.
Deposited on	:	2019-03-13
Resolution	:	2.48 Å(reported)

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

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

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

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

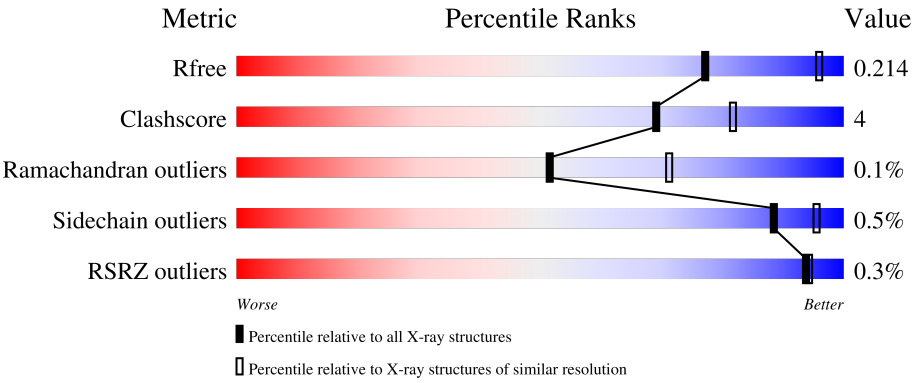
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	291	88% · 8%
1	B	291	85% 7% 8%
1	C	291	87% 5% 8%
1	D	291	88% · 8%
1	E	291	88% · 8%

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Mol	Chain	Length	Quality of chain
1	F	291	88% · 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OCA	A	301	-	-	X	X
2	OCA	B	301	-	-	X	-
2	OCA	C	301	-	-	X	X
2	OCA	D	301	-	-	X	-
2	OCA	E	301	-	-	X	X
4	NAG	D	303	-	-	-	X
4	NAG	F	303	-	-	-	X
6	PO4	A	305	-	-	X	-
6	PO4	B	302	-	-	-	X
6	PO4	B	307	-	-	-	X
6	PO4	E	305	-	-	-	X

2 Entry composition (i)

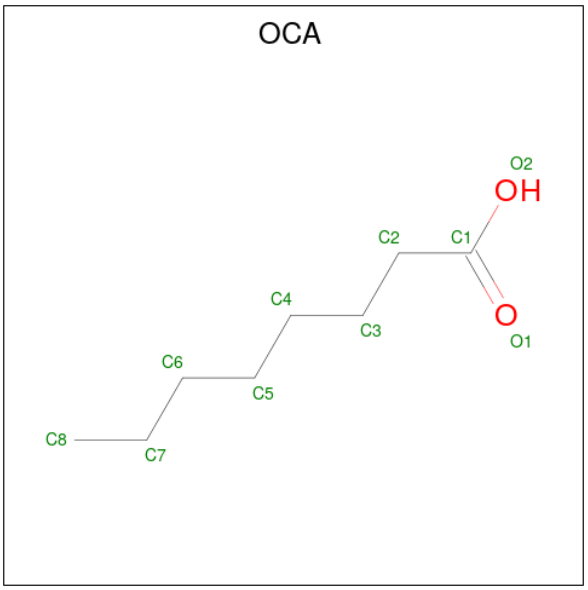
There are 7 unique types of molecules in this entry. The entry contains 25622 atoms, of which 12111 are hydrogens and 0 are deuteriums.

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 Lipase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	H	N	O	S	0	6	0
			4098	1323	2000	360	409	6			
1	B	269	Total	C	H	N	O	S	0	5	0
			4107	1327	2005	364	405	6			
1	C	269	Total	C	H	N	O	S	0	9	0
			4140	1332	2021	368	413	6			
1	E	269	Total	C	H	N	O	S	0	5	0
			4092	1325	1990	362	409	6			
1	D	269	Total	C	H	N	O	S	0	6	0
			4115	1332	2003	364	410	6			
1	F	269	Total	C	H	N	O	S	0	8	0
			4131	1335	2014	366	410	6			

- Molecule 2 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$) (labeled as "Ligand of Interest" by depositor).

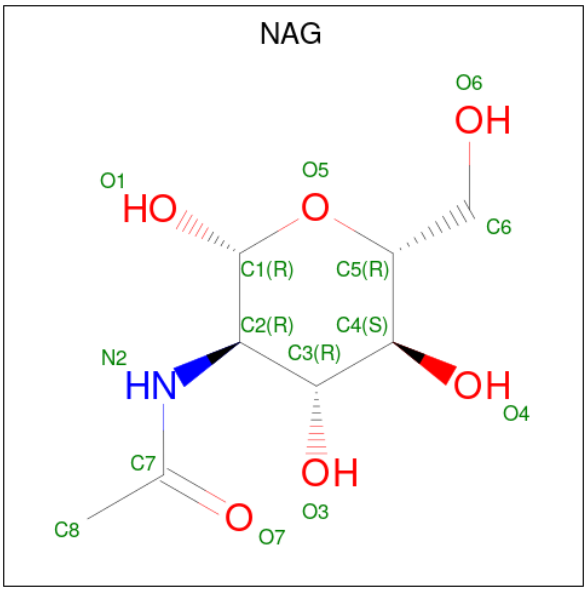


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 8 1	0	0
2	B	1	Total C O 9 8 1	0	0
2	C	1	Total C O 9 8 1	0	0
2	E	1	Total C O 9 8 1	0	0
2	D	1	Total C O 9 8 1	0	0
2	F	1	Total C O 7 6 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

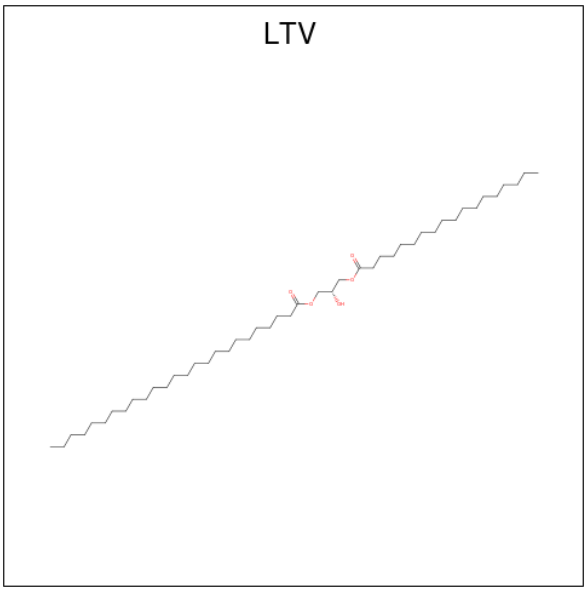
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	E	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



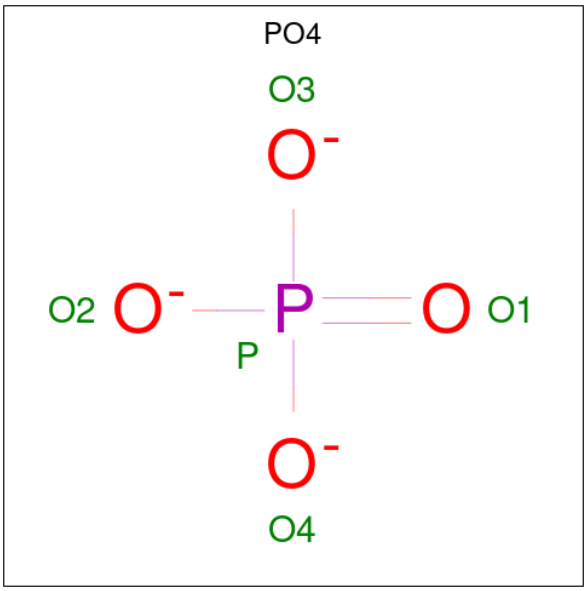
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	E	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	F	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is 2-hydroxy-3-(octadecanoyloxy)propyl pentacosanoate (three-letter code: LTV) (formula: $C_{46}H_{90}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 36 31 5	0	0
5	B	1	Total C O 43 38 5	0	0
5	C	1	Total C O 41 36 5	0	0
5	E	1	Total C O 48 43 5	0	0
5	D	1	Total C O 51 46 5	0	0
5	F	1	Total C O 43 38 5	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

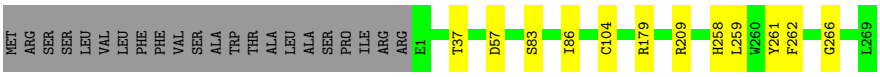
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	80	Total O 80 80	0	0
7	B	78	Total O 78 78	0	0
7	C	79	Total O 80 80	0	1
7	E	53	Total O 53 53	0	0
7	D	56	Total O 56 56	0	0
7	F	82	Total O 83 83	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

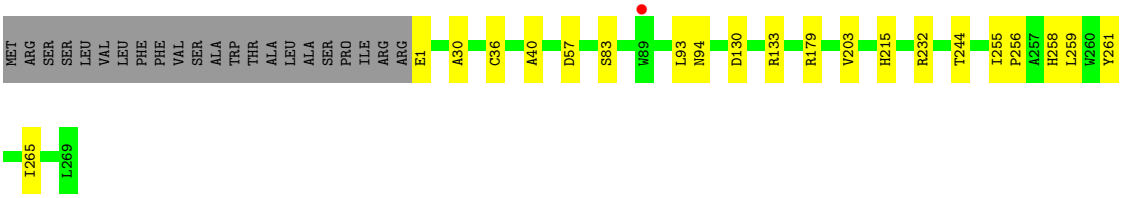
• Molecule 1: Lipase

Chain A:



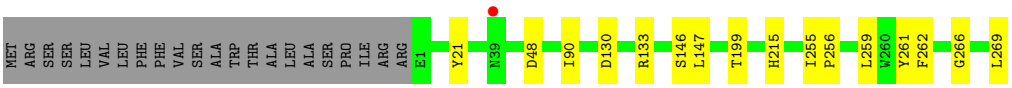
• Molecule 1: Lipase

Chain B:



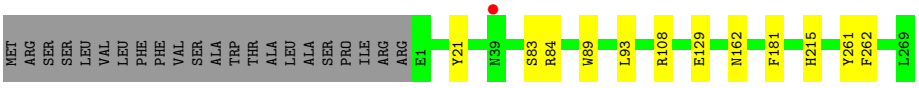
• Molecule 1: Lipase

Chain C:



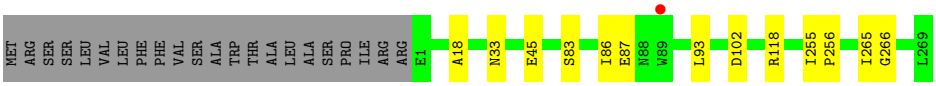
• Molecule 1: Lipase

Chain E:



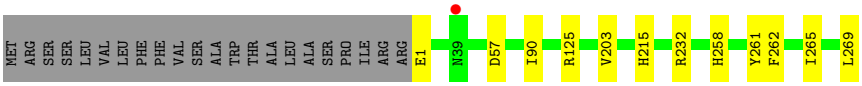
• Molecule 1: Lipase

Chain D:



• Molecule 1: Lipase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.19Å 91.37Å 124.32Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	51.27 – 2.48 51.27 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.5 (51.27-2.48) 99.5 (51.27-2.48)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	0.24	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.19rc7_4070	Depositor
R, R_{free}	0.175 , 0.214 0.174 , 0.214	Depositor DCC
R_{free} test set	3025 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25622	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: NAG, LTV, OCA, PO4, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/2169	0.51	0/2950
1	B	0.26	0/2167	0.51	0/2950
1	C	0.26	0/2200	0.51	0/2991
1	D	0.26	0/2182	0.50	0/2970
1	E	0.25	0/2171	0.49	0/2956
1	F	0.25	0/2196	0.50	0/2989
All	All	0.26	0/13085	0.50	0/17806

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	2098	2000	1994	12	0
1	B	2102	2005	2001	18	0
1	C	2119	2021	2008	15	0
1	D	2112	2003	2009	10	0
1	E	2102	1990	1986	12	0
1	F	2117	2014	2001	9	0
2	A	9	0	15	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9	0	14	10	0
2	C	9	0	15	12	0
2	D	9	0	14	6	0
2	E	9	0	13	8	0
2	F	7	0	8	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	14	13	13	0	0
4	B	14	13	13	0	0
4	C	14	13	13	0	0
4	D	14	13	13	1	0
4	E	14	13	13	0	0
4	F	14	13	13	0	0
5	A	36	0	0	4	0
5	B	43	0	0	2	0
5	C	41	0	0	4	0
5	D	51	0	0	1	0
5	E	48	0	0	2	0
5	F	43	0	0	0	0
6	A	5	0	0	2	0
6	B	10	0	0	0	0
6	D	5	0	0	1	0
6	E	5	0	0	1	0
7	A	80	0	0	4	0
7	B	78	0	0	5	0
7	C	80	0	0	4	0
7	D	56	0	0	4	0
7	E	53	0	0	1	0
7	F	83	0	0	3	0
All	All	13511	12111	12156	94	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 4.

The worst 5 of 94 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:B:93:LEU:HD13	2:C:301:OCA:H81	1.52	0.91
1:A:57:ASP:OD1	7:A:401:HOH:O	1.97	0.83
1:C:259:LEU:HD21	2:C:301:OCA:H82	1.60	0.81
6:D:305:PO4:O4	7:D:401:HOH:O	2.01	0.78
1:B:57:ASP:OD1	7:B:401:HOH:O	2.04	0.75

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	273/291 (94%)	266 (97%)	7 (3%)	0	100 100
1	B	272/291 (94%)	262 (96%)	10 (4%)	0	100 100
1	C	276/291 (95%)	265 (96%)	10 (4%)	1 (0%)	34 52
1	D	273/291 (94%)	263 (96%)	10 (4%)	0	100 100
1	E	272/291 (94%)	263 (97%)	9 (3%)	0	100 100
1	F	275/291 (94%)	263 (96%)	12 (4%)	0	100 100
All	All	1641/1746 (94%)	1582 (96%)	58 (4%)	1 (0%)	51 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	199	THR

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	226/239 (95%)	225 (100%)	1 (0%)	91 96
1	B	224/239 (94%)	223 (100%)	1 (0%)	91 96
1	C	228/239 (95%)	227 (100%)	1 (0%)	91 96
1	D	226/239 (95%)	226 (100%)	0	100 100
1	E	225/239 (94%)	223 (99%)	2 (1%)	78 91
1	F	228/239 (95%)	227 (100%)	1 (0%)	91 96
All	All	1357/1434 (95%)	1351 (100%)	6 (0%)	88 96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	181	PHE
1	E	215	HIS
1	F	215	HIS
1	B	215	HIS
1	A	104	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	LTV	D	304	-	50,50,50	0.93	2 (4%)	52,52,52	0.74	2 (3%)
5	LTV	C	305	-	40,40,50	1.01	2 (5%)	42,42,52	0.85	2 (4%)
2	OCA	A	301	1	8,8,9	0.52	0	7,7,9	0.95	0
6	PO4	D	305	-	4,4,4	0.89	0	6,6,6	0.33	0
4	NAG	B	305	1	14,14,15	0.31	0	17,19,21	0.49	0
6	PO4	B	302	-	4,4,4	0.90	0	6,6,6	0.43	0
2	OCA	F	301	1	6,6,9	0.60	0	5,5,9	0.90	0
5	LTV	E	304	-	47,47,50	0.95	2 (4%)	49,49,52	0.74	2 (4%)
6	PO4	A	305	-	4,4,4	0.90	0	6,6,6	0.44	0
5	LTV	B	306	-	42,42,50	1.00	2 (4%)	44,44,52	0.80	2 (4%)
4	NAG	E	303	-	14,14,15	0.18	0	17,19,21	0.44	0
2	OCA	E	301	1	8,8,9	0.53	0	7,7,9	1.01	0
4	NAG	A	303	1	14,14,15	0.95	1 (7%)	17,19,21	0.67	1 (5%)
5	LTV	F	304	-	42,42,50	0.99	2 (4%)	44,44,52	0.78	2 (4%)
2	OCA	B	301	1	8,8,9	1.12	1 (12%)	7,7,9	0.92	0
5	LTV	A	304	-	35,35,50	1.08	2 (5%)	37,37,52	0.86	2 (5%)
4	NAG	C	304	-	14,14,15	0.22	0	17,19,21	0.41	0
2	OCA	D	301	1	8,8,9	0.54	0	7,7,9	0.96	0
6	PO4	E	305	-	4,4,4	0.91	0	6,6,6	0.45	0
4	NAG	F	303	-	14,14,15	0.24	0	17,19,21	0.53	0
6	PO4	B	307	-	4,4,4	0.91	0	6,6,6	0.42	0
4	NAG	D	303	-	14,14,15	0.60	0	17,19,21	0.84	1 (5%)
2	OCA	C	301	-	8,8,9	1.10	1 (12%)	7,7,9	0.96	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	NAG	C	304	-	-	0/6/23/26	0/1/1/1
5	LTV	D	304	-	-	27/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LTV	C	305	-	-	19/41/41/51	-
5	LTV	B	306	-	-	25/43/43/51	-
2	OCA	A	301	1	-	4/5/6/7	-
4	NAG	E	303	-	-	1/6/23/26	0/1/1/1
4	NAG	B	305	1	-	0/6/23/26	0/1/1/1
2	OCA	E	301	1	-	2/5/6/7	-
4	NAG	A	303	1	-	0/6/23/26	0/1/1/1
4	NAG	F	303	-	-	4/6/23/26	0/1/1/1
4	NAG	D	303	-	-	2/6/23/26	0/1/1/1
2	OCA	C	301	-	-	4/6/6/7	-
5	LTV	F	304	-	-	22/43/43/51	-
2	OCA	B	301	1	-	5/6/6/7	-
5	LTV	E	304	-	-	35/48/48/51	-
2	OCA	F	301	1	-	1/3/4/7	-
2	OCA	D	301	1	-	3/5/6/7	-
5	LTV	A	304	-	-	20/36/36/51	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	304	LTV	O3-C21	3.80	1.44	1.33
5	C	305	LTV	O3-C21	3.75	1.44	1.33
5	B	306	LTV	O3-C21	3.68	1.44	1.33
5	D	304	LTV	O3-C21	3.67	1.44	1.33
5	F	304	LTV	O3-C21	3.66	1.44	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	304	LTV	O1-C17-C16	2.80	120.70	111.91
5	C	305	LTV	O3-C21-C22	2.80	120.68	111.91
5	A	304	LTV	O3-C21-C22	2.75	120.53	111.91
5	B	306	LTV	O1-C17-C16	2.64	120.18	111.91
5	C	305	LTV	O1-C17-C16	2.63	120.15	111.91

There are no chirality outliers.

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	LTV	O4-C21-O3-C20
5	A	304	LTV	C22-C21-O3-C20
5	A	304	LTV	O2-C19-C20-O3
5	A	304	LTV	C18-C19-C20-O3
5	A	304	LTV	O1-C18-C19-C20

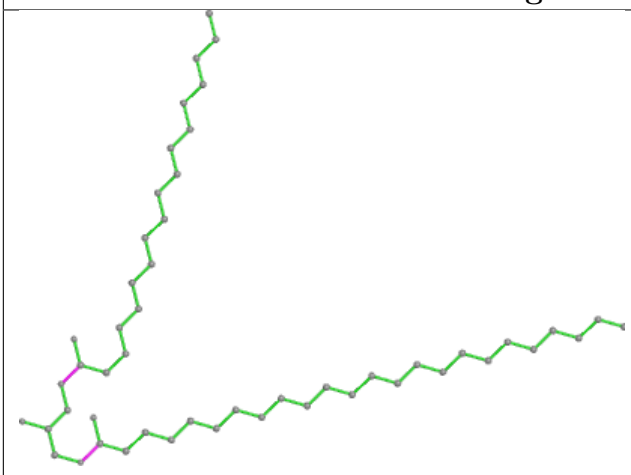
There are no ring outliers.

14 monomers are involved in 53 short contacts:

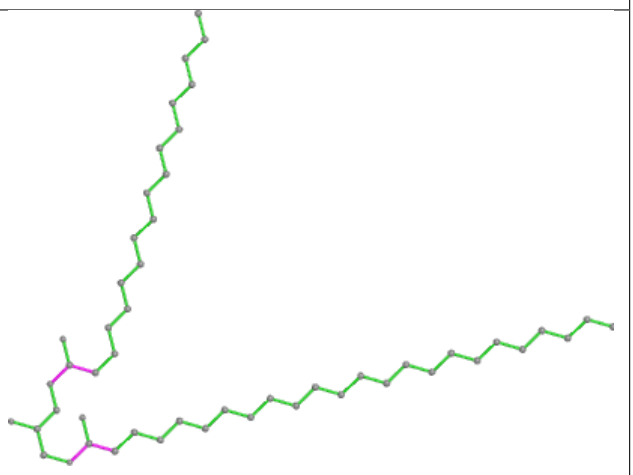
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	304	LTV	1	0
5	C	305	LTV	4	0
2	A	301	OCA	11	0
6	D	305	PO4	1	0
5	E	304	LTV	2	0
6	A	305	PO4	2	0
5	B	306	LTV	2	0
2	E	301	OCA	8	0
2	B	301	OCA	10	0
5	A	304	LTV	4	0
2	D	301	OCA	6	0
6	E	305	PO4	1	0
4	D	303	NAG	1	0
2	C	301	OCA	12	0

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.

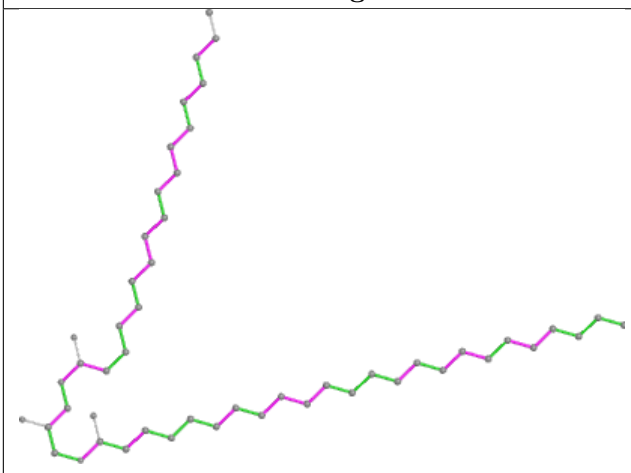
Ligand LTV D 304



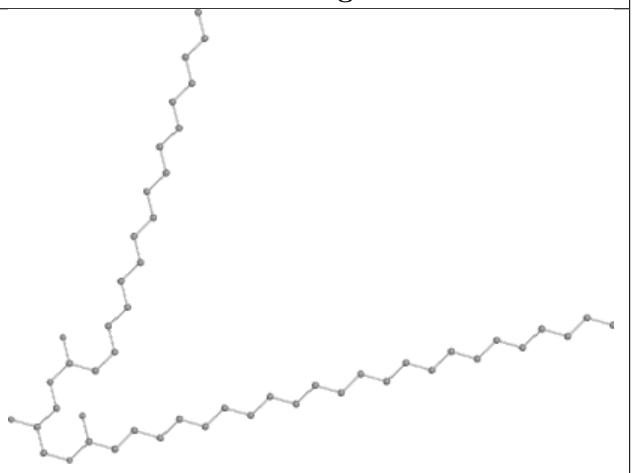
Bond lengths



Bond angles

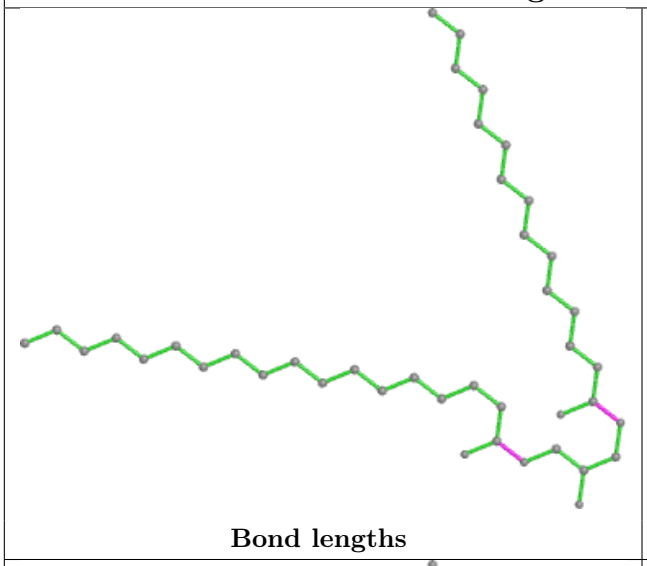


Torsions



Rings

Ligand LTV C 305



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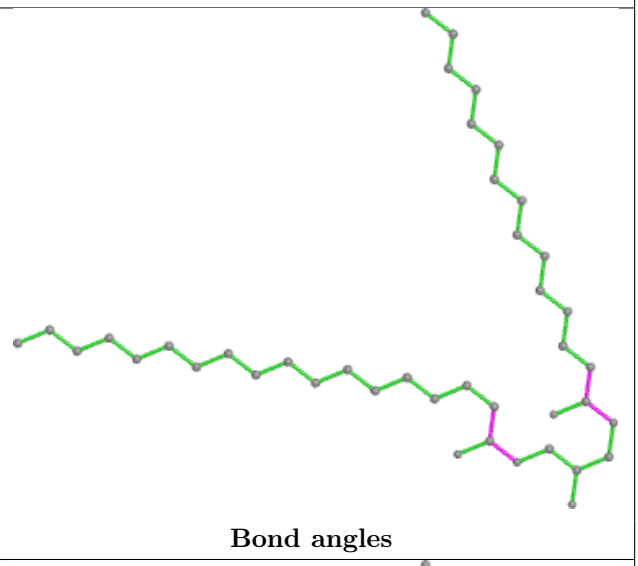
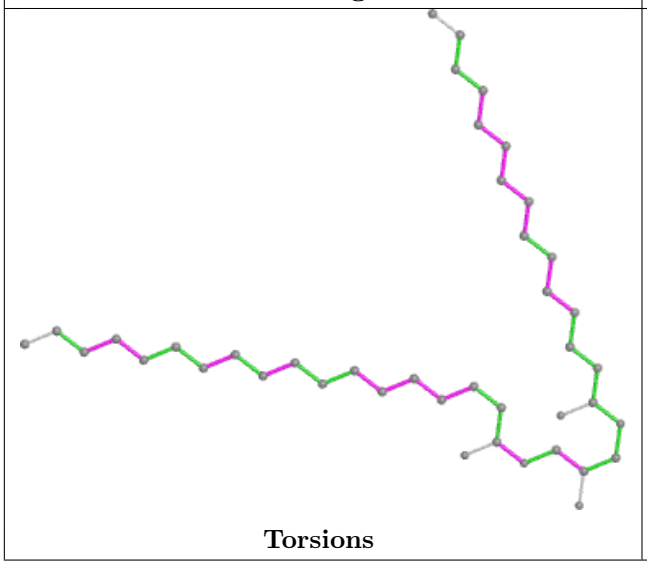


Bond angles



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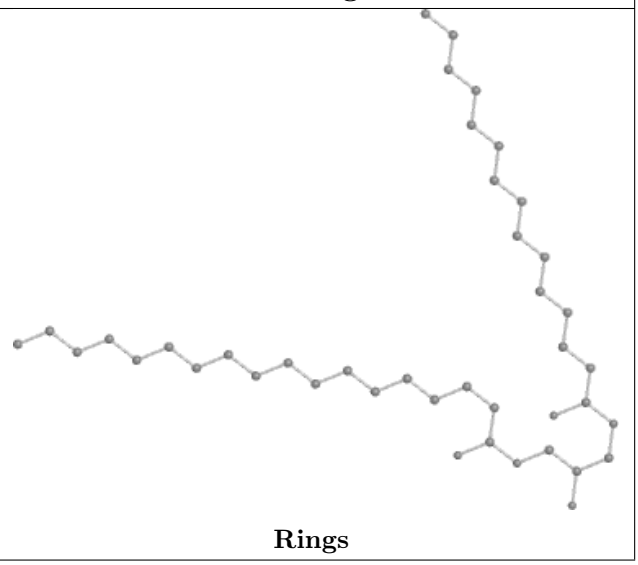
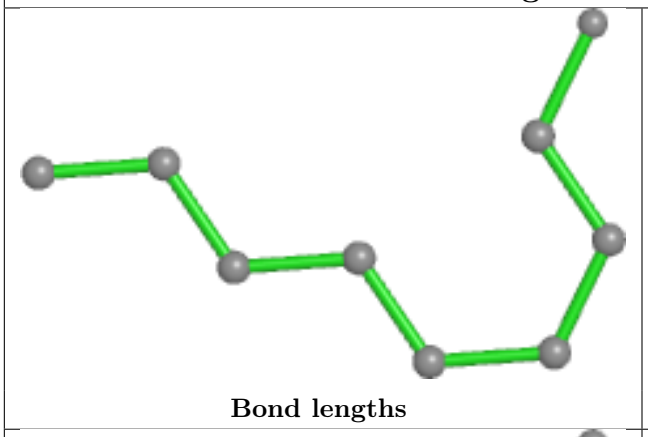


Rings

Ligand OCA A 301



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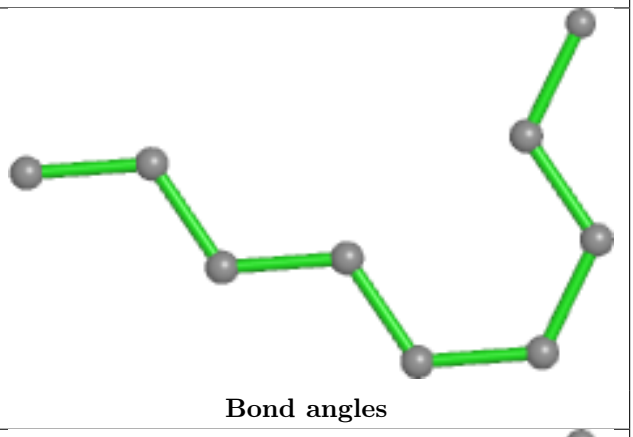

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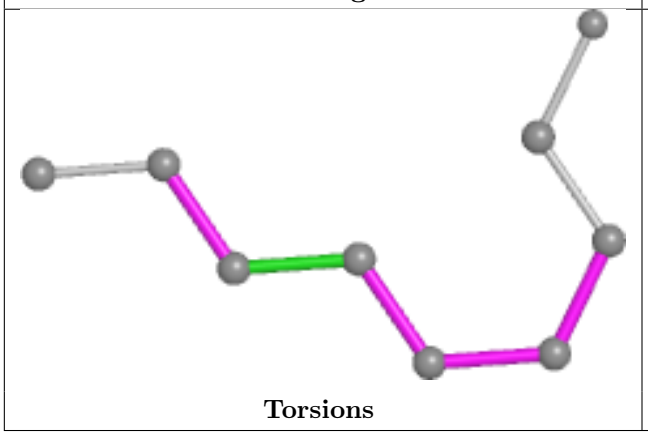

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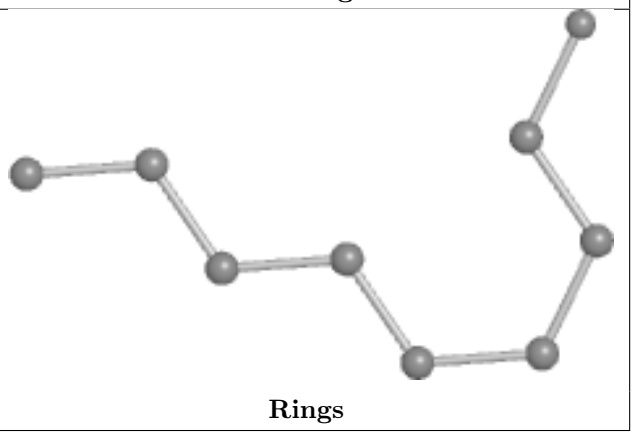
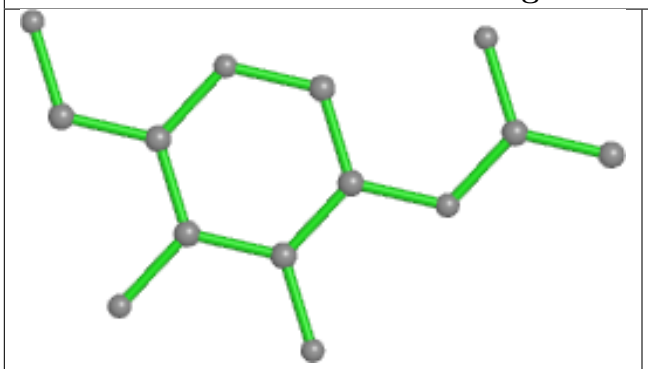


Rings

Ligand NAG B 305



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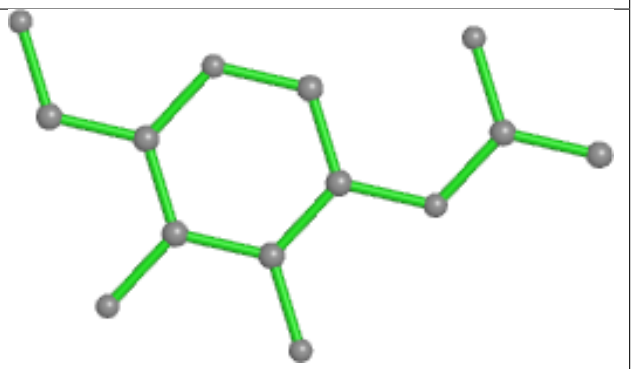
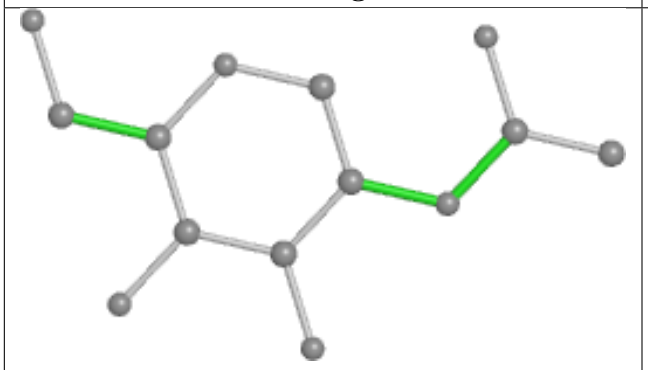
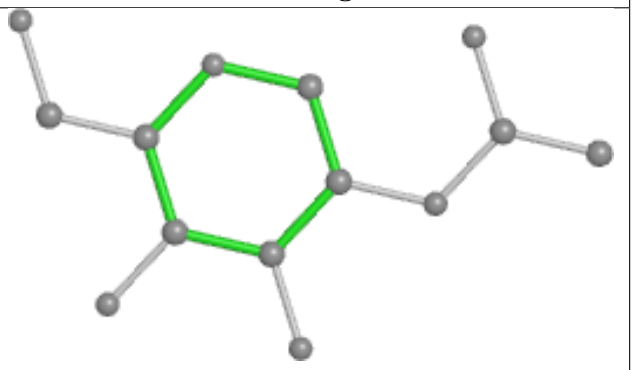


Bond angles

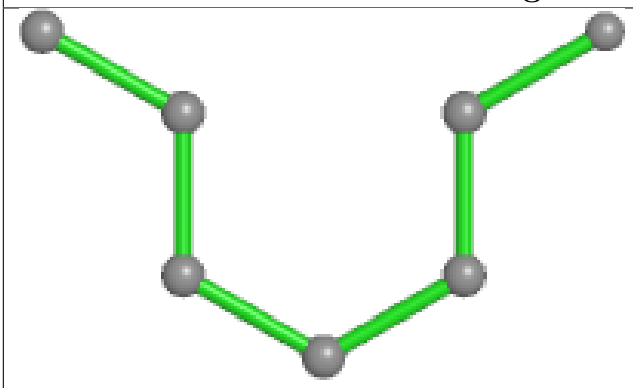


Torsions

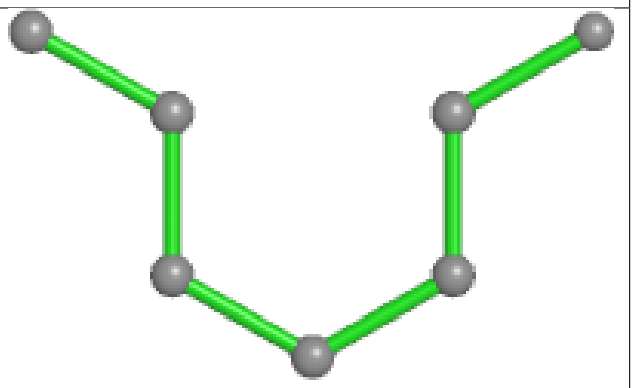


Rings

Ligand OCA F 301



Bond lengths



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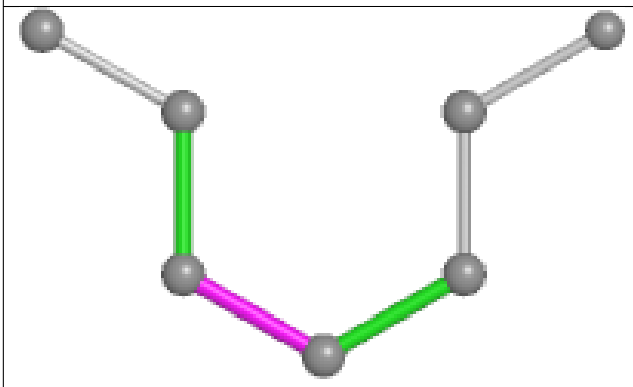

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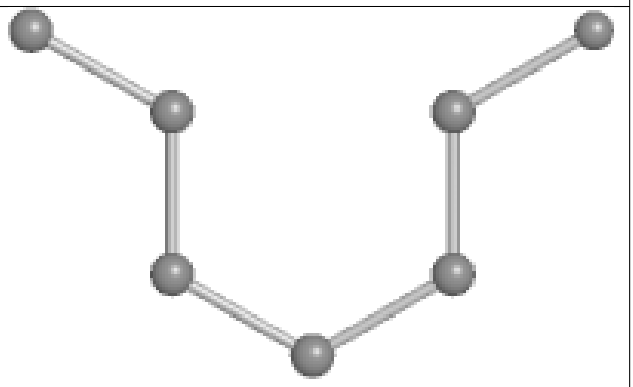
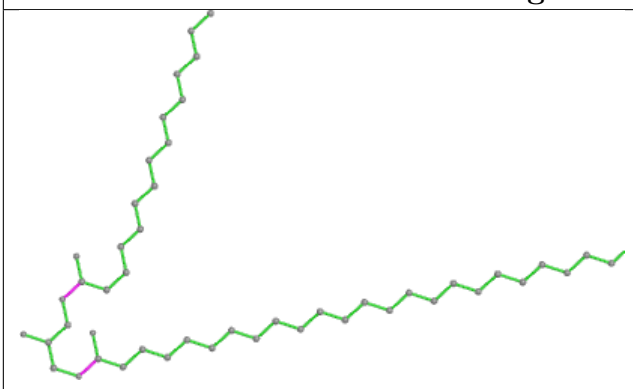


Rings

Ligand LTV E 304



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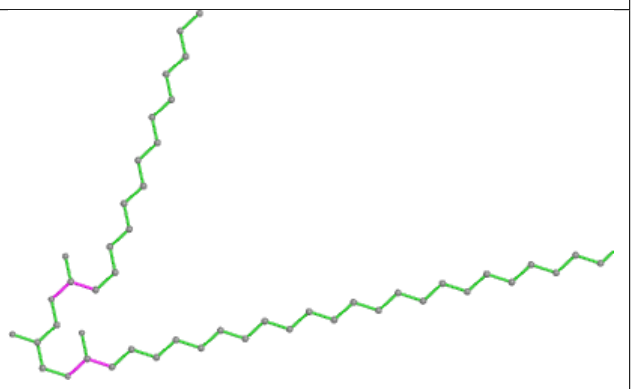
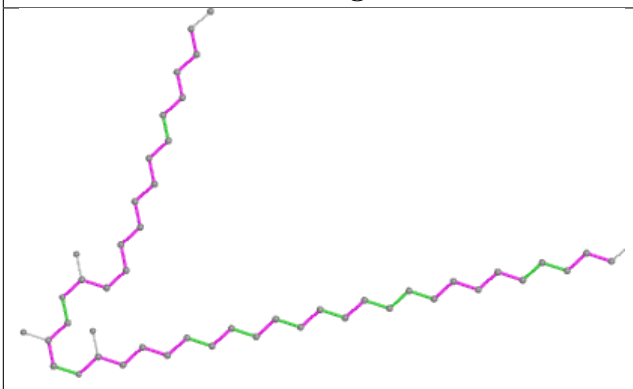


Bond angles



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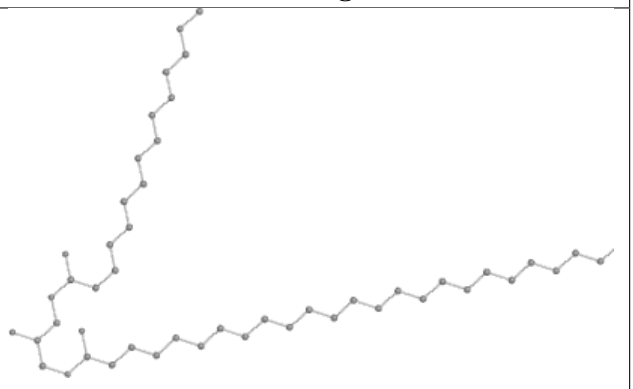
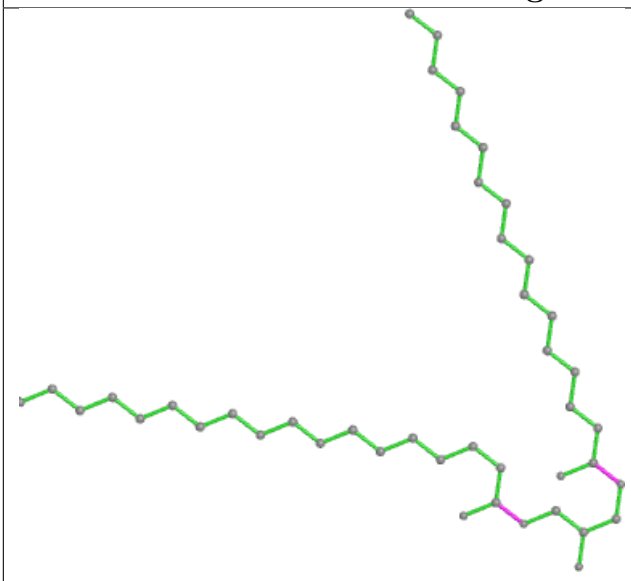


Rings

Ligand LTV B 306



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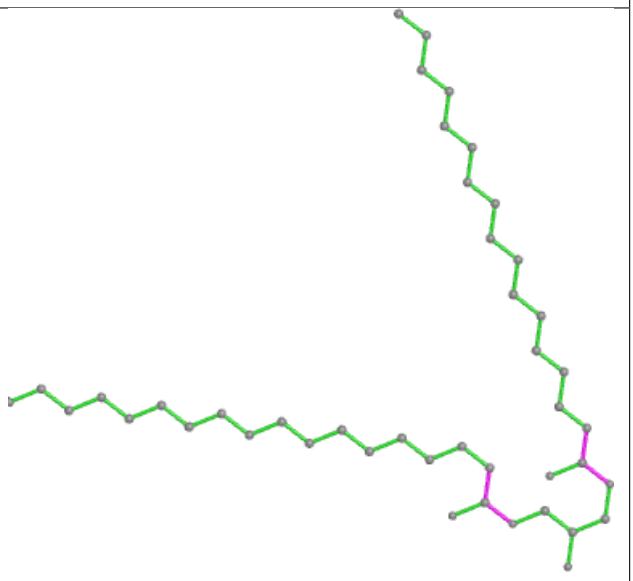

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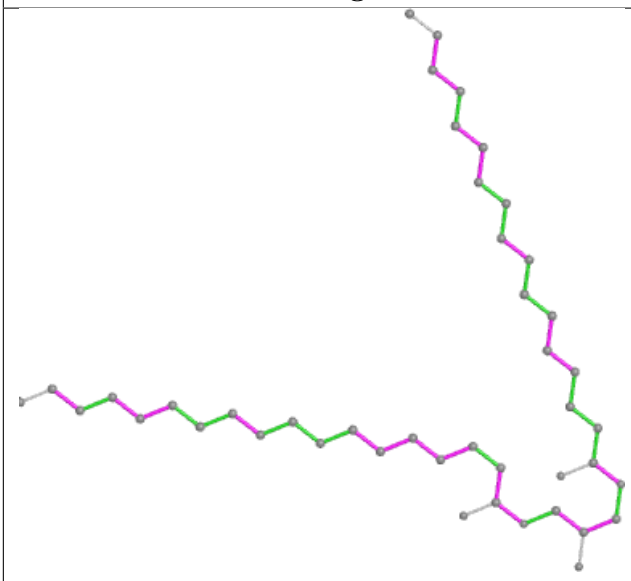

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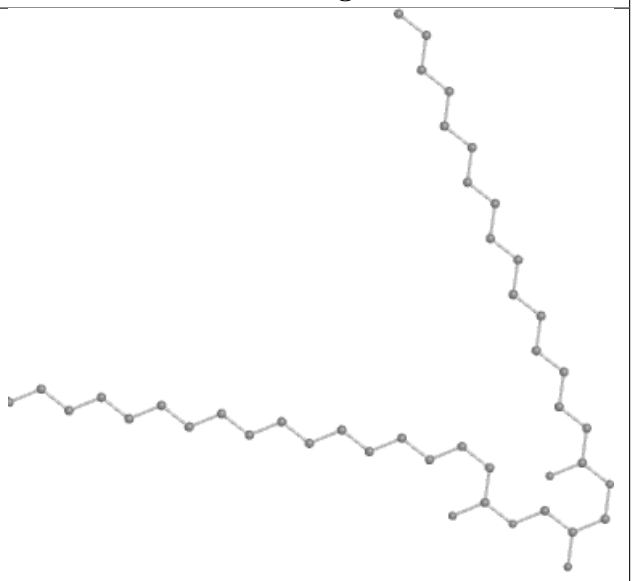
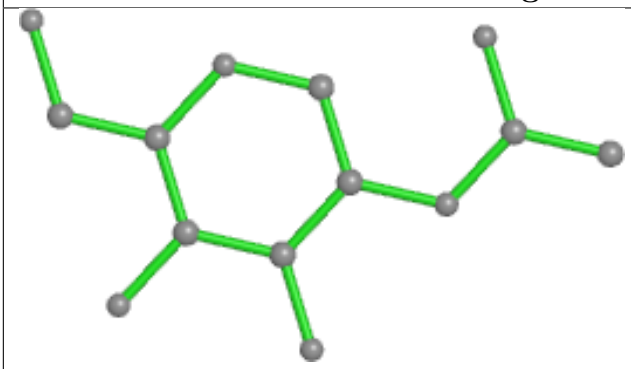


Rings

Ligand NAG E 303



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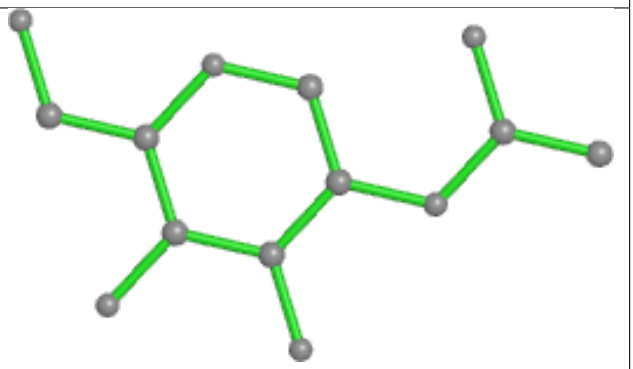

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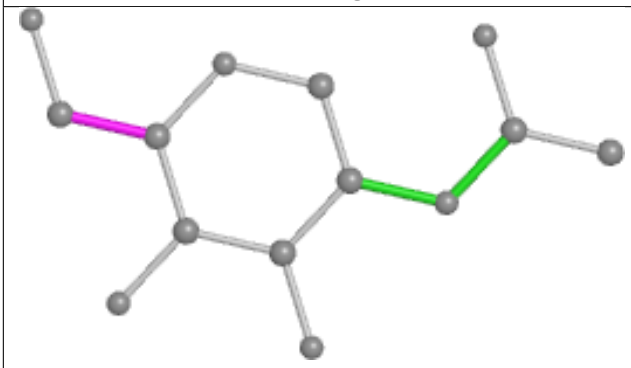

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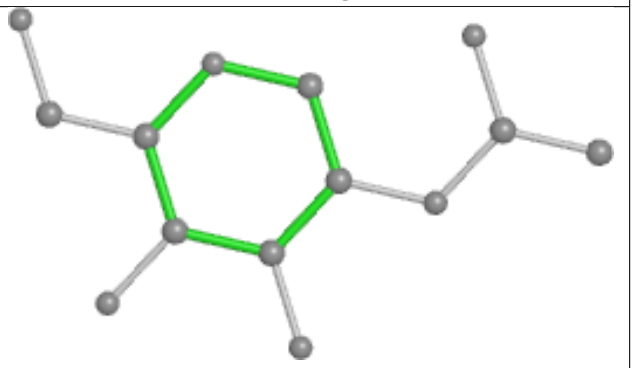
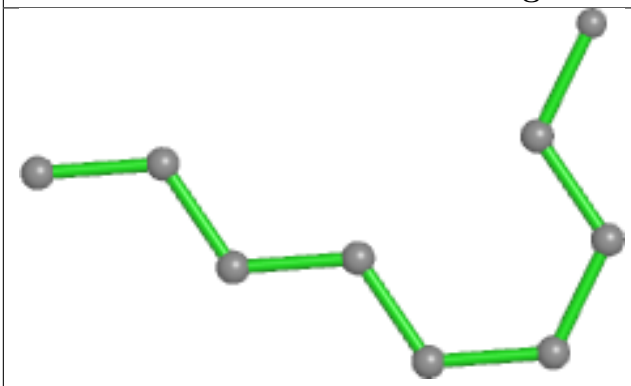


Rings

Ligand OCA E 301



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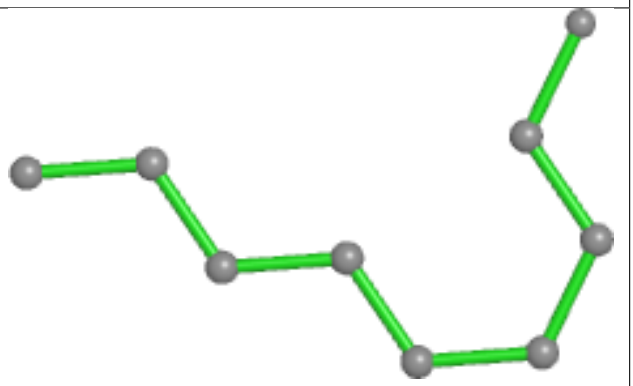

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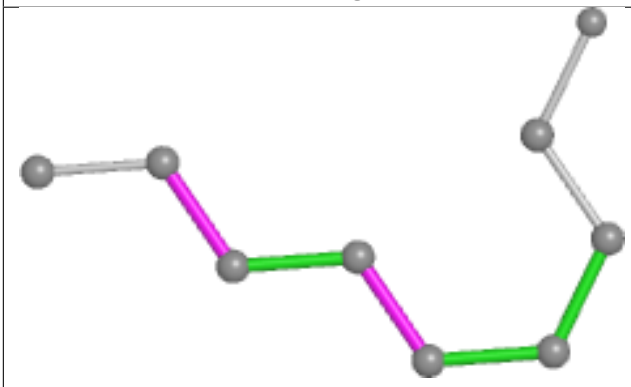

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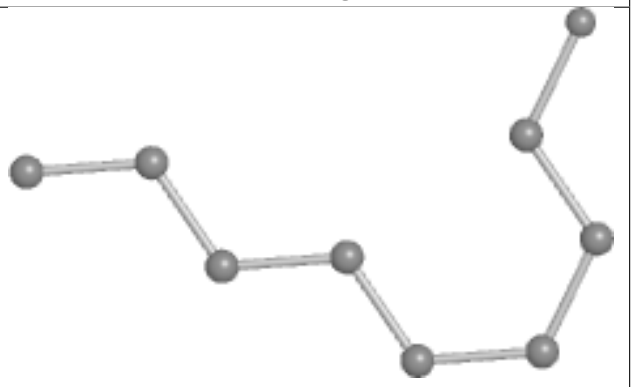
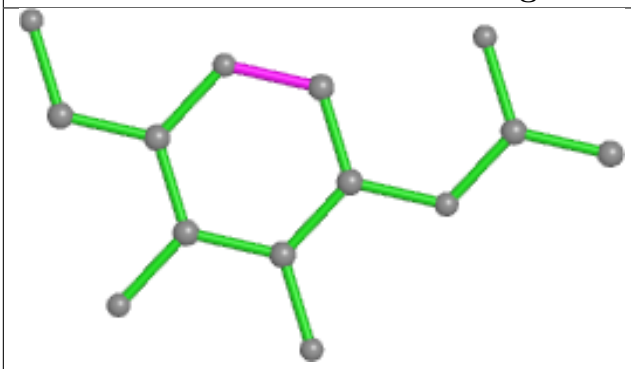


Rings

Ligand NAG A 303



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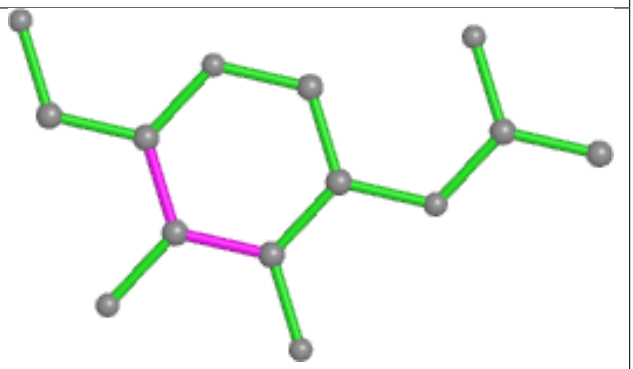

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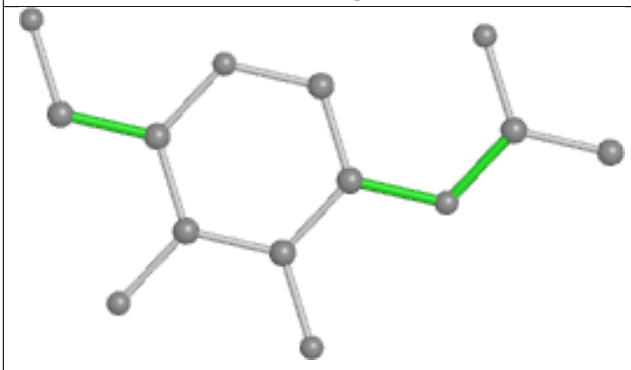

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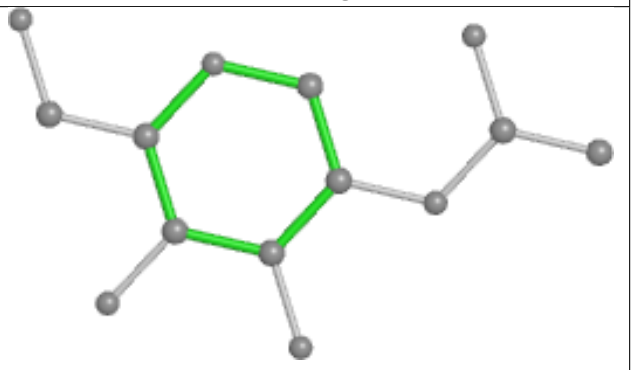
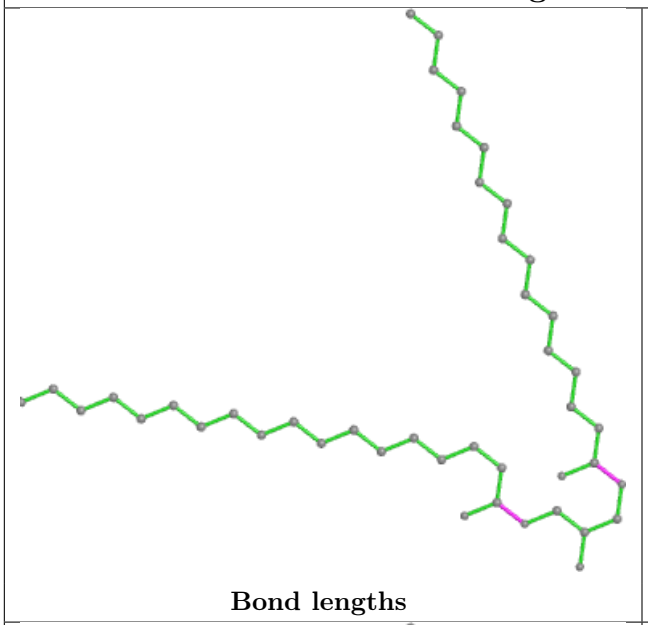


Rings

Ligand LTV F 304



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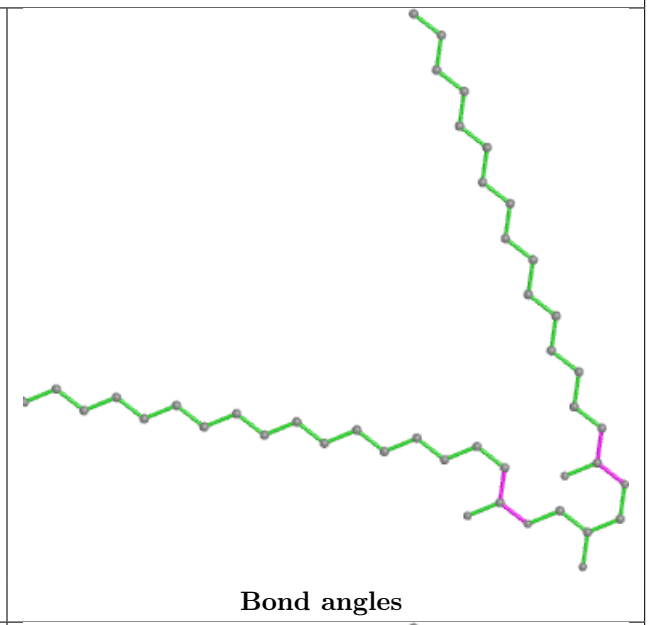
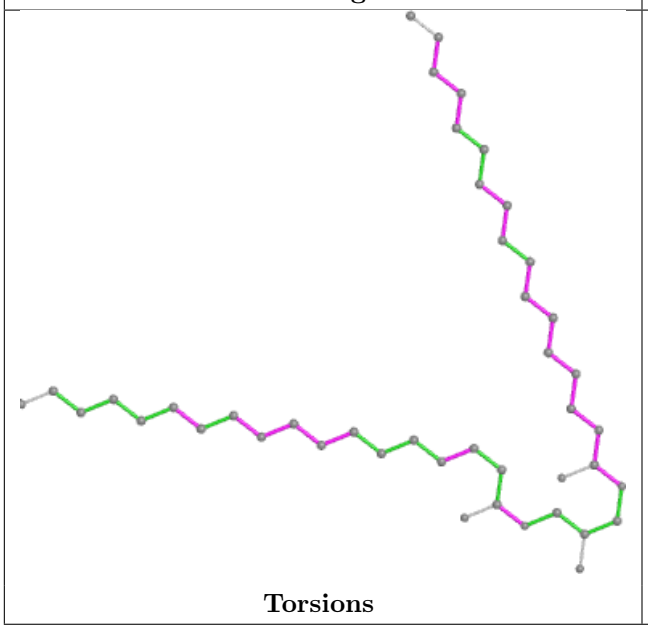
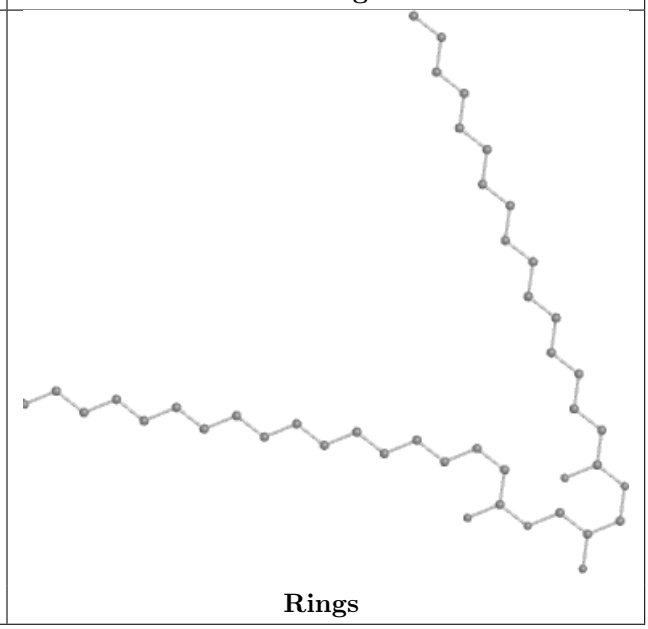


Bond angles

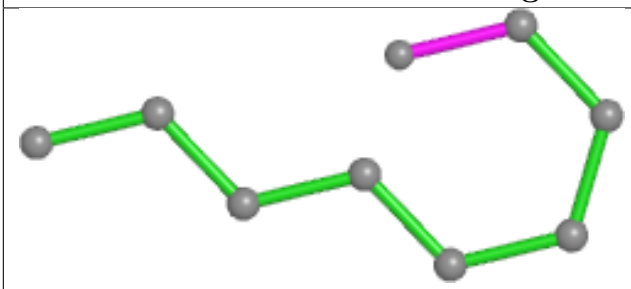


Torsions

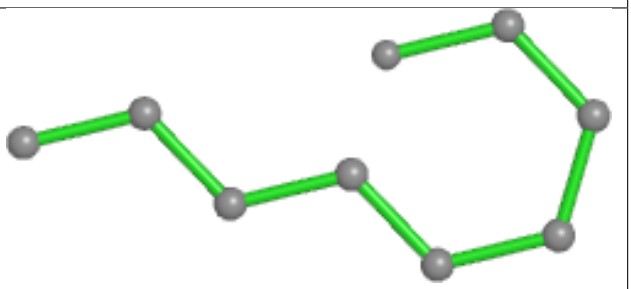


Rings

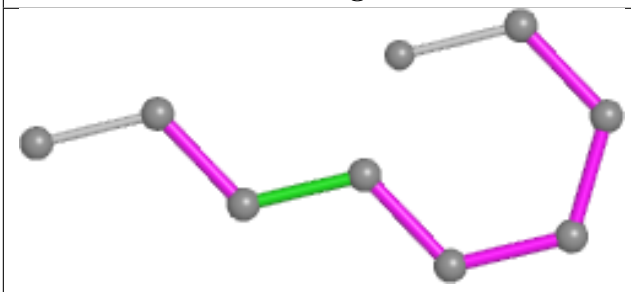
Ligand OCA B 301



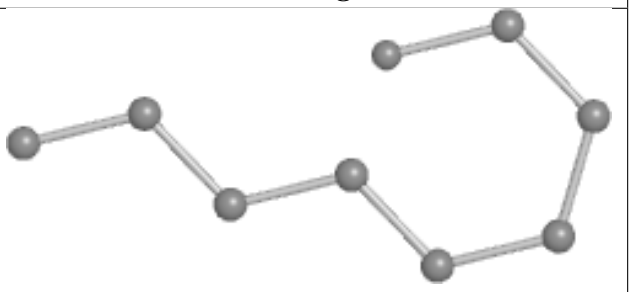
Bond lengths



Bond angles

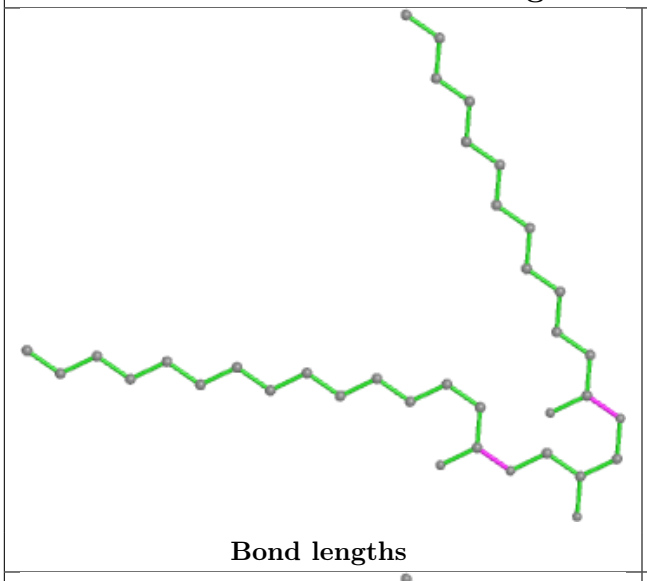


Torsions

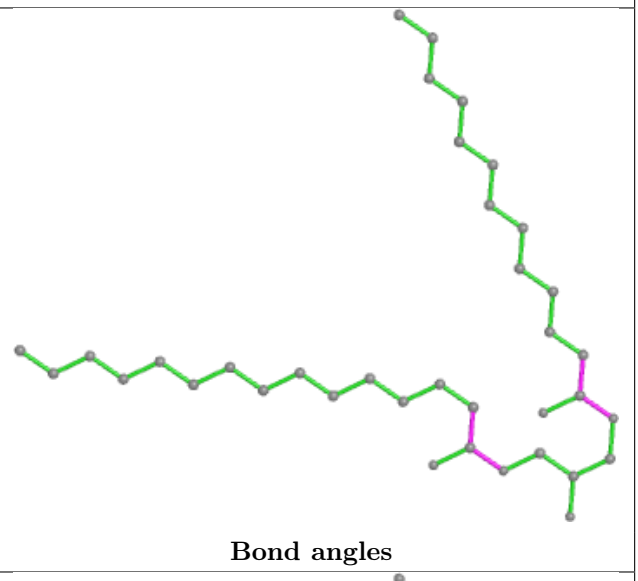


Rings

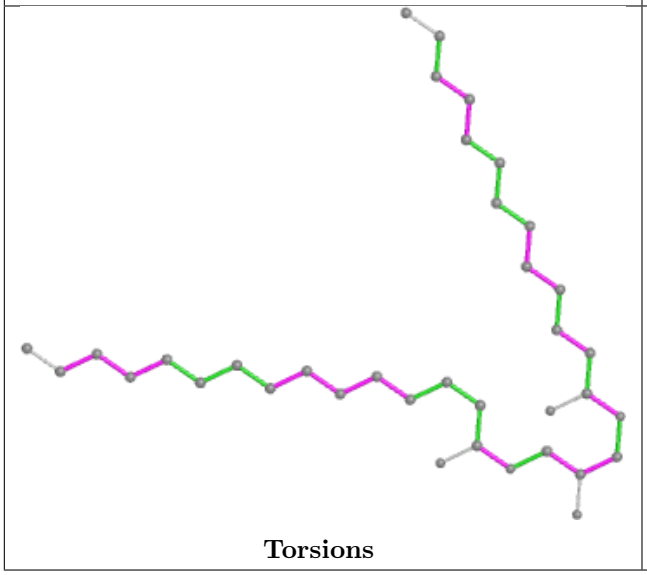
Ligand LTV A 304



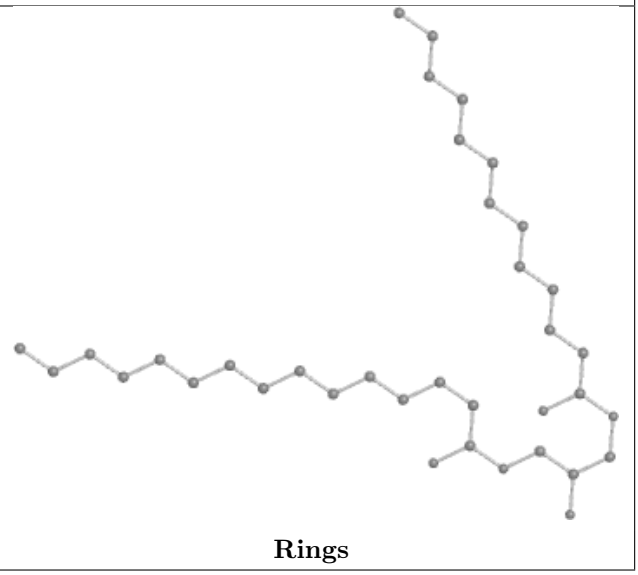
Bond lengths



Bond angles

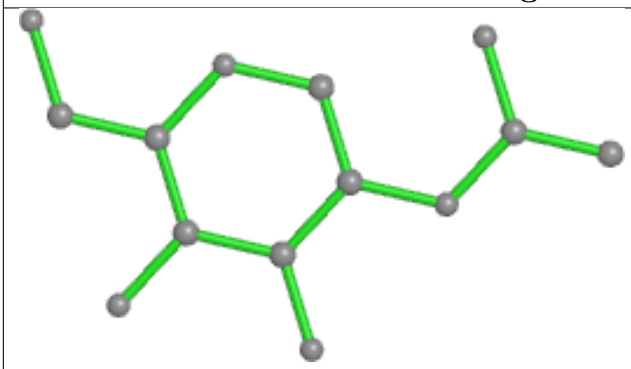


Torsions

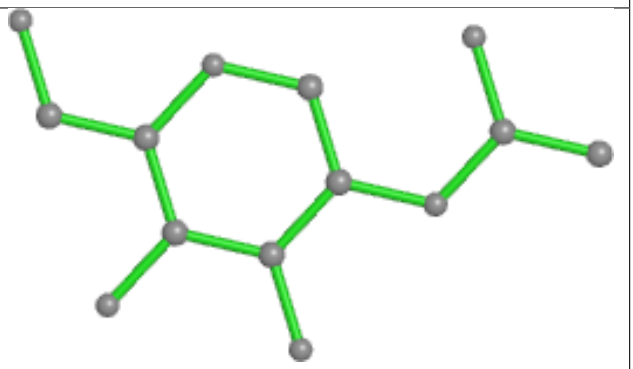


Rings

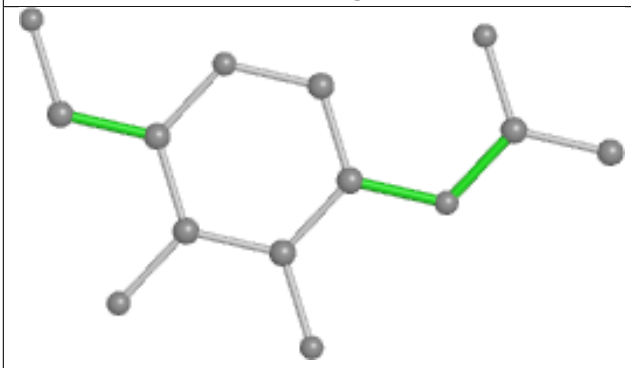
Ligand NAG C 304



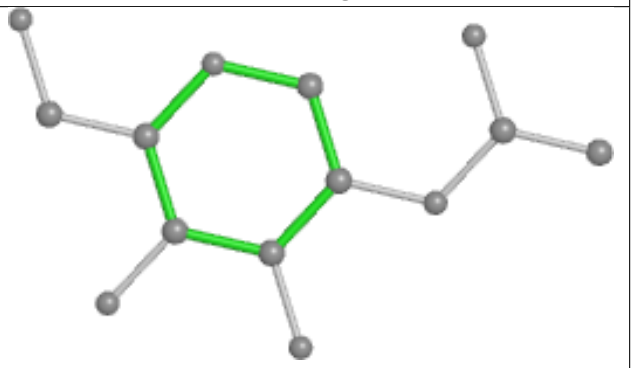
Bond lengths



Bond angles

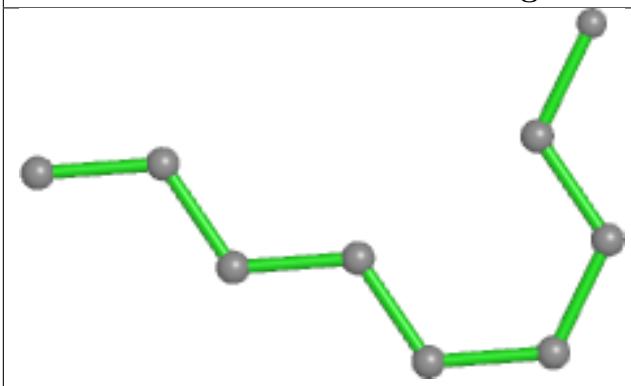


Torsions

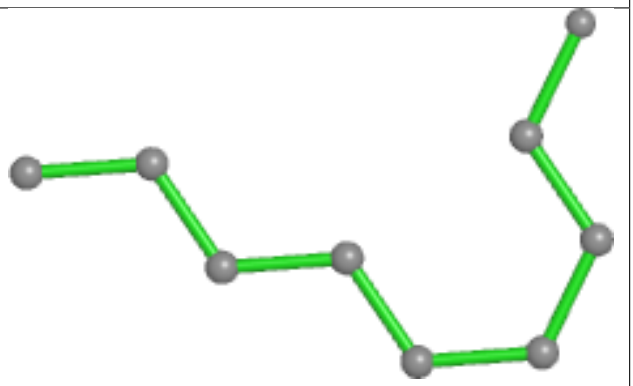


Rings

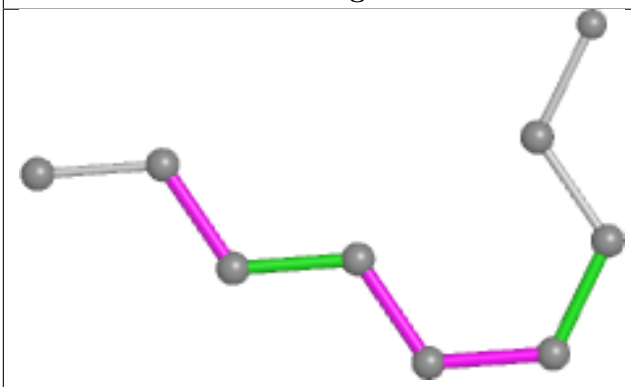
Ligand OCA D 301



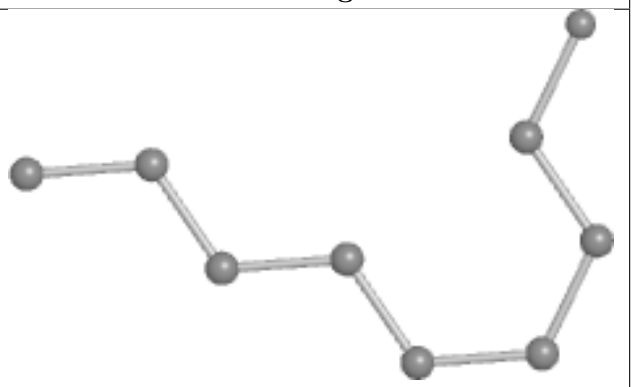
Bond lengths



Bond angles

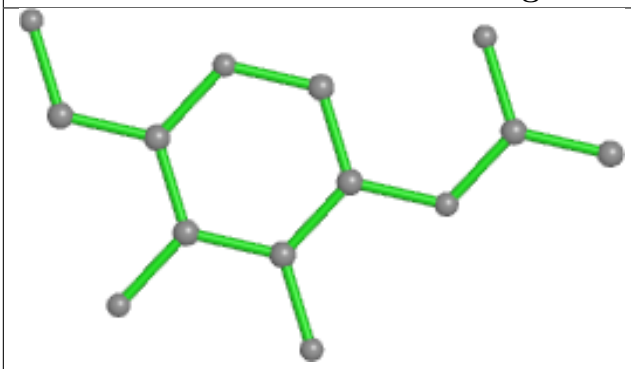


Torsions

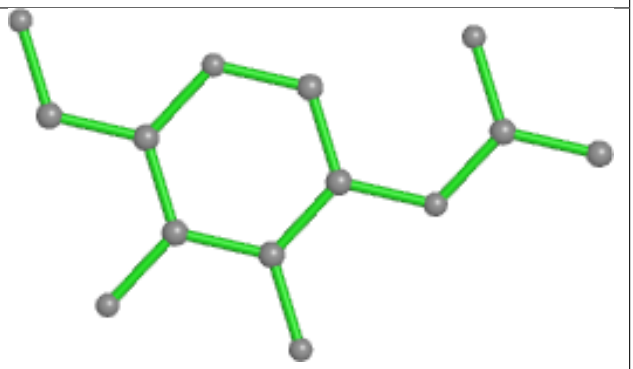


Rings

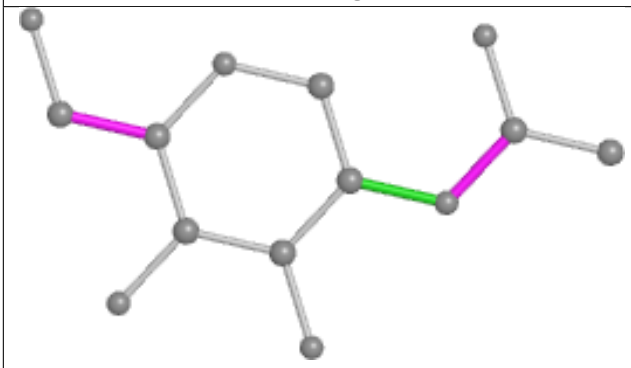
Ligand NAG F 303



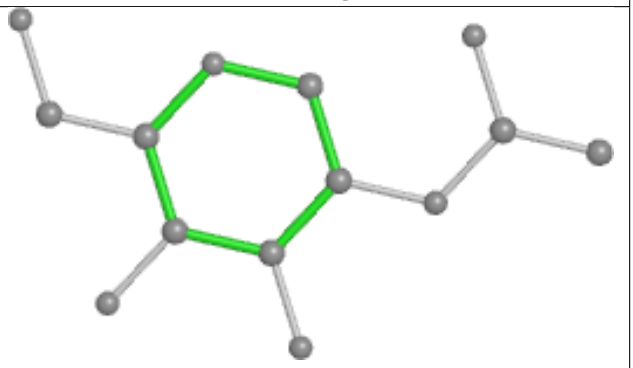
Bond lengths



Bond angles

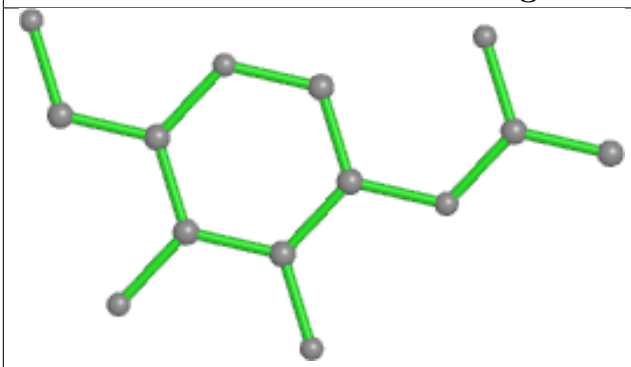


Torsions

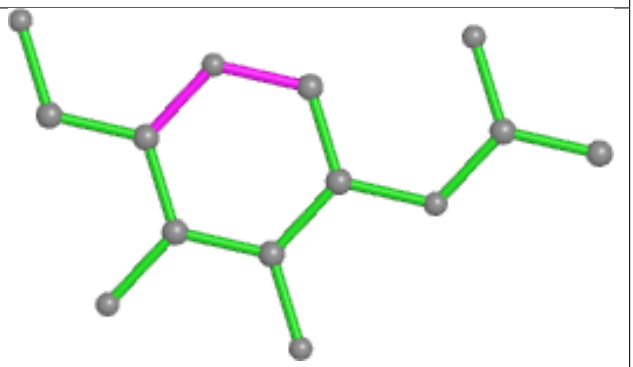


Rings

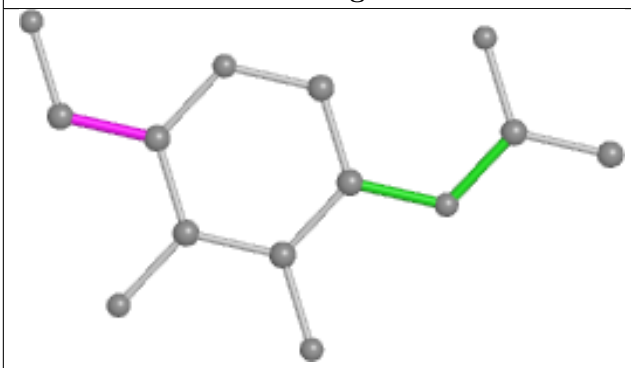
Ligand NAG D 303



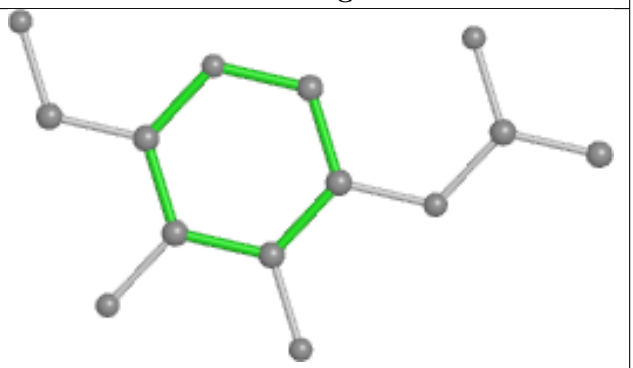
Bond lengths



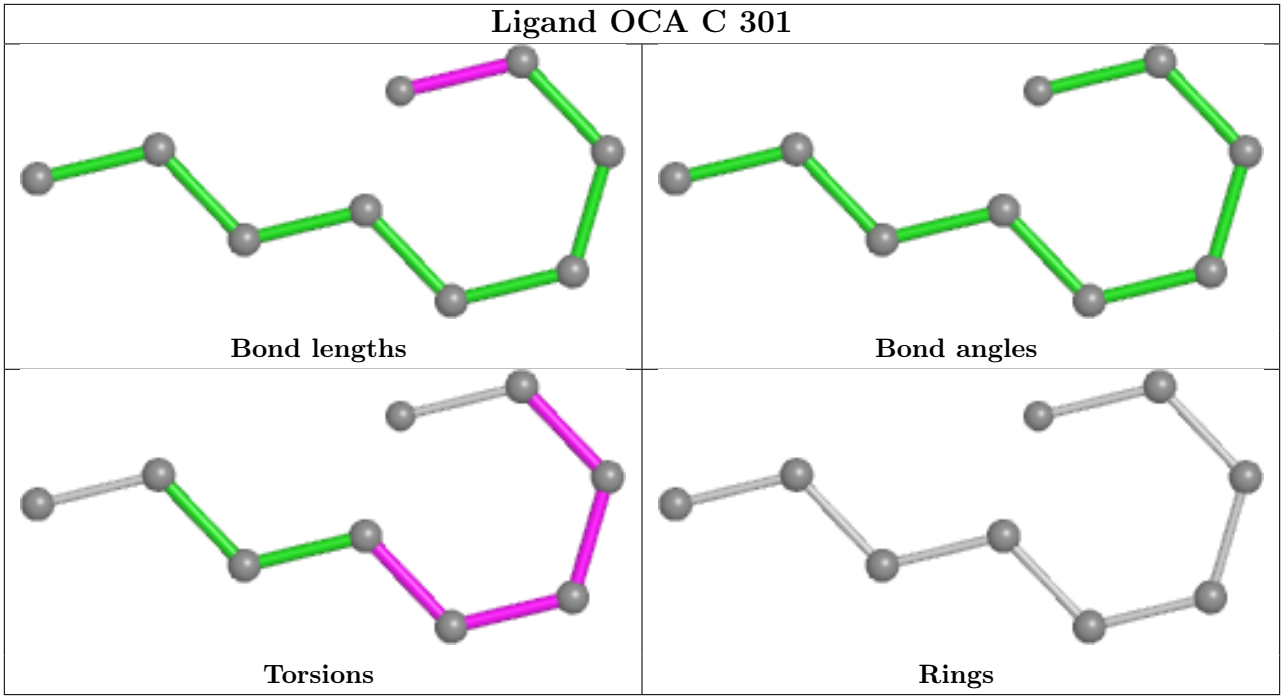
Bond angles



Torsions



Rings



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	269/291 (92%)	-0.50	0	100	100	15, 25, 45, 68	1 (0%)
1	B	269/291 (92%)	-0.46	1 (0%)	92	93	13, 24, 44, 61	0
1	C	269/291 (92%)	-0.46	1 (0%)	92	93	17, 30, 50, 72	0
1	D	269/291 (92%)	-0.45	1 (0%)	92	93	15, 26, 46, 64	1 (0%)
1	E	269/291 (92%)	-0.26	1 (0%)	92	93	22, 36, 61, 85	0
1	F	269/291 (92%)	-0.36	1 (0%)	92	93	19, 33, 56, 77	2 (0%)
All	All	1614/1746 (92%)	-0.42	5 (0%)	94	94	13, 29, 53, 85	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	39	ASN	3.9
1	C	39	ASN	3.0
1	B	89[A]	TRP	2.5
1	E	39	ASN	2.3
1	D	89[A]	TRP	2.3

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 monosaccharides in this entry.

6.4 Ligands (i)

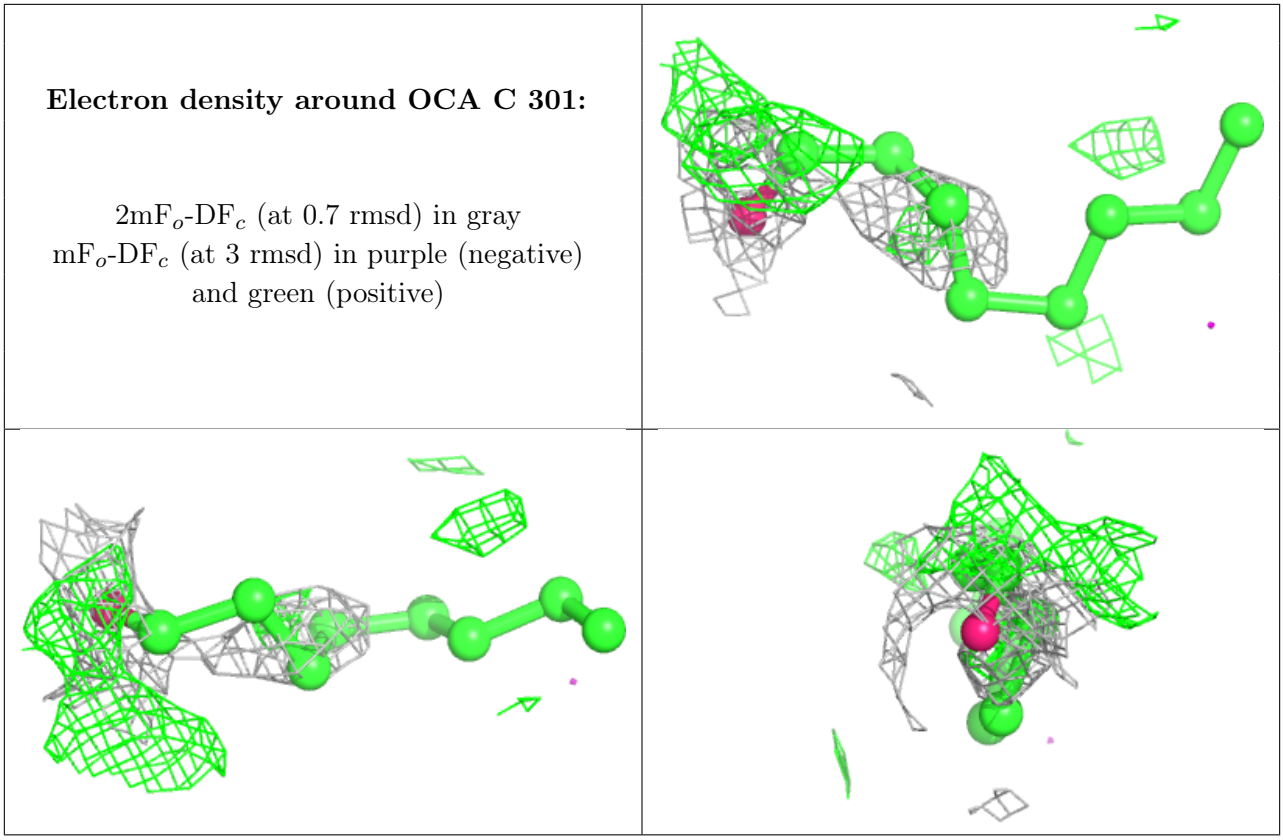
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	PO4	B	307	5/5	0.26	1.18	78,104,112,118	5
2	OCA	C	301	9/10	0.62	0.51	25,28,36,38	9
6	PO4	E	305	5/5	0.62	0.54	61,65,72,75	5
4	NAG	F	303	14/15	0.63	0.56	86,116,154,160	0
4	NAG	E	303	14/15	0.66	0.38	87,113,136,139	0
4	NAG	A	303	14/15	0.72	0.38	79,99,119,138	0
4	NAG	C	304	14/15	0.72	0.35	77,99,120,126	0
6	PO4	B	302	5/5	0.73	0.59	42,45,68,70	5
2	OCA	E	301	9/10	0.74	0.48	31,34,36,40	9
4	NAG	D	303	14/15	0.74	0.49	85,107,129,129	0
2	OCA	A	301	9/10	0.78	0.44	22,26,34,40	9
4	NAG	B	305	14/15	0.81	0.22	55,74,107,107	0
6	PO4	D	305	5/5	0.82	0.20	31,32,52,65	0
2	OCA	D	301	9/10	0.83	0.41	22,32,38,45	9
5	LTV	D	304	51/51	0.83	0.26	29,52,73,79	0
2	OCA	B	301	9/10	0.83	0.39	23,30,37,39	9
5	LTV	E	304	48/51	0.84	0.25	32,51,71,82	0
5	LTV	A	304	36/51	0.84	0.28	33,52,69,72	0
5	LTV	B	306	43/51	0.84	0.26	30,48,79,83	0
5	LTV	C	305	41/51	0.85	0.25	36,52,78,88	0
5	LTV	F	304	43/51	0.86	0.25	32,54,73,78	0
6	PO4	A	305	5/5	0.87	0.33	30,31,49,55	5
3	CA	C	303	1/1	0.92	0.09	58,58,58,58	0
3	CA	C	302	1/1	0.93	0.06	48,48,48,48	0
3	CA	E	302	1/1	0.94	0.06	66,66,66,66	0
2	OCA	F	301	7/10	0.94	0.32	26,28,31,32	5
3	CA	A	302	1/1	0.94	0.05	60,60,60,60	0
3	CA	F	302	1/1	0.95	0.07	56,56,56,56	0
3	CA	B	304	1/1	0.95	0.08	53,53,53,53	0
3	CA	D	302	1/1	0.95	0.08	50,50,50,50	0
3	CA	B	303	1/1	0.98	0.12	29,29,29,29	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.

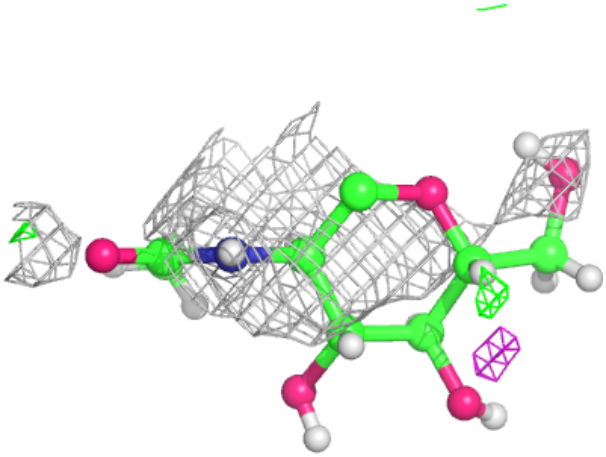
Electron density around OCA C 301:

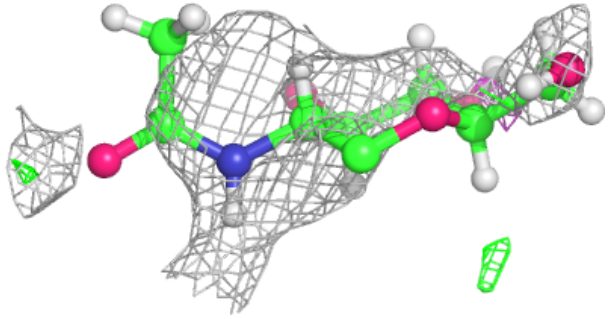
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

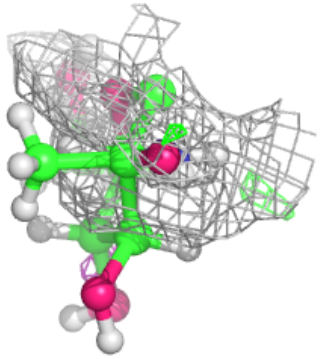


Electron density around NAG F 303:

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

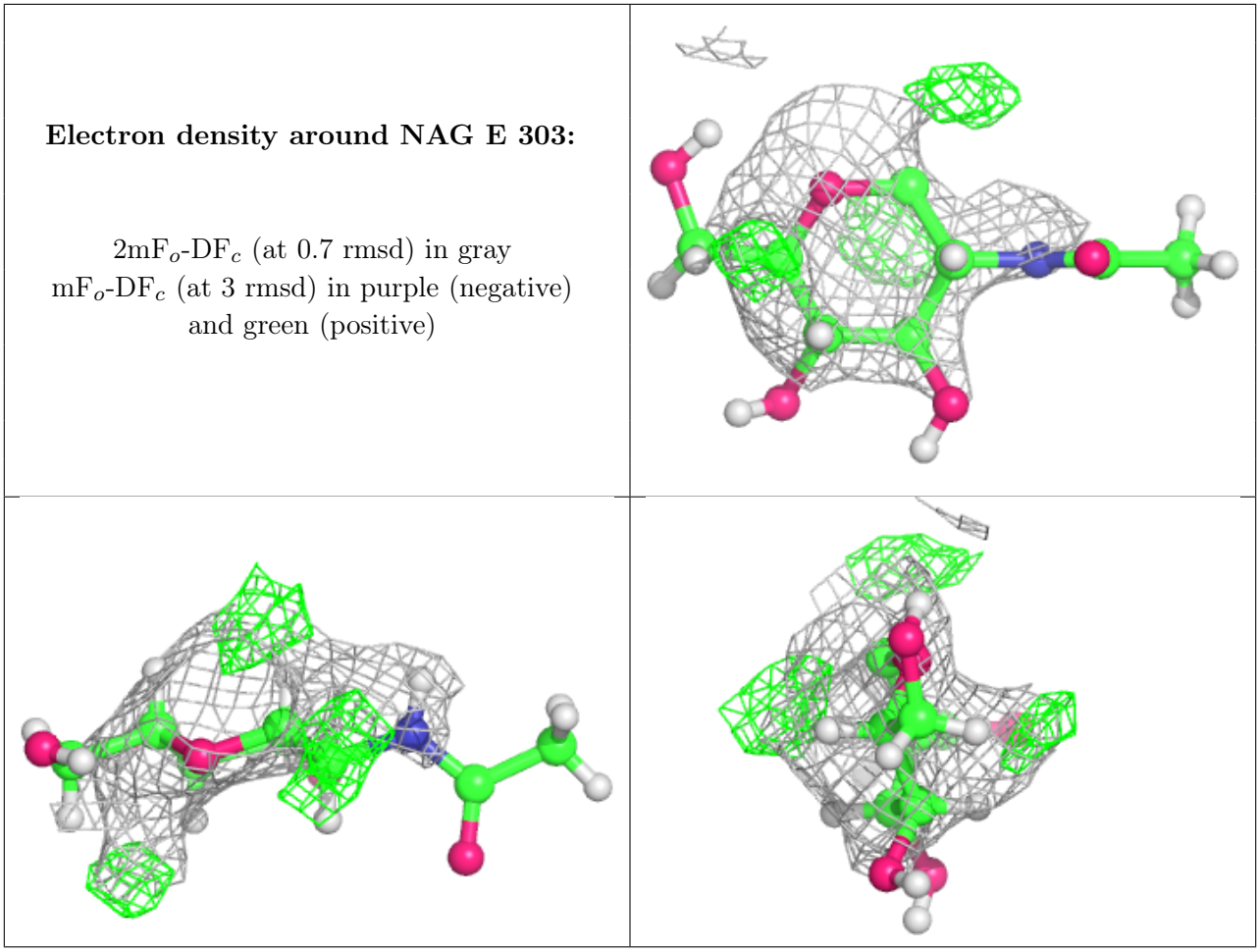






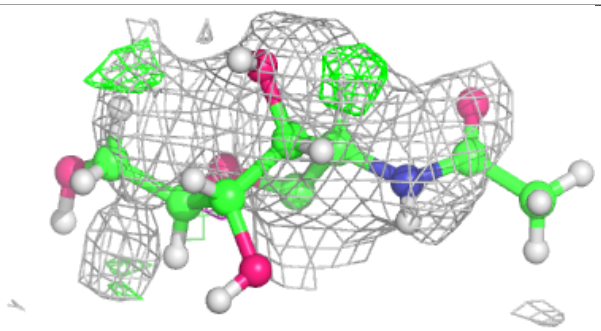
Electron density around NAG E 303:

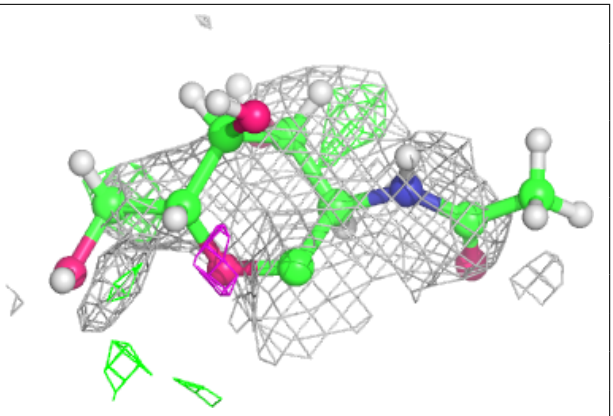
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

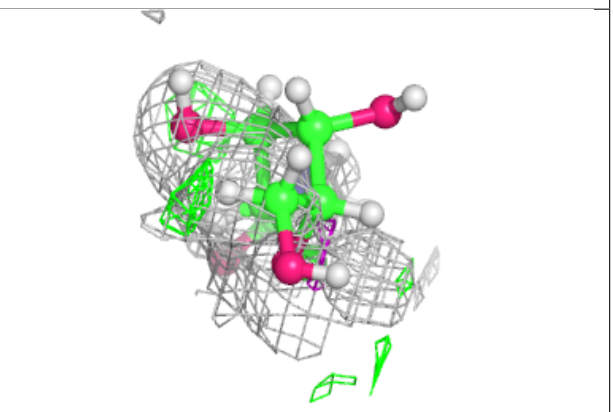


Electron density around NAG A 303:

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

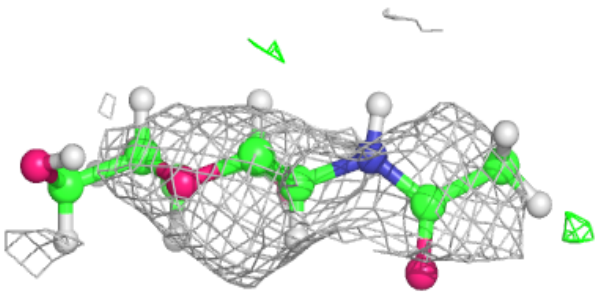


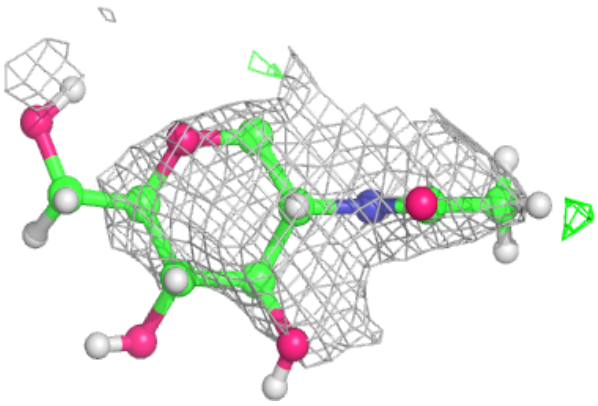


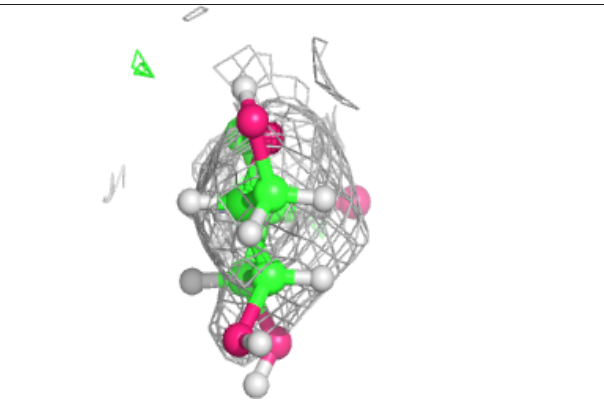


Electron density around NAG C 304:

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

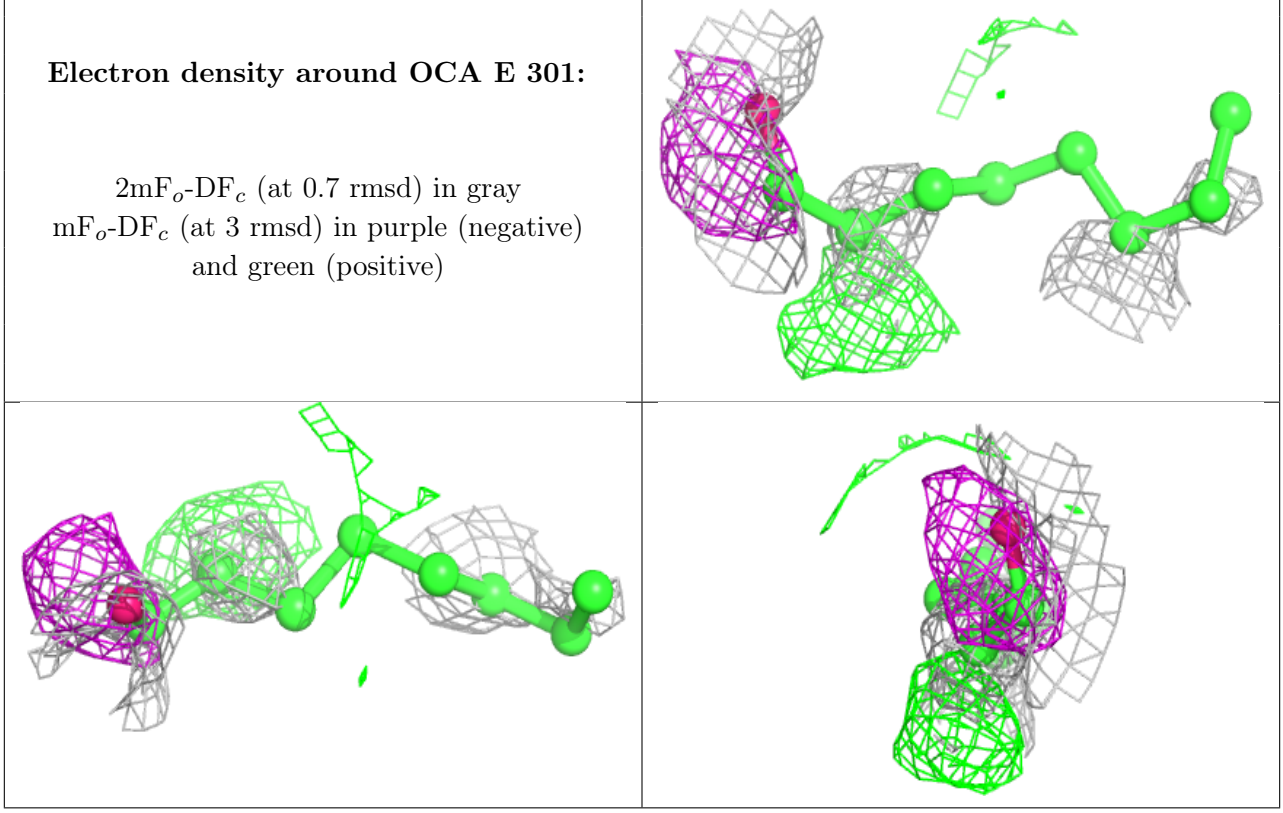






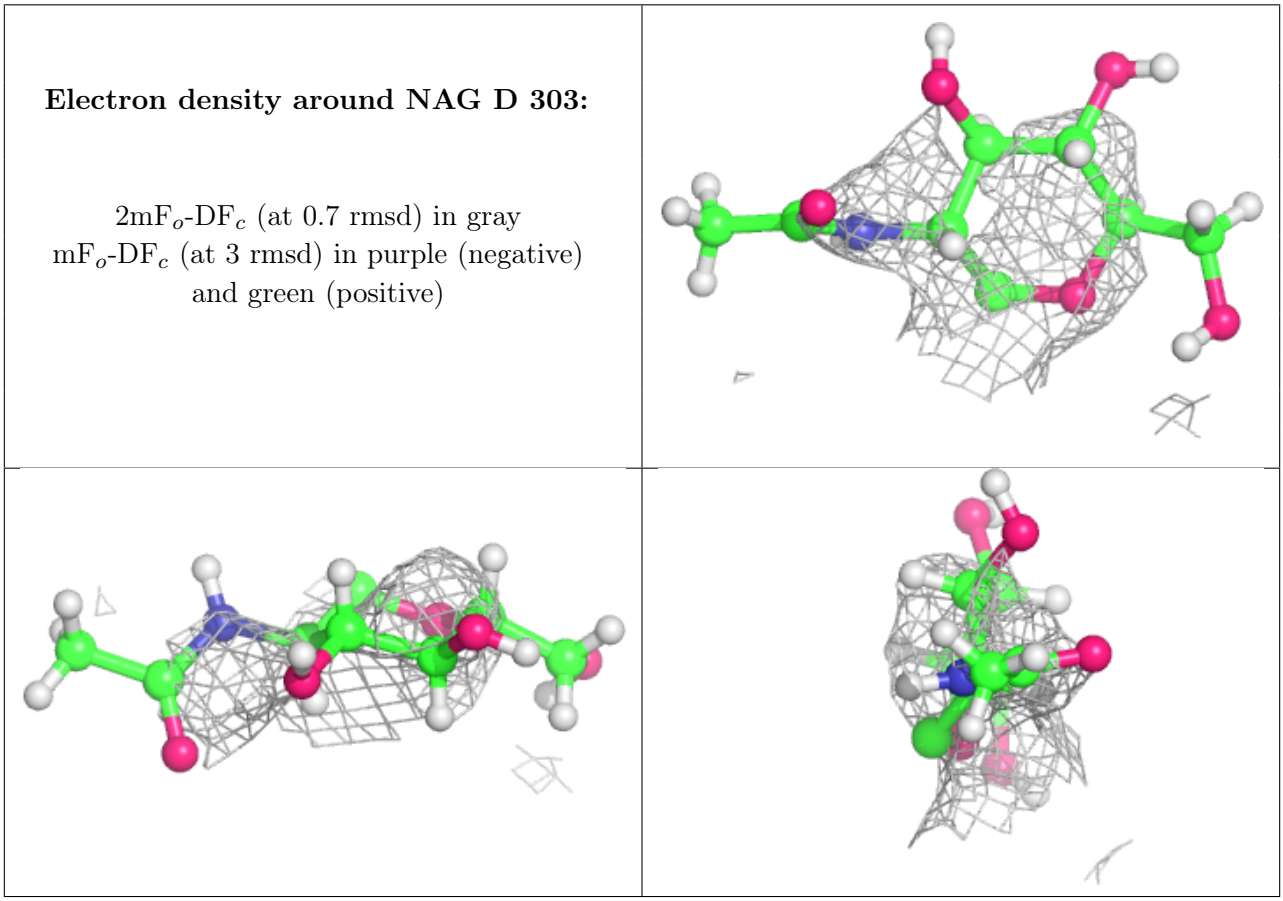
Electron density around OCA E 301:

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



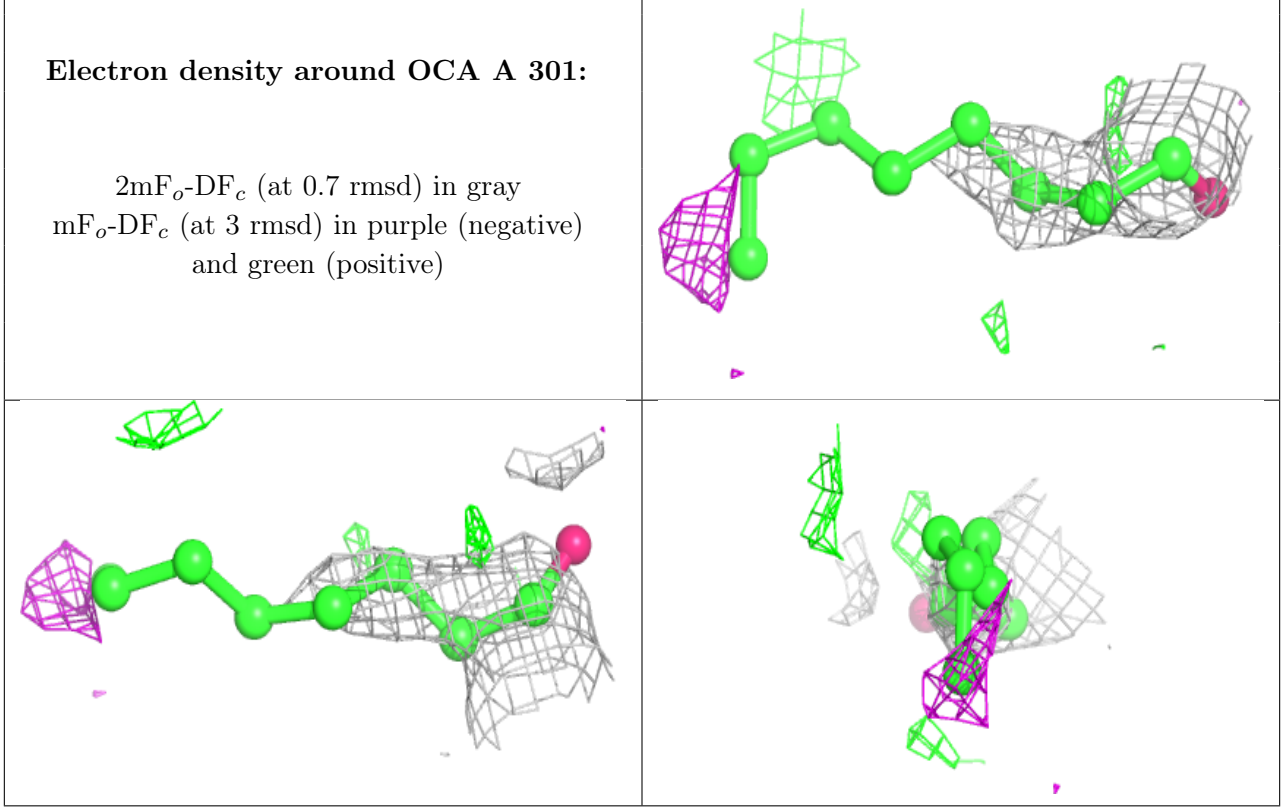
Electron density around NAG D 303:

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



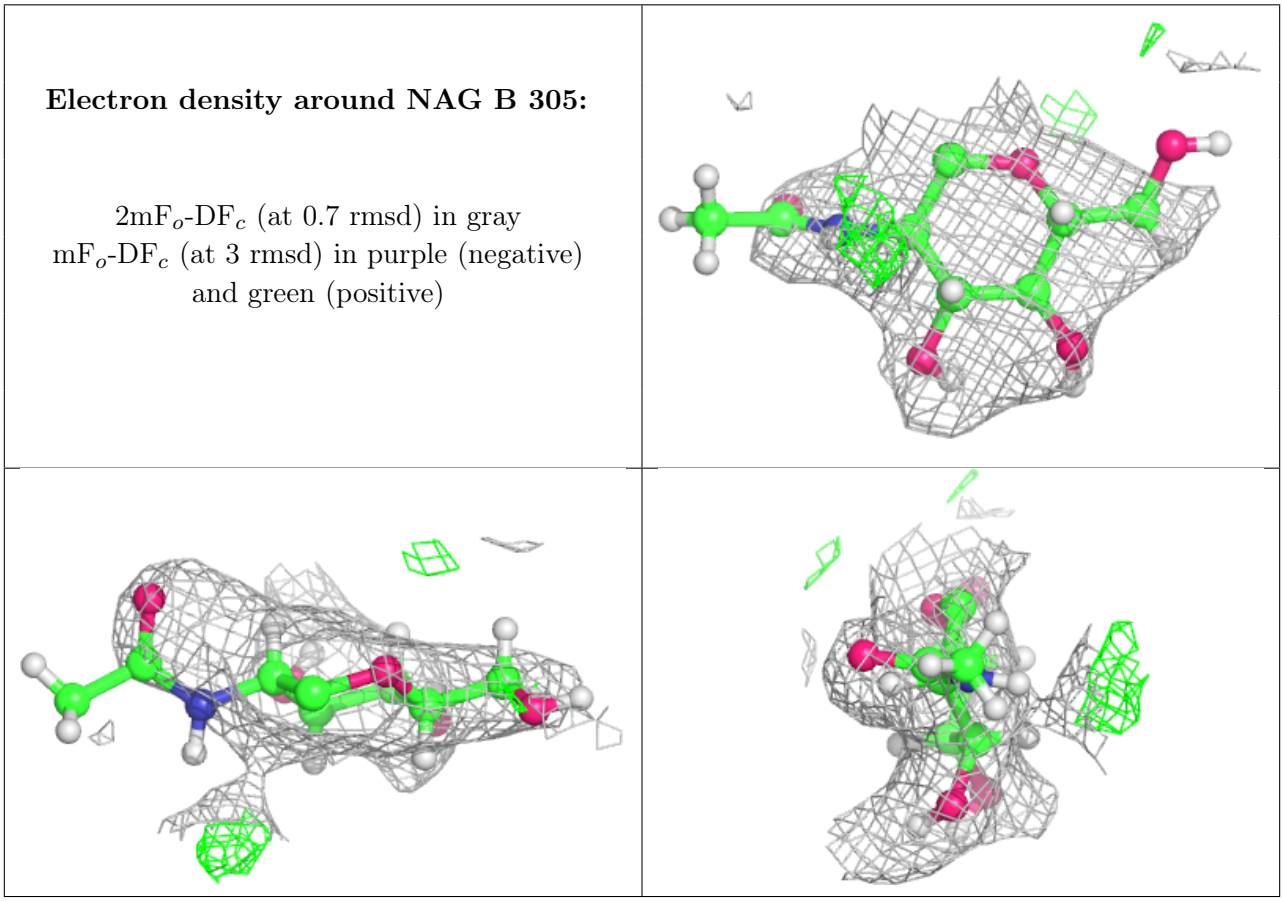
Electron density around OCA A 301:

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



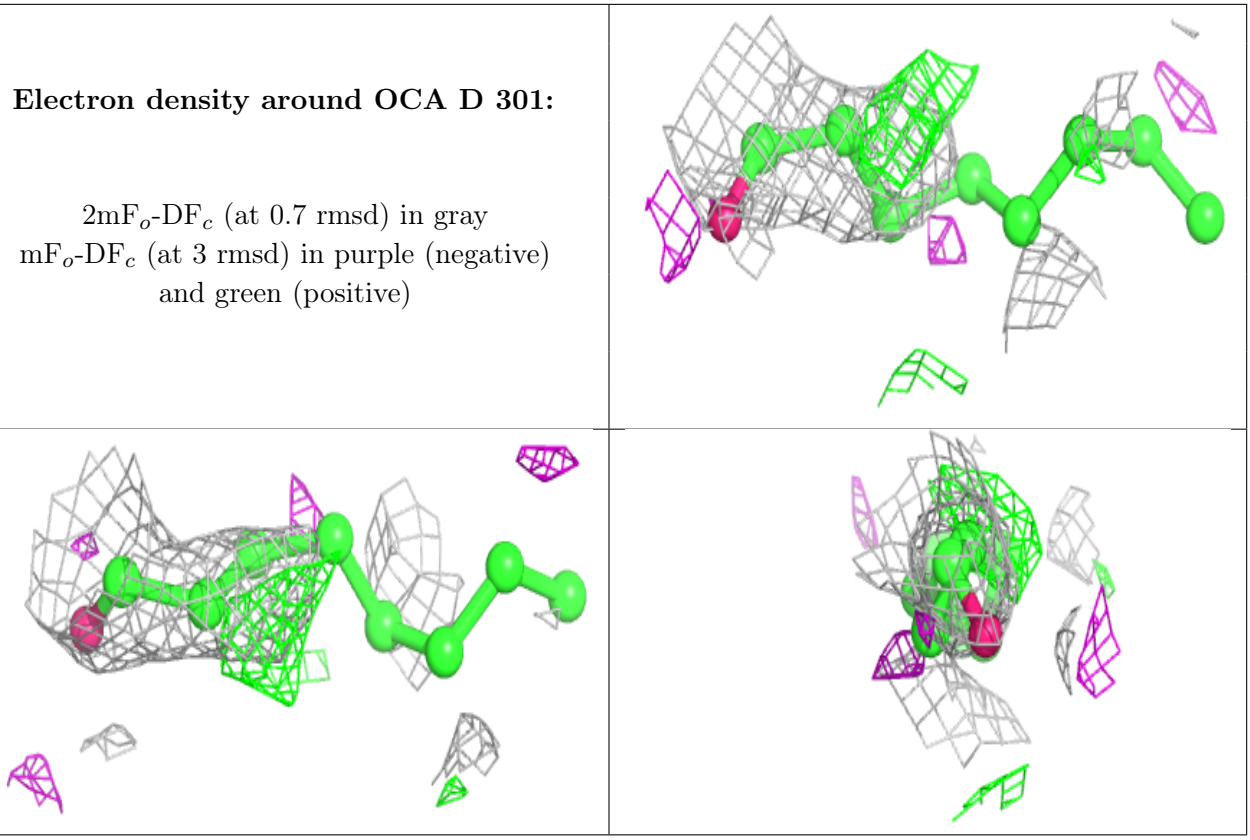
Electron density around NAG B 305:

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



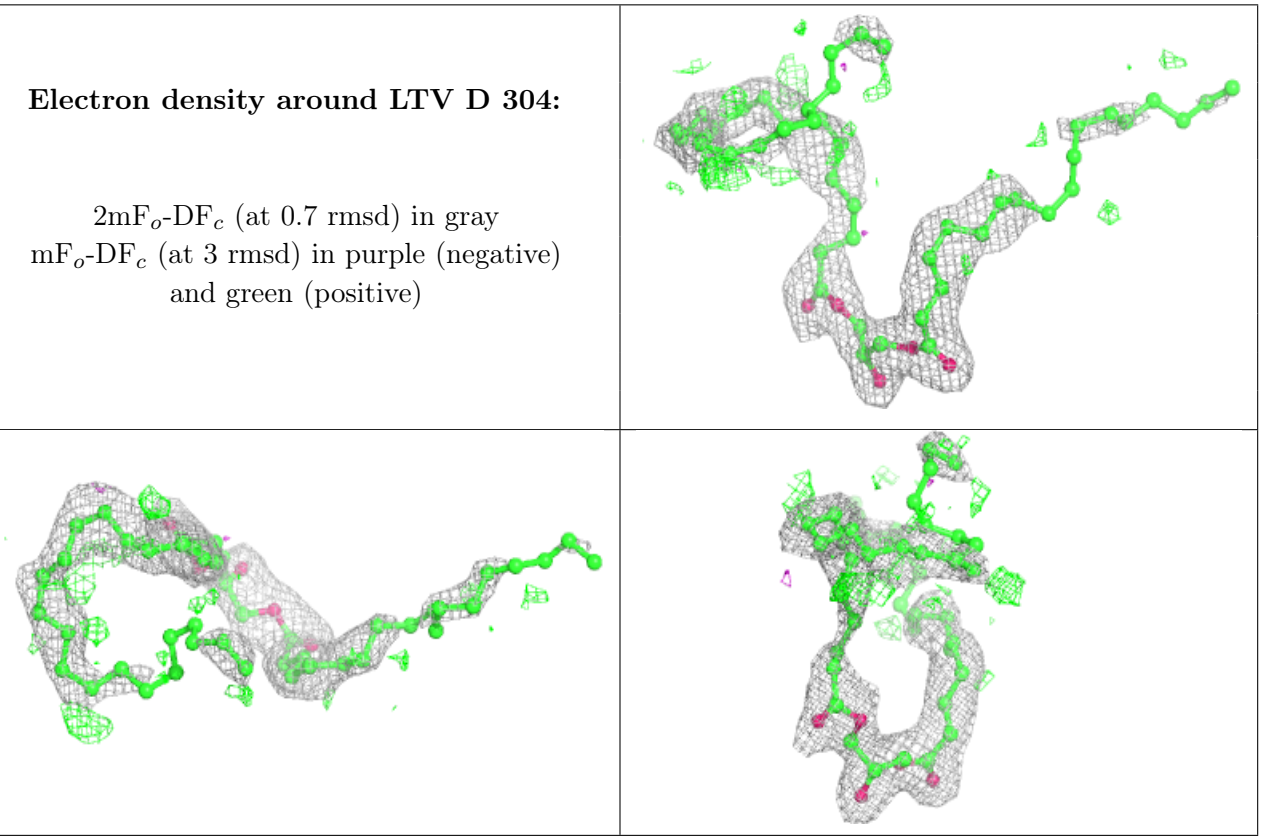
Electron density around OCA D 301:

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



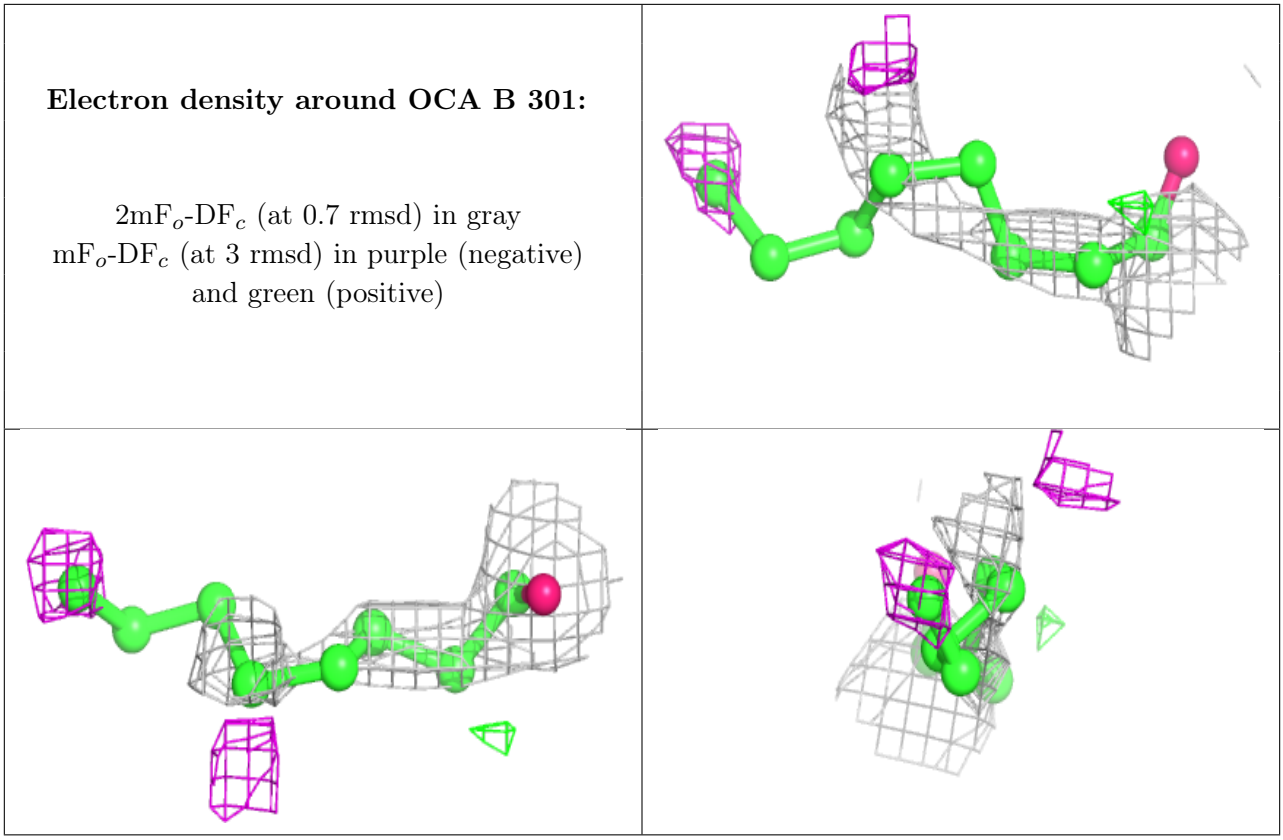
Electron density around LTV D 304:

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



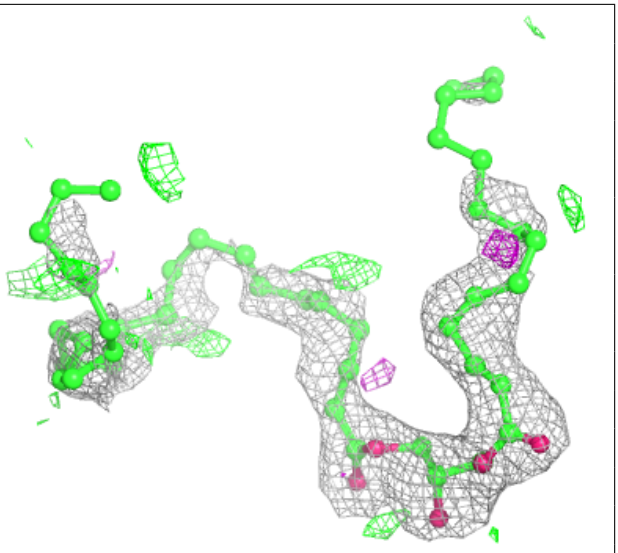
Electron density around OCA B 301:

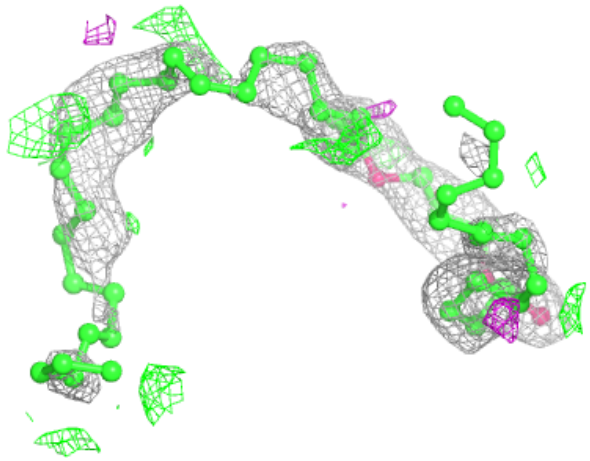
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

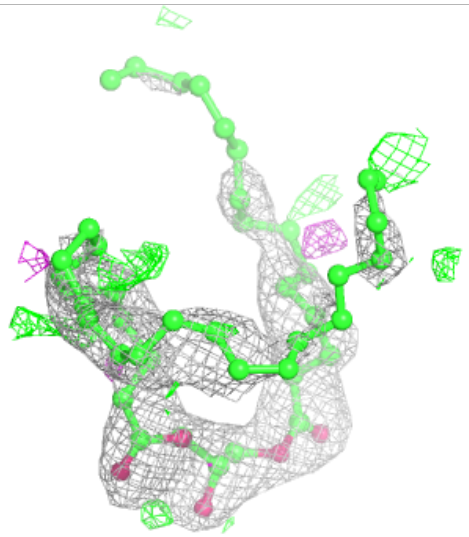


Electron density around LTV E 304:

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

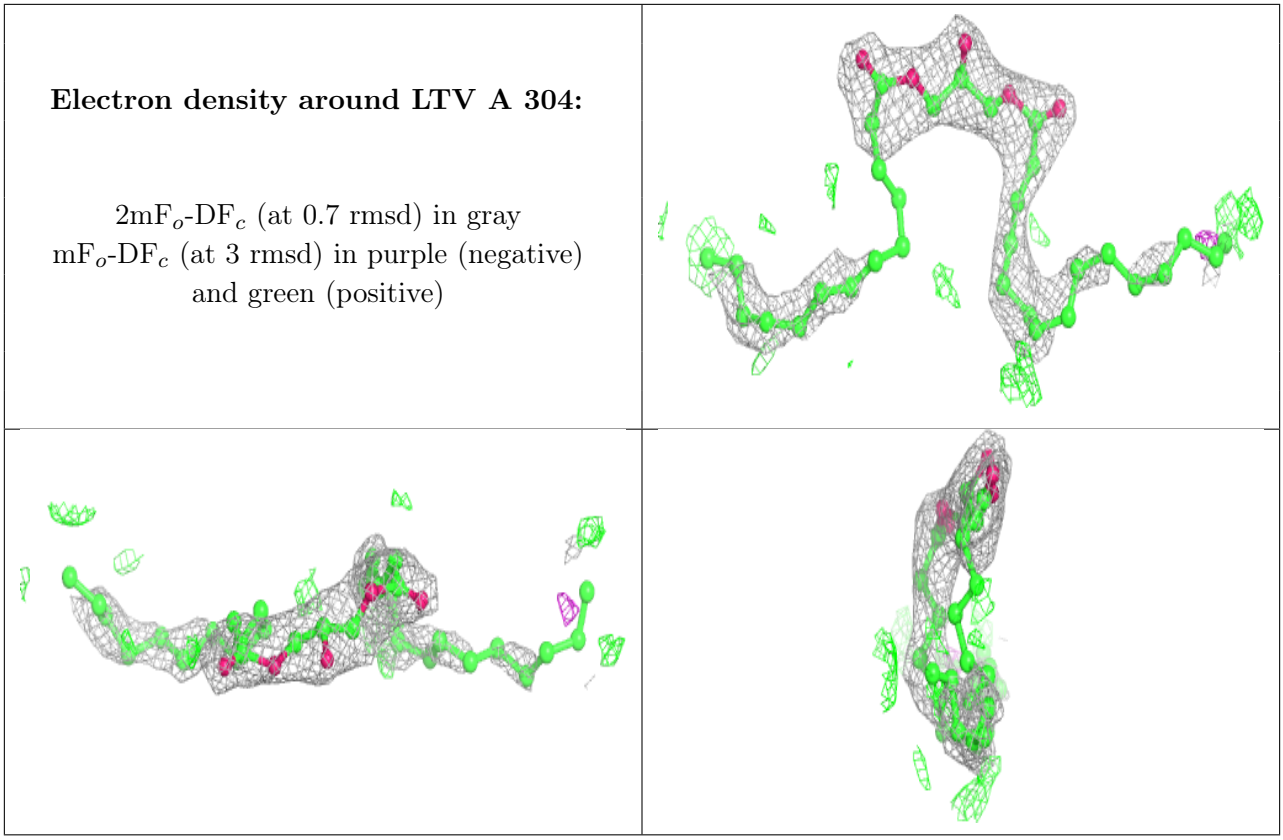






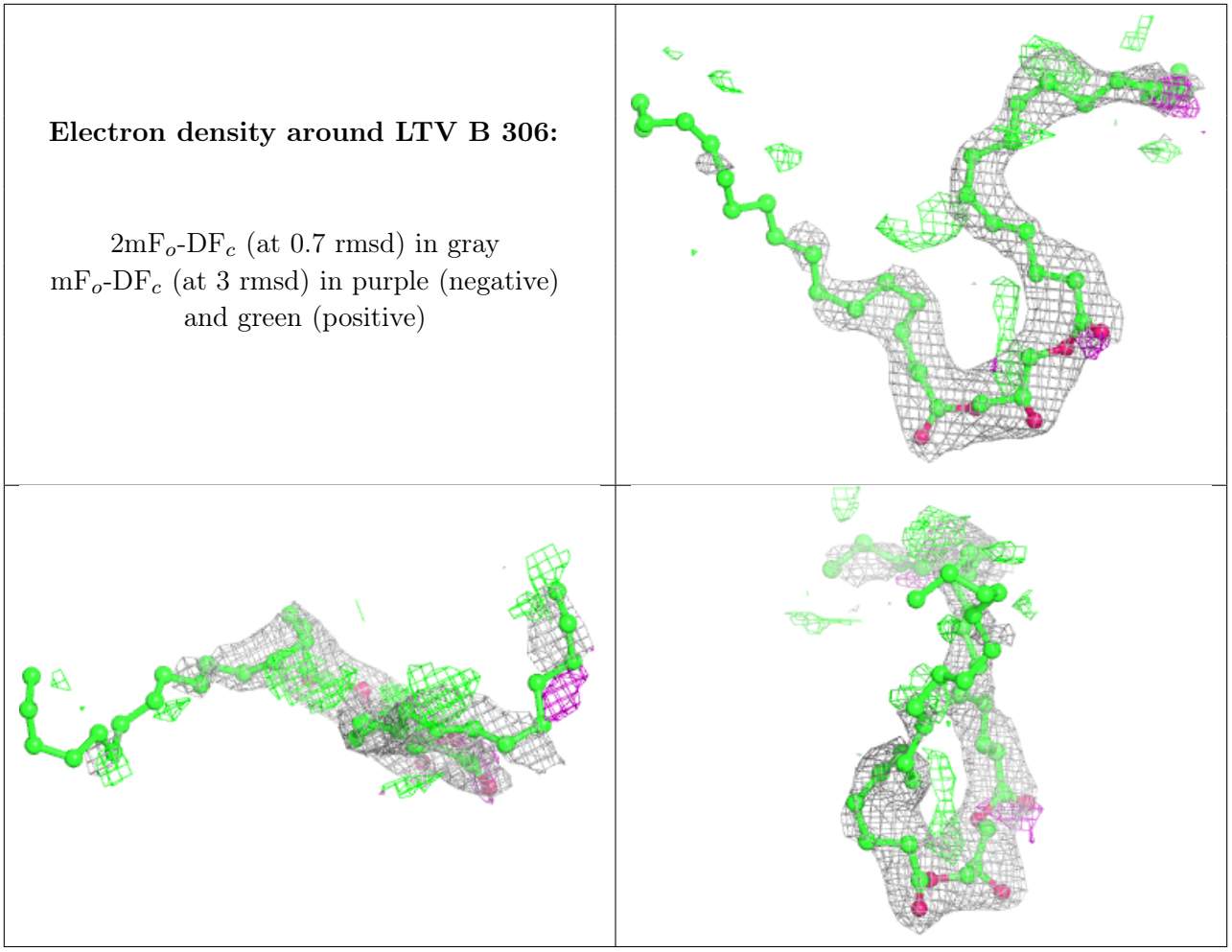
Electron density around LTV A 304:

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



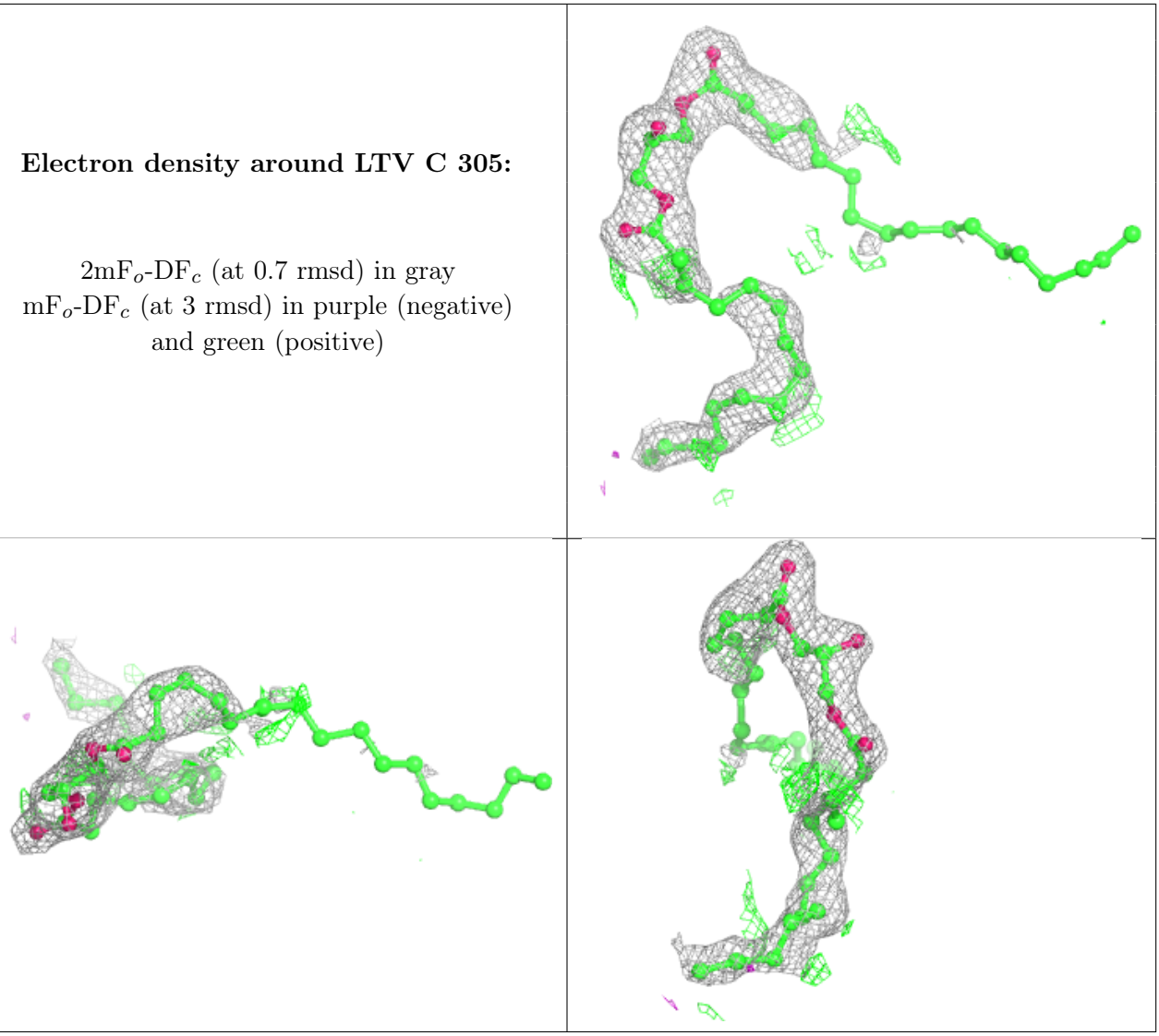
Electron density around LTV B 306:

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



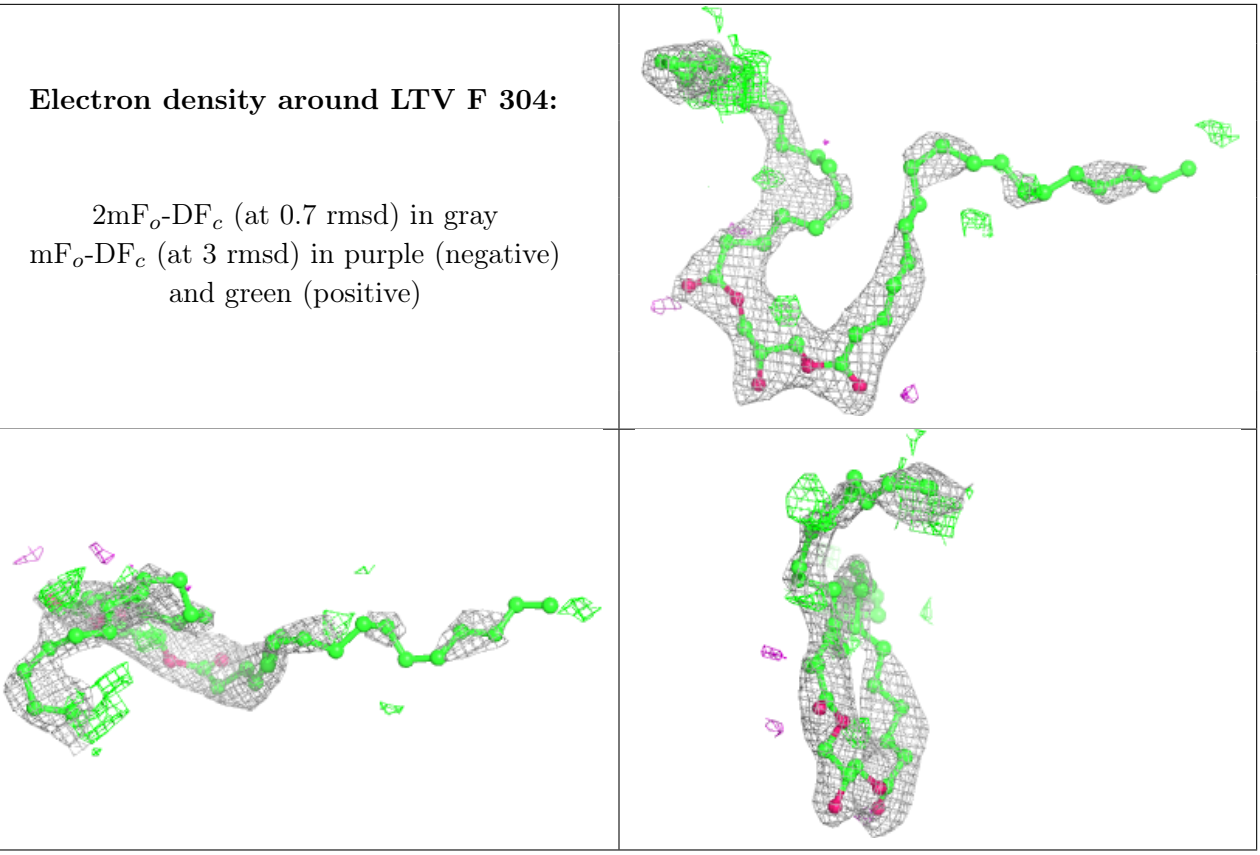
Electron density around LTV C 305:

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



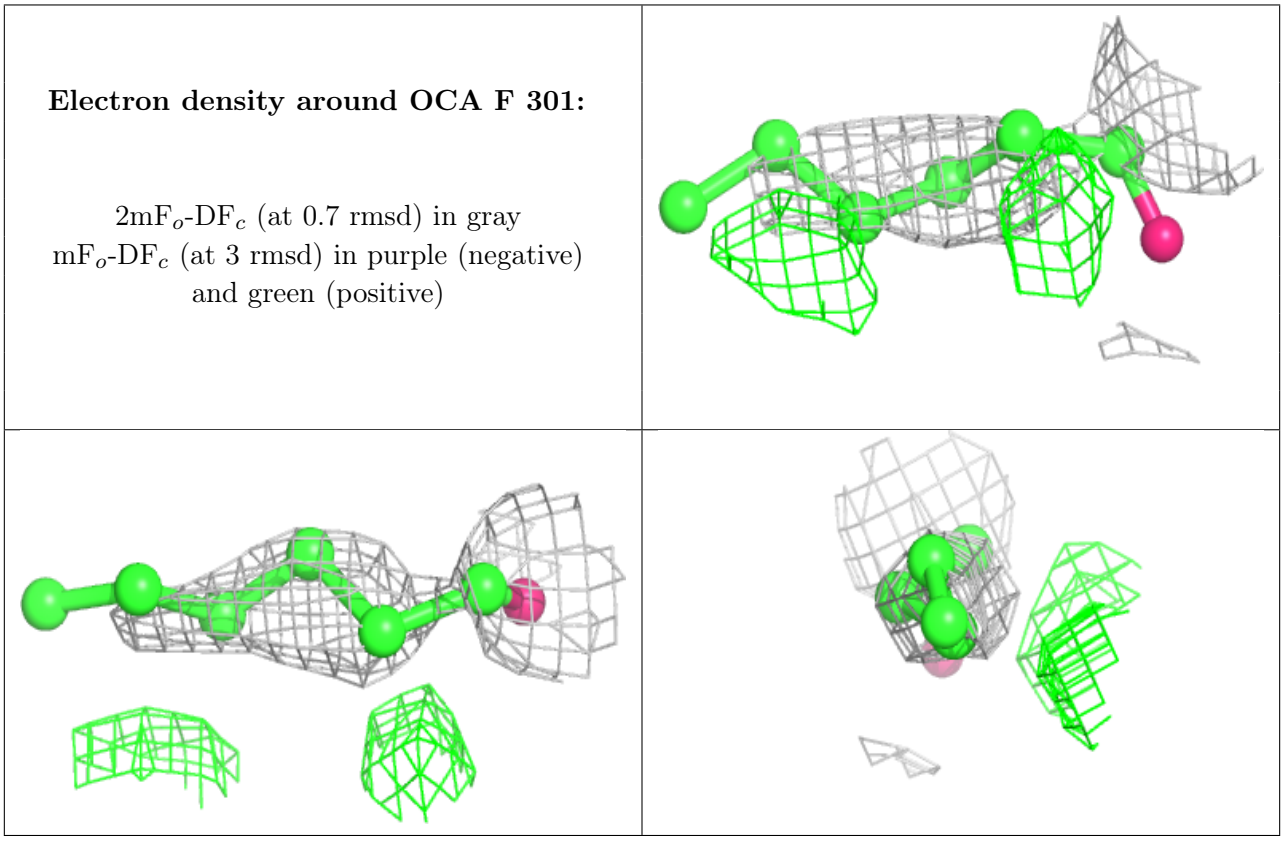
Electron density around LTV F 304:

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



Electron density around OCA F 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.