



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2020 – 12:11 PM JST

PDB ID : 6LM1
Title : The crystal structure of cyanorhodopsin (CyR) N4075R from cyanobacteria
Tolypothrix sp. NIES-4075
Authors : Hosaka, T.; Kimura-Someya, T.; Shirouzu, M.
Deposited on : 2019-12-24
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

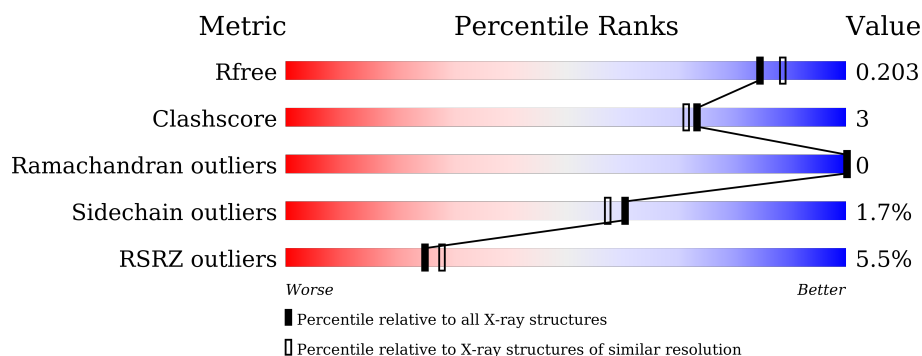
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	259	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>5%</div> <div>13%</div> </div> </div>
1	B	259	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	259	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6037 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 Rhodopsin.

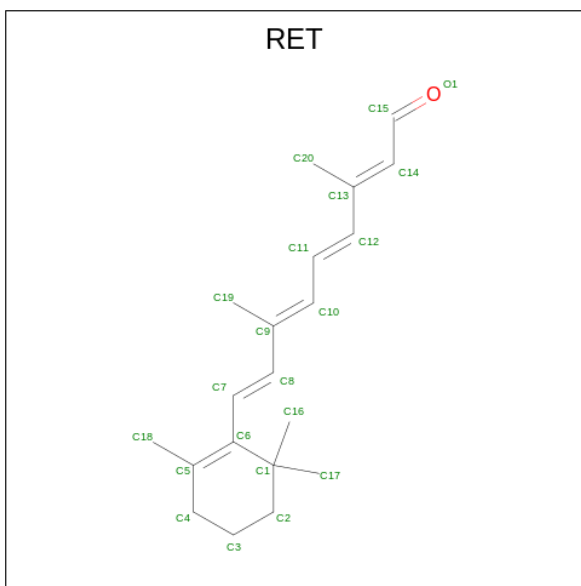
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1737	1169	273	287	8			
1	B	226	Total	C	N	O	S	0	0	0
			1733	1167	273	285	8			
1	C	226	Total	C	N	O	S	0	0	0
			1737	1169	273	287	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A0A218QMM7
A	-5	SER	-	expression tag	UNP A0A218QMM7
A	-4	SER	-	expression tag	UNP A0A218QMM7
A	-3	GLY	-	expression tag	UNP A0A218QMM7
A	-2	SER	-	expression tag	UNP A0A218QMM7
A	-1	SER	-	expression tag	UNP A0A218QMM7
A	0	GLY	-	expression tag	UNP A0A218QMM7
B	-6	GLY	-	expression tag	UNP A0A218QMM7
B	-5	SER	-	expression tag	UNP A0A218QMM7
B	-4	SER	-	expression tag	UNP A0A218QMM7
B	-3	GLY	-	expression tag	UNP A0A218QMM7
B	-2	SER	-	expression tag	UNP A0A218QMM7
B	-1	SER	-	expression tag	UNP A0A218QMM7
B	0	GLY	-	expression tag	UNP A0A218QMM7
C	-6	GLY	-	expression tag	UNP A0A218QMM7
C	-5	SER	-	expression tag	UNP A0A218QMM7
C	-4	SER	-	expression tag	UNP A0A218QMM7
C	-3	GLY	-	expression tag	UNP A0A218QMM7
C	-2	SER	-	expression tag	UNP A0A218QMM7
C	-1	SER	-	expression tag	UNP A0A218QMM7
C	0	GLY	-	expression tag	UNP A0A218QMM7

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O) (labeled as "Ligand

of Interest" by author).

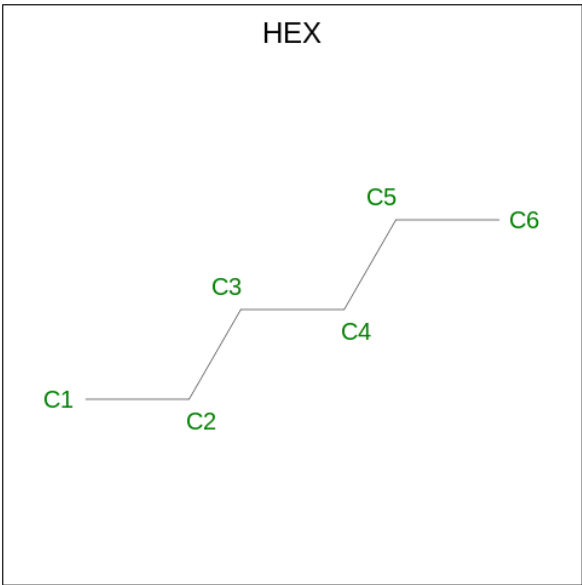


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0
2	B	1	Total C 20 20	0	0
2	C	1	Total C 20 20	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is HEXANE (three-letter code: HEX) (formula: C₆H₁₄) (labeled as "Ligand of Interest" by author).



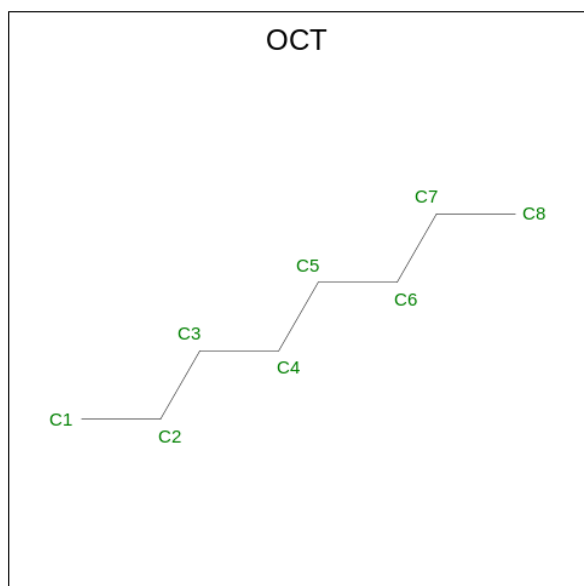
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0

- Molecule 5 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈) (labeled as "Ligand of Interest" by author).



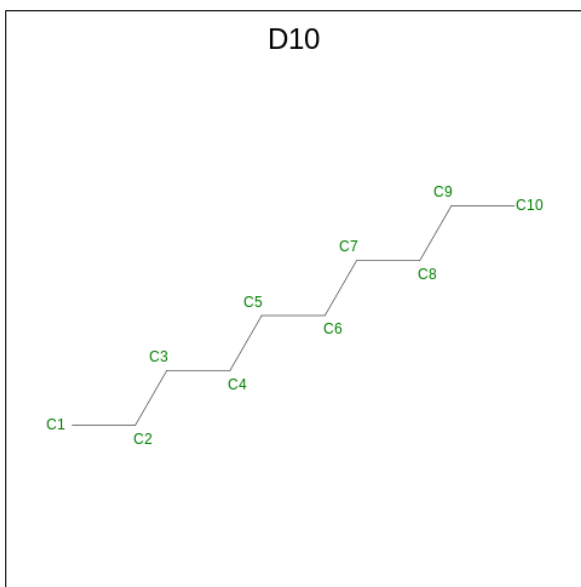
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0

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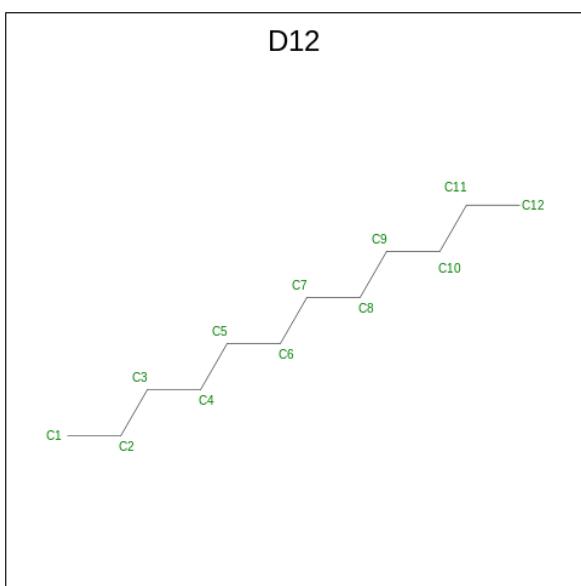
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	C	1	Total C 8 8	0	0
5	C	1	Total C 8 8	0	0
5	C	1	Total C 8 8	0	0
5	C	1	Total C 8 8	0	0
5	C	1	Total C 8 8	0	0

- Molecule 6 is DECANE (three-letter code: D10) (formula: C₁₀H₂₂) (labeled as "Ligand of Interest" by author).



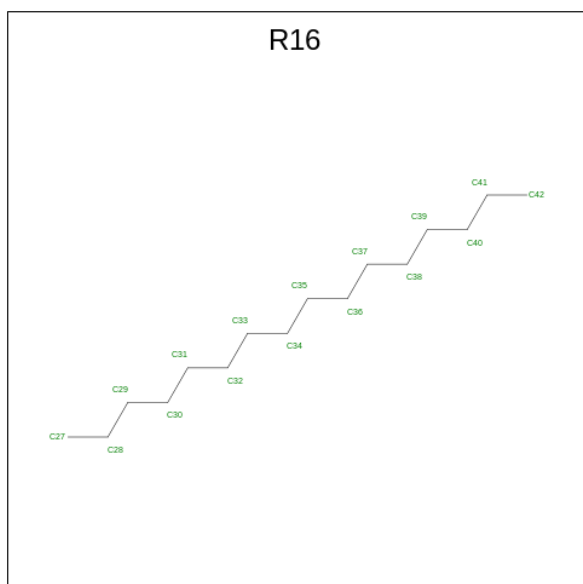
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 10 10	0	0
6	A	1	Total C 10 10	0	0
6	B	1	Total C 10 10	0	0
6	B	1	Total C 10 10	0	0

- Molecule 7 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 12 12	0	0
7	A	1	Total C 12 12	0	0
7	B	1	Total C 12 12	0	0
7	B	1	Total C 12 12	0	0
7	B	1	Total C 12 12	0	0
7	C	1	Total C 12 12	0	0

- Molecule 8 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$) (labeled as "Ligand of Interest" by author).



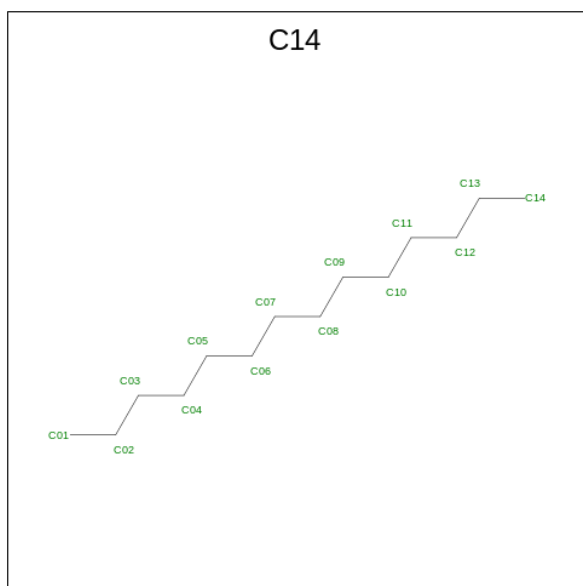
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 16 16	0	0
8	A	1	Total C 16 16	0	0
8	A	1	Total C 16 16	0	0
8	A	1	Total C 16 16	0	0
8	A	1	Total C 16 16	0	0

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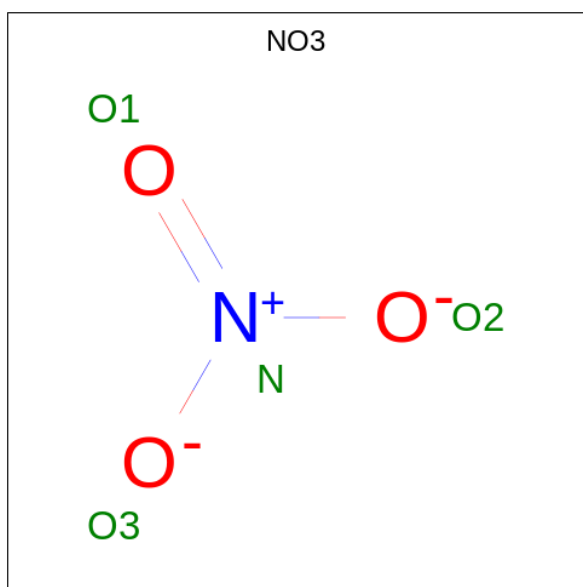
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 16 16	0	0
8	C	1	Total C 16 16	0	0
8	C	1	Total C 16 16	0	0
8	C	1	Total C 16 16	0	0

- Molecule 9 is TETRADECANE (three-letter code: C14) (formula: C₁₄H₃₀) (labeled as "Ligand of Interest" by author).



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

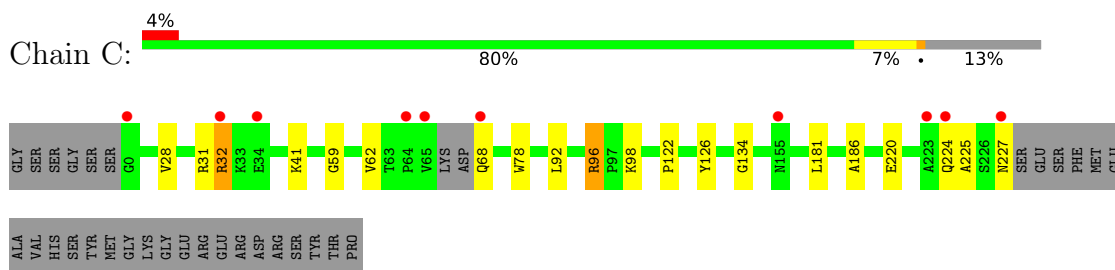
- Molecule 10 is NITRATE ION (three-letter code: NO3) (formula: NO₃) (labeled as "Ligand of Interest" by author).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	73	Total	O	0	0
			73	73		
11	B	50	Total	O	0	0
			50	50		
11	C	66	Total	O	0	0
			66	66		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.92Å 129.67Å 127.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.48 – 1.90 49.70 – 1.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.48-1.90) 82.5 (49.70-1.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.165 , 0.204 0.165 , 0.203	Depositor DCC
R_{free} test set	2000 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6037	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R16, MG, D10, D12, HEX, RET, C14, OCT, NO3

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	0.38	0/1777	0.51	0/2427
1	B	0.34	0/1773	0.47	0/2422
1	C	0.36	0/1777	0.49	0/2427
All	All	0.36	0/5327	0.49	0/7276

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1737	0	1849	8	0
1	B	1733	0	1845	5	0
1	C	1737	0	1849	15	0
2	A	20	0	27	5	0
2	B	20	0	27	3	0
2	C	20	0	27	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	30	0	70	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	70	0	0
4	C	60	0	140	2	0
5	A	64	0	144	3	0
5	B	48	0	108	0	0
5	C	40	0	90	3	0
6	A	20	0	44	0	0
6	B	20	0	44	0	0
7	A	24	0	52	1	0
7	B	36	0	78	1	0
7	C	12	0	26	1	0
8	A	80	0	170	1	0
8	B	16	0	34	0	0
8	C	48	0	102	1	0
9	A	14	0	30	0	0
9	B	14	0	30	0	0
9	C	14	0	30	0	0
10	C	8	0	0	0	0
11	A	73	0	0	1	0
11	B	50	0	0	0	0
11	C	66	0	0	2	0
All	All	6037	0	6886	42	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 3.

All (42) 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)
5:A:311:OCT:H22	1:C:98:LYS:HB3	1.62	0.82
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.49	0.78
4:A:306:HEX:H11	7:A:318:D12:H13	1.72	0.71
1:A:123:PRO:HG2	5:A:309:OCT:H32	1.72	0.71
4:C:307:HEX:H32	5:C:314:OCT:H12	1.74	0.69
1:A:40:LEU:HD23	5:A:311:OCT:H32	1.83	0.60
1:C:41:LYS:NZ	11:C:401:HOH:O	2.35	0.58
1:A:89:LEU:HD23	1:A:143:LEU:HD22	1.87	0.57
1:C:31:ARG:HG2	1:C:31:ARG:NH1	2.15	0.57
2:B:301:RET:H161	2:B:301:RET:H8	1.87	0.56
1:C:96:ARG:HD3	1:C:98:LYS:H	1.71	0.55
1:B:96:ARG:HD3	1:B:98:LYS:H	1.71	0.54
2:C:301:RET:H8	2:C:301:RET:H161	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLU:O	1:C:224:GLN:HG2	2.10	0.51
1:A:34:GLU:HG2	1:A:226:SER:OG	2.10	0.51
1:C:32:ARG:HB3	1:C:32:ARG:CZ	2.40	0.51
1:C:134:GLY:HA3	5:C:313:OCT:H22	1.95	0.49
2:A:301:RET:H161	2:A:301:RET:H8	1.95	0.49
1:C:78:TRP:CD1	2:C:301:RET:H14	2.49	0.48
1:A:78:TRP:CD1	2:A:301:RET:H14	2.49	0.48
1:C:59:GLY:HA2	1:C:62:VAL:HG22	1.96	0.47
4:C:308:HEX:H62	7:C:318:D12:H12	1.96	0.46
8:C:321:R16:H341	8:C:321:R16:H311	1.65	0.46
1:B:78:TRP:CD1	2:B:301:RET:H14	2.51	0.45
2:A:301:RET:C8	2:A:301:RET:H171	2.47	0.45
1:B:96:ARG:HD2	1:B:98:LYS:HB2	1.97	0.45
2:A:301:RET:H181	2:A:301:RET:H7	1.81	0.45
1:C:92:LEU:HD23	1:C:225:ALA:HB1	2.00	0.44
1:C:181:LEU:O	1:C:186:ALA:HB3	2.18	0.44
2:B:301:RET:C8	2:B:301:RET:H171	2.49	0.43
1:A:181:LEU:O	1:A:186:ALA:HB3	2.18	0.43
2:C:301:RET:H171	2:C:301:RET:C8	2.50	0.42
1:B:130:ILE:HG23	7:B:316:D12:H92	2.01	0.42
1:A:126:TYR:CZ	8:A:320:R16:H412	2.54	0.42
1:C:28:VAL:HA	1:C:31:ARG:HG3	2.01	0.42
1:A:184:ALA:N	11:A:401:HOH:O	2.44	0.42
1:C:68:GLN:NE2	11:C:402:HOH:O	2.39	0.41
2:A:301:RET:H8	2:A:301:RET:H171	2.02	0.41
1:B:96:ARG:CD	1:B:98:LYS:H	2.33	0.40
1:C:122:PRO:HB3	1:C:126:TYR:CZ	2.56	0.40
2:C:301:RET:H7	2:C:301:RET:H181	1.85	0.40
5:C:317:OCT:H83	5:C:317:OCT:H51	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	222/259 (86%)	220 (99%)	2 (1%)	0	100	100
1	B	222/259 (86%)	220 (99%)	2 (1%)	0	100	100
1	C	222/259 (86%)	220 (99%)	2 (1%)	0	100	100
All	All	666/777 (86%)	660 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	180/208 (86%)	177 (98%)	3 (2%)	60	57
1	B	179/208 (86%)	176 (98%)	3 (2%)	60	57
1	C	180/208 (86%)	177 (98%)	3 (2%)	60	57
All	All	539/624 (86%)	530 (98%)	9 (2%)	60	57

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	MET
1	A	96	ARG
1	A	227	ASN
1	B	31	ARG
1	B	96	ARG
1	B	224	GLN
1	C	32	ARG
1	C	96	ARG
1	C	227	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN

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Mol	Chain	Res	Type
1	C	227	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 3 are monoatomic - leaving 66 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	$\# Z > 2$
8	R16	A	321	-	15,15,15	0.31	0	14,14,14	0.85	0
10	NO3	C	323	-	1,3,3	0.67	0	0,3,3	0.00	-
8	R16	A	322	-	15,15,15	0.31	0	14,14,14	0.84	0
4	HEX	B	304	-	5,5,5	0.32	0	4,4,4	0.57	0
9	C14	C	324	-	13,13,13	0.30	0	12,12,12	0.88	0
9	C14	B	320	-	13,13,13	0.29	0	12,12,12	0.85	0
5	OCT	A	308	-	7,7,7	0.30	0	6,6,6	0.74	0
4	HEX	C	307	-	5,5,5	0.34	0	4,4,4	0.53	0
4	HEX	A	307	-	5,5,5	0.32	0	4,4,4	0.58	0
4	HEX	C	310	-	5,5,5	0.34	0	4,4,4	0.55	0
9	C14	A	325	-	13,13,13	0.29	0	12,12,12	0.79	0
5	OCT	B	312	-	7,7,7	0.32	0	6,6,6	0.66	0
6	D10	B	314	-	9,9,9	0.30	0	8,8,8	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	R16	A	320	-	15,15,15	0.31	0	14,14,14	0.77	0
5	OCT	A	315	-	7,7,7	0.30	0	6,6,6	0.74	0
4	HEX	A	305	-	5,5,5	0.29	0	4,4,4	0.64	0
5	OCT	C	315	-	7,7,7	0.30	0	6,6,6	0.75	0
4	HEX	C	312	-	5,5,5	0.31	0	4,4,4	0.57	0
4	HEX	C	306	-	5,5,5	0.31	0	4,4,4	0.55	0
4	HEX	C	308	-	5,5,5	0.31	0	4,4,4	0.57	0
8	R16	C	319	-	15,15,15	0.32	0	14,14,14	0.79	0
5	OCT	B	313	-	7,7,7	0.34	0	6,6,6	0.67	0
2	RET	A	301	1	20,20,21	0.87	1 (5%)	27,27,28	0.59	0
5	OCT	C	314	-	7,7,7	0.29	0	6,6,6	0.71	0
6	D10	A	316	-	9,9,9	0.29	0	8,8,8	0.82	0
5	OCT	A	314	-	7,7,7	0.31	0	6,6,6	0.64	0
4	HEX	B	305	-	5,5,5	0.30	0	4,4,4	0.58	0
8	R16	C	321	-	15,15,15	0.34	0	14,14,14	0.79	0
4	HEX	A	303	-	5,5,5	0.31	0	4,4,4	0.60	0
4	HEX	C	305	-	5,5,5	0.32	0	4,4,4	0.57	0
7	D12	B	318	-	11,11,11	0.29	0	10,10,10	0.81	0
8	R16	C	320	-	15,15,15	0.29	0	14,14,14	0.88	0
5	OCT	C	316	-	7,7,7	0.30	0	6,6,6	0.67	0
6	D10	B	315	-	9,9,9	0.30	0	8,8,8	0.76	0
5	OCT	A	309	-	7,7,7	0.31	0	6,6,6	0.70	0
8	R16	A	323	-	15,15,15	0.29	0	14,14,14	0.90	0
6	D10	A	317	-	9,9,9	0.32	0	8,8,8	0.76	0
7	D12	A	319	-	11,11,11	0.29	0	10,10,10	0.91	0
4	HEX	C	304	-	5,5,5	0.28	0	4,4,4	0.66	0
4	HEX	C	303	-	5,5,5	0.33	0	4,4,4	0.58	0
4	HEX	B	306	-	5,5,5	0.33	0	4,4,4	0.57	0
5	OCT	B	308	-	7,7,7	0.28	0	6,6,6	0.73	0
8	R16	A	324	-	15,15,15	0.32	0	14,14,14	0.79	0
5	OCT	A	311	-	7,7,7	0.30	0	6,6,6	0.76	0
2	RET	B	301	1	20,20,21	0.93	1 (5%)	27,27,28	0.62	1 (3%)
4	HEX	A	306	-	5,5,5	0.30	0	4,4,4	0.61	0
7	D12	A	318	-	11,11,11	0.30	0	10,10,10	0.85	0
7	D12	B	316	-	11,11,11	0.30	0	10,10,10	0.81	0
10	NO3	C	322	-	1,3,3	0.59	0	0,3,3	0.00	-
5	OCT	A	312	-	7,7,7	0.29	0	6,6,6	0.78	0
5	OCT	C	317	-	7,7,7	0.32	0	6,6,6	0.69	0
4	HEX	C	311	-	5,5,5	0.31	0	4,4,4	0.56	0
5	OCT	B	310	-	7,7,7	0.27	0	6,6,6	0.81	0
5	OCT	C	313	-	7,7,7	0.31	0	6,6,6	0.66	0
4	HEX	B	307	-	5,5,5	0.31	0	4,4,4	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	D12	C	318	-	11,11,11	0.31	0	10,10,10	0.87	0
2	RET	C	301	1	20,20,21	0.90	1 (5%)	27,27,28	0.58	0
4	HEX	B	303	-	5,5,5	0.31	0	4,4,4	0.57	0
5	OCT	A	313	-	7,7,7	0.27	0	6,6,6	0.77	0
8	R16	B	319	-	15,15,15	0.30	0	14,14,14	0.85	0
4	HEX	A	304	-	5,5,5	0.31	0	4,4,4	0.57	0
5	OCT	B	311	-	7,7,7	0.32	0	6,6,6	0.71	0
5	OCT	B	309	-	7,7,7	0.30	0	6,6,6	0.77	0
5	OCT	A	310	-	7,7,7	0.36	0	6,6,6	0.59	0
4	HEX	C	309	-	5,5,5	0.32	0	4,4,4	0.58	0
7	D12	B	317	-	11,11,11	0.31	0	10,10,10	0.86	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
8	R16	A	321	-	-	4/13/13/13	-
8	R16	A	322	-	-	3/13/13/13	-
9	C14	C	324	-	-	4/11/11/11	-
9	C14	B	320	-	-	7/11/11/11	-
5	OCT	A	308	-	-	3/5/5/5	-
4	HEX	C	307	-	-	1/3/3/3	-
4	HEX	A	307	-	-	0/3/3/3	-
4	HEX	C	310	-	-	0/3/3/3	-
9	C14	A	325	-	-	7/11/11/11	-
5	OCT	B	312	-	-	4/5/5/5	-
6	D10	B	314	-	-	2/7/7/7	-
8	R16	A	320	-	-	8/13/13/13	-
5	OCT	A	315	-	-	1/5/5/5	-
4	HEX	A	305	-	-	0/3/3/3	-
5	OCT	C	315	-	-	2/5/5/5	-
4	HEX	C	312	-	-	1/3/3/3	-
4	HEX	C	306	-	-	1/3/3/3	-
4	HEX	C	308	-	-	1/3/3/3	-
8	R16	C	319	-	-	5/13/13/13	-
5	OCT	B	313	-	-	3/5/5/5	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
5	OCT	C	314	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D10	A	316	-	-	2/7/7/7	-
5	OCT	A	314	-	-	3/5/5/5	-
4	HEX	B	305	-	-	2/3/3/3	-
8	R16	C	321	-	-	3/13/13/13	-
4	HEX	A	303	-	-	0/3/3/3	-
4	HEX	C	305	-	-	0/3/3/3	-
7	D12	B	318	-	-	3/9/9/9	-
8	R16	C	320	-	-	6/13/13/13	-
5	OCT	C	316	-	-	0/5/5/5	-
6	D10	B	315	-	-	3/7/7/7	-
5	OCT	A	309	-	-	1/5/5/5	-
8	R16	A	323	-	-	3/13/13/13	-
6	D10	A	317	-	-	4/7/7/7	-
7	D12	A	319	-	-	1/9/9/9	-
4	HEX	C	304	-	-	1/3/3/3	-
4	HEX	C	303	-	-	1/3/3/3	-
4	HEX	B	306	-	-	0/3/3/3	-
5	OCT	B	308	-	-	2/5/5/5	-
8	R16	A	324	-	-	7/13/13/13	-
5	OCT	A	311	-	-	2/5/5/5	-
2	RET	B	301	1	-	0/13/30/31	0/1/1/1
4	HEX	A	306	-	-	0/3/3/3	-
7	D12	A	318	-	-	3/9/9/9	-
7	D12	B	316	-	-	5/9/9/9	-
4	HEX	B	304	-	-	0/3/3/3	-
5	OCT	A	312	-	-	1/5/5/5	-
5	OCT	C	317	-	-	3/5/5/5	-
4	HEX	C	311	-	-	0/3/3/3	-
5	OCT	B	310	-	-	3/5/5/5	-
5	OCT	C	313	-	-	0/5/5/5	-
4	HEX	B	307	-	-	2/3/3/3	-
7	D12	C	318	-	-	1/9/9/9	-
2	RET	C	301	1	-	0/13/30/31	0/1/1/1
4	HEX	B	303	-	-	0/3/3/3	-
5	OCT	A	313	-	-	0/5/5/5	-
8	R16	B	319	-	-	5/13/13/13	-
4	HEX	A	304	-	-	1/3/3/3	-
5	OCT	B	311	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OCT	B	309	-	-	0/5/5/5	-
5	OCT	A	310	-	-	2/5/5/5	-
4	HEX	C	309	-	-	0/3/3/3	-
7	D12	B	317	-	-	3/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	RET	C14-C13	3.49	1.36	1.33
2	B	301	RET	C14-C13	3.40	1.36	1.33
2	A	301	RET	C14-C13	3.14	1.36	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RET	C7-C8-C9	2.03	129.30	126.23

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	321	R16	C31-C32-C33-C34
8	A	322	R16	C35-C36-C37-C38
7	B	318	D12	C2-C3-C4-C5
8	A	323	R16	C35-C36-C37-C38
8	A	320	R16	C35-C36-C37-C38
8	A	321	R16	C30-C31-C32-C33
5	B	312	OCT	C3-C4-C5-C6
8	A	320	R16	C29-C30-C31-C32
5	A	310	OCT	C3-C4-C5-C6
9	B	320	C14	C10-C11-C12-C13
5	B	311	OCT	C2-C3-C4-C5
9	A	325	C14	C09-C10-C11-C12
8	C	320	R16	C35-C36-C37-C38
8	B	319	R16	C35-C36-C37-C38
6	B	315	D10	C3-C4-C5-C6
7	B	316	D12	C6-C7-C8-C9
8	A	320	R16	C38-C39-C40-C41
8	A	324	R16	C30-C31-C32-C33
8	A	322	R16	C33-C34-C35-C36
5	B	310	OCT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	B	316	D12	C2-C3-C4-C5
4	B	305	HEX	C2-C3-C4-C5
9	B	320	C14	C08-C09-C10-C11
6	A	317	D10	C3-C4-C5-C6
5	B	308	OCT	C3-C4-C5-C6
5	C	317	OCT	C3-C4-C5-C6
8	C	319	R16	C32-C33-C34-C35
6	B	315	D10	C6-C7-C8-C9
5	B	308	OCT	C4-C5-C6-C7
5	B	313	OCT	C3-C4-C5-C6
8	A	321	R16	C34-C35-C36-C37
9	A	325	C14	C05-C06-C07-C08
8	C	320	R16	C31-C32-C33-C34
9	C	324	C14	C09-C10-C11-C12
9	B	320	C14	C04-C05-C06-C07
8	C	320	R16	C32-C33-C34-C35
7	A	318	D12	C4-C5-C6-C7
8	B	319	R16	C34-C35-C36-C37
9	B	320	C14	C07-C08-C09-C10
8	B	319	R16	C39-C40-C41-C42
8	C	319	R16	C31-C32-C33-C34
8	C	319	R16	C33-C34-C35-C36
9	A	325	C14	C03-C04-C05-C06
9	A	325	C14	C08-C09-C10-C11
5	B	310	OCT	C1-C2-C3-C4
7	B	318	D12	C1-C2-C3-C4
7	B	317	D12	C1-C2-C3-C4
9	B	320	C14	C11-C12-C13-C14
8	A	320	R16	C30-C31-C32-C33
6	B	314	D10	C1-C2-C3-C4
8	C	320	R16	C33-C34-C35-C36
6	A	316	D10	C2-C3-C4-C5
5	C	315	OCT	C4-C5-C6-C7
7	B	316	D12	C7-C8-C9-C10
4	A	304	HEX	C3-C4-C5-C6
8	A	320	R16	C32-C33-C34-C35
5	B	310	OCT	C3-C4-C5-C6
7	B	317	D12	C9-C10-C11-C12
8	A	321	R16	C31-C32-C33-C34
6	A	317	D10	C7-C8-C9-C10
5	A	315	OCT	C1-C2-C3-C4
5	A	314	OCT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
8	A	324	R16	C33-C34-C35-C36
5	B	311	OCT	C5-C6-C7-C8
5	C	317	OCT	C2-C3-C4-C5
9	A	325	C14	C02-C03-C04-C05
5	B	311	OCT	C4-C5-C6-C7
8	A	323	R16	C37-C38-C39-C40
8	C	321	R16	C28-C29-C30-C31
8	C	320	R16	C27-C28-C29-C30
5	C	315	OCT	C5-C6-C7-C8
4	B	307	HEX	C2-C3-C4-C5
5	B	312	OCT	C2-C3-C4-C5
5	A	314	OCT	C2-C3-C4-C5
8	A	320	R16	C37-C38-C39-C40
4	C	308	HEX	C3-C4-C5-C6
5	A	308	OCT	C3-C4-C5-C6
5	A	308	OCT	C4-C5-C6-C7
6	B	315	D10	C5-C6-C7-C8
6	A	317	D10	C6-C7-C8-C9
7	A	318	D12	C5-C6-C7-C8
9	B	320	C14	C03-C04-C05-C06
5	B	312	OCT	C5-C6-C7-C8
5	A	311	OCT	C4-C5-C6-C7
9	C	324	C14	C08-C09-C10-C11
8	A	324	R16	C32-C33-C34-C35
7	B	318	D12	C9-C10-C11-C12
4	B	305	HEX	C3-C4-C5-C6
8	A	323	R16	C28-C29-C30-C31
8	B	319	R16	C30-C31-C32-C33
5	A	310	OCT	C2-C3-C4-C5
8	A	320	R16	C33-C34-C35-C36
5	A	309	OCT	C2-C3-C4-C5
5	A	311	OCT	C3-C4-C5-C6
5	A	308	OCT	C2-C3-C4-C5
8	A	321	R16	C39-C40-C41-C42
9	C	324	C14	C05-C06-C07-C08
8	C	319	R16	C30-C31-C32-C33
5	A	312	OCT	C1-C2-C3-C4
4	C	303	HEX	C2-C3-C4-C5
4	B	307	HEX	C3-C4-C5-C6
7	B	316	D12	C3-C4-C5-C6
7	C	318	D12	C3-C4-C5-C6
5	B	313	OCT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	B	320	C14	C06-C07-C08-C09
9	A	325	C14	C10-C11-C12-C13
5	B	311	OCT	C3-C4-C5-C6
8	A	322	R16	C32-C33-C34-C35
6	A	316	D10	C5-C6-C7-C8
4	C	304	HEX	C1-C2-C3-C4
5	C	314	OCT	C3-C4-C5-C6
5	A	314	OCT	C3-C4-C5-C6
4	C	312	HEX	C3-C4-C5-C6
5	B	313	OCT	C2-C3-C4-C5
4	C	307	HEX	C3-C4-C5-C6
8	A	324	R16	C27-C28-C29-C30
8	C	320	R16	C36-C37-C38-C39
7	B	316	D12	C5-C6-C7-C8
6	A	317	D10	C5-C6-C7-C8
6	B	314	D10	C2-C3-C4-C5
8	A	324	R16	C28-C29-C30-C31
7	B	317	D12	C11-C10-C9-C8
8	A	324	R16	C36-C37-C38-C39
9	A	325	C14	C11-C12-C13-C14
7	A	318	D12	C6-C7-C8-C9
8	C	319	R16	C35-C36-C37-C38
5	C	317	OCT	C4-C5-C6-C7
9	C	324	C14	C10-C11-C12-C13
5	B	312	OCT	C4-C5-C6-C7
8	A	320	R16	C39-C40-C41-C42
8	A	324	R16	C38-C39-C40-C41
8	C	321	R16	C30-C31-C32-C33
4	C	306	HEX	C2-C3-C4-C5
7	A	319	D12	C2-C3-C4-C5
8	B	319	R16	C36-C37-C38-C39

There are no ring outliers.

16 monomers are involved in 23 short contacts:

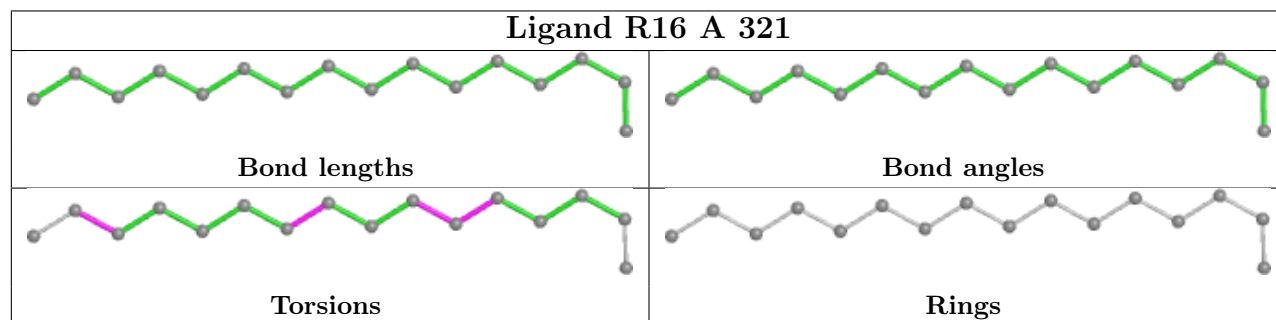
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	307	HEX	1	0
8	A	320	R16	1	0
4	C	308	HEX	1	0
2	A	301	RET	5	0
5	C	314	OCT	1	0
8	C	321	R16	1	0

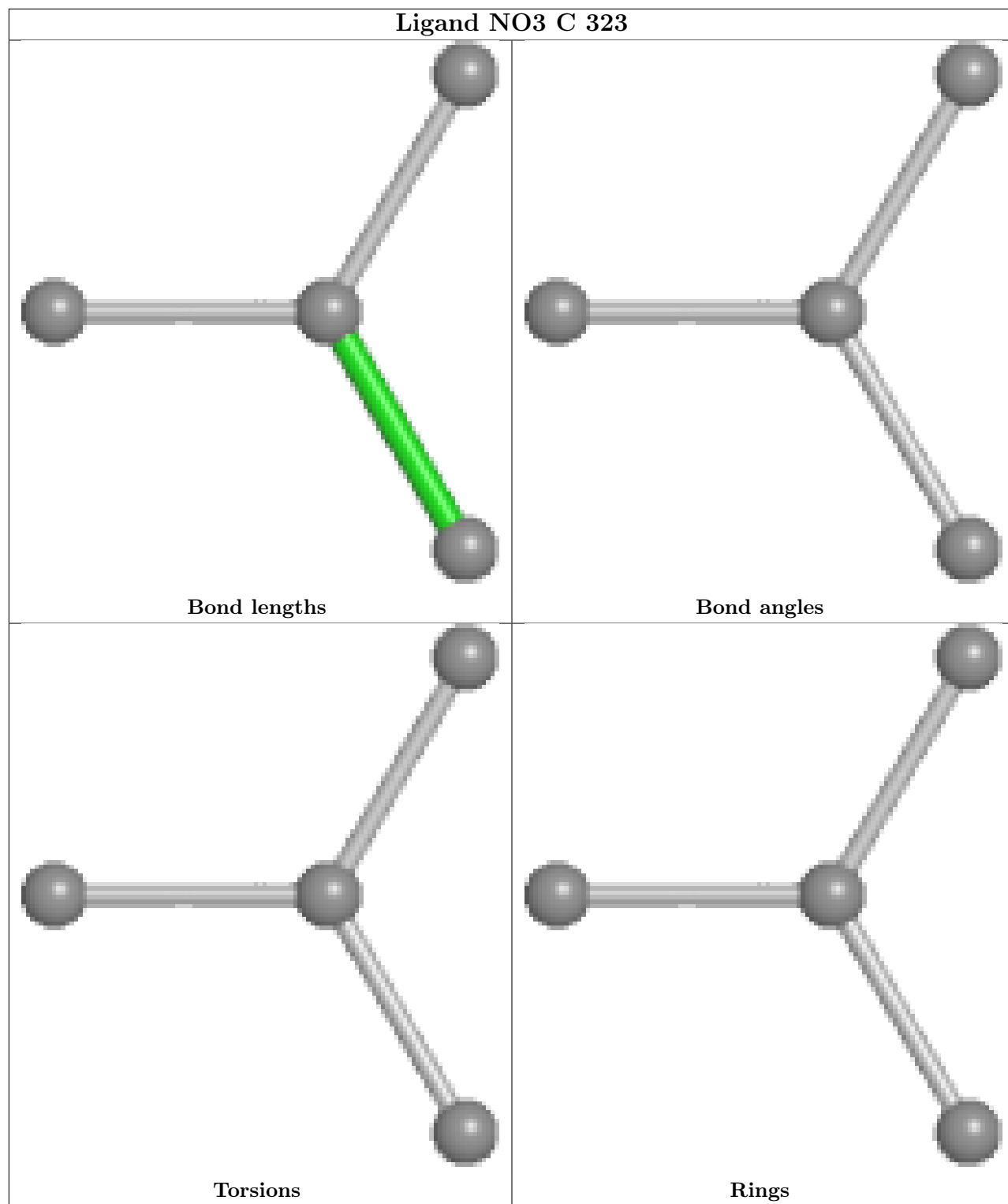
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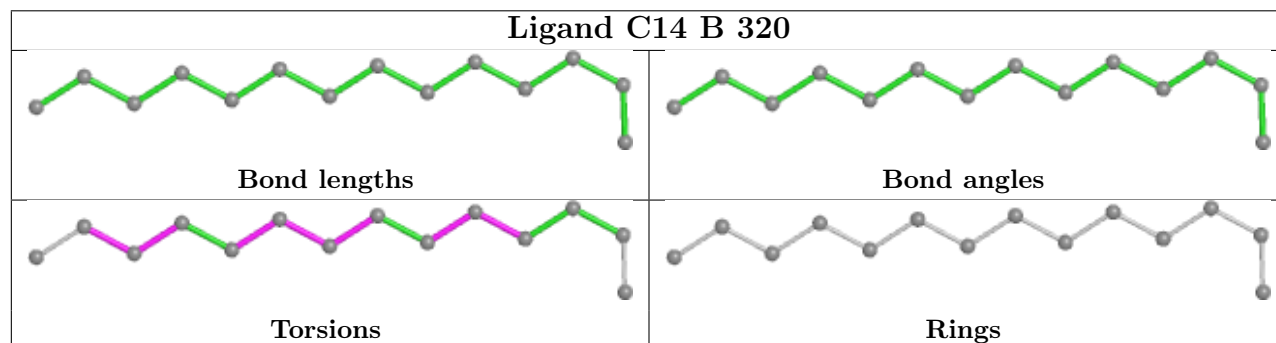
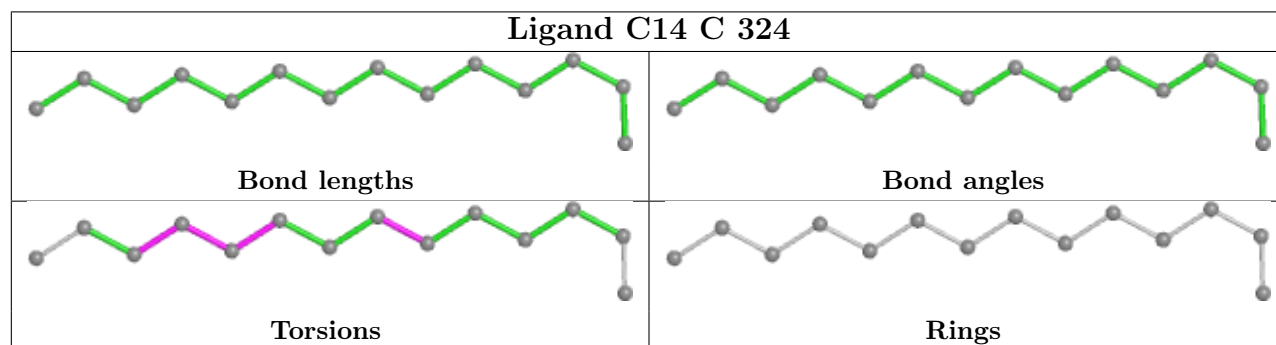
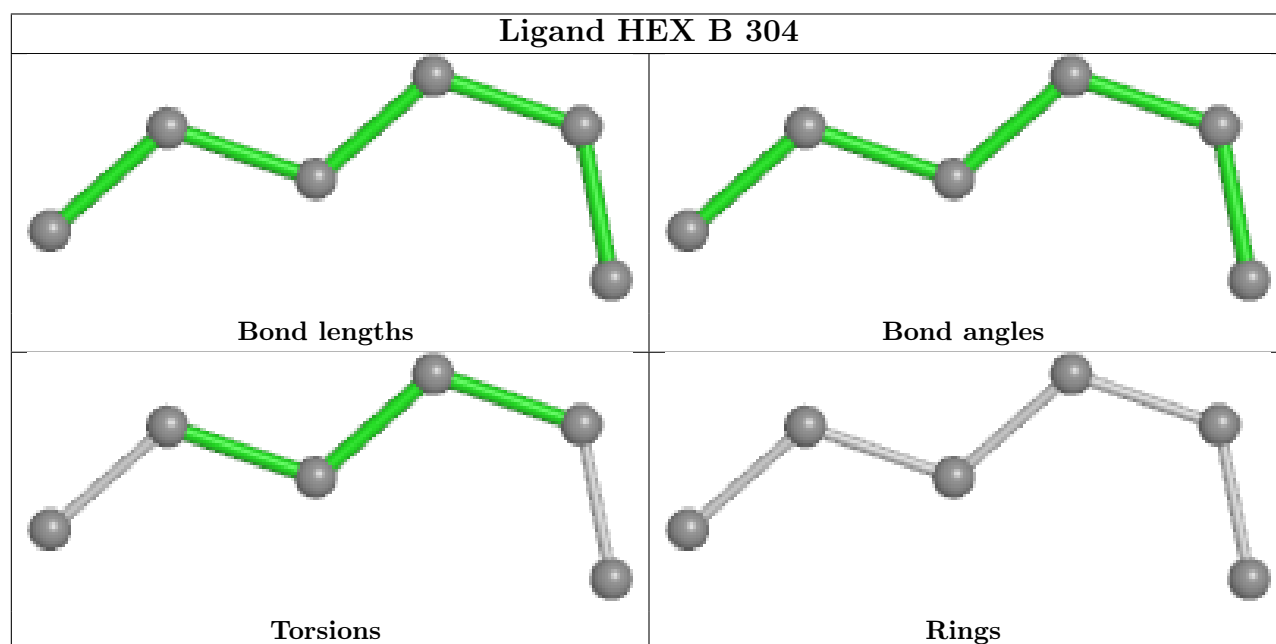
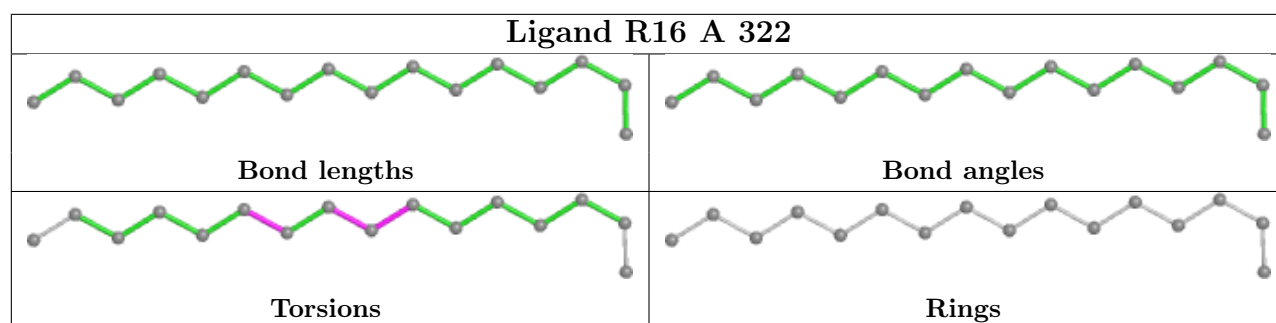
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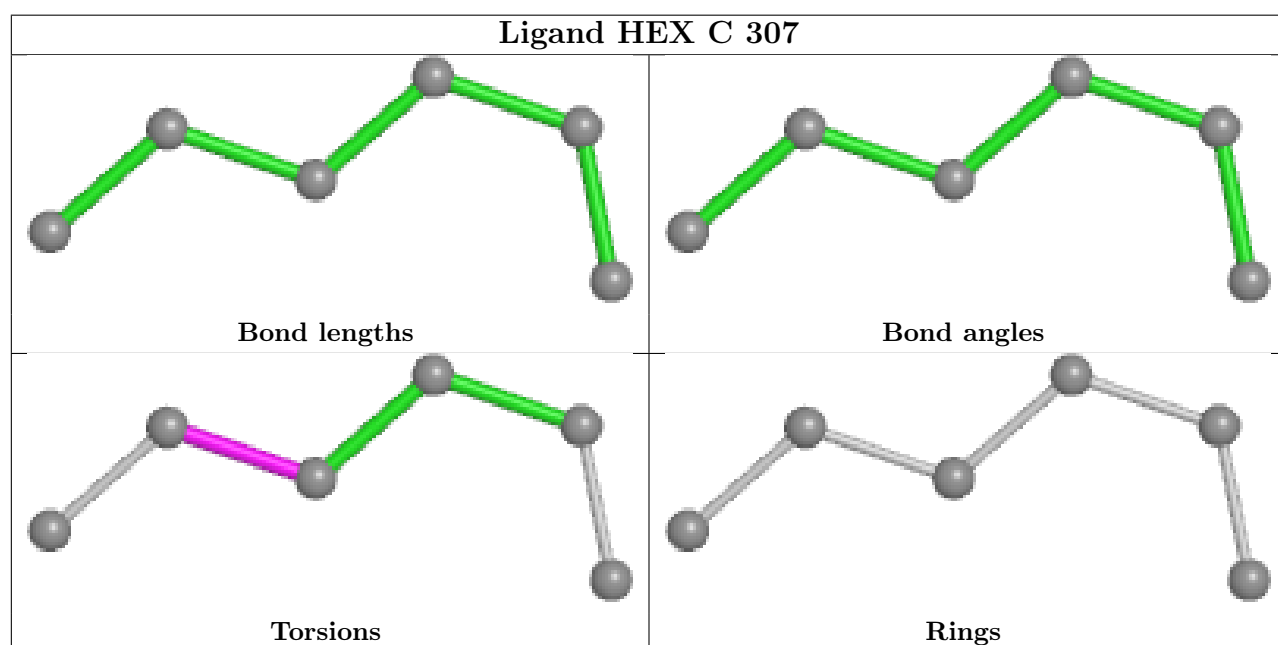
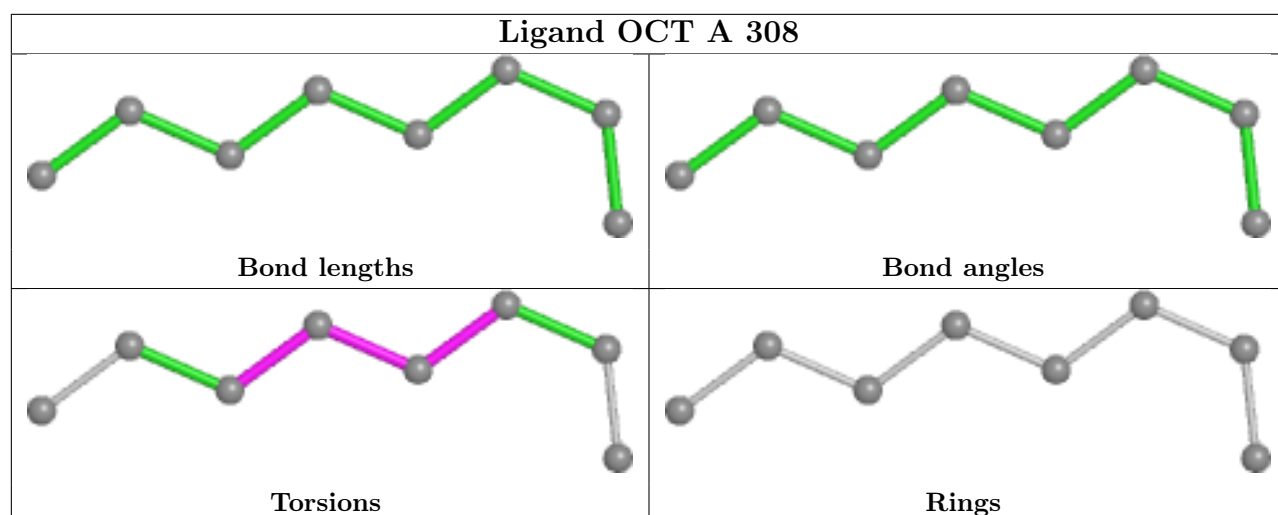
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	309	OCT	1	0
5	A	311	OCT	2	0
2	B	301	RET	3	0
4	A	306	HEX	1	0
7	A	318	D12	1	0
7	B	316	D12	1	0
5	C	317	OCT	1	0
5	C	313	OCT	1	0
7	C	318	D12	1	0
2	C	301	RET	4	0

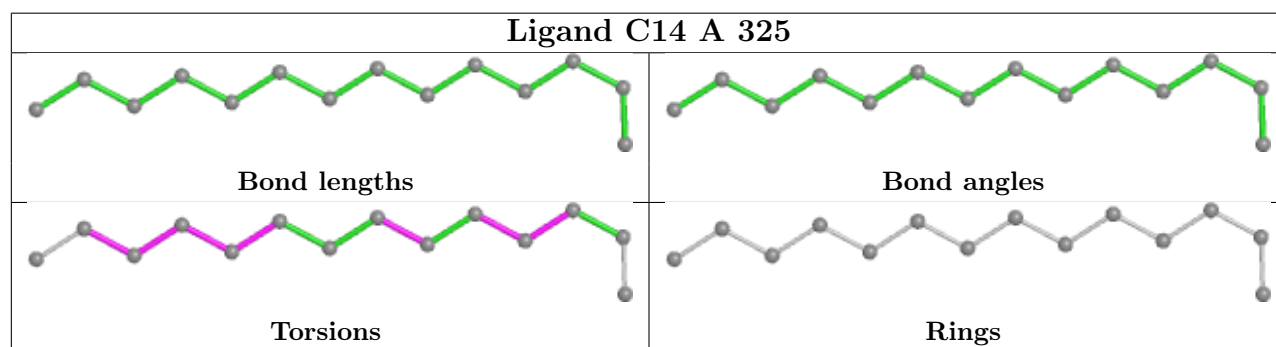
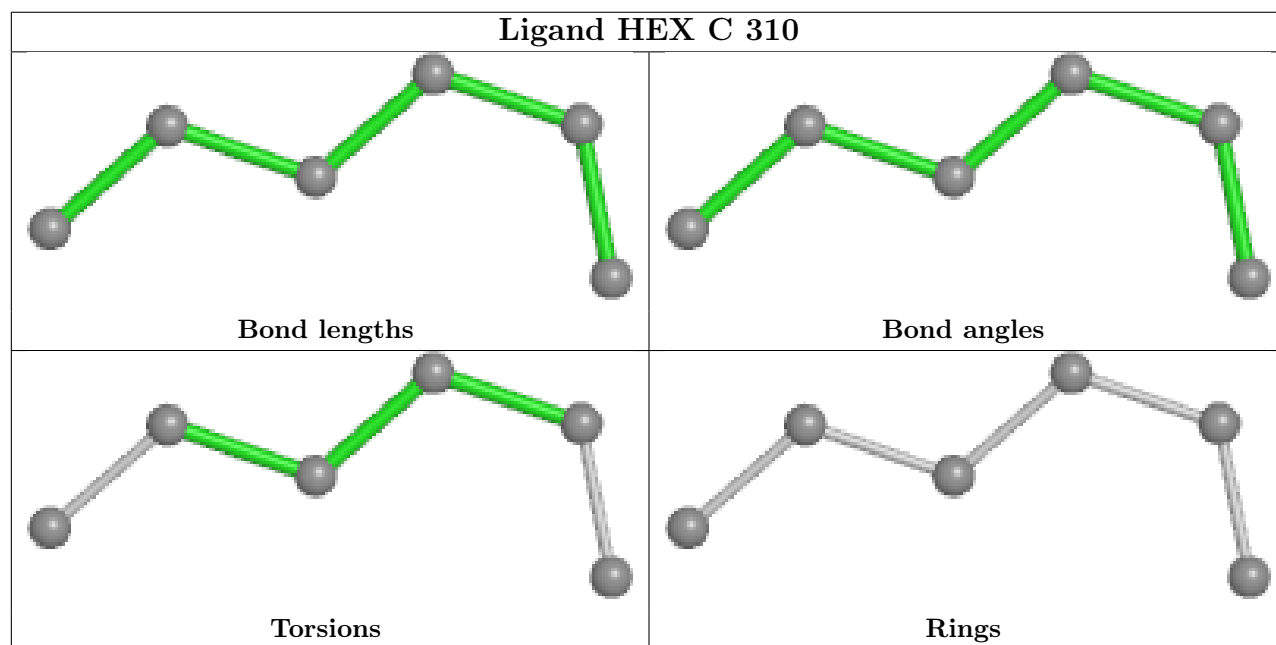
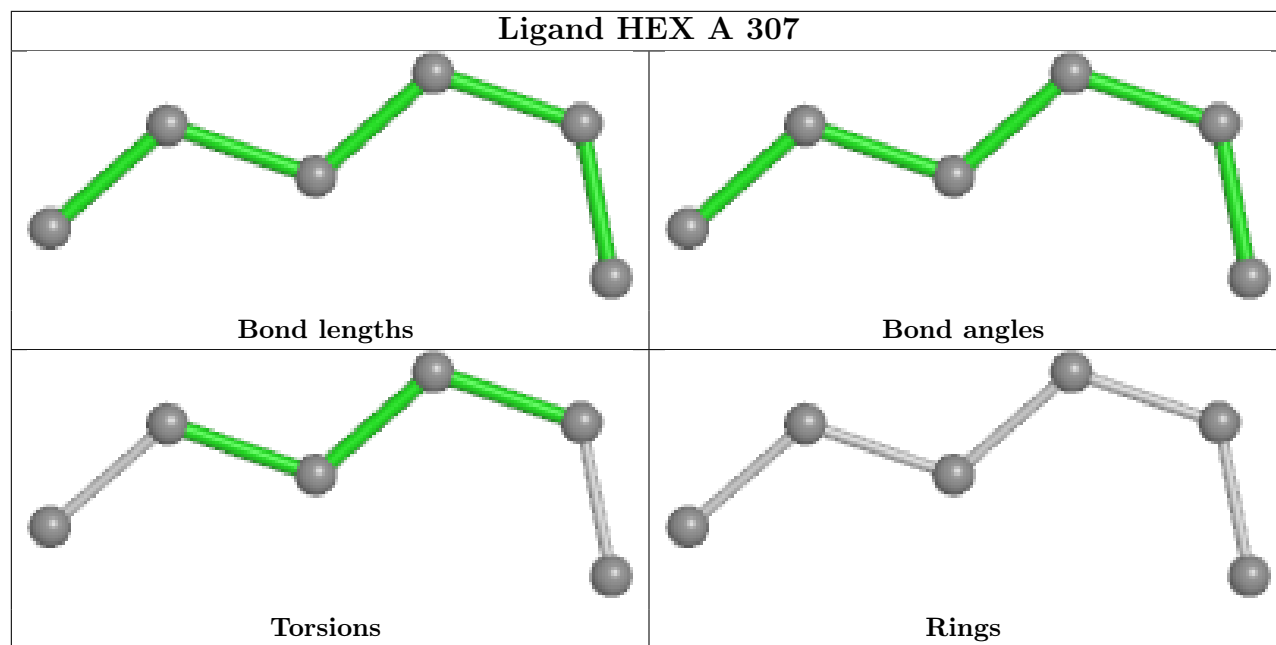
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

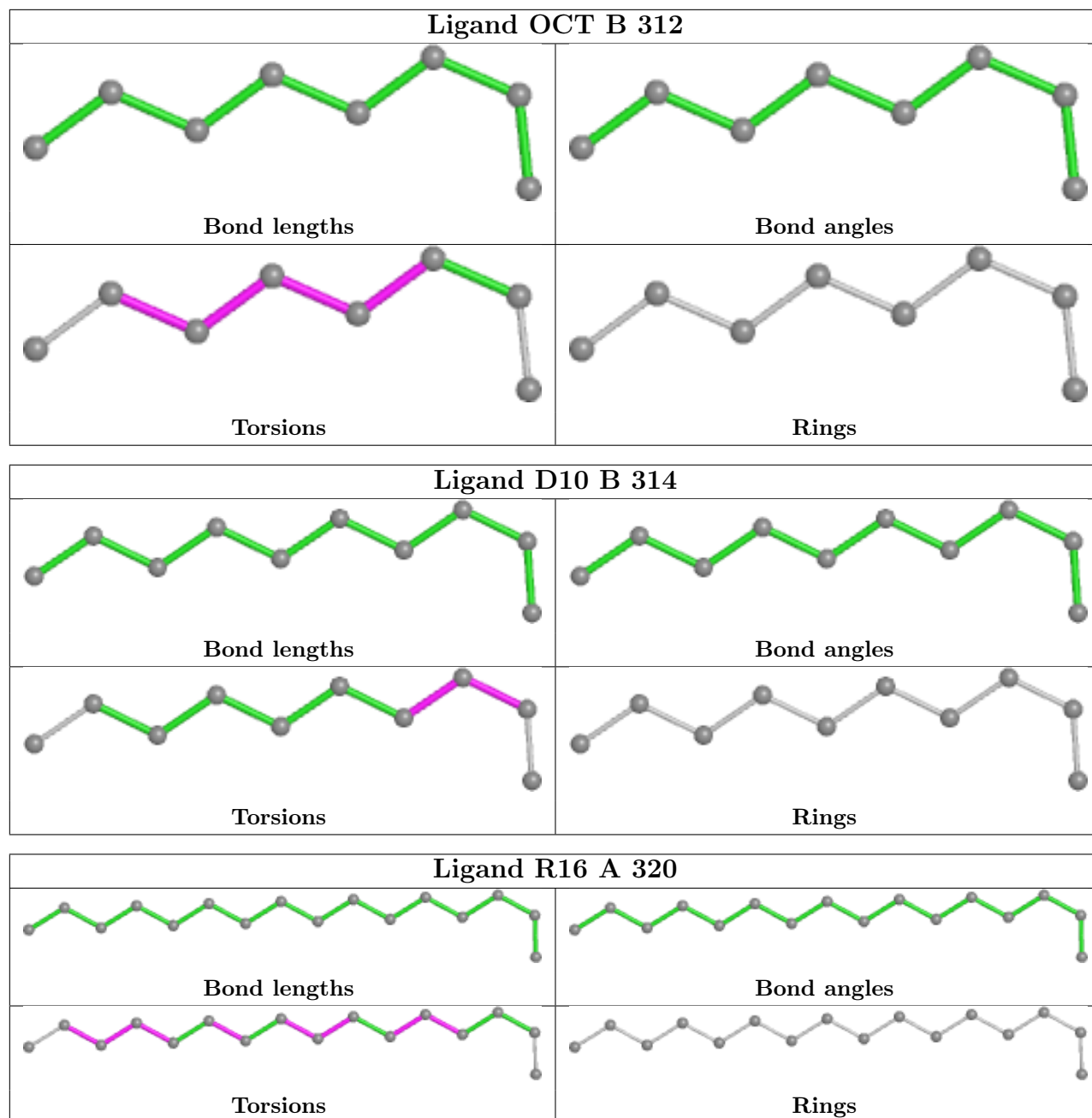


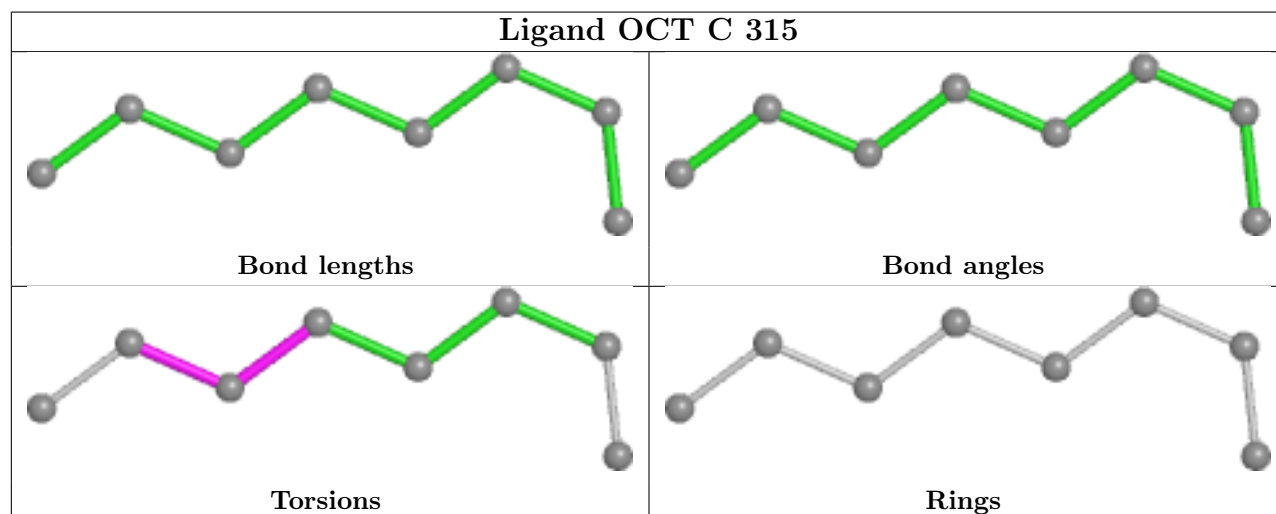
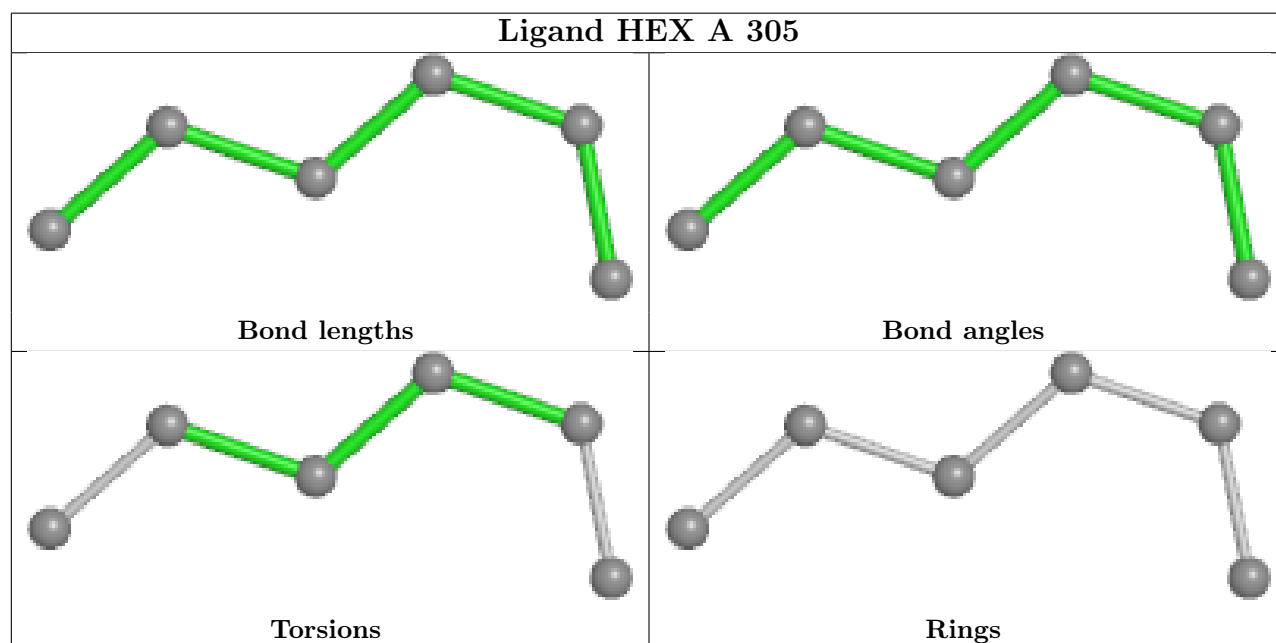
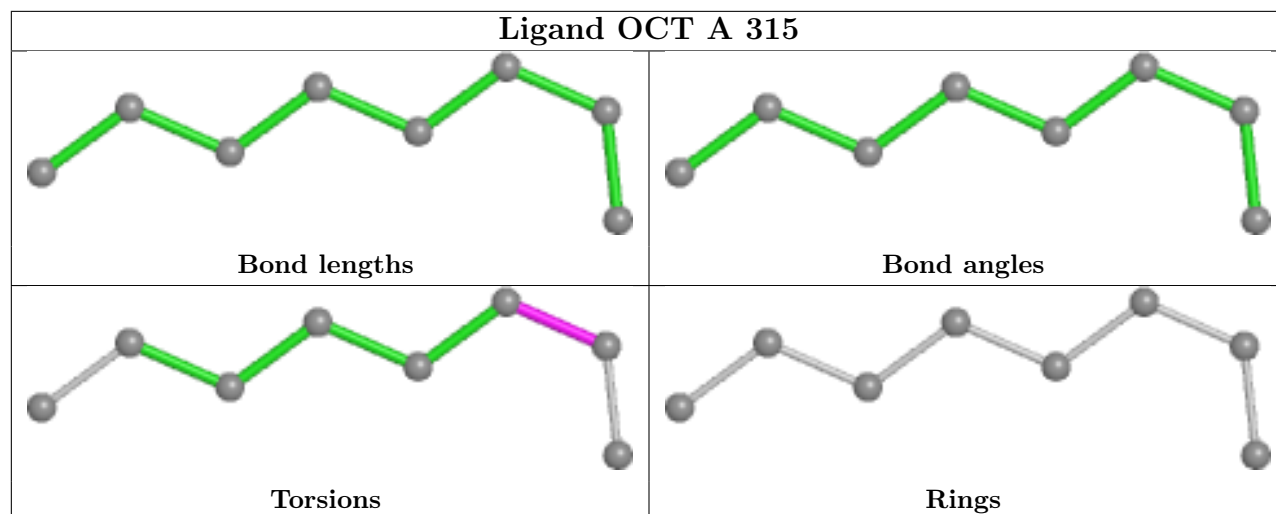


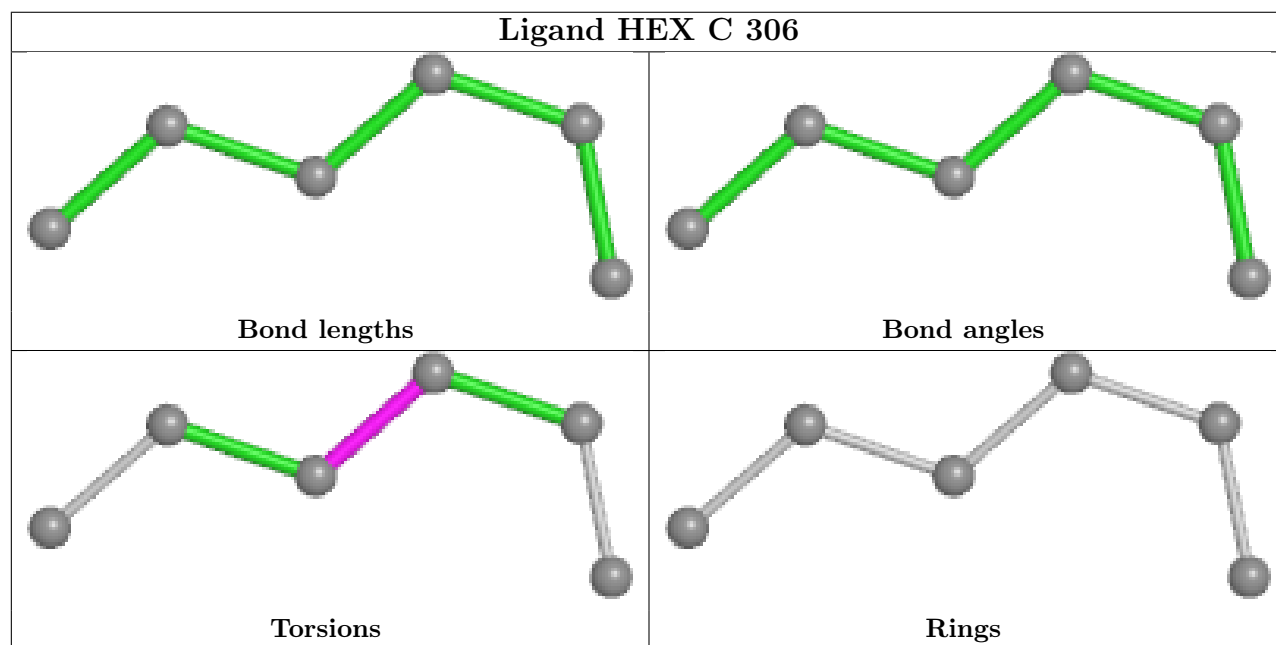
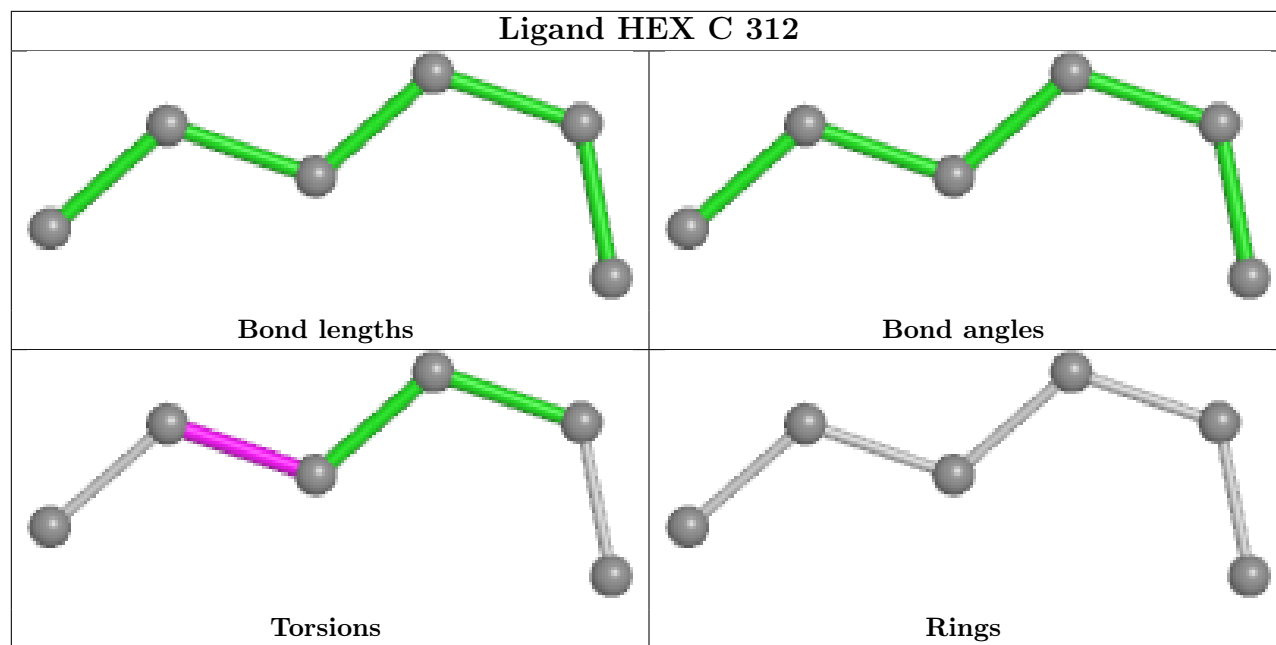


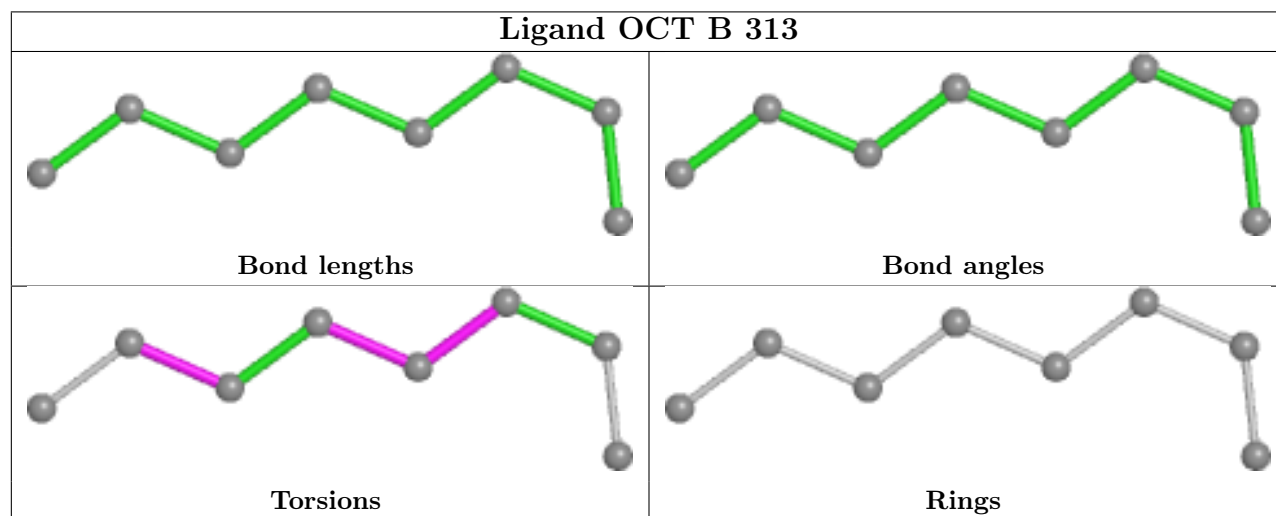
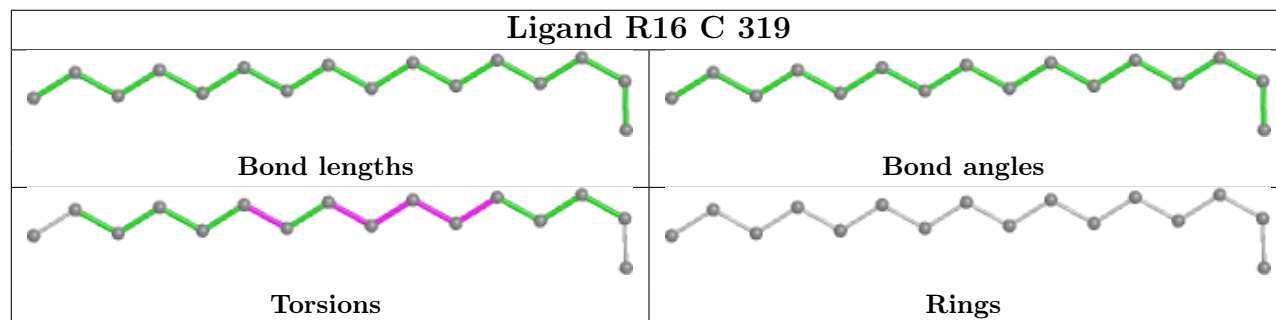
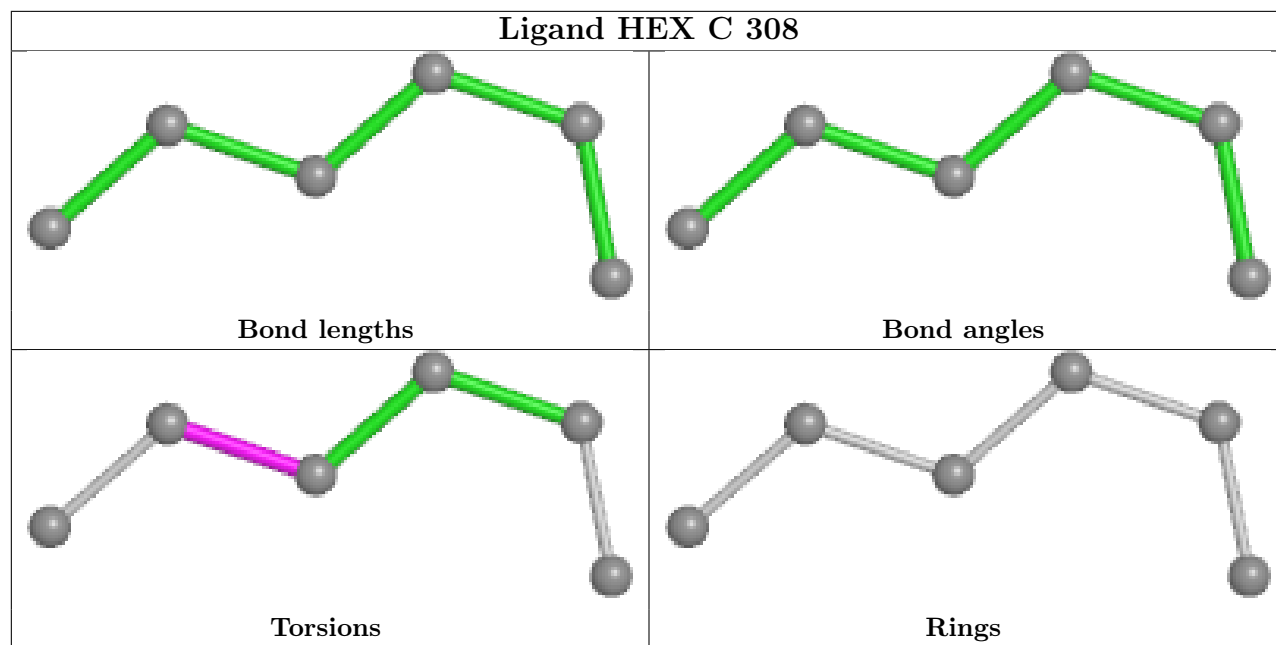


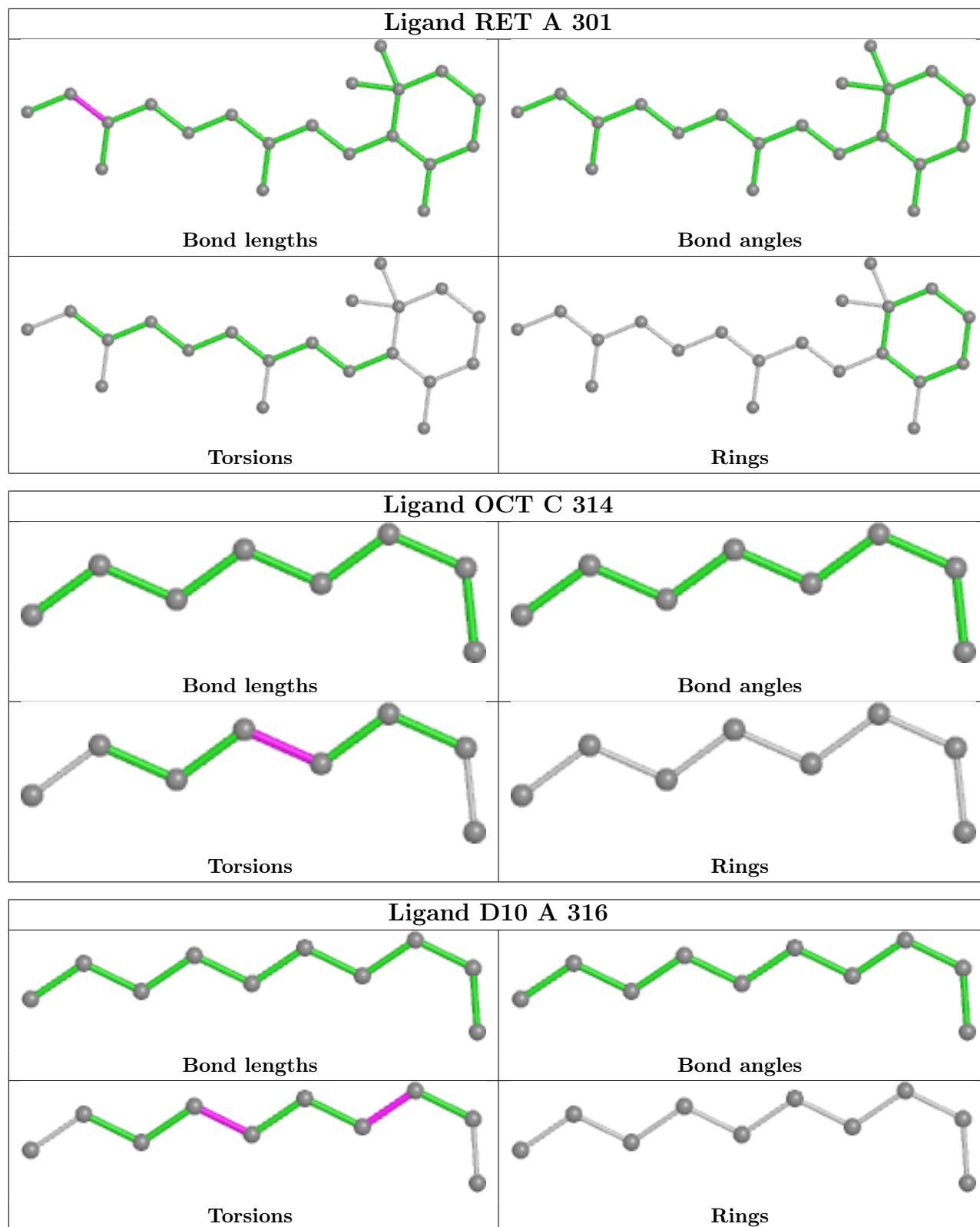


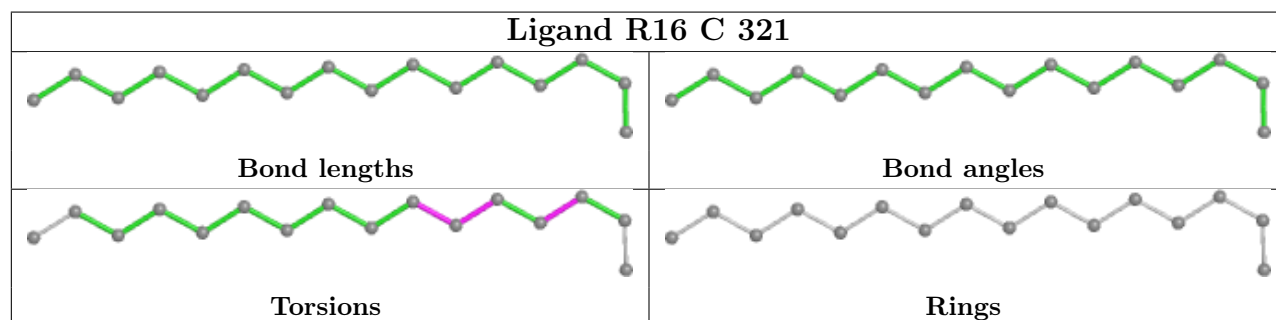
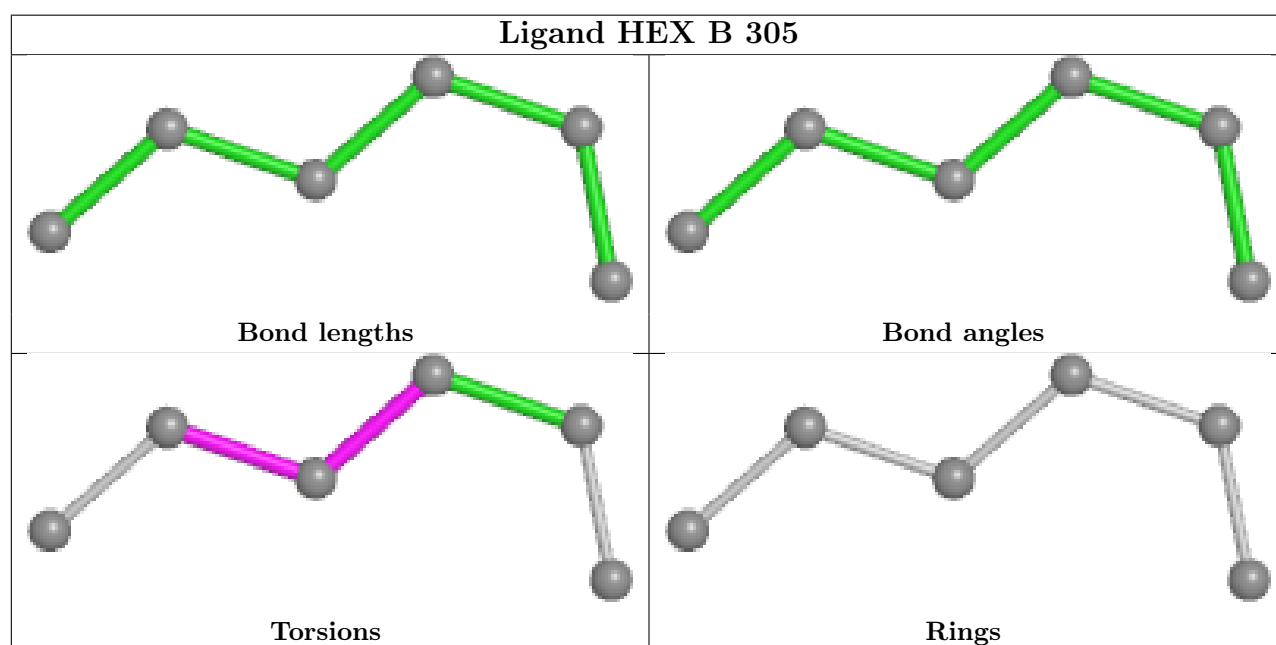
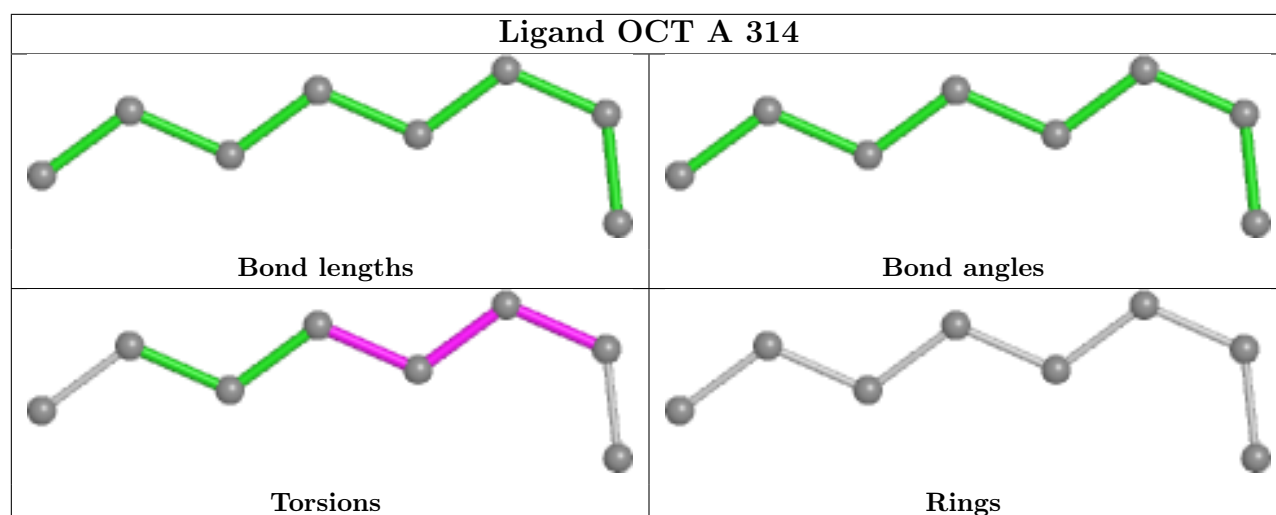


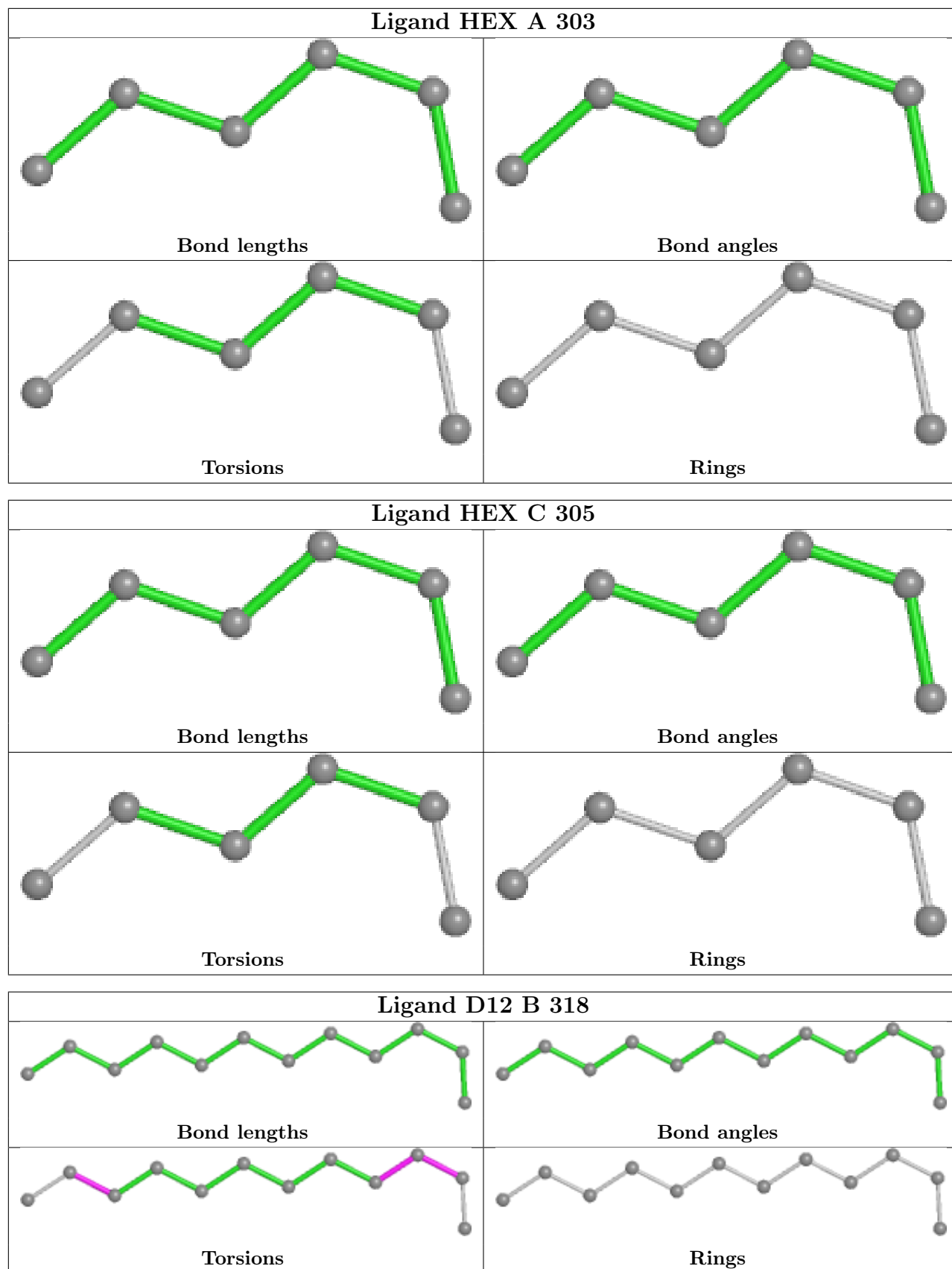


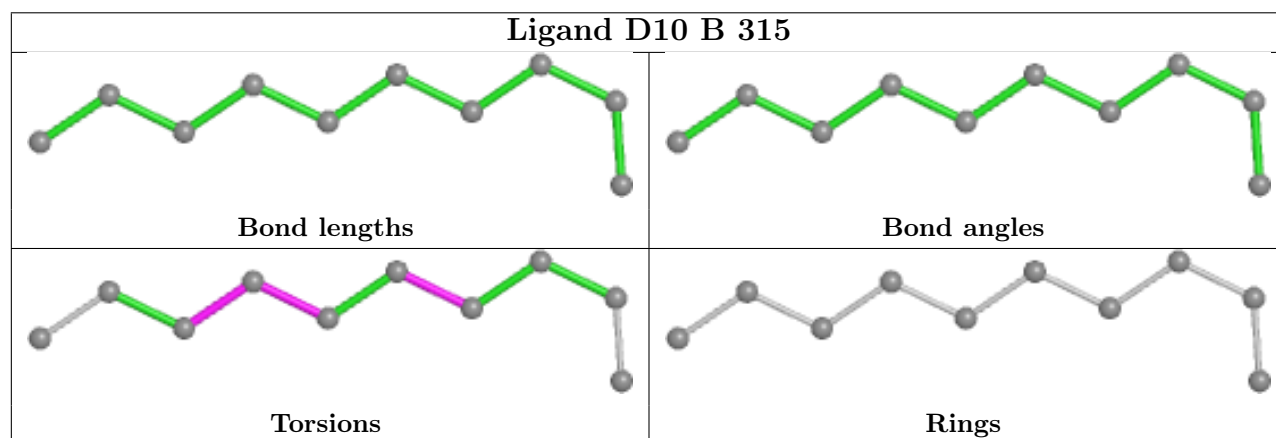
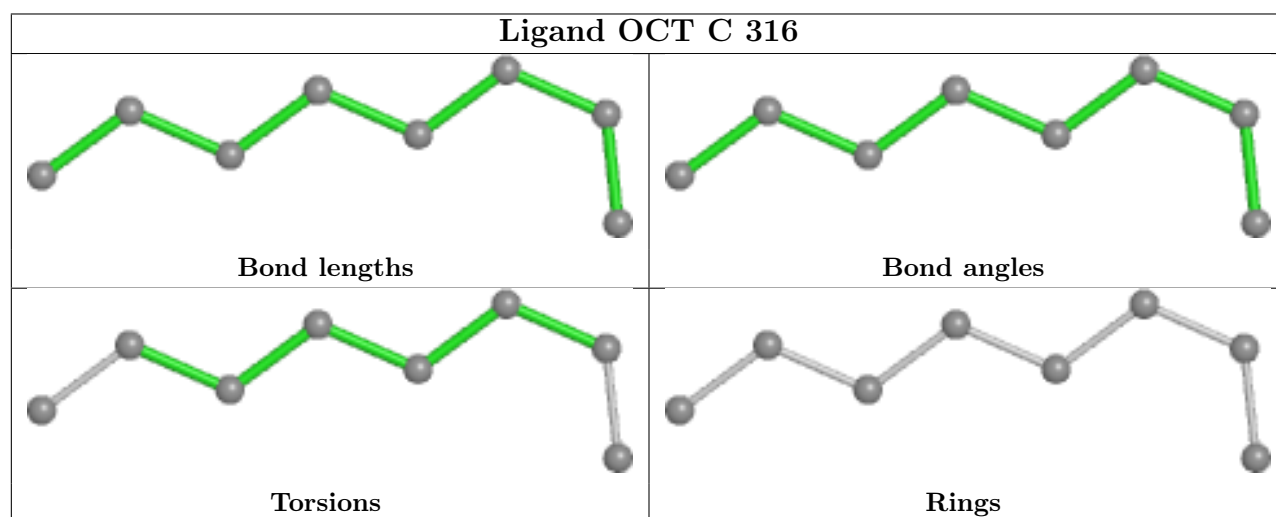
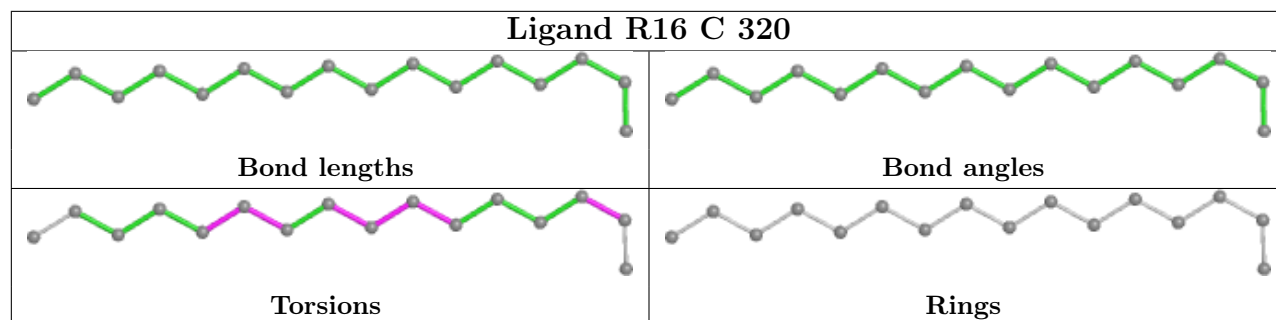


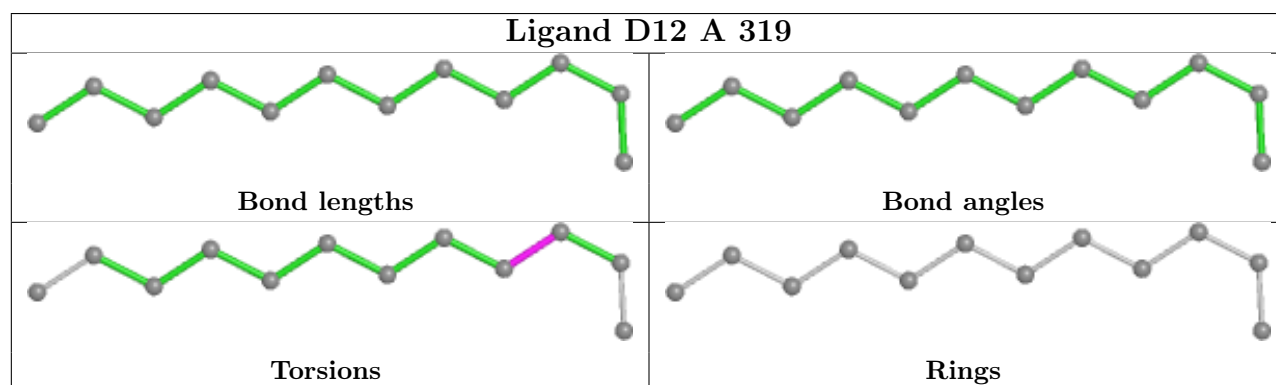
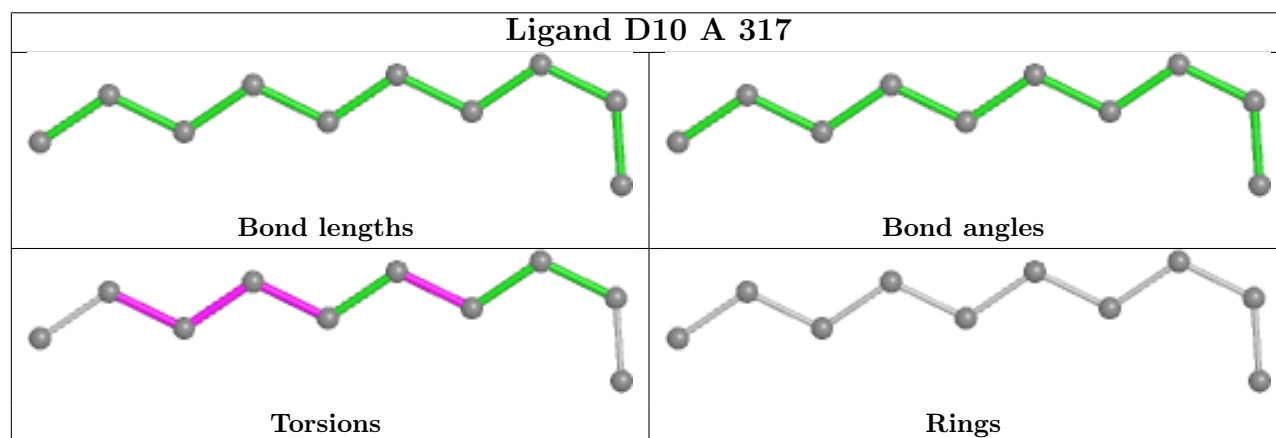
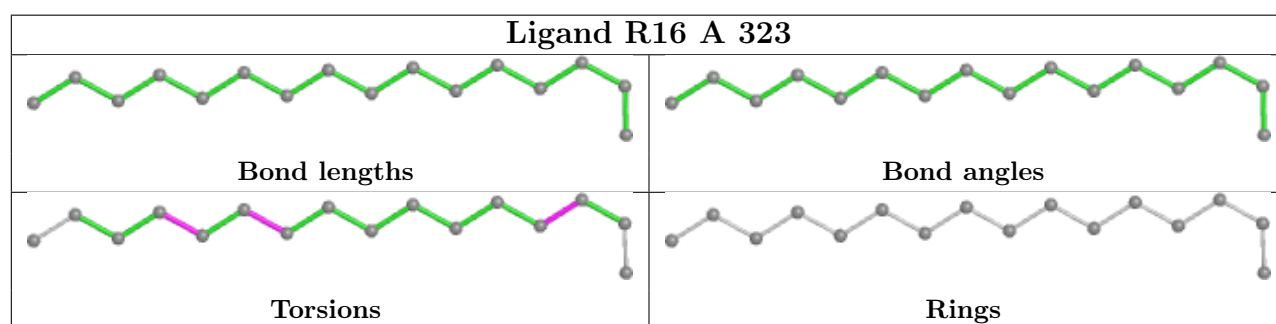
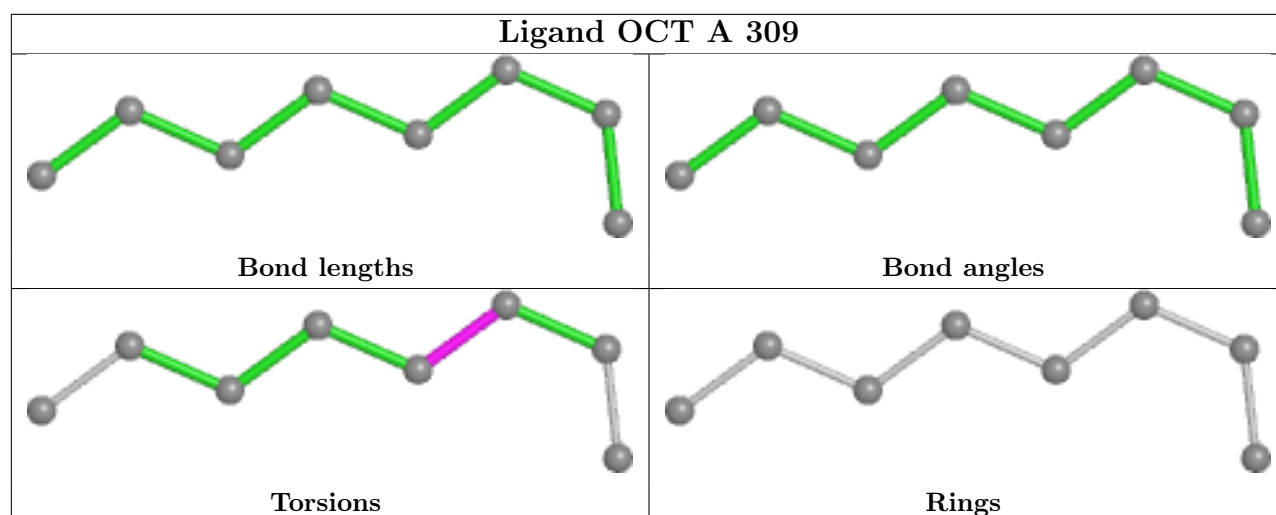


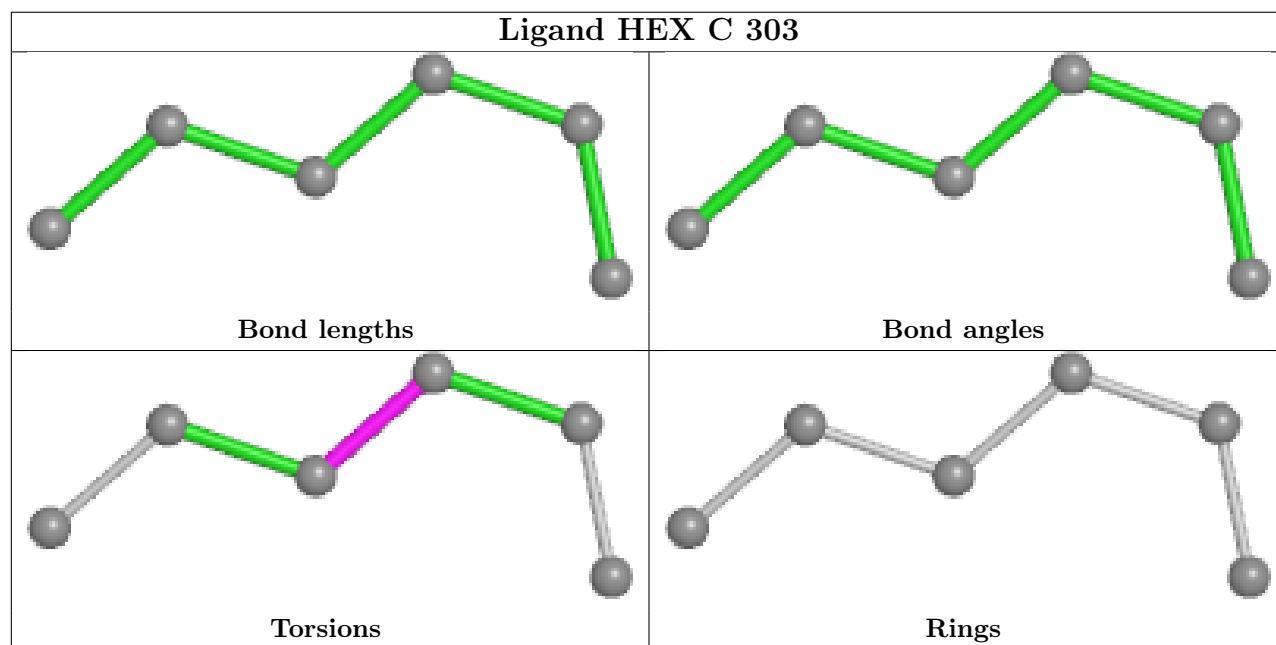
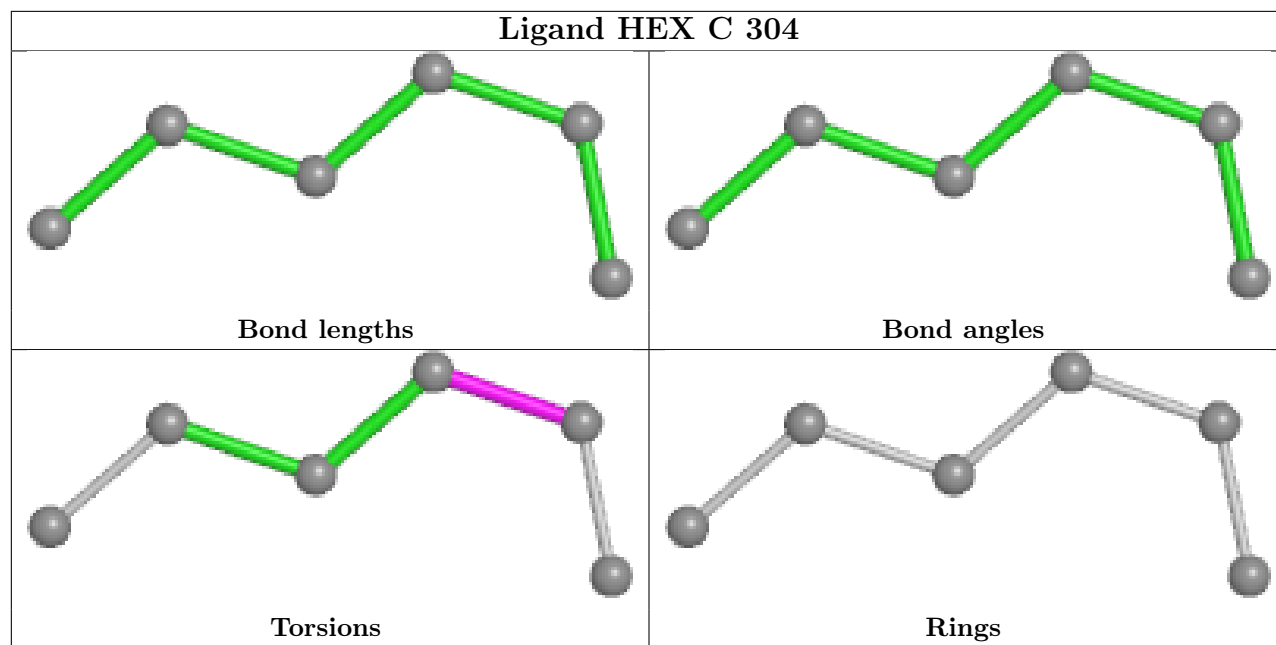


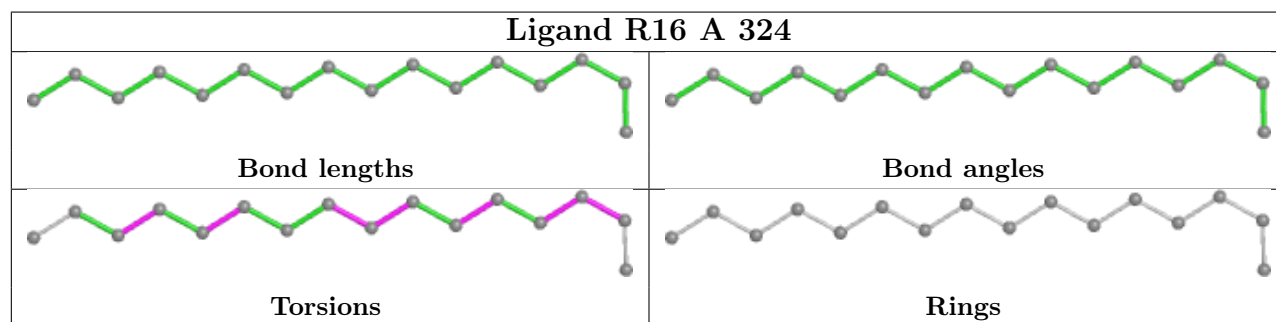
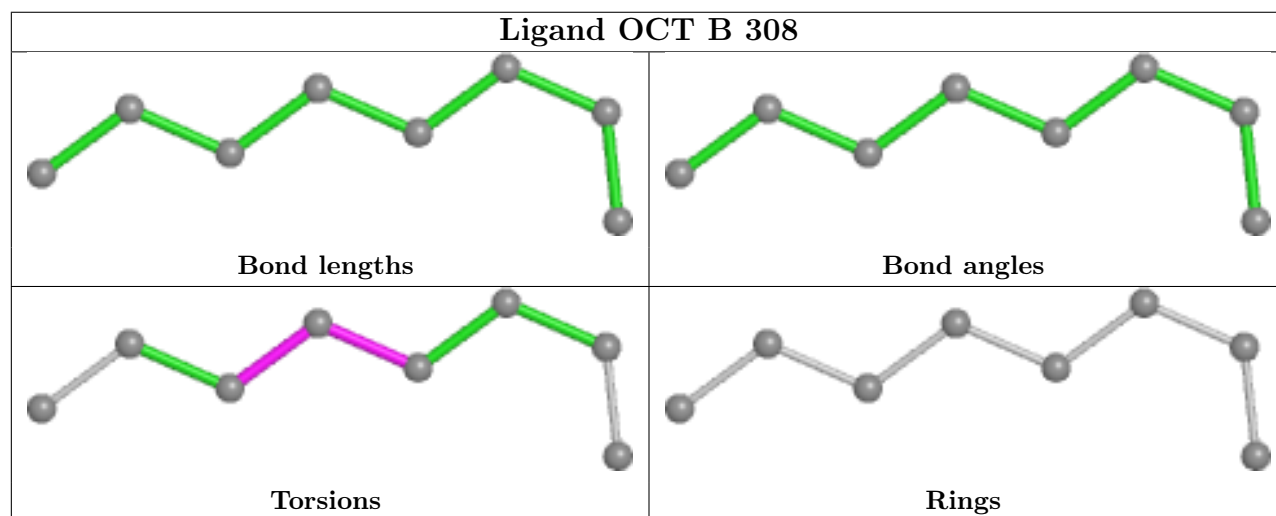
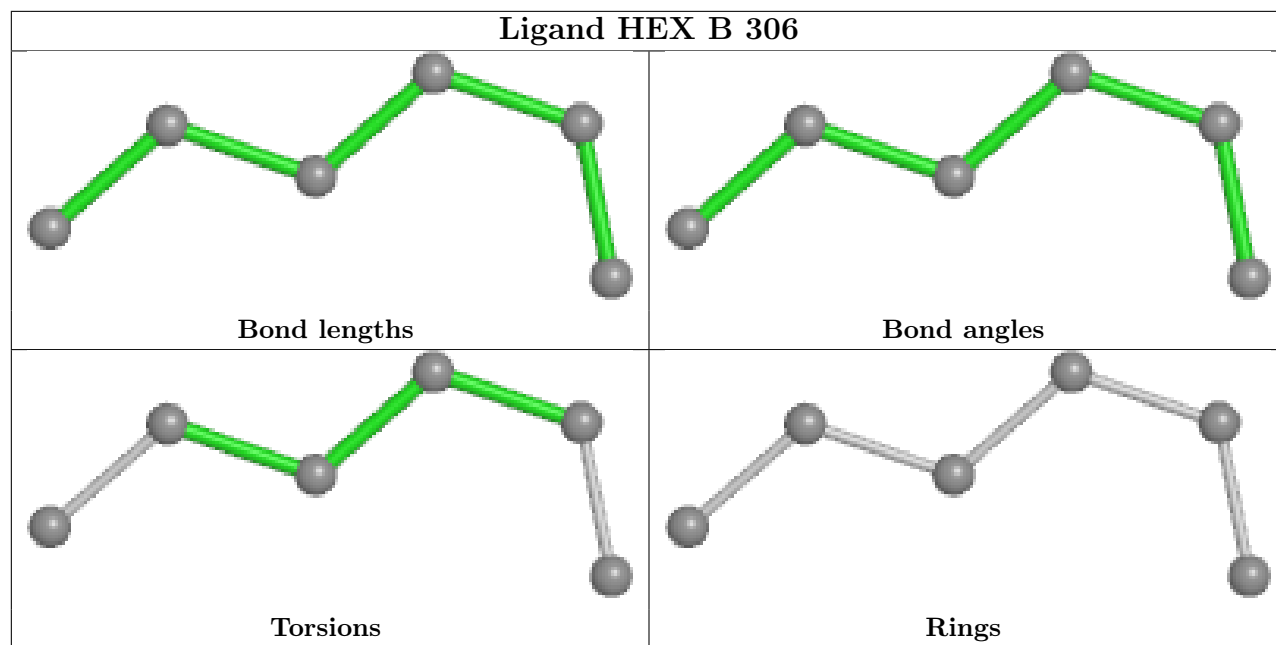


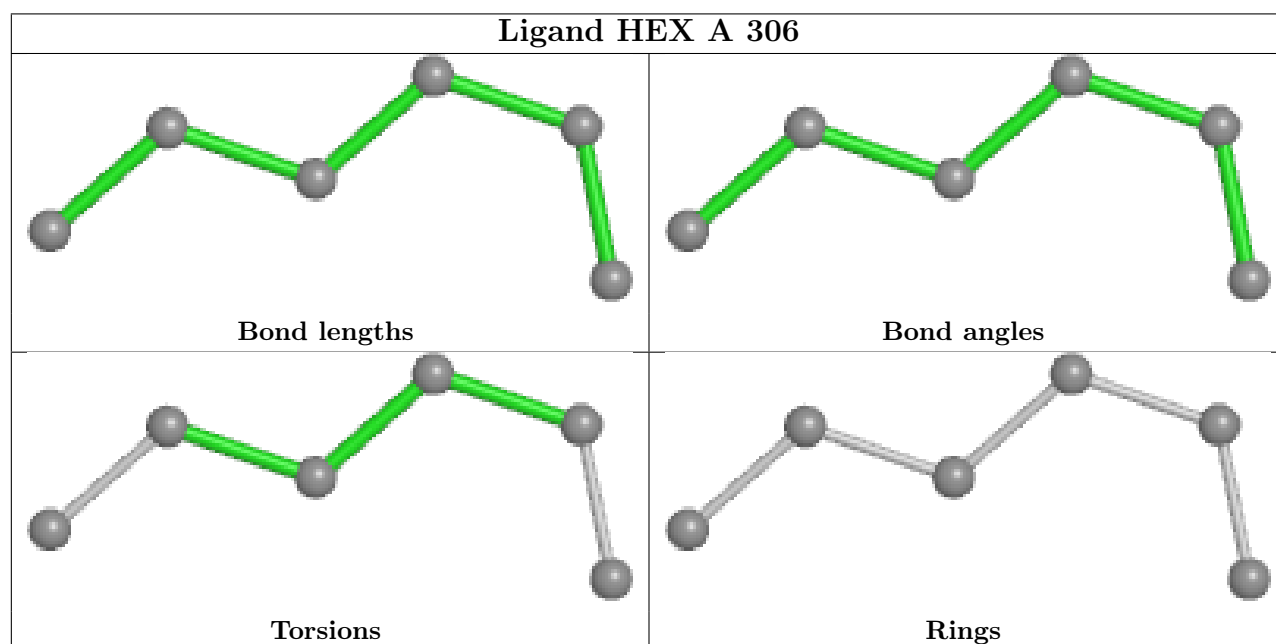
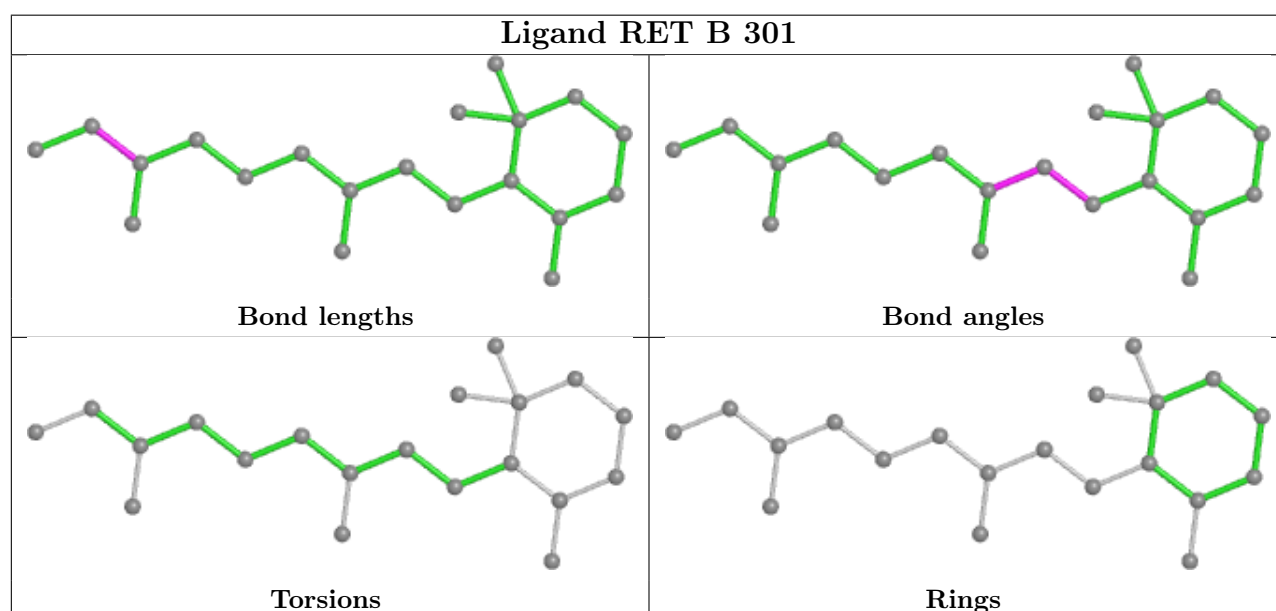
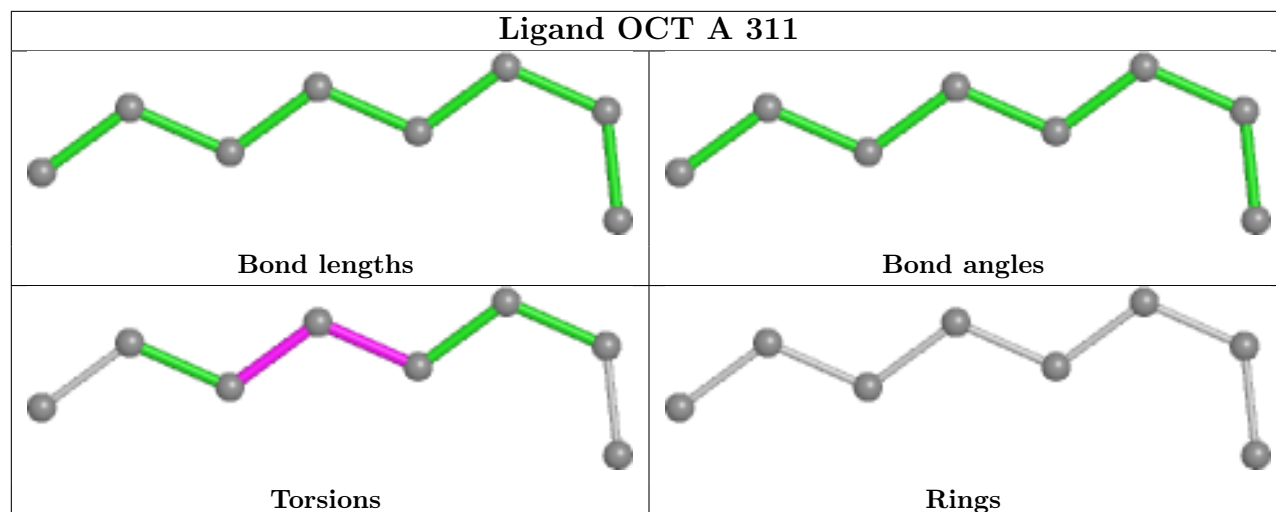


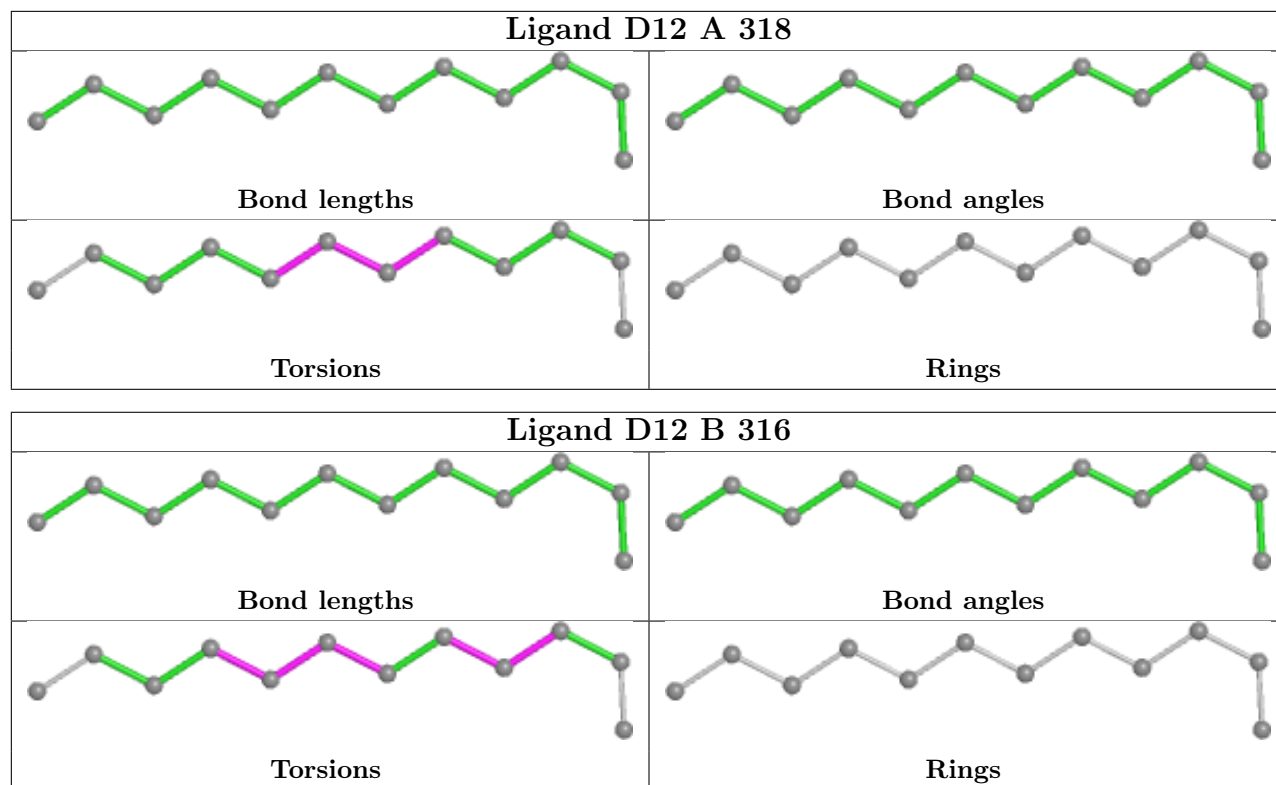


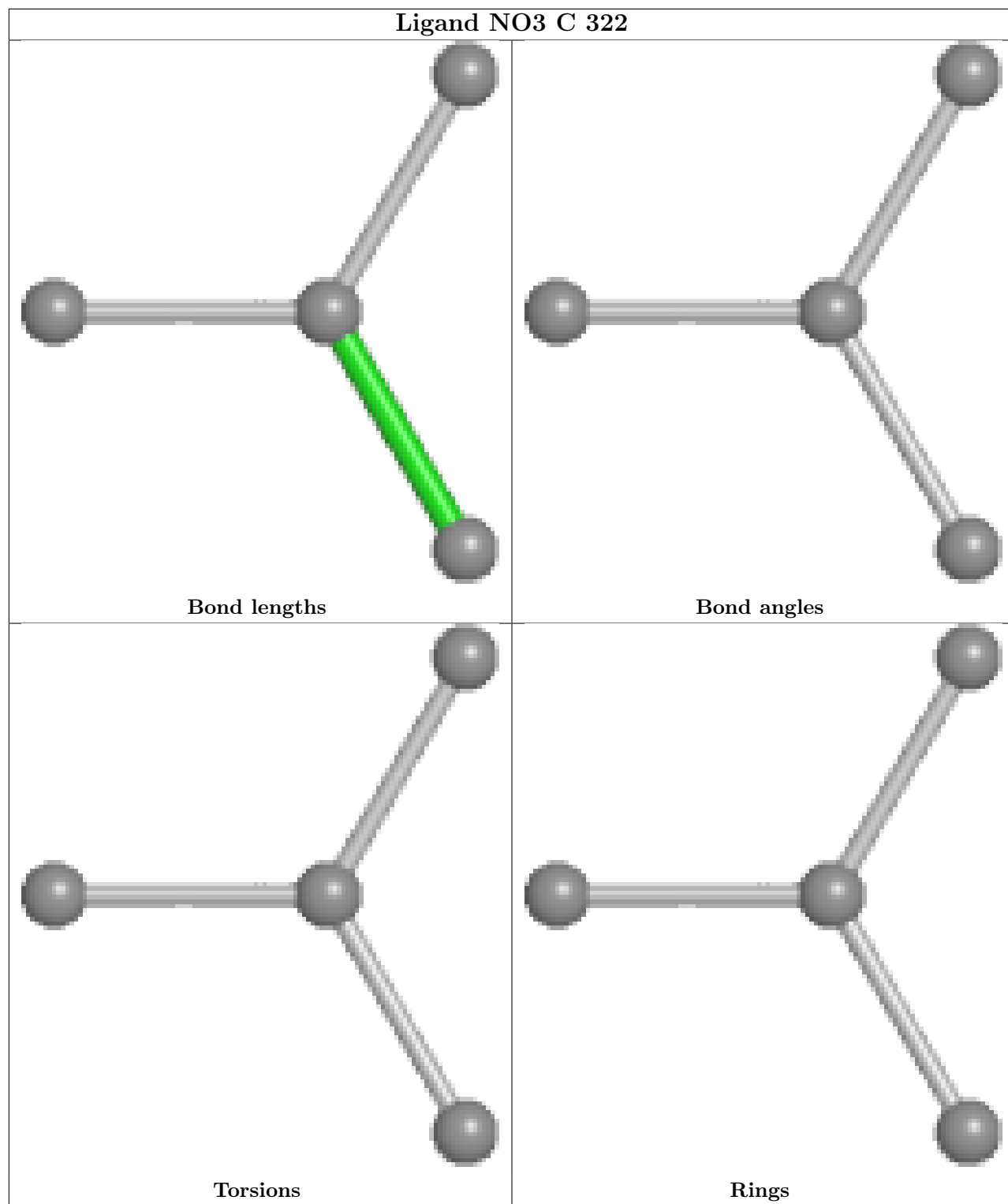


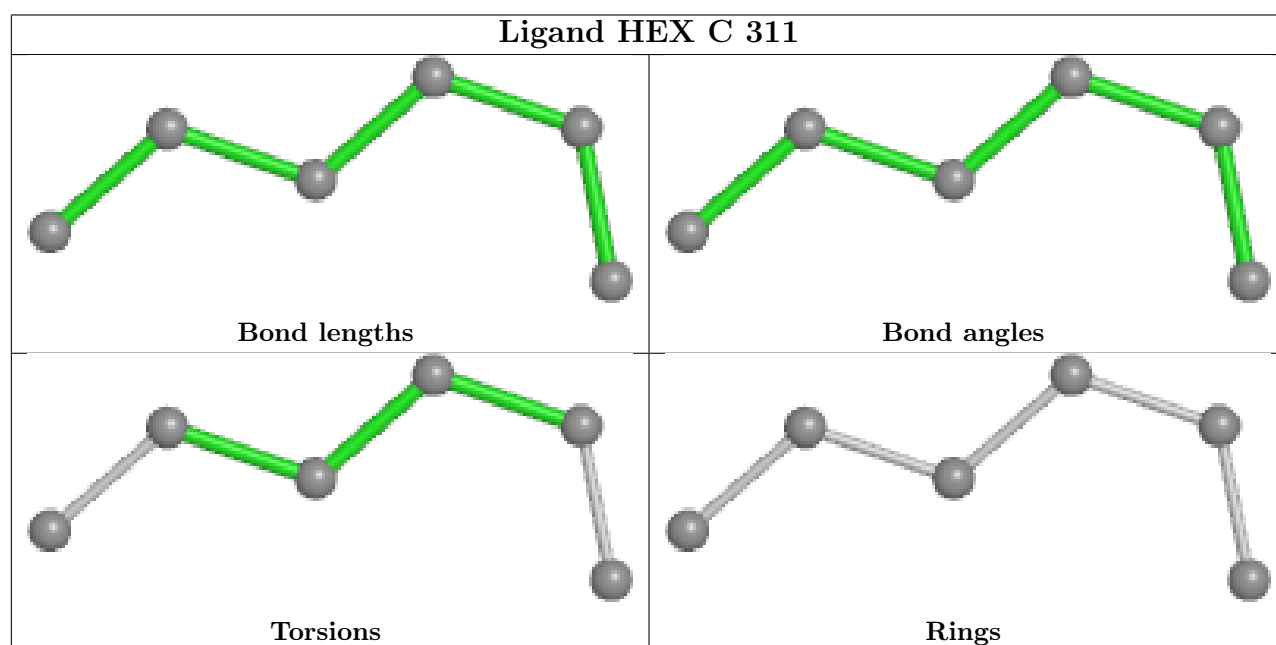
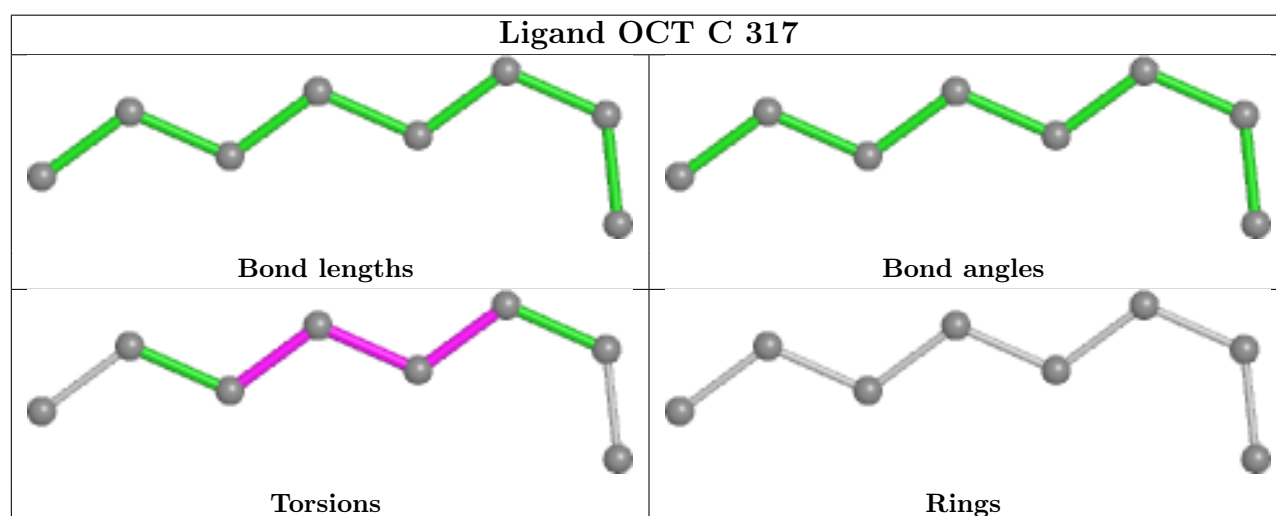
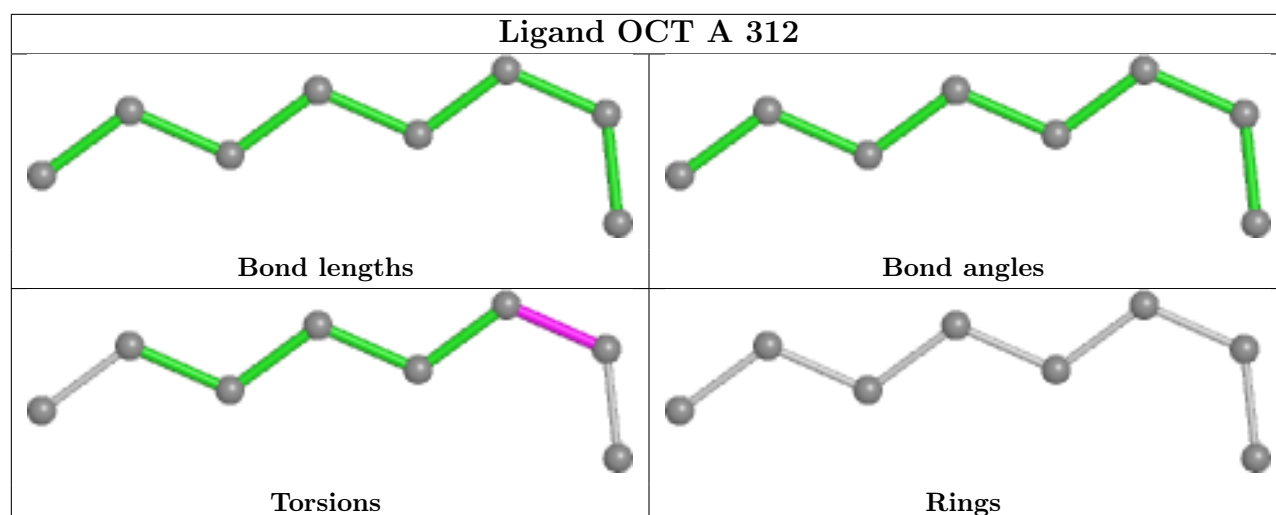


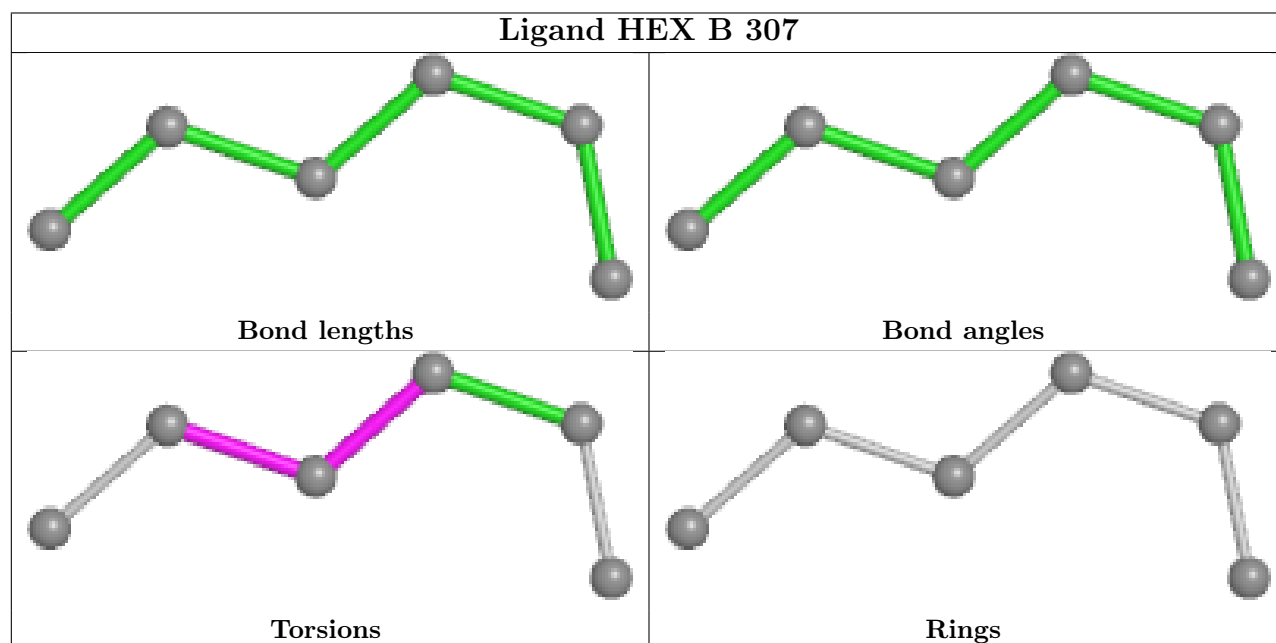
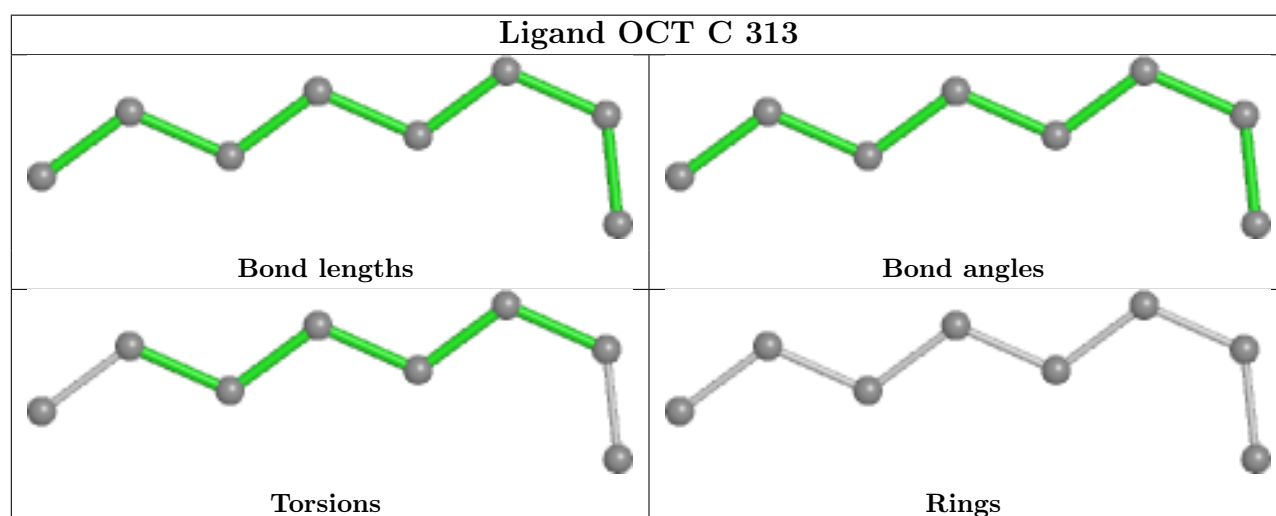
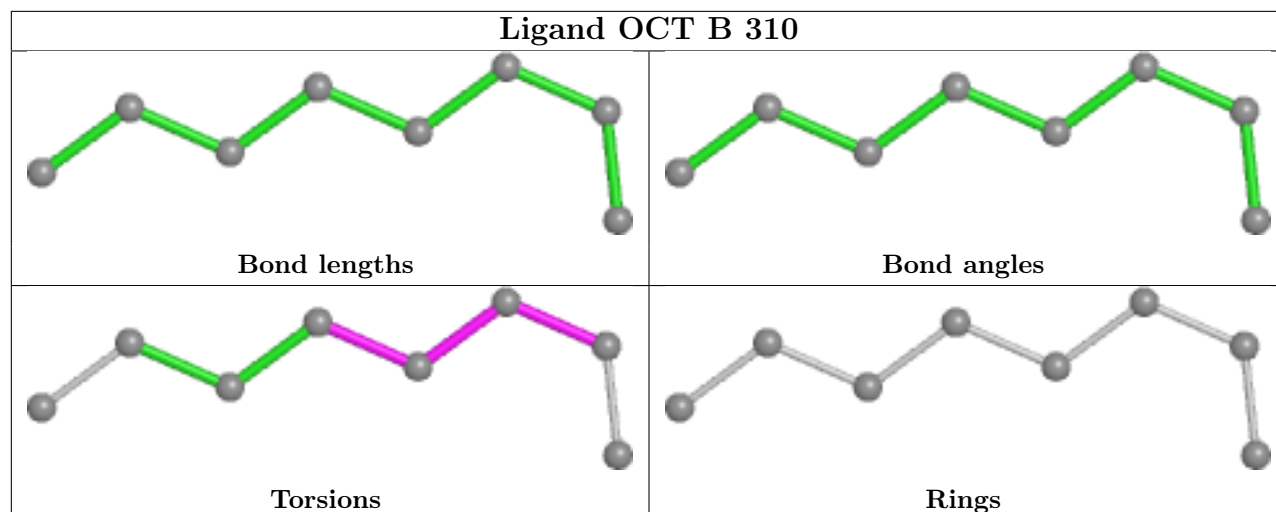


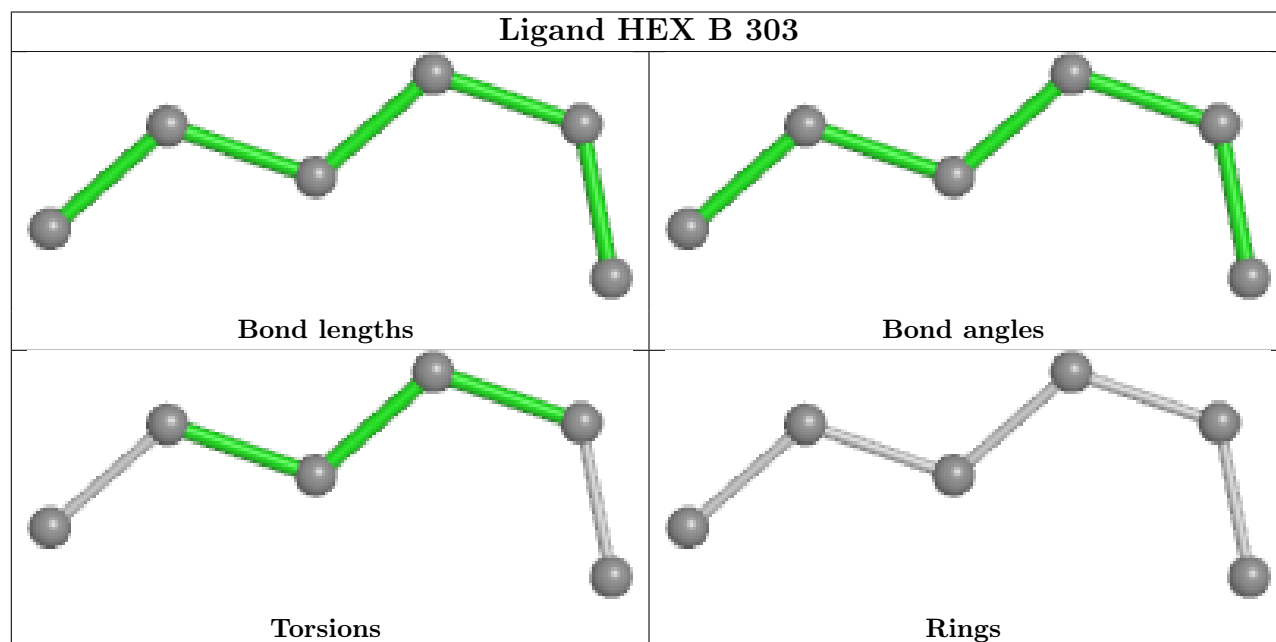
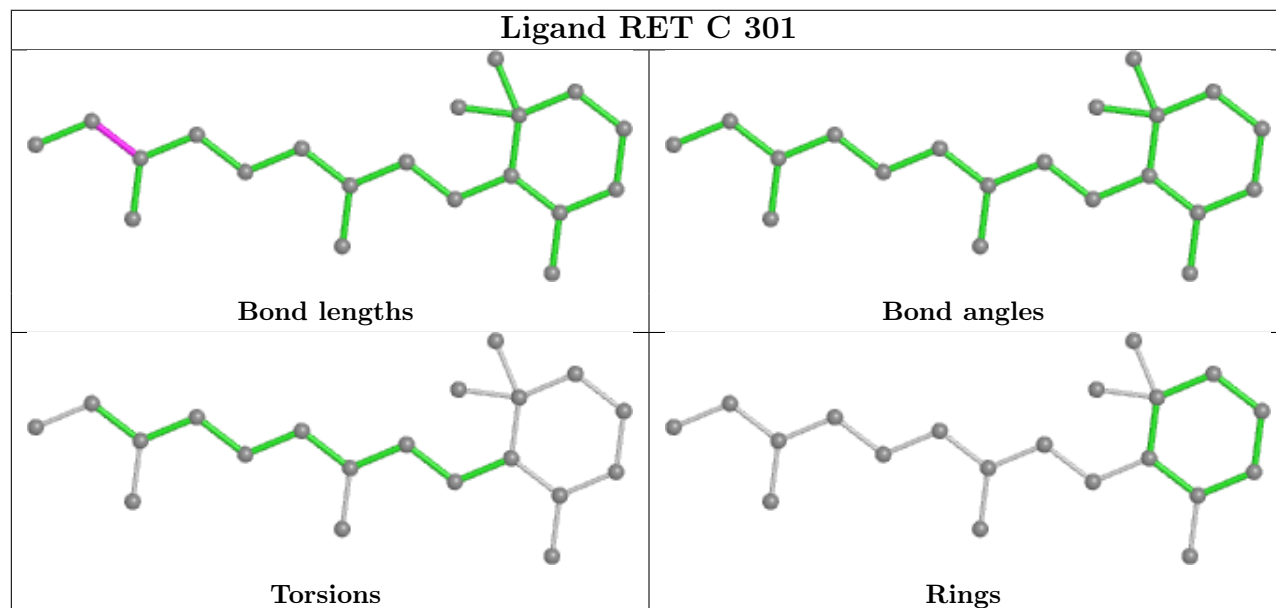
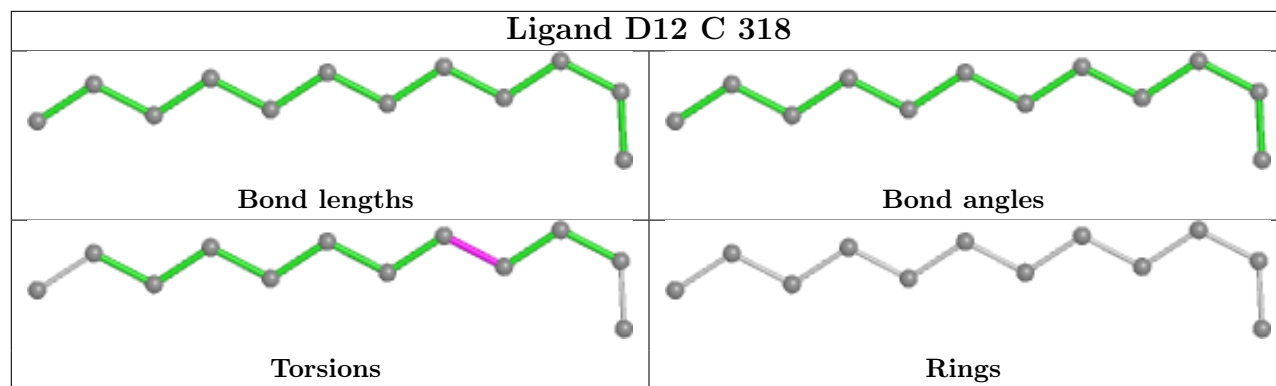


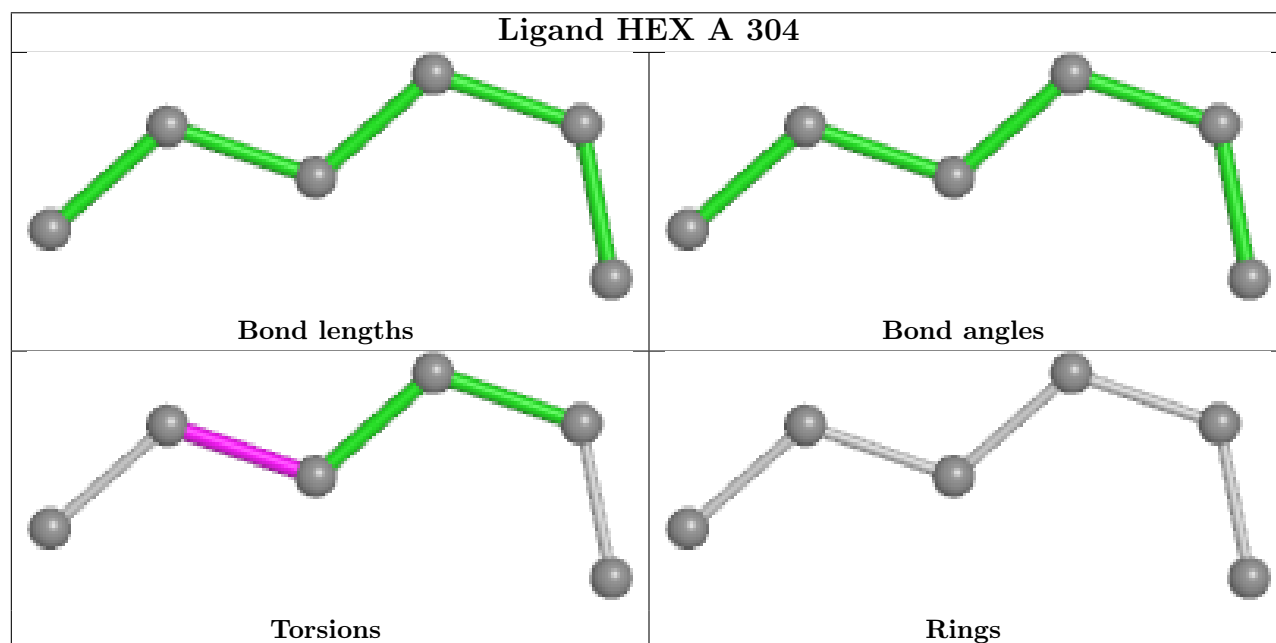
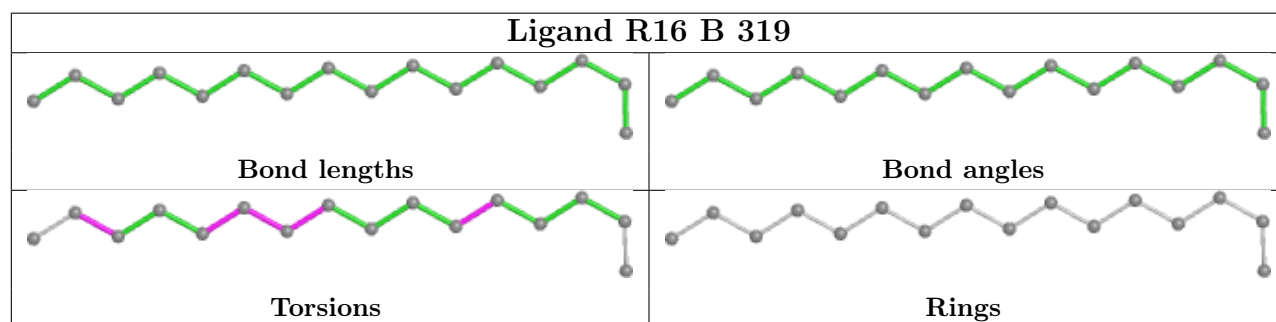
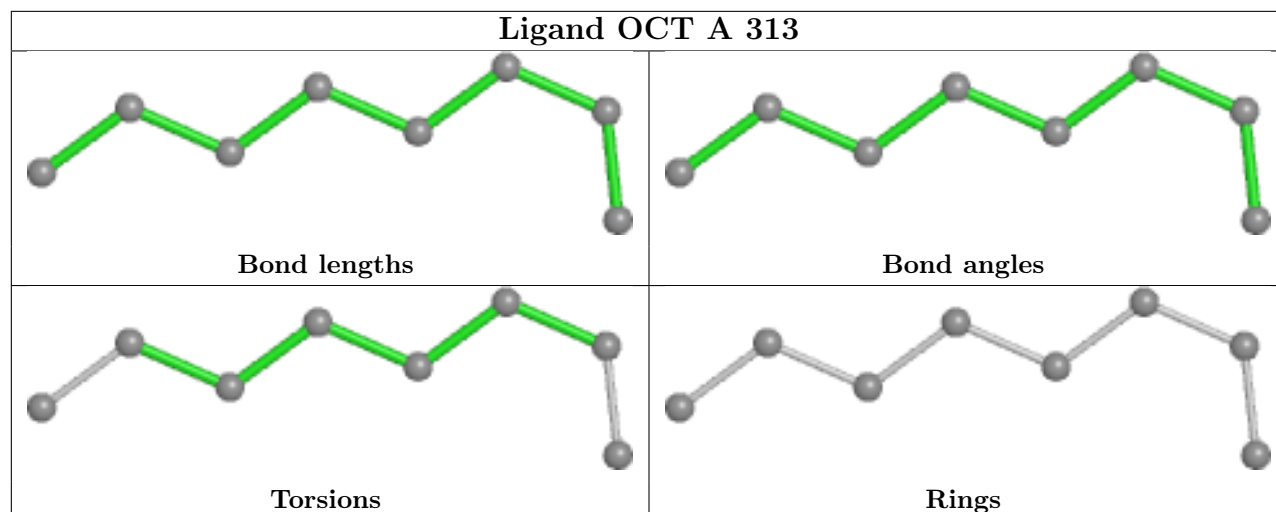


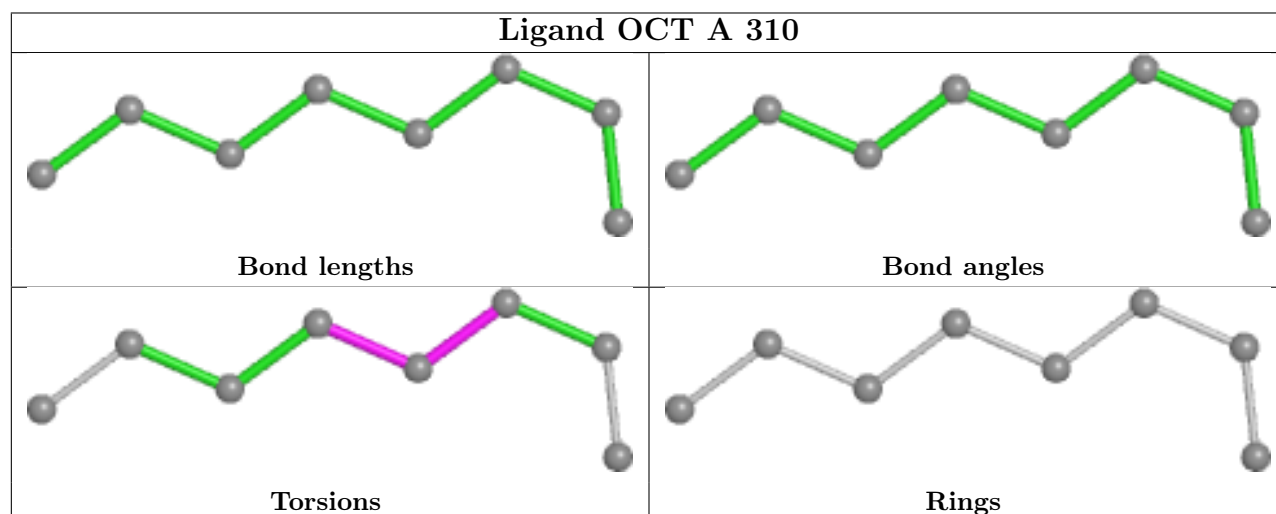
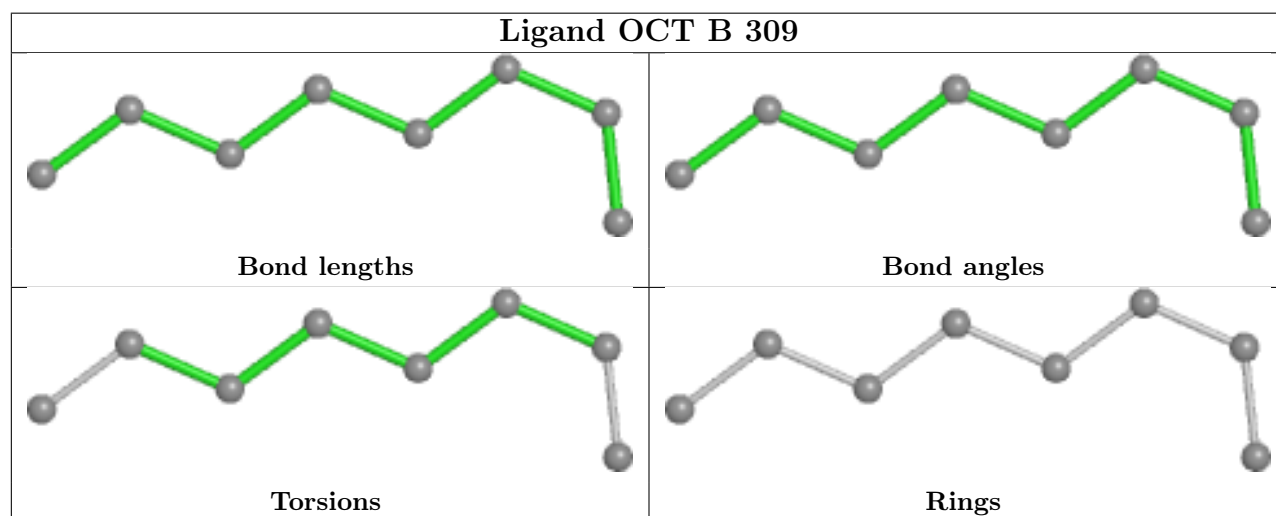
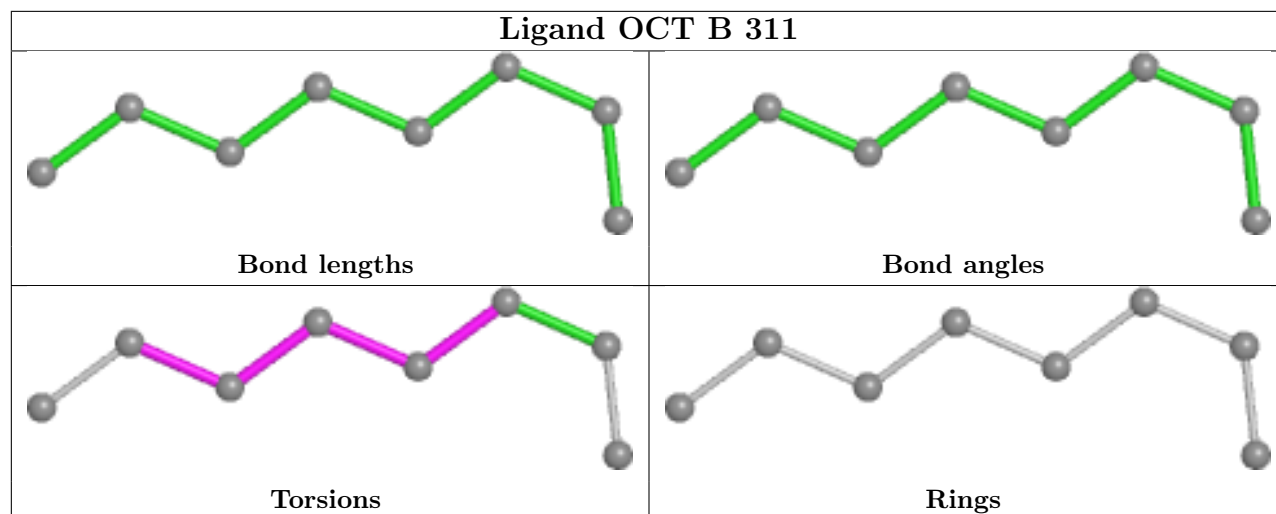


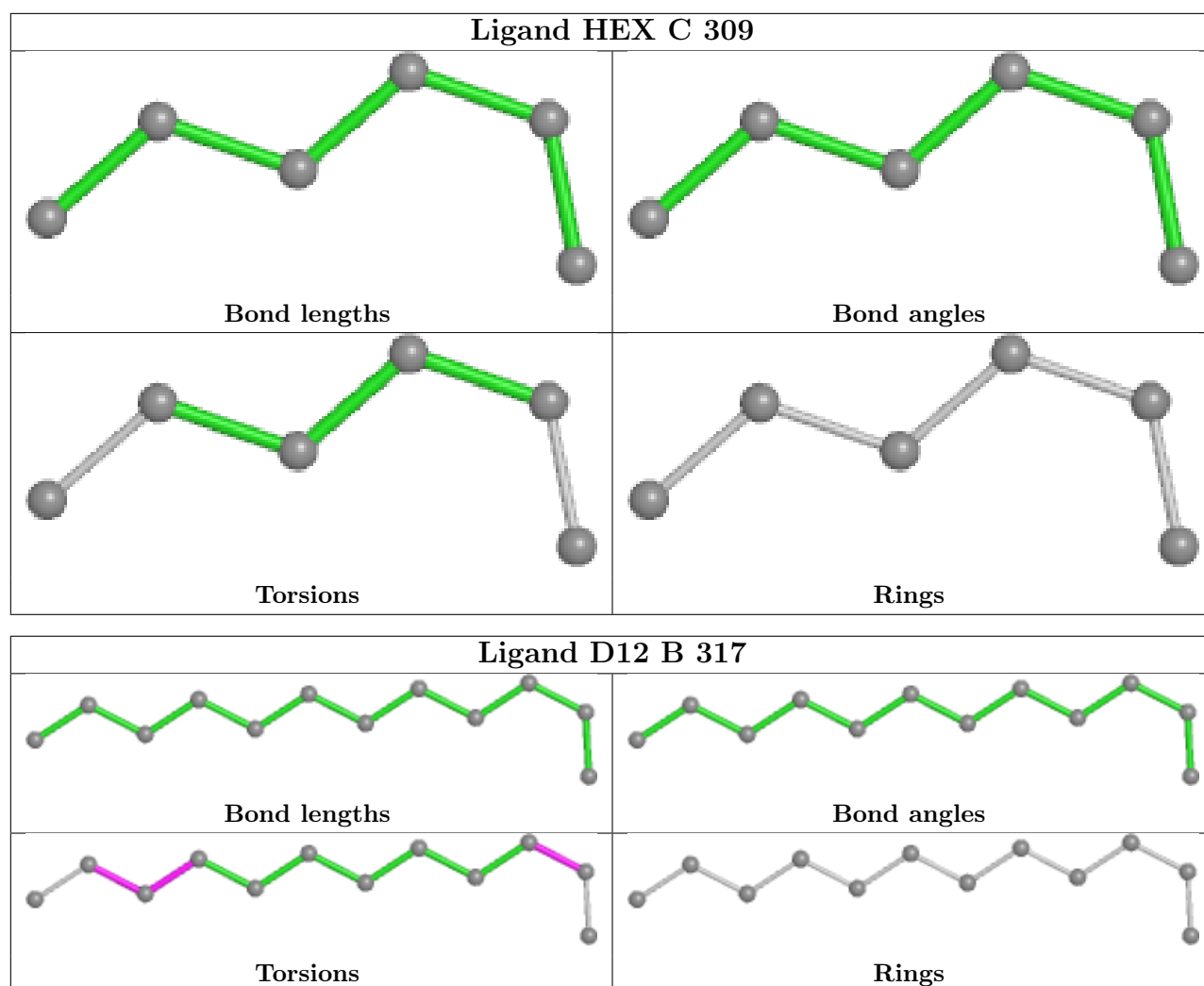












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/259 (87%)	-0.59	5 (2%) 62 64	19, 27, 55, 90	0
1	B	226/259 (87%)	-0.11	22 (9%) 7 9	21, 35, 74, 109	0
1	C	226/259 (87%)	-0.43	10 (4%) 34 37	19, 28, 59, 101	0
All	All	678/777 (87%)	-0.38	37 (5%) 25 28	19, 29, 65, 109	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	VAL	8.8
1	C	65	VAL	5.8
1	C	32	ARG	5.7
1	B	224	GLN	5.6
1	C	227	ASN	5.6
1	A	65	VAL	5.4
1	B	223	ALA	5.0
1	B	32	ARG	4.6
1	B	68	GLN	4.4
1	C	0	GLY	4.4
1	B	219	PRO	4.3
1	B	31	ARG	4.2
1	B	221	ILE	4.2
1	A	0	GLY	4.2
1	B	0	GLY	4.2
1	B	227	ASN	3.9
1	C	68	GLN	3.5
1	B	155	ASN	3.4
1	B	225	ALA	3.4
1	B	220	GLU	3.3
1	C	224	GLN	3.1
1	A	68	GLN	3.0
1	B	157	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	155	ASN	2.8
1	A	64	PRO	2.8
1	B	218	ALA	2.7
1	B	34	GLU	2.6
1	B	156	VAL	2.6
1	B	33	LYS	2.4
1	C	223	ALA	2.3
1	C	64	PRO	2.1
1	B	153	ARG	2.1
1	B	36	MET	2.1
1	B	1	MET	2.0
1	B	28	VAL	2.0
1	A	227	ASN	2.0
1	C	34	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	OCT	A	311	8/8	0.17	0.37	51,66,68,68	0
4	HEX	C	307	6/6	0.50	0.23	60,62,65,66	0
5	OCT	A	310	8/8	0.53	0.23	43,55,58,59	0
5	OCT	B	313	8/8	0.61	0.27	48,58,68,68	0
8	R16	C	321	16/16	0.65	0.16	42,54,57,59	0
4	HEX	B	306	6/6	0.65	0.18	60,64,64,70	0
5	OCT	A	309	8/8	0.69	0.13	55,59,63,64	0
5	OCT	B	312	8/8	0.70	0.13	49,56,59,62	0
7	D12	B	317	12/12	0.70	0.19	49,52,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	C14	C	324	14/14	0.71	0.20	48,53,60,61	0
5	OCT	C	317	8/8	0.72	0.14	55,61,64,70	0
4	HEX	C	310	6/6	0.73	0.26	51,56,63,63	0
6	D10	B	315	10/10	0.73	0.14	52,65,68,69	0
8	R16	A	320	16/16	0.74	0.17	47,55,64,64	0
4	HEX	A	306	6/6	0.74	0.12	49,52,54,56	0
4	HEX	B	304	6/6	0.74	0.16	67,67,68,68	0
5	OCT	B	311	8/8	0.75	0.18	51,66,67,69	0
8	R16	C	319	16/16	0.76	0.17	46,58,61,62	0
4	HEX	C	305	6/6	0.76	0.23	55,56,61,62	0
4	HEX	B	307	6/6	0.77	0.18	57,59,65,68	0
8	R16	A	322	16/16	0.77	0.27	54,61,68,68	0
8	R16	A	321	16/16	0.77	0.16	40,50,56,56	0
8	R16	A	324	16/16	0.78	0.19	37,54,62,63	0
5	OCT	A	308	8/8	0.78	0.19	51,53,57,58	0
6	D10	A	317	10/10	0.78	0.16	52,60,72,72	0
4	HEX	C	312	6/6	0.78	0.13	51,53,54,55	0
4	HEX	B	305	6/6	0.79	0.13	32,54,60,64	0
9	C14	A	325	14/14	0.79	0.18	44,51,58,59	0
8	R16	B	319	16/16	0.80	0.24	51,61,69,71	0
7	D12	A	319	12/12	0.80	0.19	48,55,61,63	0
7	D12	B	318	12/12	0.80	0.11	41,55,62,63	0
4	HEX	C	309	6/6	0.81	0.18	49,52,58,62	0
5	OCT	A	314	8/8	0.81	0.26	33,42,49,49	0
7	D12	A	318	12/12	0.82	0.13	38,50,56,57	0
5	OCT	C	314	8/8	0.82	0.20	49,53,55,57	0
4	HEX	C	308	6/6	0.82	0.21	55,60,64,65	0
8	R16	A	323	16/16	0.82	0.17	47,55,69,70	0
4	HEX	B	303	6/6	0.83	0.16	50,53,53,55	0
5	OCT	A	312	8/8	0.84	0.12	45,51,56,59	0
4	HEX	A	303	6/6	0.85	0.11	42,49,50,54	0
4	HEX	C	303	6/6	0.85	0.16	46,47,50,56	0
5	OCT	C	315	8/8	0.85	0.11	49,58,65,65	0
5	OCT	C	316	8/8	0.86	0.30	36,41,50,52	0
5	OCT	C	313	8/8	0.86	0.18	33,41,51,54	0
6	D10	B	314	10/10	0.86	0.28	34,46,60,62	0
7	D12	C	318	12/12	0.86	0.11	39,46,57,60	0
4	HEX	C	311	6/6	0.87	0.15	48,50,53,53	0
4	HEX	A	307	6/6	0.87	0.16	58,58,61,61	0
7	D12	B	316	12/12	0.88	0.15	47,55,59,63	0
8	R16	C	320	16/16	0.88	0.28	49,56,63,64	0
6	D10	A	316	10/10	0.88	0.16	53,56,66,66	0

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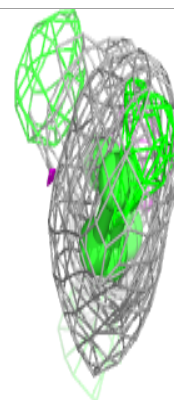
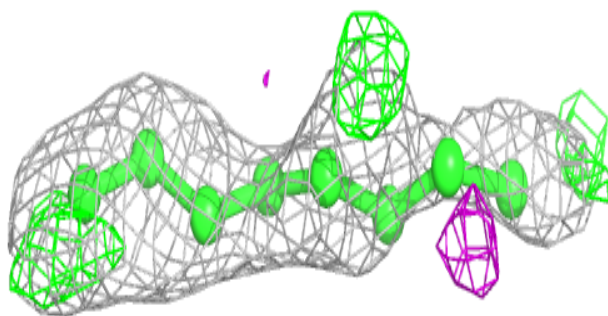
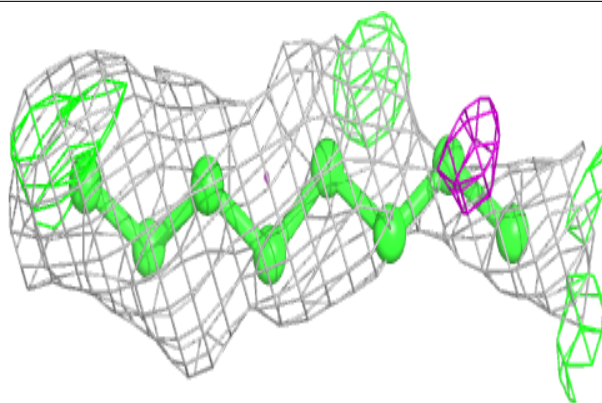
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	OCT	B	308	8/8	0.89	0.11	50,53,58,60	0
9	C14	B	320	14/14	0.89	0.11	47,53,62,65	0
5	OCT	B	309	8/8	0.89	0.12	48,52,59,60	0
4	HEX	C	304	6/6	0.90	0.34	44,47,56,57	0
5	OCT	B	310	8/8	0.90	0.13	55,58,62,63	0
3	MG	B	302	1/1	0.91	0.17	52,52,52,52	0
3	MG	C	302	1/1	0.91	0.28	47,47,47,47	0
5	OCT	A	313	8/8	0.92	0.16	35,46,57,59	0
4	HEX	C	306	6/6	0.92	0.29	45,49,56,57	0
5	OCT	A	315	8/8	0.92	0.19	45,50,57,61	0
10	NO3	C	323	4/4	0.93	0.24	50,53,57,60	0
4	HEX	A	304	6/6	0.93	0.12	41,47,56,60	0
4	HEX	A	305	6/6	0.93	0.23	37,42,55,64	0
3	MG	A	302	1/1	0.94	0.18	46,46,46,46	0
2	RET	C	301	20/21	0.95	0.09	16,19,23,24	0
10	NO3	C	322	4/4	0.96	0.22	58,58,59,60	0
2	RET	A	301	20/21	0.96	0.07	18,20,23,25	0
2	RET	B	301	20/21	0.97	0.06	19,21,25,26	0

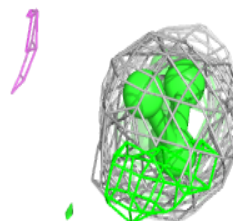
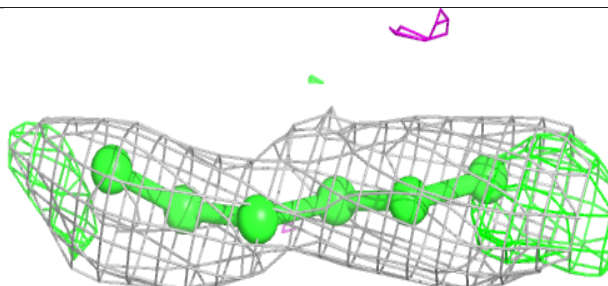
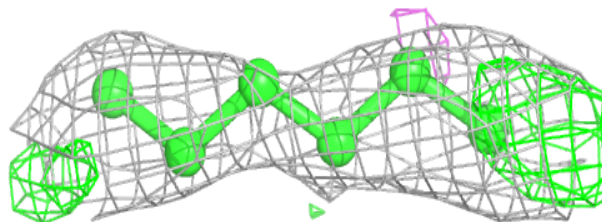
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OCT A 311:

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

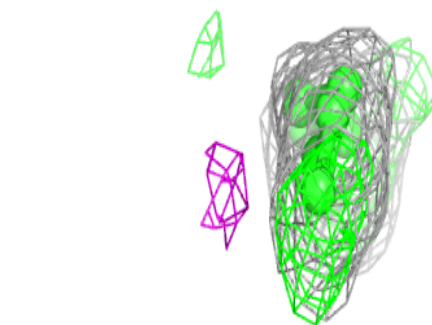
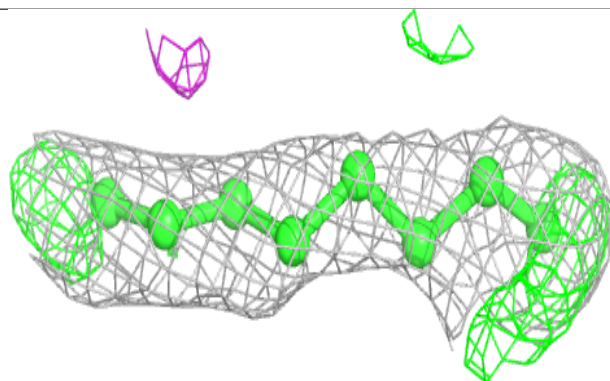
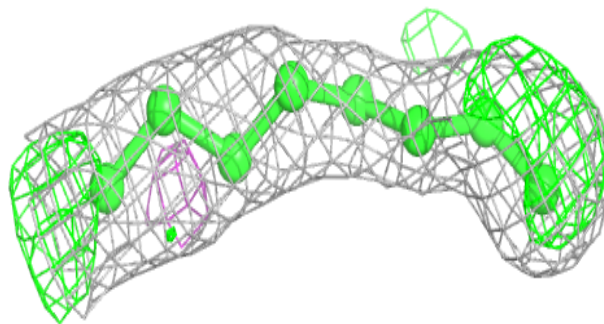
**Electron density around HEX C 307:**

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

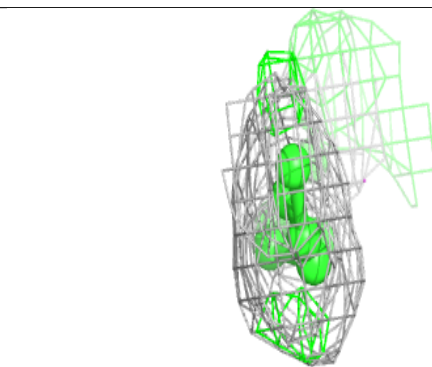
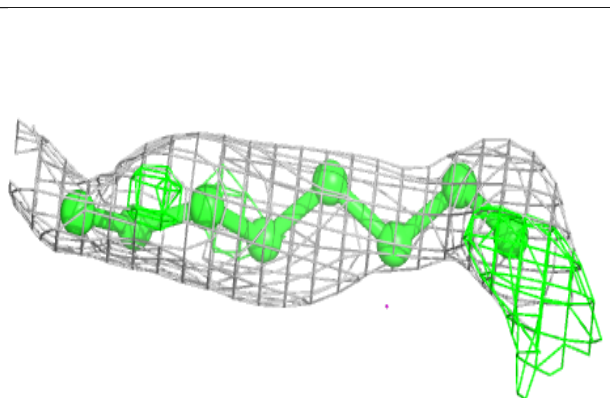
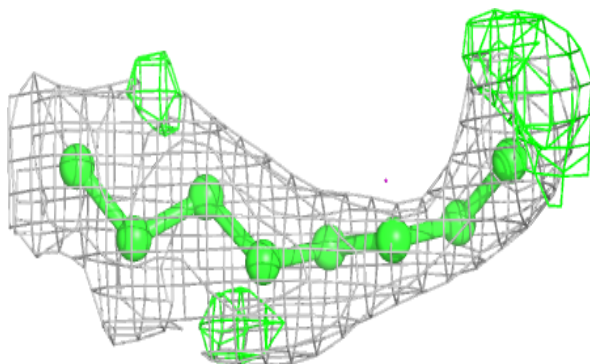


Electron density around OCT A 310:

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

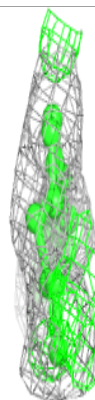
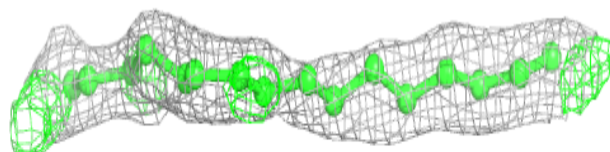
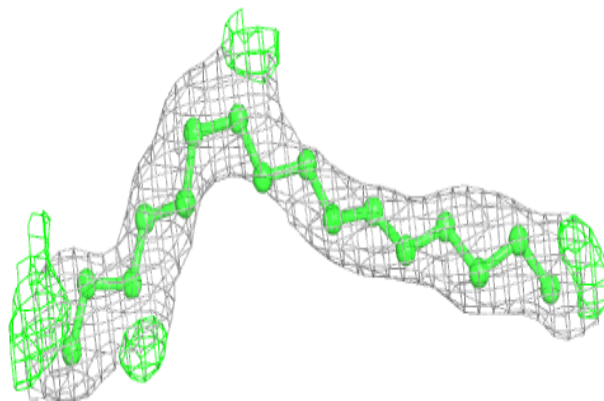
**Electron density around OCT B 313:**

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

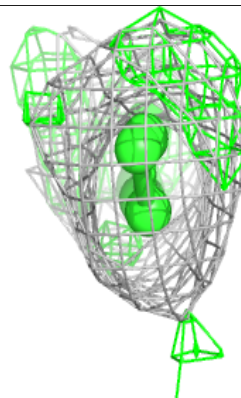
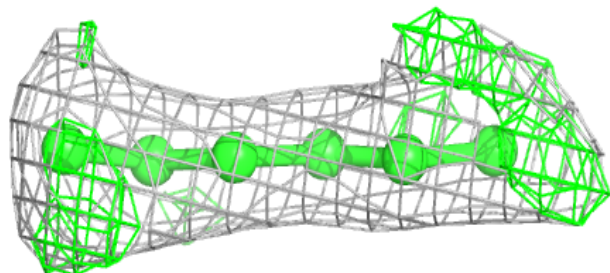
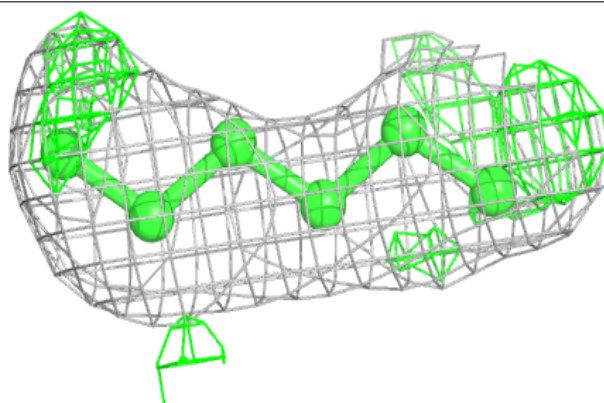


Electron density around R16 C 321:

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

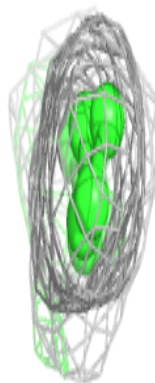
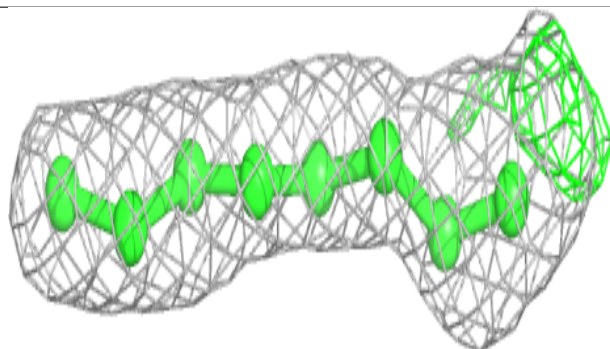
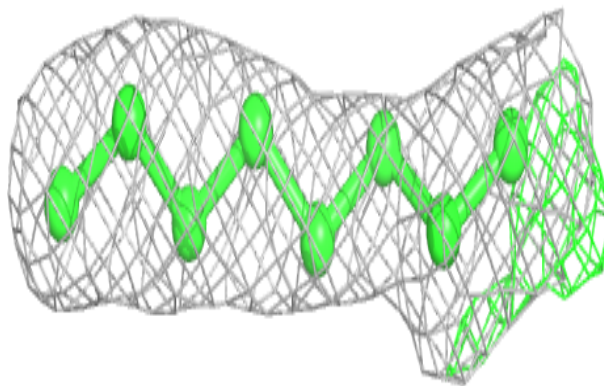
**Electron density around HEX B 306:**

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

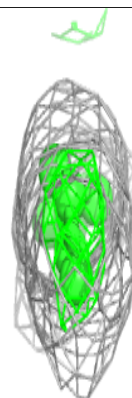
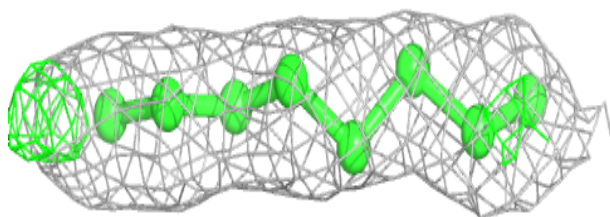
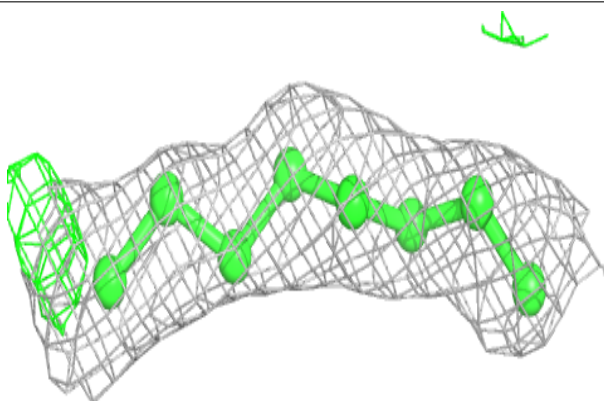


Electron density around OCT A 309:

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

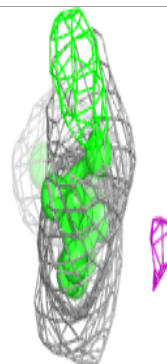
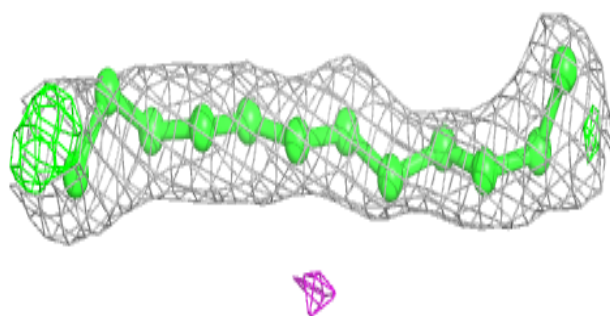
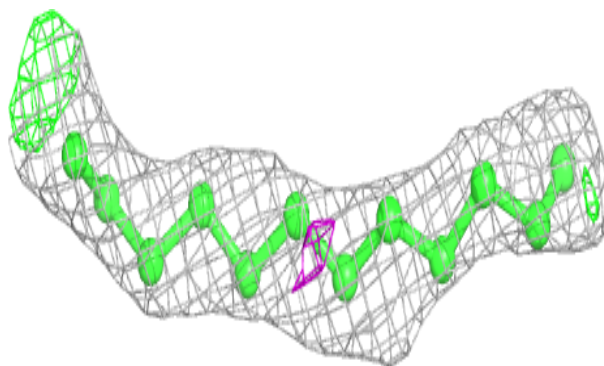
**Electron density around OCT B 312:**

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

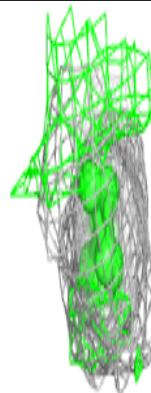
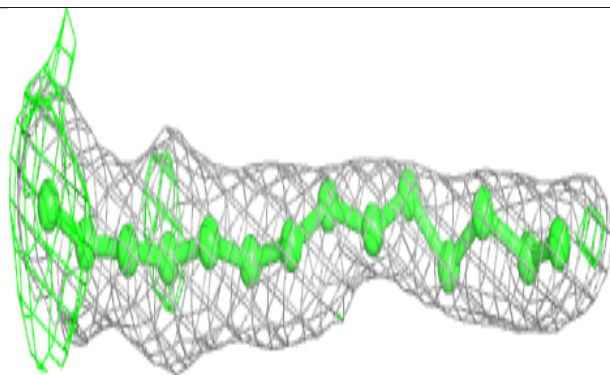
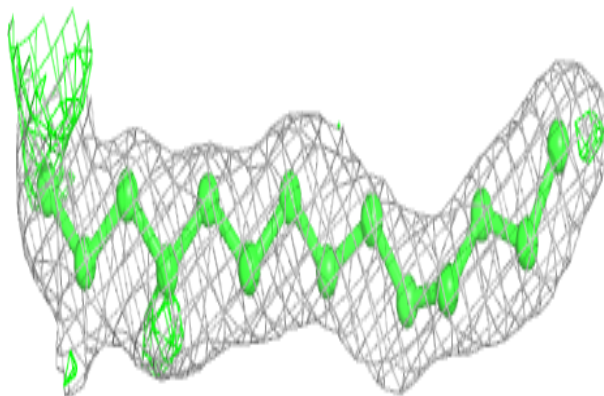


Electron density around D12 B 317:

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

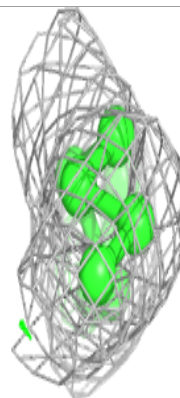
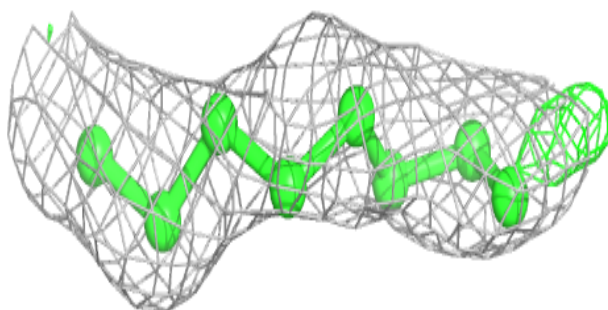
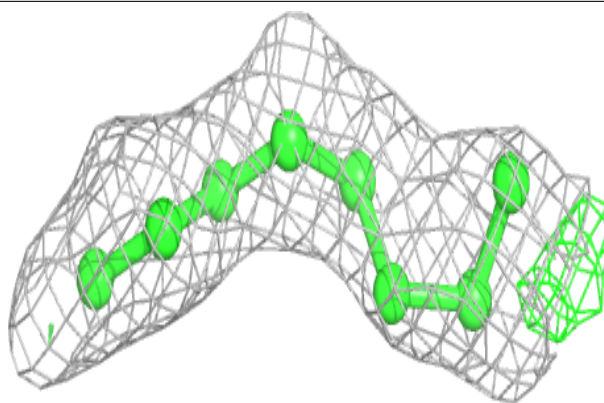
**Electron density around C14 C 324:**

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

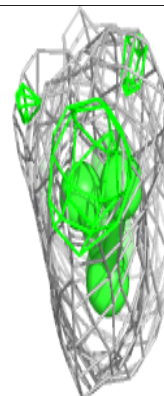
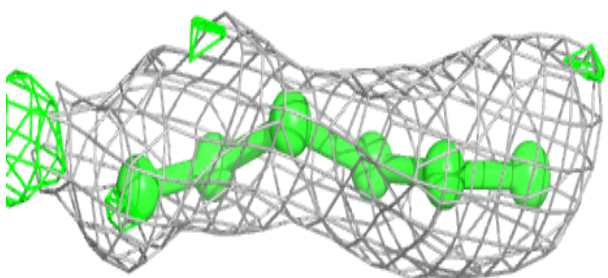
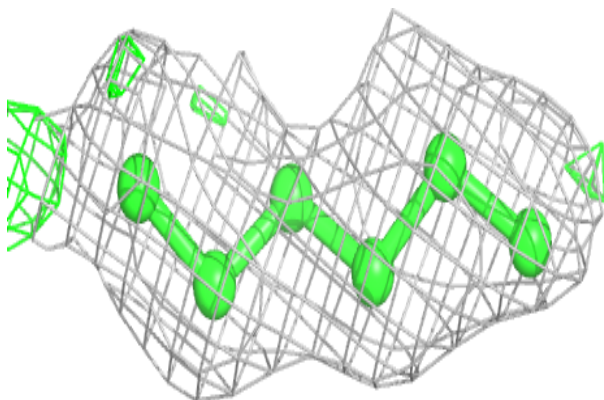


Electron density around OCT C 317:

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

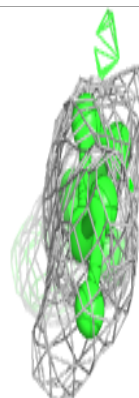
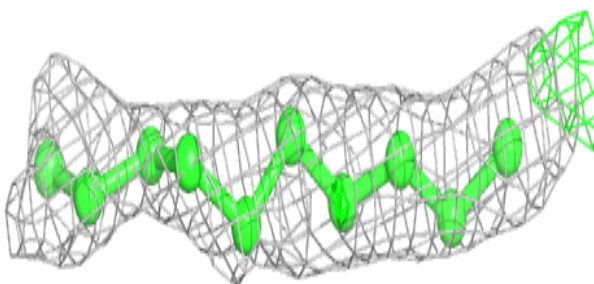
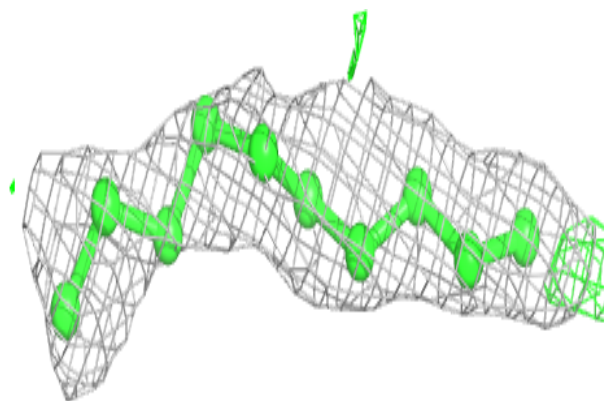
**Electron density around HEX C 310:**

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

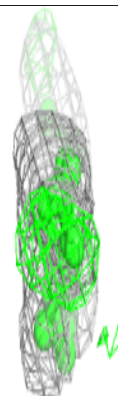
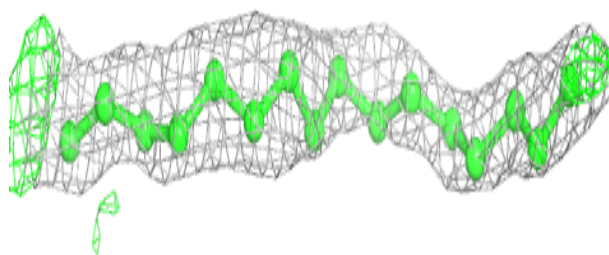
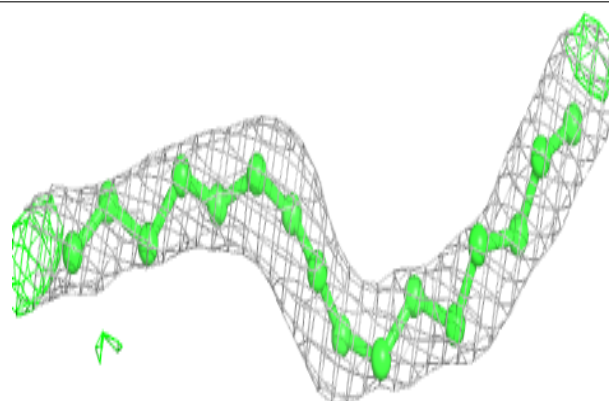


Electron density around D10 B 315:

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

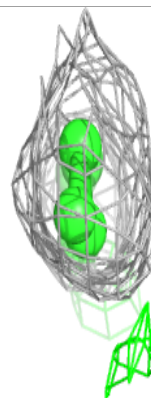
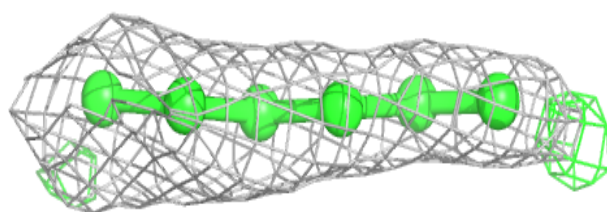
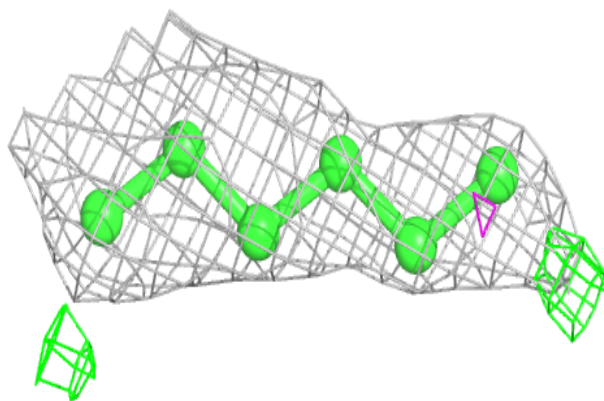
**Electron density around R16 A 320:**

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

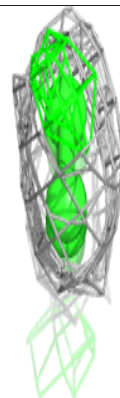
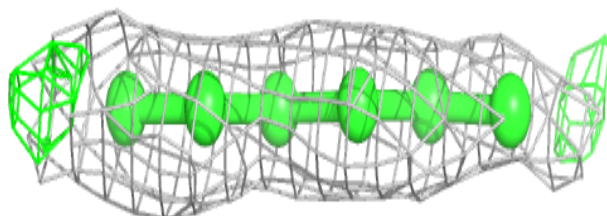
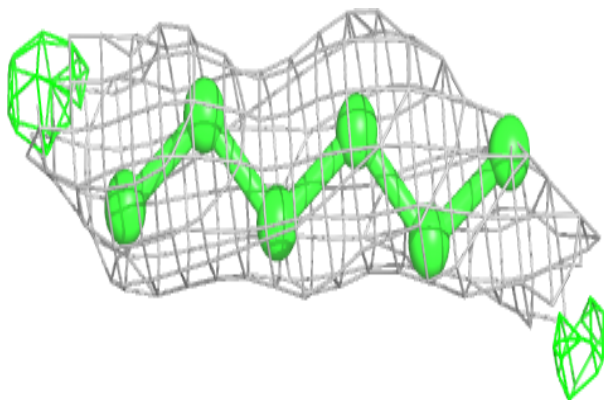


Electron density around HEX A 306:

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

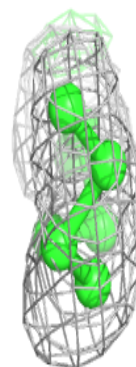
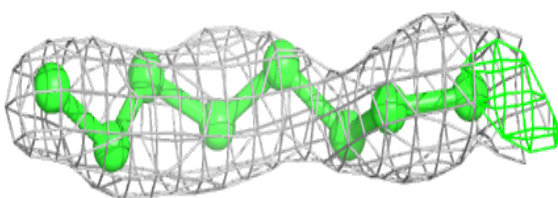
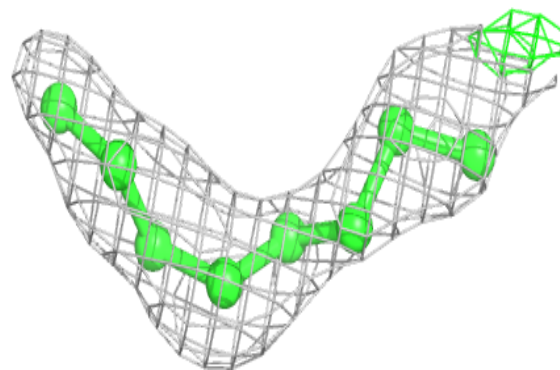
**Electron density around HEX B 304:**

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

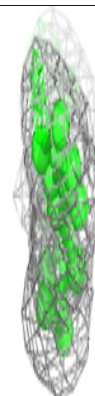
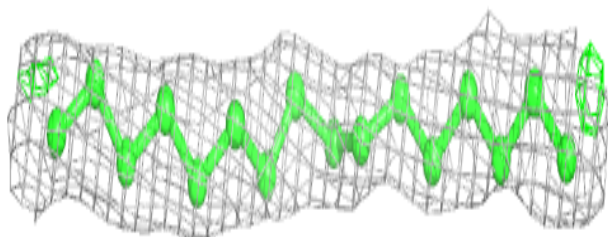
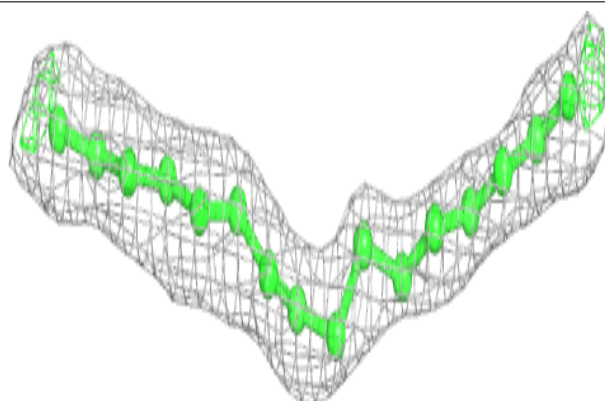


Electron density around OCT B 311:

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

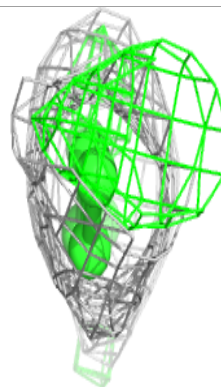
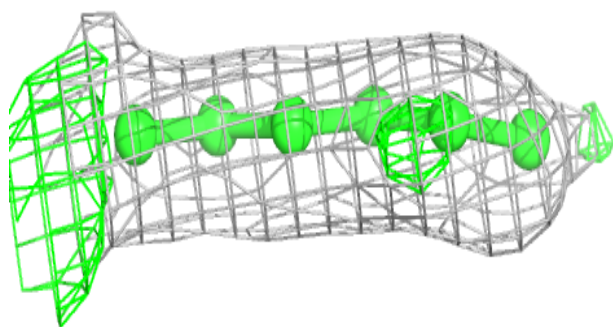
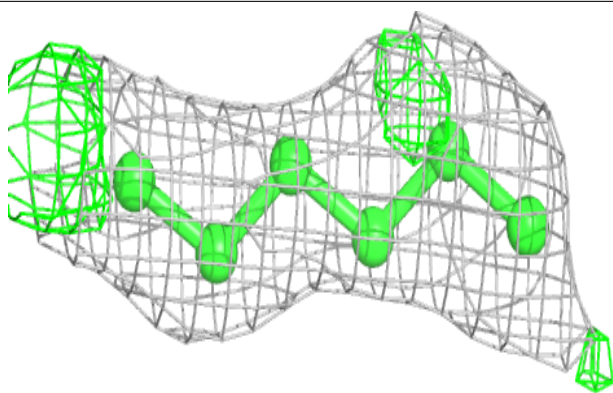
**Electron density around R16 C 319:**

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

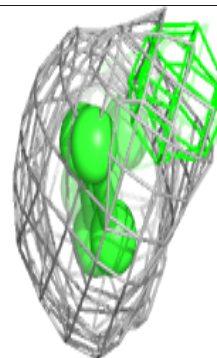
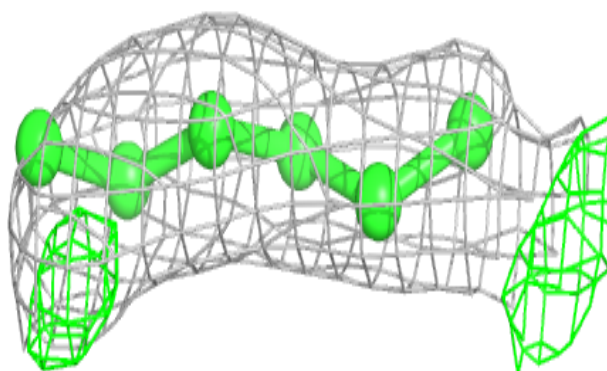
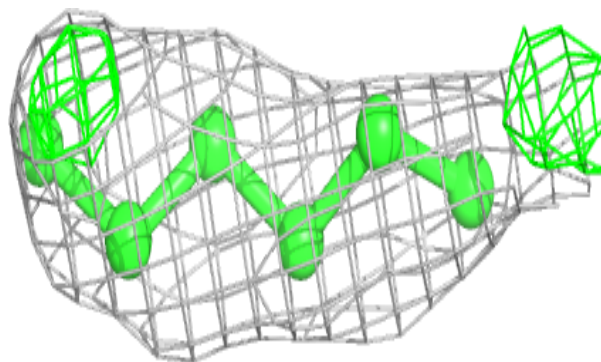


Electron density around HEX C 305:

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

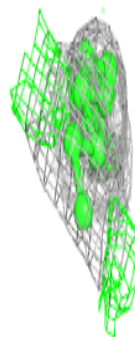
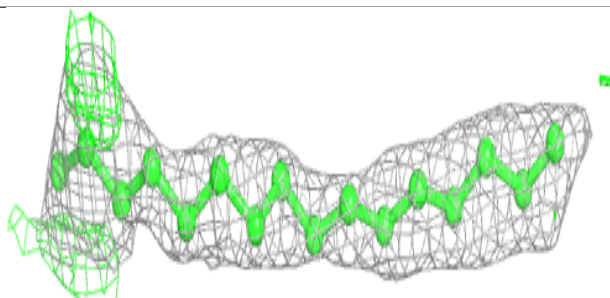
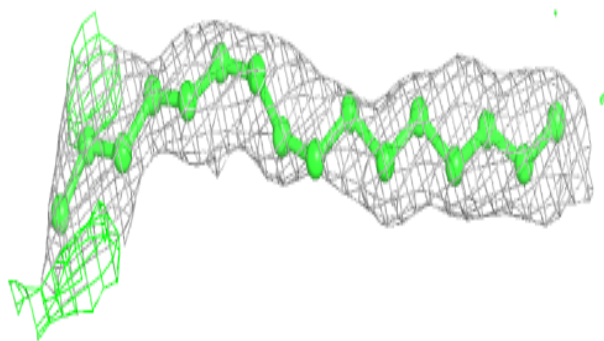
**Electron density around HEX B 307:**

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

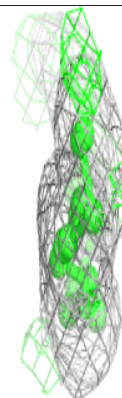
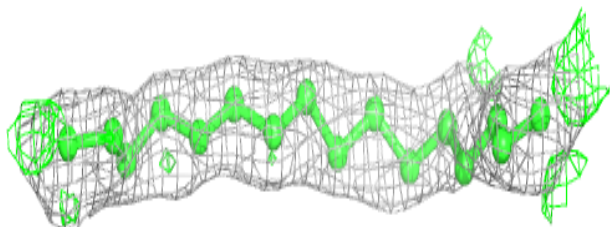
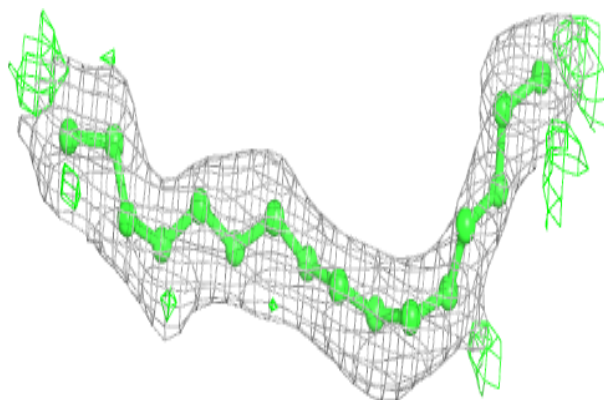


Electron density around R16 A 322:

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

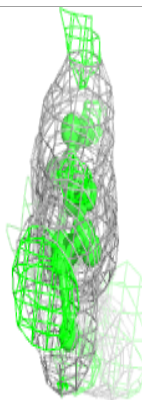
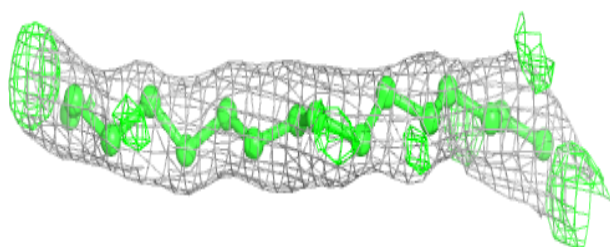
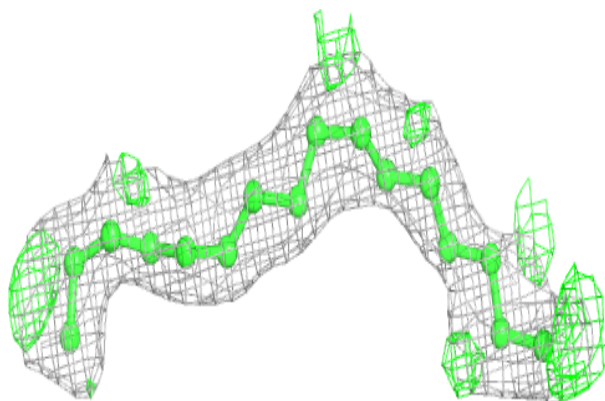
**Electron density around R16 A 321:**

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

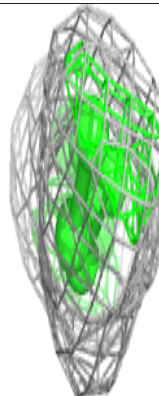
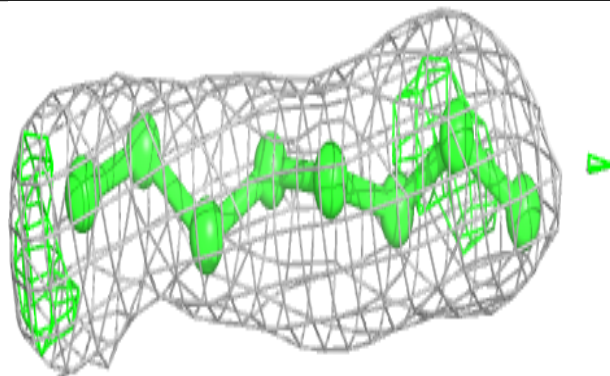
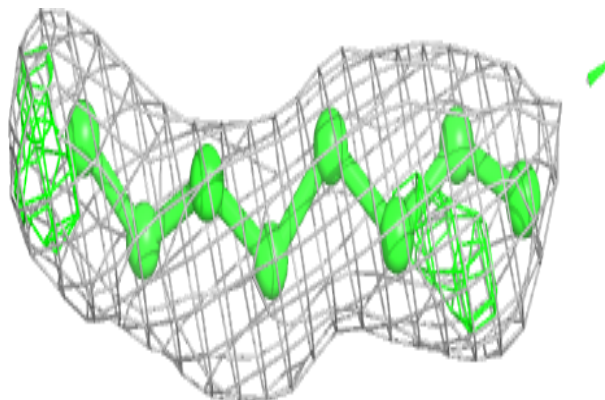


Electron density around R16 A 324:

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

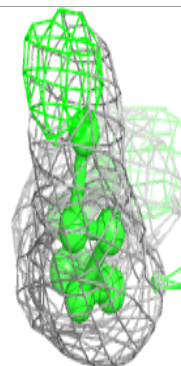
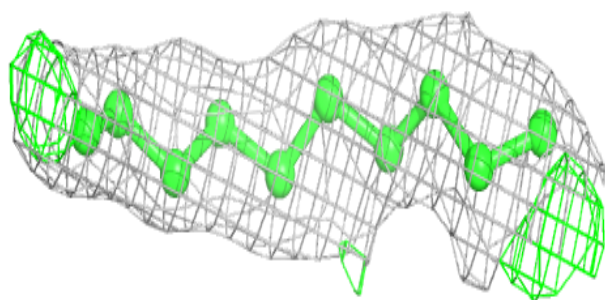
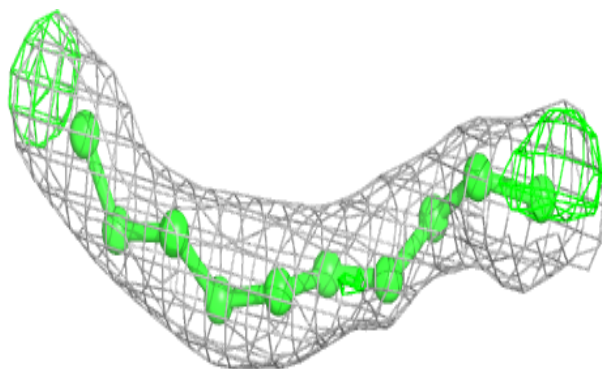
**Electron density around OCT A 308:**

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

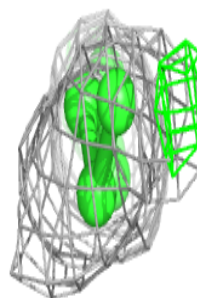
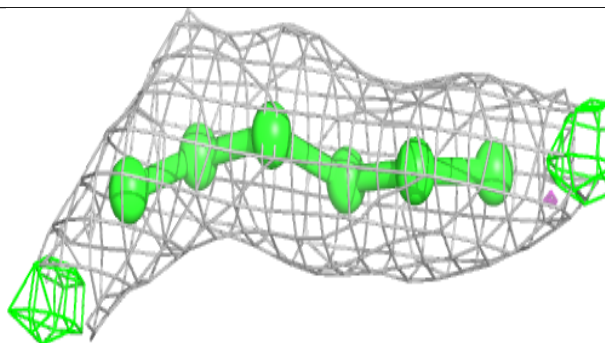
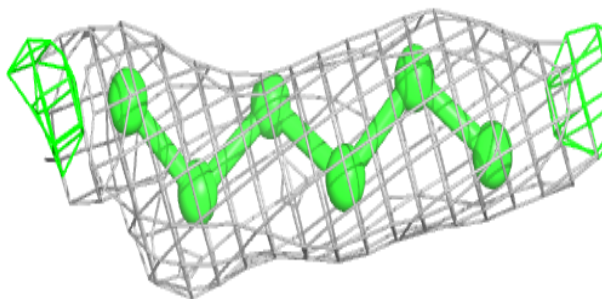


Electron density around D10 A 317:

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

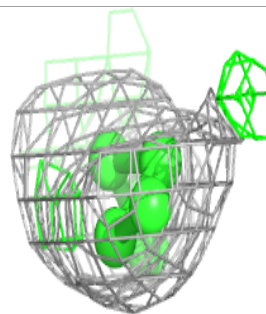
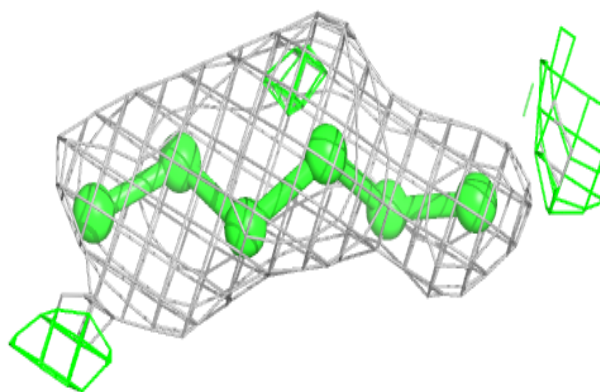
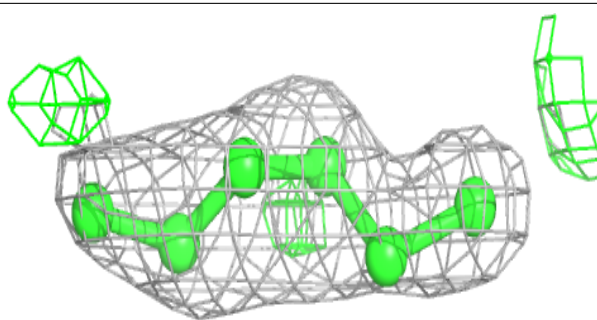
**Electron density around HEX C 312:**

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

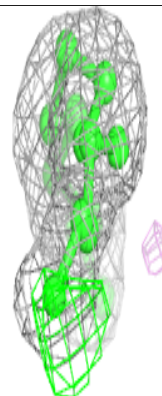
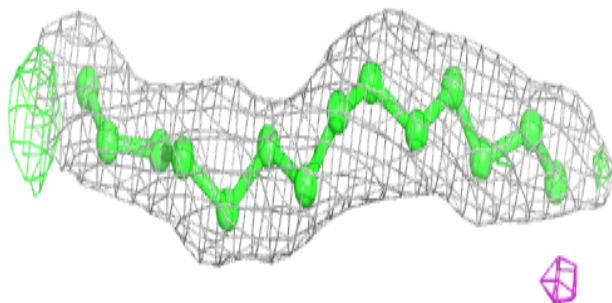
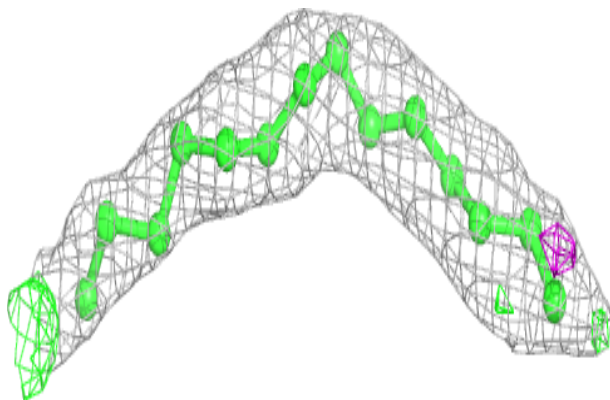


Electron density around HEX B 305:

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

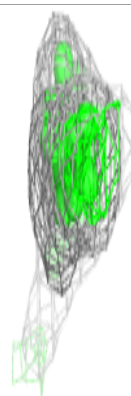
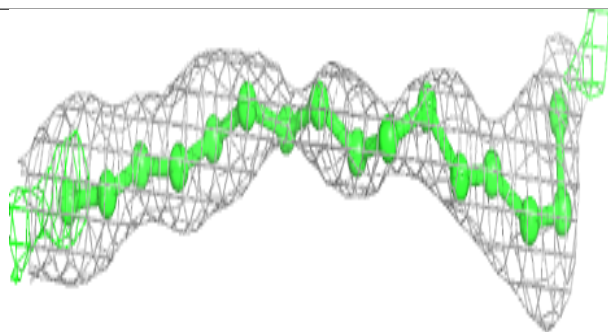
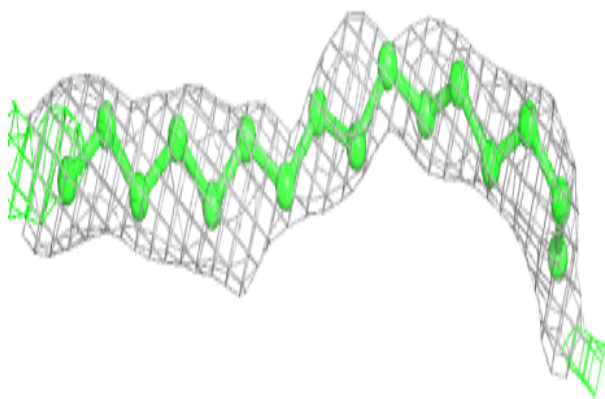
**Electron density around C14 A 325:**

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

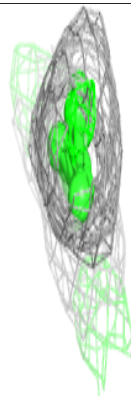
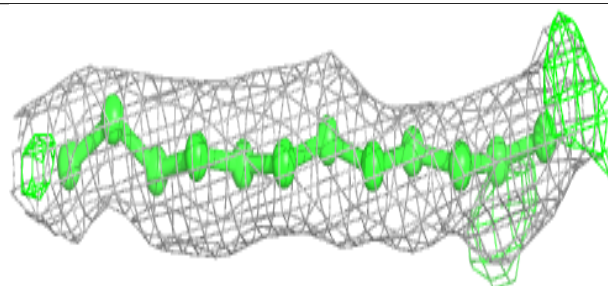
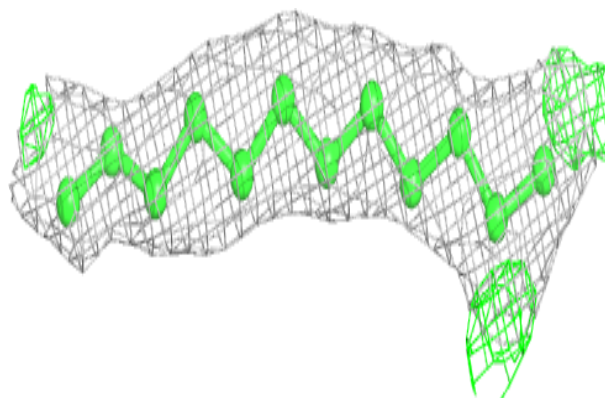


Electron density around R16 B 319:

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

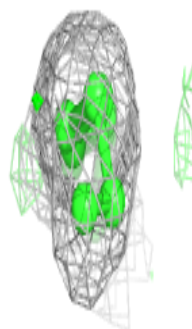
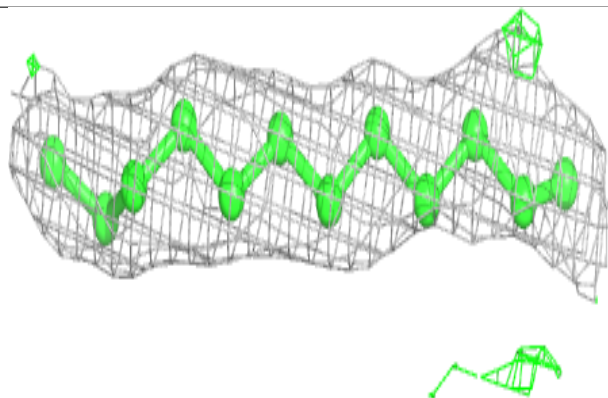
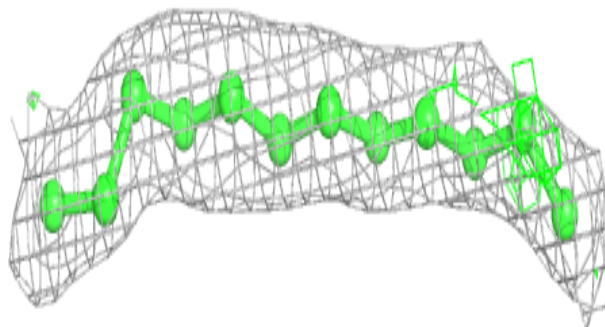
**Electron density around D12 A 319:**

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

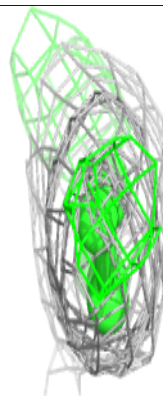
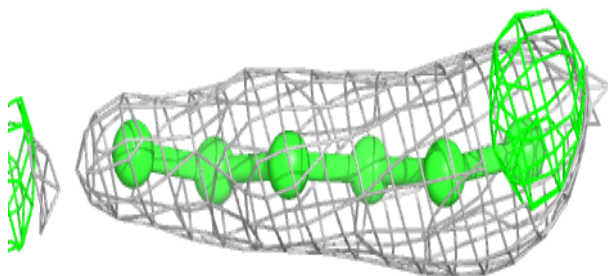
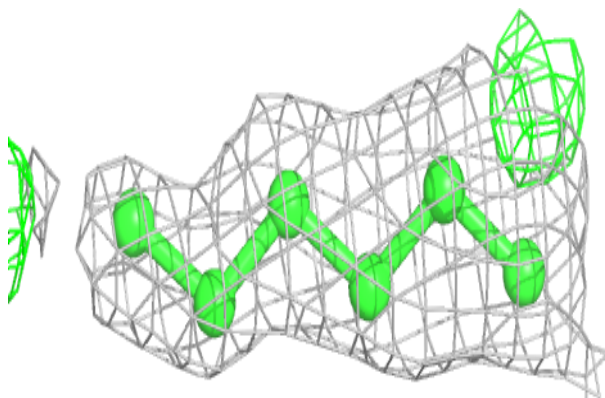


Electron density around D12 B 318:

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

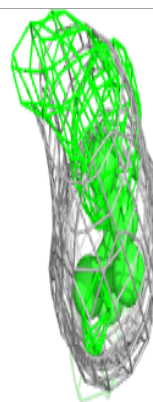
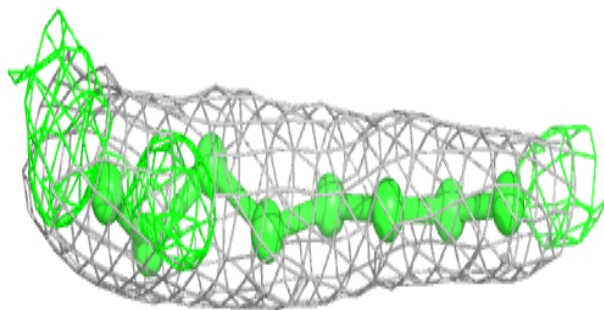
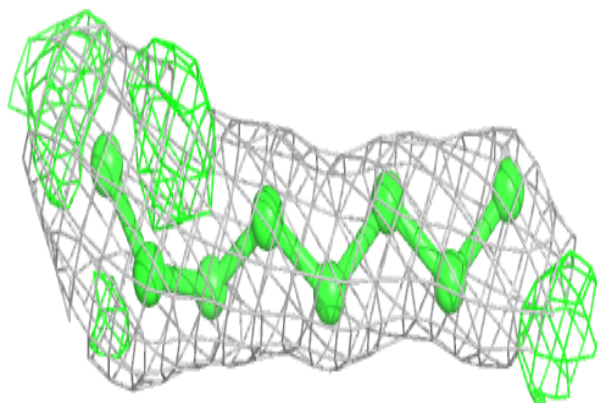
**Electron density around HEX C 309:**

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

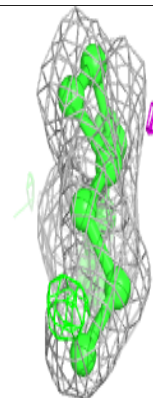
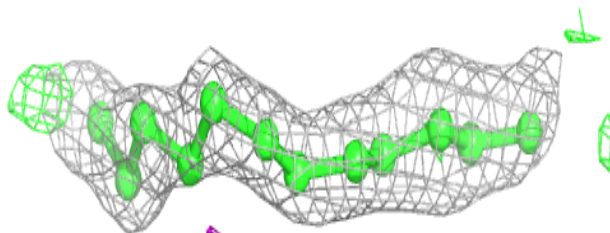
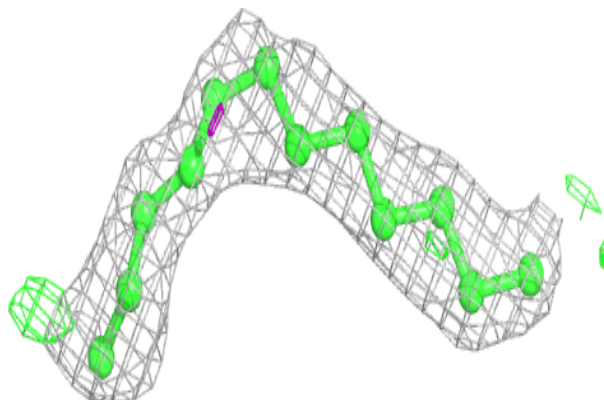


Electron density around OCT A 314:

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

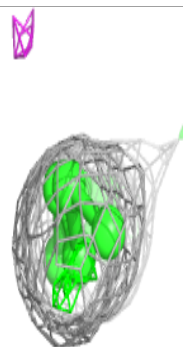
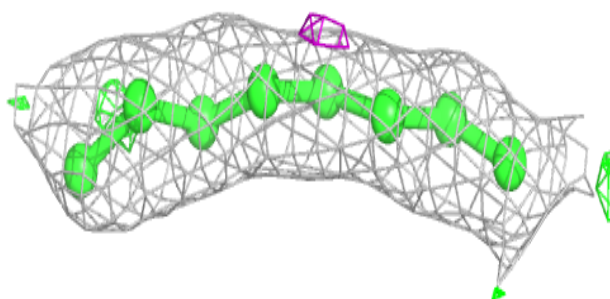
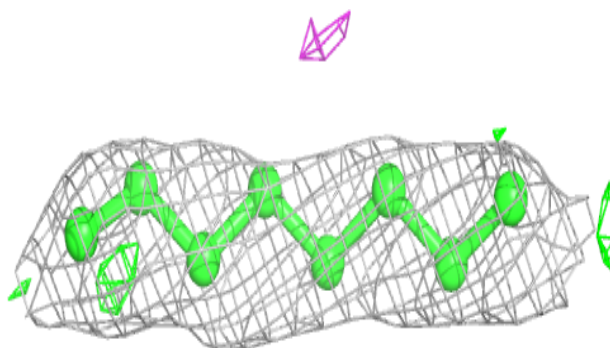
**Electron density around D12 A 318:**

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

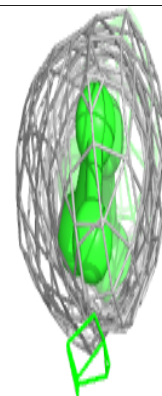
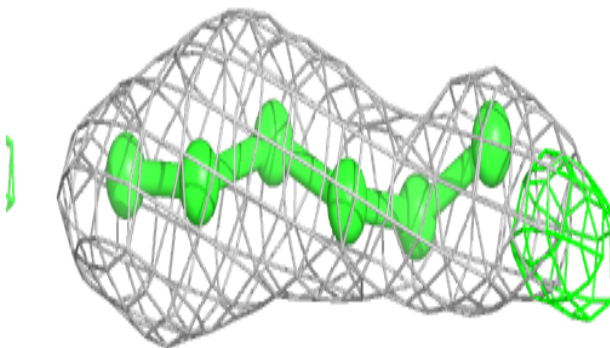
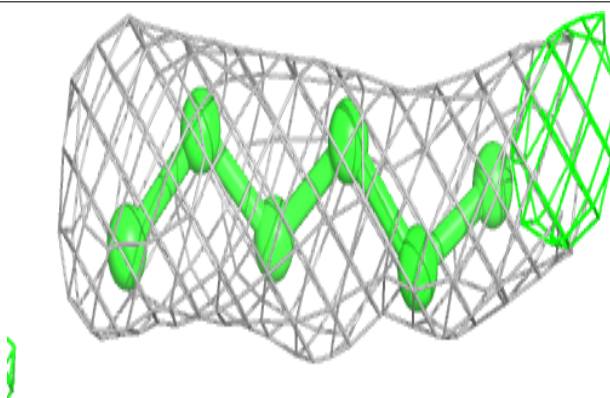


Electron density around OCT C 314:

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

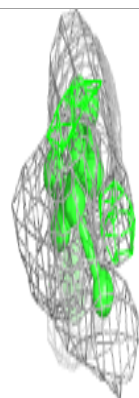
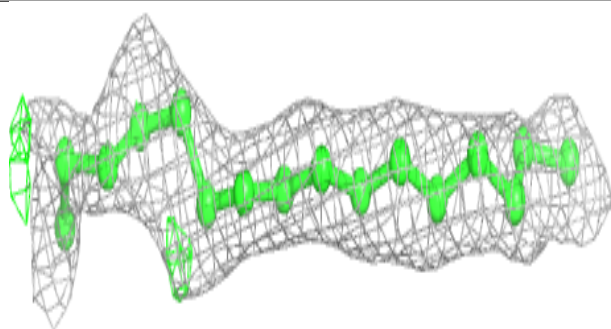
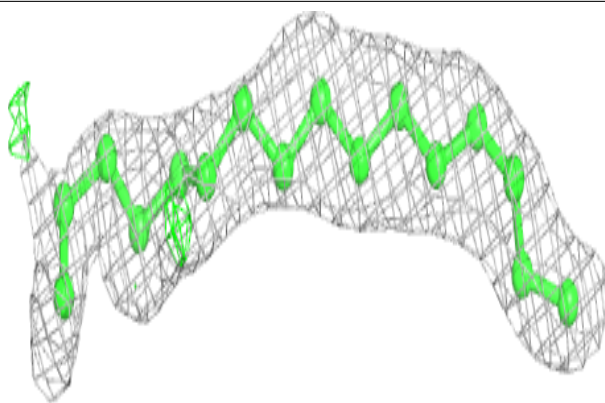
**Electron density around HEX C 308:**

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

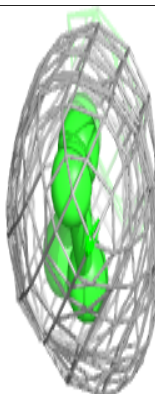
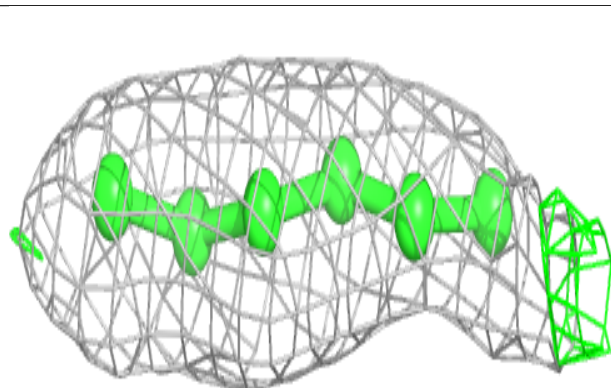
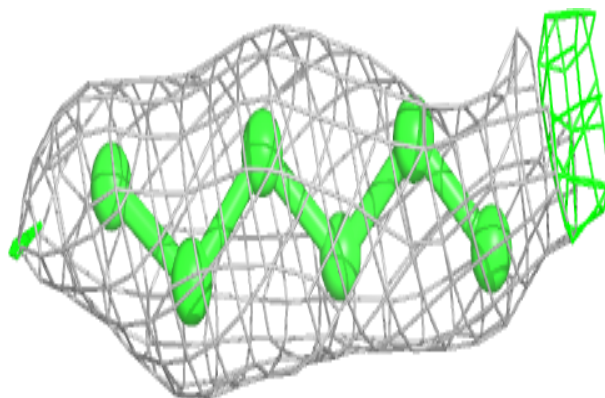


Electron density around R16 A 323:

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

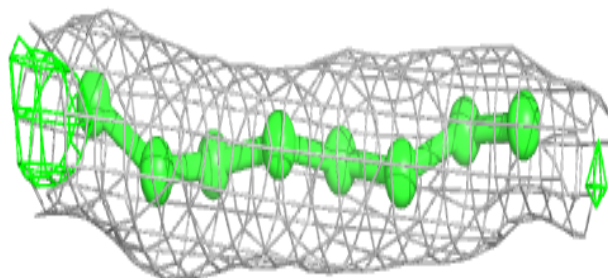
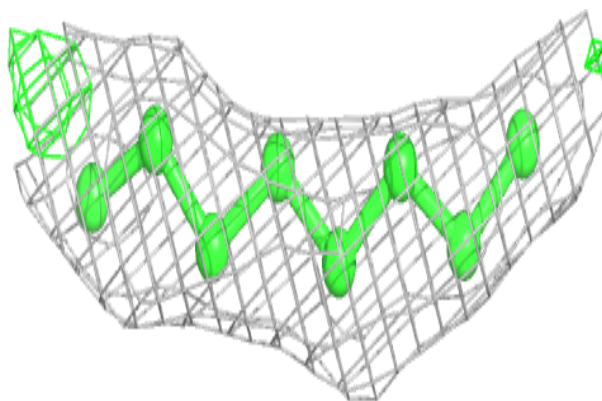
**Electron density around HEX B 303:**

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

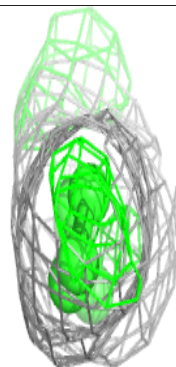
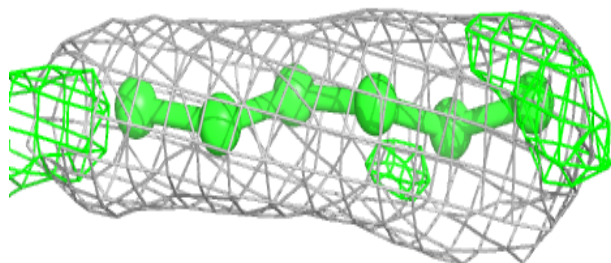
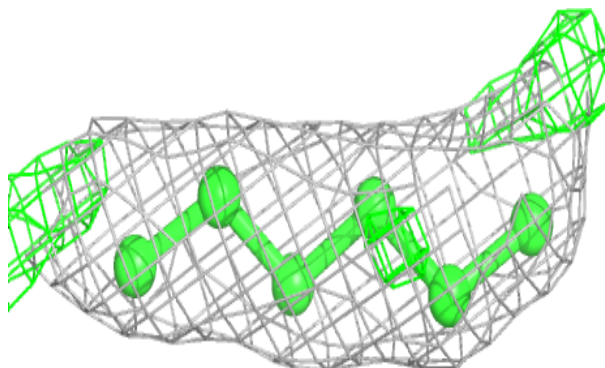


Electron density around OCT A 312:

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

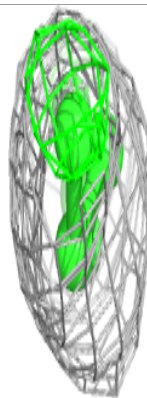
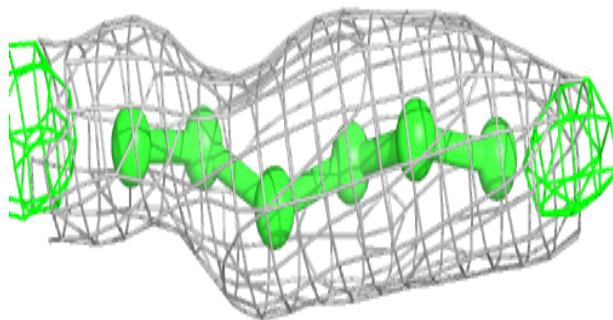
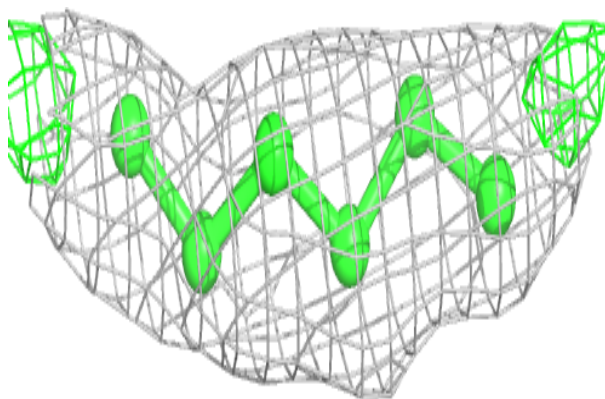
**Electron density around HEX A 303:**

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

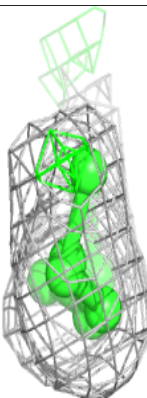
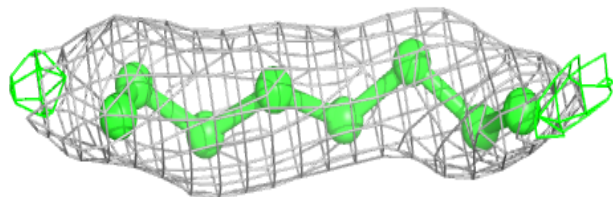
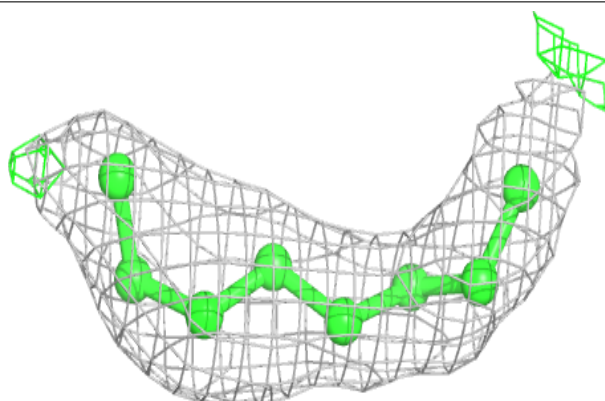


Electron density around HEX C 303:

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

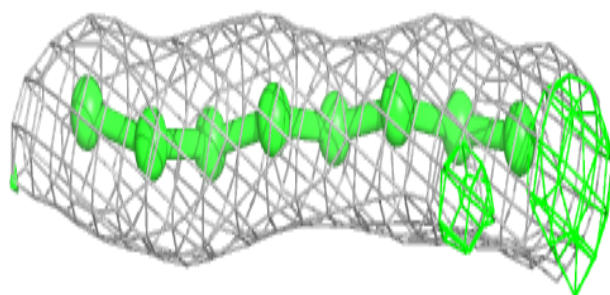
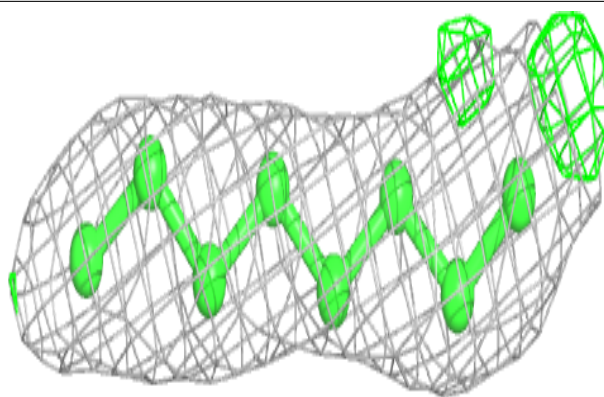
**Electron density around OCT C 315:**

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

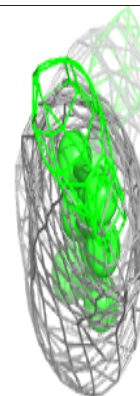
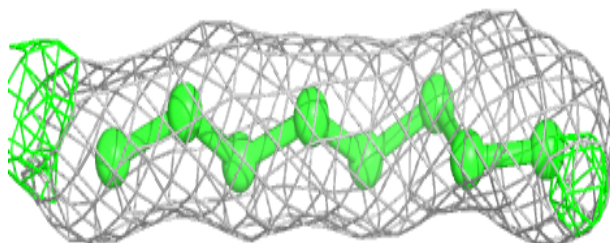
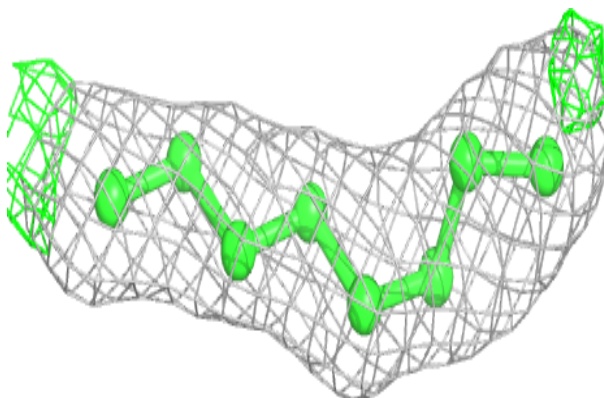


Electron density around OCT C 316:

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

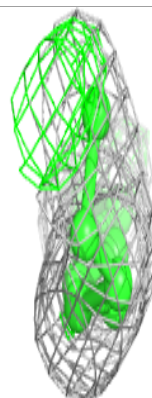
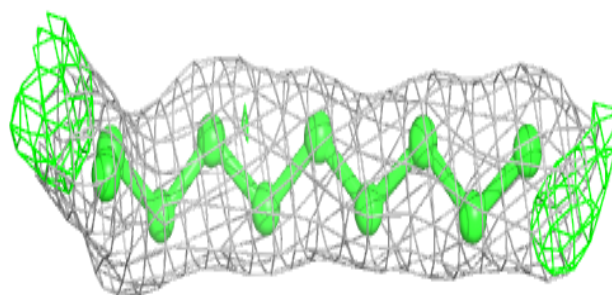
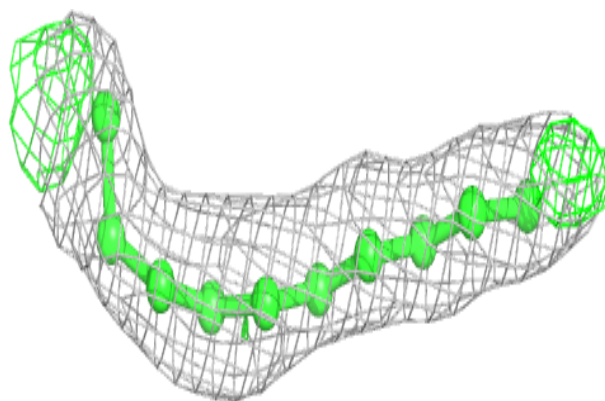
**Electron density around OCT C 313:**

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

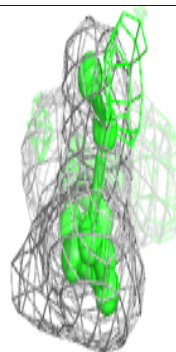
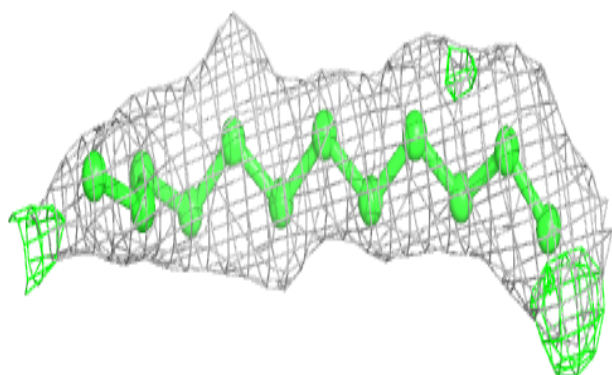
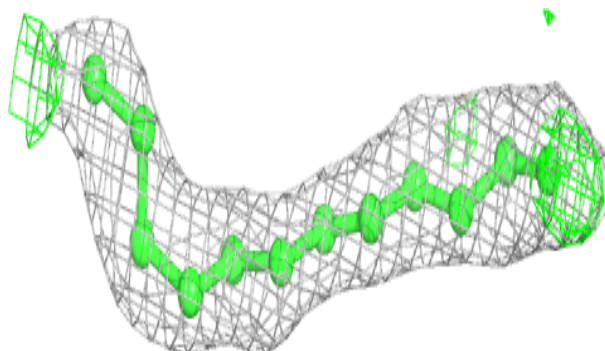


Electron density around D10 B 314:

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

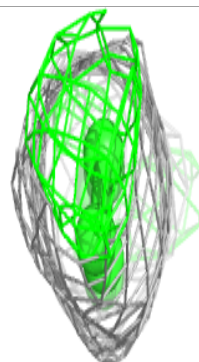
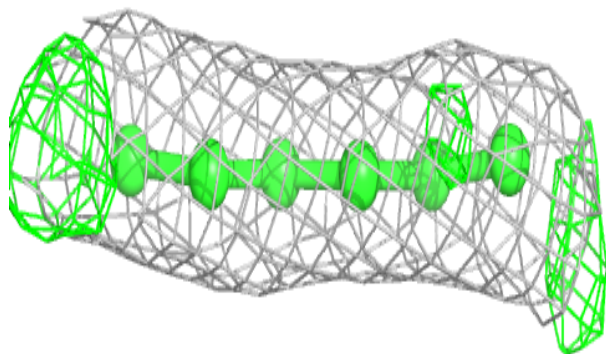
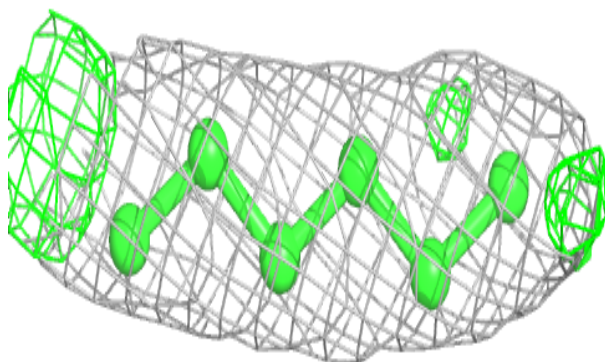
**Electron density around D12 C 318:**

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

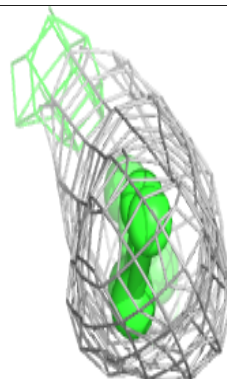
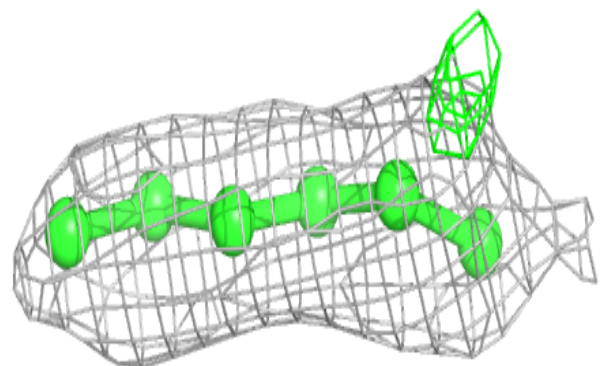
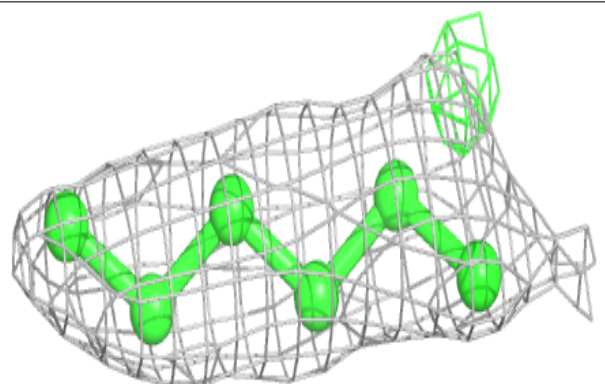


Electron density around HEX C 311:

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

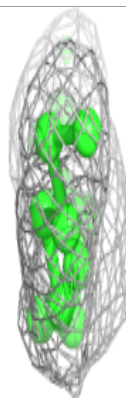
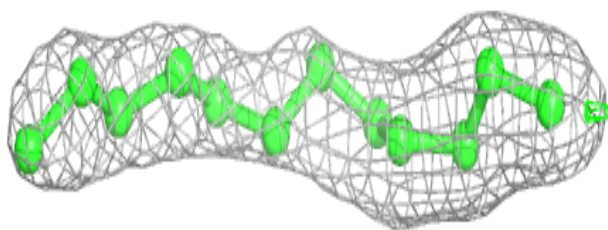
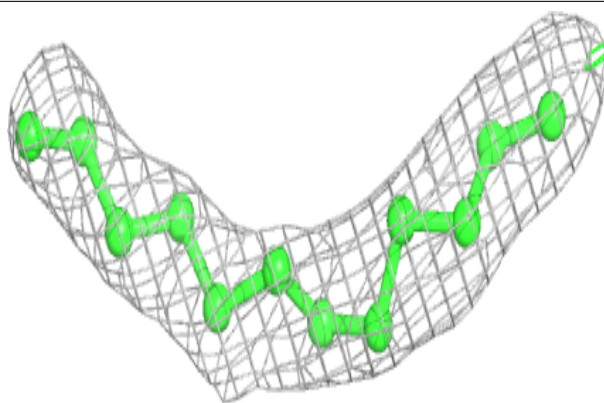
**Electron density around HEX A 307:**

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

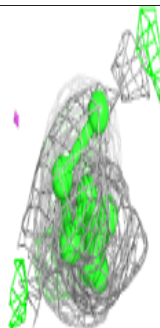
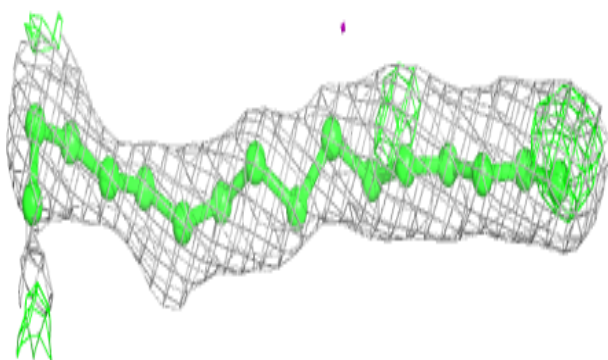
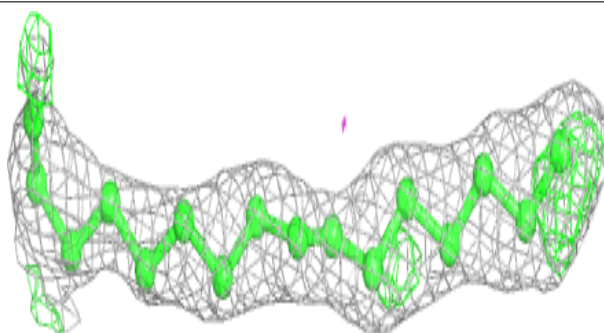


Electron density around D12 B 316:

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

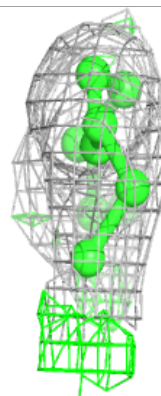
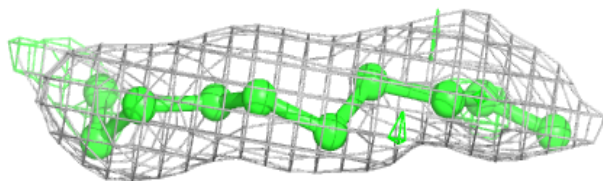
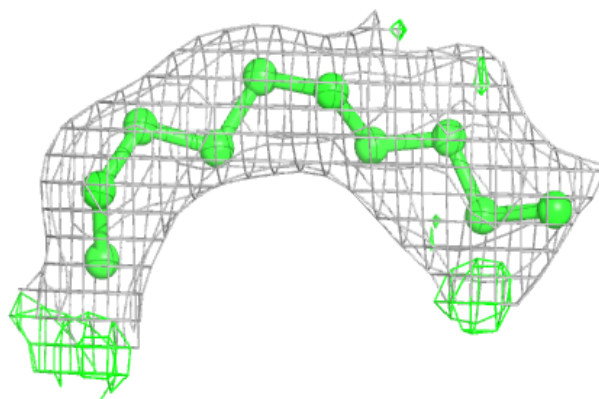
**Electron density around R16 C 320:**

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

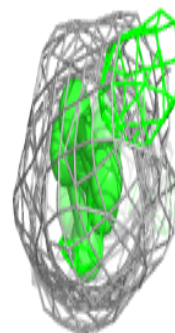
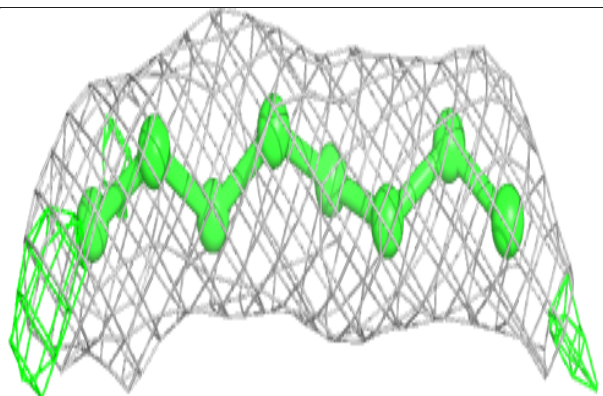
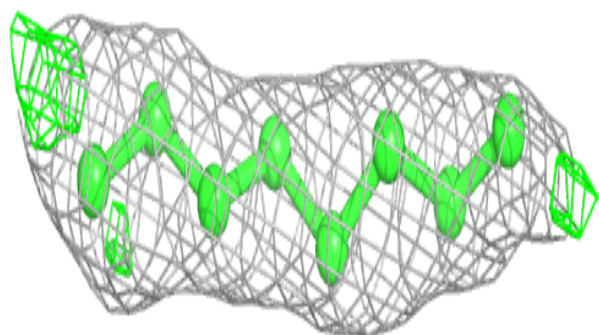


Electron density around D10 A 316:

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

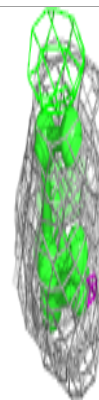
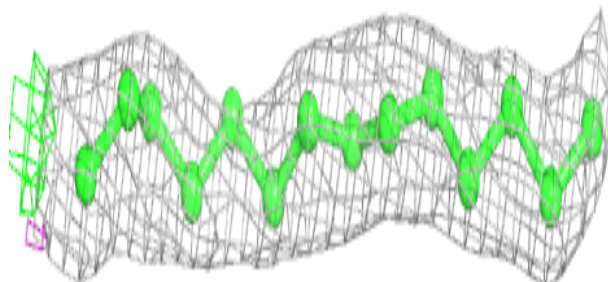
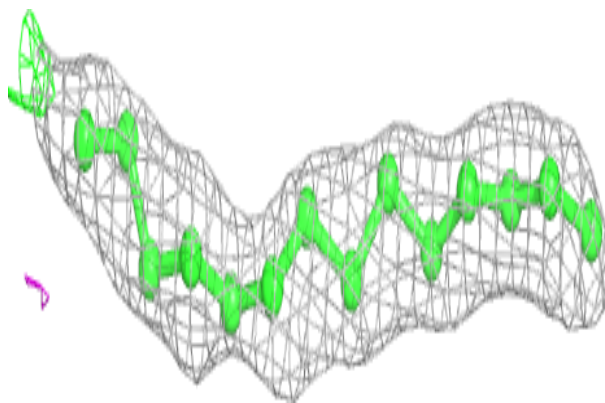
**Electron density around OCT B 308:**

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

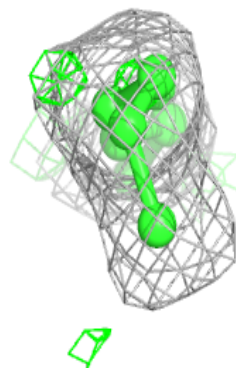
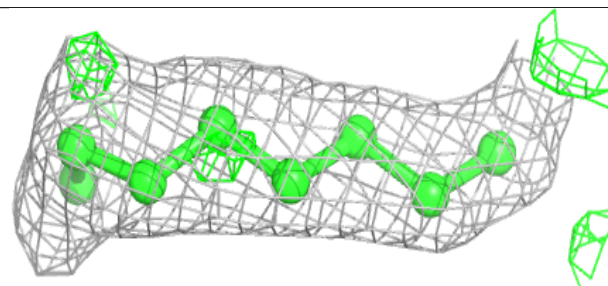
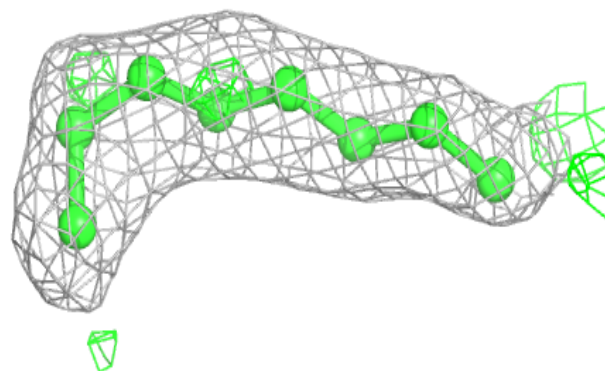


Electron density around C14 B 320:

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

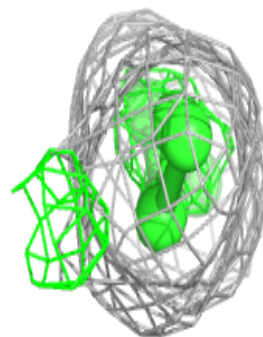
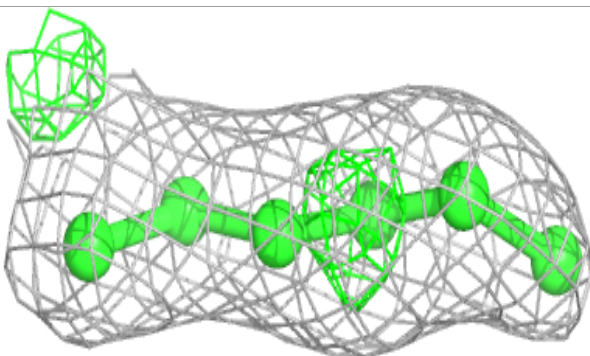
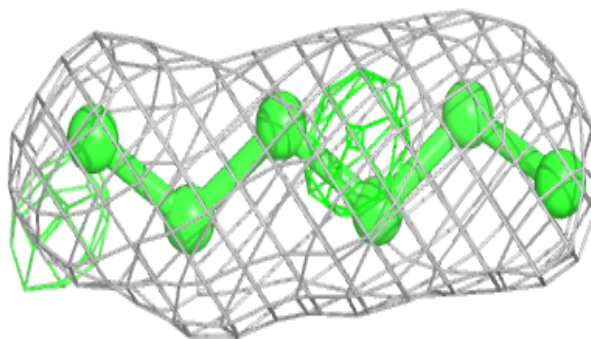
**Electron density around OCT B 309:**

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

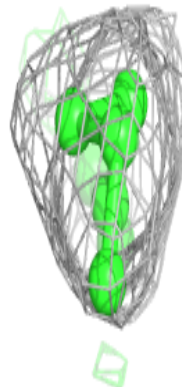
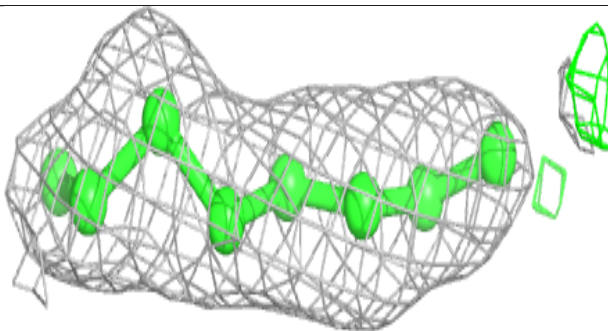
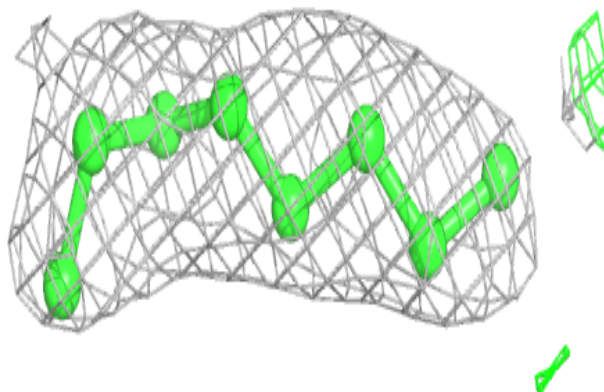


Electron density around HEX C 304:

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

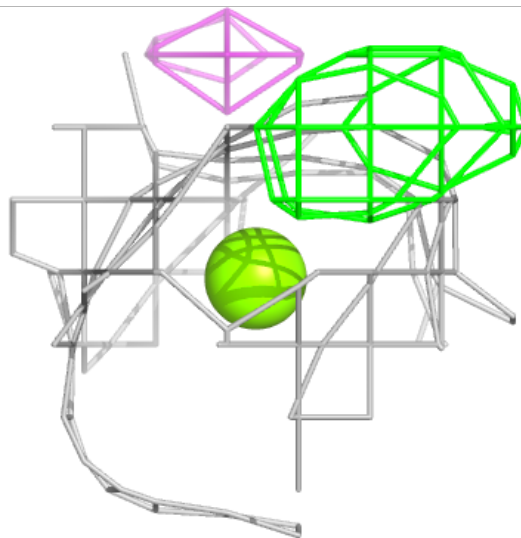
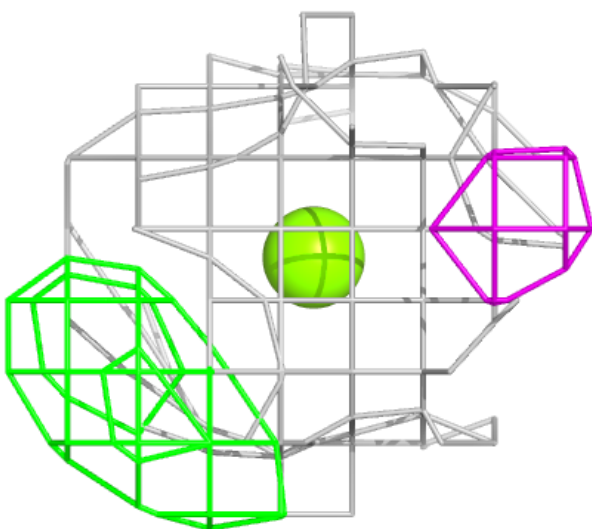
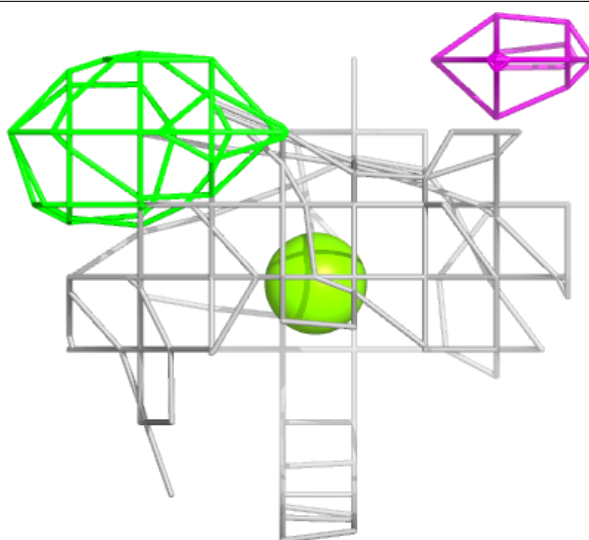
**Electron density around OCT B 310:**

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



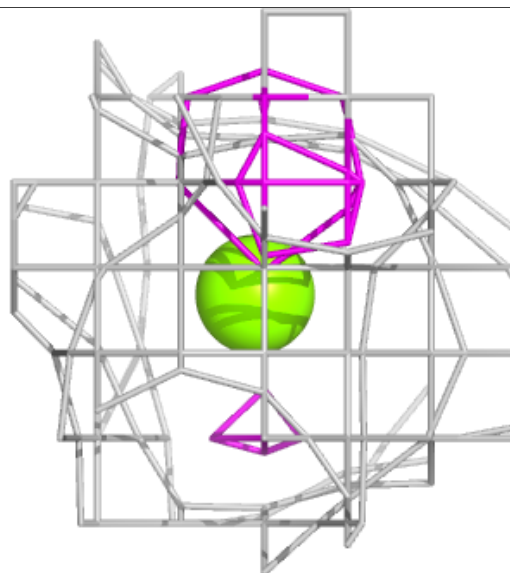
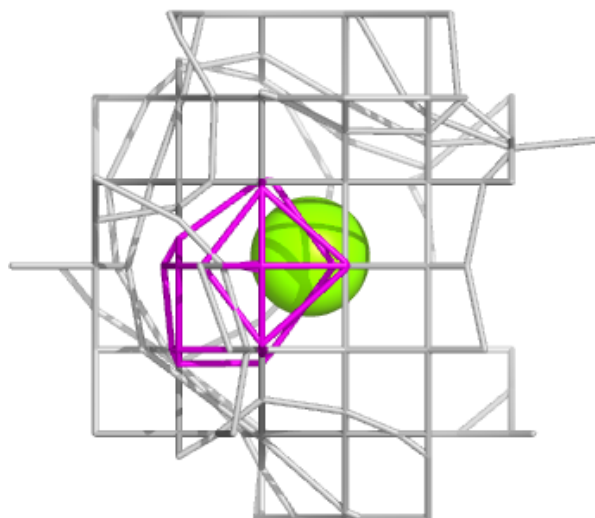
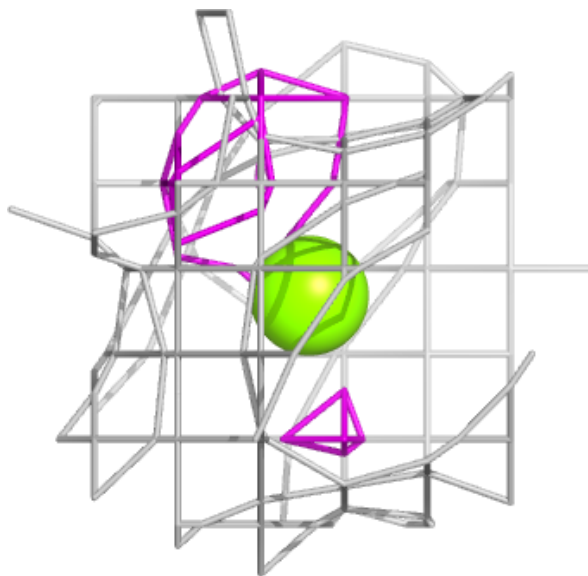
Electron density around MG B 302:

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



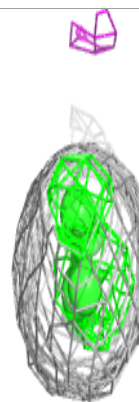
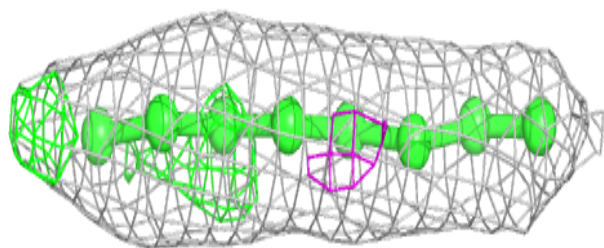
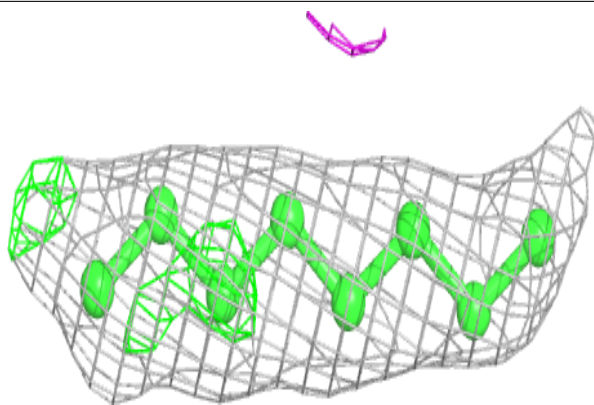
Electron density around MG C 302:

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

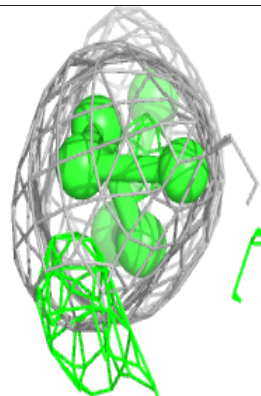
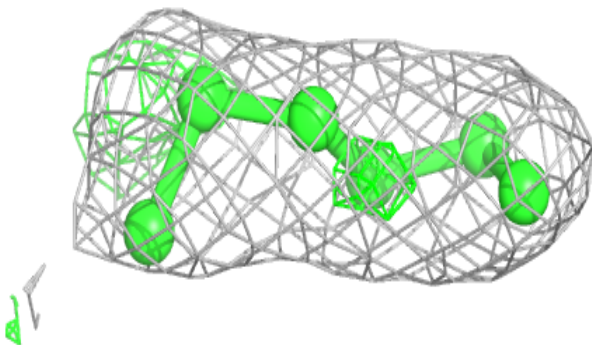
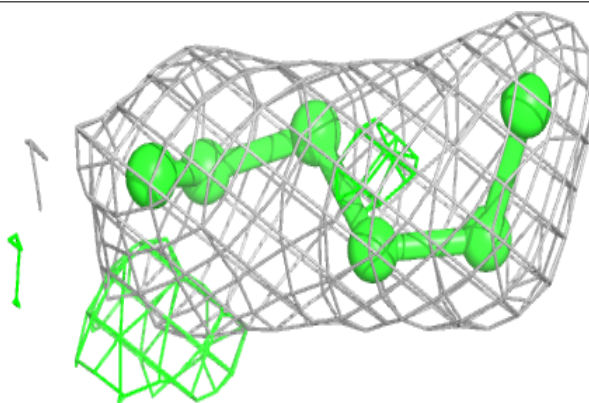


Electron density around OCT A 313:

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

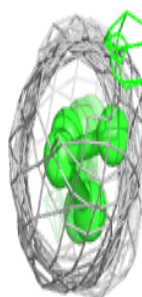
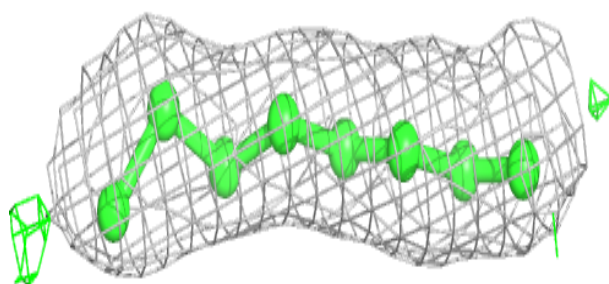
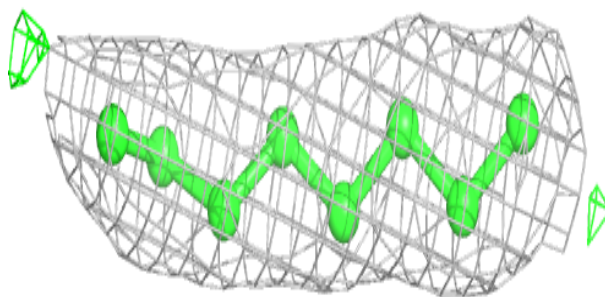
**Electron density around HEX C 306:**

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



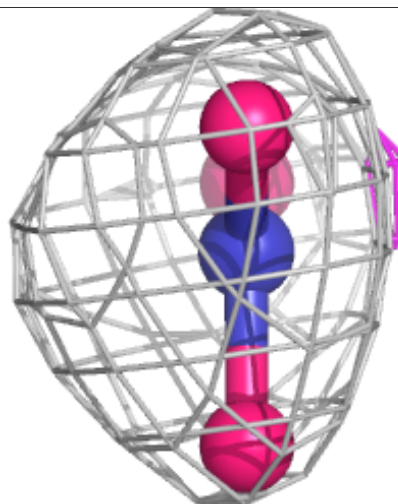
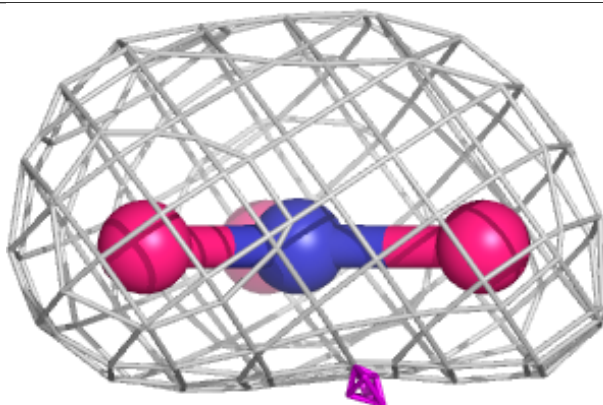
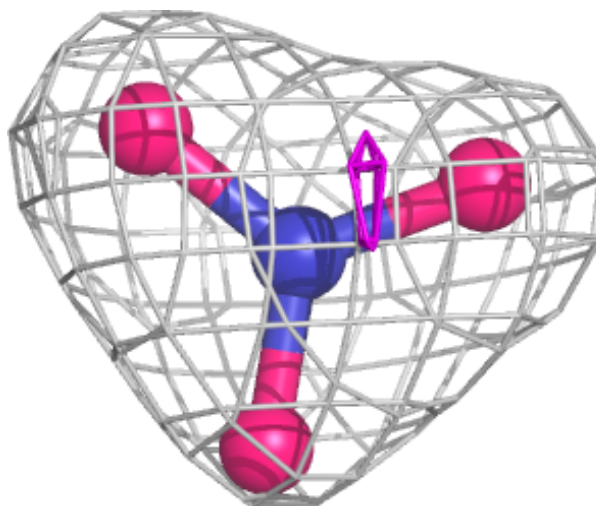
Electron density around OCT A 315:

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



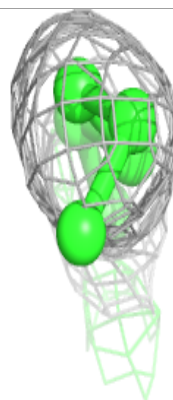
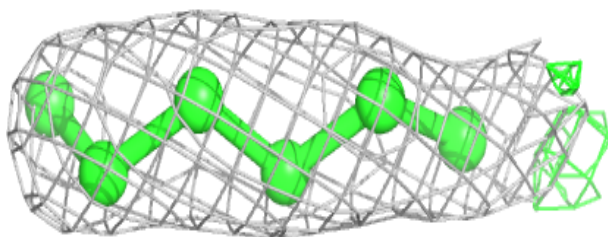
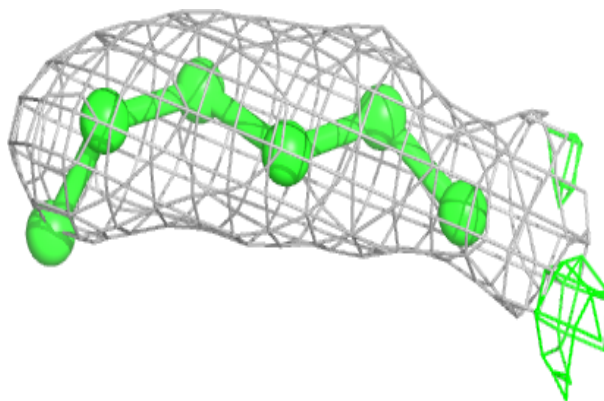
Electron density around NO3 C 323:

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

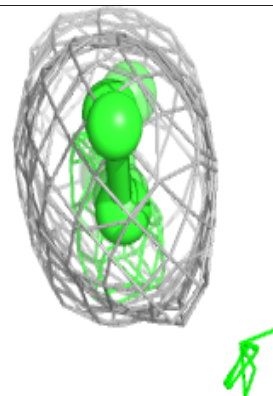
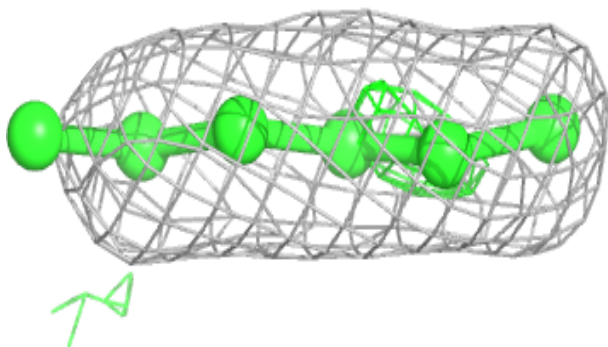
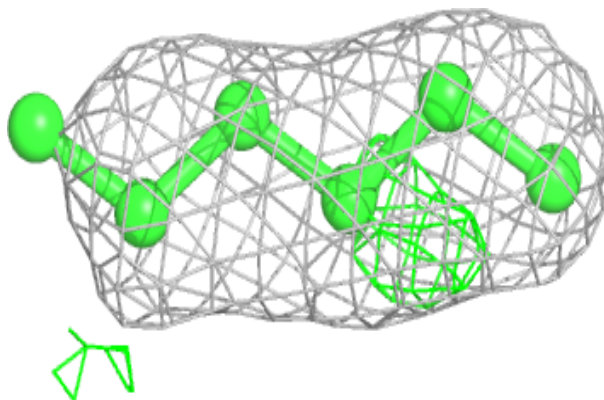


Electron density around HEX A 304:

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

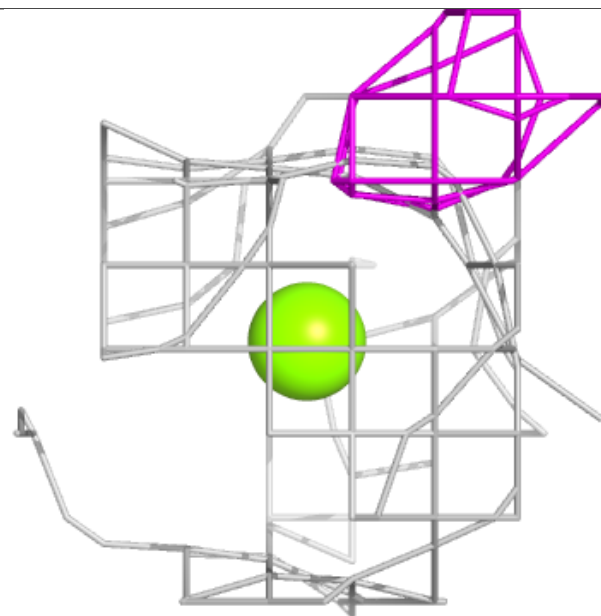
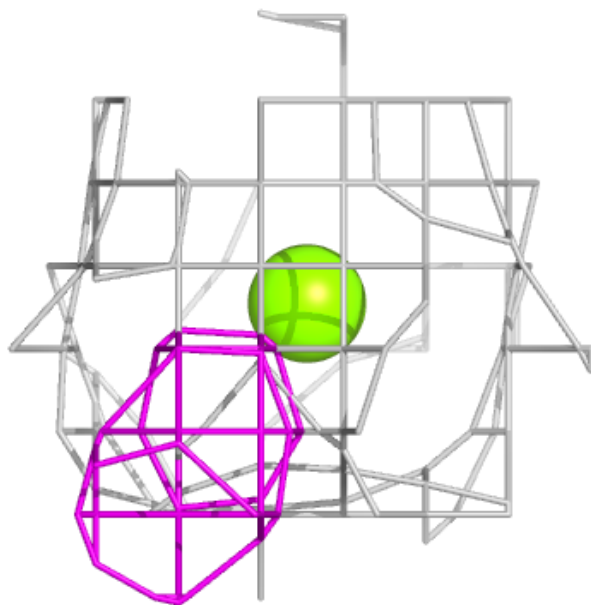
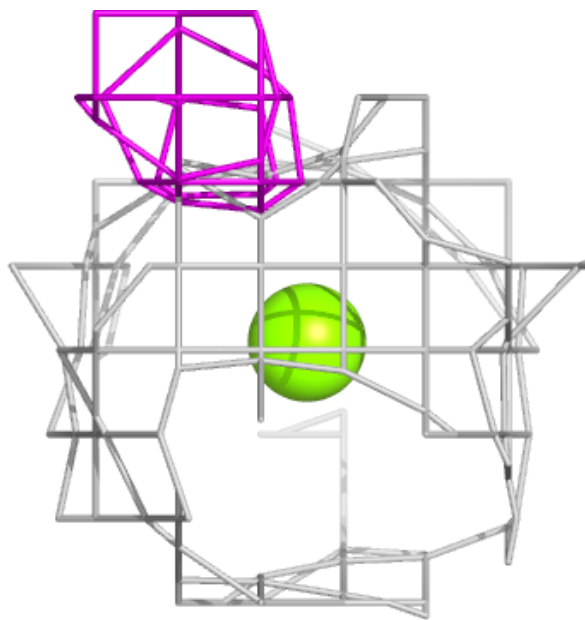
**Electron density around HEX A 305:**

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



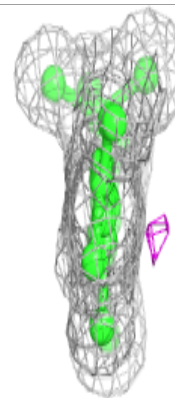
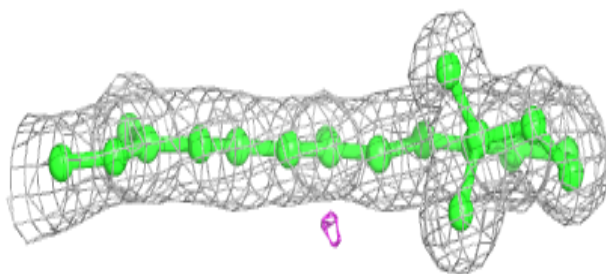
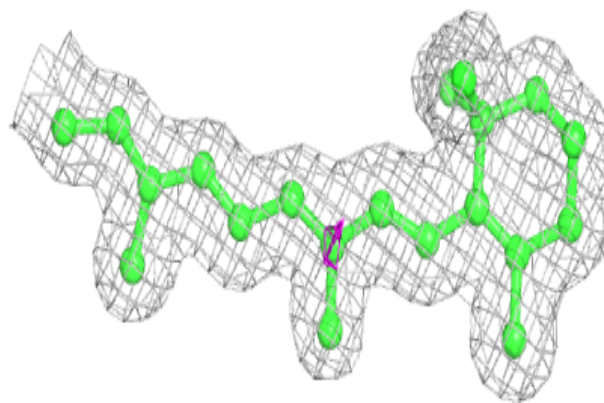
Electron density around MG A 302:

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



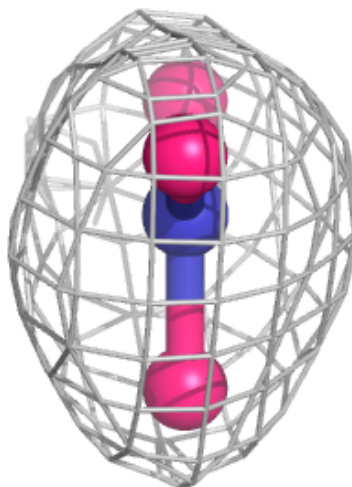
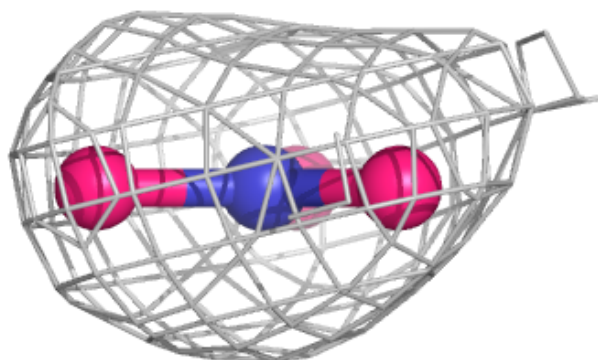
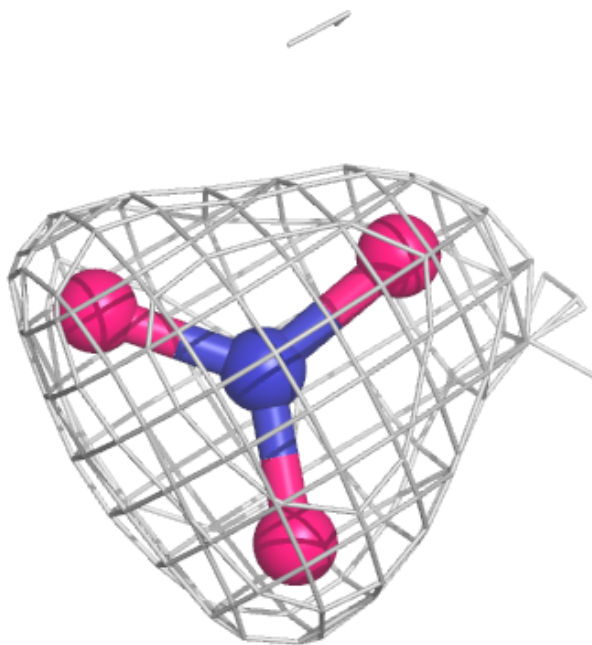
Electron density around RET C 301:

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



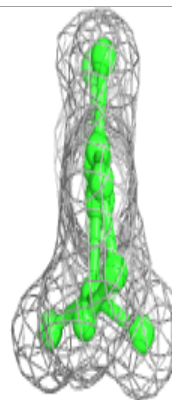
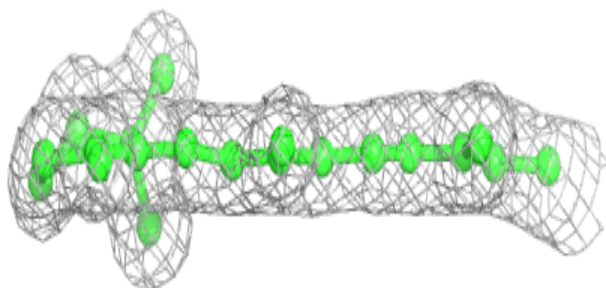
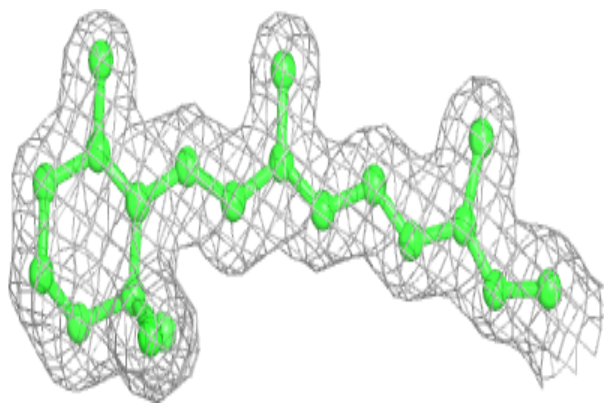
Electron density around NO3 C 322:

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

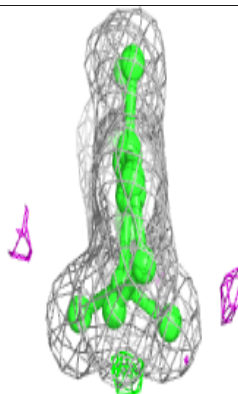
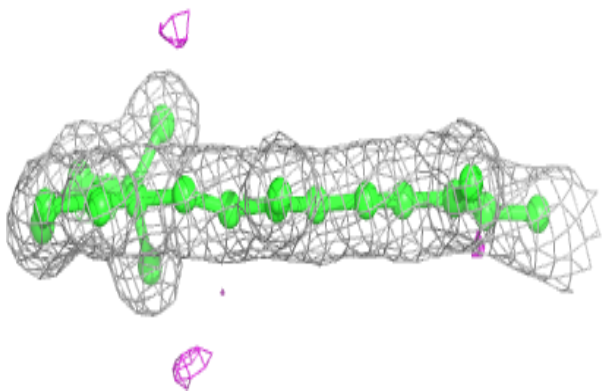
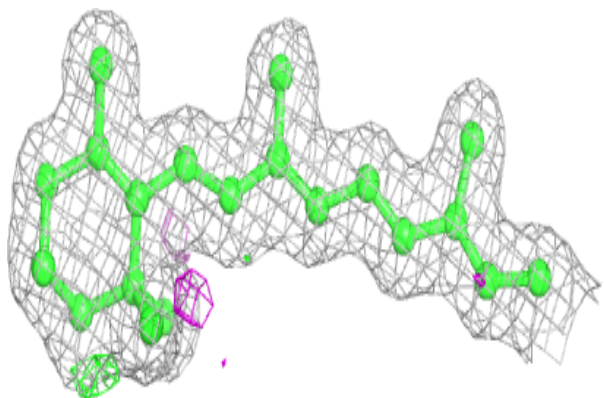


Electron density around RET A 301:

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

**Electron density around RET 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.