



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:58 AM UTC

PDB ID : 6LM1 / pdb_00006lm1
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

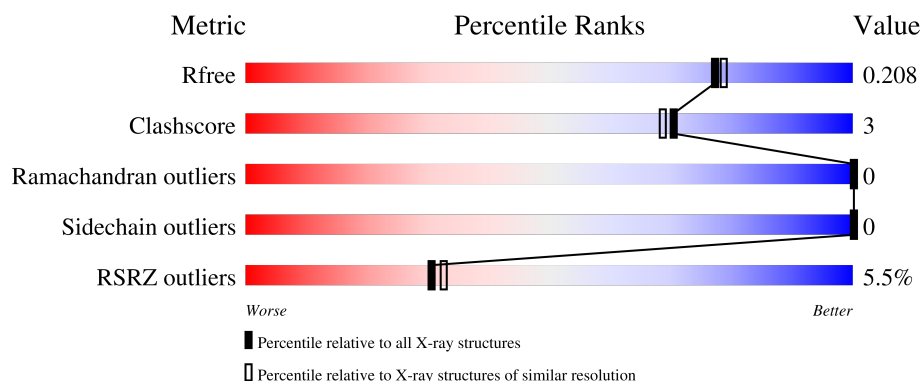
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	259	
1	C	259	

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.

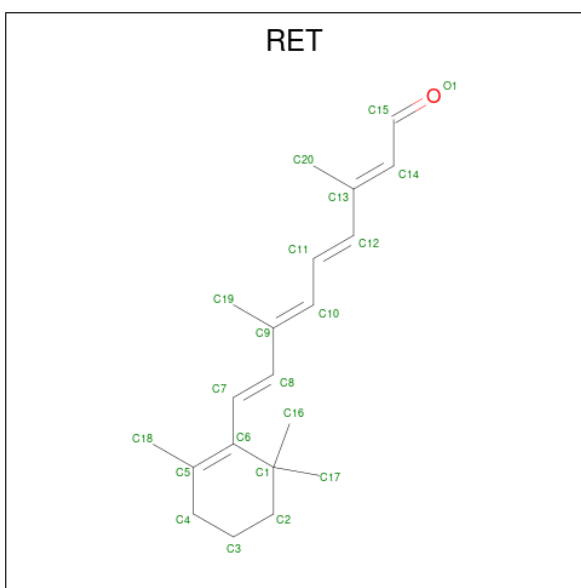
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1737	1169	273	287	8			
1	B	226	Total	C	N	O	S	0	0	0
			1733	1167	273	285	8			
1	C	226	Total	C	N	O	S	0	0	0
			1737	1169	273	287	8			

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 (CCD ID: RET) (formula: C₂₀H₂₈O) (labeled as "Ligand of Interest")

by depositor).

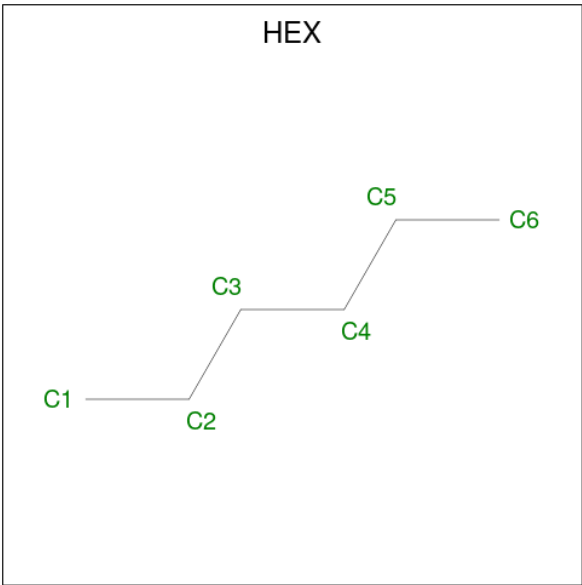


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0
2	B	1	Total C 20 20	0	0
2	C	1	Total C 20 20	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄) (labeled as "Ligand of Interest" by depositor).



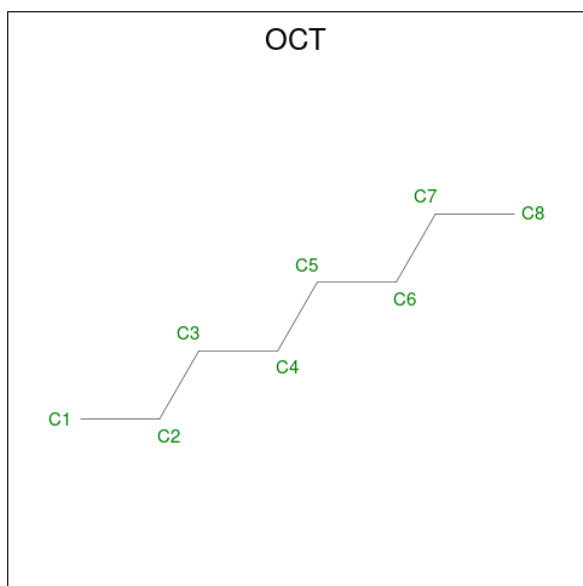
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 6 6	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 6 6	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 (CCD ID: OCT) (formula: C₈H₁₈) (labeled as "Ligand of Interest" by depositor).



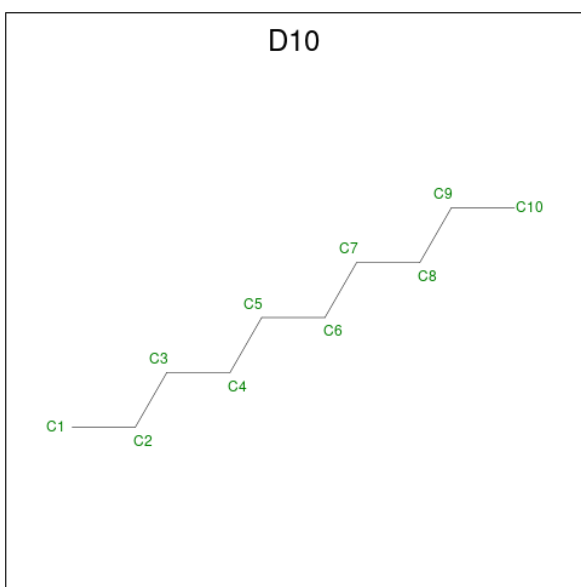
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0

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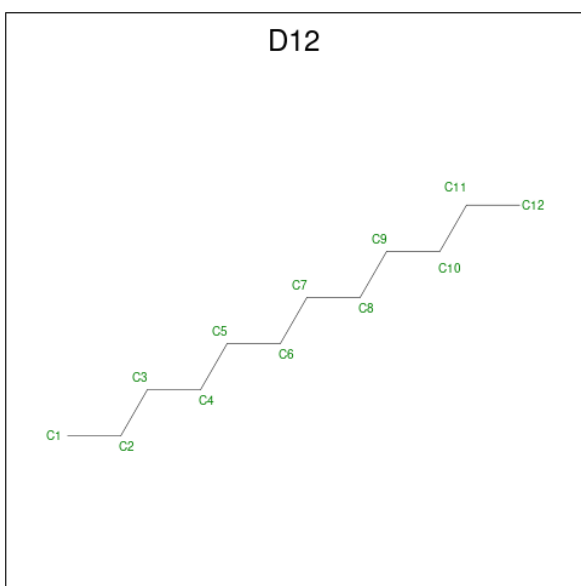
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 8 8	0	0
5	C	1	Total C 8 8	0	0
5	C	1	Total C 8 8	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 (CCD ID: D10) (formula: C₁₀H₂₂) (labeled as "Ligand of Interest" by depositor).



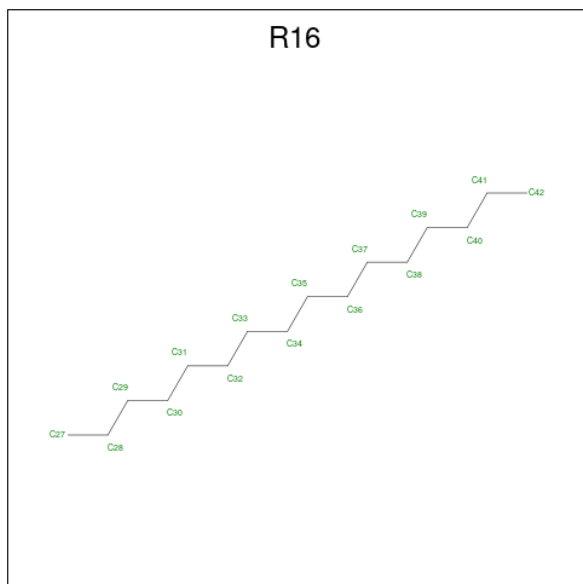
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 10 10	0	0
6	A	1	Total C 10 10	0	0
6	B	1	Total C 10 10	0	0
6	B	1	Total C 10 10	0	0

- Molecule 7 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: R16) (formula: $C_{16}H_{34}$) (labeled as "Ligand of Interest" by depositor).



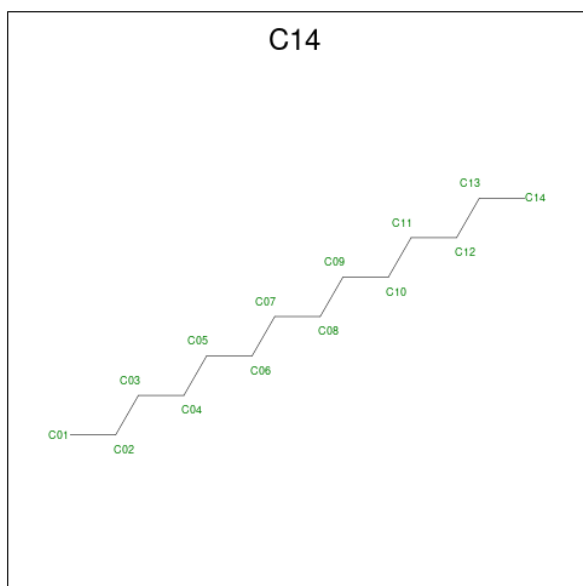
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 16 16	0	0
8	A	1	Total C 16 16	0	0
8	A	1	Total C 16 16	0	0
8	A	1	Total C 16 16	0	0
8	A	1	Total C 16 16	0	0

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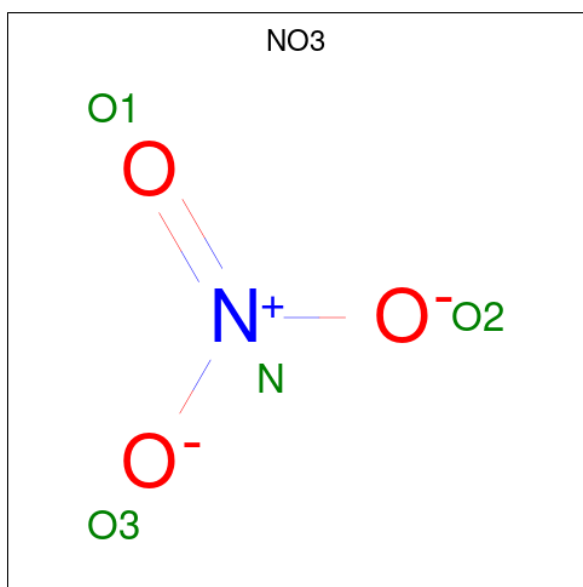
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 16 16	0	0
8	C	1	Total C 16 16	0	0
8	C	1	Total C 16 16	0	0
8	C	1	Total C 16 16	0	0

- Molecule 9 is TETRADECANE (CCD ID: C14) (formula: $C_{14}H_{30}$) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: NO3) (formula: NO_3) (labeled as "Ligand of Interest" by depositor).



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		

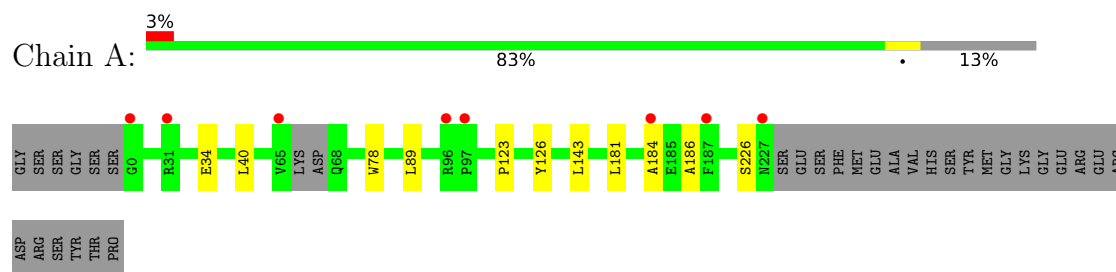
- Molecule 11 is water.

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		

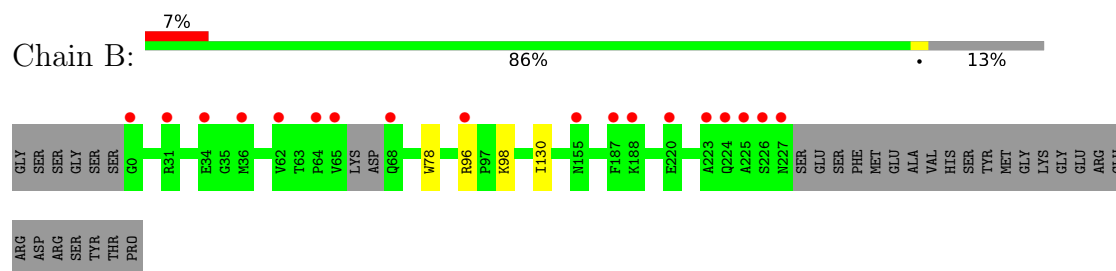
3 Residue-property plots [i](#)

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

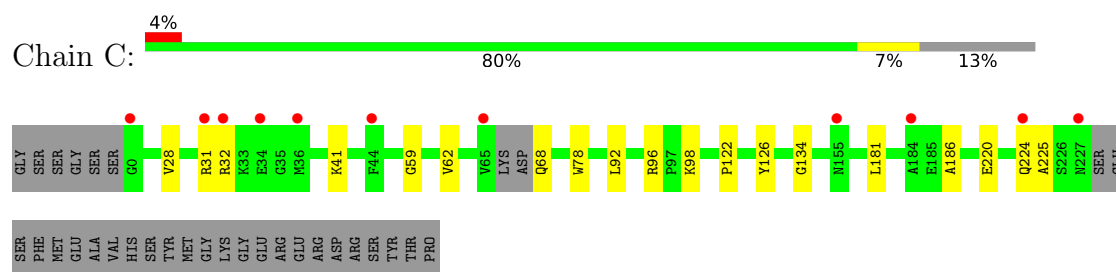
• Molecule 1: Rhodopsin



• Molecule 1: Rhodopsin



• Molecule 1: Rhodopsin



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 45.48 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.48-1.90) 100.0 (45.48-1.90)	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 0.168 , 0.208	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)	0.36 , 76.8	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	0.96	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: HEX, NO3, D10, OCT, D12, RET, R16, C14, MG

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	0.30	0/1777	0.46	0/2427
1	B	0.25	0/1773	0.41	0/2422
1	C	0.29	0/1777	0.43	0/2427
All	All	0.28	0/5327	0.43	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	16	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	43	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 (43) 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:HH11	1:C:31:ARG:HG2	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:H8	2:B:301:RET:H161	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:H161	2:C:301:RET:H8	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:H8	2:A:301:RET:H161	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:H171	2:A:301:RET:C8	2.47	0.45
1:B:96:ARG:HD2	1:B:98:LYS:HB2	1.97	0.45
2:A:301:RET:H7	2:A:301:RET:H181	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
1:C:220:GLU:H	1:C:220:GLU:CD	2.26	0.43
2:C:301:RET:C8	2:C:301:RET:H171	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:H51	5:C:317:OCT:H83	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	180 (100%)	0	100	100
1	B	179/208 (86%)	179 (100%)	0	100	100
1	C	180/208 (86%)	180 (100%)	0	100	100
All	All	539/624 (86%)	539 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	227	ASN
1	B	3	GLN
1	B	224	GLN
1	B	227	ASN
1	C	3	GLN
1	C	159	ASN
1	C	224	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
4	HEX	A	304	-	5,5,5	0.31	0	4,4,4	0.61	0
5	OCT	B	313	-	7,7,7	0.35	0	6,6,6	0.68	0
6	D10	A	316	-	9,9,9	0.29	0	8,8,8	0.83	0
4	HEX	A	306	-	5,5,5	0.31	0	4,4,4	0.66	0
4	HEX	C	307	-	5,5,5	0.35	0	4,4,4	0.57	0
5	OCT	C	316	-	7,7,7	0.30	0	6,6,6	0.69	0
4	HEX	C	309	-	5,5,5	0.33	0	4,4,4	0.62	0
4	HEX	C	305	-	5,5,5	0.33	0	4,4,4	0.62	0
8	R16	A	320	-	15,15,15	0.32	0	14,14,14	0.77	0
9	C14	B	320	-	13,13,13	0.29	0	12,12,12	0.85	0
7	D12	B	316	-	11,11,11	0.30	0	10,10,10	0.82	0
2	RET	A	301	1	20,20,21	0.95	1 (5%)	27,27,28	0.62	0
4	HEX	C	308	-	5,5,5	0.32	0	4,4,4	0.61	0
7	D12	C	318	-	11,11,11	0.31	0	10,10,10	0.87	0
6	D10	B	315	-	9,9,9	0.31	0	8,8,8	0.77	0
5	OCT	A	314	-	7,7,7	0.31	0	6,6,6	0.65	0
4	HEX	B	306	-	5,5,5	0.34	0	4,4,4	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEX	B	304	-	5,5,5	0.33	0	4,4,4	0.61	0
7	D12	A	319	-	11,11,11	0.30	0	10,10,10	0.92	0
4	HEX	C	311	-	5,5,5	0.32	0	4,4,4	0.60	0
4	HEX	C	312	-	5,5,5	0.32	0	4,4,4	0.62	0
4	HEX	A	303	-	5,5,5	0.32	0	4,4,4	0.64	0
4	HEX	C	310	-	5,5,5	0.35	0	4,4,4	0.59	0
5	OCT	A	309	-	7,7,7	0.32	0	6,6,6	0.72	0
4	HEX	C	303	-	5,5,5	0.34	0	4,4,4	0.62	0
5	OCT	A	311	-	7,7,7	0.30	0	6,6,6	0.78	0
5	OCT	B	308	-	7,7,7	0.29	0	6,6,6	0.75	0
10	NO3	C	323	-	1,3,3	0.57	0	0,3,3	-	-
8	R16	A	322	-	15,15,15	0.31	0	14,14,14	0.85	0
5	OCT	B	309	-	7,7,7	0.30	0	6,6,6	0.79	0
4	HEX	A	307	-	5,5,5	0.33	0	4,4,4	0.62	0
5	OCT	C	317	-	7,7,7	0.32	0	6,6,6	0.71	0
7	D12	A	318	-	11,11,11	0.30	0	10,10,10	0.86	0
9	C14	C	324	-	13,13,13	0.31	0	12,12,12	0.88	0
10	NO3	C	322	-	1,3,3	0.50	0	0,3,3	-	-
5	OCT	A	310	-	7,7,7	0.37	0	6,6,6	0.60	0
4	HEX	B	305	-	5,5,5	0.31	0	4,4,4	0.62	0
4	HEX	B	307	-	5,5,5	0.32	0	4,4,4	0.61	0
5	OCT	B	312	-	7,7,7	0.32	0	6,6,6	0.68	0
6	D10	B	314	-	9,9,9	0.31	0	8,8,8	0.78	0
5	OCT	A	315	-	7,7,7	0.30	0	6,6,6	0.76	0
5	OCT	C	313	-	7,7,7	0.31	0	6,6,6	0.67	0
5	OCT	C	315	-	7,7,7	0.31	0	6,6,6	0.77	0
5	OCT	B	310	-	7,7,7	0.27	0	6,6,6	0.83	0
9	C14	A	325	-	13,13,13	0.30	0	12,12,12	0.80	0
4	HEX	C	304	-	5,5,5	0.29	0	4,4,4	0.71	0
8	R16	B	319	-	15,15,15	0.31	0	14,14,14	0.85	0
2	RET	B	301	1	20,20,21	1.02	1 (5%)	27,27,28	0.66	1 (3%)
4	HEX	A	305	-	5,5,5	0.30	0	4,4,4	0.70	0
5	OCT	A	308	-	7,7,7	0.30	0	6,6,6	0.76	0
8	R16	A	321	-	15,15,15	0.32	0	14,14,14	0.85	0
8	R16	A	324	-	15,15,15	0.32	0	14,14,14	0.79	0
4	HEX	B	303	-	5,5,5	0.31	0	4,4,4	0.61	0
4	HEX	C	306	-	5,5,5	0.32	0	4,4,4	0.59	0
5	OCT	A	313	-	7,7,7	0.27	0	6,6,6	0.79	0
8	R16	C	319	-	15,15,15	0.33	0	14,14,14	0.80	0
5	OCT	B	311	-	7,7,7	0.33	0	6,6,6	0.72	0
7	D12	B	318	-	11,11,11	0.29	0	10,10,10	0.82	0
8	R16	A	323	-	15,15,15	0.30	0	14,14,14	0.90	0
8	R16	C	320	-	15,15,15	0.29	0	14,14,14	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RET	C	301	1	20,20,21	0.99	1 (5%)	27,27,28	0.61	0
7	D12	B	317	-	11,11,11	0.31	0	10,10,10	0.87	0
8	R16	C	321	-	15,15,15	0.35	0	14,14,14	0.79	0
5	OCT	C	314	-	7,7,7	0.29	0	6,6,6	0.72	0
6	D10	A	317	-	9,9,9	0.32	0	8,8,8	0.77	0
5	OCT	A	312	-	7,7,7	0.30	0	6,6,6	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEX	A	304	-	-	1/3/3/3	-
5	OCT	B	313	-	-	3/5/5/5	-
6	D10	A	316	-	-	2/7/7/7	-
4	HEX	A	306	-	-	0/3/3/3	-
4	HEX	C	307	-	-	1/3/3/3	-
5	OCT	C	316	-	-	0/5/5/5	-
4	HEX	C	309	-	-	0/3/3/3	-
4	HEX	C	305	-	-	0/3/3/3	-
8	R16	A	320	-	-	8/13/13/13	-
9	C14	B	320	-	-	7/11/11/11	-
7	D12	B	316	-	-	5/9/9/9	-
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
4	HEX	C	308	-	-	1/3/3/3	-
7	D12	C	318	-	-	1/9/9/9	-
6	D10	B	315	-	-	3/7/7/7	-
5	OCT	A	314	-	-	3/5/5/5	-
4	HEX	B	306	-	-	0/3/3/3	-
4	HEX	B	304	-	-	0/3/3/3	-
7	D12	A	319	-	-	0/9/9/9	-
4	HEX	C	311	-	-	0/3/3/3	-
4	HEX	C	312	-	-	1/3/3/3	-
4	HEX	A	303	-	-	0/3/3/3	-
4	HEX	C	310	-	-	0/3/3/3	-
5	OCT	A	309	-	-	1/5/5/5	-
4	HEX	C	303	-	-	1/3/3/3	-
5	OCT	A	311	-	-	2/5/5/5	-
5	OCT	B	308	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	R16	A	322	-	-	3/13/13/13	-
5	OCT	B	309	-	-	0/5/5/5	-
4	HEX	A	307	-	-	0/3/3/3	-
5	OCT	C	317	-	-	3/5/5/5	-
7	D12	A	318	-	-	3/9/9/9	-
9	C14	C	324	-	-	4/11/11/11	-
5	OCT	A	310	-	-	2/5/5/5	-
4	HEX	B	305	-	-	2/3/3/3	-
4	HEX	B	307	-	-	2/3/3/3	-
5	OCT	B	312	-	-	4/5/5/5	-
6	D10	B	314	-	-	2/7/7/7	-
5	OCT	A	315	-	-	1/5/5/5	-
5	OCT	C	313	-	-	0/5/5/5	-
5	OCT	C	315	-	-	2/5/5/5	-
5	OCT	B	310	-	-	3/5/5/5	-
9	C14	A	325	-	-	7/11/11/11	-
4	HEX	C	304	-	-	1/3/3/3	-
8	R16	B	319	-	-	4/13/13/13	-
2	RET	B	301	1	-	0/13/30/31	0/1/1/1
4	HEX	A	305	-	-	0/3/3/3	-
5	OCT	A	308	-	-	3/5/5/5	-
8	R16	A	321	-	-	4/13/13/13	-
8	R16	A	324	-	-	7/13/13/13	-
4	HEX	B	303	-	-	0/3/3/3	-
4	HEX	C	306	-	-	0/3/3/3	-
5	OCT	A	313	-	-	0/5/5/5	-
8	R16	C	319	-	-	5/13/13/13	-
5	OCT	B	311	-	-	4/5/5/5	-
7	D12	B	318	-	-	3/9/9/9	-
8	R16	A	323	-	-	3/13/13/13	-
8	R16	C	320	-	-	6/13/13/13	-
2	RET	C	301	1	-	0/13/30/31	0/1/1/1
7	D12	B	317	-	-	3/9/9/9	-
8	R16	C	321	-	-	3/13/13/13	-
5	OCT	C	314	-	-	1/5/5/5	-
6	D10	A	317	-	-	4/7/7/7	-
5	OCT	A	312	-	-	1/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	RET	C14-C13	3.95	1.36	1.33
2	B	301	RET	C14-C13	3.86	1.36	1.33
2	A	301	RET	C14-C13	3.57	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	2.07	129.30	126.23

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	321	R16	C31-C32-C33-C34
8	A	323	R16	C35-C36-C37-C38
7	B	318	D12	C2-C3-C4-C5
8	A	322	R16	C35-C36-C37-C38
5	B	311	OCT	C2-C3-C4-C5
8	A	320	R16	C35-C36-C37-C38
9	A	325	C14	C09-C10-C11-C12
8	A	321	R16	C30-C31-C32-C33
5	B	312	OCT	C3-C4-C5-C6
8	A	320	R16	C29-C30-C31-C32
8	A	322	R16	C33-C34-C35-C36
5	A	310	OCT	C3-C4-C5-C6
9	B	320	C14	C10-C11-C12-C13
4	B	305	HEX	C2-C3-C4-C5
7	B	316	D12	C6-C7-C8-C9
8	B	319	R16	C35-C36-C37-C38
6	B	315	D10	C3-C4-C5-C6
8	C	320	R16	C35-C36-C37-C38
5	C	317	OCT	C3-C4-C5-C6
8	A	320	R16	C38-C39-C40-C41
8	A	324	R16	C30-C31-C32-C33
5	B	310	OCT	C2-C3-C4-C5
7	B	316	D12	C2-C3-C4-C5
9	A	325	C14	C05-C06-C07-C08
9	B	320	C14	C08-C09-C10-C11
5	B	308	OCT	C3-C4-C5-C6
6	A	317	D10	C3-C4-C5-C6
9	C	324	C14	C09-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	C	319	R16	C32-C33-C34-C35
8	B	319	R16	C39-C40-C41-C42
6	B	315	D10	C6-C7-C8-C9
7	A	318	D12	C4-C5-C6-C7
5	B	308	OCT	C4-C5-C6-C7
5	B	313	OCT	C3-C4-C5-C6
8	C	319	R16	C33-C34-C35-C36
8	C	320	R16	C31-C32-C33-C34
8	A	321	R16	C34-C35-C36-C37
8	C	320	R16	C32-C33-C34-C35
9	B	320	C14	C04-C05-C06-C07
8	B	319	R16	C34-C35-C36-C37
9	B	320	C14	C07-C08-C09-C10
8	C	319	R16	C31-C32-C33-C34
9	A	325	C14	C03-C04-C05-C06
9	A	325	C14	C08-C09-C10-C11
6	B	314	D10	C1-C2-C3-C4
5	B	310	OCT	C1-C2-C3-C4
9	B	320	C14	C11-C12-C13-C14
7	B	318	D12	C1-C2-C3-C4
7	B	317	D12	C1-C2-C3-C4
8	A	320	R16	C30-C31-C32-C33
8	A	320	R16	C32-C33-C34-C35
8	C	320	R16	C33-C34-C35-C36
4	A	304	HEX	C3-C4-C5-C6
6	A	316	D10	C2-C3-C4-C5
7	B	316	D12	C7-C8-C9-C10
7	B	317	D12	C9-C10-C11-C12
5	C	315	OCT	C4-C5-C6-C7
5	A	314	OCT	C1-C2-C3-C4
6	A	317	D10	C7-C8-C9-C10
5	B	310	OCT	C3-C4-C5-C6
8	A	321	R16	C31-C32-C33-C34
8	C	320	R16	C27-C28-C29-C30
5	A	315	OCT	C1-C2-C3-C4
8	A	324	R16	C33-C34-C35-C36
5	C	317	OCT	C2-C3-C4-C5
5	B	311	OCT	C5-C6-C7-C8
8	A	323	R16	C37-C38-C39-C40
5	B	311	OCT	C4-C5-C6-C7
9	A	325	C14	C02-C03-C04-C05
8	C	321	R16	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
4	B	307	HEX	C2-C3-C4-C5
5	C	315	OCT	C5-C6-C7-C8
5	B	312	OCT	C2-C3-C4-C5
5	A	314	OCT	C2-C3-C4-C5
8	A	320	R16	C37-C38-C39-C40
5	A	308	OCT	C3-C4-C5-C6
5	A	308	OCT	C4-C5-C6-C7
6	B	315	D10	C5-C6-C7-C8
4	C	308	HEX	C3-C4-C5-C6
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	A	311	OCT	C4-C5-C6-C7
5	B	312	OCT	C5-C6-C7-C8
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
8	A	321	R16	C39-C40-C41-C42
5	A	308	OCT	C2-C3-C4-C5
5	A	312	OCT	C1-C2-C3-C4
8	C	319	R16	C30-C31-C32-C33
9	C	324	C14	C05-C06-C07-C08
4	C	303	HEX	C2-C3-C4-C5
4	B	307	HEX	C3-C4-C5-C6
7	B	316	D12	C3-C4-C5-C6
5	B	313	OCT	C5-C6-C7-C8
7	C	318	D12	C3-C4-C5-C6
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
4	C	312	HEX	C3-C4-C5-C6

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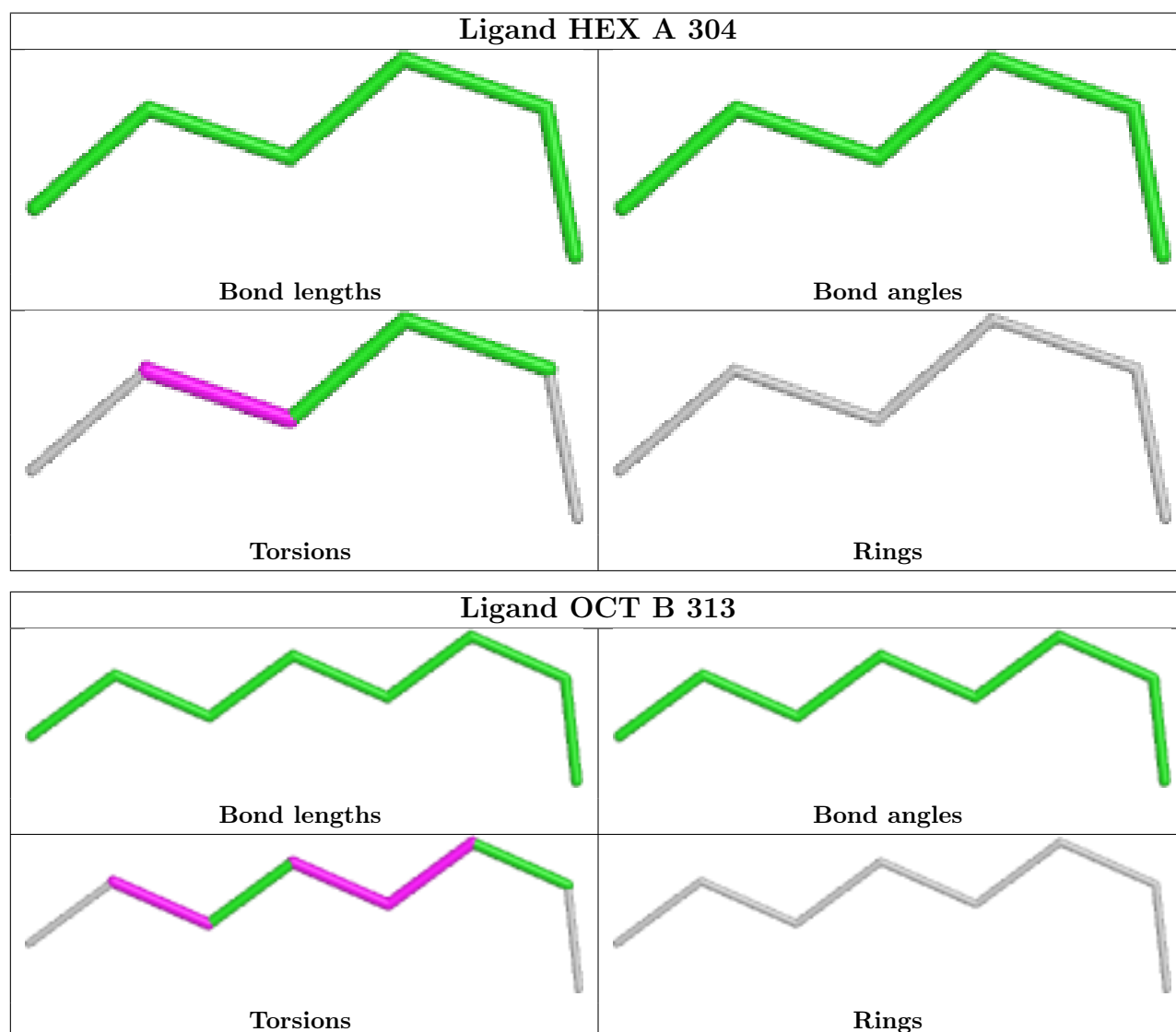
Mol	Chain	Res	Type	Atoms
5	A	314	OCT	C3-C4-C5-C6
8	A	324	R16	C27-C28-C29-C30
5	B	313	OCT	C2-C3-C4-C5
4	C	307	HEX	C3-C4-C5-C6
8	C	320	R16	C36-C37-C38-C39
7	B	316	D12	C5-C6-C7-C8
6	A	317	D10	C5-C6-C7-C8
6	B	314	D10	C2-C3-C4-C5
8	A	324	R16	C28-C29-C30-C31
7	B	317	D12	C11-C10-C9-C8
8	A	324	R16	C36-C37-C38-C39
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

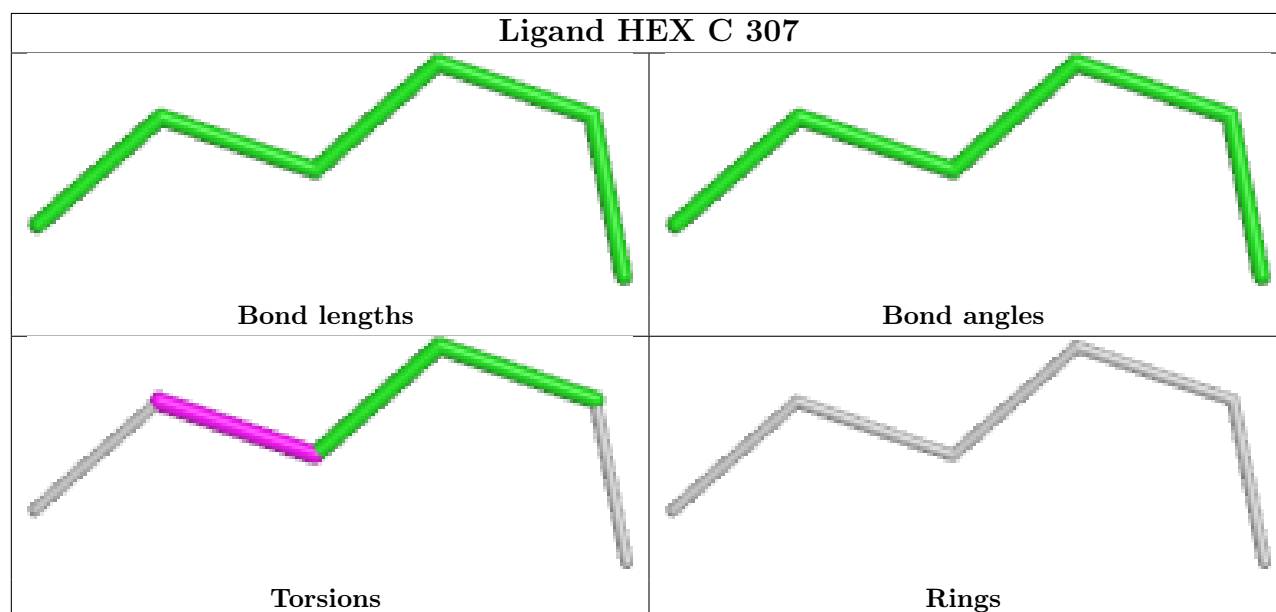
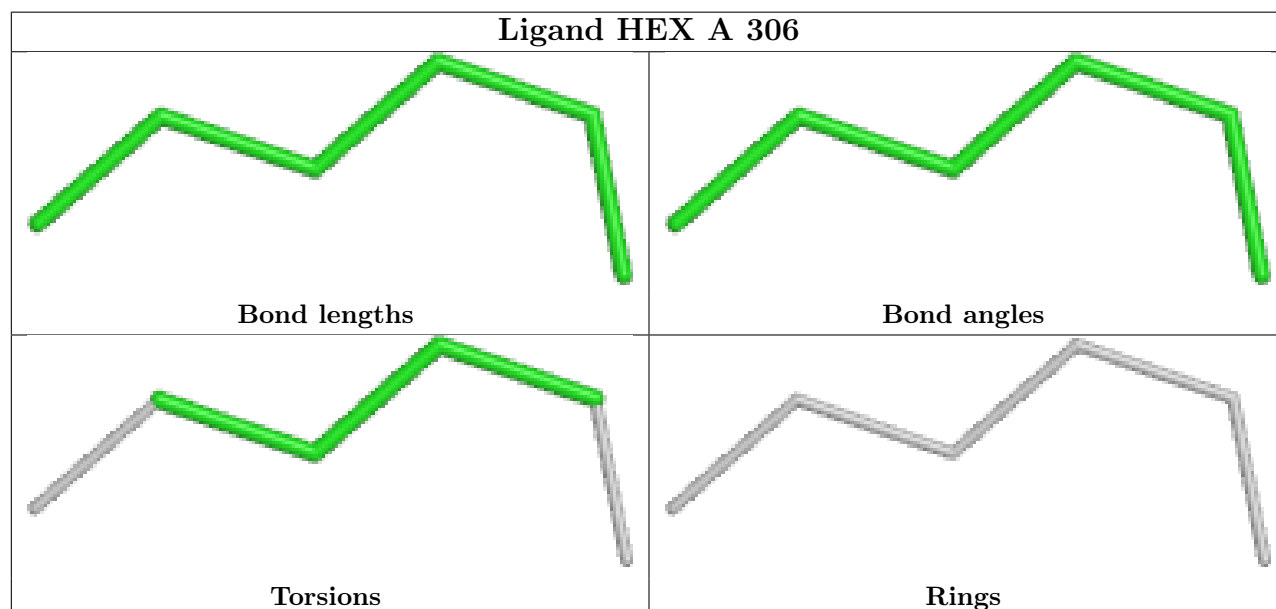
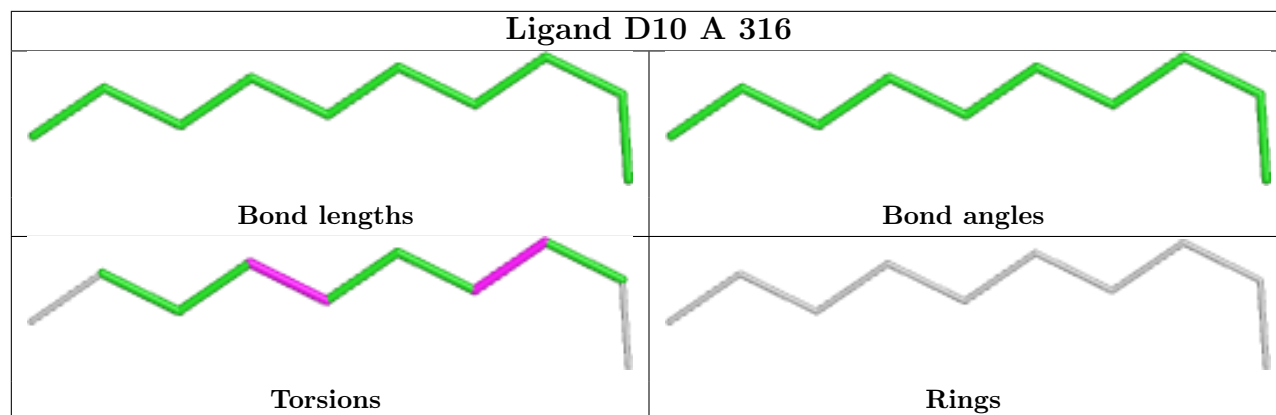
There are no ring outliers.

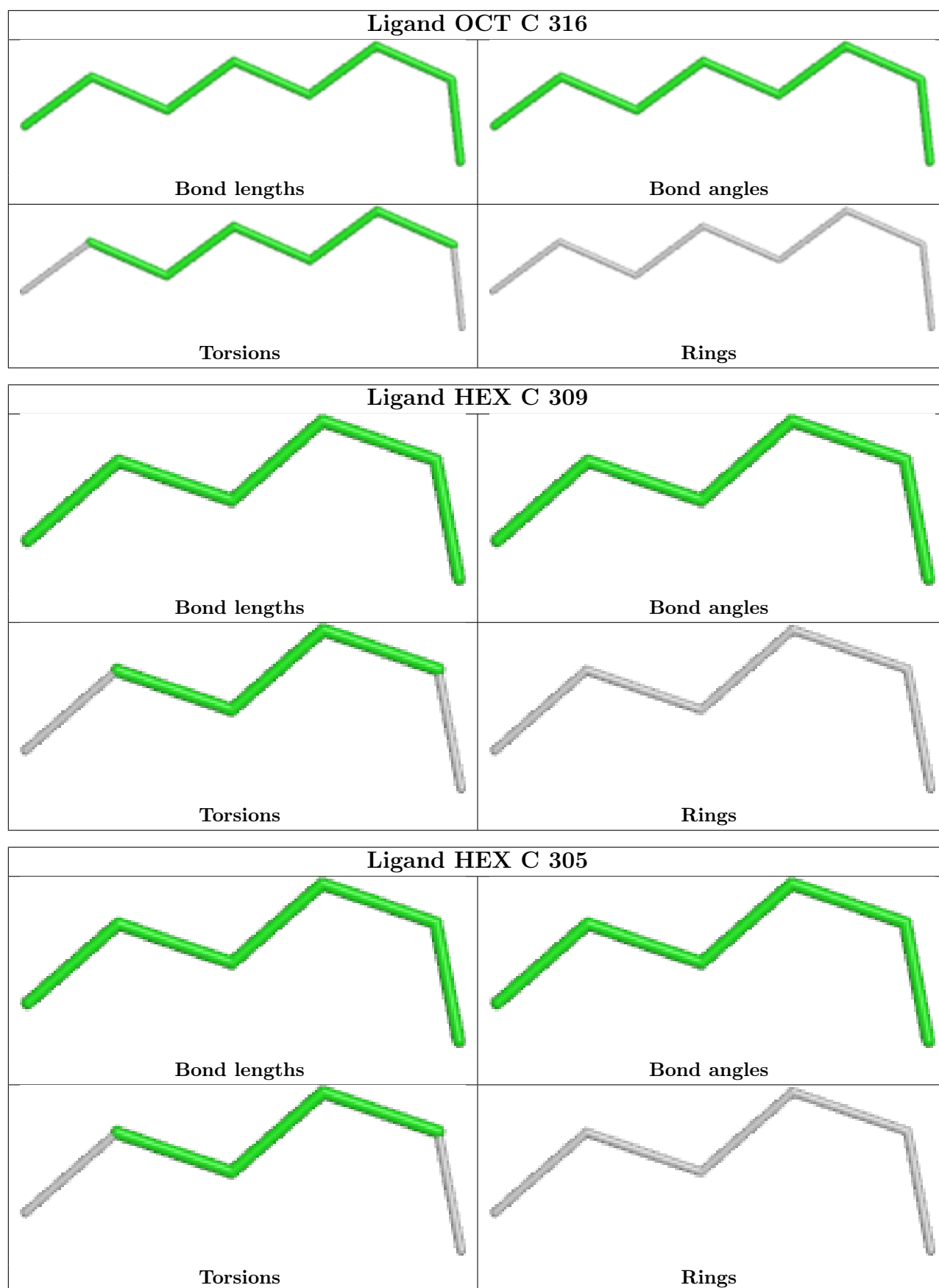
16 monomers are involved in 23 short contacts:

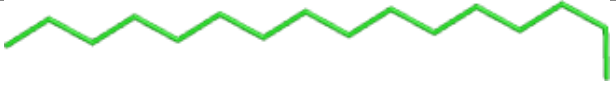
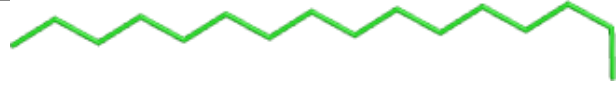
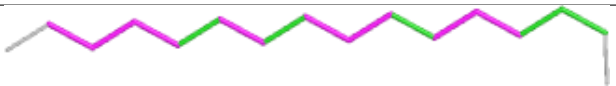
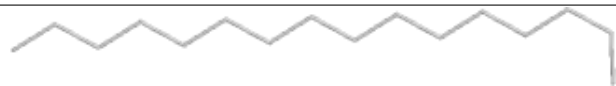
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	HEX	1	0
4	C	307	HEX	1	0
8	A	320	R16	1	0
7	B	316	D12	1	0
2	A	301	RET	5	0
4	C	308	HEX	1	0
7	C	318	D12	1	0
5	A	309	OCT	1	0
5	A	311	OCT	2	0
5	C	317	OCT	1	0
7	A	318	D12	1	0
5	C	313	OCT	1	0
2	B	301	RET	3	0
2	C	301	RET	4	0
8	C	321	R16	1	0
5	C	314	OCT	1	0

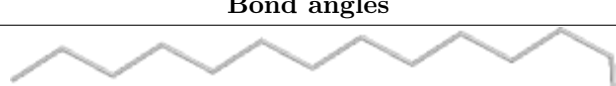
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

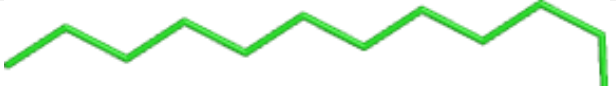
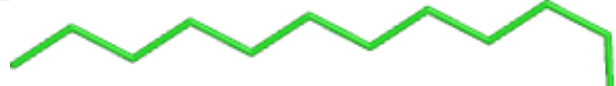
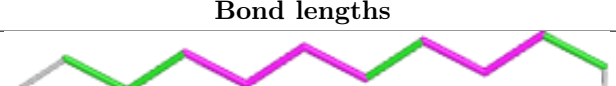
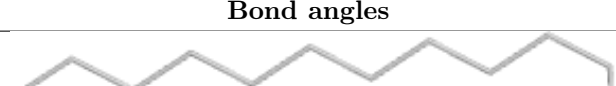


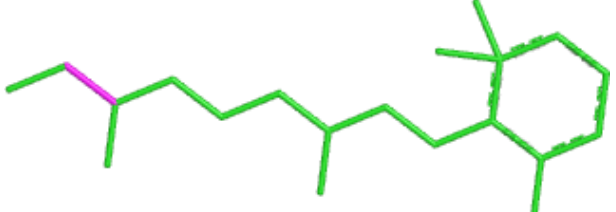
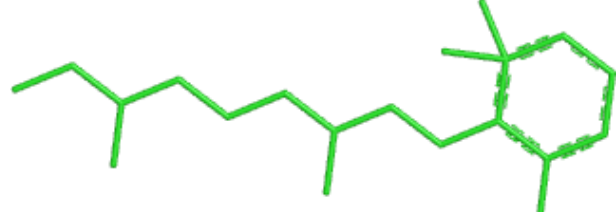
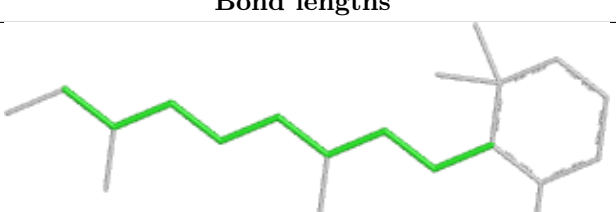
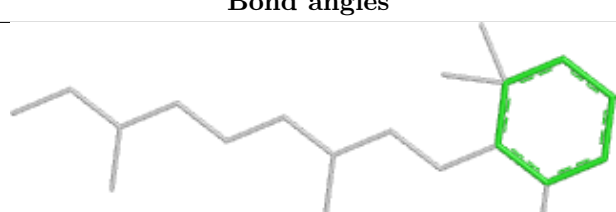


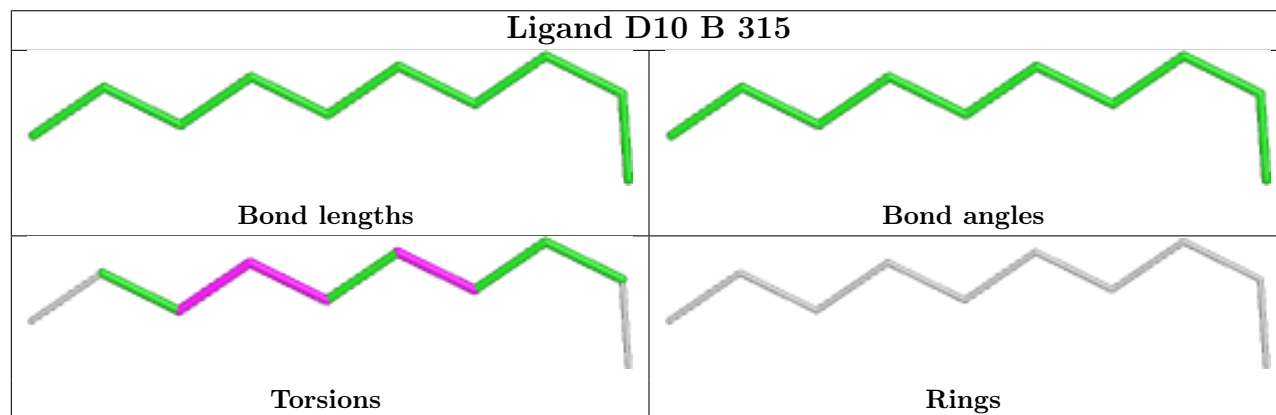
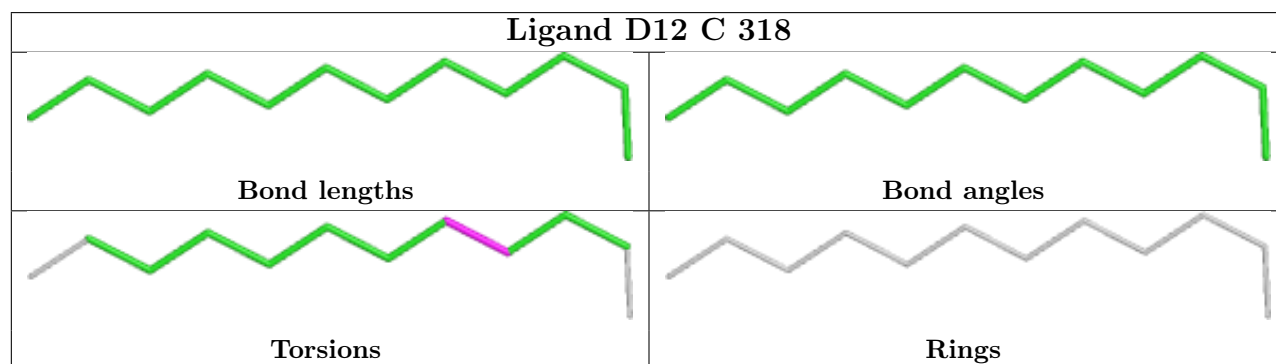
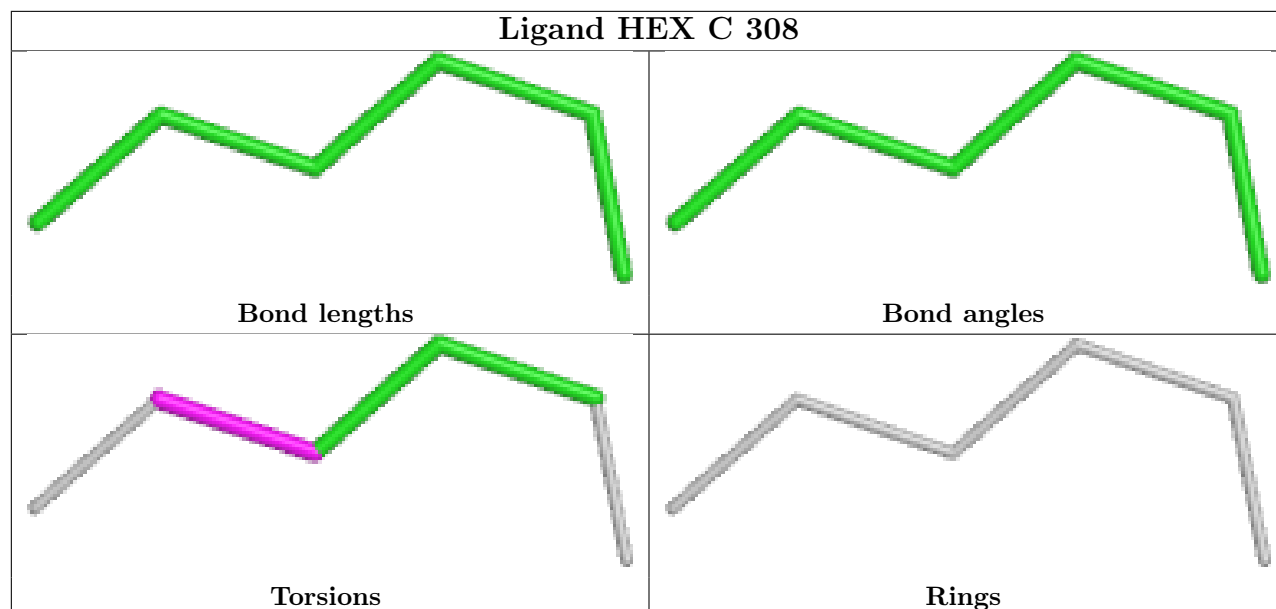


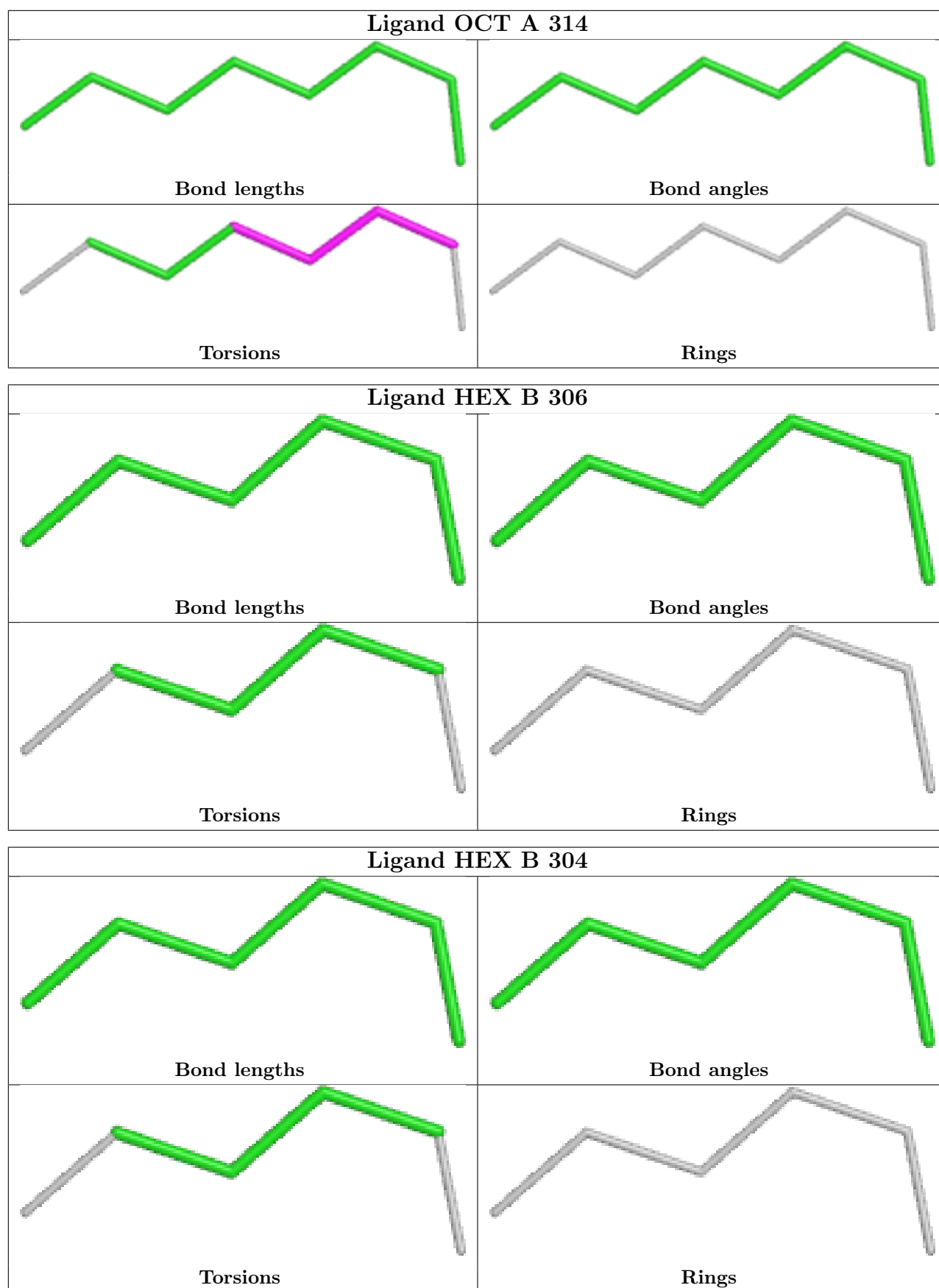
Ligand R16 A 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

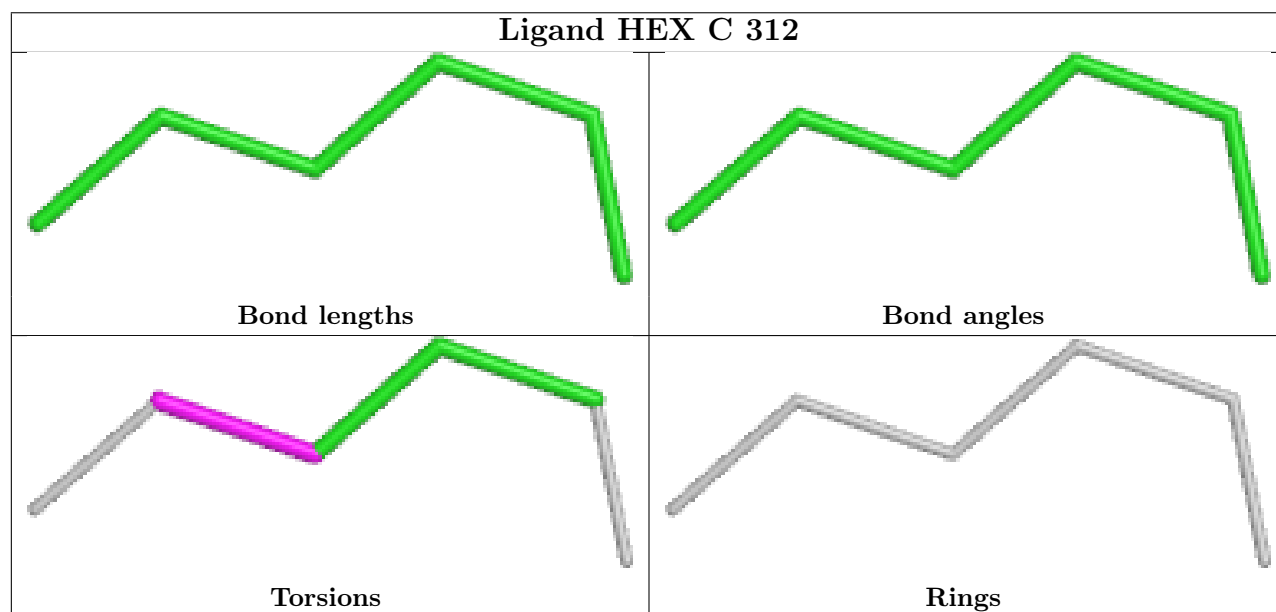
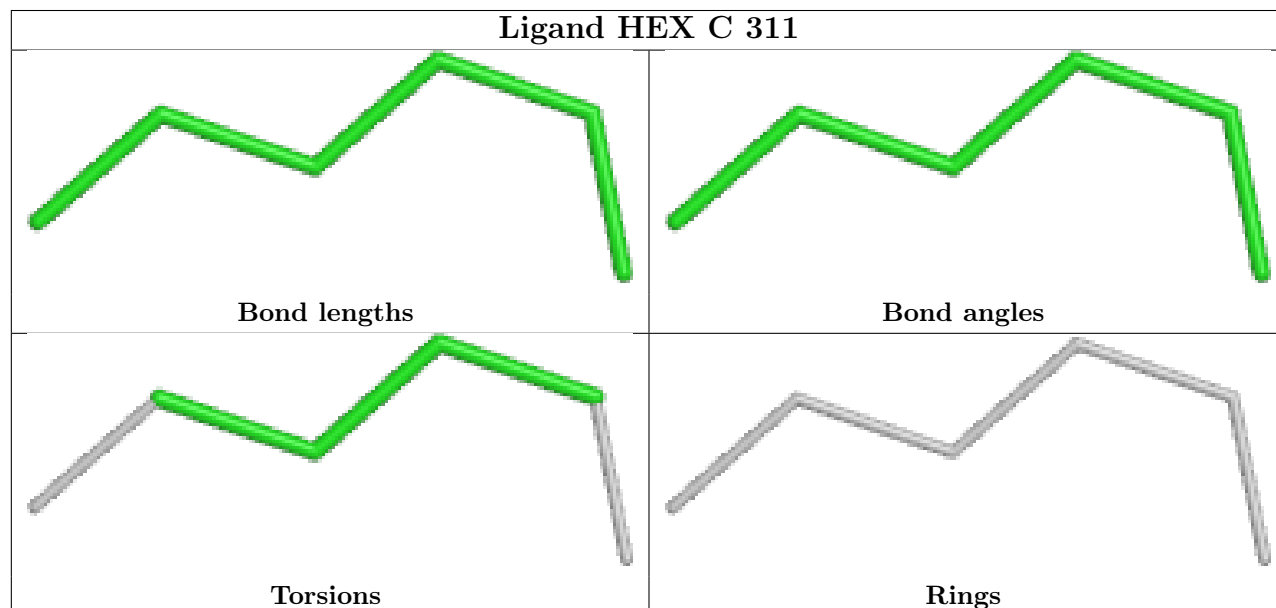
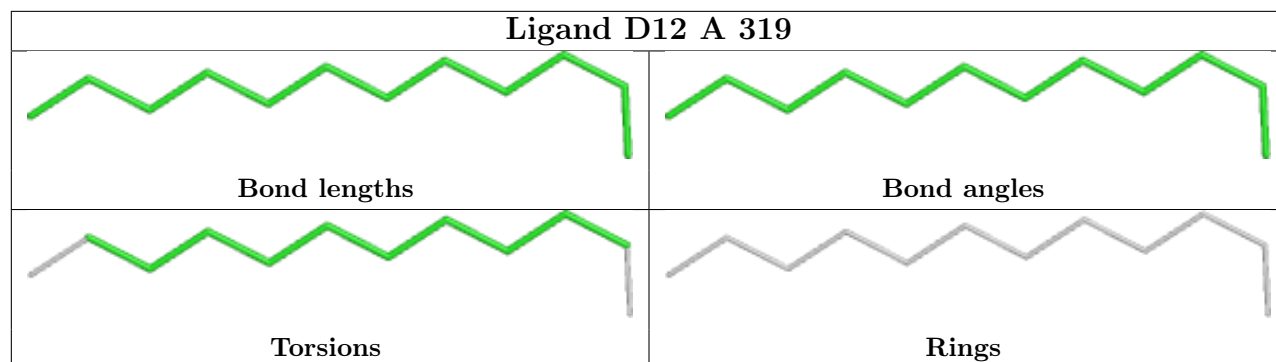
Ligand C14 B 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

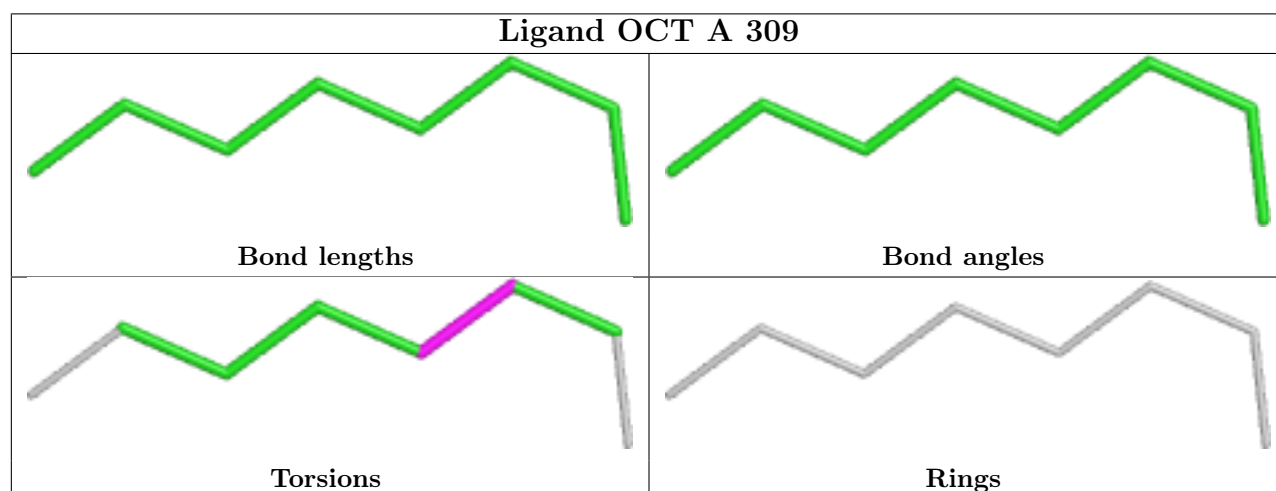
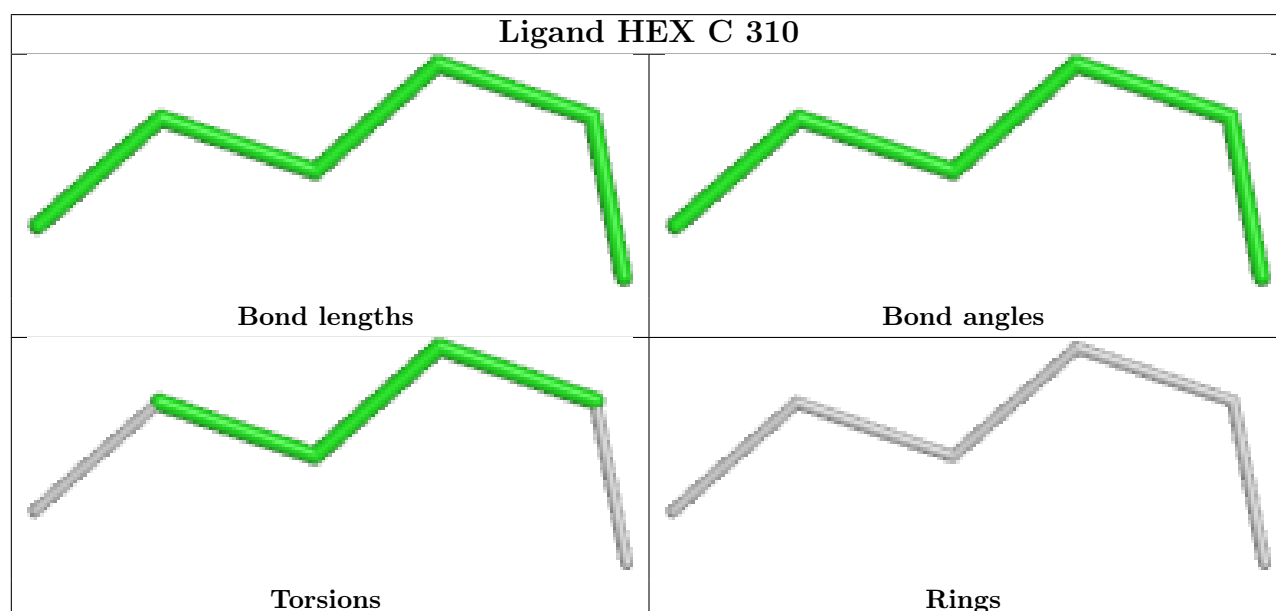
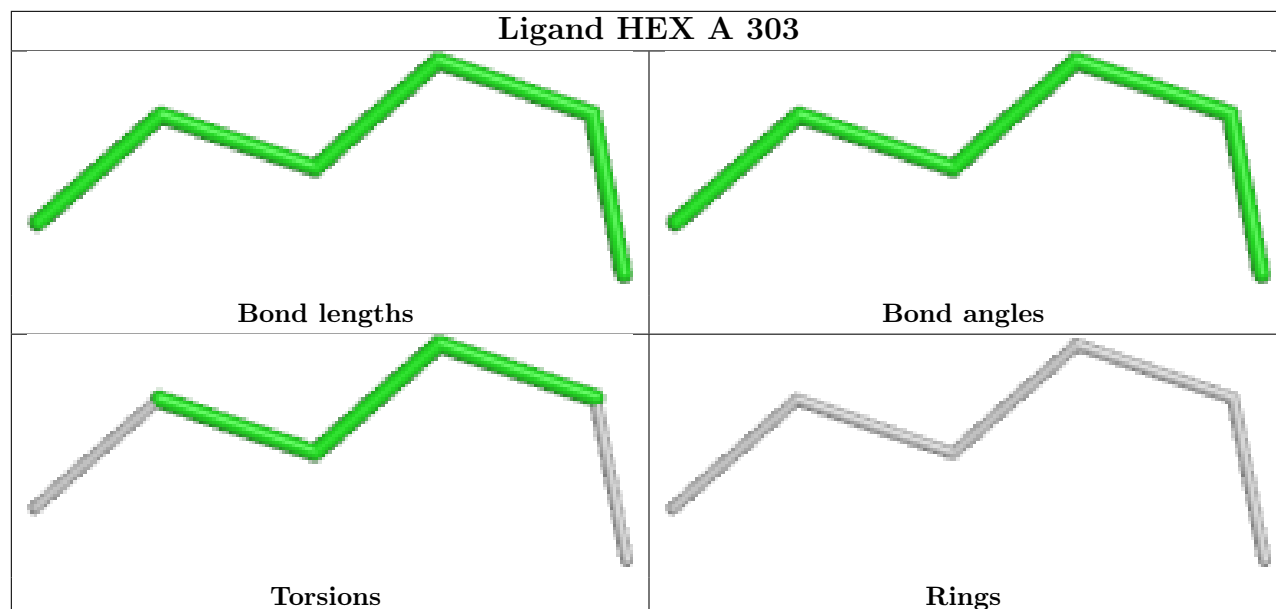
Ligand D12 B 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

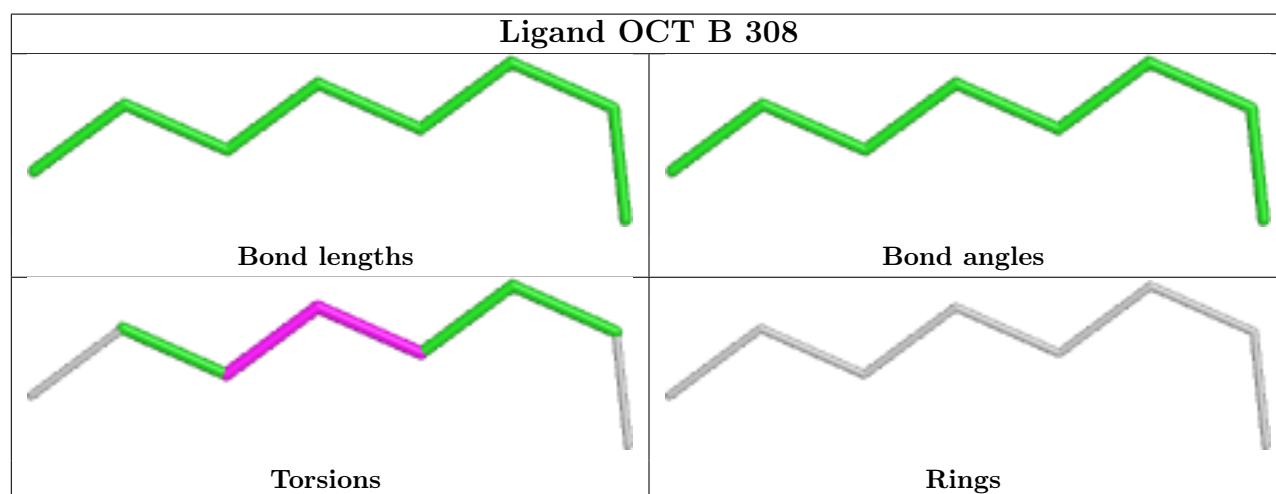
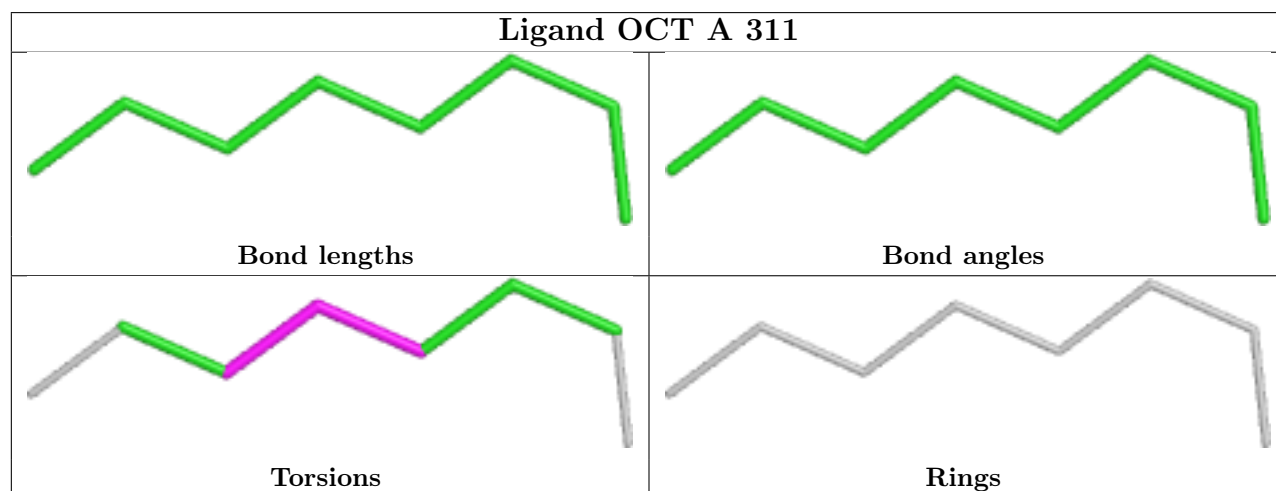
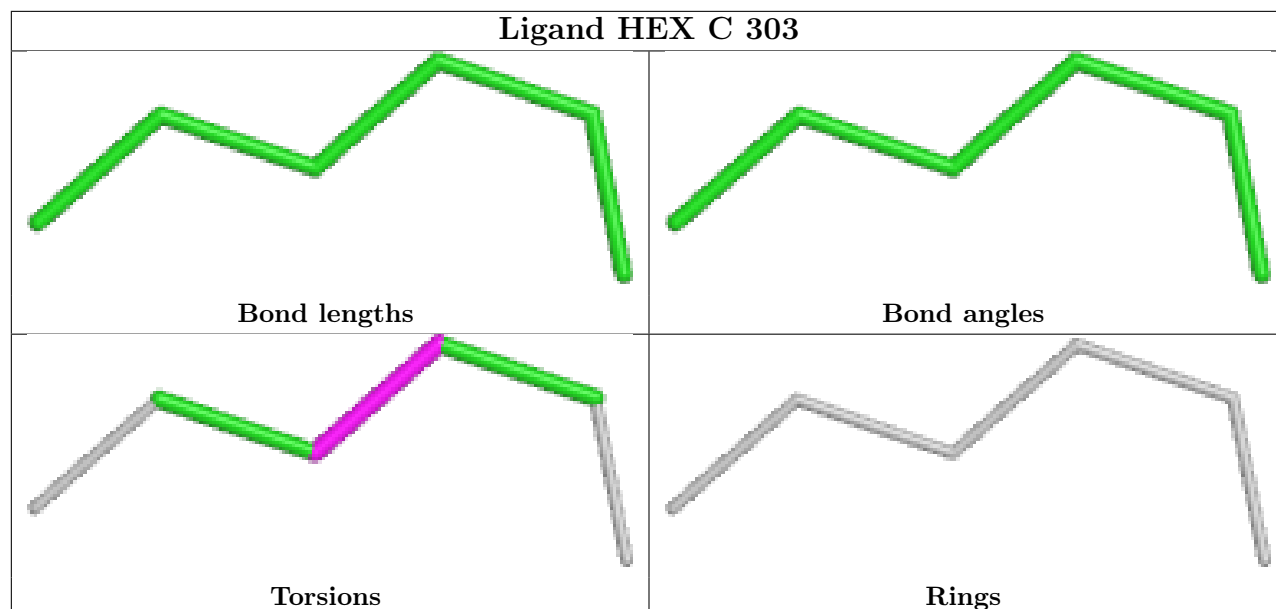
Ligand RET A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

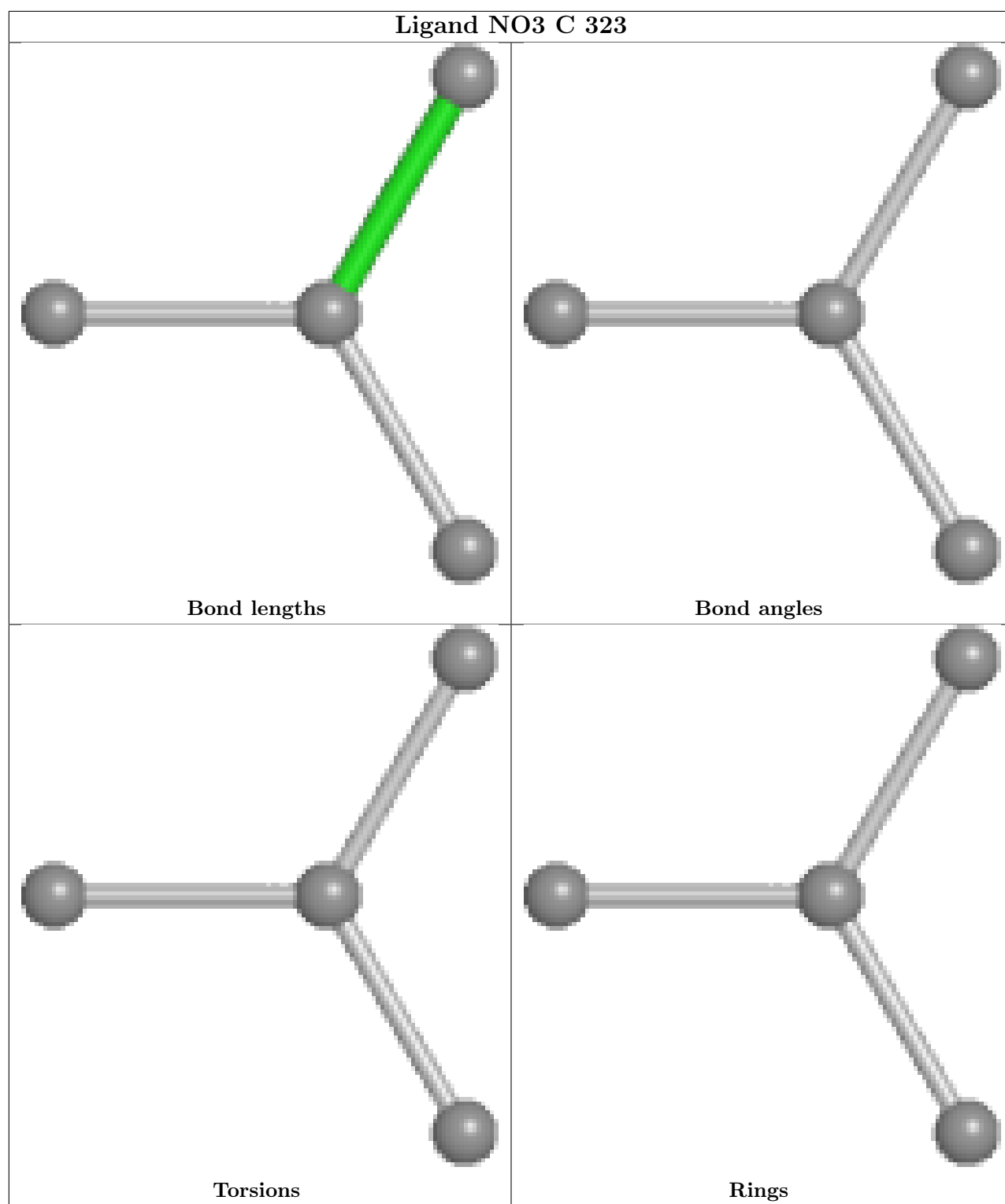


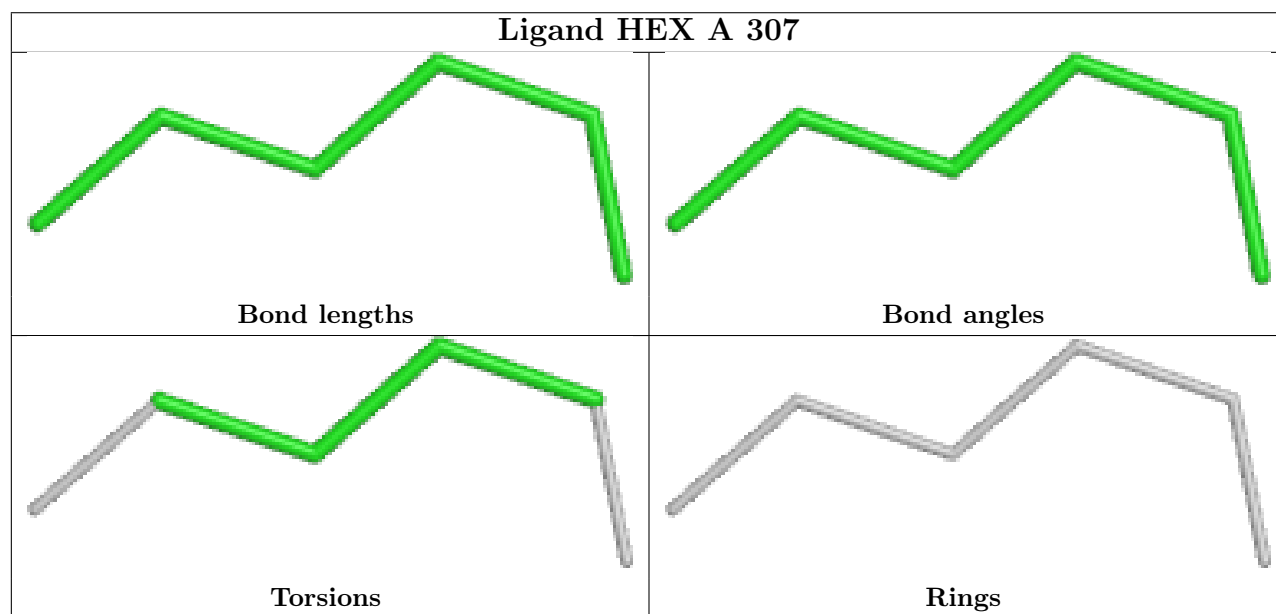
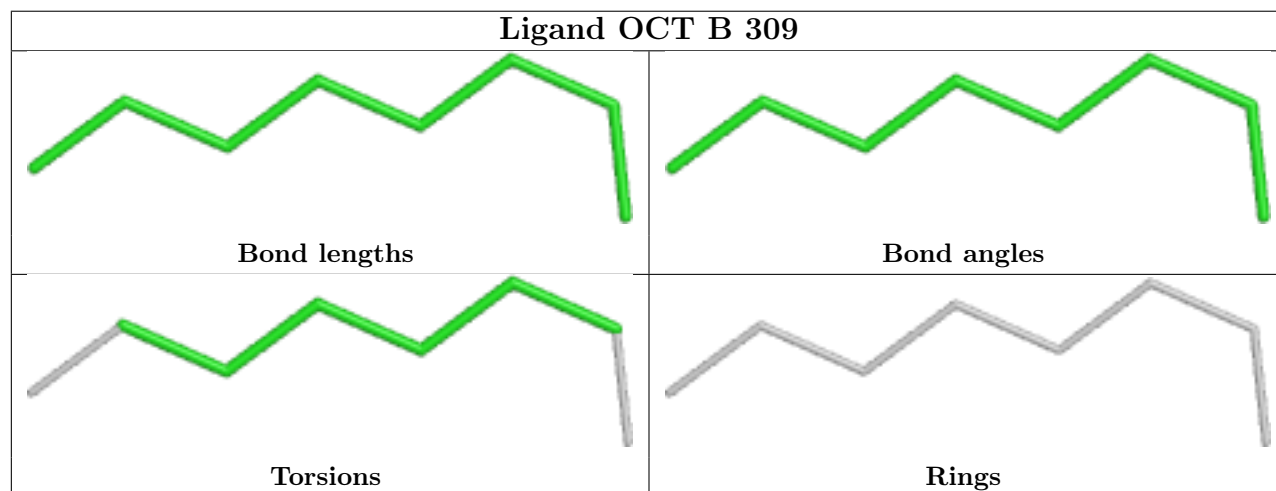
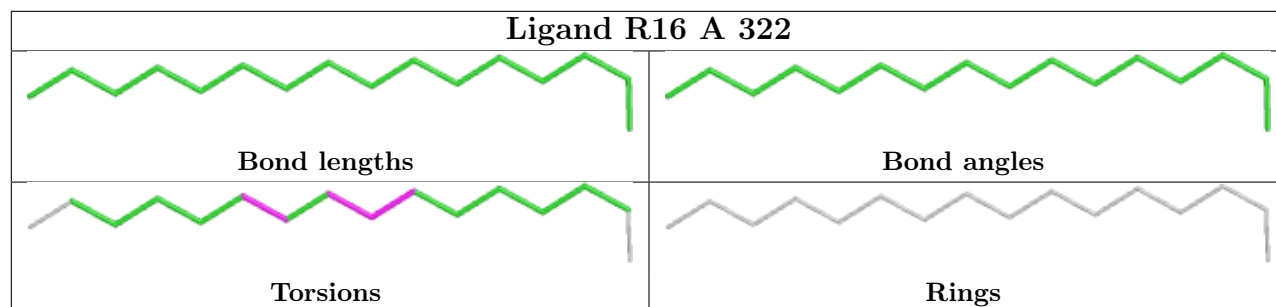


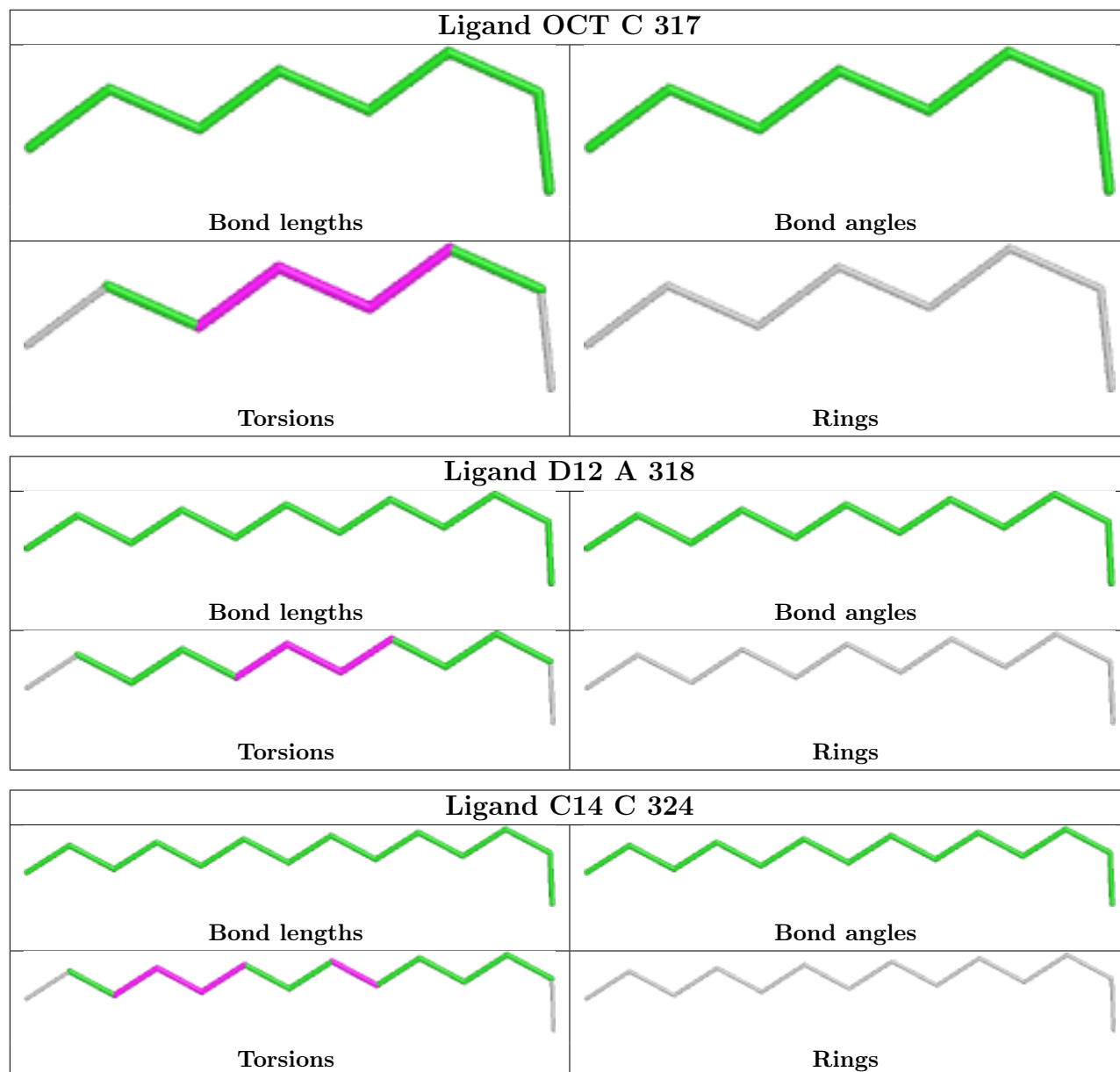


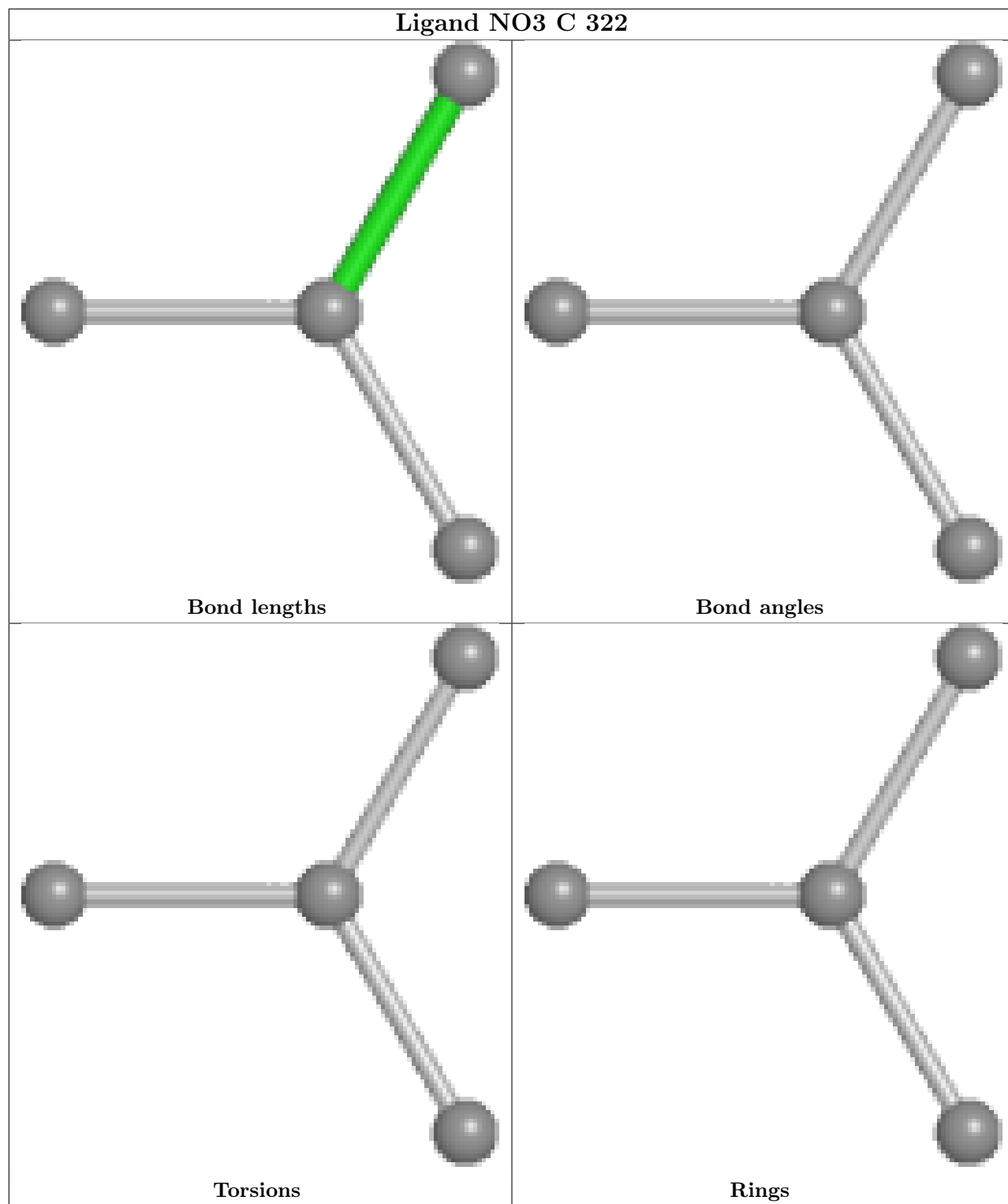


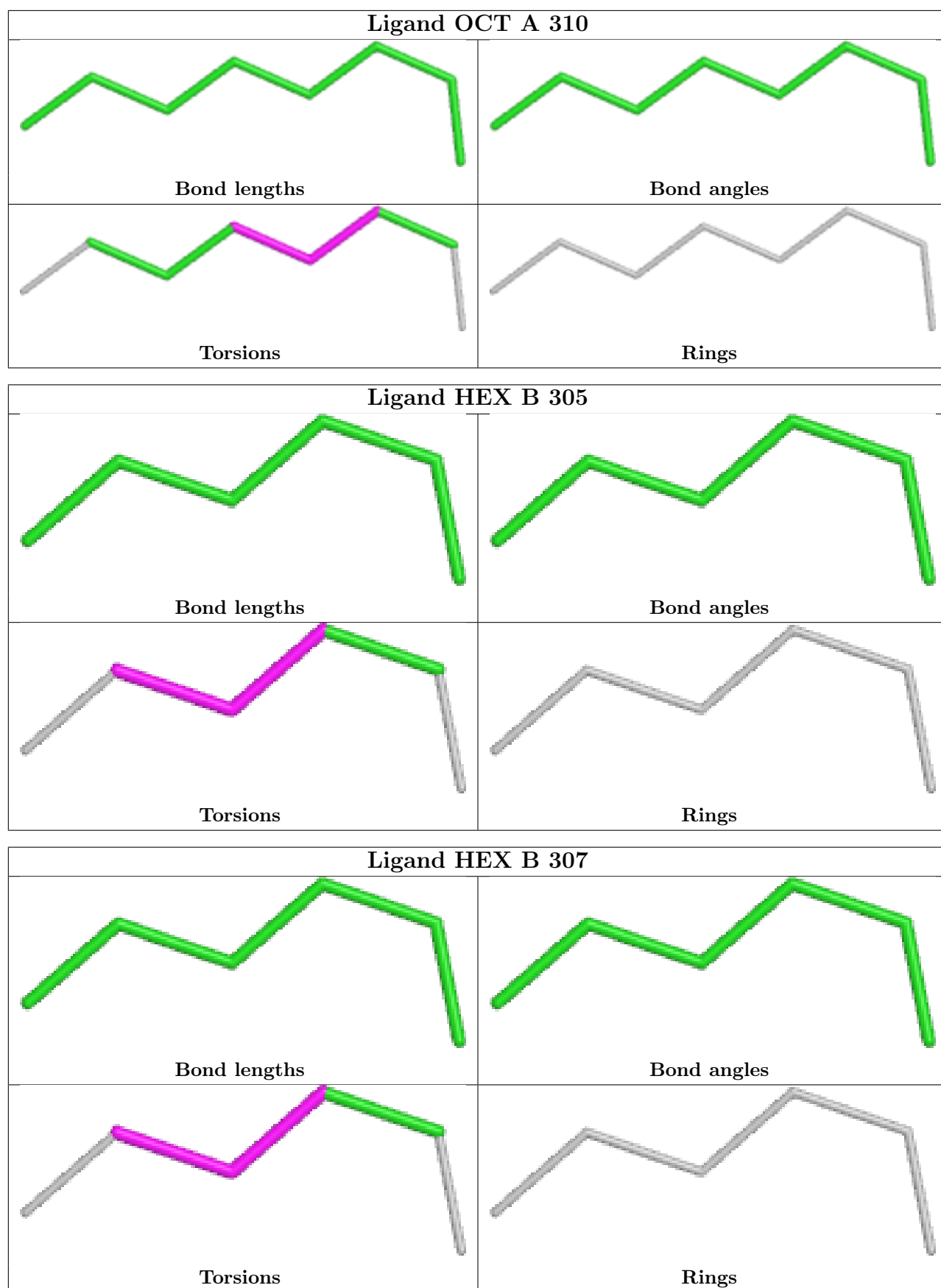


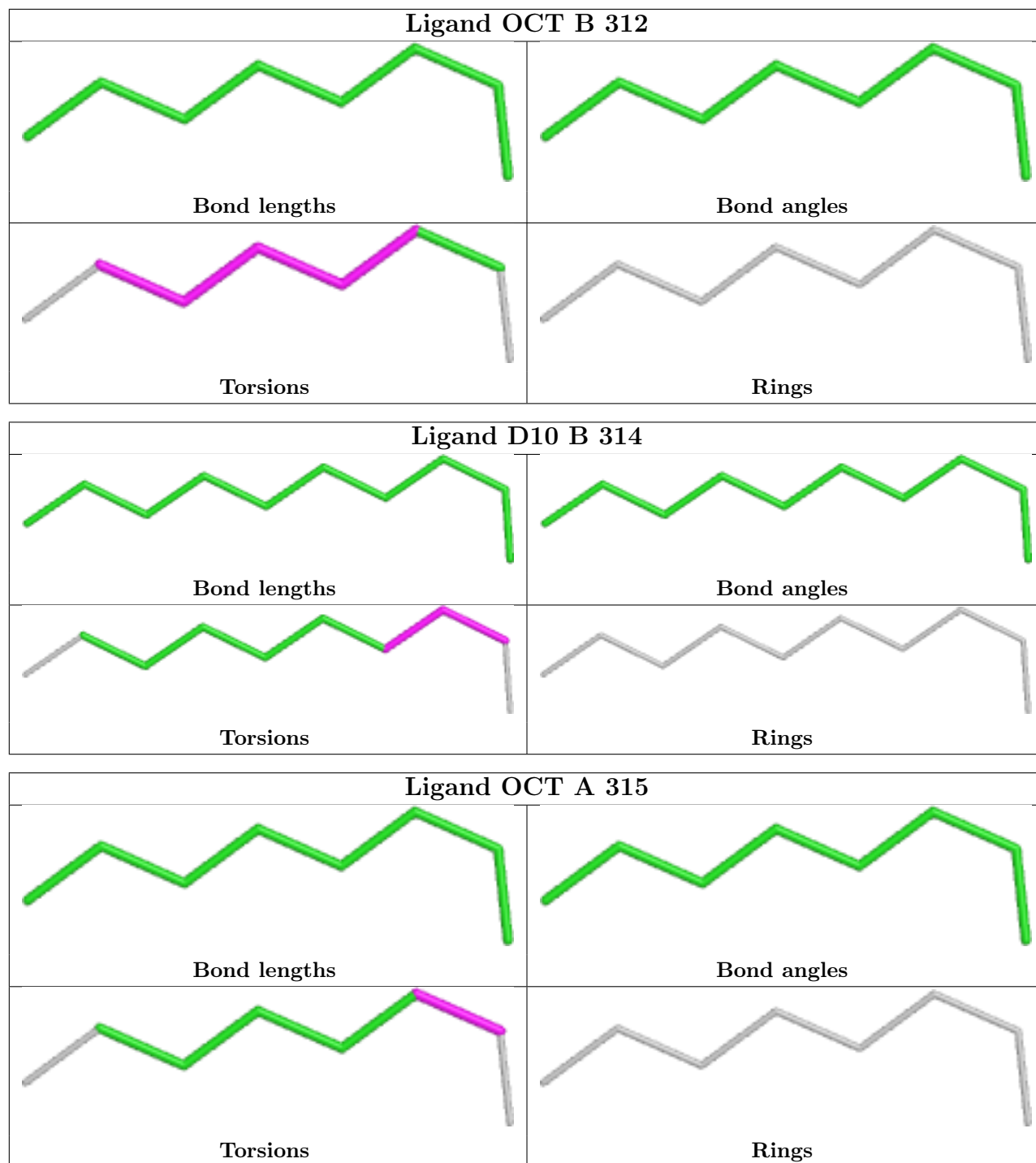


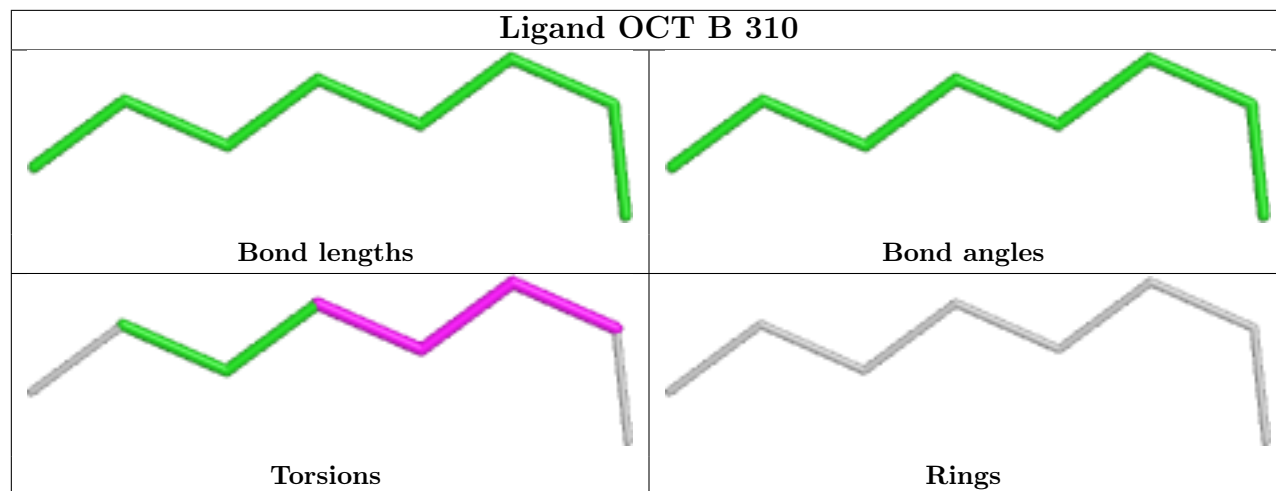
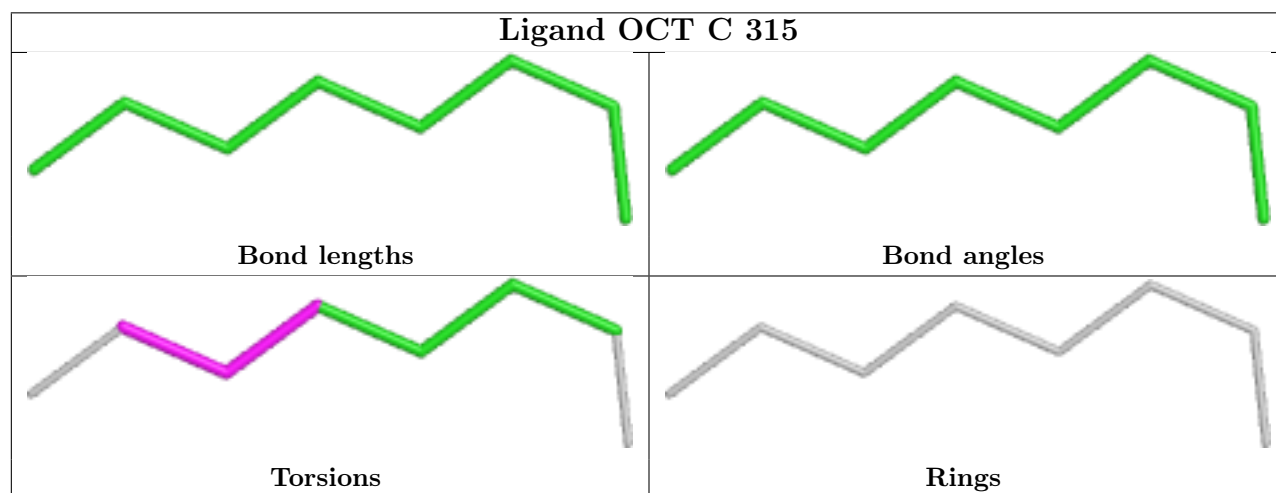
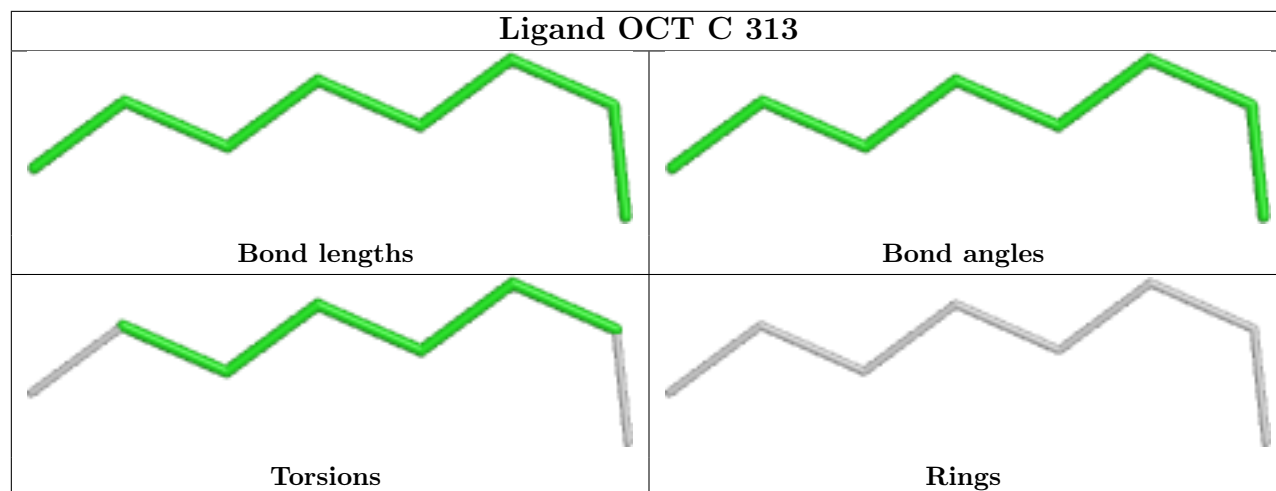


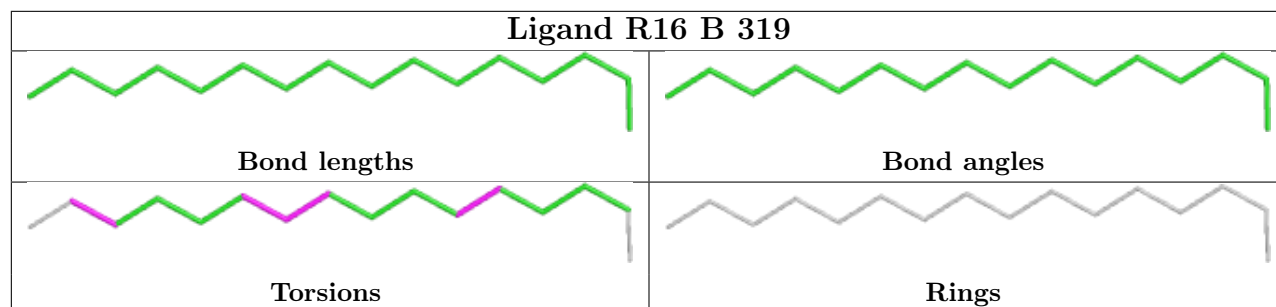
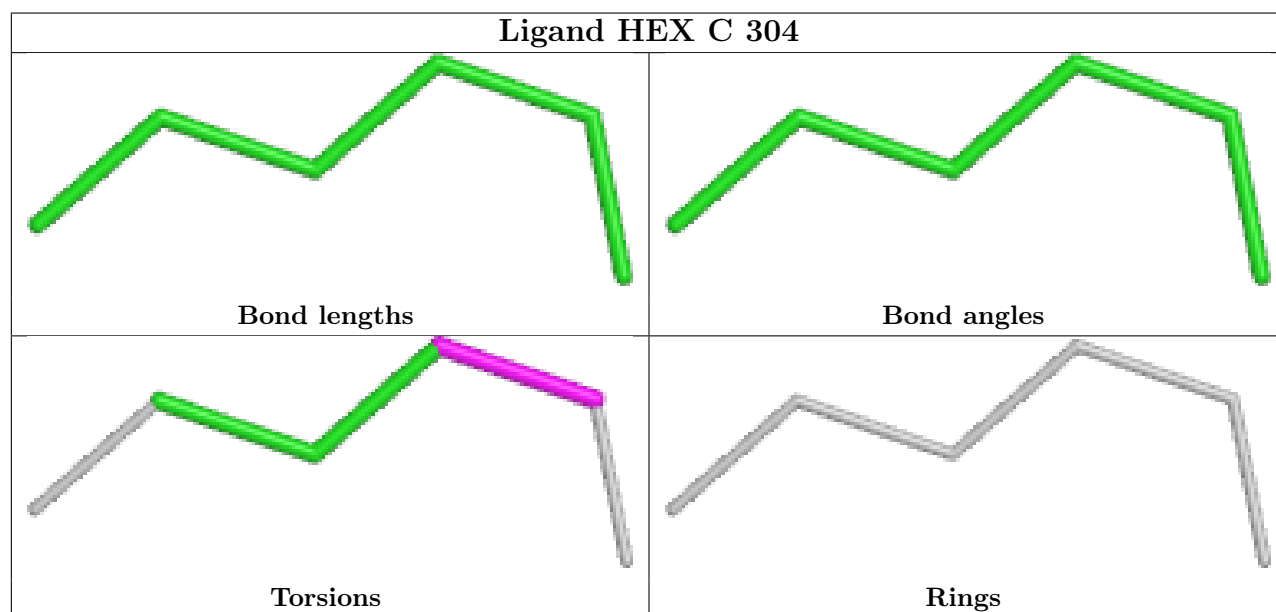
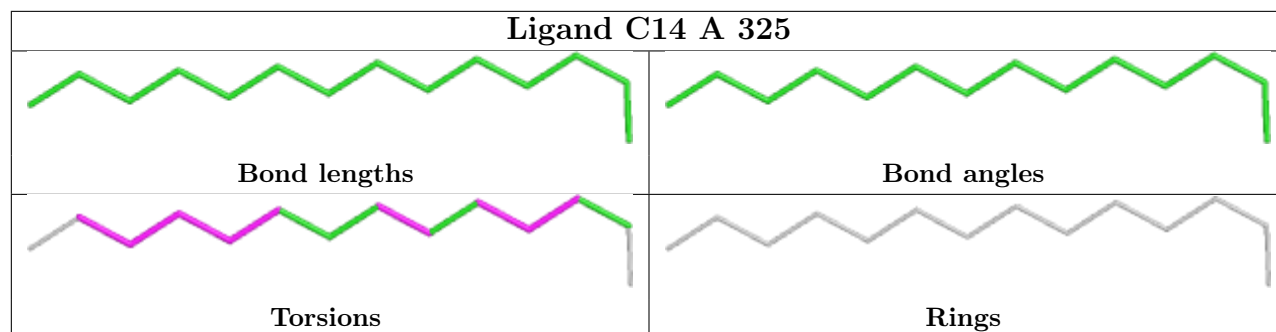


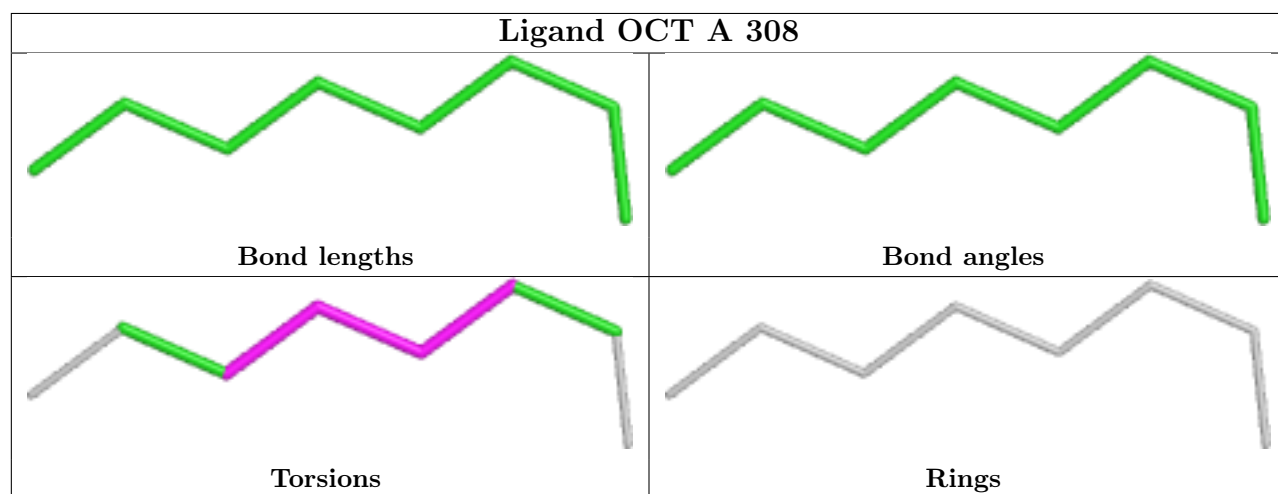
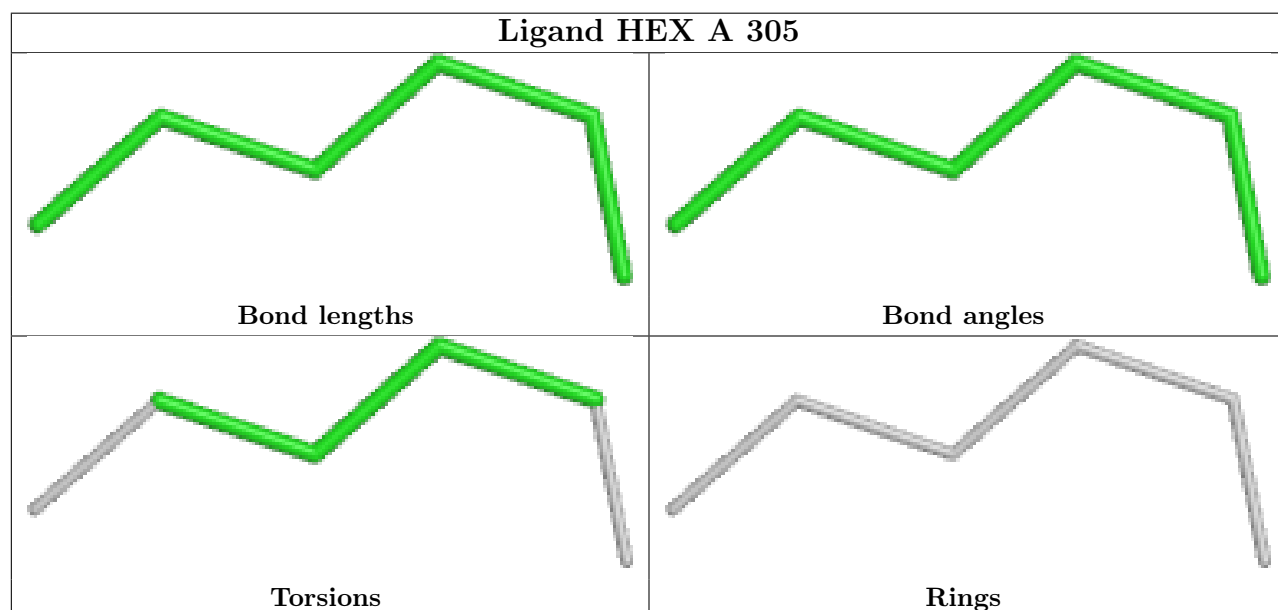
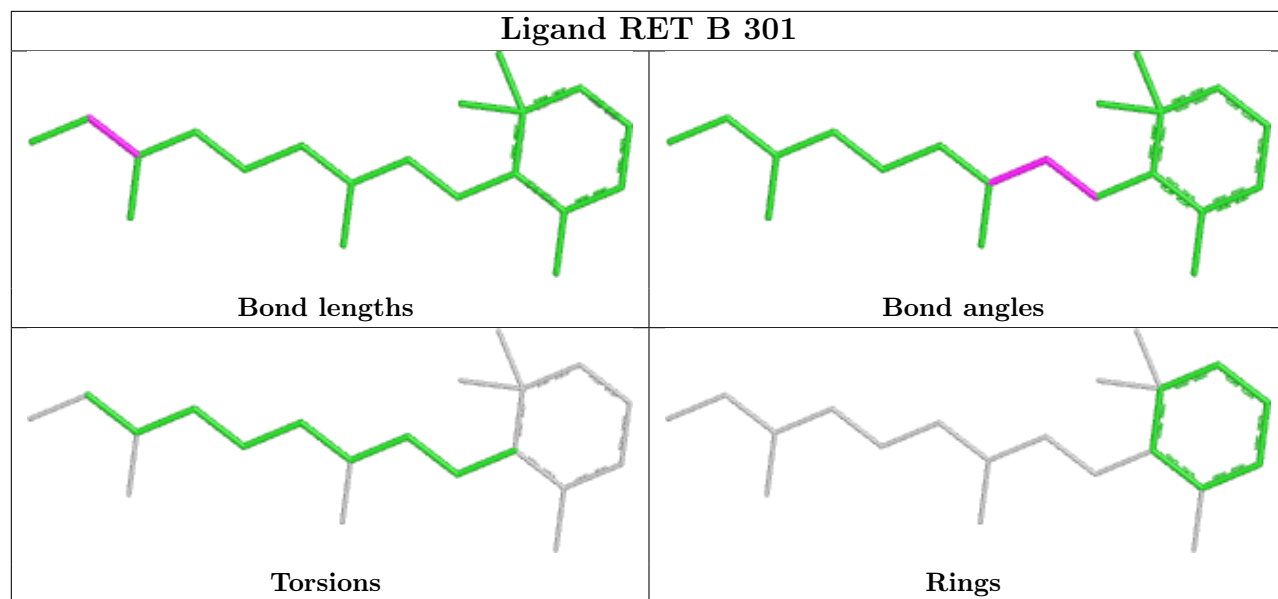


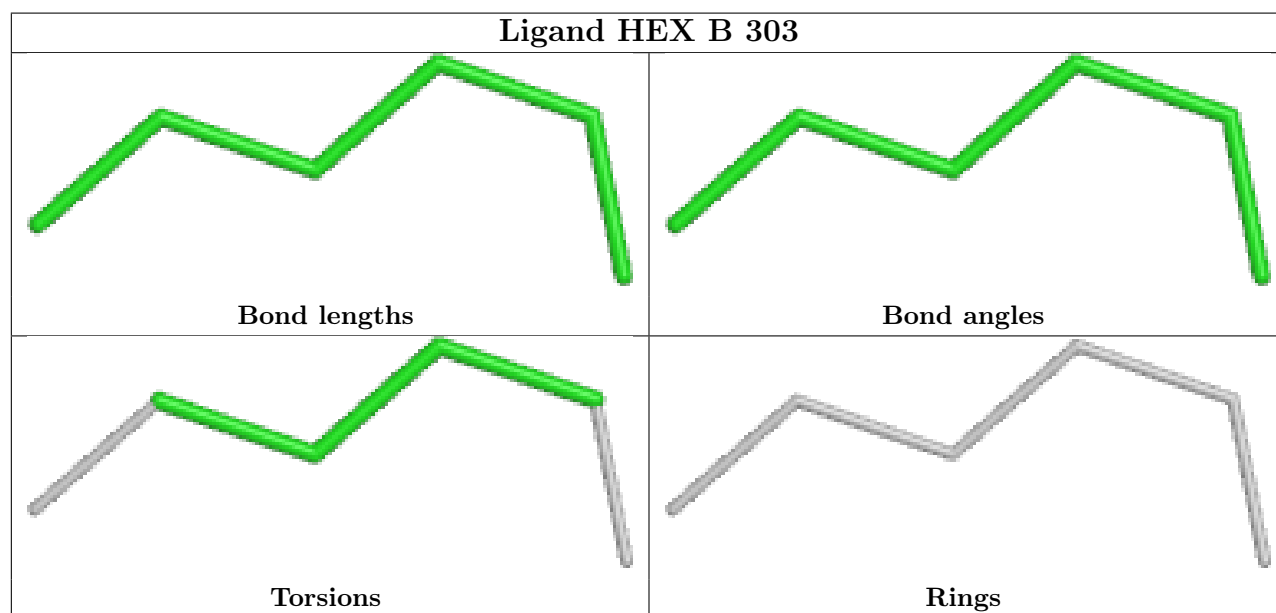
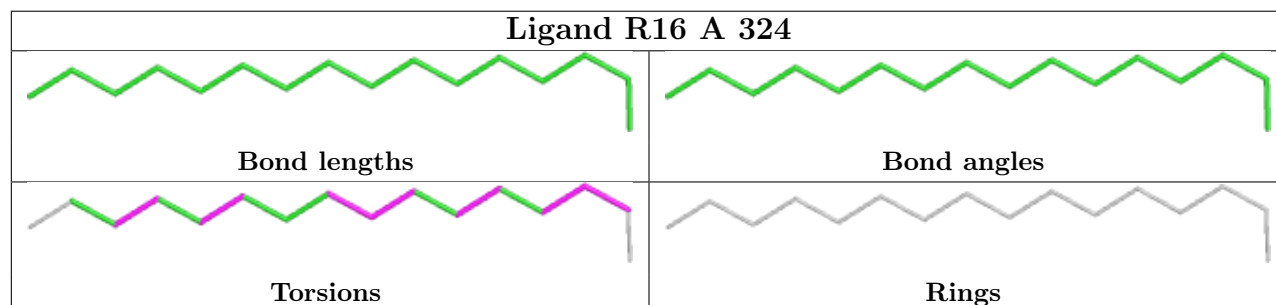
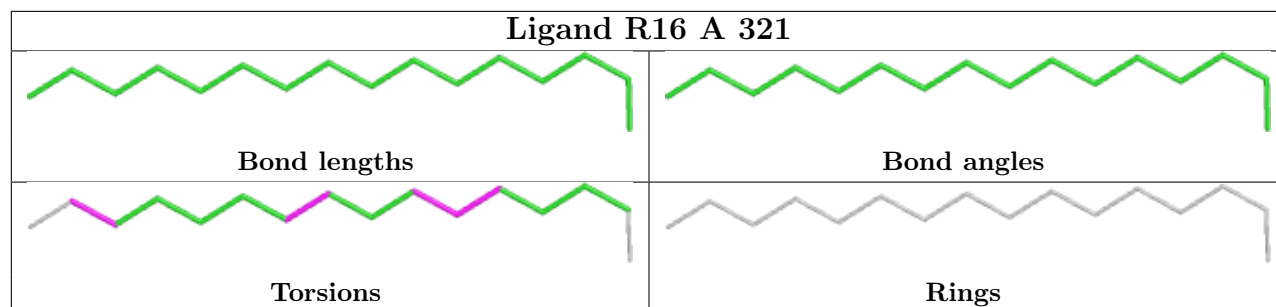


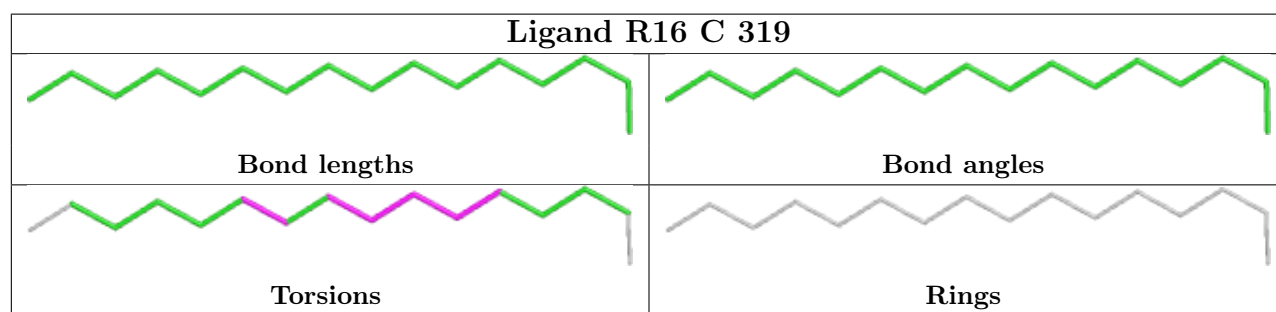
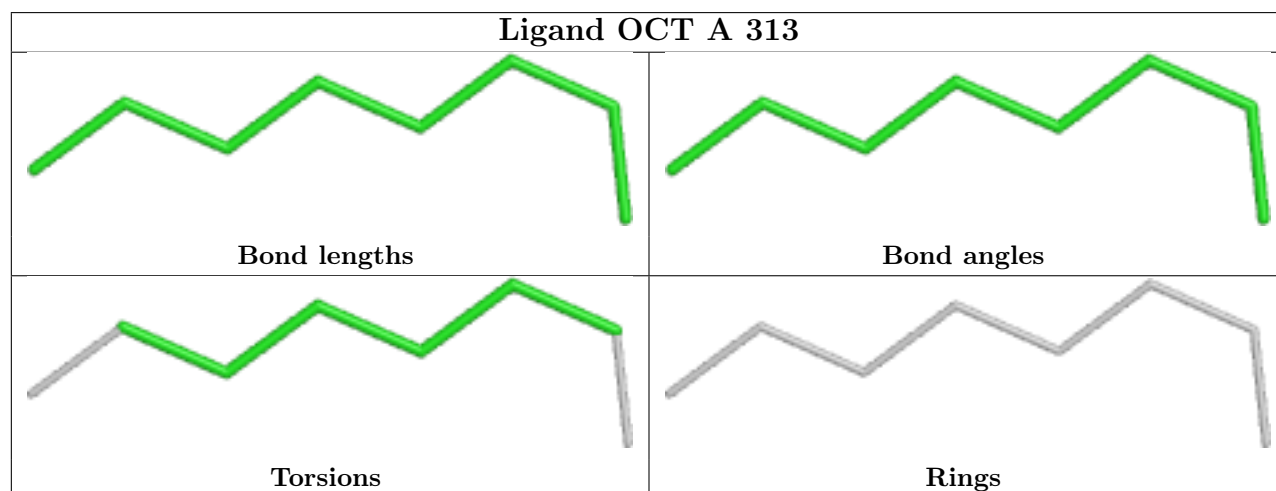
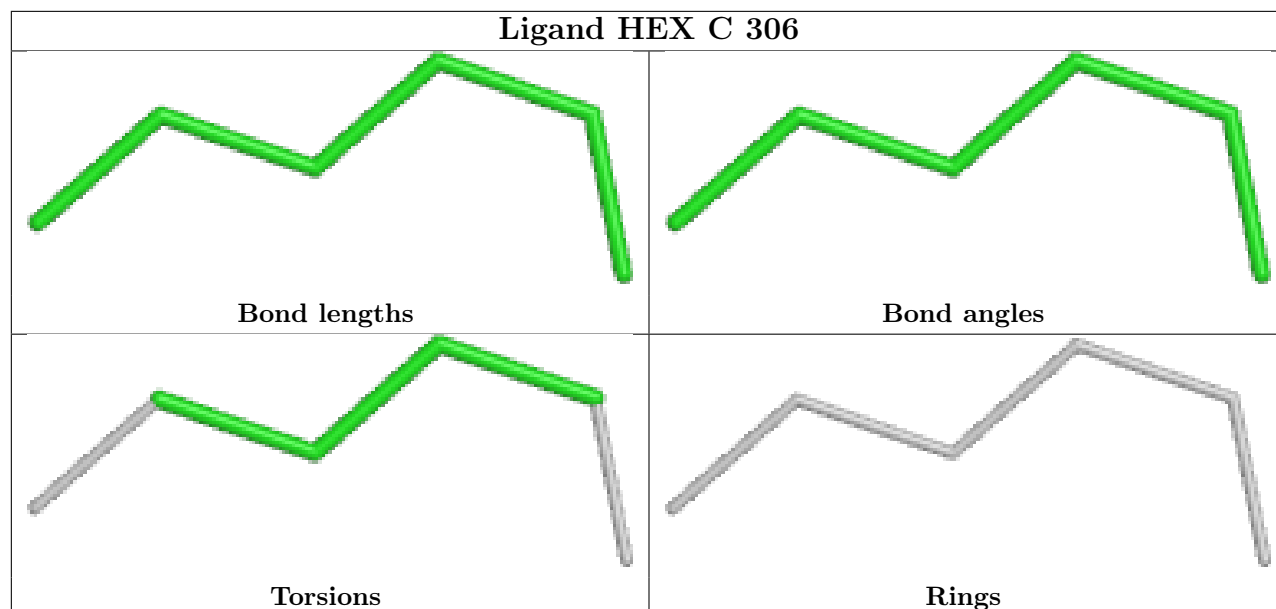


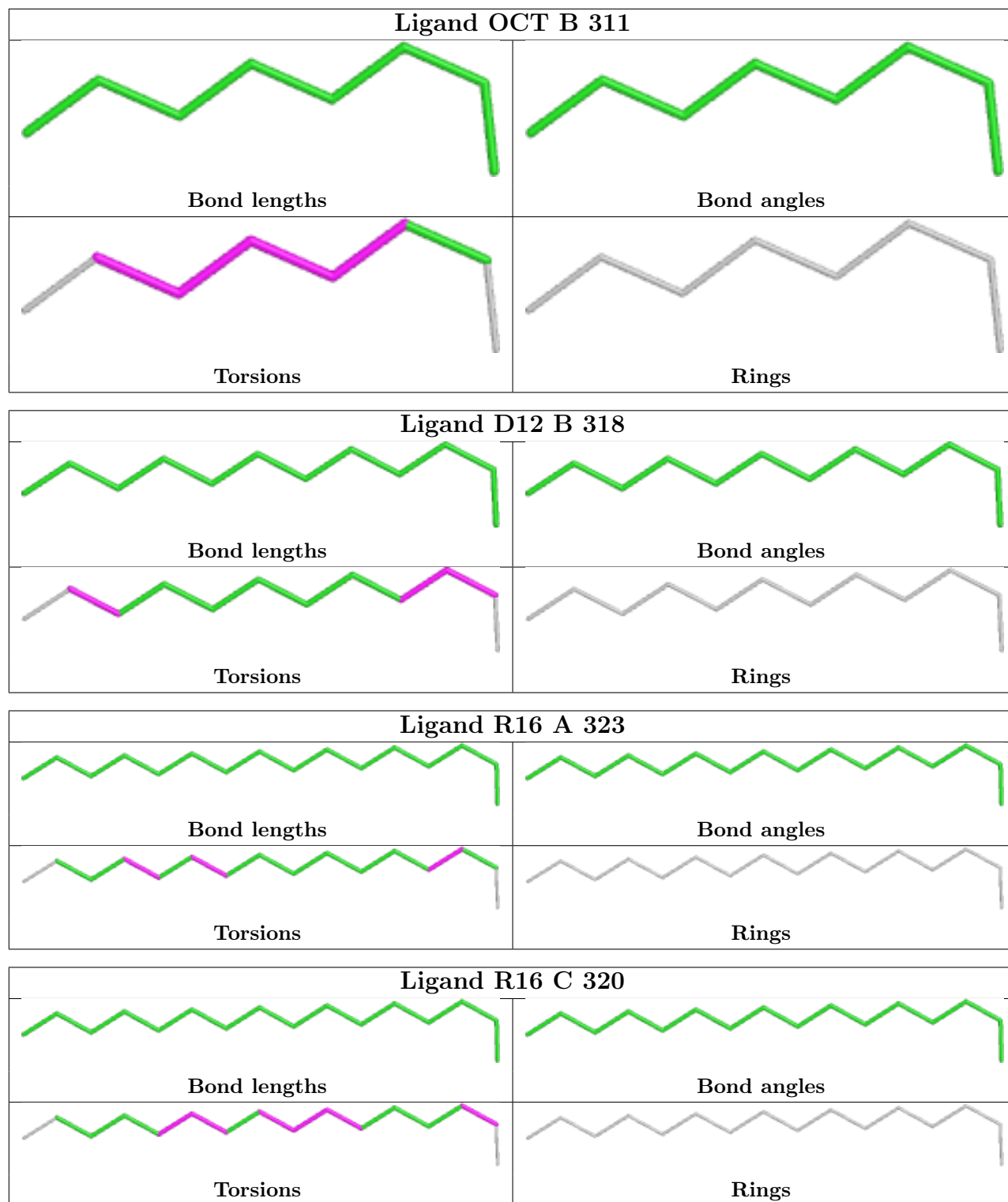


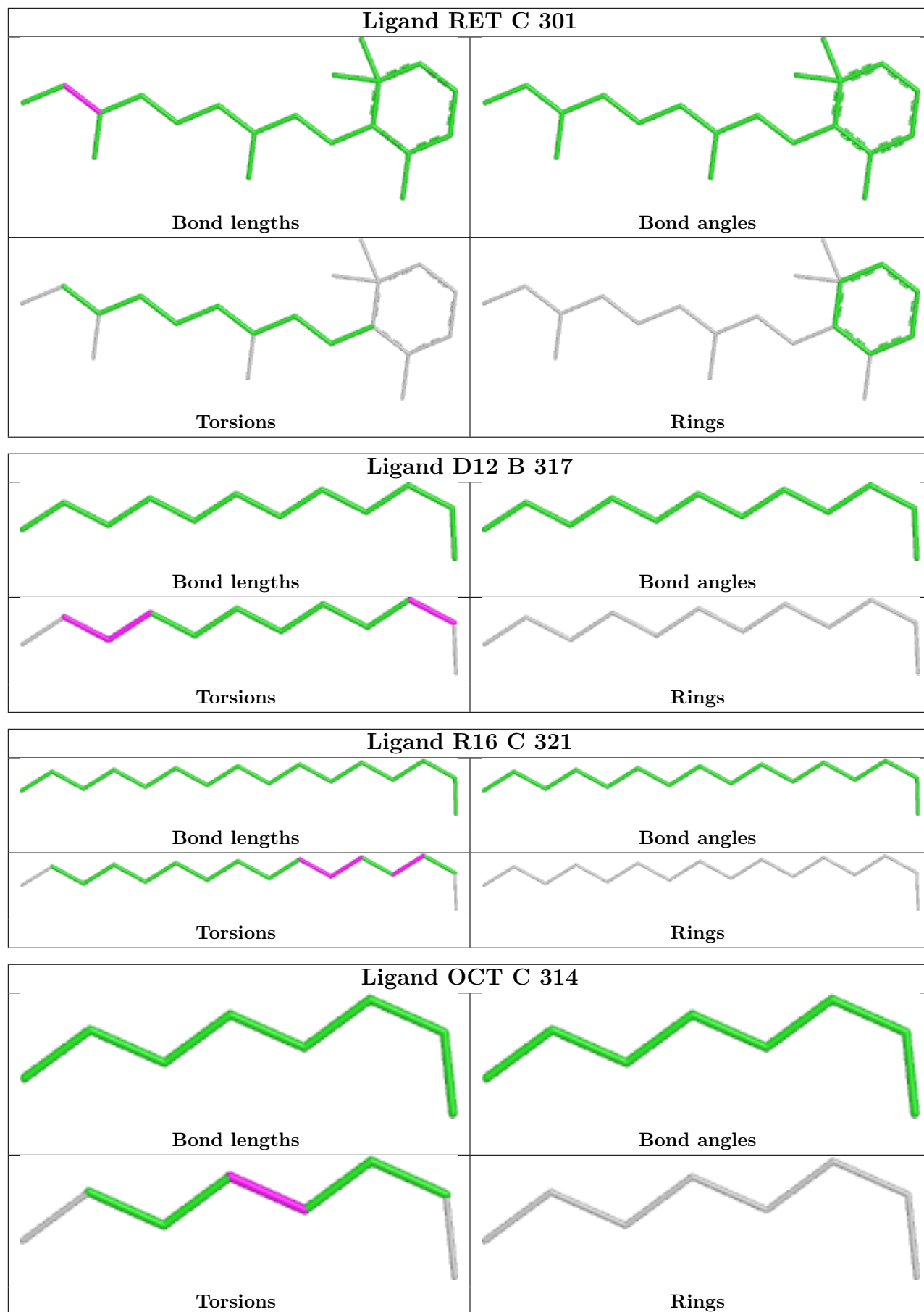


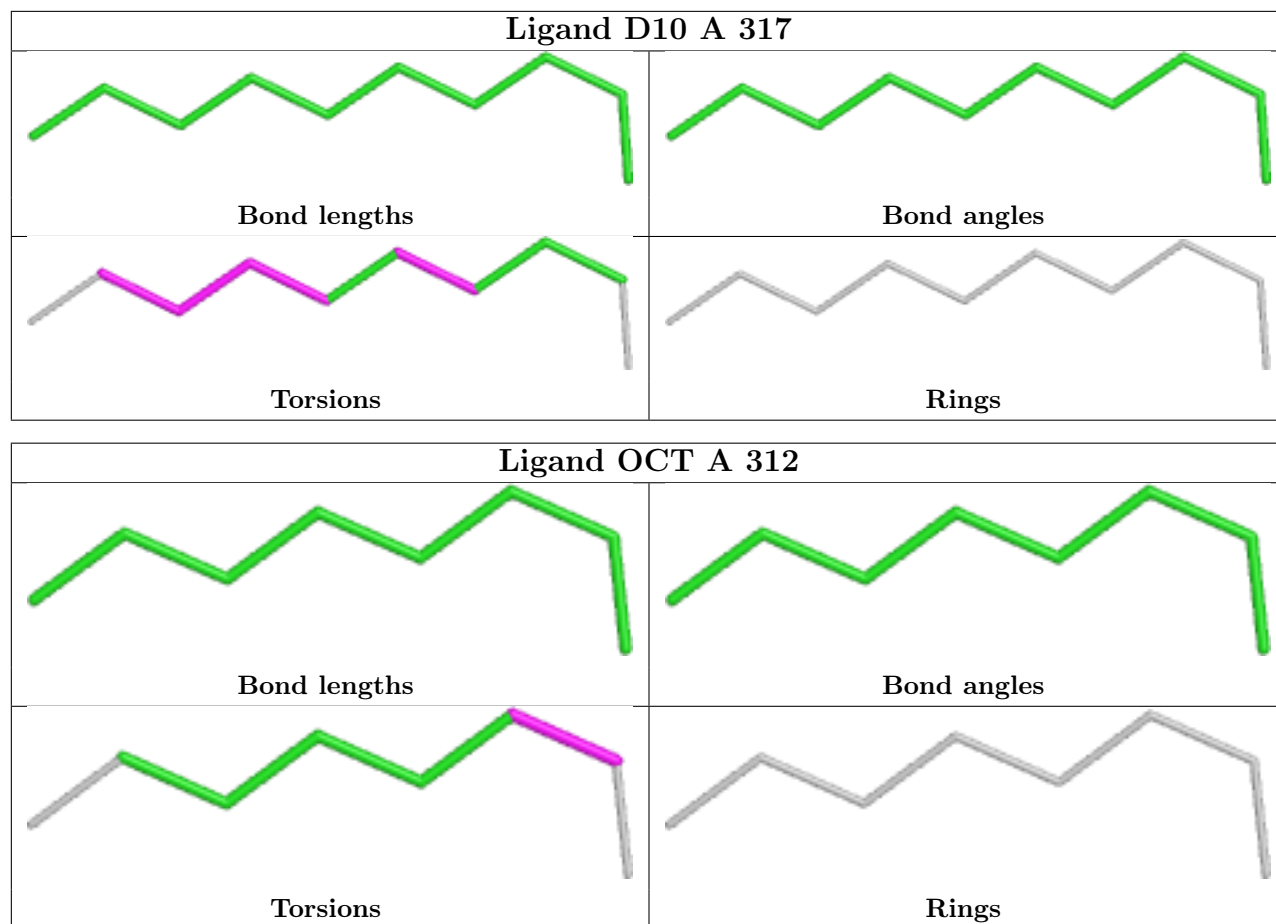












5.7 Other polymers [i](#)

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%)	0.02	8 (3%) 47 50	19, 27, 55, 90	0
1	B	226/259 (87%)	0.45	18 (7%) 18 19	21, 35, 74, 109	0
1	C	226/259 (87%)	0.09	11 (4%) 35 37	19, 28, 59, 101	0
All	All	678/777 (87%)	0.19	37 (5%) 30 32	19, 29, 65, 109	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	65	VAL	5.6
1	B	65	VAL	5.5
1	A	65	VAL	5.3
1	B	223	ALA	4.4
1	B	227	ASN	3.3
1	C	227	ASN	3.1
1	A	227	ASN	3.0
1	B	31	ARG	3.0
1	A	0	GLY	2.9
1	C	0	GLY	2.9
1	B	224	GLN	2.8
1	C	32	ARG	2.8
1	B	62	VAL	2.8
1	C	155	ASN	2.8
1	B	36	MET	2.8
1	A	184	ALA	2.7
1	C	44	PHE	2.5
1	B	64	PRO	2.5
1	A	187	PHE	2.4
1	B	187	PHE	2.4
1	B	0	GLY	2.4
1	B	96	ARG	2.4
1	B	68	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	34	GLU	2.3
1	B	225	ALA	2.3
1	A	31	ARG	2.3
1	C	224	GLN	2.3
1	B	155	ASN	2.3
1	A	96	ARG	2.2
1	B	226	SER	2.2
1	A	97	PRO	2.2
1	C	36	MET	2.1
1	C	31	ARG	2.1
1	B	220	GLU	2.0
1	C	34	GLU	2.0
1	C	184	ALA	2.0
1	B	188	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	OCT	A	311	8/8	0.67	0.36	51,66,68,68	0
5	OCT	B	313	8/8	0.68	0.32	48,58,68,68	0
4	HEX	B	306	6/6	0.71	0.33	60,64,64,70	0
8	R16	C	321	16/16	0.71	0.24	42,54,57,59	0
4	HEX	C	305	6/6	0.72	0.25	55,56,61,62	0
4	HEX	C	307	6/6	0.73	0.29	60,62,65,66	0
9	C14	C	324	14/14	0.73	0.23	48,53,60,61	0
4	HEX	B	304	6/6	0.76	0.23	67,67,68,68	0
6	D10	B	315	10/10	0.77	0.24	52,65,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OCT	A	309	8/8	0.77	0.23	55,59,63,64	0
5	OCT	A	310	8/8	0.77	0.23	43,55,58,59	0
4	HEX	A	306	6/6	0.79	0.21	49,52,54,56	0
7	D12	A	319	12/12	0.80	0.21	48,55,61,63	0
7	D12	C	318	12/12	0.80	0.20	39,46,57,60	0
8	R16	A	320	16/16	0.80	0.19	47,55,64,64	0
8	R16	A	321	16/16	0.80	0.21	40,50,56,56	0
4	HEX	C	310	6/6	0.80	0.24	51,56,63,63	0
4	HEX	B	305	6/6	0.80	0.19	32,54,60,64	0
5	OCT	B	312	8/8	0.81	0.20	49,56,59,62	0
7	D12	B	317	12/12	0.82	0.20	49,52,63,65	0
4	HEX	C	308	6/6	0.82	0.22	55,60,64,65	0
5	OCT	C	317	8/8	0.83	0.22	55,61,64,70	0
8	R16	A	322	16/16	0.83	0.24	54,61,68,68	0
8	R16	A	323	16/16	0.83	0.21	47,55,69,70	0
8	R16	A	324	16/16	0.83	0.20	37,54,62,63	0
4	HEX	C	312	6/6	0.83	0.20	51,53,54,55	0
5	OCT	A	314	8/8	0.83	0.18	33,42,49,49	0
8	R16	C	319	16/16	0.84	0.20	46,58,61,62	0
4	HEX	C	309	6/6	0.84	0.21	49,52,58,62	0
8	R16	B	319	16/16	0.84	0.22	51,61,69,71	0
5	OCT	C	315	8/8	0.85	0.23	49,58,65,65	0
5	OCT	C	316	8/8	0.85	0.17	36,41,50,52	0
5	OCT	A	312	8/8	0.85	0.18	45,51,56,59	0
6	D10	A	316	10/10	0.85	0.23	53,56,66,66	0
8	R16	C	320	16/16	0.85	0.23	49,56,63,64	0
6	D10	A	317	10/10	0.85	0.20	52,60,72,72	0
5	OCT	C	314	8/8	0.85	0.19	49,53,55,57	0
5	OCT	B	308	8/8	0.86	0.20	50,53,58,60	0
7	D12	A	318	12/12	0.86	0.16	38,50,56,57	0
5	OCT	A	308	8/8	0.86	0.24	51,53,57,58	0
4	HEX	B	307	6/6	0.86	0.23	57,59,65,68	0
6	D10	B	314	10/10	0.86	0.18	34,46,60,62	0
7	D12	B	318	12/12	0.87	0.17	41,55,62,63	0
5	OCT	B	311	8/8	0.87	0.21	51,66,67,69	0
4	HEX	C	311	6/6	0.87	0.17	48,50,53,53	0
4	HEX	C	304	6/6	0.87	0.22	44,47,56,57	0
5	OCT	C	313	8/8	0.87	0.14	33,41,51,54	0
3	MG	B	302	1/1	0.87	0.12	52,52,52,52	0
7	D12	B	316	12/12	0.88	0.17	47,55,59,63	0
9	C14	B	320	14/14	0.88	0.17	47,53,62,65	0
4	HEX	A	307	6/6	0.88	0.17	58,58,61,61	0

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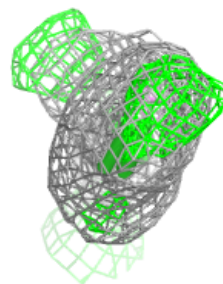
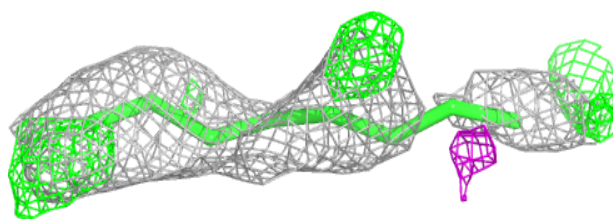
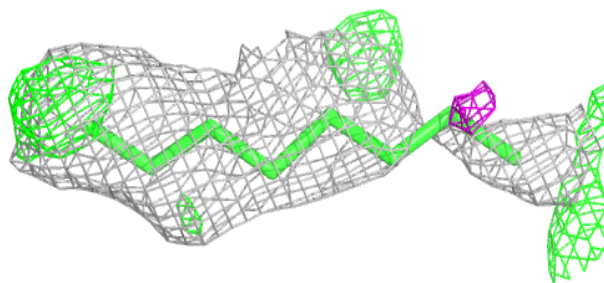
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HEX	C	303	6/6	0.89	0.17	46,47,50,56	0
4	HEX	A	303	6/6	0.89	0.19	42,49,50,54	0
4	HEX	A	304	6/6	0.89	0.15	41,47,56,60	0
9	C14	A	325	14/14	0.89	0.18	44,51,58,59	0
4	HEX	C	306	6/6	0.89	0.21	45,49,56,57	0
5	OCT	A	315	8/8	0.89	0.17	45,50,57,61	0
4	HEX	B	303	6/6	0.90	0.17	50,53,53,55	0
5	OCT	B	309	8/8	0.90	0.18	48,52,59,60	0
10	NO3	C	322	4/4	0.90	0.10	58,58,59,60	0
10	NO3	C	323	4/4	0.90	0.11	50,53,57,60	0
4	HEX	A	305	6/6	0.91	0.17	37,42,55,64	0
5	OCT	B	310	8/8	0.91	0.17	55,58,62,63	0
5	OCT	A	313	8/8	0.92	0.16	35,46,57,59	0
3	MG	C	302	1/1	0.92	0.24	47,47,47,47	0
2	RET	C	301	20/21	0.94	0.07	16,19,23,24	0
2	RET	A	301	20/21	0.95	0.06	18,20,23,25	0
3	MG	A	302	1/1	0.96	0.14	46,46,46,46	0
2	RET	B	301	20/21	0.96	0.06	19,21,25,26	0

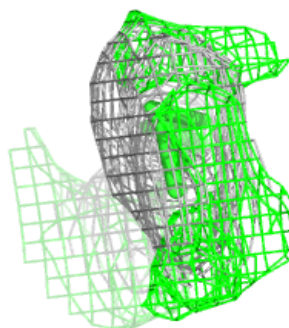
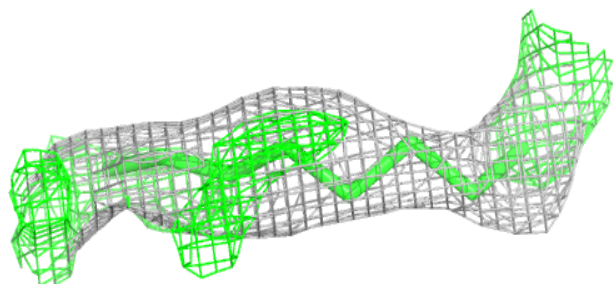
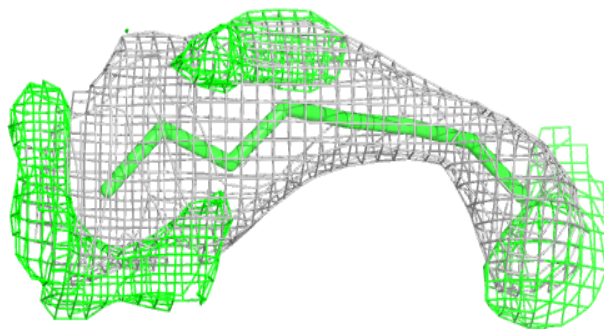
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

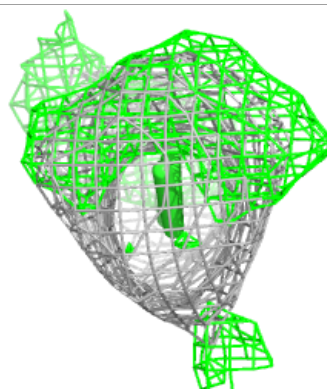
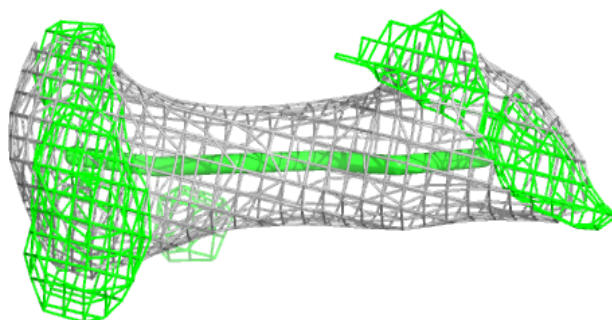
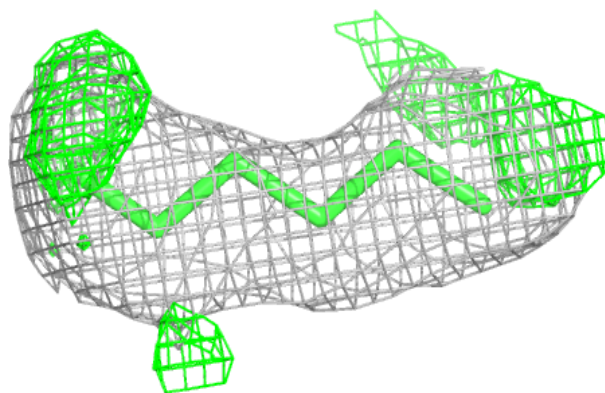
**Electron density around OCT B 313:**

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

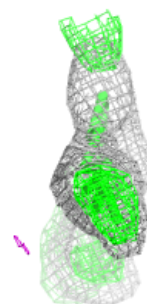
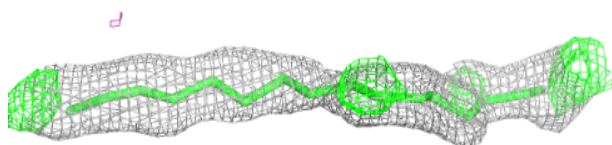
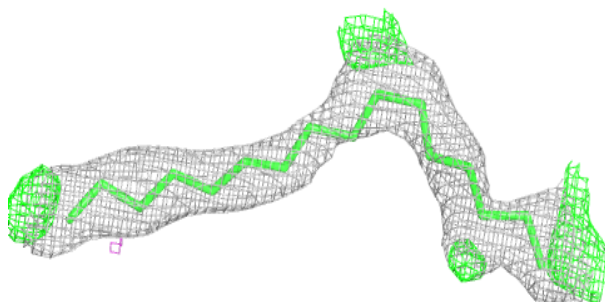


Electron density around HEX B 306:

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

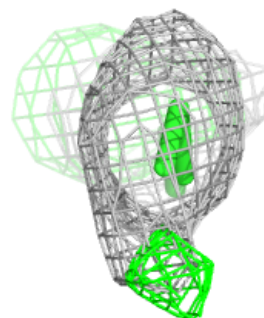
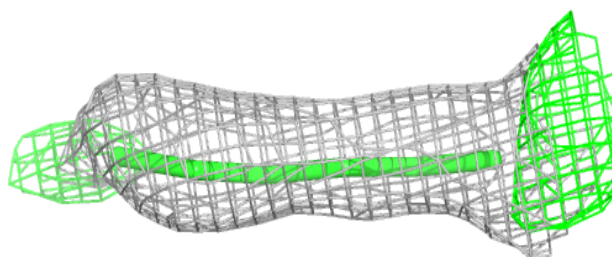
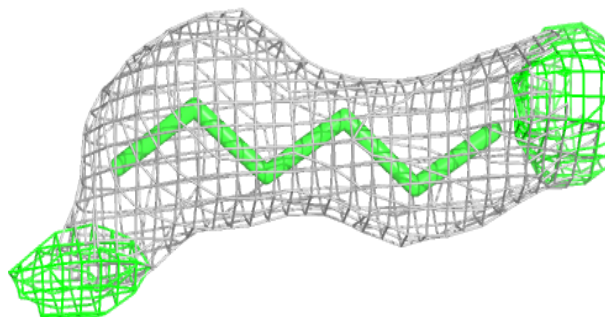
**Electron density around R16 C 321:**

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

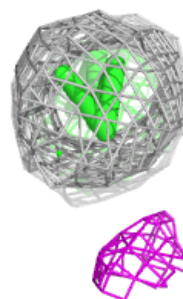
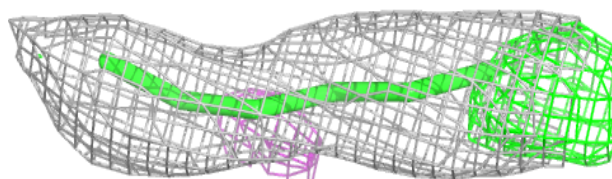
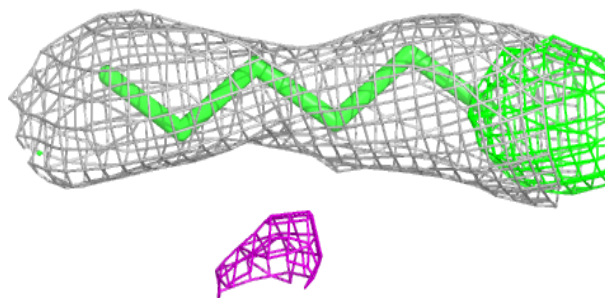


Electron density around HEX C 305:

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

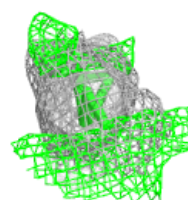
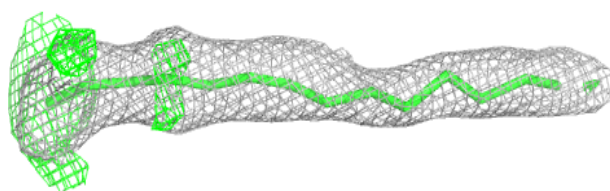
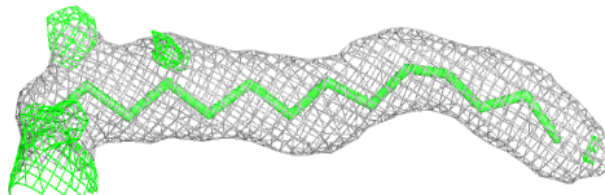
**Electron density around HEX C 307:**

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

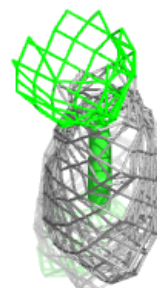
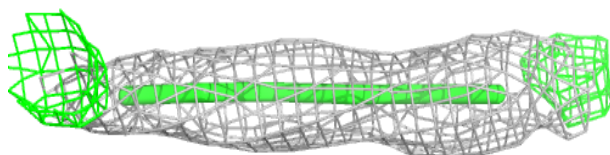
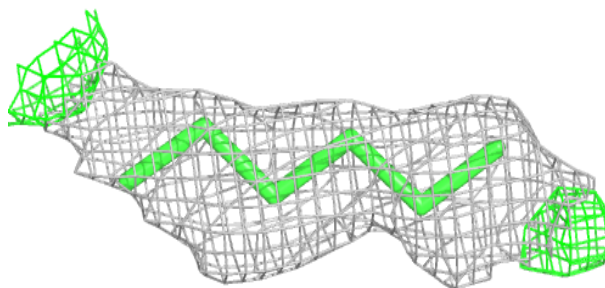


Electron density around C14 C 324:

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

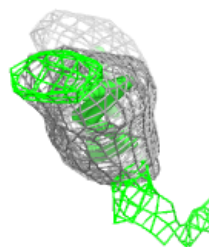
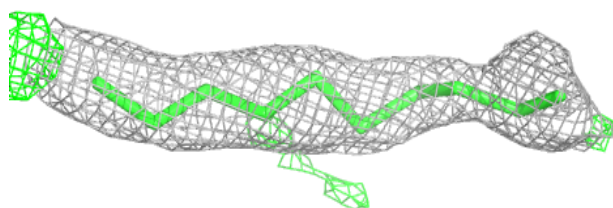
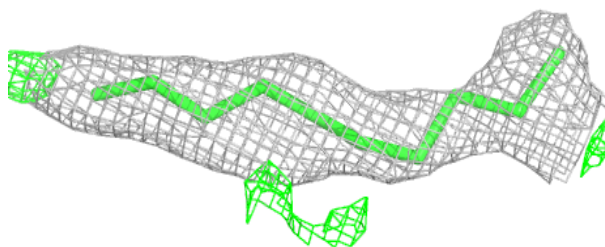
**Electron density around HEX B 304:**

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

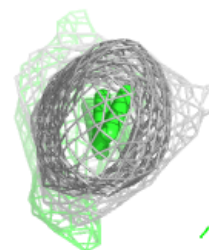
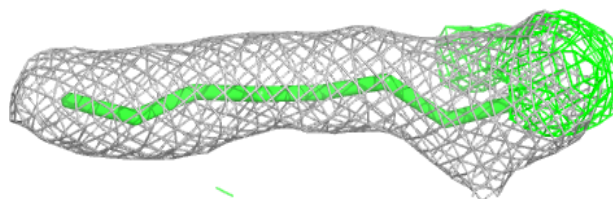
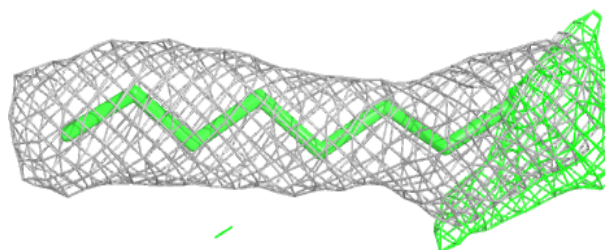


Electron density around D10 B 315:

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

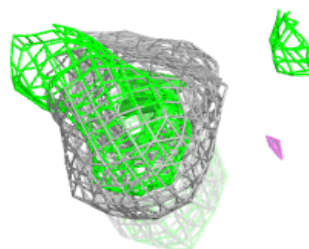
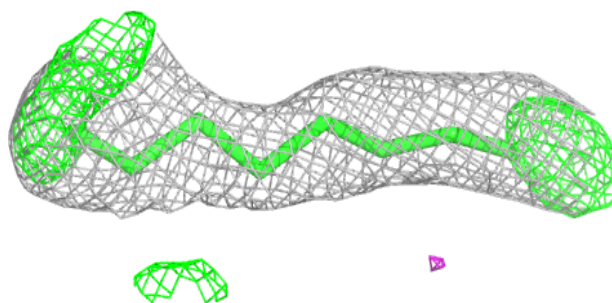
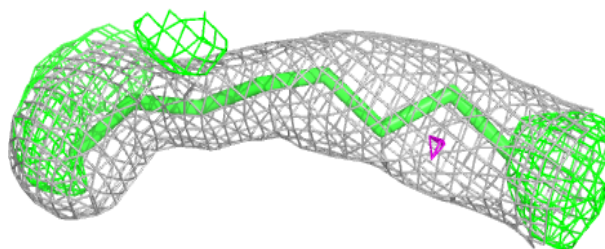
**Electron density around OCT A 309:**

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

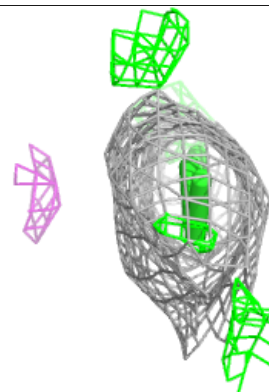
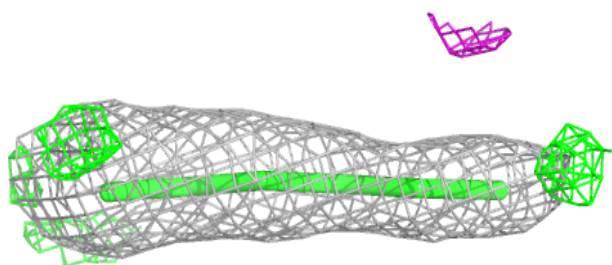
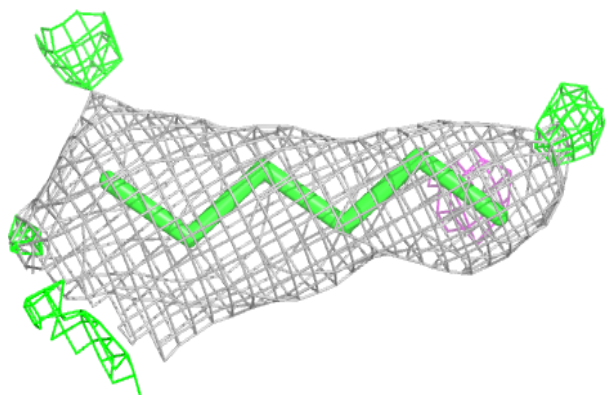


Electron density around OCT A 310:

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

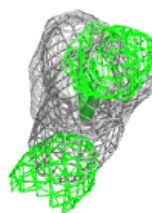
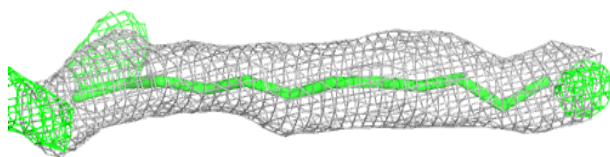
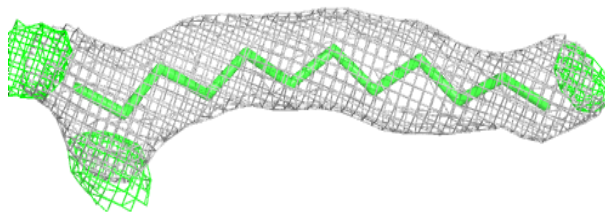
**Electron density around HEX A 306:**

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

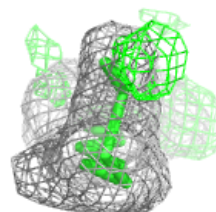
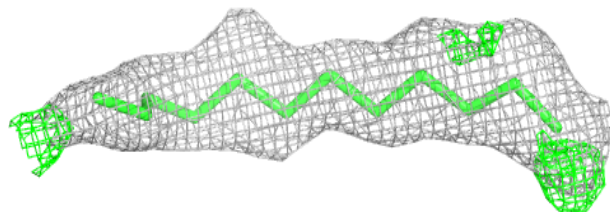
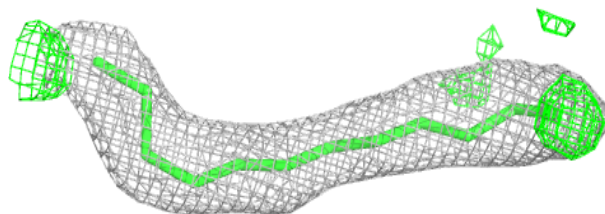


Electron density around D12 A 319:

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

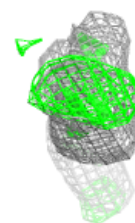
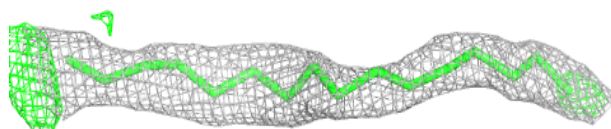
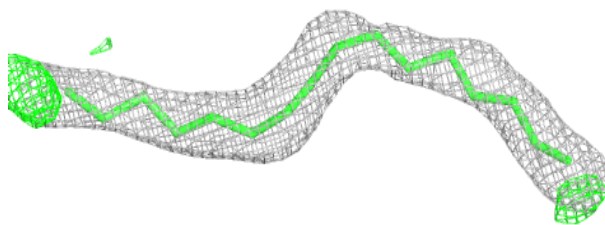
**Electron density around D12 C 318:**

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

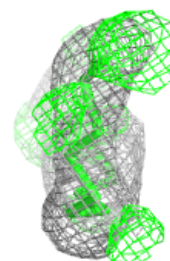
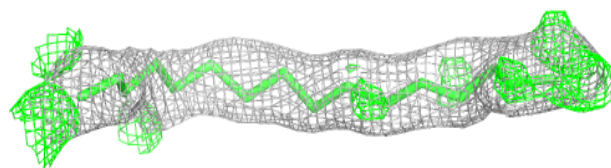
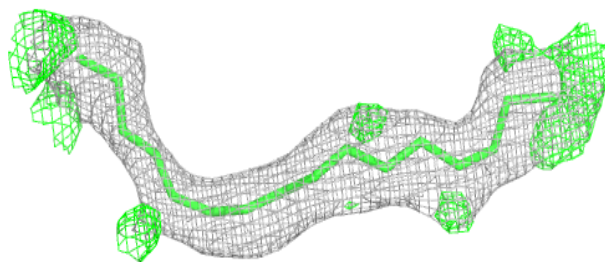


Electron density around R16 A 320:

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

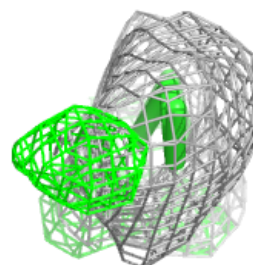
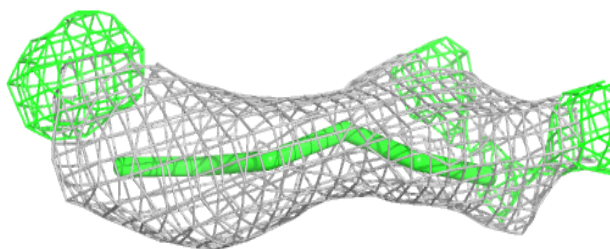
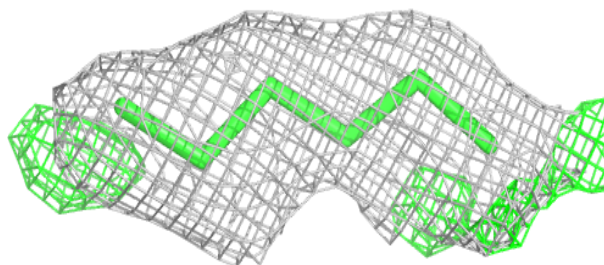
**Electron density around R16 A 321:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

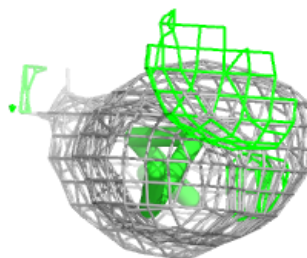
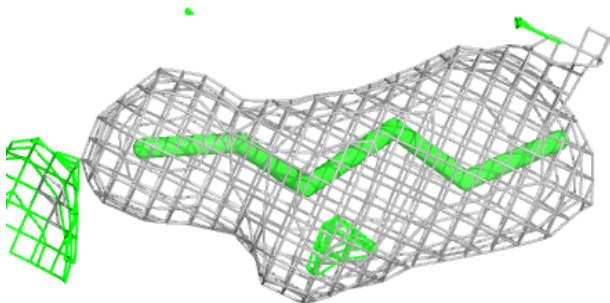
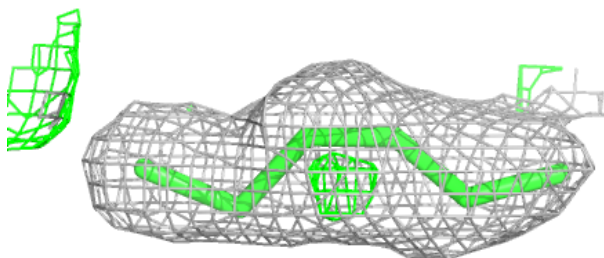


Electron density around HEX C 310:

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

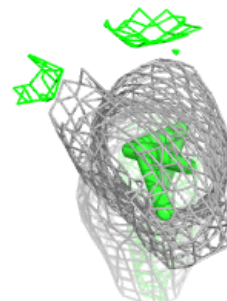
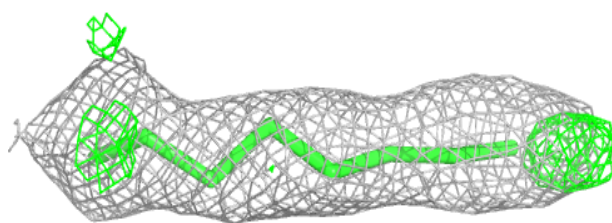
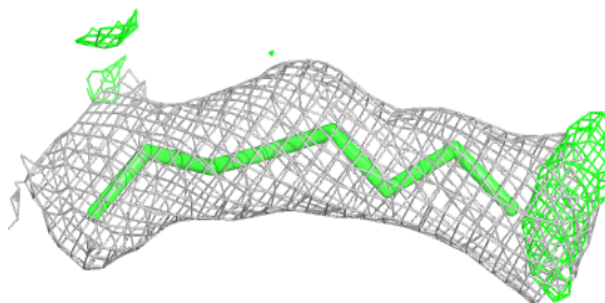
**Electron density around HEX B 305:**

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

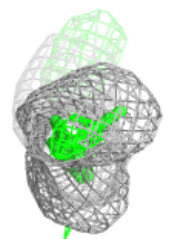
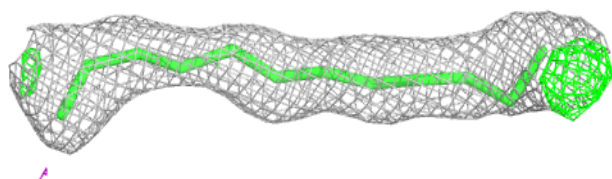
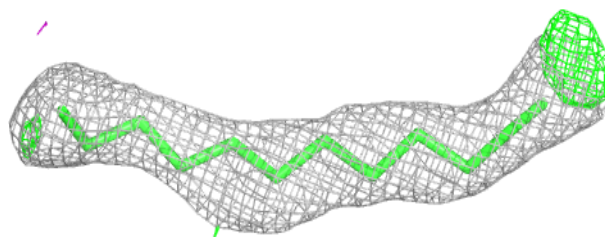


Electron density around OCT B 312:

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

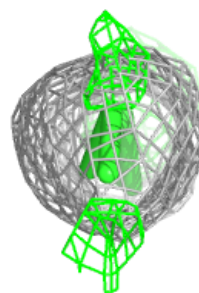
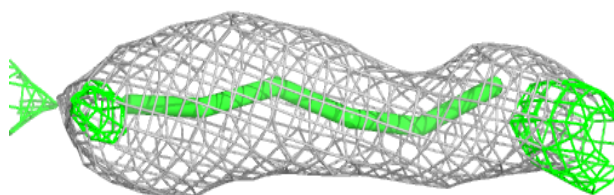
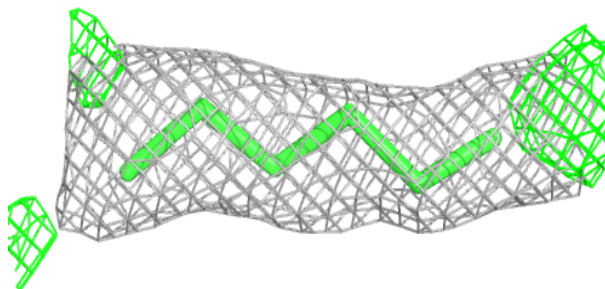
**Electron density around D12 B 317:**

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

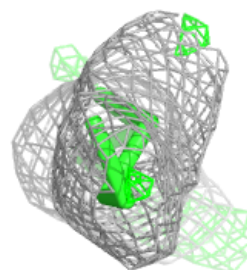
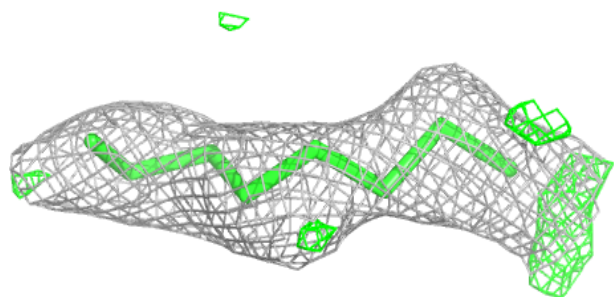
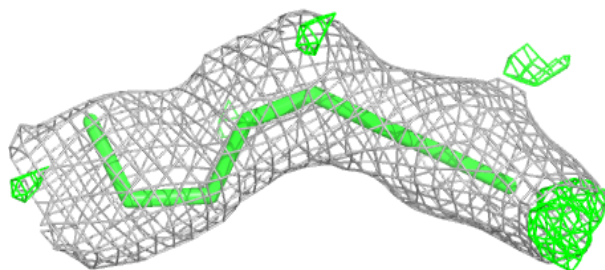


Electron density around HEX C 308:

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

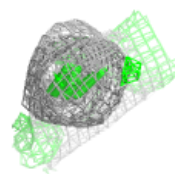
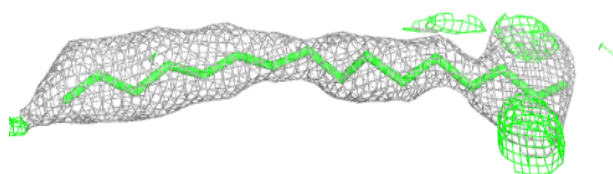
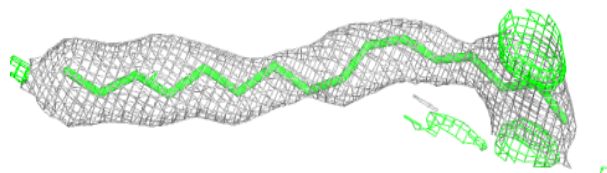
**Electron density around OCT C 317:**

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

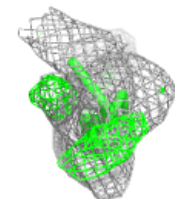
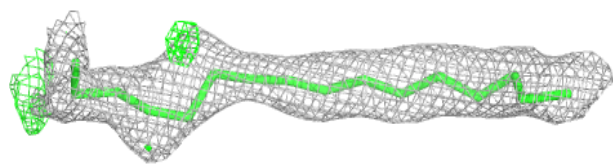
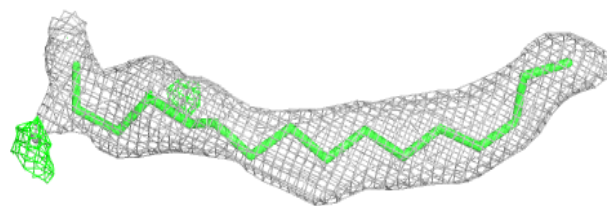


Electron density around R16 A 322:

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

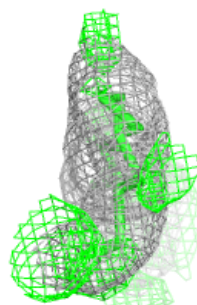
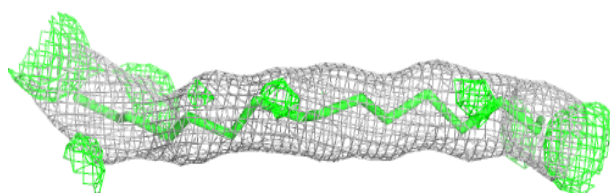
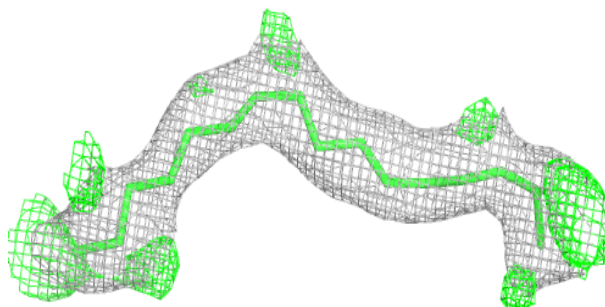
**Electron density around R16 A 323:**

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

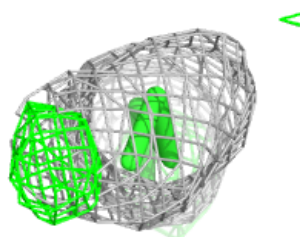
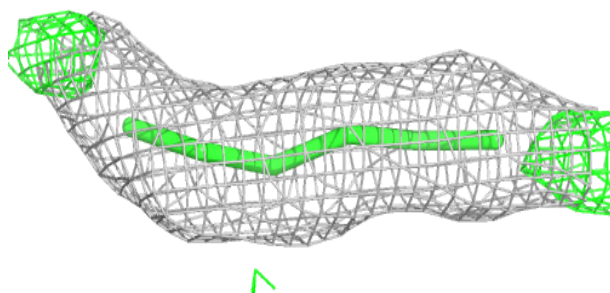
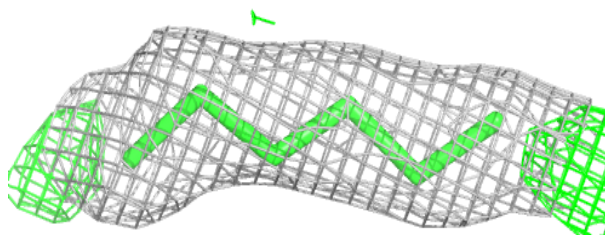


Electron density around R16 A 324:

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

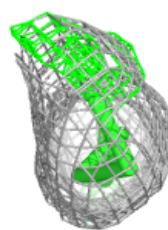
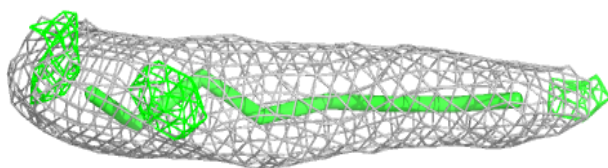
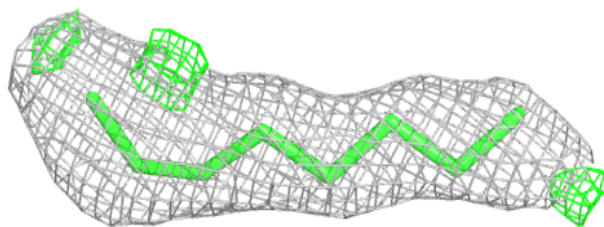
**Electron density around HEX C 312:**

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

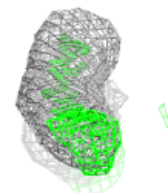
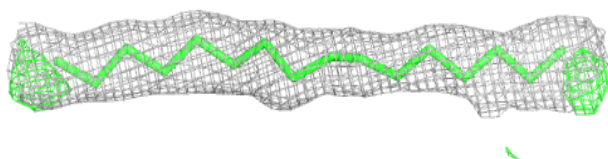
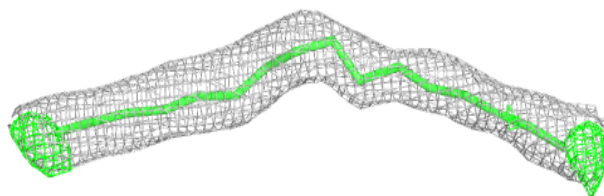


Electron density around OCT A 314:

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

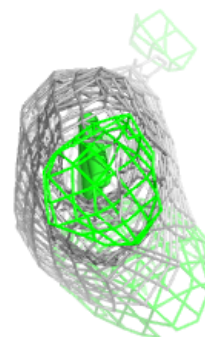
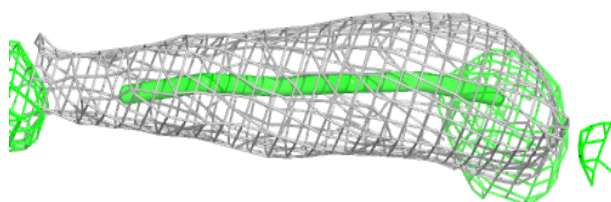
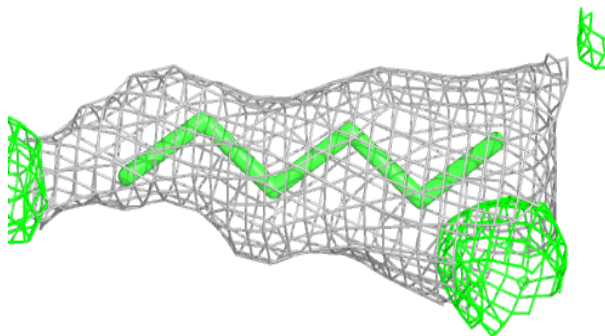
**Electron density around R16 C 319:**

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

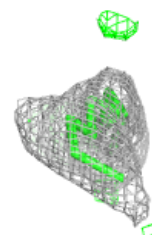
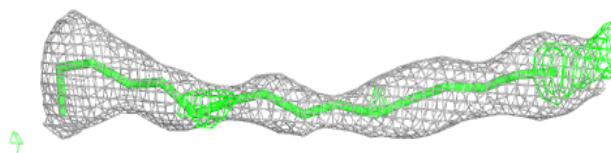
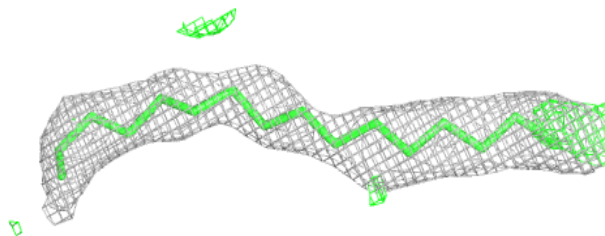


Electron density around HEX C 309:

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

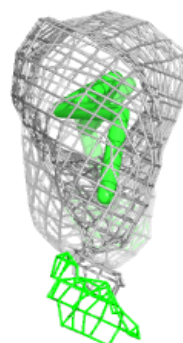
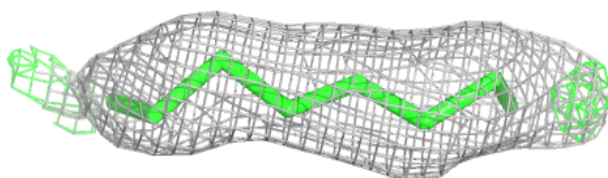
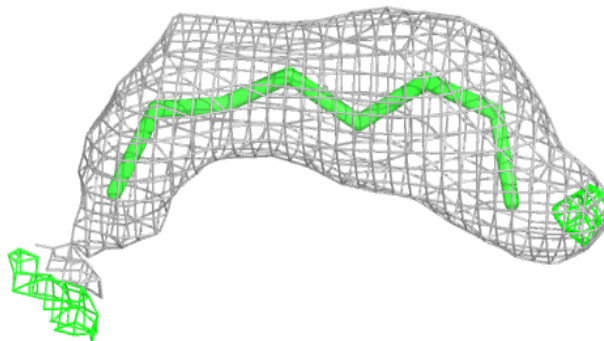
**Electron density around R16 B 319:**

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

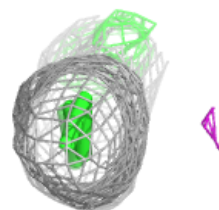
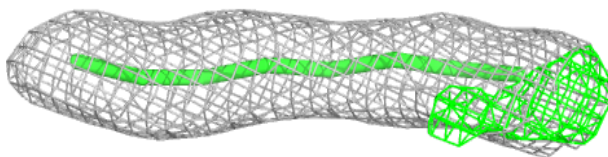
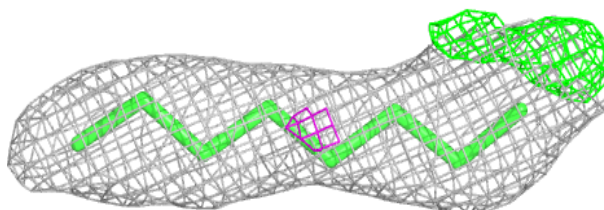


Electron density around OCT C 315:

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

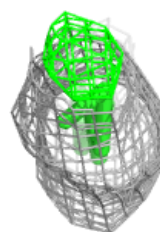
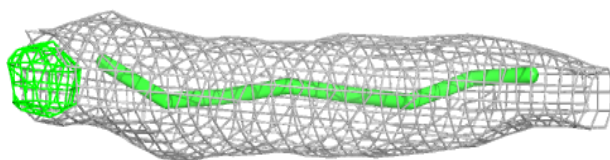
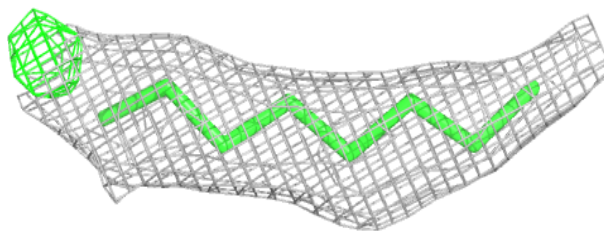
**Electron density around OCT C 316:**

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

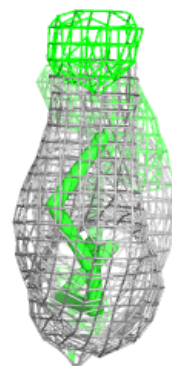
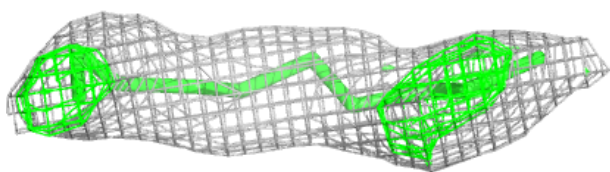
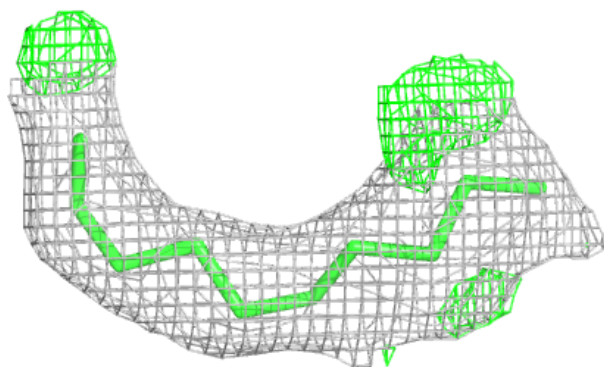


Electron density around OCT A 312:

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

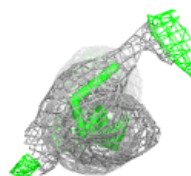
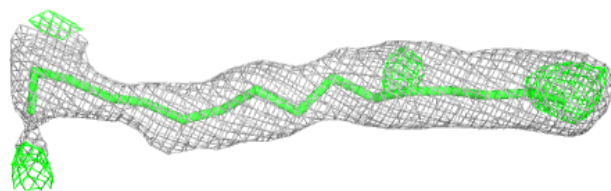
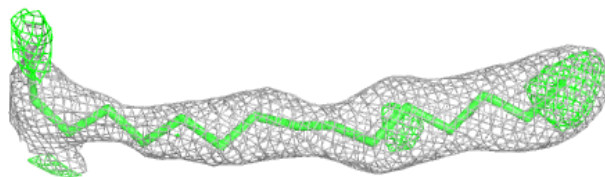
**Electron density around D10 A 316:**

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

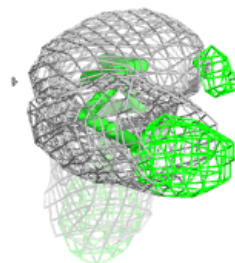
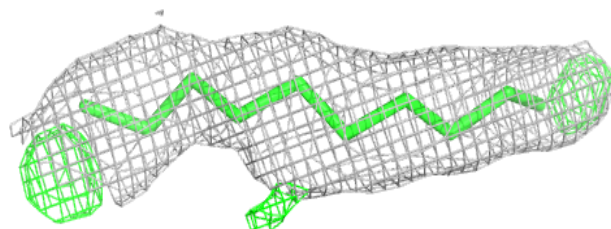
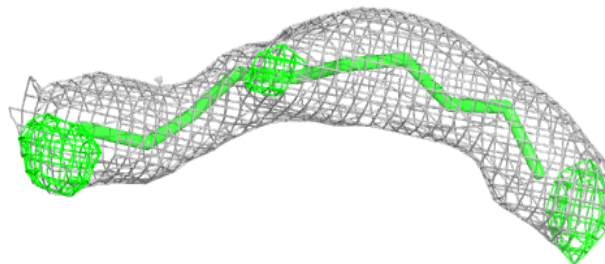


Electron density around R16 C 320:

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

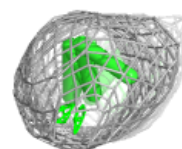
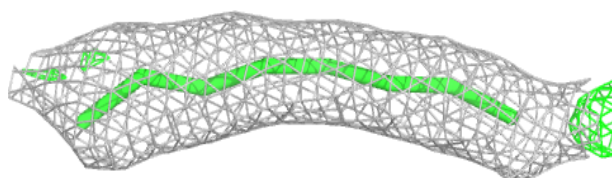
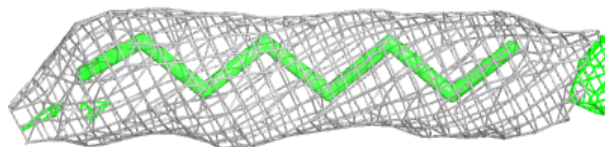
**Electron density around D10 A 317:**

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

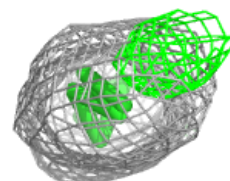
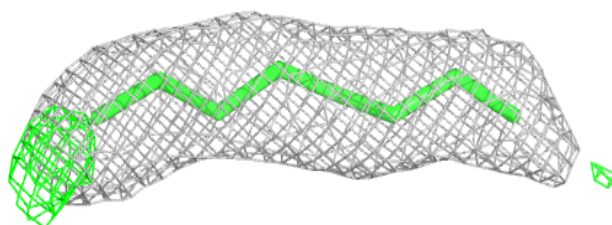
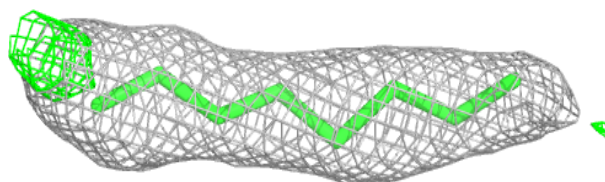


Electron density around OCT C 314:

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

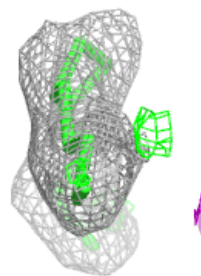
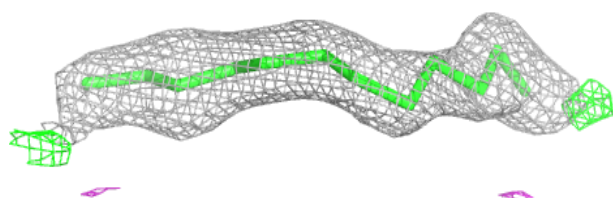
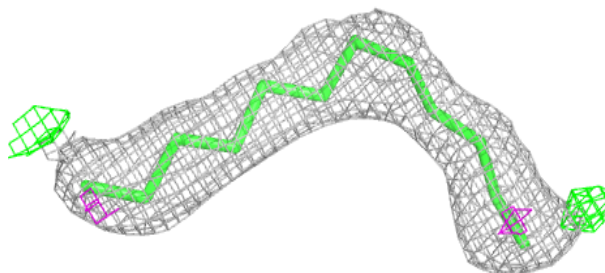
**Electron density around OCT B 308:**

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

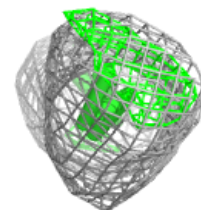
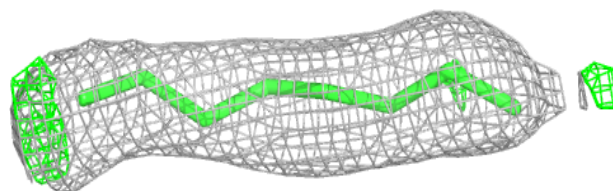
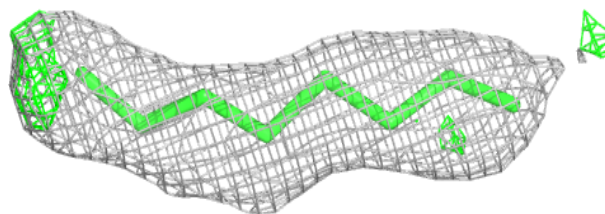


Electron density around D12 A 318:

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

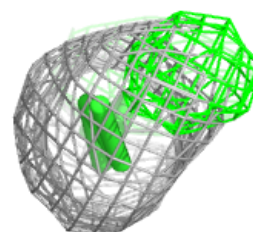
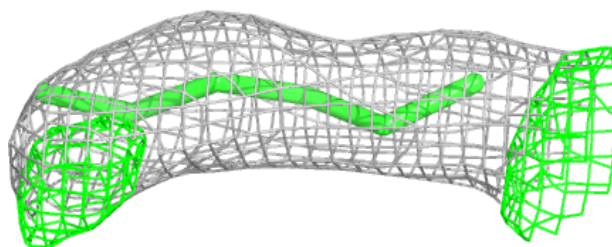
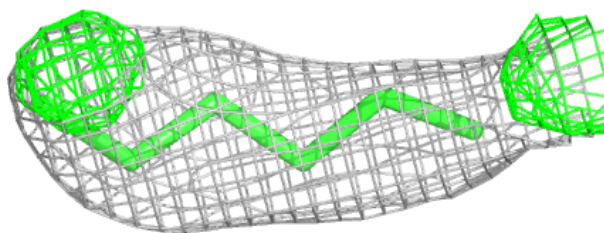
**Electron density around OCT A 308:**

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

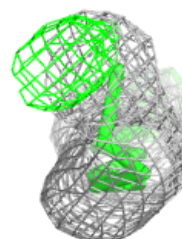
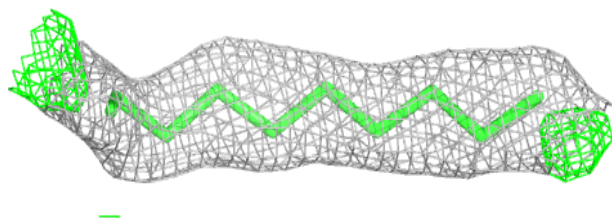
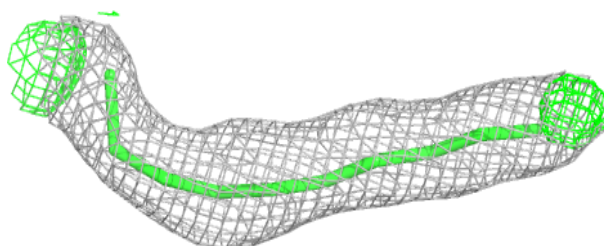


Electron density around HEX B 307:

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

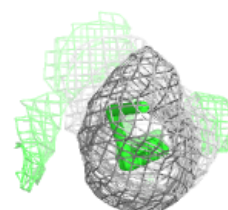
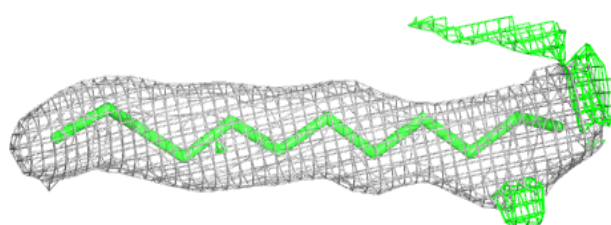
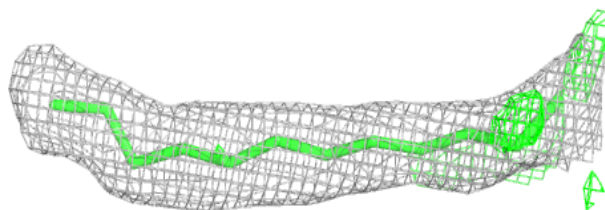
**Electron density around D10 B 314:**

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

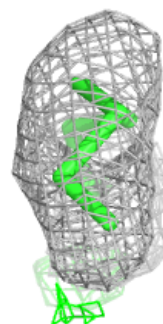
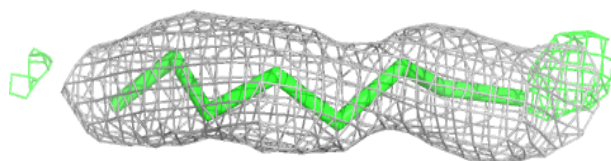
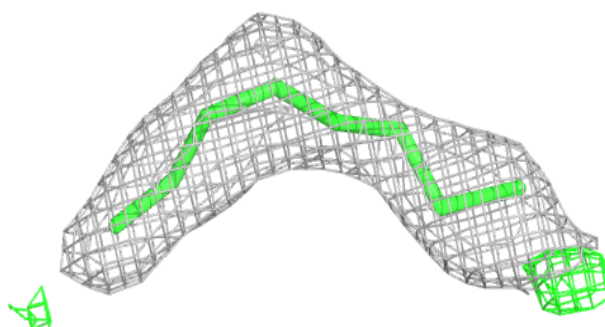


Electron density around D12 B 318:

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

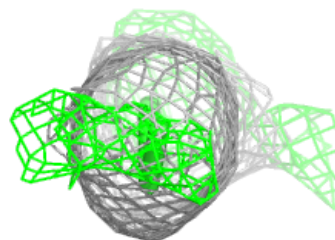
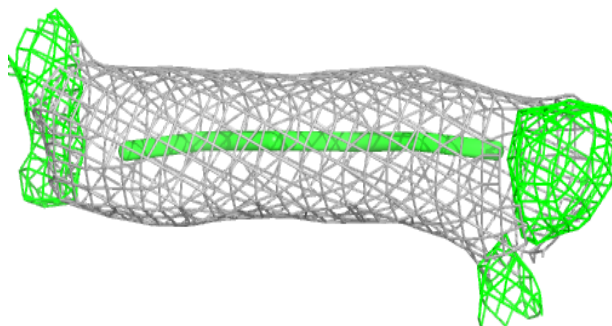
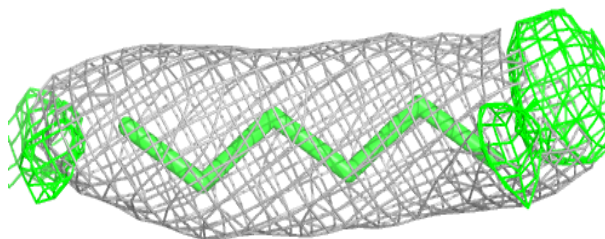
**Electron density around OCT B 311:**

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

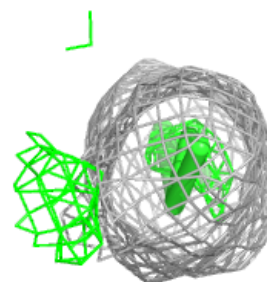
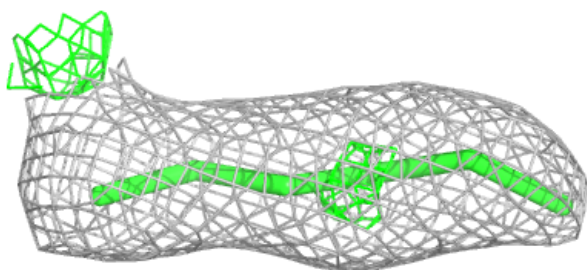
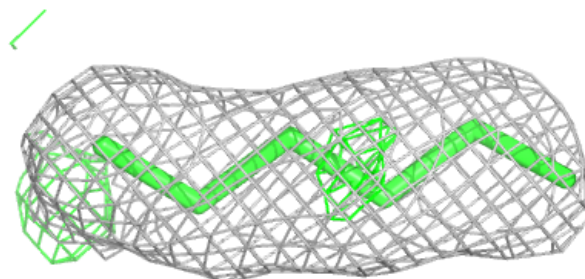


Electron density around HEX C 311:

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

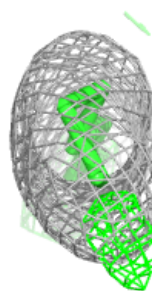
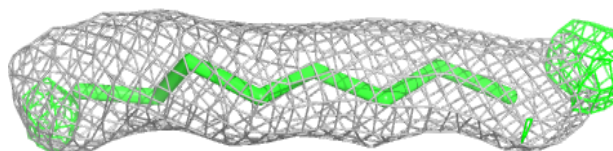
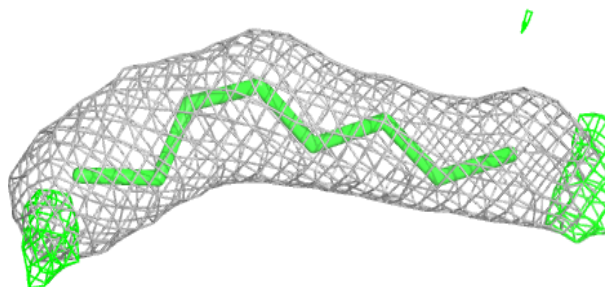
**Electron density around HEX C 304:**

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



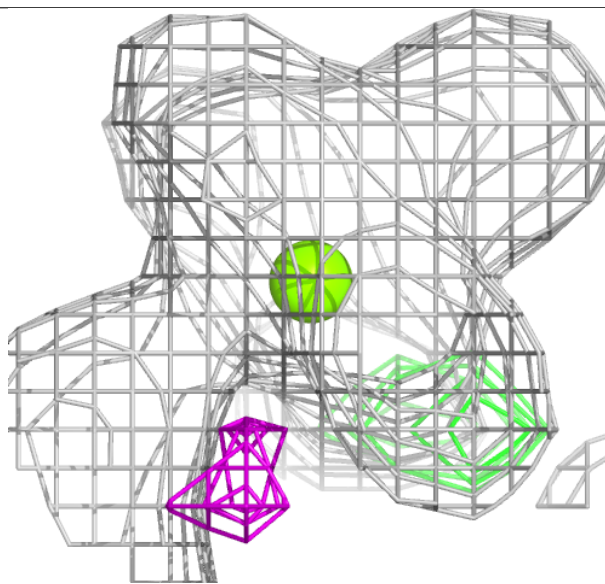
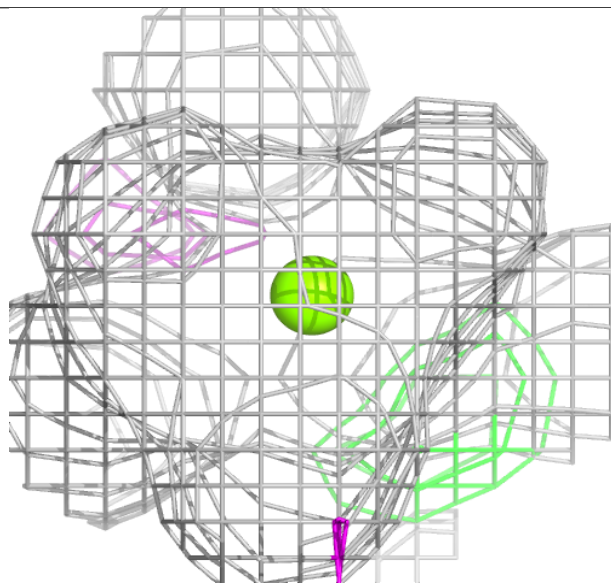
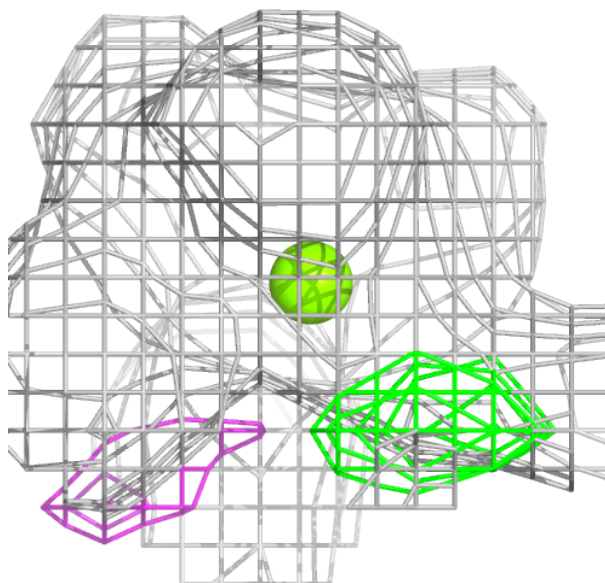
Electron density around OCT C 313:

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



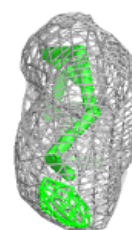
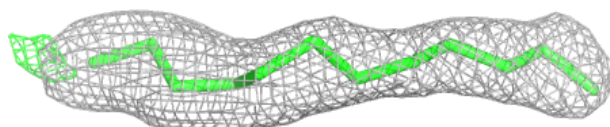
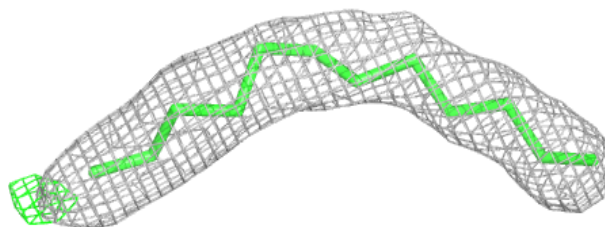
Electron density around MG B 302:

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

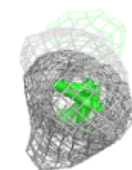
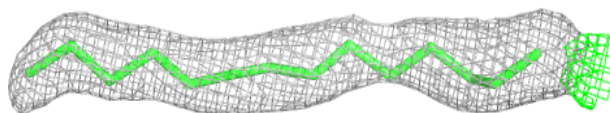
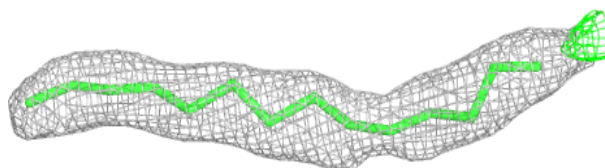


Electron density around D12 B 316:

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

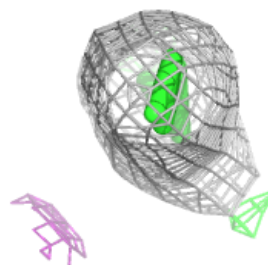
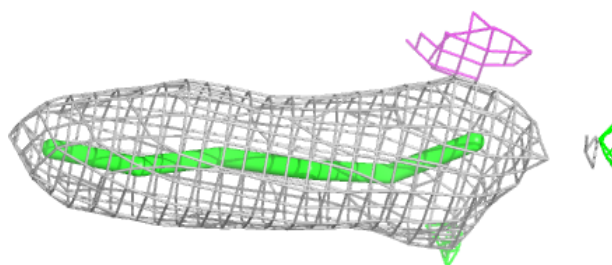
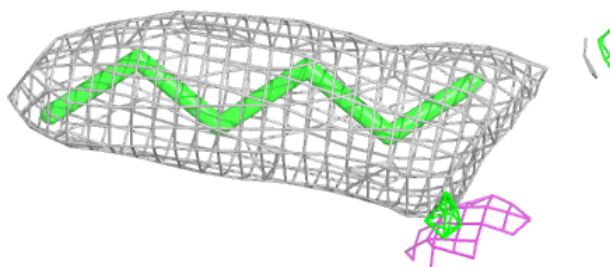
**Electron density around C14 B 320:**

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

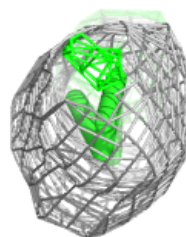
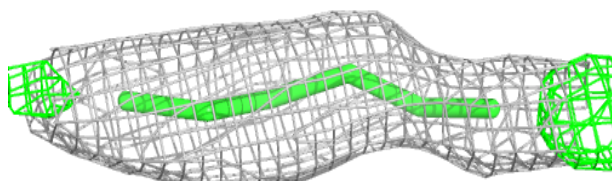
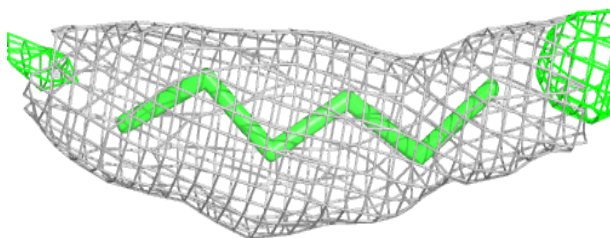


Electron density around HEX A 307:

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

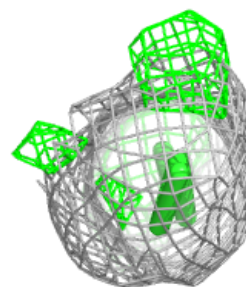
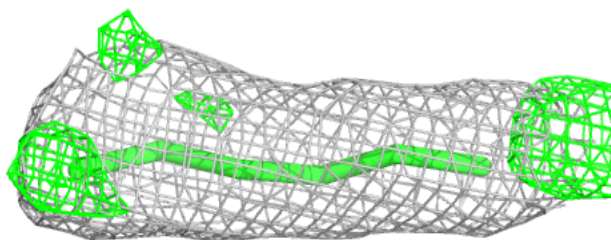
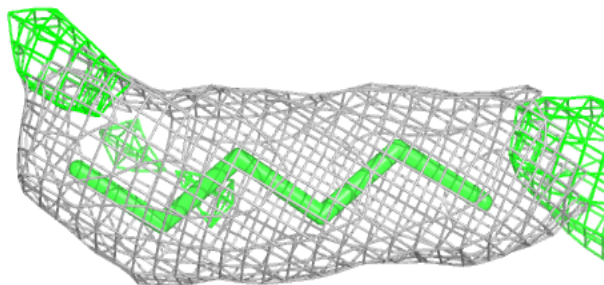
**Electron density around HEX C 303:**

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

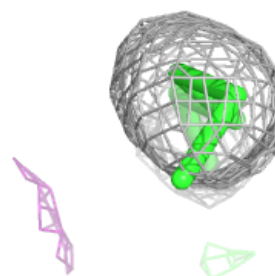
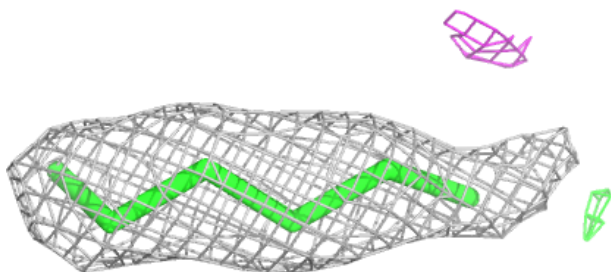
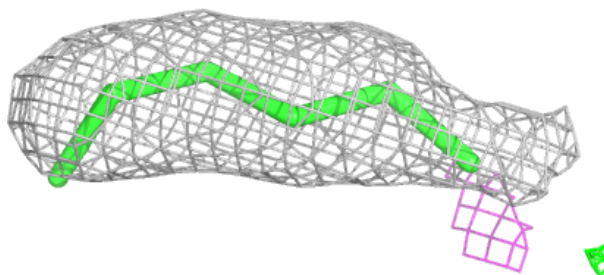


Electron density around HEX A 303:

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

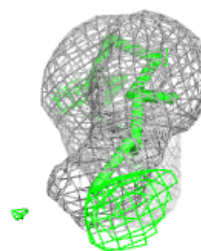
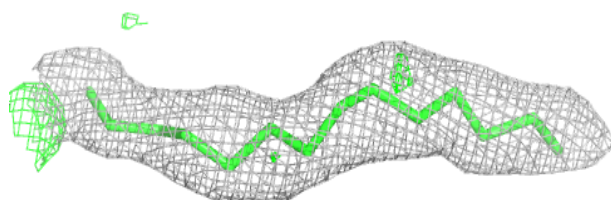
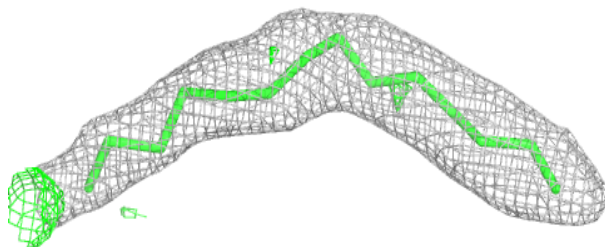
**Electron density around HEX A 304:**

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

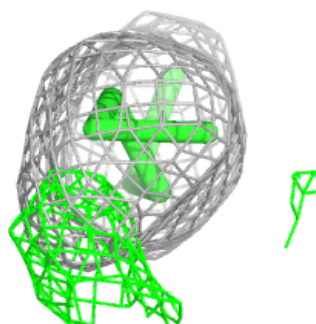
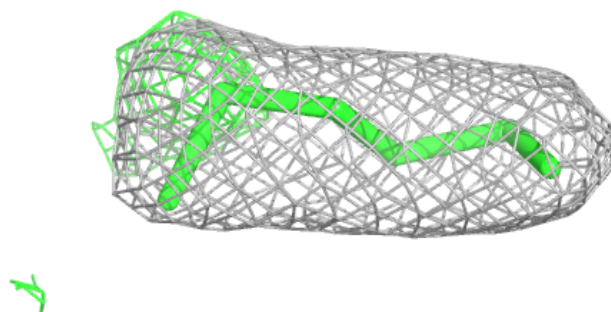
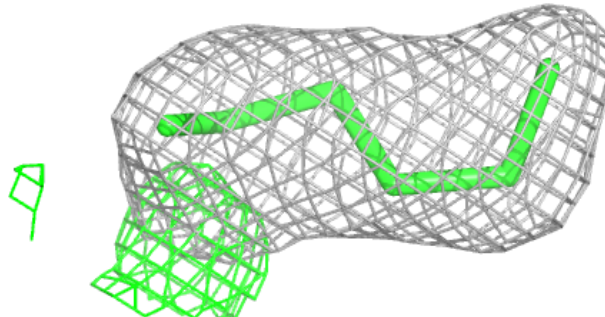


Electron density around C14 A 325:

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

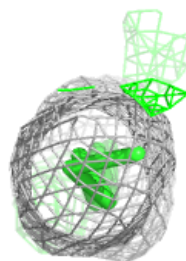
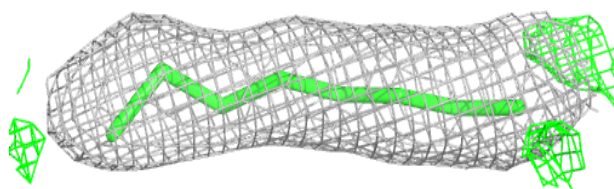
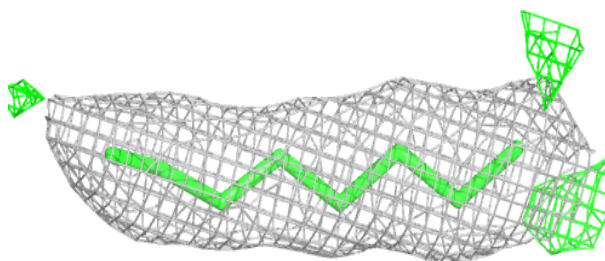
**Electron density around HEX C 306:**

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

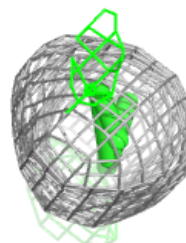
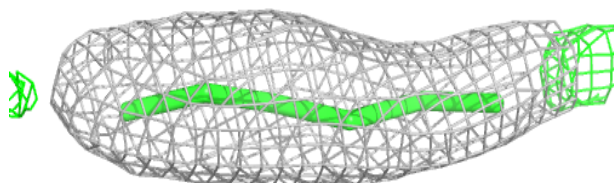
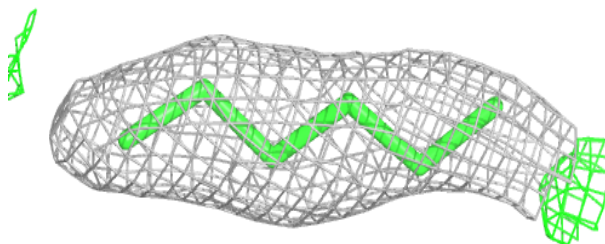


Electron density around OCT A 315:

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

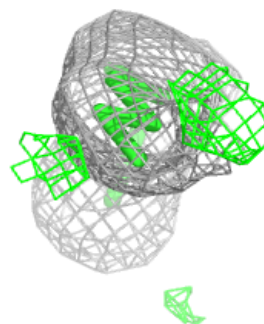
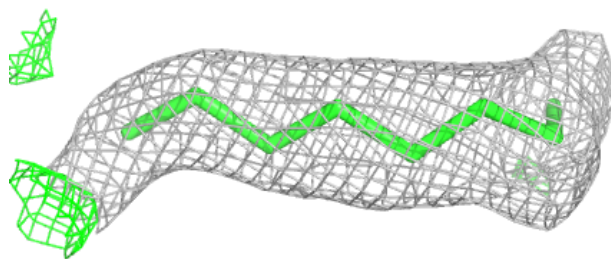
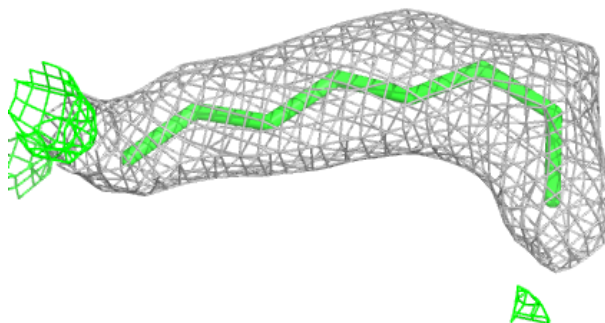
**Electron density around HEX B 303:**

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



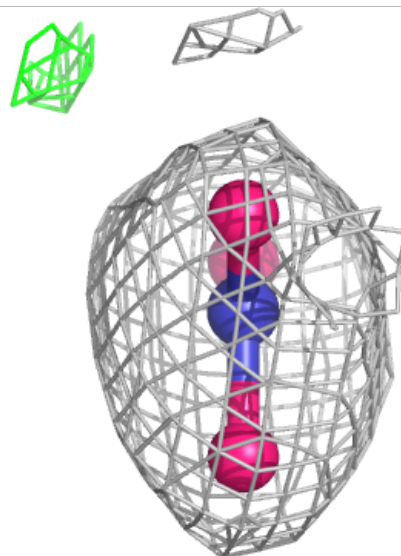
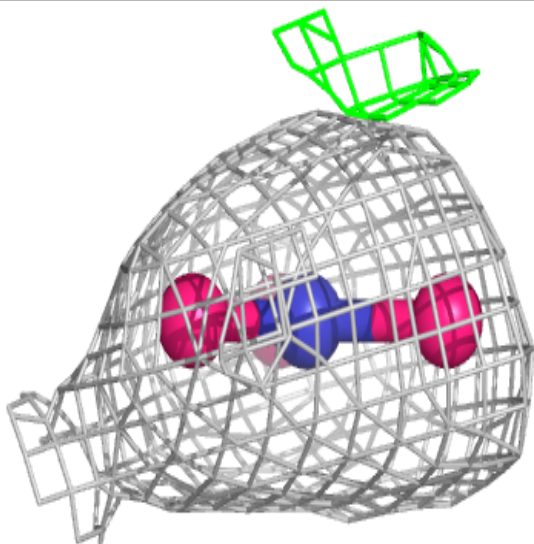
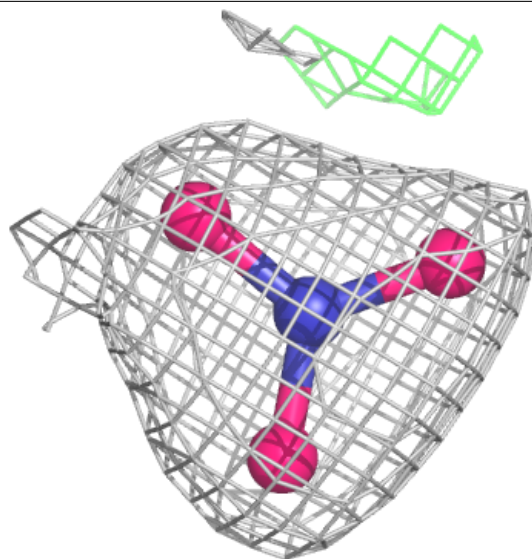
Electron density around OCT B 309:

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



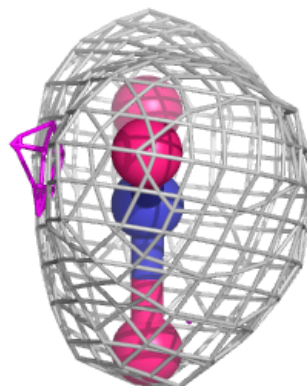
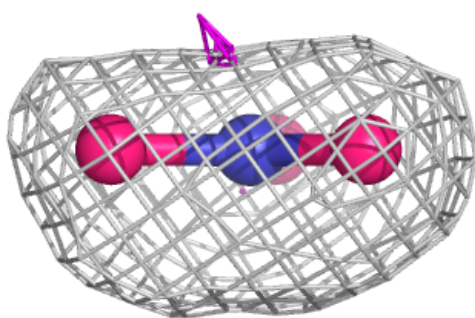
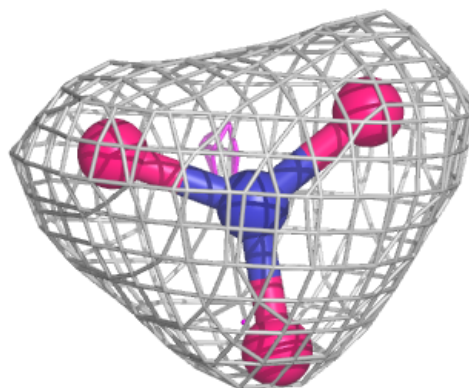
Electron density around NO3 C 322:

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

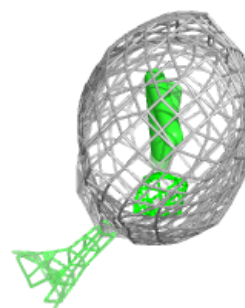
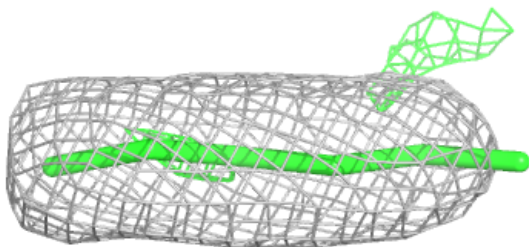
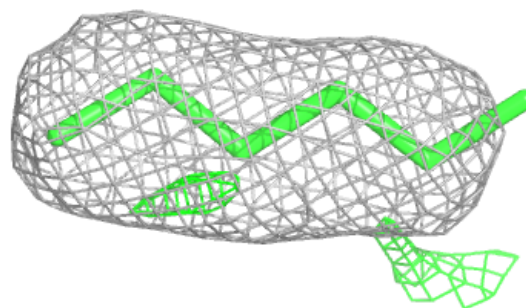


Electron density around NO3 C 323:

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

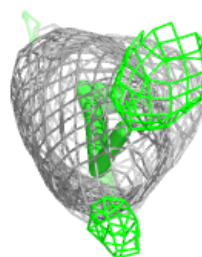
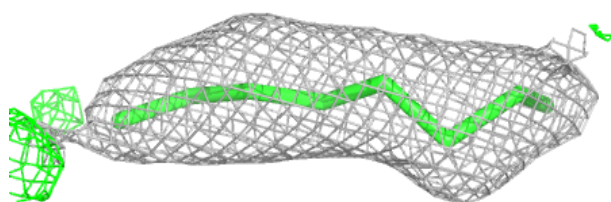
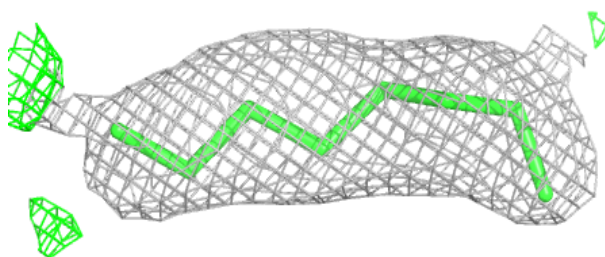
**Electron density around HEX A 305:**

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

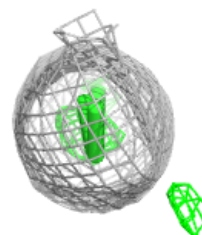
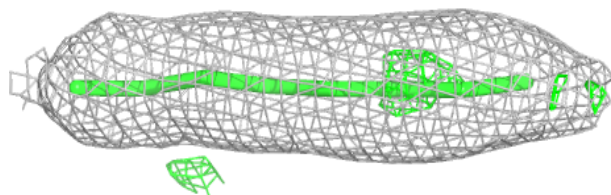
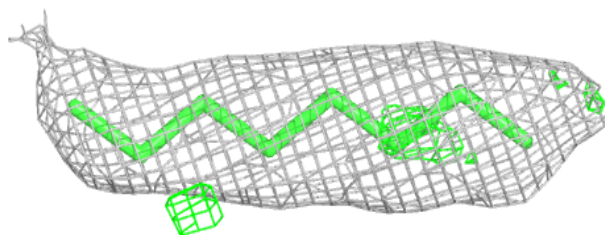


Electron density around OCT B 310:

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

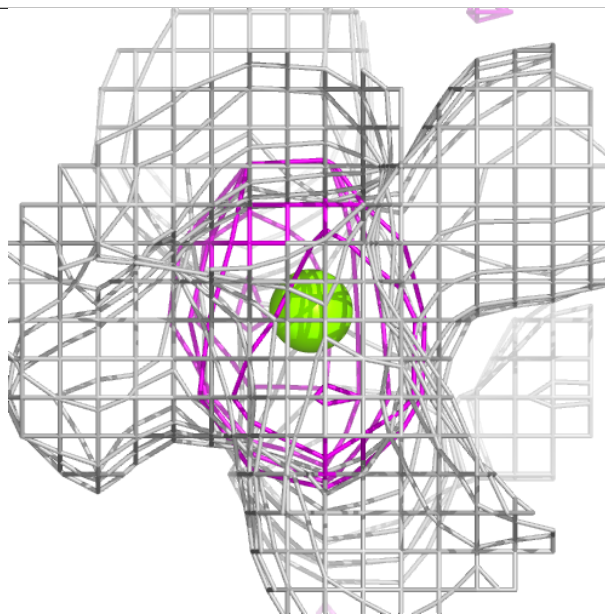
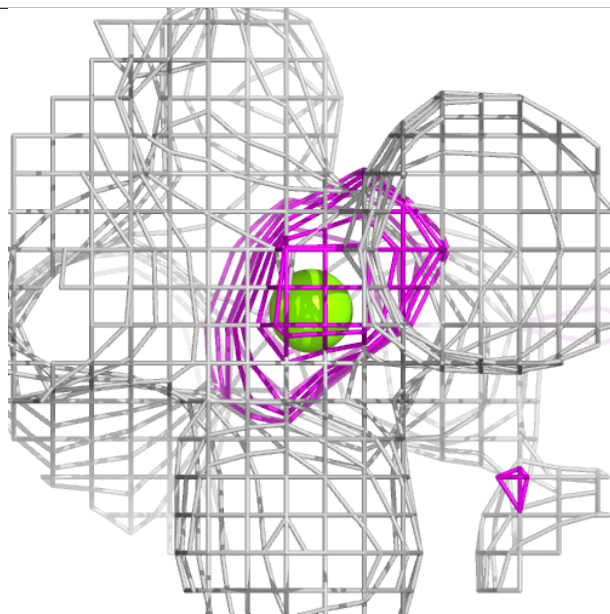
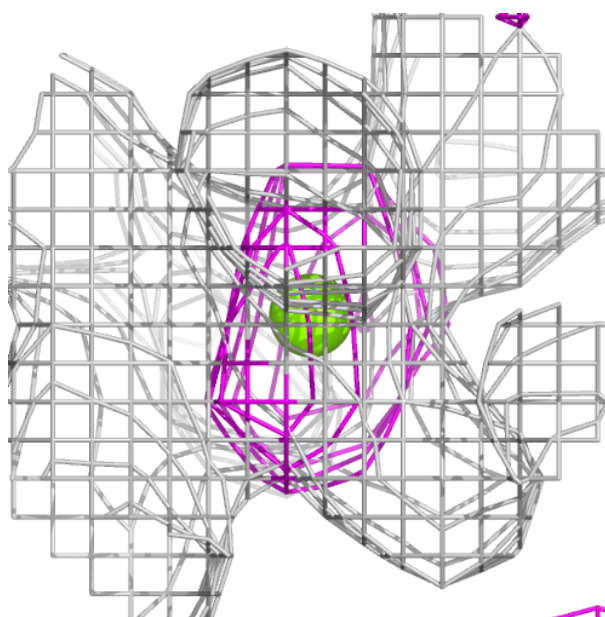
**Electron density around OCT A 313:**

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



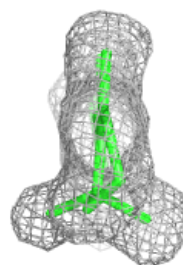
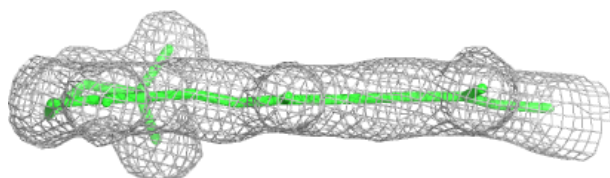
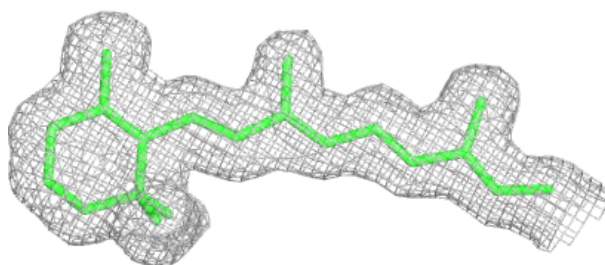
Electron density around MG C 302:

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

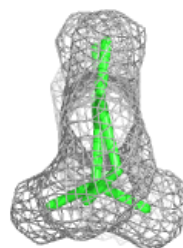
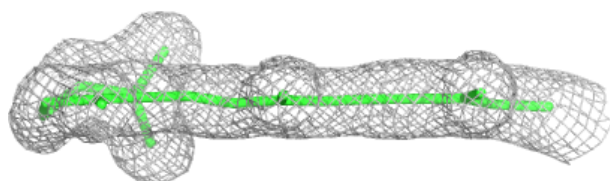
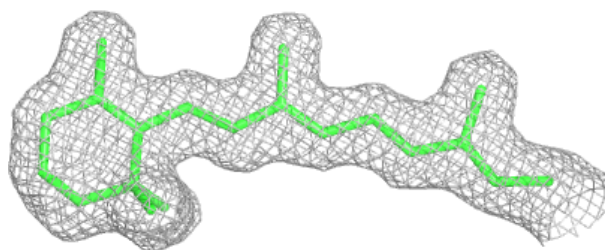


Electron density around RET C 301:

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

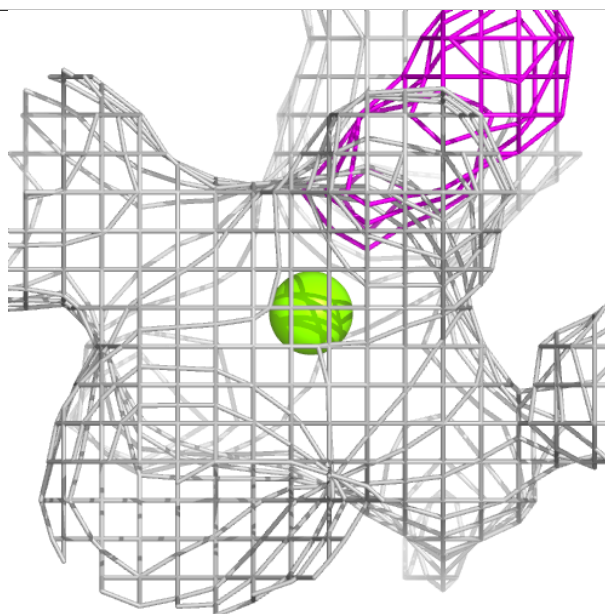
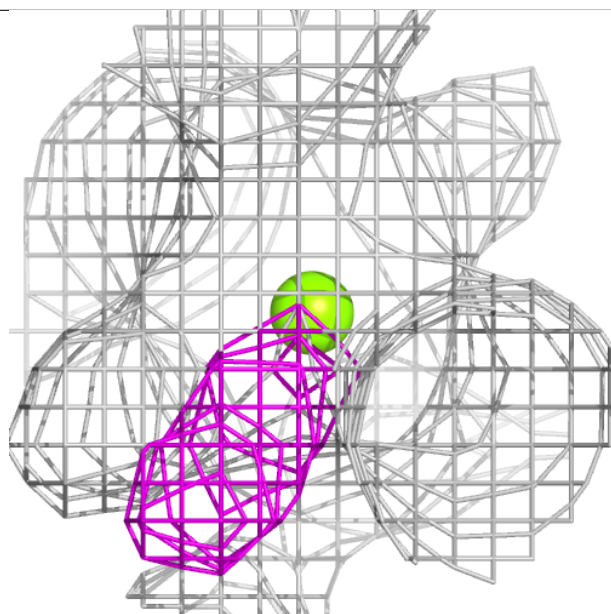
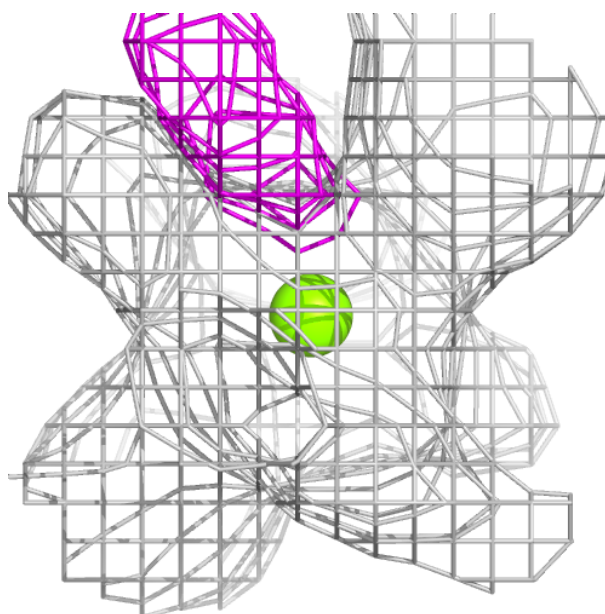
**Electron density around RET A 301:**

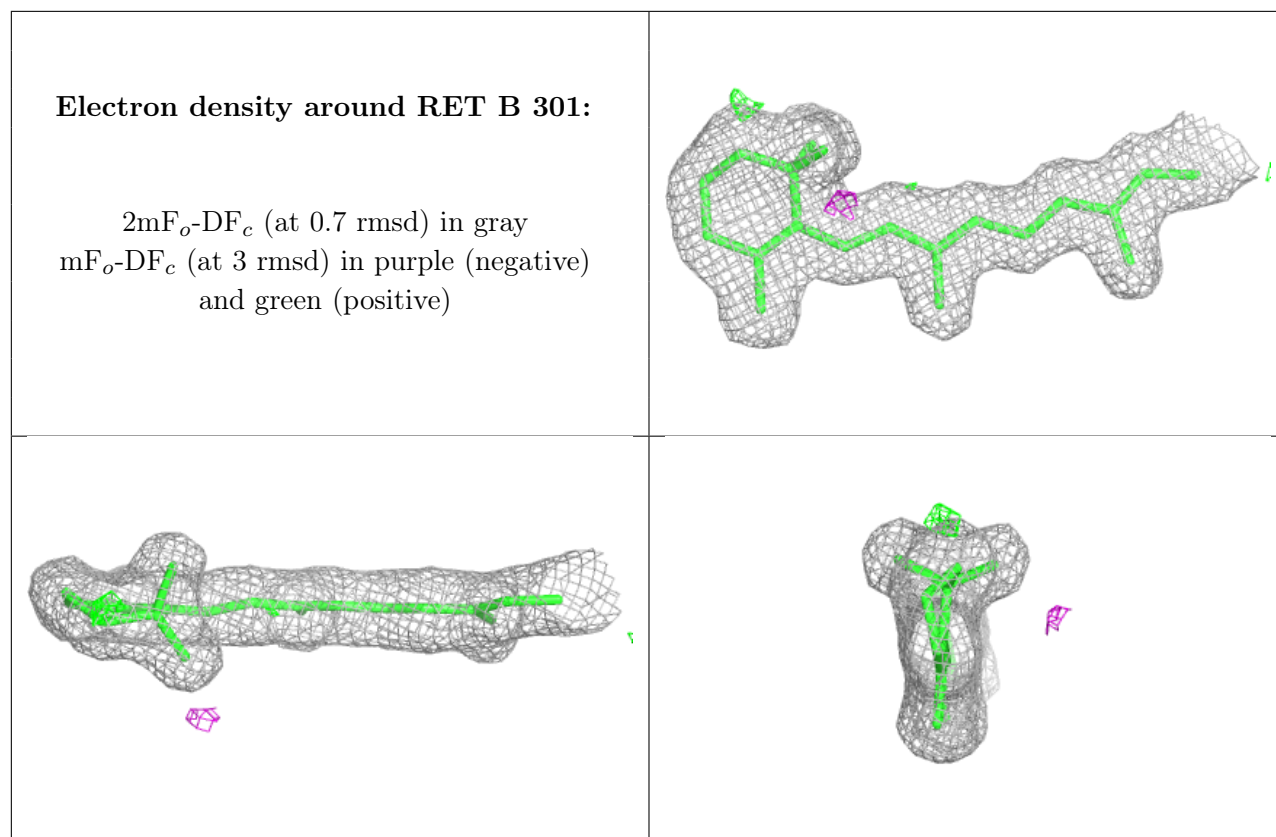
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.