



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 23, 2024 – 02:22 PM EDT

PDB ID : 6OSZ
Title : High Resolution Structure of the Monoclinic Form of Thermomyces Lanuginosa Lipase Complexed with Its Catalytic Products
Authors : McPherson, A.
Deposited on : 2019-05-02
Resolution : 1.43 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

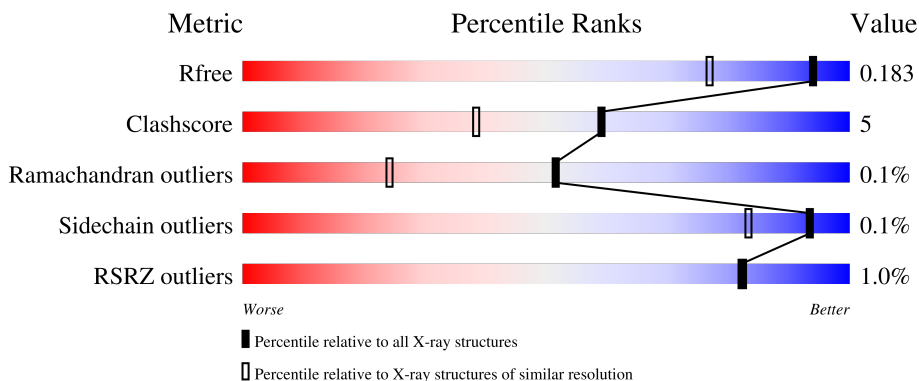
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	291	88% 5% 8%
1	B	291	86% 7% 8%
1	C	291	87% 5% 8%
1	D	291	88% 5% 8%
1	E	291	88% 5% 8%

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Mol	Chain	Length	Quality of chain
1	F	291	 % 87% 5% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OCA	A	301	-	-	X	-
2	OCA	B	301	-	-	X	X
2	OCA	C	301	-	-	X	X
2	OCA	D	301	-	-	X	-
2	OCA	E	301	-	-	X	X
2	OCA	F	301	-	-	X	-

2 Entry composition [i](#)

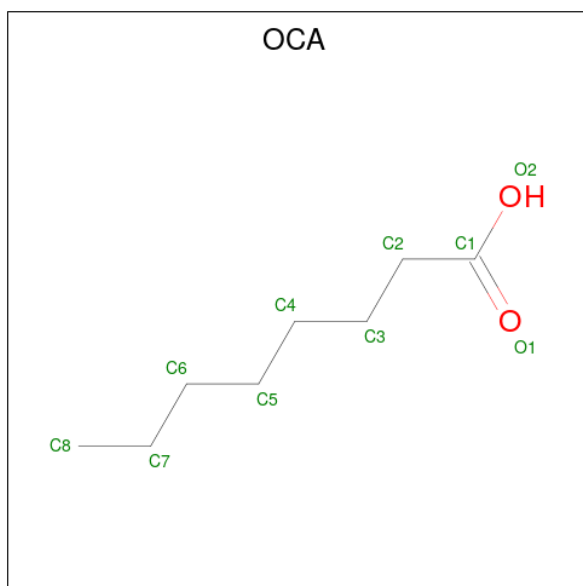
There are 7 unique types of molecules in this entry. The entry contains 27446 atoms, of which 12612 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipase.

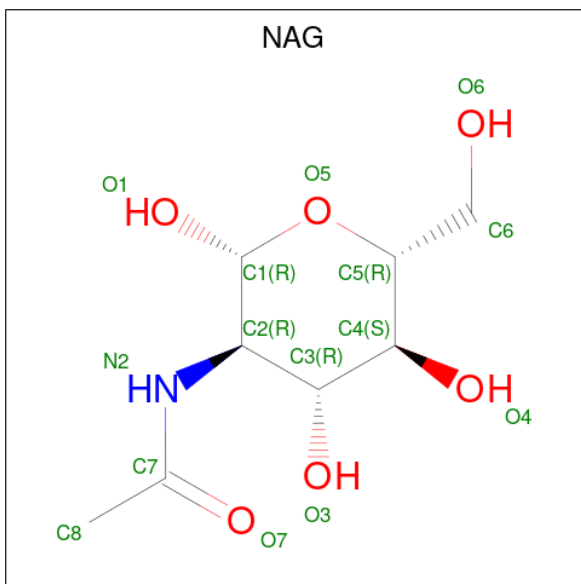
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	269	Total 4126	C 1329	H 2018	N 364	O 409	S 6	0	7	0
1	B	269	Total 4107	C 1327	H 2005	N 364	O 405	S 6	0	5	0
1	C	269	Total 4137	C 1332	H 2018	N 368	O 413	S 6	10	9	0
1	E	269	Total 4096	C 1321	H 1994	N 365	O 410	S 6	0	5	0
1	D	269	Total 4086	C 1317	H 1992	N 364	O 407	S 6	0	4	0
1	F	269	Total 4121	C 1332	H 2009	N 365	O 409	S 6	0	7	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	H	O	0	0
			24	8	15	1		
2	B	1	Total	C	H	O	0	0
			24	8	15	1		
2	C	1	Total	C	H	O	0	0
			24	8	15	1		
2	E	1	Total	C	H	O	0	0
			24	8	15	1		
2	D	1	Total	C	H	O	0	0
			24	8	15	1		
2	F	1	Total	C	H	O	0	0
			24	8	15	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



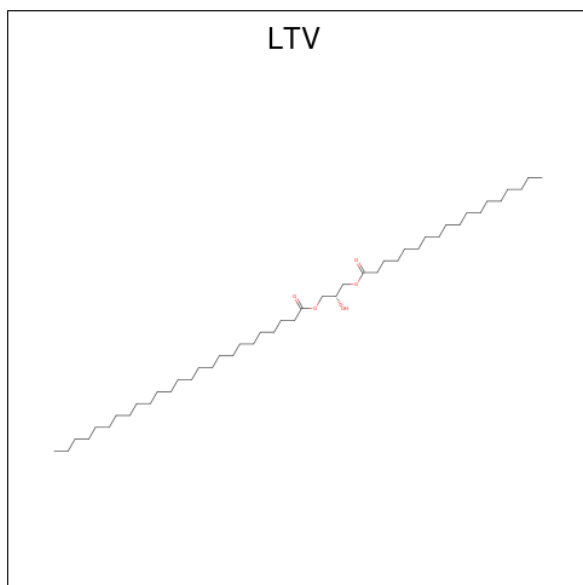
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	E	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	F	1	27	8	13	1	5	0	0

- Molecule 4 is 2-hydroxy-3-(octadecanoyloxy)propyl pentacosanoate (three-letter code: LTV) (formula: $C_{46}H_{90}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	83	31	47	5	0	0	
4	B	1	107	38	64	5	0	0	
4	C	1	99	36	58	5	0	0	
4	E	1	141	46	90	5	0	0	
4	D	1	141	46	90	5	0	0	
4	F	1	101	37	59	5	0	0	

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Ca 2 2	0	0
6	C	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0

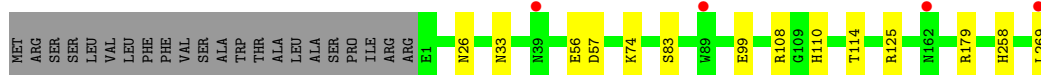
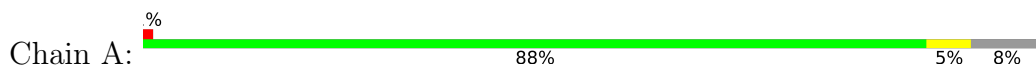
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	325	Total O 328 328	0	3
7	B	330	Total O 333 333	0	4
7	C	264	Total O 264 264	0	1
7	E	224	Total O 224 224	0	1
7	D	260	Total O 262 262	0	2
7	F	326	Total O 328 328	0	3

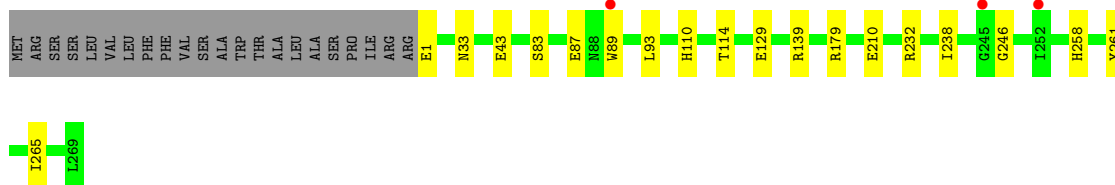
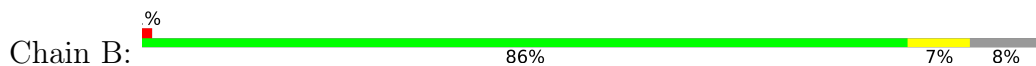
3 Residue-property plots [i](#)

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

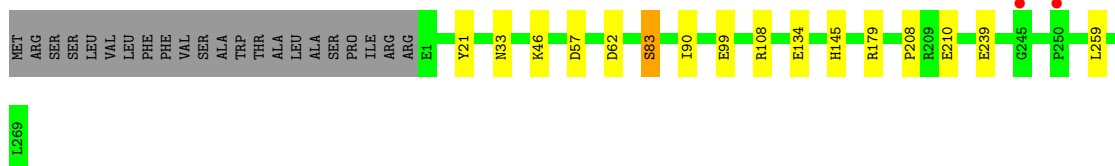
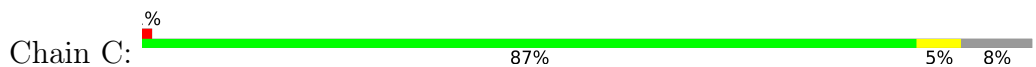
- Molecule 1: Lipase



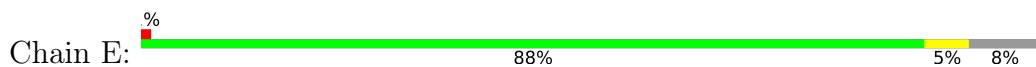
- Molecule 1: Lipase



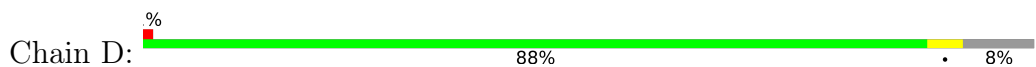
- Molecule 1: Lipase



- Molecule 1: Lipase

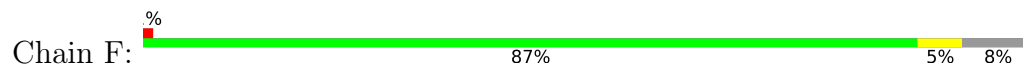


- Molecule 1: Lipase





- Molecule 1: Lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.93Å 89.94Å 123.42Å 90.00° 94.49° 90.00°	Depositor
Resolution (Å)	76.69 – 1.43 76.69 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.4 (76.69-1.43) 99.4 (76.69-1.43)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.43Å)	Xtrriage
Refinement program	PHENIX 1.19rc7_4070	Depositor
R, R_{free}	0.149 , 0.185 0.146 , 0.183	Depositor DCC
R_{free} test set	15362 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtrriage
Anisotropy	0.215	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	27446	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCA, CA, NAG, LTV, PO4

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	0.34	0/2179	0.66	0/2964
1	B	0.34	0/2167	0.65	0/2950
1	C	0.34	0/2200	0.64	0/2991
1	D	0.33	0/2156	0.62	0/2934
1	E	0.32	0/2166	0.60	0/2947
1	F	0.35	0/2188	0.64	0/2978
All	All	0.34	0/13056	0.64	0/17764

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	125	ARG	Sidechain
1	E	133[A]	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2108	2018	2012	18	2
1	B	2102	2005	2002	19	1
1	C	2119	2018	2006	20	2
1	D	2094	1992	1993	19	0
1	E	2102	1994	1987	20	1
1	F	2112	2009	1995	18	0
2	A	9	15	15	6	0
2	B	9	15	15	9	0
2	C	9	15	15	12	0
2	D	9	15	15	6	0
2	E	9	15	15	10	0
2	F	9	15	15	6	0
3	A	14	13	13	1	0
3	B	14	13	13	3	0
3	C	14	13	13	2	0
3	D	14	13	13	3	0
3	E	14	13	13	0	0
3	F	14	13	13	3	0
4	A	36	47	0	0	0
4	B	43	64	0	0	0
4	C	41	58	0	1	0
4	D	51	90	0	0	0
4	E	51	90	0	4	0
4	F	42	59	0	0	0
5	A	10	0	0	0	0
5	B	10	0	0	1	0
5	C	5	0	0	0	0
5	D	10	0	0	1	0
5	E	10	0	0	2	0
5	F	5	0	0	1	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	328	0	0	4	0
7	B	333	0	0	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	264	0	0	4	1
7	D	262	0	0	9	4
7	E	224	0	0	2	1
7	F	328	0	0	9	3
All	All	14834	12612	12163	120	8

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

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLU:OE2	7:D:401:HOH:O	1.84	0.96
1:B:33:ASN:HD21	3:B:305:NAG:C1	1.81	0.92
1:D:125:ARG:NH2	7:D:404:HOH:O	2.05	0.90
1:D:94[A]:ASN:OD1	7:D:402:HOH:O	1.89	0.90
1:D:130[A]:ASP:OD1	7:D:403:HOH:O	1.93	0.86
1:B:129:GLU:OE1	7:B:401:HOH:O	1.96	0.83
1:F:38:GLY:O	7:F:401:HOH:O	1.96	0.83
1:F:33:ASN:HD21	3:F:303:NAG:C1	1.92	0.82
1:D:33:ASN:HD21	3:D:303:NAG:C1	1.95	0.79
1:C:33:ASN:OD1	7:C:401:HOH:O	2.03	0.76
1:F:266:GLY:HA3	2:F:301:OCA:H82	1.68	0.75
1:F:125[A]:ARG:NH2	7:F:405:HOH:O	2.19	0.75
1:B:33:ASN:ND2	3:B:305:NAG:C1	2.50	0.75
1:B:93:LEU:HD13	2:C:301:OCA:H81	1.69	0.74
1:C:83:SER:H	2:C:301:OCA:C2	2.01	0.74
1:C:208:PRO:HB2	1:C:210[B]:GLU:OE1	1.89	0.72
5:B:302:PO4:O4	7:B:402:HOH:O	2.07	0.71
1:F:102:ASP:OD2	7:F:402:HOH:O	2.09	0.71
1:B:139[B]:ARG:NE	7:B:405:HOH:O	2.23	0.70
1:C:33:ASN:OD1	3:C:303:NAG:H2	1.91	0.70
1:B:210:GLU:OE2	7:B:403:HOH:O	2.10	0.70
2:B:301:OCA:H82	1:E:93:LEU:HD13	1.74	0.69
1:F:33:ASN:ND2	3:F:303:NAG:C1	2.57	0.67
1:B:179:ARG:NH1	7:B:406:HOH:O	2.29	0.66
1:A:125:ARG:NH1	7:A:403:HOH:O	2.22	0.66
1:A:57:ASP:OD1	7:A:401:HOH:O	2.13	0.66
1:F:259:LEU:HD22	2:F:301:OCA:H83	1.76	0.66
1:A:33:ASN:OD1	7:A:402:HOH:O	2.15	0.65
5:F:305:PO4:O3	7:F:403:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD21	2:C:301:OCA:H82	1.78	0.65
1:B:93:LEU:CD1	2:C:301:OCA:H81	2.27	0.64
1:B:83:SER:HB2	2:B:301:OCA:H32	1.81	0.62
1:C:33:ASN:OD1	3:C:303:NAG:C2	2.42	0.62
1:C:83:SER:H	2:C:301:OCA:H21	1.65	0.61
1:C:259:LEU:HD21	2:C:301:OCA:H61	1.83	0.60
1:D:179:ARG:NH1	7:D:411:HOH:O	2.35	0.60
1:D:83:SER:H	2:D:301:OCA:H21	1.66	0.59
1:A:83:SER:O	2:A:301:OCA:H82	2.02	0.58
1:A:99[A]:GLU:HG3	1:A:108[A]:ARG:NH1	2.18	0.58
1:B:93:LEU:HD13	2:C:301:OCA:C8	2.34	0.57
1:C:99[A]:GLU:HG3	1:C:108[A]:ARG:HH11	1.70	0.57
1:F:57[B]:ASP:OD1	7:F:404:HOH:O	2.17	0.57
1:F:259:LEU:CD2	2:F:301:OCA:H83	2.36	0.56
2:B:301:OCA:C8	1:E:93:LEU:HD13	2.36	0.56
1:A:269:LEU:HD21	7:D:405:HOH:O	2.06	0.55
1:E:83:SER:H	2:E:301:OCA:C3	2.20	0.55
1:C:259:LEU:CD2	2:C:301:OCA:H61	2.37	0.54
1:A:269:LEU:HD23	1:D:90:ILE:HG21	1.90	0.54
1:C:83:SER:N	2:C:301:OCA:H21	2.23	0.54
1:B:110:HIS:O	1:B:114[B]:THR:HG22	2.07	0.54
1:B:261:TYR:HB2	1:B:265[B]:ILE:HD12	1.90	0.53
1:E:89:TRP:HZ2	4:E:304:LTV:C32	2.22	0.53
1:E:89:TRP:HZ2	4:E:304:LTV:C33	2.22	0.53
1:F:118:ARG:NH1	7:F:406:HOH:O	2.36	0.52
1:A:83:SER:HB2	2:A:301:OCA:H32	1.92	0.52
1:E:83:SER:CB	2:E:301:OCA:H31	2.39	0.52
1:A:83:SER:OG	2:A:301:OCA:H21	2.10	0.52
1:B:1:GLU:OE2	1:B:232:ARG:NH1	2.43	0.52
1:C:179:ARG:NH2	7:C:408:HOH:O	2.44	0.51
1:F:135:HIS:HD2	7:F:685[B]:HOH:O	1.93	0.51
1:E:83:SER:H	2:E:301:OCA:H31	1.74	0.51
1:C:83:SER:H	2:C:301:OCA:C1	2.23	0.51
1:E:83:SER:HB2	2:E:301:OCA:H31	1.93	0.51
1:A:110:HIS:O	1:A:114[B]:THR:HG22	2.12	0.50
1:E:83:SER:OG	2:E:301:OCA:C2	2.59	0.50
1:B:238:ILE:HD12	1:B:246:GLY:HA3	1.93	0.50
1:F:179:ARG:NH1	7:F:408:HOH:O	2.43	0.50
1:D:83:SER:H	2:D:301:OCA:C2	2.25	0.50
1:B:33:ASN:HD21	3:B:305:NAG:C2	2.25	0.49
2:B:301:OCA:C8	1:E:93:LEU:CD1	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ASP:OD1	7:C:403:HOH:O	2.20	0.49
1:B:258:HIS:NE2	2:B:301:OCA:H21	2.27	0.49
1:C:239:GLU:OE1	7:C:402:HOH:O	2.19	0.49
1:D:83:SER:HB2	2:D:301:OCA:H21	1.94	0.49
1:A:33:ASN:OD1	3:A:302:NAG:H2	2.13	0.49
1:E:4:GLN:OE1	1:E:232:ARG:HD3	2.13	0.49
1:F:261:TYR:HB2	1:F:265[B]:ILE:HD12	1.94	0.49
1:D:81:ARG:HH12	5:D:305:PO4:P	2.35	0.48
1:E:266:GLY:HA3	2:E:301:OCA:H72	1.96	0.48
1:A:83:SER:H	2:A:301:OCA:C2	2.26	0.48
1:D:33:ASN:ND2	3:D:303:NAG:C1	2.70	0.48
1:C:210[B]:GLU:H	1:C:210[B]:GLU:CD	2.17	0.48
1:E:85:SER:O	1:E:89:TRP:HD1	1.97	0.47
1:F:266:GLY:CA	2:F:301:OCA:H82	2.41	0.47
1:F:33:ASN:OD1	3:F:303:NAG:C1	2.63	0.47
1:D:208:PRO:HB2	1:D:210:GLU:HG2	1.97	0.46
1:E:108:ARG:NH2	5:E:305:PO4:O2	2.40	0.46
1:C:21:TYR:OH	2:C:301:OCA:H41	2.15	0.46
1:C:90:ILE:HD11	4:E:304:LTV:C34	2.46	0.45
1:D:33:ASN:HD21	3:D:303:NAG:C2	2.29	0.45
1:A:83:SER:HB2	2:A:301:OCA:C3	2.46	0.45
1:E:147:LEU:H	2:E:301:OCA:C1	2.30	0.45
1:A:269:LEU:HD13	7:D:401:HOH:O	2.16	0.45
1:E:83:SER:OG	2:E:301:OCA:H22	2.17	0.45
1:D:94[A]:ASN:ND2	7:D:417:HOH:O	2.50	0.45
1:C:145:HIS:HE1	2:C:301:OCA:H42	1.82	0.44
1:F:87[A]:GLU:HG3	7:F:410:HOH:O	2.18	0.44
1:D:83:SER:O	2:D:301:OCA:H42	2.16	0.44
1:E:134:GLU:HG3	7:E:556:HOH:O	2.17	0.44
1:A:258:HIS:NE2	2:A:301:OCA:C1	2.81	0.43
1:A:74:LYS:NZ	7:A:415:HOH:O	2.50	0.43
1:D:83:SER:CB	2:D:301:OCA:H21	2.48	0.43
1:A:269:LEU:HD23	1:D:90:ILE:CG2	2.48	0.43
1:E:35:THR:HA	1:E:45:GLU:HG2	2.01	0.43
1:D:99:GLU:HG3	1:D:101:ASN:ND2	2.33	0.43
1:E:258:HIS:NE2	2:E:301:OCA:H41	2.34	0.42
5:E:306:PO4:O3	7:E:401[A]:HOH:O	2.21	0.42
1:C:57:ASP:HA	1:C:62:ASP:OD1	2.19	0.42
1:B:87:GLU:CD	7:B:422:HOH:O	2.58	0.42
1:B:83:SER:O	2:B:301:OCA:H51	2.20	0.42
1:E:85:SER:O	1:E:89:TRP:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:OCA:H82	7:D:517:HOH:O	2.20	0.41
1:A:26:ASN:HB3	1:A:56:GLU:HB3	2.03	0.41
1:F:83:SER:N	2:F:301:OCA:O1	2.47	0.41
1:F:147:LEU:H	2:F:301:OCA:C1	2.34	0.40
1:B:89[B]:TRP:HZ3	4:C:304:LTV:C32	2.35	0.40
2:E:301:OCA:O1	4:E:304:LTV:C22	2.70	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:638:HOH:O	7:D:573:HOH:O[1_554]	1.69	0.51
1:E:4:GLN:OE1	7:D:629:HOH:O[1_654]	1.89	0.31
1:A:179:ARG:NH2	7:D:500:HOH:O[2_647]	2.04	0.16
1:B:43:GLU:OE2	7:F:589:HOH:O[1_655]	2.05	0.15
1:A:179:ARG:HH22	7:D:500:HOH:O[2_647]	1.46	0.14
7:B:694:HOH:O	7:F:710:HOH:O[1_655]	2.08	0.12
1:C:46:LYS:HZ3	7:E:582:HOH:O[1_455]	1.55	0.05
1:C:134:GLU:OE2	7:F:711:HOH:O[2_646]	2.15	0.05

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	274/291 (94%)	267 (97%)	7 (3%)	0	100	100
1	B	272/291 (94%)	264 (97%)	8 (3%)	0	100	100
1	C	276/291 (95%)	268 (97%)	8 (3%)	0	100	100
1	D	271/291 (93%)	263 (97%)	8 (3%)	0	100	100
1	E	272/291 (94%)	265 (97%)	7 (3%)	0	100	100
1	F	274/291 (94%)	265 (97%)	8 (3%)	1 (0%)	34	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1639/1746 (94%)	1592 (97%)	46 (3%)	1 (0%)	51 24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	199	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	227/239 (95%)	227 (100%)	0	100 100
1	B	224/239 (94%)	224 (100%)	0	100 100
1	C	228/239 (95%)	227 (100%)	1 (0%)	91 80
1	D	224/239 (94%)	224 (100%)	0	100 100
1	E	225/239 (94%)	225 (100%)	0	100 100
1	F	227/239 (95%)	227 (100%)	0	100 100
All	All	1355/1434 (94%)	1354 (100%)	1 (0%)	93 83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	83	SER

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

Mol	Chain	Res	Type
1	B	33	ASN
1	D	33	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 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	D	306	-	4,4,4	0.84	0	6,6,6	0.51	0
5	PO4	D	305	-	4,4,4	0.92	0	6,6,6	0.44	0
5	PO4	C	305	-	4,4,4	1.01	0	6,6,6	0.77	0
4	LTV	A	303	-	35,35,50	0.94	3 (8%)	37,37,52	0.80	2 (5%)
3	NAG	D	303	-	14,14,15	0.57	0	17,19,21	0.78	0
5	PO4	A	305	-	4,4,4	0.89	0	6,6,6	0.69	0
3	NAG	C	303	1	14,14,15	1.35	2 (14%)	17,19,21	0.97	2 (11%)
4	LTV	C	304	-	40,40,50	0.88	3 (7%)	42,42,52	0.76	2 (4%)
5	PO4	F	305	-	4,4,4	0.89	0	6,6,6	0.37	0
4	LTV	F	304	-	41,41,50	0.88	3 (7%)	43,43,52	0.74	0
2	OCA	F	301	1	8,8,9	0.55	0	7,7,9	1.06	1 (14%)
5	PO4	E	305	-	4,4,4	0.94	0	6,6,6	0.36	0
5	PO4	B	302	-	4,4,4	0.86	0	6,6,6	0.60	0
2	OCA	E	301	1	8,8,9	0.47	0	7,7,9	0.90	0
3	NAG	A	302	1	14,14,15	0.43	0	17,19,21	0.75	1 (5%)
5	PO4	A	304	-	4,4,4	0.90	0	6,6,6	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OCA	C	301	1	8,8,9	1.14	1 (12%)	7,7,9	1.36	2 (28%)
3	NAG	B	305	-	14,14,15	0.45	0	17,19,21	1.13	2 (11%)
4	LTV	B	306	-	42,42,50	0.87	2 (4%)	44,44,52	0.86	2 (4%)
2	OCA	B	301	1	8,8,9	1.12	1 (12%)	7,7,9	0.83	0
4	LTV	D	304	-	50,50,50	0.84	3 (6%)	52,52,52	0.75	2 (3%)
5	PO4	E	306	-	4,4,4	0.94	0	6,6,6	0.23	0
5	PO4	B	307	-	4,4,4	0.91	0	6,6,6	0.47	0
2	OCA	D	301	1	8,8,9	0.50	0	7,7,9	1.29	1 (14%)
2	OCA	A	301	1	8,8,9	0.49	0	7,7,9	1.00	0
3	NAG	F	303	-	14,14,15	0.61	0	17,19,21	0.77	0
4	LTV	E	304	-	50,50,50	0.81	3 (6%)	52,52,52	0.74	2 (3%)
3	NAG	E	303	1	14,14,15	0.36	0	17,19,21	0.40	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	LTV	F	304	-	-	23/42/42/51	-
2	OCA	F	301	1	-	3/5/6/7	-
4	LTV	A	303	-	-	24/36/36/51	-
3	NAG	D	303	-	-	1/6/23/26	0/1/1/1
2	OCA	E	301	1	-	1/5/6/7	-
3	NAG	A	302	1	-	0/6/23/26	0/1/1/1
2	OCA	D	301	1	-	1/5/6/7	-
2	OCA	C	301	1	-	2/6/6/7	-
3	NAG	E	303	1	-	2/6/23/26	0/1/1/1
2	OCA	A	301	1	-	3/5/6/7	-
3	NAG	B	305	-	-	0/6/23/26	0/1/1/1
3	NAG	F	303	-	-	2/6/23/26	0/1/1/1
4	LTV	B	306	-	-	22/43/43/51	-
4	LTV	E	304	-	-	21/51/51/51	-
2	OCA	B	301	1	-	2/6/6/7	-
4	LTV	D	304	-	-	24/51/51/51	-
3	NAG	C	303	1	-	0/6/23/26	0/1/1/1
4	LTV	C	304	-	-	23/41/41/51	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	NAG	C1-C2	4.08	1.58	1.52
2	B	301	OCA	O2-C1	-3.10	1.26	1.42
2	C	301	OCA	O2-C1	-3.02	1.26	1.42
4	D	304	LTV	O1-C17	2.85	1.41	1.33
3	C	303	NAG	O5-C1	2.84	1.48	1.43
4	C	304	LTV	O1-C17	2.62	1.41	1.33
4	A	303	LTV	O1-C17	2.62	1.41	1.33
4	E	304	LTV	O1-C17	2.61	1.41	1.33
4	B	306	LTV	O1-C17	2.58	1.40	1.33
4	F	304	LTV	O1-C17	2.57	1.40	1.33
4	B	306	LTV	O3-C21	2.51	1.40	1.33
4	D	304	LTV	O3-C21	2.41	1.40	1.33
4	F	304	LTV	O3-C20	-2.41	1.39	1.45
4	C	304	LTV	O3-C21	2.36	1.40	1.33
4	A	303	LTV	O3-C21	2.32	1.40	1.33
4	E	304	LTV	O3-C21	2.31	1.40	1.33
4	A	303	LTV	O3-C20	-2.17	1.40	1.45
4	F	304	LTV	O3-C21	2.15	1.39	1.33
4	D	304	LTV	O3-C20	-2.13	1.40	1.45
4	C	304	LTV	O3-C20	-2.07	1.40	1.45
4	E	304	LTV	O3-C20	-2.04	1.40	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	306	LTV	O3-C21-C22	3.12	121.70	111.91
4	E	304	LTV	O3-C21-C22	2.88	120.93	111.91
4	C	304	LTV	O3-C21-C22	2.81	120.72	111.91
4	D	304	LTV	O3-C21-C22	2.70	120.37	111.91
4	D	304	LTV	O1-C17-C16	2.57	119.98	111.91
4	B	306	LTV	O1-C17-C16	2.57	119.96	111.91
2	D	301	OCA	C4-C3-C2	-2.51	102.84	113.79
4	A	303	LTV	O3-C21-C22	2.51	119.77	111.91
3	C	303	NAG	C1-C2-N2	2.38	114.55	110.49
3	B	305	NAG	C4-C3-C2	-2.36	107.57	111.02
4	A	303	LTV	O1-C17-C16	2.31	119.17	111.91
4	C	304	LTV	O1-C17-C16	2.31	119.16	111.91
2	C	301	OCA	C6-C5-C4	-2.29	102.78	114.42
3	C	303	NAG	C1-O5-C5	2.20	115.17	112.19
2	F	301	OCA	O1-C1-C2	-2.20	112.47	126.89
4	E	304	LTV	O1-C17-C16	2.19	118.79	111.91
2	C	301	OCA	C4-C3-C2	-2.19	103.31	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	305	NAG	C1-O5-C5	-2.09	109.36	112.19
3	A	302	NAG	C3-C4-C5	2.07	113.93	110.24

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	LTV	O1-C18-C19-O2
4	B	306	LTV	O4-C21-O3-C20
4	B	306	LTV	C22-C21-O3-C20
4	B	306	LTV	O2-C19-C20-O3
4	B	306	LTV	C18-C19-C20-O3
4	C	304	LTV	C18-C19-C20-O3
4	C	304	LTV	O1-C18-C19-O2
4	E	304	LTV	C18-C19-C20-O3
4	B	306	LTV	O-C17-O1-C18
4	C	304	LTV	O-C17-O1-C18
4	D	304	LTV	O-C17-O1-C18
4	F	304	LTV	O-C17-O1-C18
4	B	306	LTV	C16-C17-O1-C18
4	C	304	LTV	C22-C21-O3-C20
4	C	304	LTV	C16-C17-O1-C18
4	E	304	LTV	C22-C21-O3-C20
4	D	304	LTV	C16-C17-O1-C18
4	A	303	LTV	O4-C21-O3-C20
4	D	304	LTV	C22-C21-O3-C20
4	F	304	LTV	C16-C17-O1-C18
4	A	303	LTV	O-C17-O1-C18
4	C	304	LTV	O4-C21-O3-C20
4	D	304	LTV	O4-C21-O3-C20
4	F	304	LTV	O4-C21-O3-C20
4	A	303	LTV	C16-C17-O1-C18
4	E	304	LTV	O4-C21-O3-C20
4	A	303	LTV	O2-C19-C20-O3
4	C	304	LTV	O2-C19-C20-O3
4	A	303	LTV	C23-C24-C25-C26
4	A	303	LTV	C22-C21-O3-C20
4	F	304	LTV	C22-C21-O3-C20
4	E	304	LTV	C1-C2-C3-C4
4	A	303	LTV	O1-C18-C19-C20
4	B	306	LTV	O1-C18-C19-C20
3	F	303	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	F	303	NAG	O7-C7-N2-C2
4	E	304	LTV	O2-C19-C20-O3
4	B	306	LTV	C21-C22-C23-C24
4	B	306	LTV	C23-C24-C25-C26
4	C	304	LTV	C6-C7-C8-C9
4	B	306	LTV	O1-C18-C19-O2
4	D	304	LTV	O2-C19-C20-O3
4	F	304	LTV	O2-C19-C20-O3
4	A	303	LTV	C29-C30-C31-C32
4	D	304	LTV	C28-C29-C30-C31
4	A	303	LTV	C11-C10-C9-C8
4	B	306	LTV	C29-C30-C31-C32
4	E	304	LTV	C25-C26-C27-C28
4	F	304	LTV	C22-C23-C24-C25
4	C	304	LTV	O1-C18-C19-C20
4	D	304	LTV	C18-C19-C20-O3
4	F	304	LTV	C18-C19-C20-O3
2	D	301	OCA	C2-C3-C4-C5
4	F	304	LTV	C5-C6-C7-C8
3	D	303	NAG	O5-C5-C6-O6
2	C	301	OCA	C2-C3-C4-C5
4	E	304	LTV	C13-C14-C15-C16
4	F	304	LTV	C24-C25-C26-C27
4	C	304	LTV	C31-C32-C33-C34
4	C	304	LTV	C9-C10-C11-C12
4	A	303	LTV	C25-C26-C27-C28
4	D	304	LTV	C31-C32-C33-C34
4	C	304	LTV	C30-C31-C32-C33
4	A	303	LTV	C9-C10-C11-C12
4	C	304	LTV	C3-C4-C5-C6
4	A	303	LTV	C21-C22-C23-C24
4	B	306	LTV	C5-C6-C7-C8
4	E	304	LTV	C9-C10-C11-C12
4	E	304	LTV	C28-C29-C30-C31
4	D	304	LTV	C10-C11-C12-C13
4	E	304	LTV	C3-C4-C5-C6
2	A	301	OCA	C3-C4-C5-C6
2	F	301	OCA	C3-C4-C5-C6
4	E	304	LTV	C41-C42-C43-C44
4	B	306	LTV	C33-C34-C35-C36
4	D	304	LTV	C35-C36-C37-C38
3	E	303	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	304	LTV	C5-C6-C7-C8
4	A	303	LTV	C18-C19-C20-O3
2	A	301	OCA	C4-C5-C6-C7
4	C	304	LTV	C26-C27-C28-C29
4	C	304	LTV	C13-C14-C15-C16
4	A	303	LTV	C24-C25-C26-C27
4	F	304	LTV	C6-C7-C8-C9
4	D	304	LTV	C33-C34-C35-C36
2	F	301	OCA	C5-C6-C7-C8
4	B	306	LTV	C6-C7-C8-C9
4	B	306	LTV	C22-C23-C24-C25
4	F	304	LTV	C2-C3-C4-C5
4	F	304	LTV	O3-C21-C22-C23
2	C	301	OCA	O2-C1-C2-C3
4	D	304	LTV	C22-C23-C24-C25
4	E	304	LTV	O3-C21-C22-C23
4	F	304	LTV	C34-C35-C36-C37
4	E	304	LTV	C40-C41-C42-C43
2	B	301	OCA	C5-C6-C7-C8
4	E	304	LTV	C10-C11-C12-C13
4	C	304	LTV	C11-C10-C9-C8
4	A	303	LTV	C12-C13-C14-C15
4	C	304	LTV	C25-C26-C27-C28
4	E	304	LTV	C11-C12-C13-C14
4	A	303	LTV	C26-C27-C28-C29
4	C	304	LTV	C23-C24-C25-C26
4	C	304	LTV	C2-C3-C4-C5
2	B	301	OCA	C4-C5-C6-C7
4	B	306	LTV	C9-C10-C11-C12
4	B	306	LTV	C31-C32-C33-C34
4	F	304	LTV	C26-C27-C28-C29
4	F	304	LTV	C13-C14-C15-C16
2	E	301	OCA	C3-C4-C5-C6
4	E	304	LTV	C22-C23-C24-C25
4	D	304	LTV	C29-C30-C31-C32
4	E	304	LTV	C15-C16-C17-O1
4	D	304	LTV	C21-C22-C23-C24
4	F	304	LTV	C27-C28-C29-C30
4	D	304	LTV	C11-C10-C9-C8
4	F	304	LTV	C32-C33-C34-C35
4	B	306	LTV	C1-C2-C3-C4
2	A	301	OCA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	E	304	LTV	C36-C37-C38-C39
4	E	304	LTV	C34-C35-C36-C37
4	A	303	LTV	C10-C11-C12-C13
4	C	304	LTV	C11-C12-C13-C14
4	D	304	LTV	C9-C10-C11-C12
4	F	304	LTV	O4-C21-C22-C23
4	A	303	LTV	C7-C8-C9-C10
4	B	306	LTV	C12-C13-C14-C15
4	C	304	LTV	C24-C25-C26-C27
4	E	304	LTV	O4-C21-C22-C23
4	F	304	LTV	C1-C2-C3-C4
4	A	303	LTV	C3-C4-C5-C6
4	D	304	LTV	C32-C33-C34-C35
4	A	303	LTV	C30-C31-C32-C33
4	F	304	LTV	C30-C31-C32-C33
4	B	306	LTV	C24-C25-C26-C27
4	B	306	LTV	C30-C31-C32-C33
4	D	304	LTV	C38-C39-C40-C41
4	B	306	LTV	C26-C27-C28-C29
4	C	304	LTV	C12-C13-C14-C15
4	A	303	LTV	C4-C5-C6-C7
4	D	304	LTV	C27-C28-C29-C30
2	F	301	OCA	C4-C5-C6-C7
4	E	304	LTV	C32-C33-C34-C35
4	A	303	LTV	C15-C16-C17-O1
4	F	304	LTV	C15-C16-C17-O1
4	D	304	LTV	C11-C12-C13-C14
4	A	303	LTV	C15-C16-C17-O
4	F	304	LTV	C3-C4-C5-C6
4	D	304	LTV	C-C1-C2-C3
4	D	304	LTV	C34-C35-C36-C37
4	C	304	LTV	O3-C21-C22-C23
4	F	304	LTV	C15-C16-C17-O
4	D	304	LTV	C15-C16-C17-O1
3	E	303	NAG	C4-C5-C6-O6

There are no ring outliers.

18 monomers are involved in 70 short contacts:

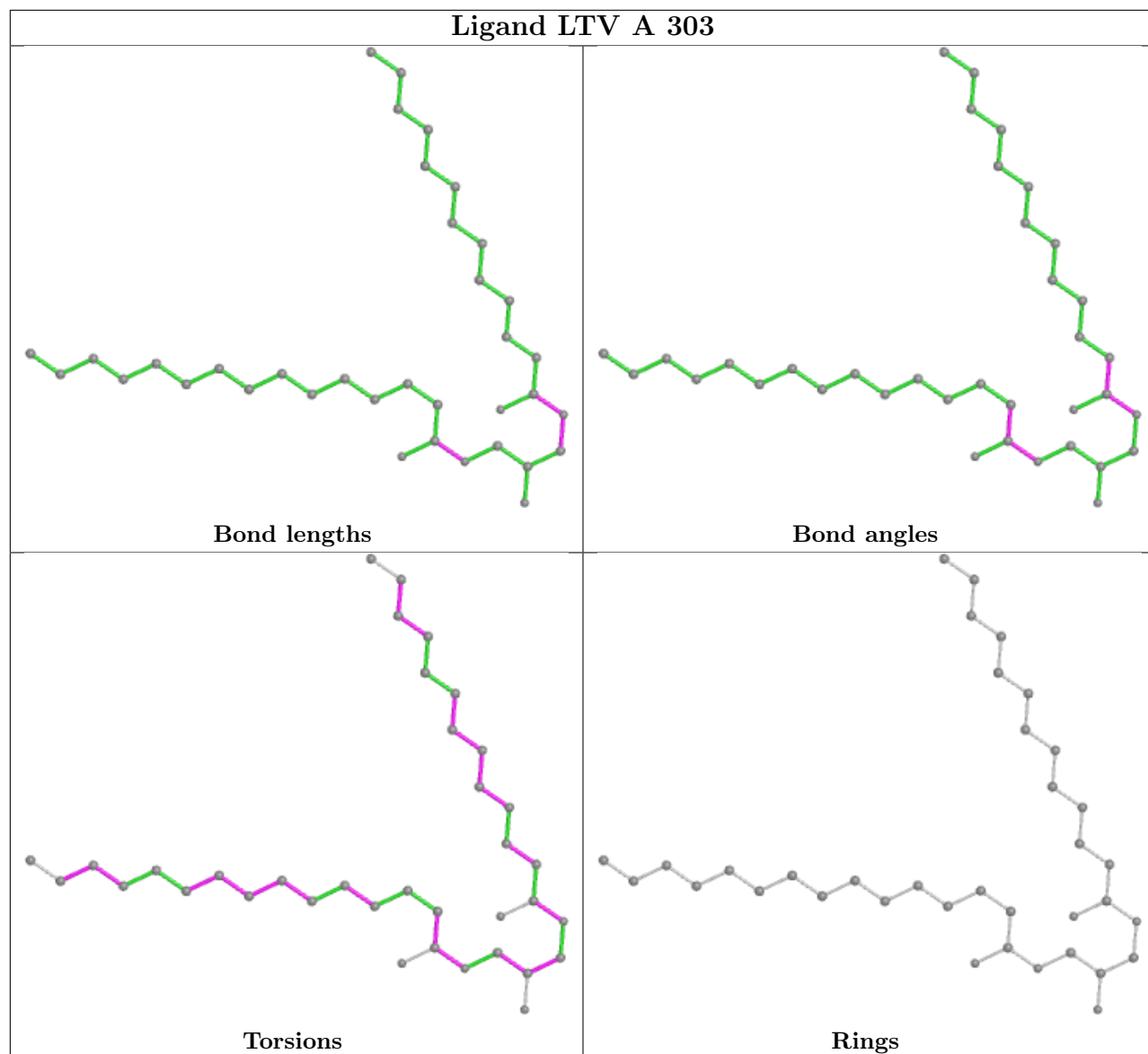
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	305	PO4	1	0
3	D	303	NAG	3	0

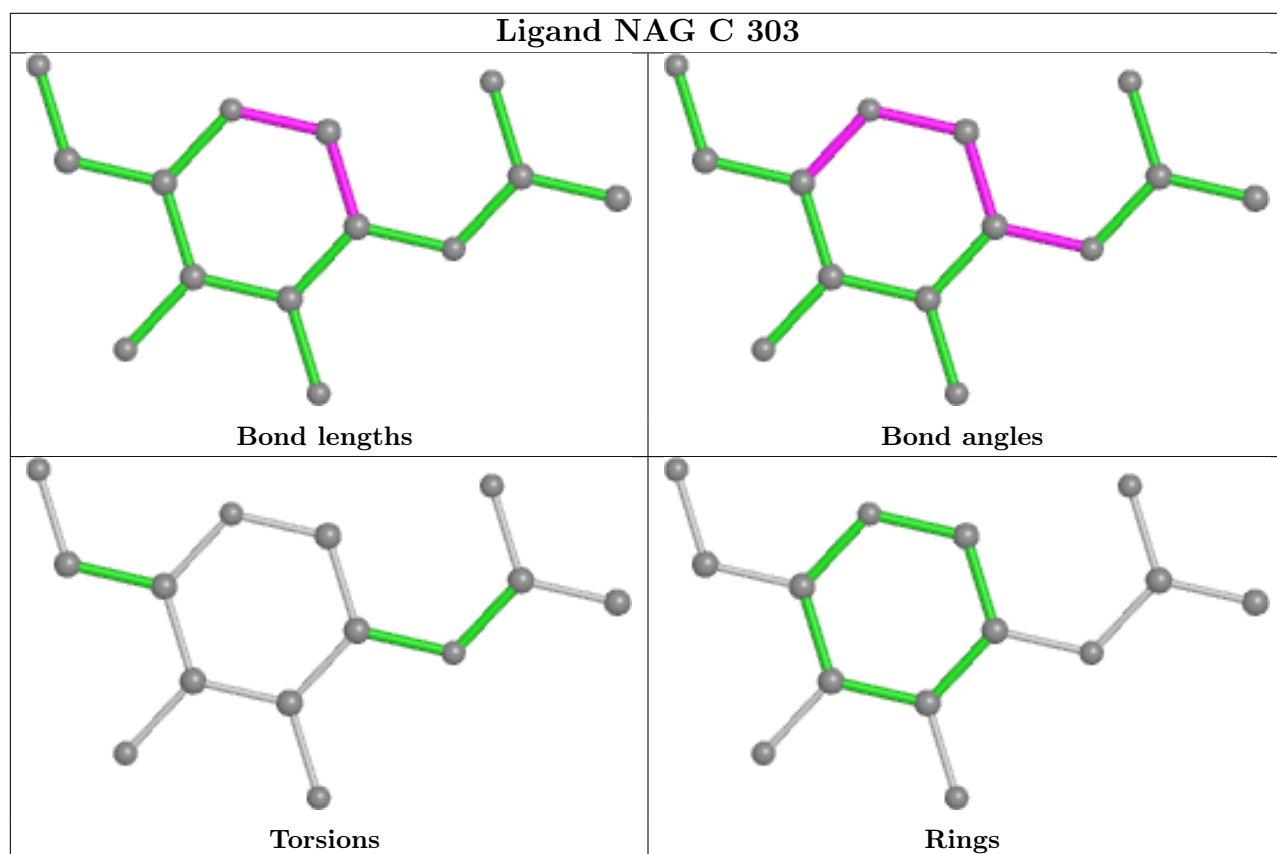
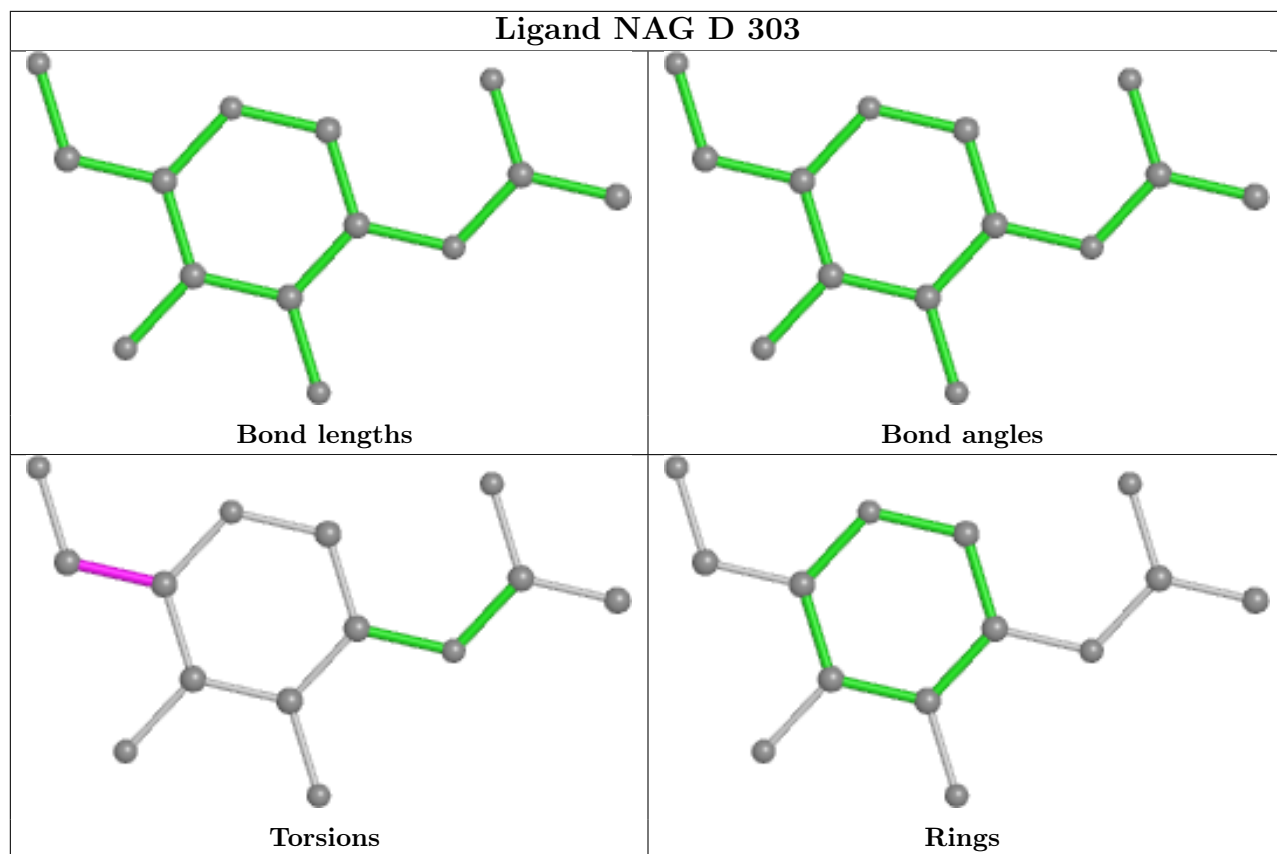
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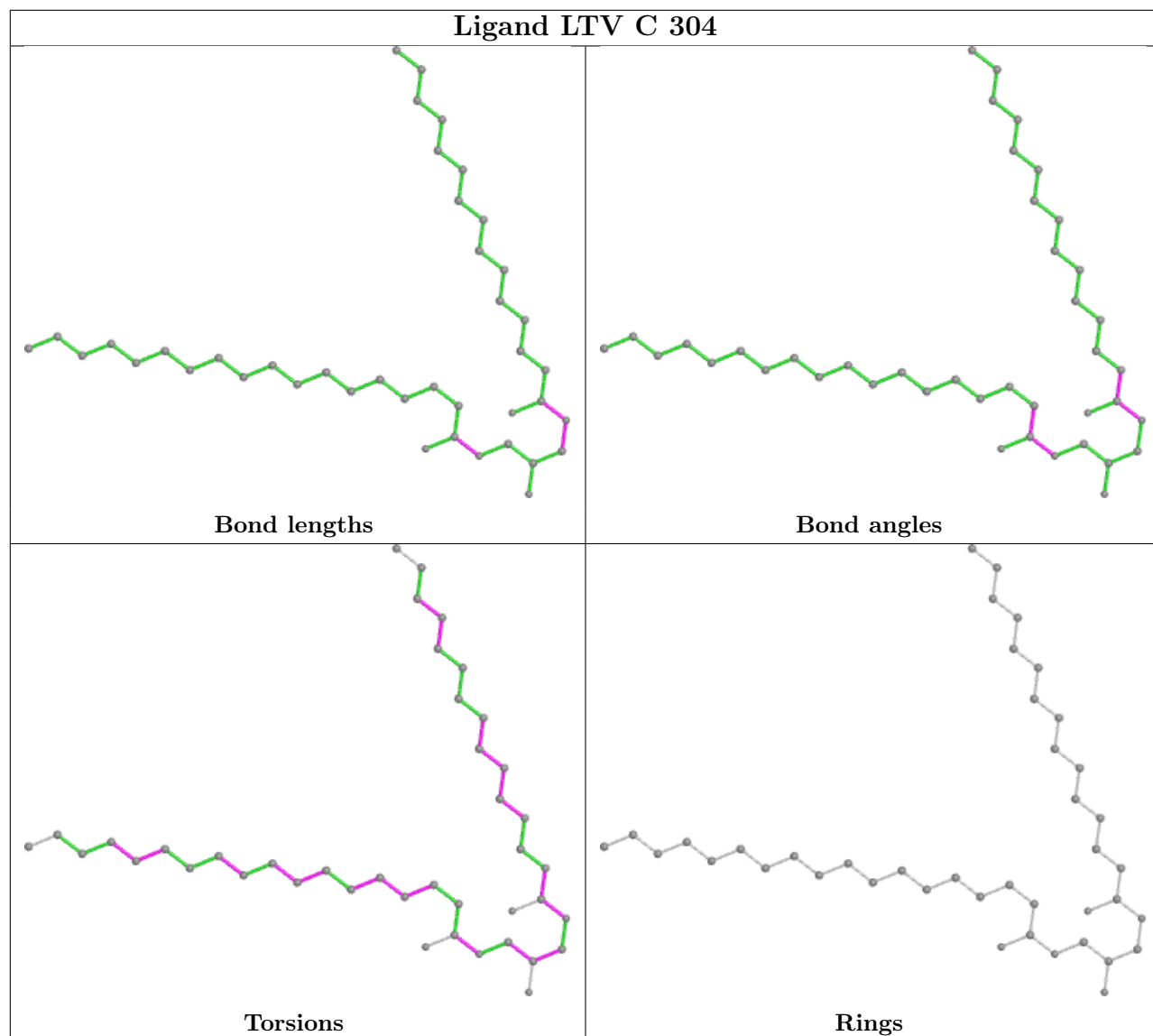
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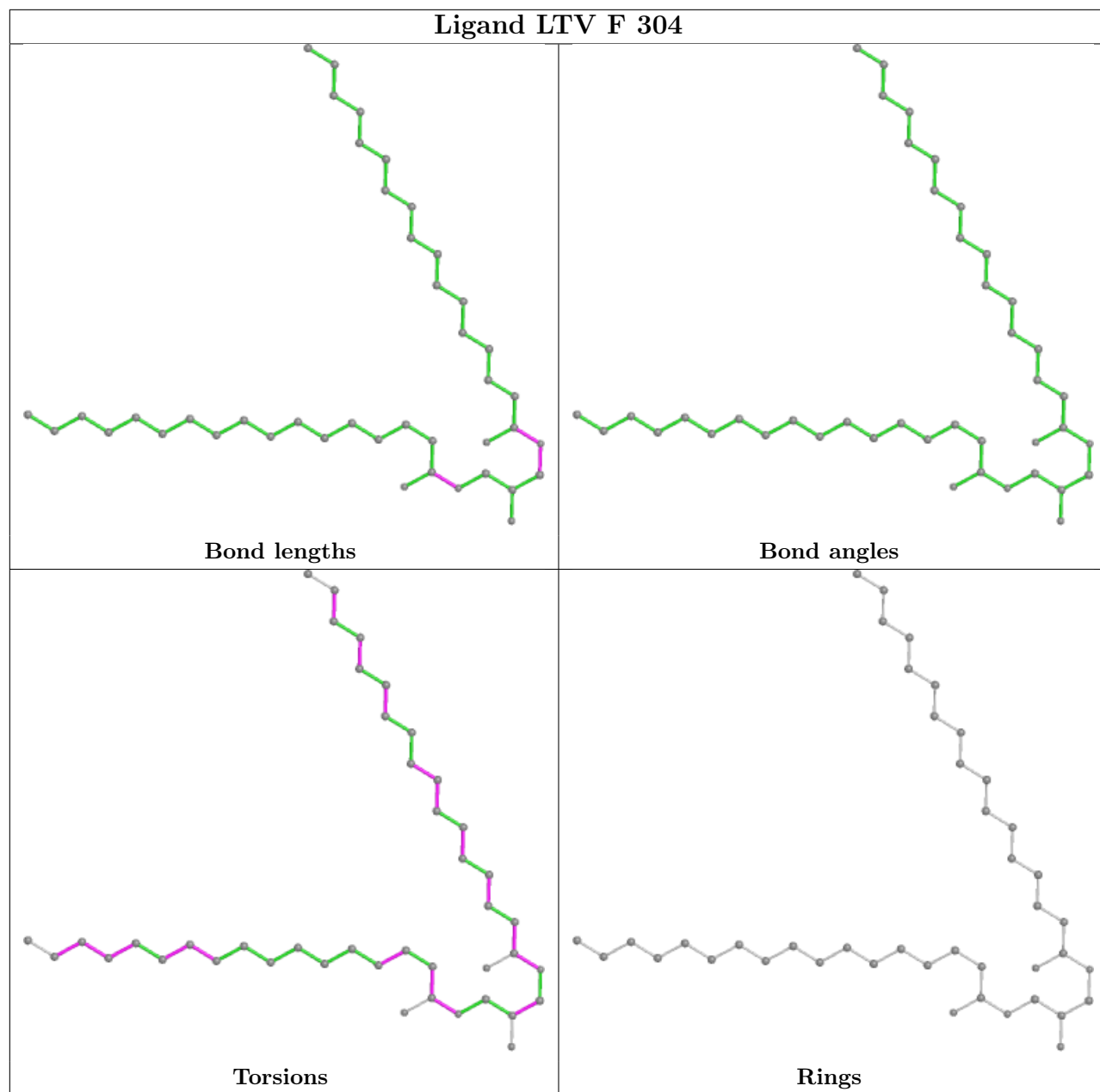
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	NAG	2	0
4	C	304	LTV	1	0
5	F	305	PO4	1	0
2	F	301	OCA	6	0
5	E	305	PO4	1	0
5	B	302	PO4	1	0
2	E	301	OCA	10	0
3	A	302	NAG	1	0
2	C	301	OCA	12	0
3	B	305	NAG	3	0
2	B	301	OCA	9	0
5	E	306	PO4	1	0
2	D	301	OCA	6	0
2	A	301	OCA	6	0
3	F	303	NAG	3	0
4	E	304	LTV	4	0

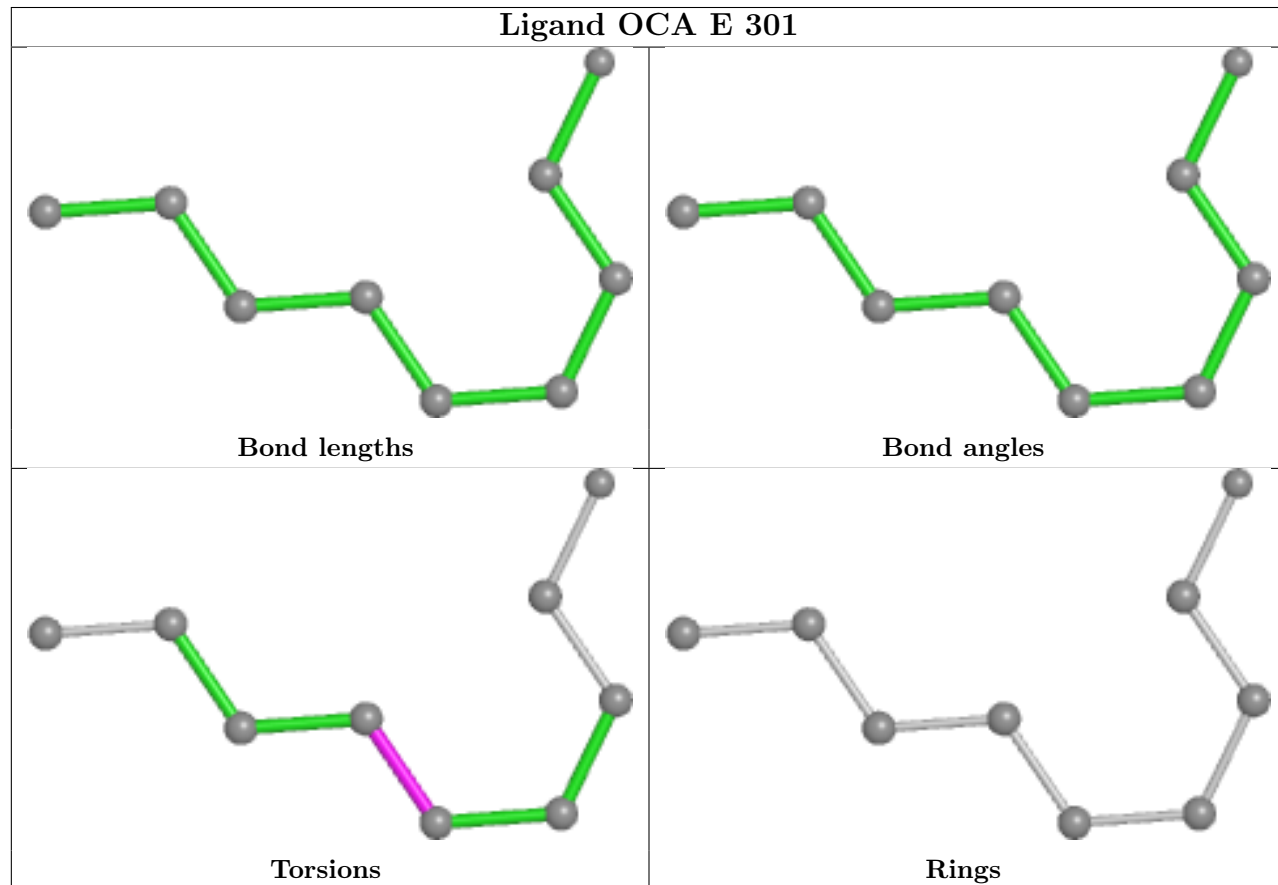
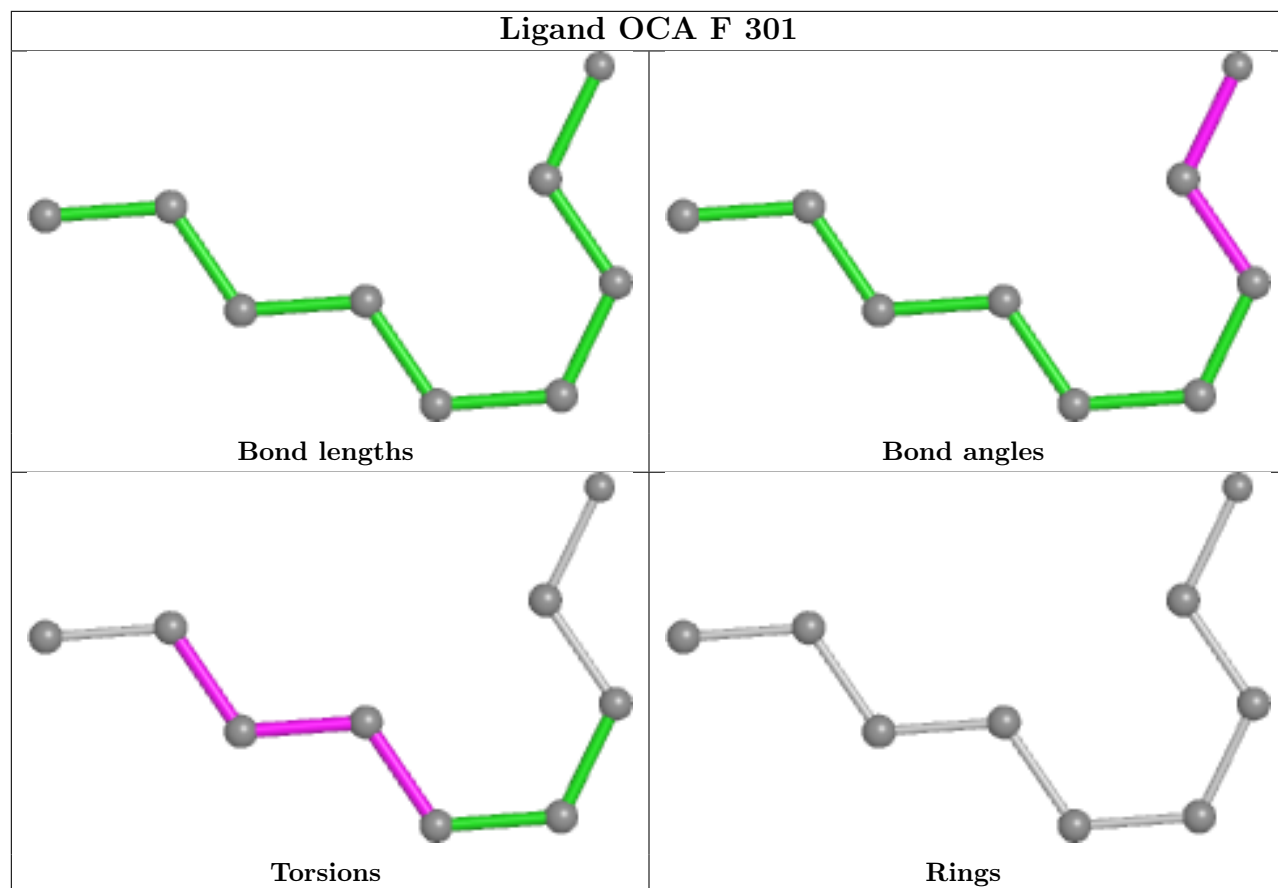
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

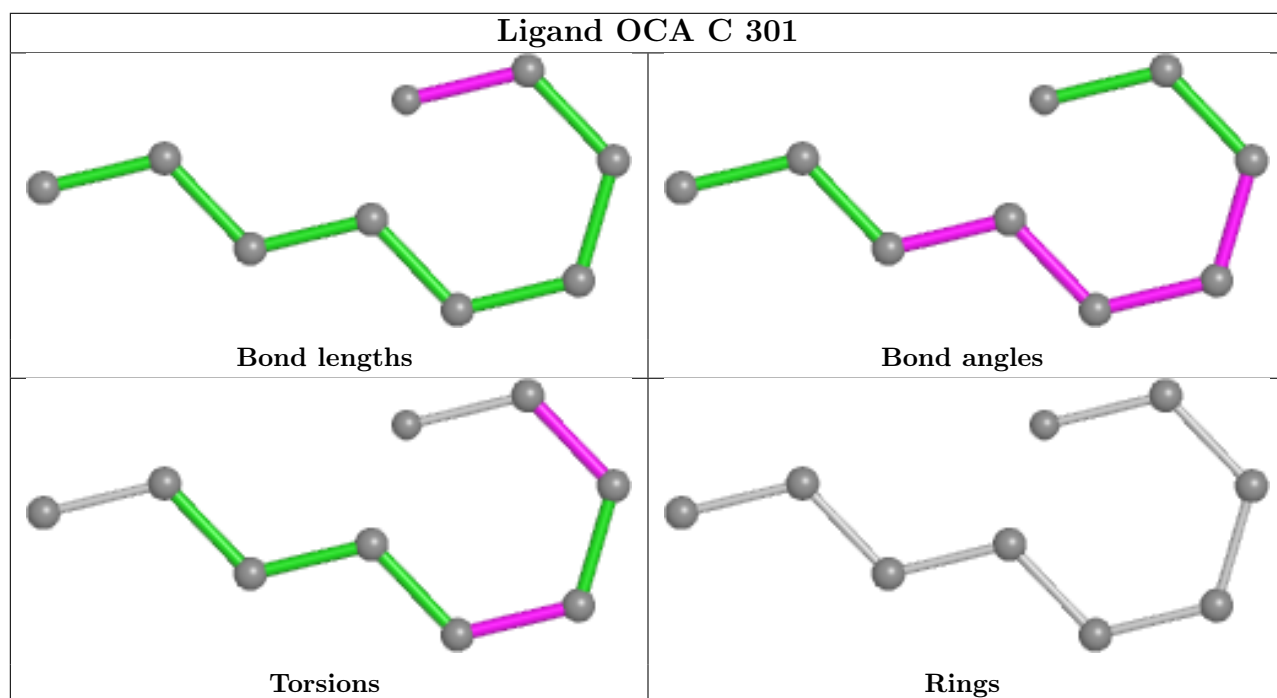
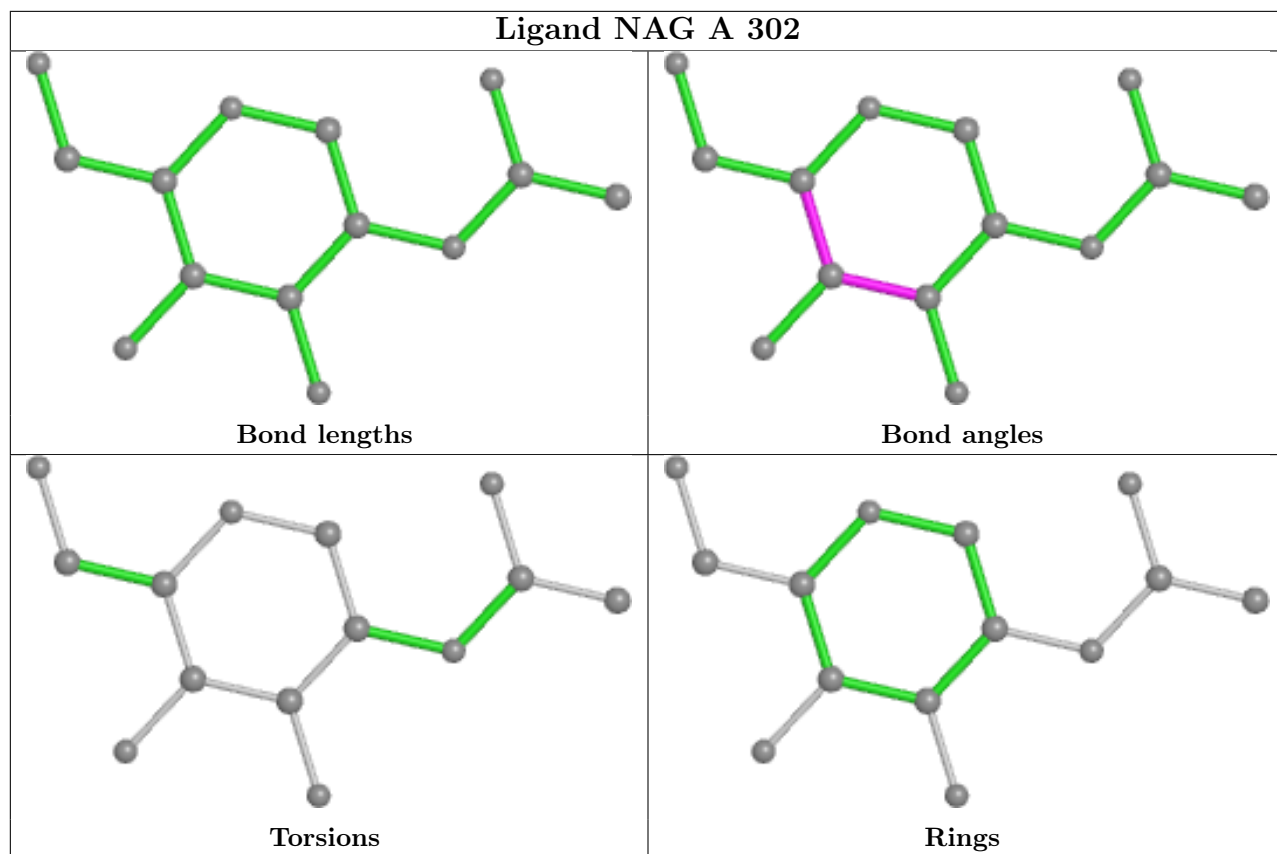


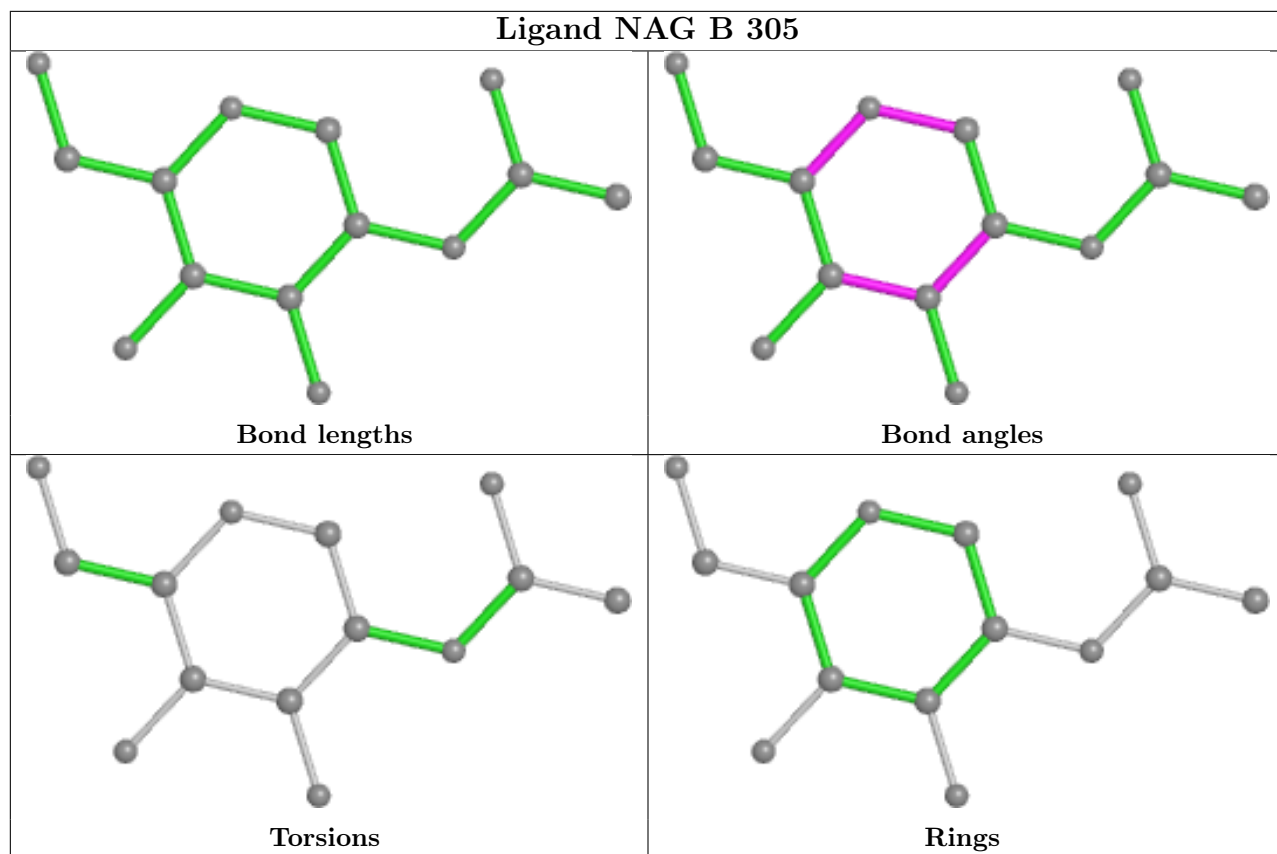


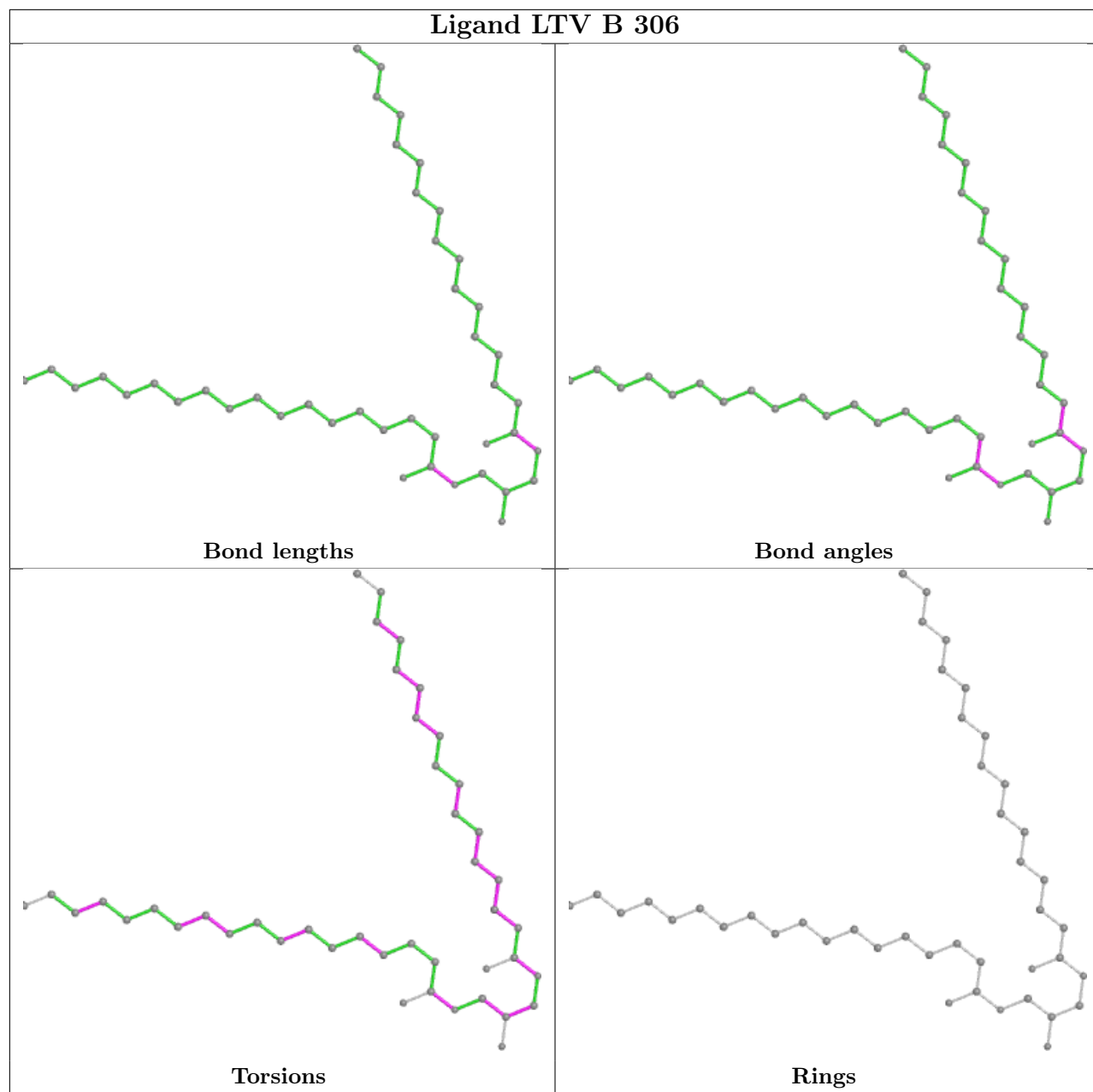


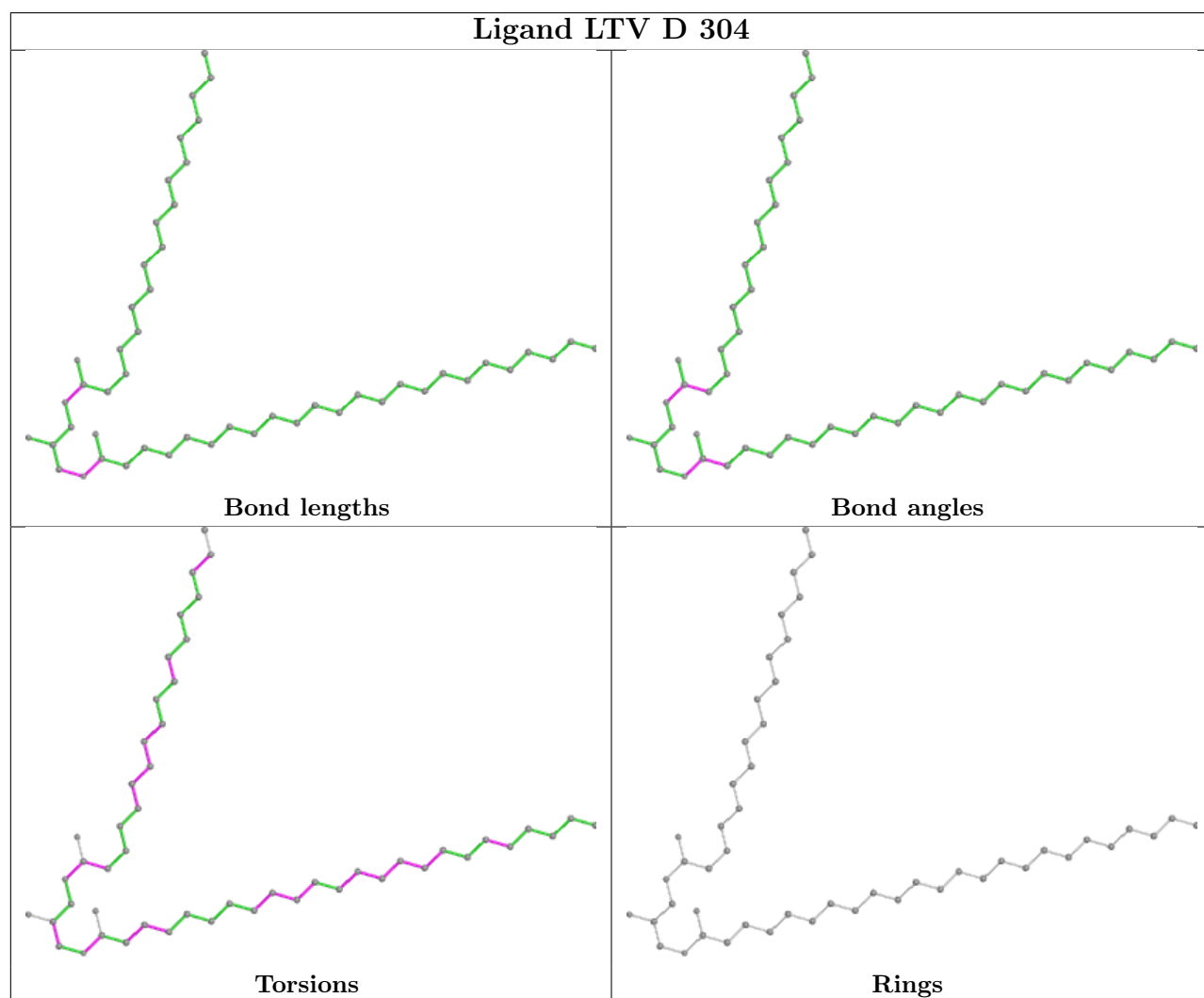
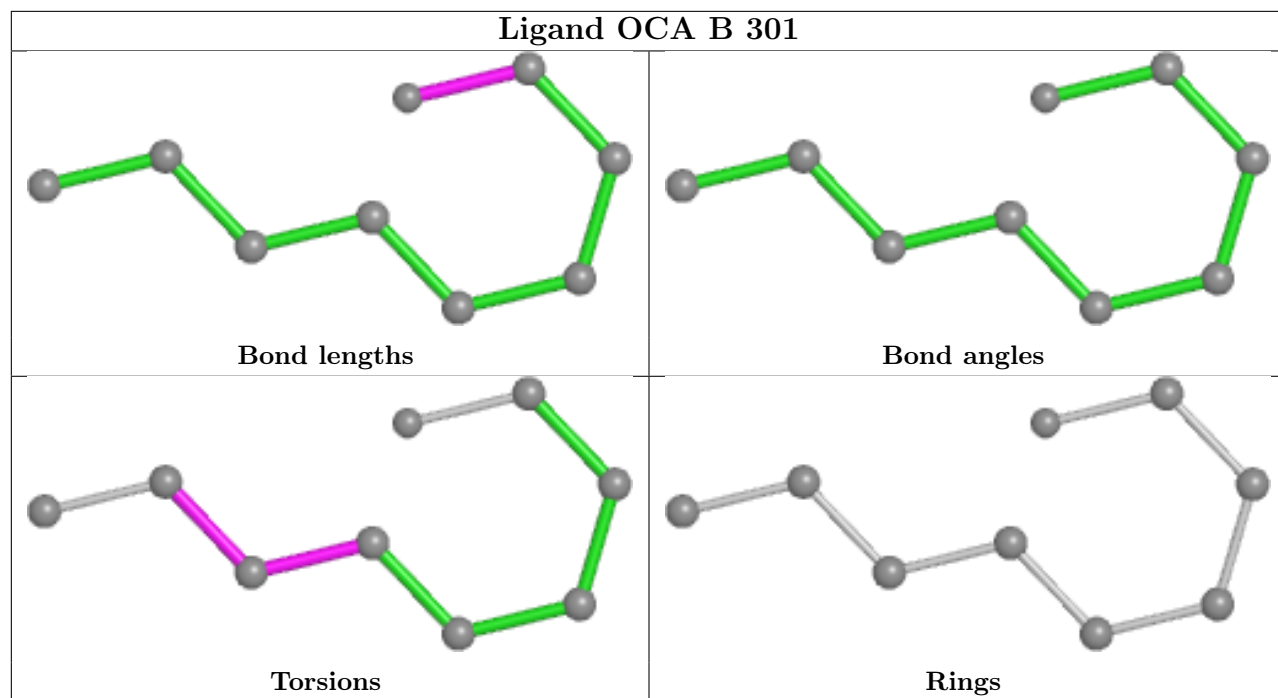


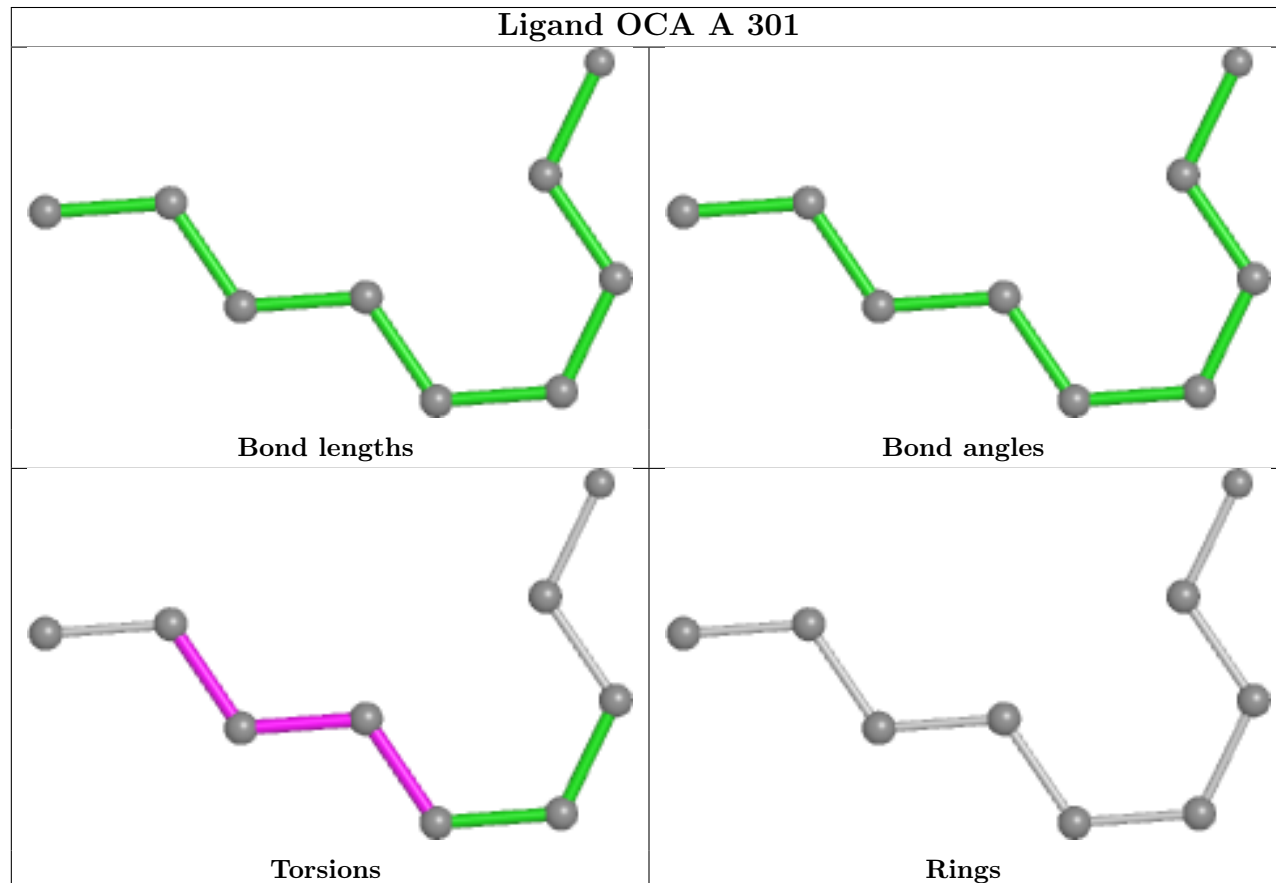
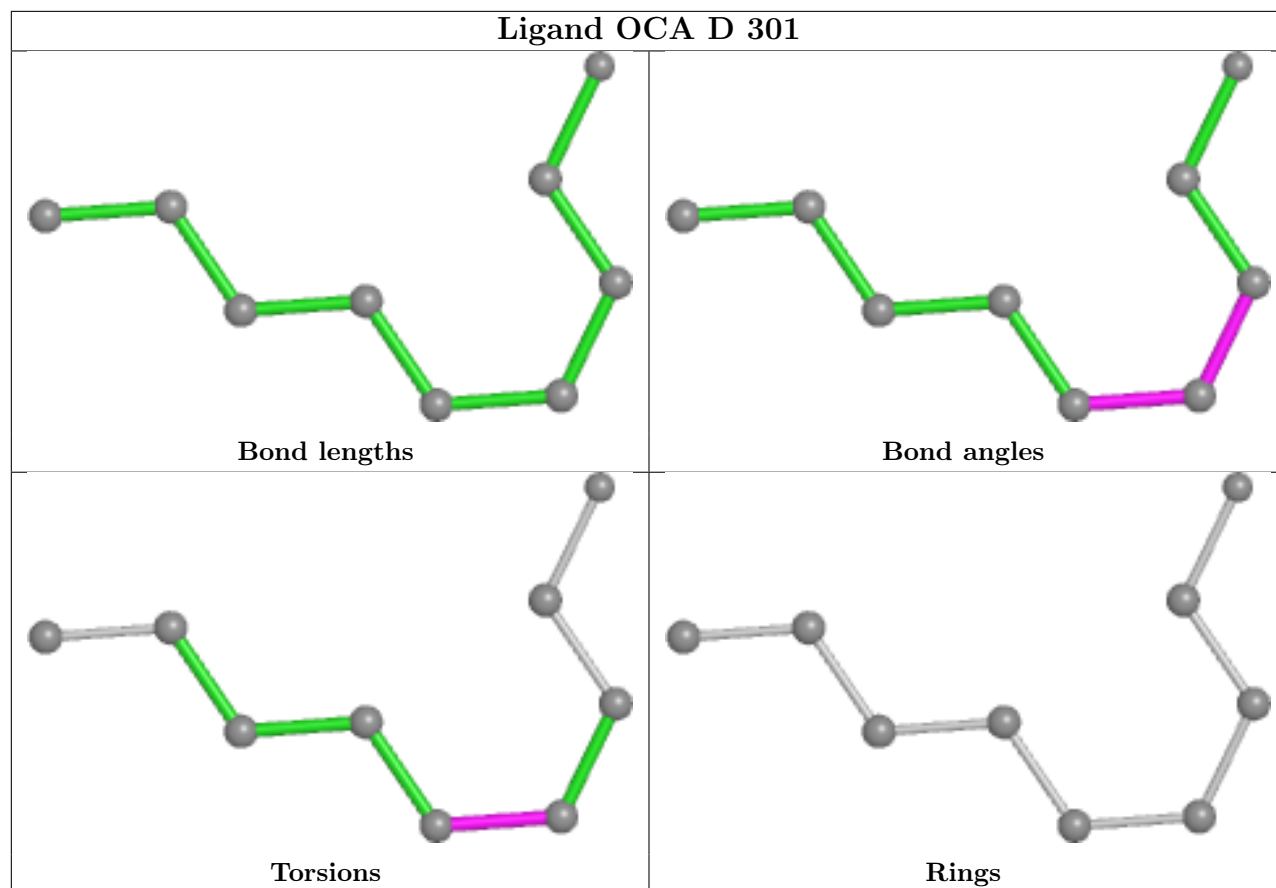


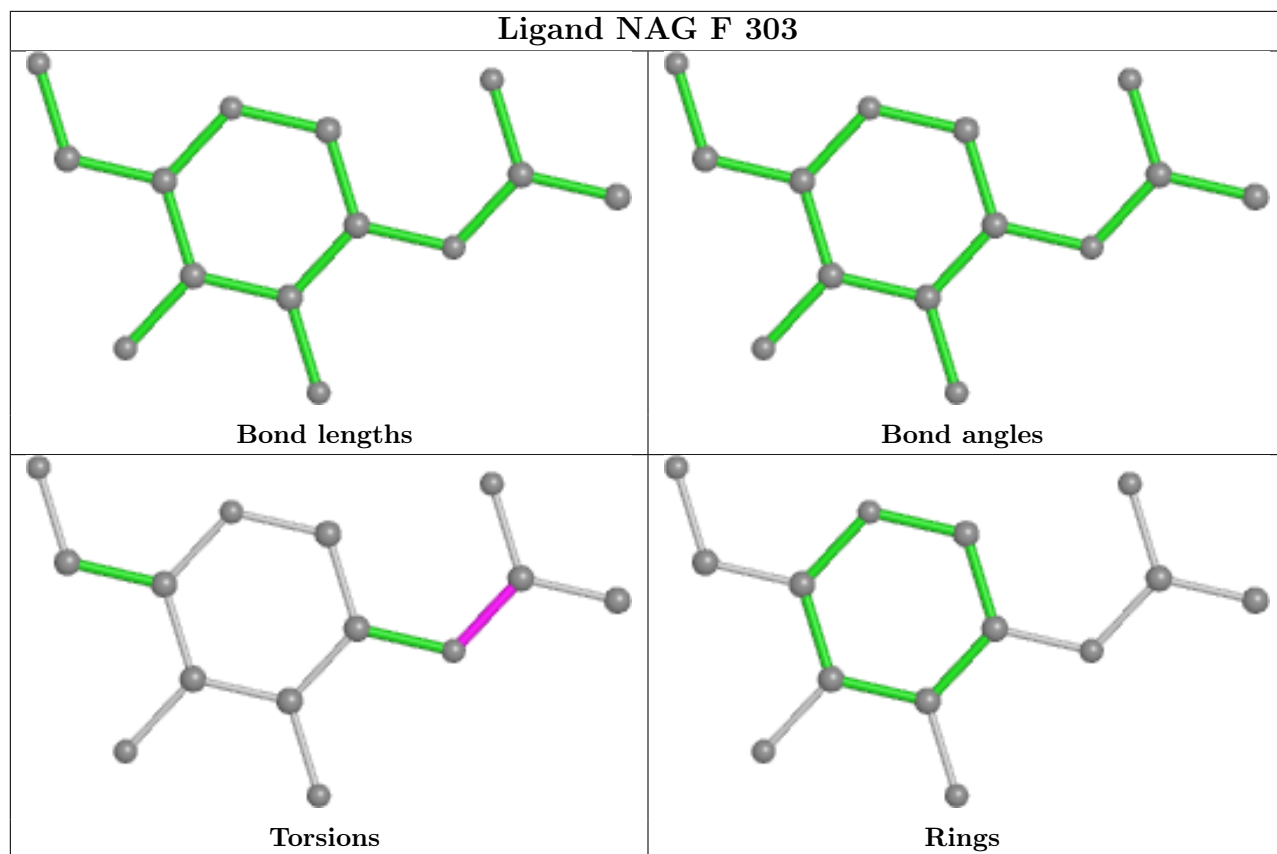


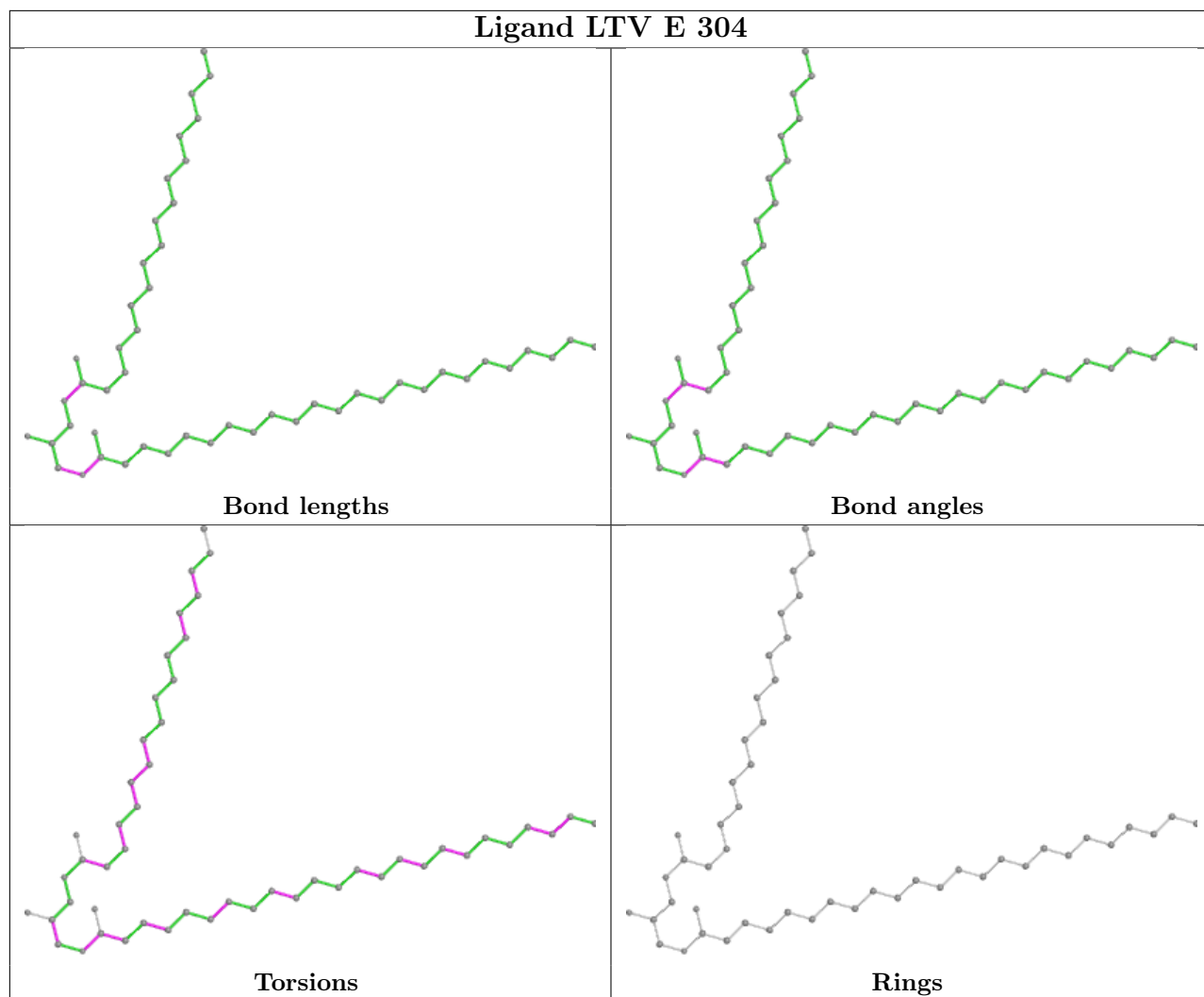


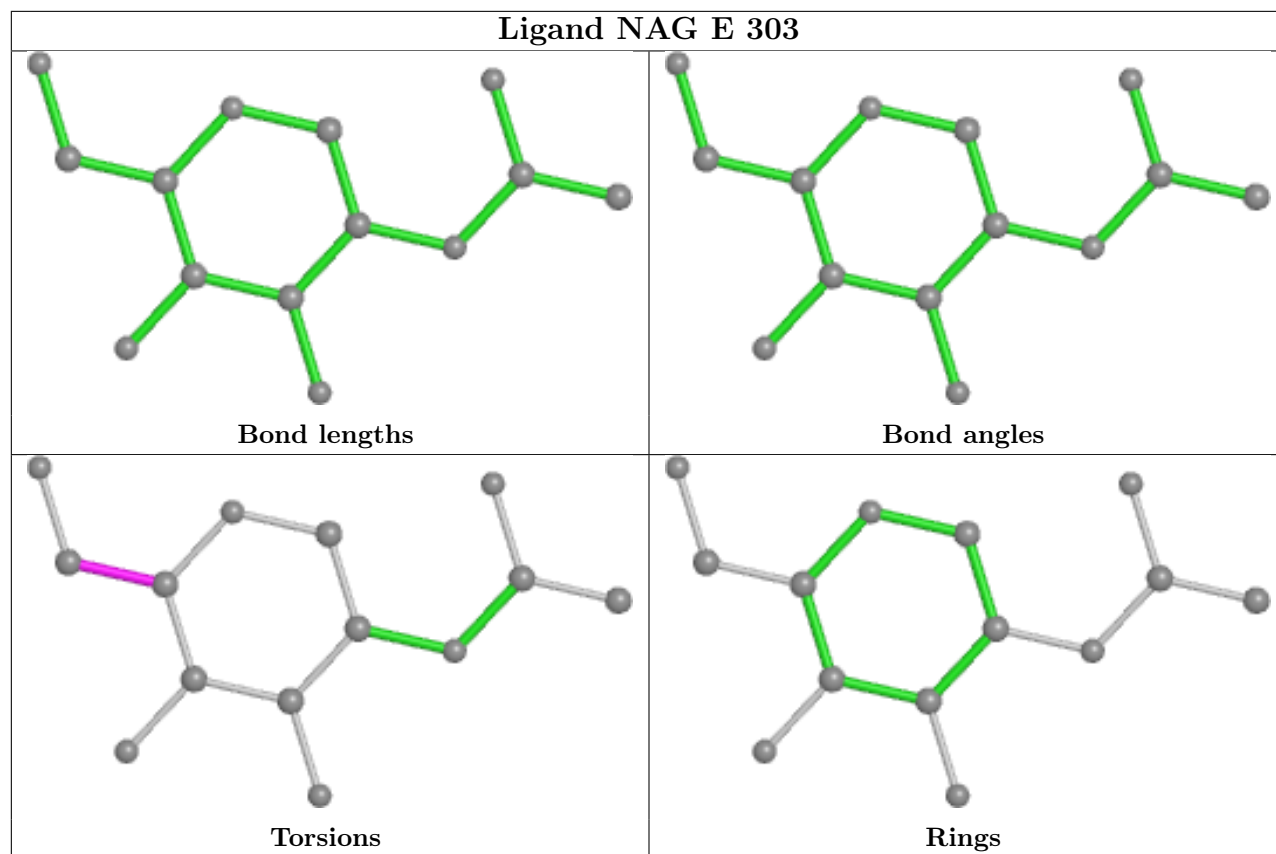












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	269/291 (92%)	-0.36	4 (1%) 73 73	14, 21, 36, 45	3 (1%)
1	B	269/291 (92%)	-0.33	3 (1%) 80 81	15, 23, 37, 47	0
1	C	269/291 (92%)	-0.24	2 (0%) 87 88	15, 26, 42, 51	1 (0%)
1	D	269/291 (92%)	-0.33	3 (1%) 80 81	15, 24, 37, 45	2 (0%)
1	E	269/291 (92%)	-0.25	2 (0%) 87 88	18, 28, 41, 48	1 (0%)
1	F	269/291 (92%)	-0.45	2 (0%) 87 88	15, 22, 34, 40	2 (0%)
All	All	1614/1746 (92%)	-0.33	16 (0%) 82 82	14, 24, 39, 51	9 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	89	TRP	4.3
1	B	89[A]	TRP	4.3
1	D	252	ILE	4.0
1	A	269	LEU	3.9
1	D	89	TRP	3.9
1	C	245	GLY	3.8
1	C	250	PRO	3.1
1	A	89	TRP	2.9
1	F	89[A]	TRP	2.8
1	B	245	GLY	2.6
1	B	252	ILE	2.6
1	D	250	PRO	2.4
1	E	252	ILE	2.3
1	A	162	ASN	2.2
1	F	252	ILE	2.1
1	A	39	ASN	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.

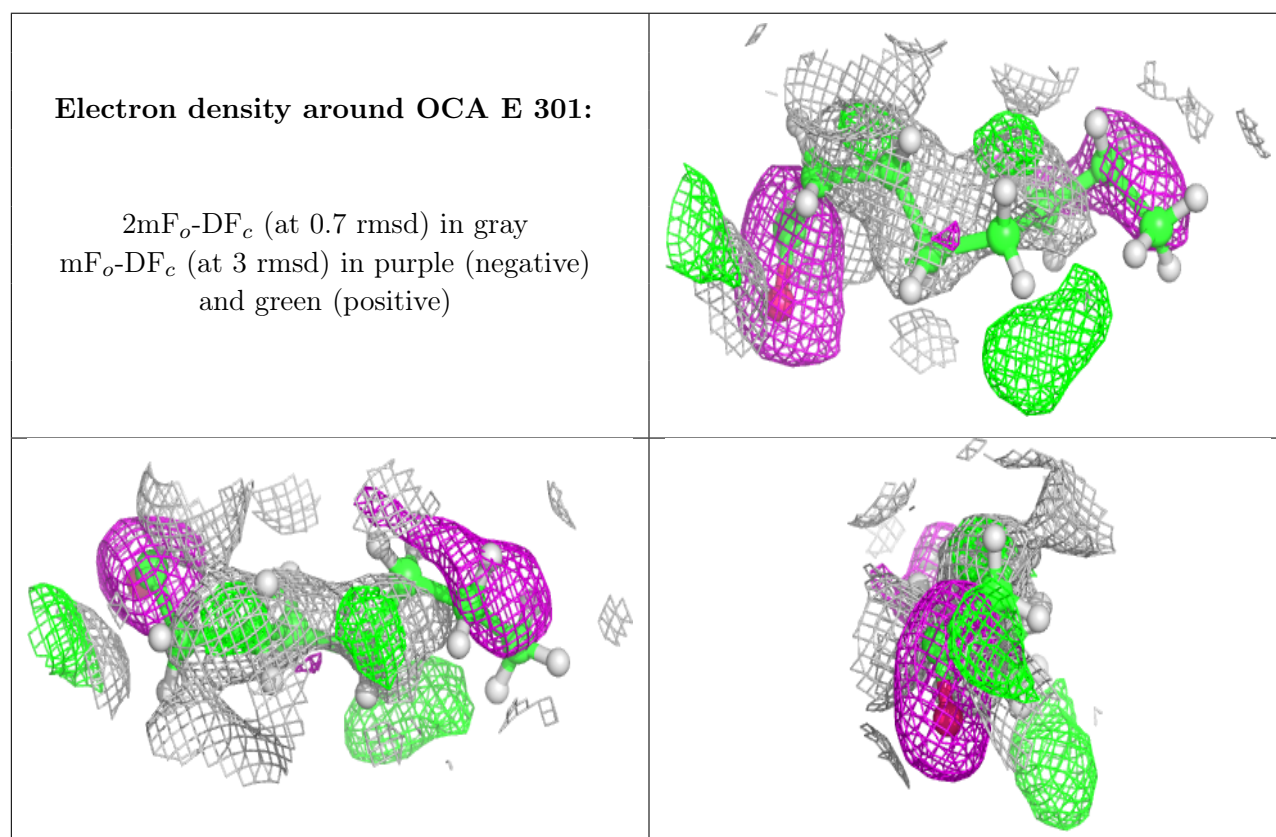
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OCA	E	301	9/10	0.25	0.59	35,46,55,55	24
2	OCA	C	301	9/10	0.41	0.59	30,41,47,47	24
2	OCA	A	301	9/10	0.56	0.33	28,41,48,48	24
2	OCA	D	301	9/10	0.60	0.37	30,45,53,53	24
2	OCA	B	301	9/10	0.62	0.46	32,49,59,59	24
2	OCA	F	301	9/10	0.62	0.35	29,42,52,52	24
3	NAG	A	302	14/15	0.64	0.30	56,59,71,72	0
3	NAG	C	303	14/15	0.68	0.29	48,53,64,64	0
3	NAG	D	303	14/15	0.68	0.26	50,54,65,65	0
4	LTV	E	304	51/51	0.70	0.35	54,70,80,81	0
4	LTV	D	304	51/51	0.72	0.30	52,66,73,73	0
3	NAG	F	303	14/15	0.73	0.20	42,45,54,55	0
4	LTV	A	303	36/51	0.76	0.26	46,61,73,74	0
4	LTV	F	304	42/51	0.76	0.29	44,59,71,71	0
4	LTV	C	304	41/51	0.77	0.29	52,66,74,75	0
3	NAG	E	303	14/15	0.77	0.21	55,59,71,71	0
4	LTV	B	306	43/51	0.78	0.29	48,63,75,76	0
3	NAG	B	305	14/15	0.84	0.14	36,40,49,49	0
5	PO4	B	307	5/5	0.84	0.19	55,56,56,56	5
5	PO4	D	305	5/5	0.84	0.28	51,53,54,54	5
5	PO4	F	305	5/5	0.87	0.13	41,43,43,44	5
5	PO4	C	305	5/5	0.88	0.23	58,61,71,76	0
5	PO4	E	306	5/5	0.88	0.14	38,41,42,43	5
5	PO4	A	305	5/5	0.90	0.11	26,29,30,30	5
5	PO4	D	306	5/5	0.91	0.11	45,45,46,47	5
5	PO4	E	305	5/5	0.91	0.15	54,54,55,55	5
5	PO4	B	302	5/5	0.92	0.11	37,39,40,41	5

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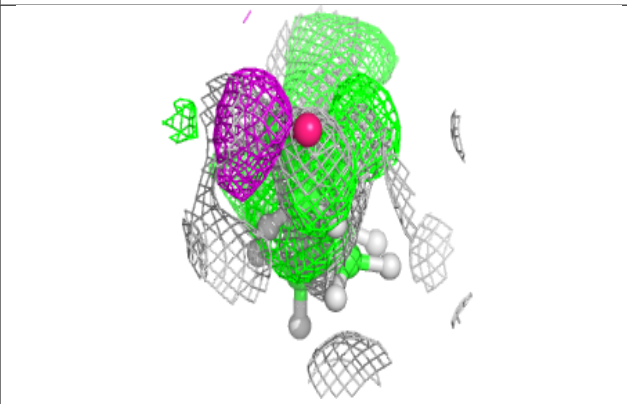
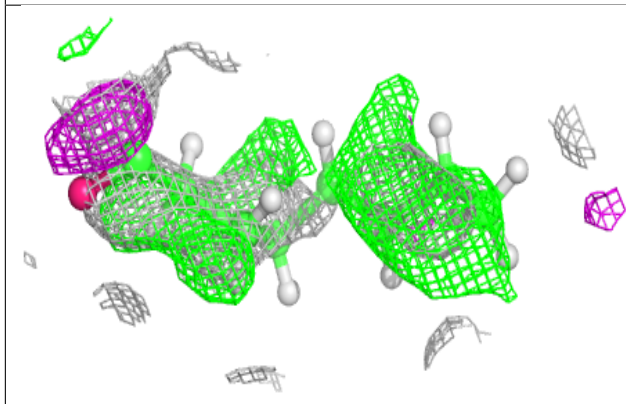
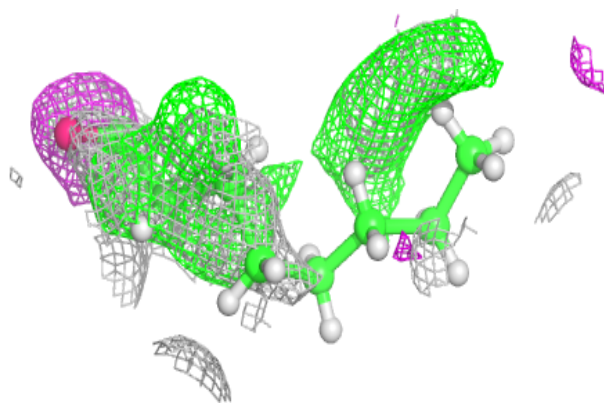
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PO4	A	304	5/5	0.92	0.14	47,49,50,50	5
6	CA	B	304	1/1	0.98	0.09	52,52,52,52	0
6	CA	F	302	1/1	0.98	0.06	39,39,39,39	1
6	CA	C	302	1/1	0.99	0.07	37,37,37,37	1
6	CA	E	302	1/1	0.99	0.04	50,50,50,50	0
6	CA	B	303	1/1	0.99	0.10	20,20,20,20	0
6	CA	D	302	1/1	1.00	0.04	28,28,28,28	1

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

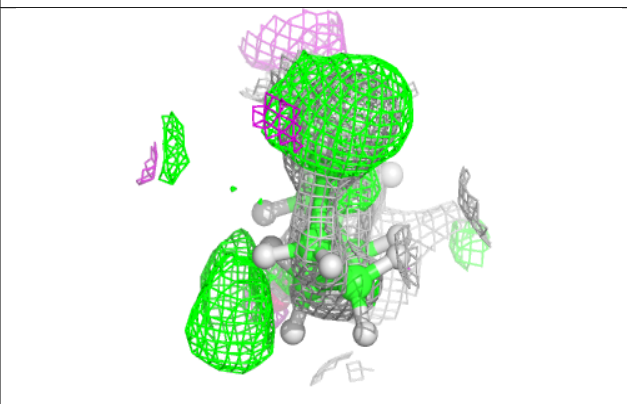
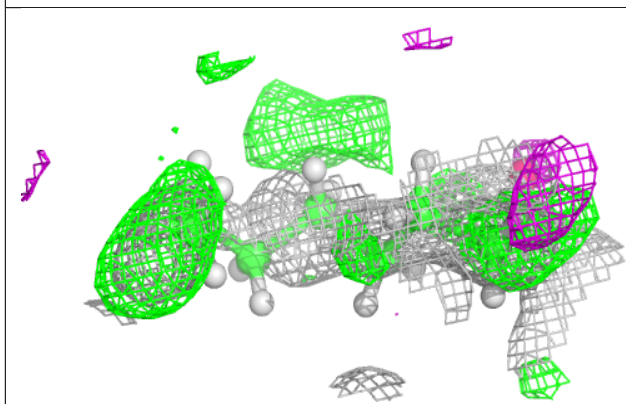
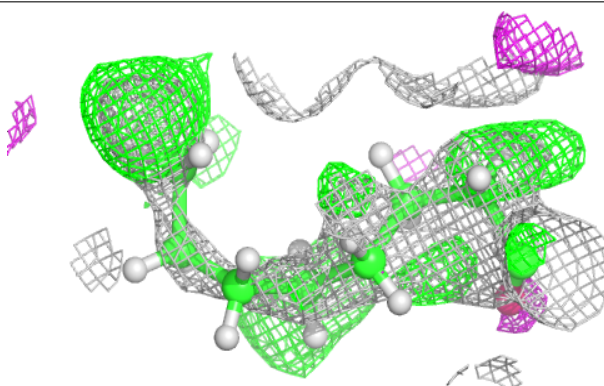


Electron density around OCA C 301:

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

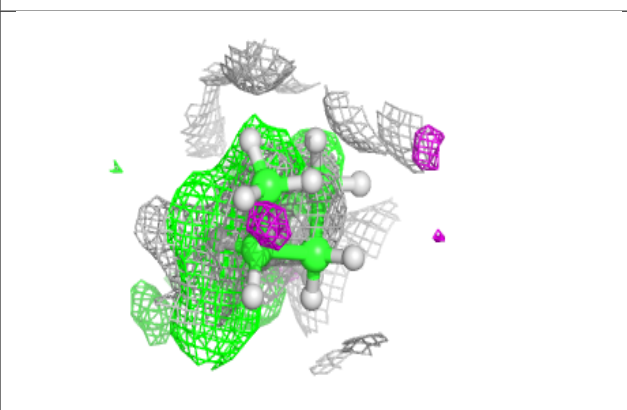
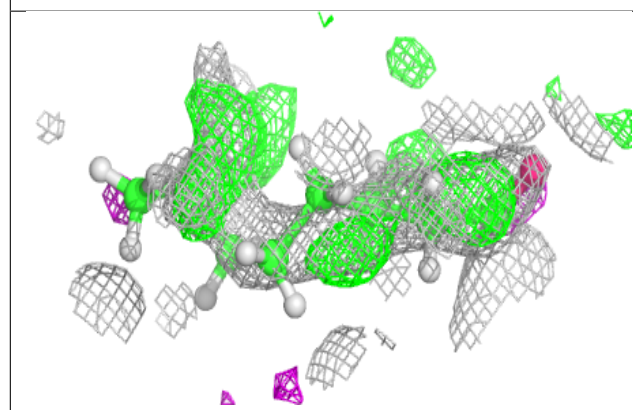
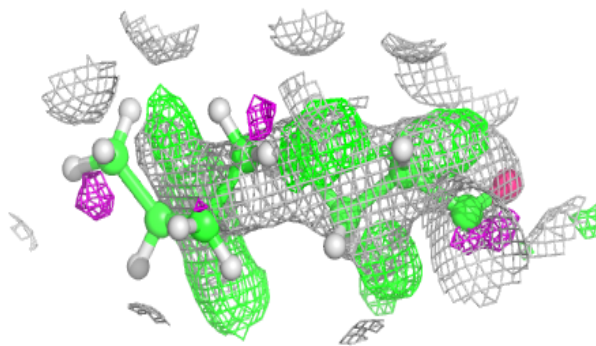
**Electron density around OCA A 301:**

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

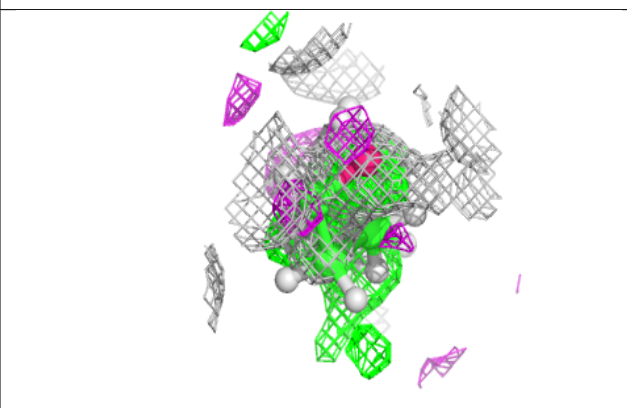
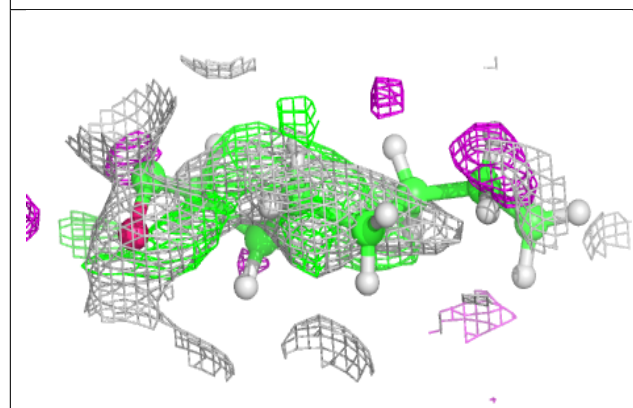
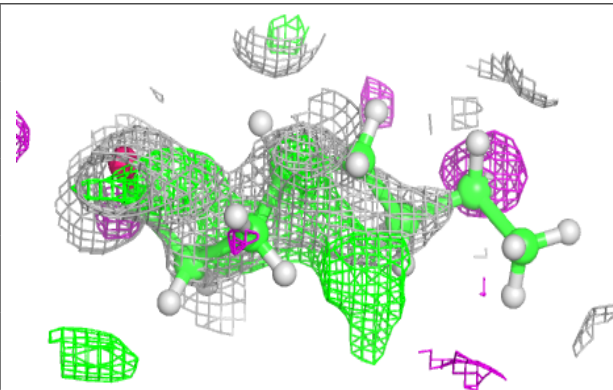


Electron density around OCA D 301:

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

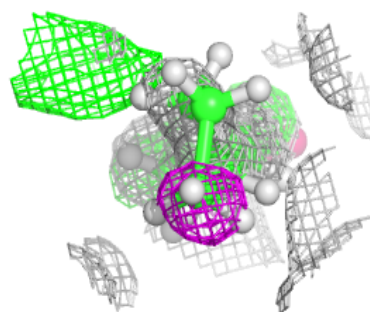
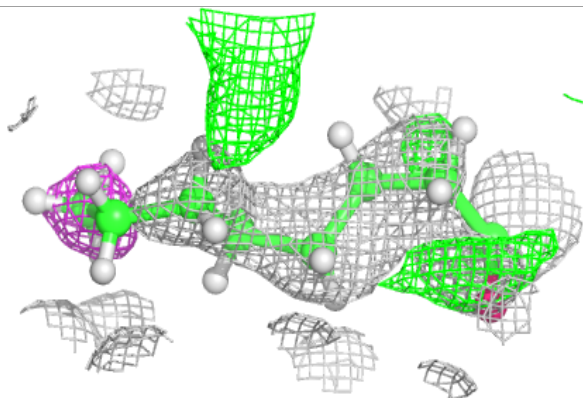
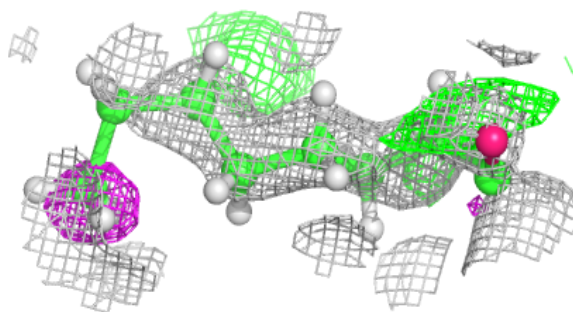
**Electron density around OCA B 301:**

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

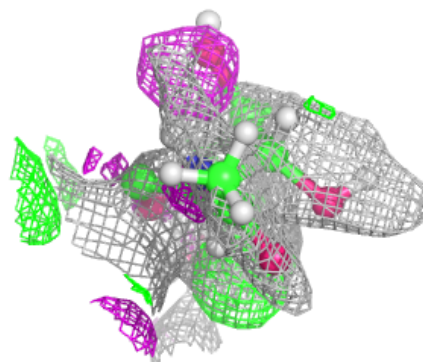
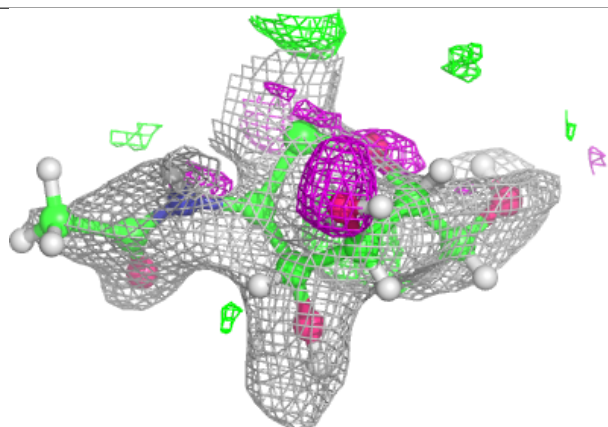
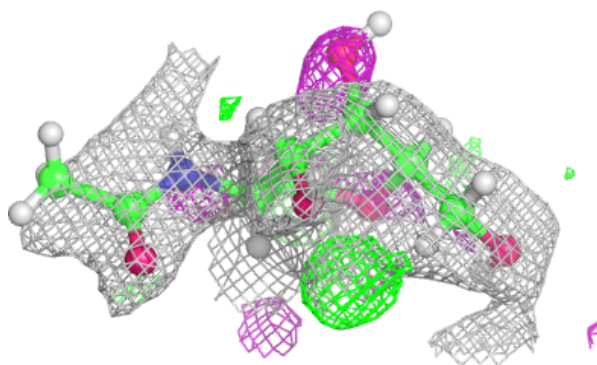


Electron density around OCA F 301:

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

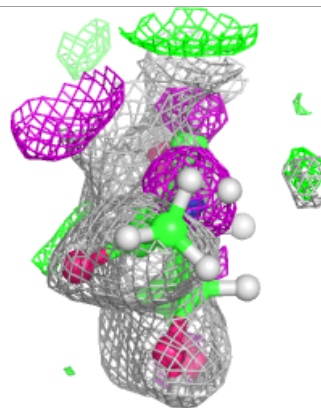
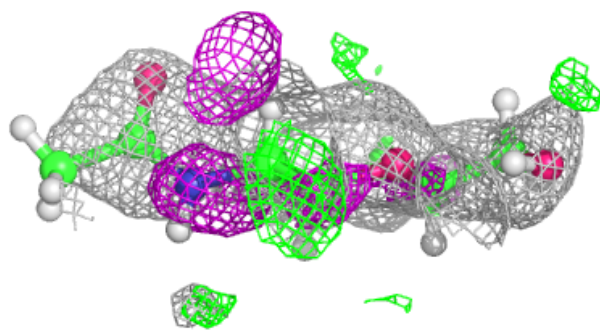
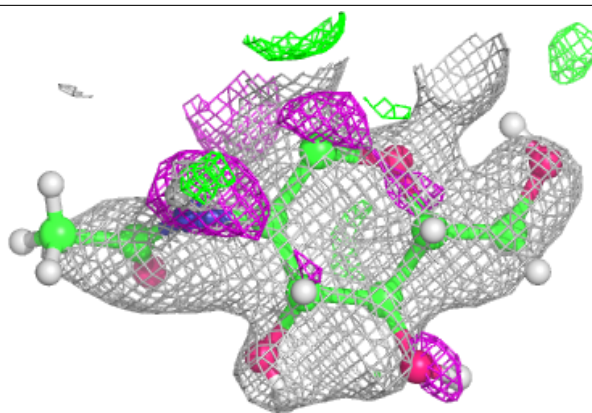
**Electron density around NAG A 302:**

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

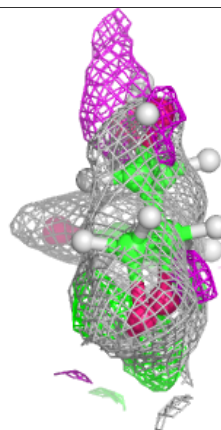
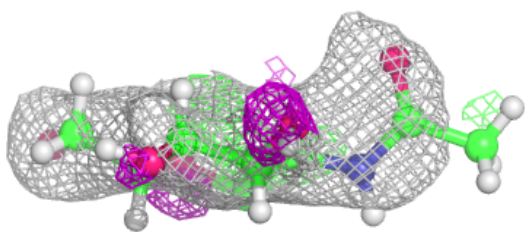
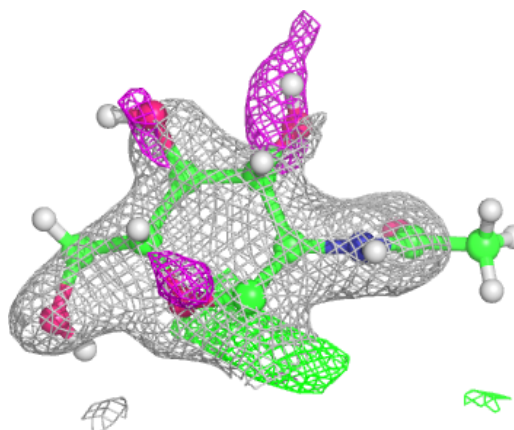


Electron density around NAG C 303:

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

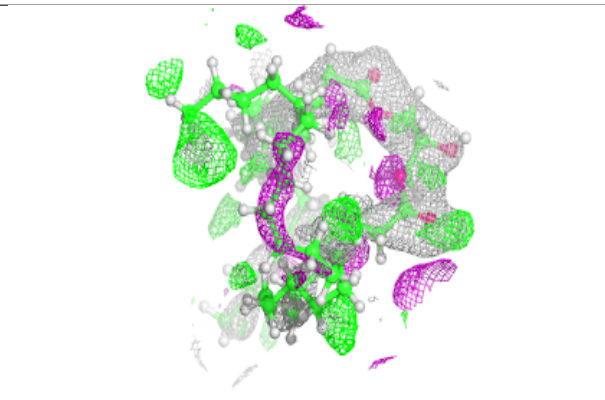
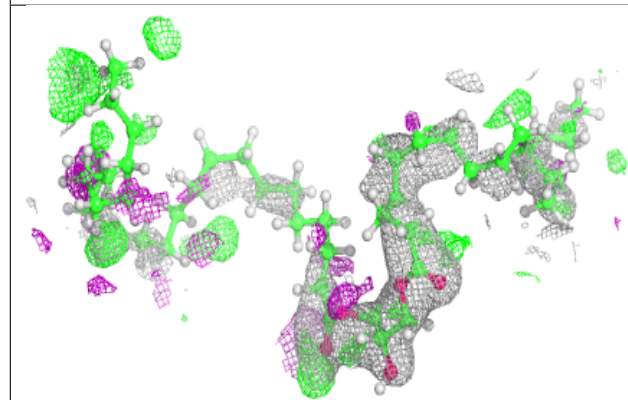
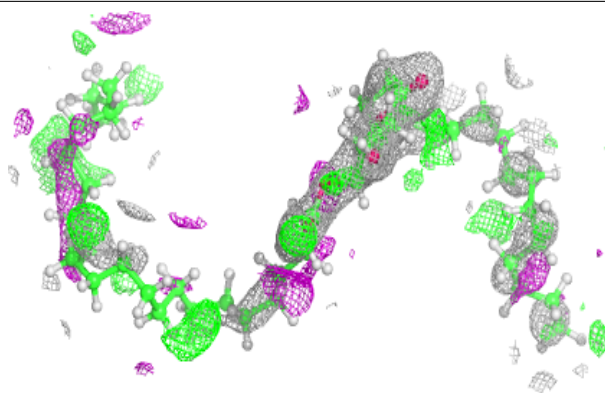
**Electron density around NAG D 303:**

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

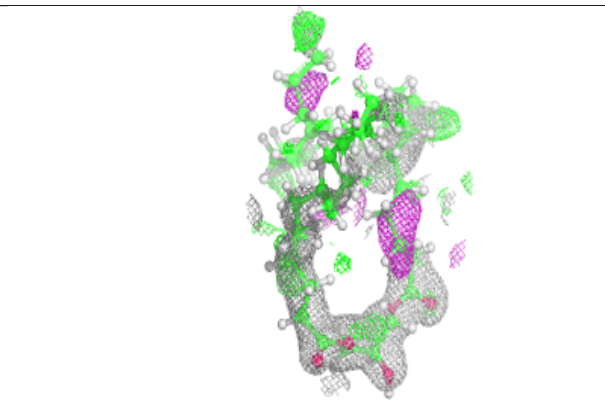
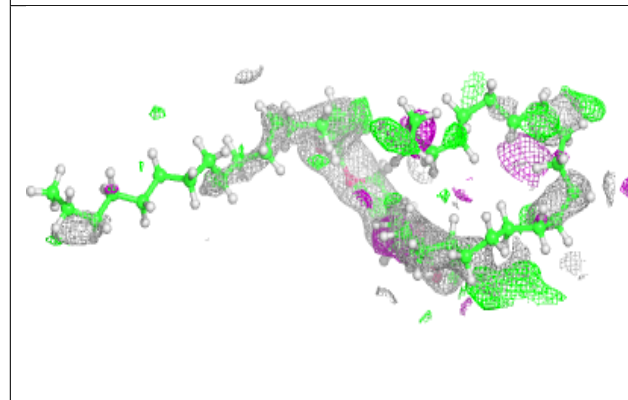
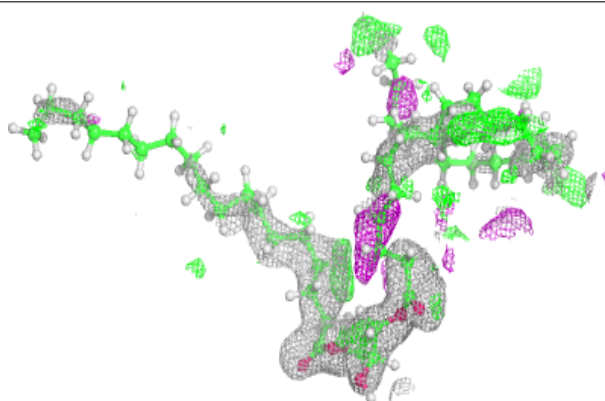


Electron density around LTV E 304:

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

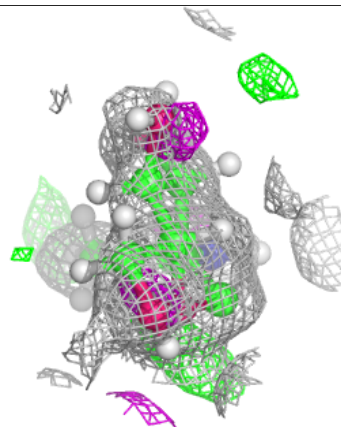
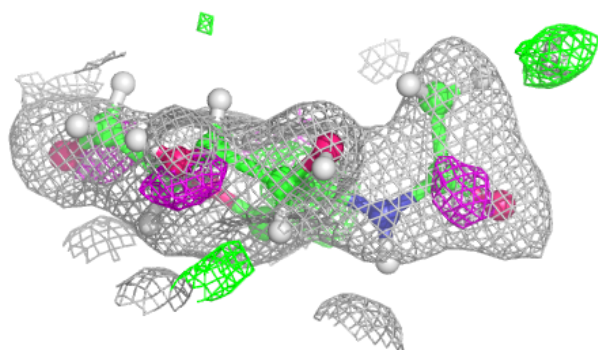
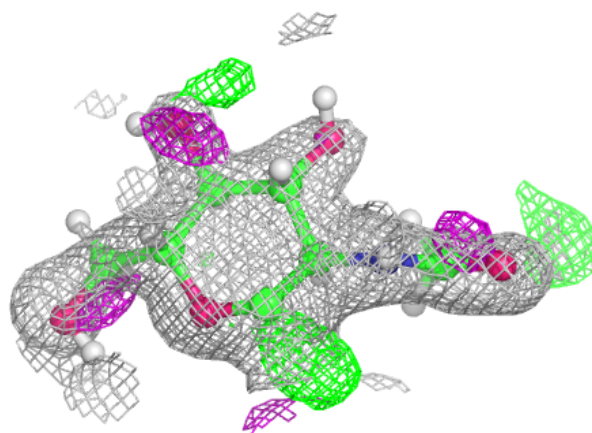
**Electron density around LTV D 304:**

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

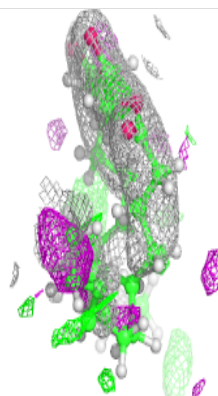
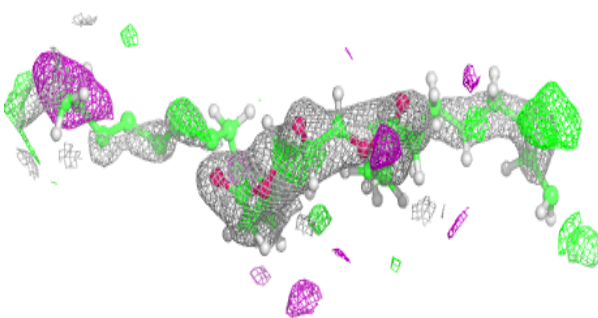
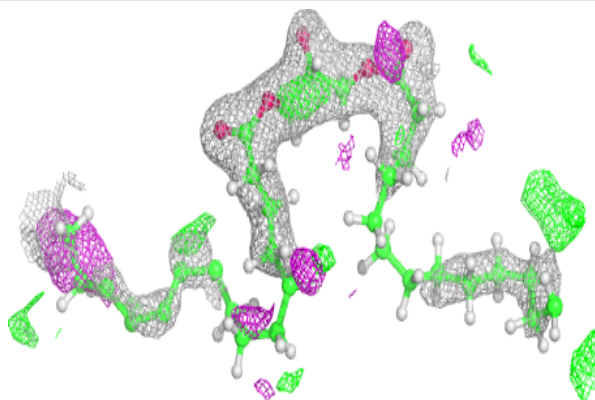


Electron density around NAG F 303:

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

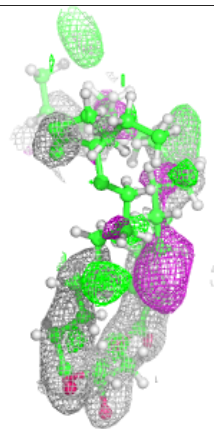
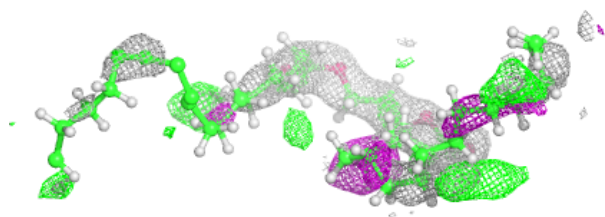
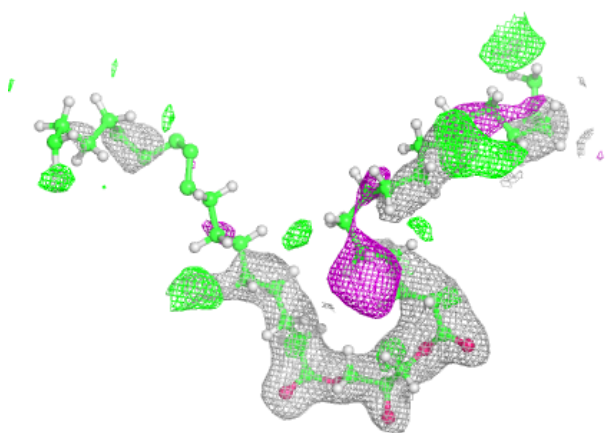
**Electron density around LTV A 303:**

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



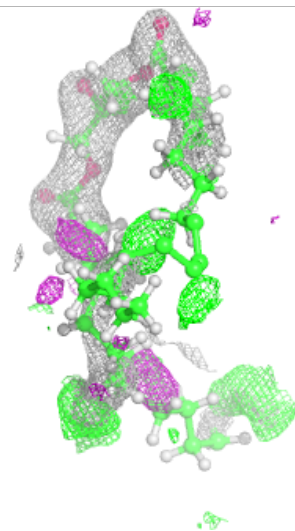
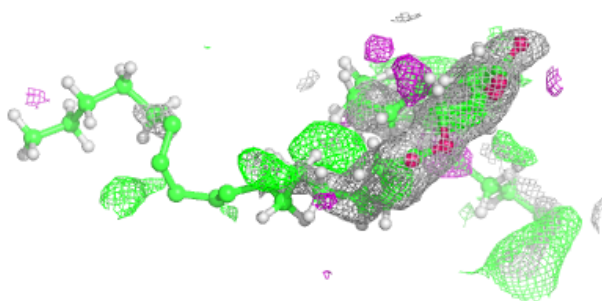
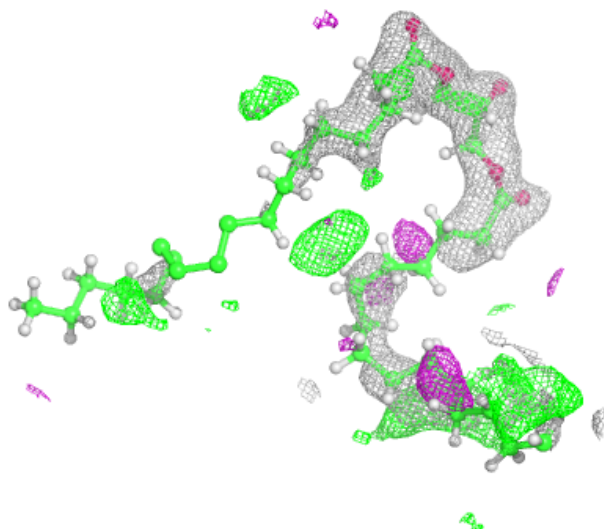
Electron density around LTV F 304:

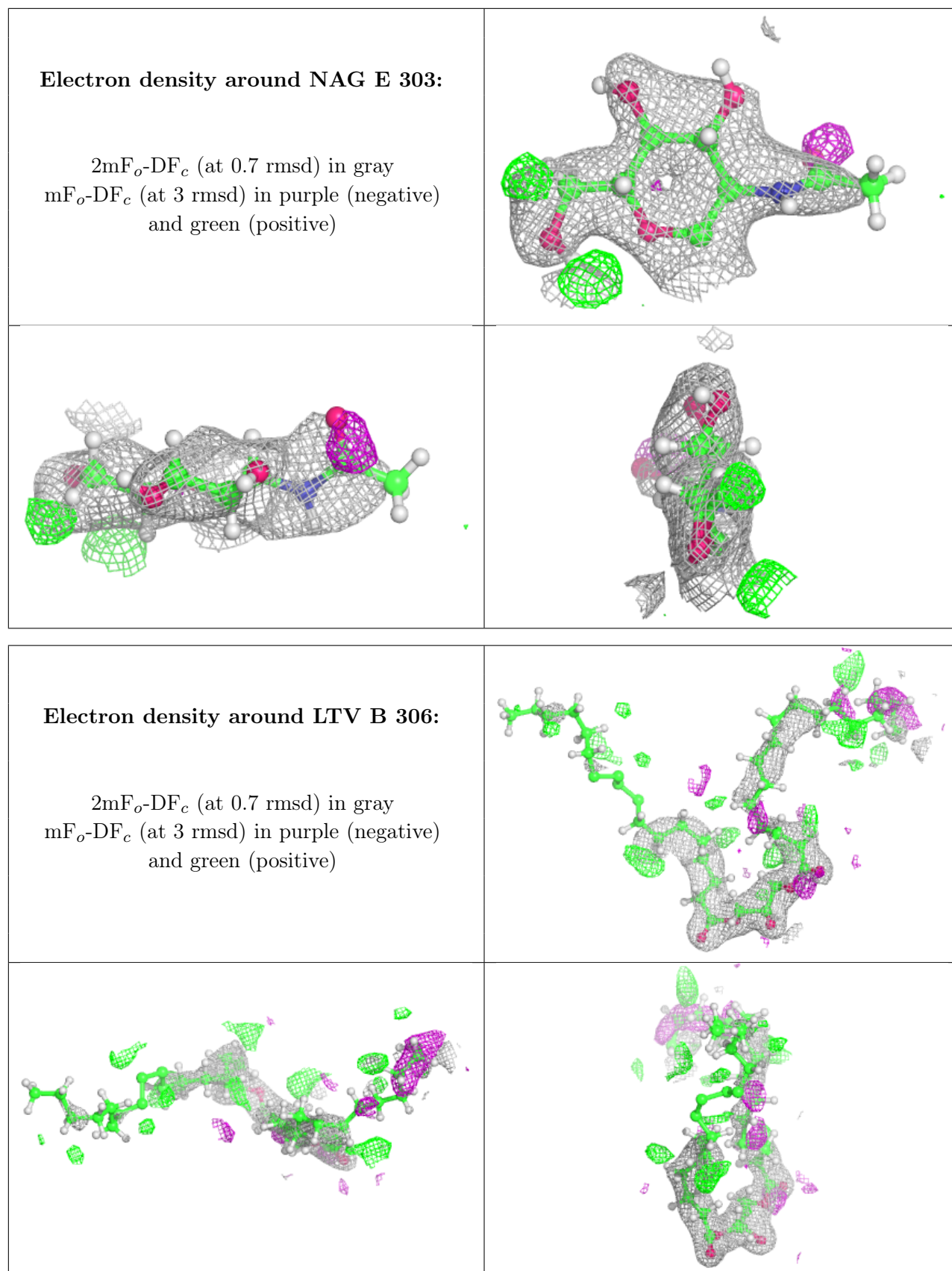
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

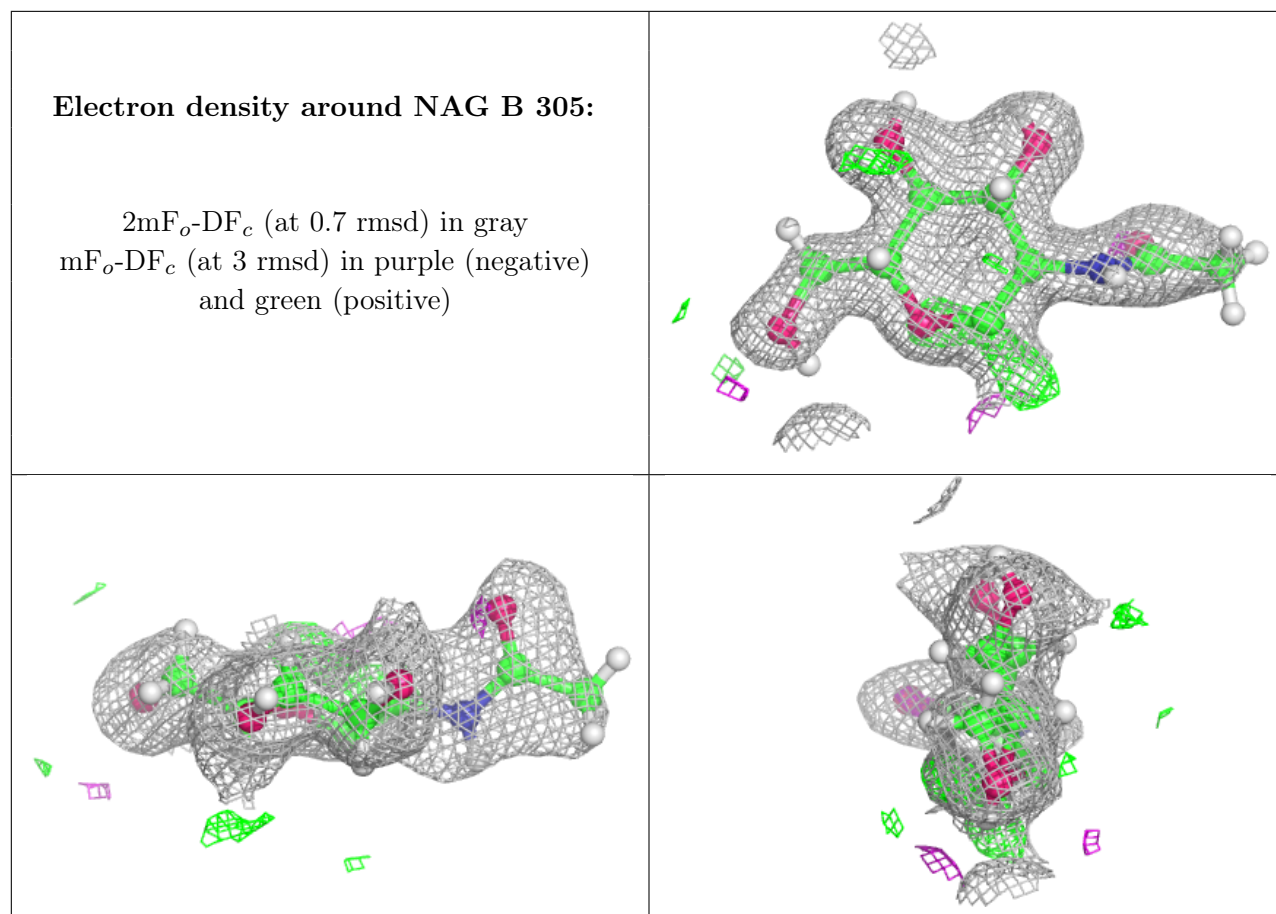


Electron density around LTV C 304:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.