



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 28, 2026 – 12:24 PM EDT

PDB ID : 37DS / pdb_000037ds
Title : Crystal Structure of Thermomyces lanuginosa Lipase With Bound 1,3 diacylglycerol and Fatty Acid Acyl intermediates: Monoclinic Crystals
Authors : McPherson, A.
Deposited on : 2026-07-15
Resolution : 1.43 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

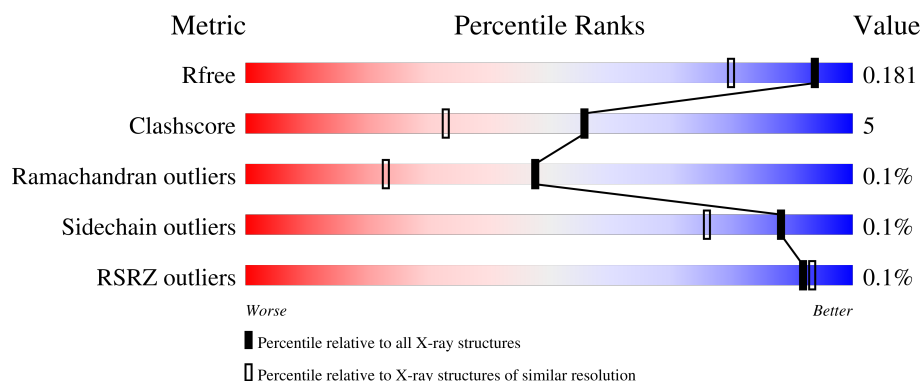
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

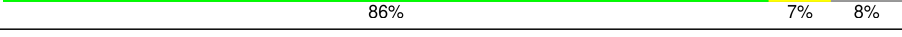
The reported resolution of this entry is 1.43 Å.

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}	180053	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (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	 87% 6% 8%
1	B	291	 85% 7% 8%
1	C	291	 86% 7% 8%
1	D	291	 86% 7% 8%
1	E	291	 87% 5% 8%

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Mol	Chain	Length	Quality of chain
1	F	291	 88% 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
3	ACT	A	302	-	-	X	-

2 Entry composition [i](#)

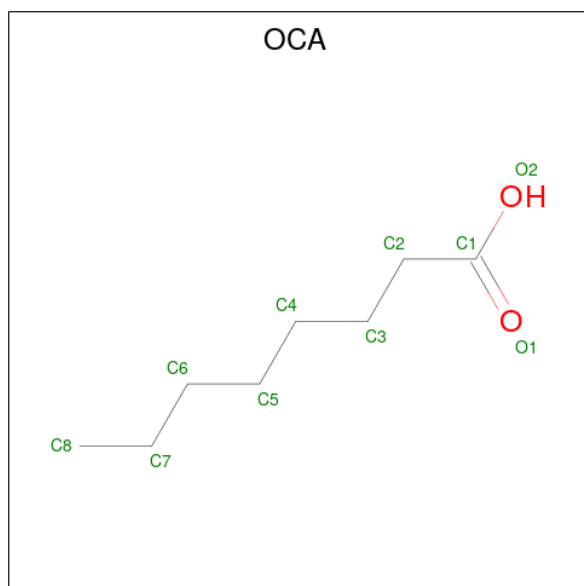
There are 12 unique types of molecules in this entry. The entry contains 29081 atoms, of which 13186 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lipase.

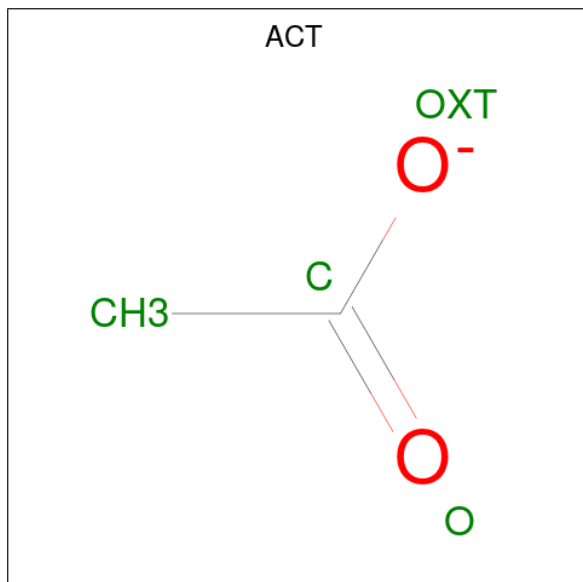
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	H	N	O	S	0	7	0
			4126	1329	2018	364	409	6			
1	B	269	Total	C	H	N	O	S	0	7	0
			4133	1336	2019	364	408	6			
1	C	269	Total	C	H	N	O	S	0	13	0
			4181	1350	2038	372	415	6			
1	E	269	Total	C	H	N	O	S	0	8	0
			4133	1336	2011	367	413	6			
1	D	269	Total	C	H	N	O	S	0	5	0
			4100	1322	2001	364	407	6			
1	F	269	Total	C	H	N	O	S	1	6	0
			4102	1328	1996	365	407	6			

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



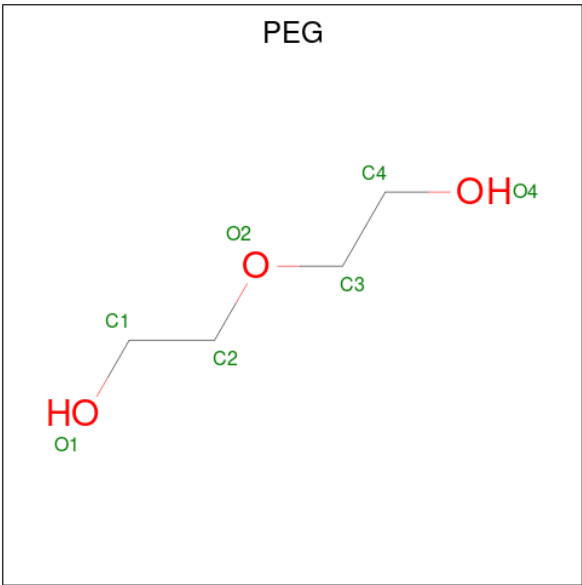
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	8	15	1		
2	B	1	Total	C	H	O	0	0
			17	6	10	1		
2	C	1	Total	C	H	O	0	0
			11	4	6	1		
2	E	1	Total	C	H	O	0	0
			17	6	10	1		
2	D	1	Total	C	H	O	0	0
			11	4	6	1		
2	F	1	Total	C	H	O	1	0
			20	7	12	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	C	1	Total	C	H	O	0	0
			7	2	3	2		
3	C	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		

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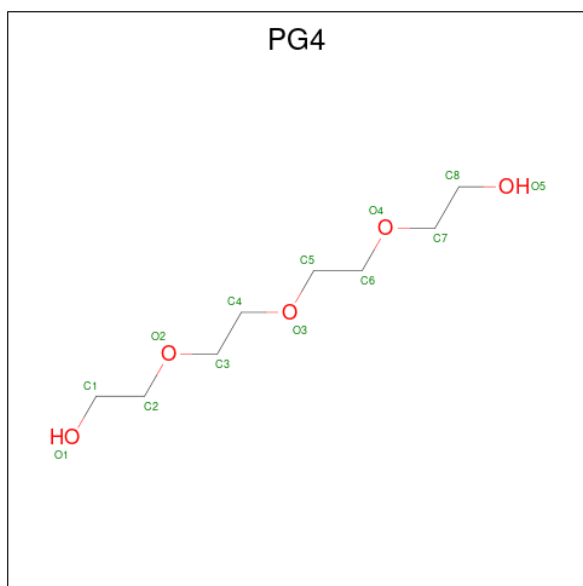
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	E	1	Total	C	H	O	0	0
			17	4	10	3		
4	E	1	Total	C	H	O	0	0
			17	4	10	3		
4	E	1	Total	C	H	O	0	0
			17	4	10	3		
4	E	1	Total	C	H	O	0	0
			17	4	10	3		
4	E	1	Total	C	H	O	0	0
			17	4	10	3		
4	E	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		

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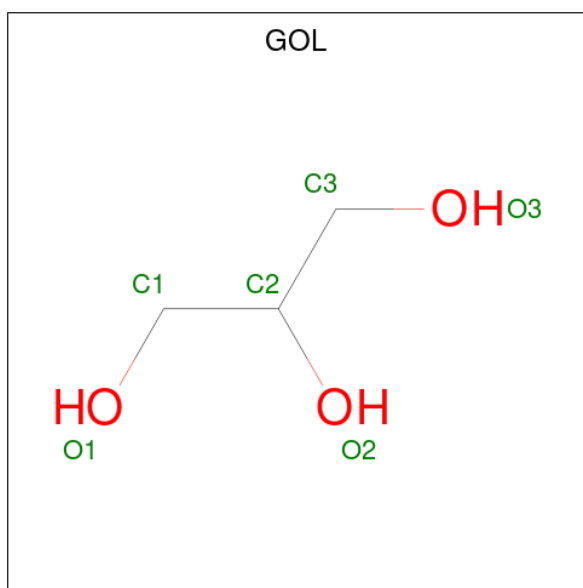
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	F	1	Total	C	H	O	0	0
			17	4	10	3		
4	F	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			25	7	14	4		
5	B	1	Total	C	H	O	0	0
			31	8	18	5		
5	C	1	Total	C	H	O	0	0
			31	8	18	5		
5	C	1	Total	C	H	O	0	0
			31	8	18	5		
5	C	1	Total	C	H	O	0	0
			23	6	13	4		
5	E	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

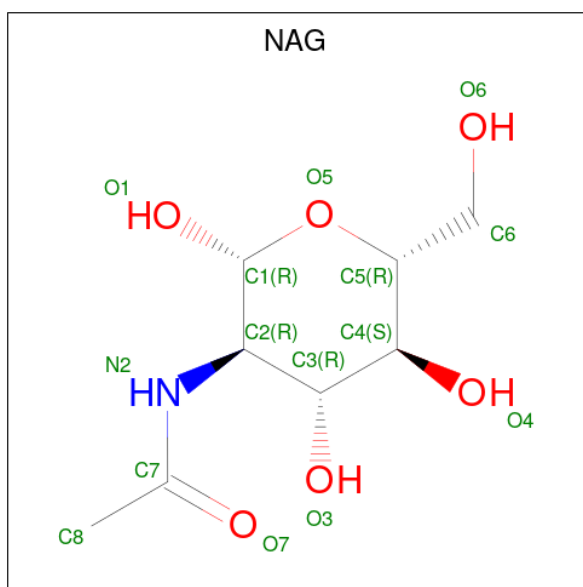


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

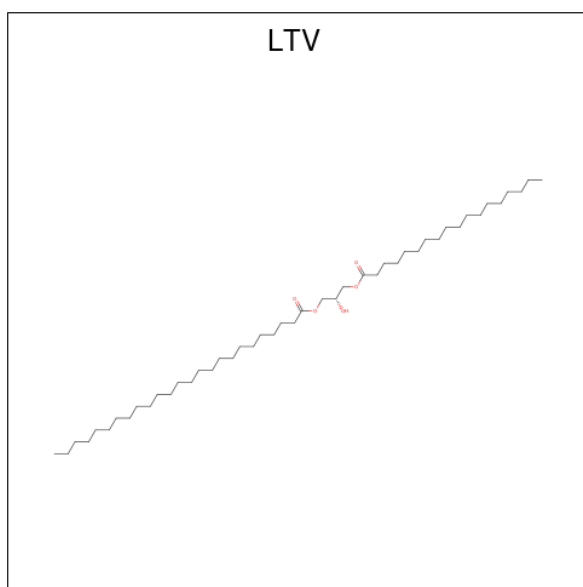
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Ca	0	0
			3	3		
7	B	2	Total	Ca	0	0
			2	2		
7	C	2	Total	Ca	0	0
			2	2		
7	E	2	Total	Ca	0	0
			2	2		
7	D	2	Total	Ca	0	0
			2	2		
7	F	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



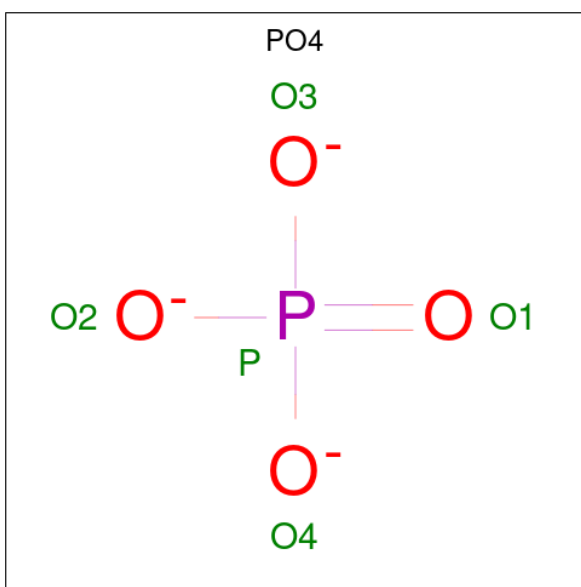
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 27	C 8	H 13	N 1	O 5	0	0
8	B	1	Total 27	C 8	H 13	N 1	O 5	0	0
8	C	1	Total 27	C 8	H 13	N 1	O 5	0	0
8	E	1	Total 27	C 8	H 13	N 1	O 5	0	0
8	D	1	Total 27	C 8	H 13	N 1	O 5	0	0
8	F	1	Total 27	C 8	H 13	N 1	O 5	0	0

- Molecule 9 is 2-hydroxy-3-(octadecanoyloxy)propyl pentacosanoate (CCD ID: LTV) (formula: $C_{46}H_{90}O_5$) (labeled as "Ligand of Interest" by depositor).



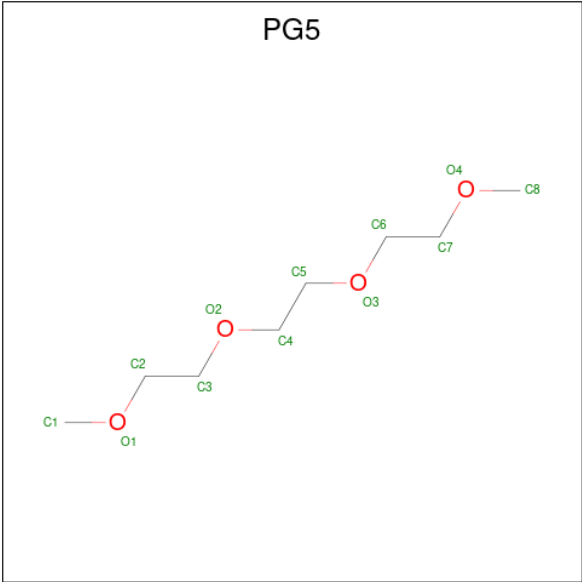
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			94	31	58	5		
9	C	1	Total	C	H	O	0	0
			107	35	67	5		
9	E	1	Total	C	H	O	0	0
			137	45	87	5		
9	E	1	Total	C	H	O	0	0
			116	38	73	5		
9	D	1	Total	C	H	O	0	0
			116	38	73	5		
9	F	1	Total	C	H	O	0	0
			106	35	66	5		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 11 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (CCD ID: PG5) (formula: C₈H₁₈O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	H	O	0	0
			30	8	18	4		

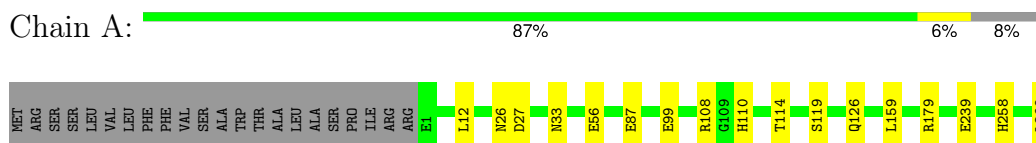
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	424	Total	O	0	3
			427	427		
12	B	445	Total	O	0	2
			446	446		
12	C	375	Total	O	0	2
			377	377		
12	E	340	Total	O	0	0
			340	340		
12	D	362	Total	O	0	4
			365	365		
12	F	413	Total	O	0	3
			415	415		

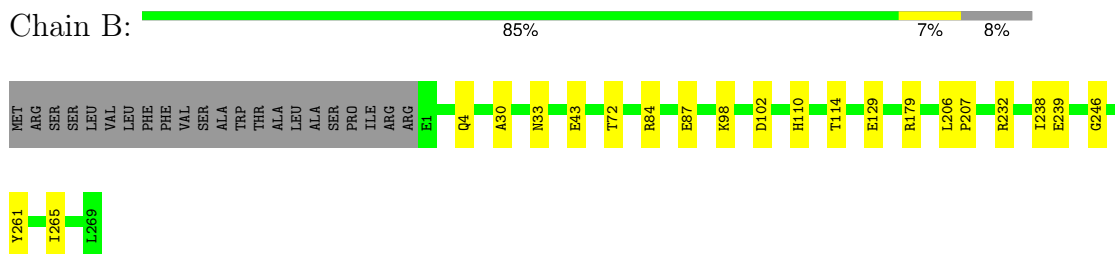
3 Residue-property plots [i](#)

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.

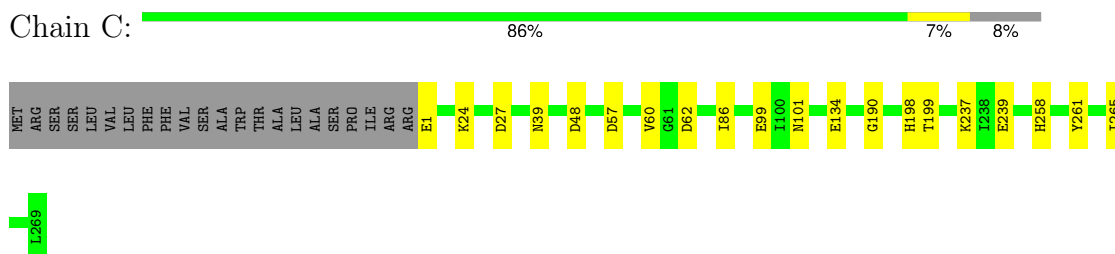
- Molecule 1: Lipase



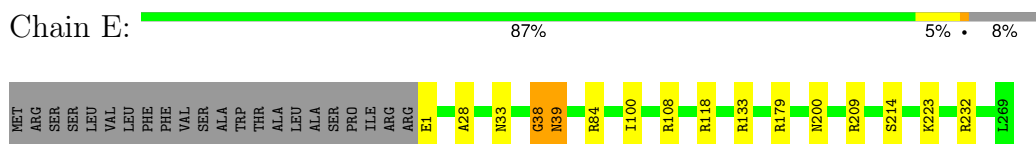
- Molecule 1: Lipase



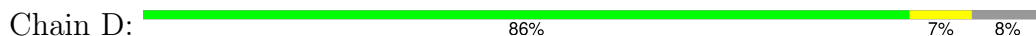
- Molecule 1: Lipase

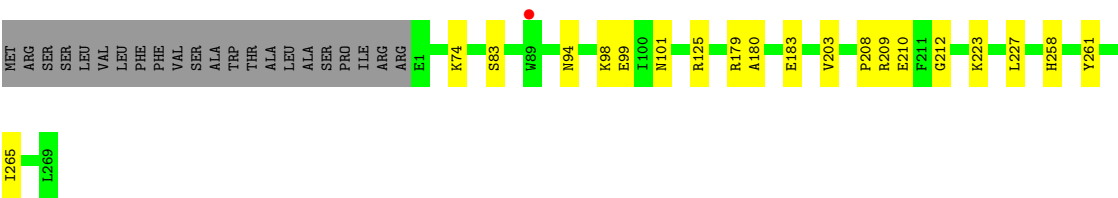


- Molecule 1: Lipase

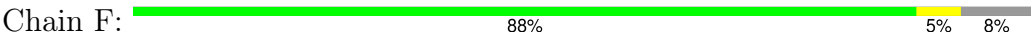


- Molecule 1: Lipase





• 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)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.130 , 0.181 0.131 , 0.181	Depositor DCC
R_{free} test set	15410 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	29081	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG5, ACT, LTV, NAG, PEG, CA, OCA, PG4, 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	0.40	0/2179	0.61	0/2964
1	B	0.40	0/2182	0.59	0/2969
1	C	0.36	0/2229	0.54	0/3032
1	D	0.46	1/2164 (0.0%)	0.54	0/2945
1	E	0.34	0/2194	0.55	0/2986
1	F	0.40	0/2179	0.57	0/2966
All	All	0.39	1/13127 (0.0%)	0.57	0/17862

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	VAL	CA-CB	-12.27	1.47	1.54

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	2108	2018	2012	16	2
1	B	2114	2019	2015	19	1
1	C	2143	2038	2029	20	0
1	D	2099	2001	2003	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2122	2011	2006	19	0
1	F	2106	1996	1988	14	0
2	A	9	15	15	1	0
2	B	7	10	8	0	0
2	C	5	6	4	1	0
2	D	5	6	4	3	0
2	E	7	10	8	0	0
2	F	8	12	10	2	0
3	A	4	3	3	3	0
3	C	8	6	6	0	0
4	A	49	70	70	4	0
4	B	49	70	70	4	0
4	C	56	80	80	10	0
4	D	63	90	90	5	0
4	E	49	70	70	4	0
4	F	14	20	20	5	0
5	A	11	14	13	1	0
5	B	13	18	18	1	0
5	C	36	49	49	4	0
5	E	13	18	18	1	0
6	A	6	8	8	0	0
6	F	6	8	8	1	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
8	A	14	13	13	2	0
8	B	14	13	13	1	0
8	C	14	13	13	3	0
8	D	14	13	13	0	0
8	E	14	13	13	2	0
8	F	14	13	13	0	0
9	A	36	58	0	0	0
9	C	40	67	0	0	0
9	D	43	73	0	0	0
9	E	93	160	0	4	0
9	F	40	66	0	0	0
10	A	10	0	0	0	0
10	B	15	0	0	0	0
10	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	10	0	0	2	0
10	E	10	0	0	2	0
10	F	5	0	0	1	0
11	C	12	18	18	0	0
12	A	427	0	0	8	0
12	B	446	0	0	7	6
12	C	377	0	0	6	2
12	D	365	0	0	12	3
12	E	340	0	0	5	4
12	F	415	0	0	7	8
All	All	15895	13186	12721	124	13

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

The worst 5 of 124 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)
3:A:302:ACT:OXT	12:A:401:HOH:O	1.75	1.05
1:B:179:ARG:NE	12:B:402:HOH:O	1.95	0.97
1:B:129:GLU:OE1	12:B:401:HOH:O	1.86	0.93
1:F:210:GLU:HG2	12:F:423:HOH:O	1.68	0.93
1:D:94[A]:ASN:OD1	12:D:401:HOH:O	1.93	0.86

The worst 5 of 13 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)
12:C:604:HOH:O	12:E:651:HOH:O[2_746]	1.93	0.27
12:C:464:HOH:O	12:D:660:HOH:O[1_554]	1.95	0.25
12:B:786:HOH:O	12:F:798:HOH:O[1_655]	1.98	0.22
12:B:792:HOH:O	12:E:734:HOH:O[2_756]	1.99	0.21
12:B:503:HOH:O	12:F:580:HOH:O[1_655]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/291 (94%)	267 (97%)	7 (3%)	0	100	100
1	B	274/291 (94%)	266 (97%)	8 (3%)	0	100	100
1	C	279/291 (96%)	271 (97%)	8 (3%)	0	100	100
1	D	272/291 (94%)	264 (97%)	8 (3%)	0	100	100
1	E	275/291 (94%)	267 (97%)	6 (2%)	2 (1%)	18	4
1	F	273/291 (94%)	265 (97%)	8 (3%)	0	100	100
All	All	1647/1746 (94%)	1600 (97%)	45 (3%)	2 (0%)	48	23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	39	ASN
1	E	38	GLY

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	227/239 (95%)	227 (100%)	0	100	100
1	B	225/239 (94%)	225 (100%)	0	100	100
1	C	231/239 (97%)	231 (100%)	0	100	100
1	D	225/239 (94%)	224 (100%)	1 (0%)	84	69
1	E	228/239 (95%)	228 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	226/239 (95%)	226 (100%)	0	100	100
All	All	1362/1434 (95%)	1361 (100%)	1 (0%)	88	76

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

Mol	Chain	Res	Type
1	D	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	92	ASN
1	A	126	GLN
1	B	11	ASN
1	F	71	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 12 are monoatomic - leaving 81 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	PEG	A	305	-	6,6,6	0.31	0	5,5,5	0.68	0
9	LTV	F	307	-	39,39,50	1.03	3 (7%)	41,41,52	1.06	3 (7%)
8	NAG	D	310	1	14,14,15	0.66	0	17,19,21	1.20	1 (5%)
4	PEG	A	306	-	6,6,6	0.26	0	5,5,5	0.72	0
4	PEG	B	308	-	6,6,6	0.24	0	5,5,5	0.24	0
6	GOL	F	304	-	5,5,5	0.38	0	5,5,5	0.83	0
4	PEG	D	306	-	6,6,6	0.26	0	5,5,5	0.30	0
4	PEG	E	302	-	6,6,6	0.25	0	5,5,5	0.45	0
8	NAG	A	315	1	14,14,15	0.98	1 (7%)	17,19,21	2.29	2 (11%)
4	PEG	F	303	-	6,6,6	0.24	0	5,5,5	0.24	0
10	PO4	D	313	-	4,4,4	1.74	1 (25%)	6,6,6	0.48	0
4	PEG	A	308	-	6,6,6	0.26	0	5,5,5	0.25	0
4	PEG	D	305	-	6,6,6	0.25	0	5,5,5	0.28	0
4	PEG	B	315	-	6,6,6	0.26	0	5,5,5	0.21	0
5	PG4	A	304	-	10,10,12	0.32	0	9,9,11	0.33	0
4	PEG	E	305	-	6,6,6	0.25	0	5,5,5	0.23	0
4	PEG	E	306	-	6,6,6	0.24	0	5,5,5	0.23	0
4	PEG	B	303	-	6,6,6	0.28	0	5,5,5	0.30	0
9	LTV	C	315	-	39,39,50	1.02	2 (5%)	41,41,52	1.06	2 (4%)
10	PO4	F	308	-	4,4,4	1.83	1 (25%)	6,6,6	0.53	0
4	PEG	E	316	-	6,6,6	0.25	0	5,5,5	0.26	0
2	OCA	A	301	1	7,8,9	0.45	0	6,7,9	0.79	0
8	NAG	B	311	-	14,14,15	1.01	1 (7%)	17,19,21	1.82	3 (17%)
4	PEG	E	315	-	6,6,6	0.25	0	5,5,5	0.19	0
4	PEG	C	320	-	6,6,6	0.23	0	5,5,5	0.27	0
5	PG4	C	310	-	12,12,12	0.30	0	11,11,11	0.22	0
2	OCA	D	301	1	3,4,9	0.49	0	2,3,9	1.14	0
4	PEG	F	301	-	6,6,6	0.24	0	5,5,5	0.28	0
9	LTV	A	316	1	35,35,50	1.08	2 (5%)	37,37,52	1.15	3 (8%)
4	PEG	D	314	-	6,6,6	0.24	0	5,5,5	0.24	0
6	GOL	A	311	-	5,5,5	0.32	0	5,5,5	0.76	0
4	PEG	C	303	-	6,6,6	0.26	0	5,5,5	0.31	0
5	PG4	B	307	-	12,12,12	0.29	0	11,11,11	0.31	0
10	PO4	C	316	-	4,4,4	1.53	1 (25%)	6,6,6	0.46	0
2	OCA	C	301	1	4,4,9	1.64	1 (25%)	3,3,9	0.39	0
4	PEG	B	306	-	6,6,6	0.25	0	5,5,5	0.19	0
5	PG4	E	307	-	12,12,12	0.29	0	11,11,11	0.33	0
10	PO4	B	314	-	4,4,4	1.55	1 (25%)	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	C	309	-	12,12,12	0.29	0	11,11,11	0.21	0
10	PO4	E	314	-	4,4,4	1.59	1 (25%)	6,6,6	0.33	0
4	PEG	C	305	-	6,6,6	0.25	0	5,5,5	0.38	0
9	LTV	D	311	-	42,42,50	1.05	2 (4%)	44,44,52	1.04	2 (4%)
10	PO4	E	313	-	4,4,4	1.56	1 (25%)	6,6,6	0.47	0
3	ACT	A	302	-	3,3,3	1.33	0	3,3,3	0.98	0
4	PEG	C	304	-	6,6,6	0.24	0	5,5,5	0.56	0
4	PEG	D	302	-	6,6,6	0.25	0	5,5,5	0.24	0
4	PEG	C	317	-	6,6,6	0.26	0	5,5,5	0.31	0
10	PO4	A	317	-	4,4,4	1.46	1 (25%)	6,6,6	0.44	0
3	ACT	C	302	-	3,3,3	1.29	0	3,3,3	1.10	0
4	PEG	D	307	-	6,6,6	0.26	0	5,5,5	0.28	0
4	PEG	B	312	-	6,6,6	0.26	0	5,5,5	0.21	0
4	PEG	C	318	7	6,6,6	0.24	0	5,5,5	0.33	0
2	OCA	E	301	1	5,6,9	0.47	0	4,5,9	1.03	1 (25%)
8	NAG	C	314	1	14,14,15	1.15	2 (14%)	17,19,21	1.47	3 (17%)
4	PEG	D	315	-	6,6,6	0.26	0	5,5,5	0.27	0
11	PG5	C	308	-	11,11,11	0.36	0	10,10,10	0.14	0
4	PEG	D	304	-	6,6,6	0.24	0	5,5,5	0.32	0
4	PEG	A	303	-	6,6,6	0.27	0	5,5,5	0.24	0
4	PEG	D	316	-	6,6,6	0.26	0	5,5,5	0.25	0
2	OCA	B	301	1	6,6,9	1.33	1 (16%)	5,5,9	0.25	0
10	PO4	A	318	-	4,4,4	1.86	1 (25%)	6,6,6	0.63	0
4	PEG	A	309	-	6,6,6	0.26	0	5,5,5	0.26	0
4	PEG	D	303	-	6,6,6	0.27	0	5,5,5	0.53	0
5	PG4	C	311	-	9,9,12	0.28	0	8,8,11	0.21	0
10	PO4	B	313	-	4,4,4	1.59	1 (25%)	6,6,6	0.46	0
4	PEG	E	303	-	6,6,6	0.23	0	5,5,5	0.30	0
4	PEG	B	305	-	6,6,6	0.25	0	5,5,5	0.23	0
4	PEG	A	310	7	6,6,6	0.29	0	5,5,5	0.29	0
10	PO4	D	312	7	4,4,4	1.41	1 (25%)	6,6,6	0.52	0
4	PEG	C	319	-	6,6,6	0.26	0	5,5,5	0.21	0
4	PEG	B	304	-	6,6,6	0.24	0	5,5,5	0.15	0
2	OCA	F	302	1	6,7,9	0.40	0	5,6,9	0.92	0
4	PEG	E	304	-	6,6,6	0.26	0	5,5,5	0.28	0
3	ACT	C	307	-	3,3,3	1.29	0	3,3,3	1.19	0
9	LTV	E	311	-	49,49,50	0.97	2 (4%)	51,51,52	1.13	3 (5%)
4	PEG	C	306	-	6,6,6	0.24	0	5,5,5	0.28	0
9	LTV	E	312	-	42,42,50	0.99	2 (4%)	44,44,52	1.11	2 (4%)
4	PEG	A	307	-	6,6,6	0.24	0	5,5,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	E	310	1	14,14,15	1.00	1 (7%)	17,19,21	1.87	3 (17%)
10	PO4	B	302	-	4,4,4	1.46	1 (25%)	6,6,6	0.56	0
8	NAG	F	306	1	14,14,15	0.66	0	17,19,21	1.43	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	309	-	-	2/4/4/4	-
4	PEG	A	305	-	-	2/4/4/4	-
4	PEG	C	305	-	-	3/4/4/4	-
9	LTV	D	311	-	-	22/43/43/51	-
4	PEG	D	303	-	-	4/4/4/4	-
9	LTV	F	307	-	-	26/40/40/51	-
4	PEG	E	316	-	-	1/4/4/4	-
5	PG4	C	311	-	-	5/7/7/10	-
4	PEG	E	303	-	-	1/4/4/4	-
8	NAG	D	310	1	-	0/6/23/26	0/1/1/1
4	PEG	B	305	-	-	1/4/4/4	-
4	PEG	A	310	7	-	2/4/4/4	-
4	PEG	A	306	-	-	3/4/4/4	-
4	PEG	C	304	-	-	2/4/4/4	-
4	PEG	B	308	-	-	2/4/4/4	-
4	PEG	C	319	-	-	1/4/4/4	-
6	GOL	F	304	-	-	2/4/4/4	-
4	PEG	D	306	-	-	1/4/4/4	-
4	PEG	E	302	-	-	1/4/4/4	-
4	PEG	D	302	-	-	2/4/4/4	-
4	PEG	B	304	-	-	1/4/4/4	-
2	OCA	A	301	1	-	5/6/6/7	-
2	OCA	F	302	1	-	2/5/5/7	-
4	PEG	E	304	-	-	2/4/4/4	-
4	PEG	C	317	-	-	2/4/4/4	-
8	NAG	B	311	-	-	0/6/23/26	0/1/1/1
4	PEG	E	315	-	-	1/4/4/4	-
4	PEG	C	320	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	315	1	-	0/6/23/26	0/1/1/1
4	PEG	F	303	-	-	3/4/4/4	-
5	PG4	C	310	-	-	5/10/10/10	-
2	OCA	D	301	1	-	1/2/2/7	-
9	LTV	E	311	-	-	22/50/50/51	-
4	PEG	A	308	-	-	1/4/4/4	-
4	PEG	C	306	-	-	2/4/4/4	-
4	PEG	F	301	-	-	2/4/4/4	-
4	PEG	D	305	-	-	3/4/4/4	-
9	LTV	A	316	1	-	14/36/36/51	-
9	LTV	E	312	-	-	25/43/43/51	-
4	PEG	B	315	-	-	0/4/4/4	-
4	PEG	A	307	-	-	1/4/4/4	-
4	PEG	D	307	-	-	1/4/4/4	-
4	PEG	B	312	-	-	0/4/4/4	-
4	PEG	C	318	7	-	3/4/4/4	-
5	PG4	A	304	-	-	4/8/8/10	-
4	PEG	E	305	-	-	0/4/4/4	-
2	OCA	E	301	1	-	2/4/4/7	-
4	PEG	E	306	-	-	0/4/4/4	-
4	PEG	D	314	-	-	2/4/4/4	-
4	PEG	B	303	-	-	1/4/4/4	-
4	PEG	C	303	-	-	1/4/4/4	-
5	PG4	B	307	-	-	5/10/10/10	-
5	PG4	C	309	-	-	6/10/10/10	-
6	GOL	A	311	-	-	2/4/4/4	-
8	NAG	E	310	1	-	1/6/23/26	0/1/1/1
2	OCA	C	301	1	-	2/2/2/7	-
4	PEG	B	306	-	-	2/4/4/4	-
5	PG4	E	307	-	-	7/10/10/10	-
8	NAG	C	314	1	-	2/6/23/26	0/1/1/1
9	LTV	C	315	-	-	19/40/40/51	-
4	PEG	D	315	-	-	3/4/4/4	-
11	PG5	C	308	-	-	5/9/9/9	-
4	PEG	D	304	-	-	3/4/4/4	-
8	NAG	F	306	1	-	2/6/23/26	0/1/1/1
4	PEG	A	303	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	D	316	-	-	0/4/4/4	-
2	OCA	B	301	1	-	3/4/4/7	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	308	PO4	P-O1	3.38	1.58	1.50
9	D	311	LTV	O1-C17	3.32	1.43	1.33
10	A	318	PO4	P-O1	3.31	1.58	1.50
2	C	301	OCA	O2-C1	-3.19	1.25	1.42
2	B	301	OCA	O2-C1	-3.17	1.25	1.42

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	315	NAG	C1-C2-N2	6.05	119.96	110.43
8	A	315	NAG	O5-C1-C2	-5.91	102.14	111.29
8	E	310	NAG	O5-C1-C2	-5.31	103.08	111.29
8	B	311	NAG	C1-O5-C5	-4.66	105.94	112.19
9	E	311	LTV	O3-C21-C22	4.22	124.70	111.83

There are no chirality outliers.

5 of 255 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	316	LTV	O1-C18-C19-C20
9	C	315	LTV	C18-C19-C20-O3
9	C	315	LTV	O1-C18-C19-C20
9	E	312	LTV	O4-C21-O3-C20
9	E	312	LTV	C22-C21-O3-C20

There are no ring outliers.

39 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305	PEG	1	0
4	A	306	PEG	1	0
6	F	304	GOL	1	0
8	A	315	NAG	2	0
4	F	303	PEG	2	0
10	D	313	PO4	1	0

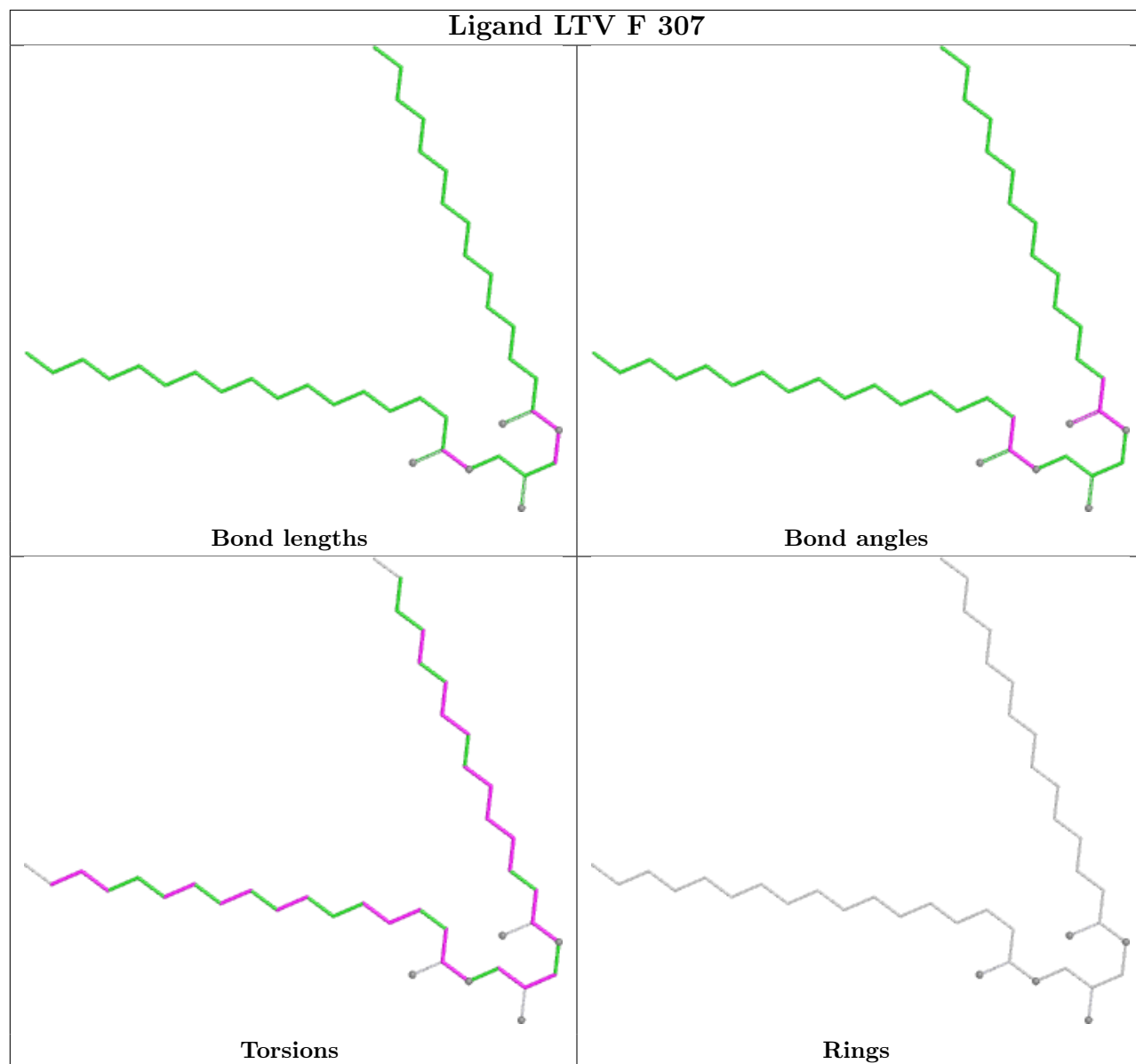
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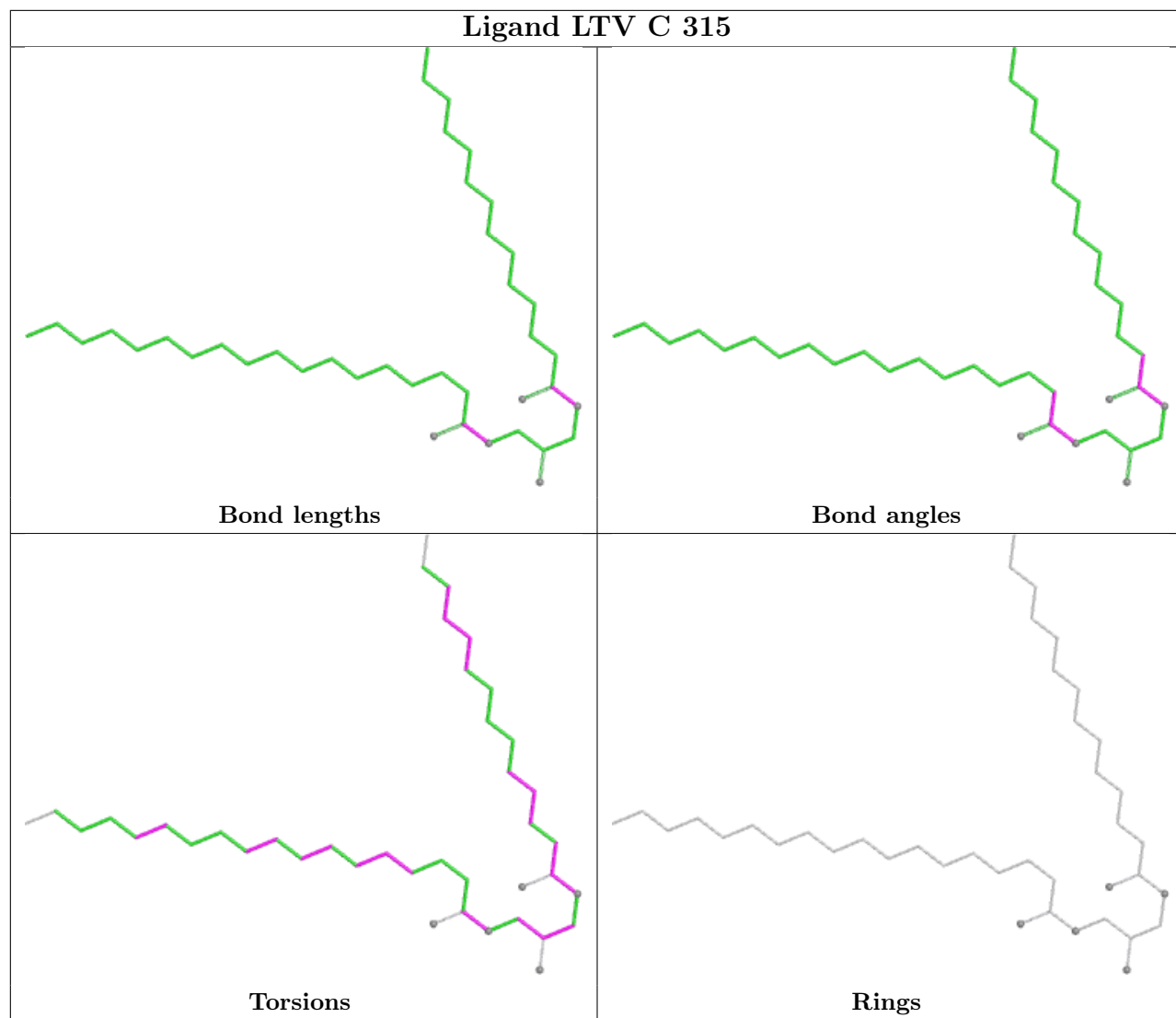
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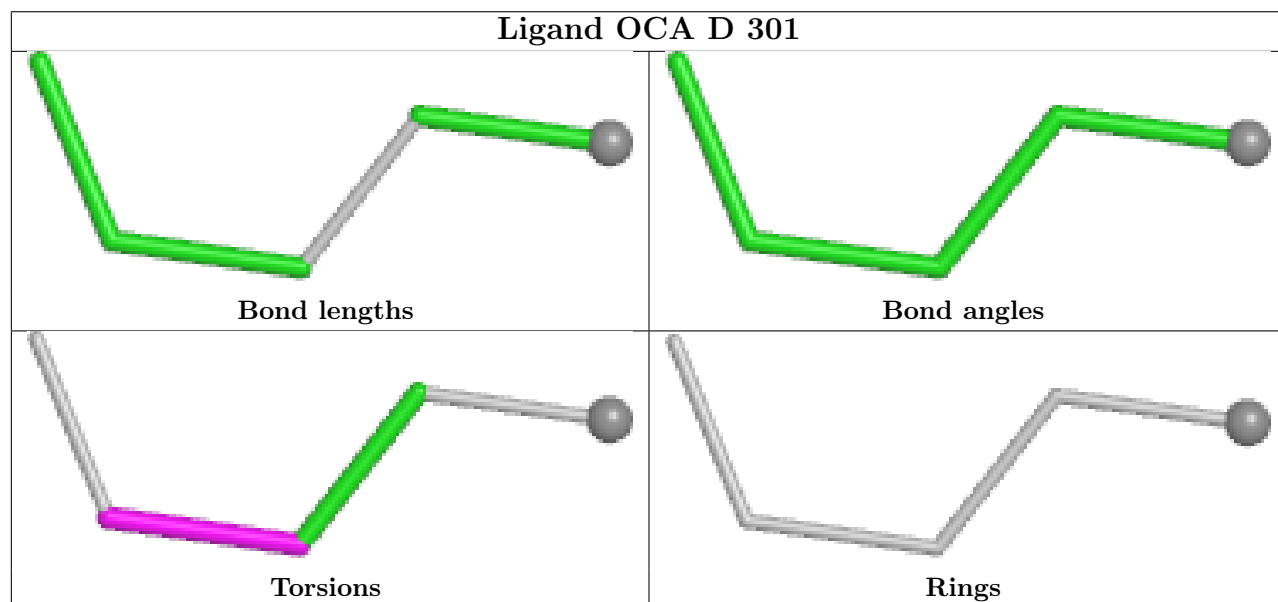
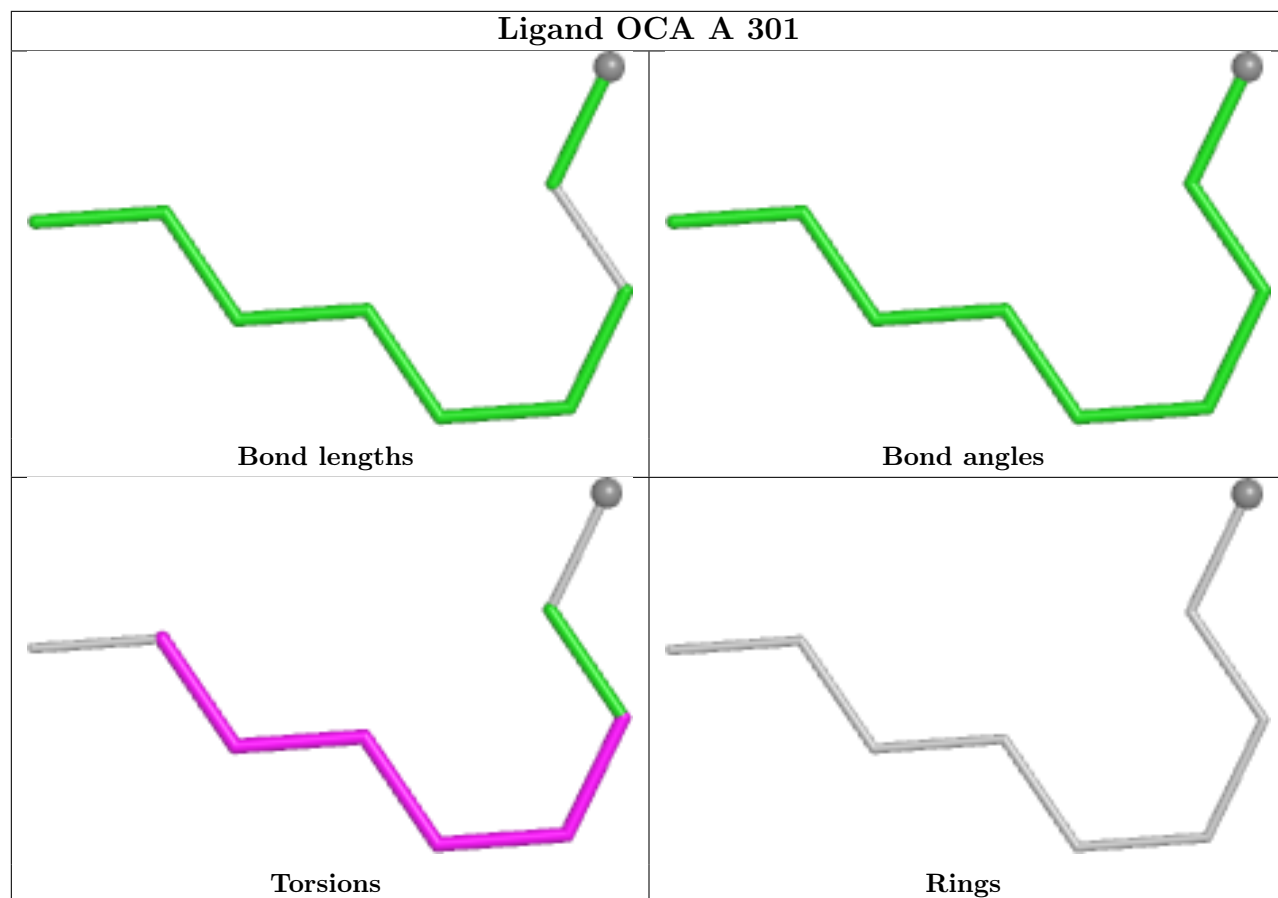
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	308	PEG	1	0
4	B	315	PEG	2	0
5	A	304	PG4	1	0
10	F	308	PO4	1	0
2	A	301	OCA	1	0
8	B	311	NAG	1	0
5	C	310	PG4	3	0
2	D	301	OCA	3	0
4	F	301	PEG	3	0
5	B	307	PG4	1	0
2	C	301	OCA	1	0
4	B	306	PEG	2	0
5	E	307	PG4	1	0
10	E	314	PO4	1	0
4	C	305	PEG	3	0
10	E	313	PO4	1	0
3	A	302	ACT	3	0
4	C	304	PEG	3	0
4	C	317	PEG	3	0
8	C	314	NAG	3	0
4	D	304	PEG	3	0
4	A	303	PEG	1	0
4	A	309	PEG	1	0
4	D	303	PEG	2	0
5	C	311	PG4	1	0
4	E	303	PEG	1	0
10	D	312	PO4	1	0
4	C	319	PEG	1	0
2	F	302	OCA	2	0
4	E	304	PEG	3	0
9	E	311	LTV	2	0
9	E	312	LTV	2	0
8	E	310	NAG	2	0

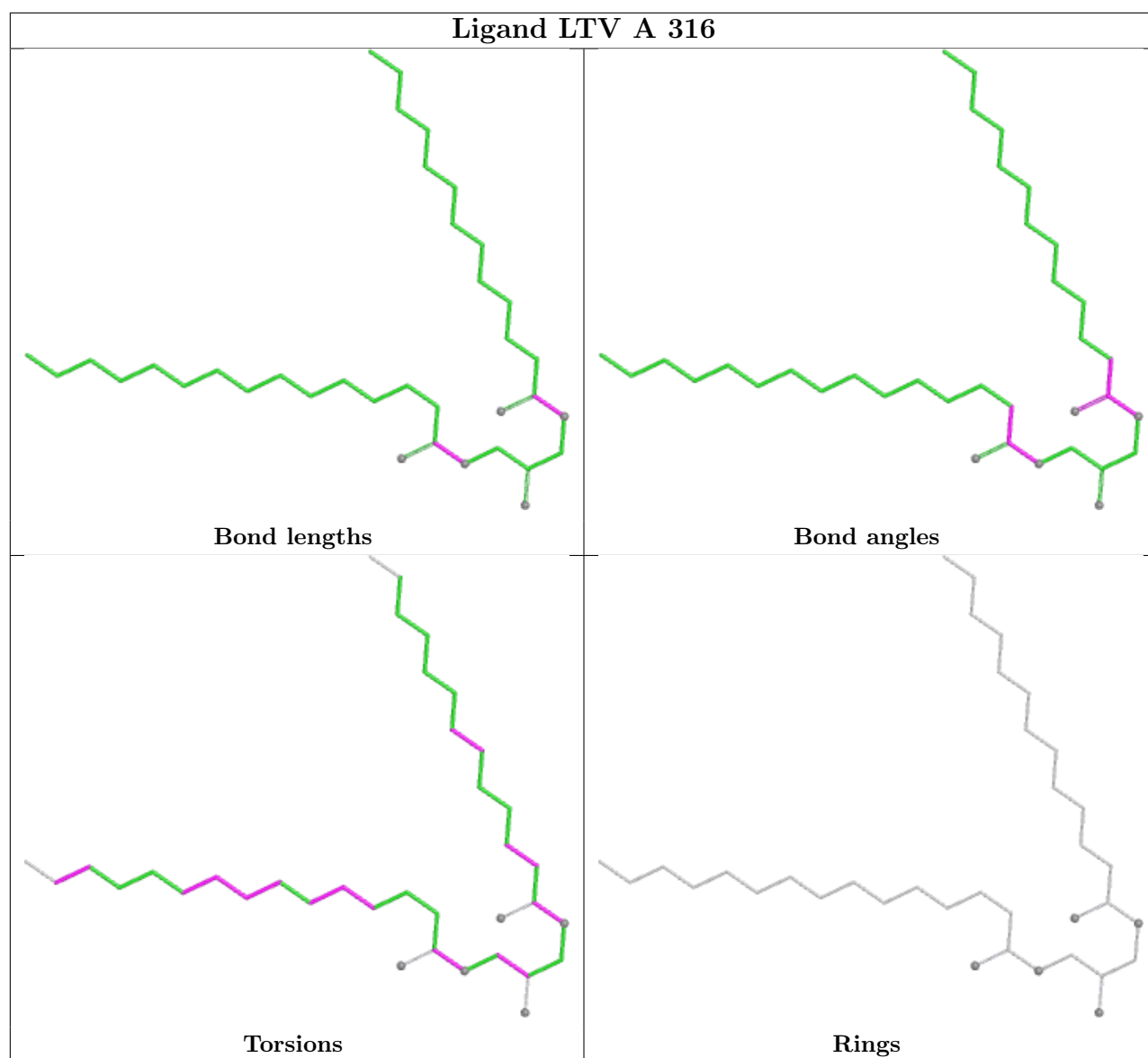
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

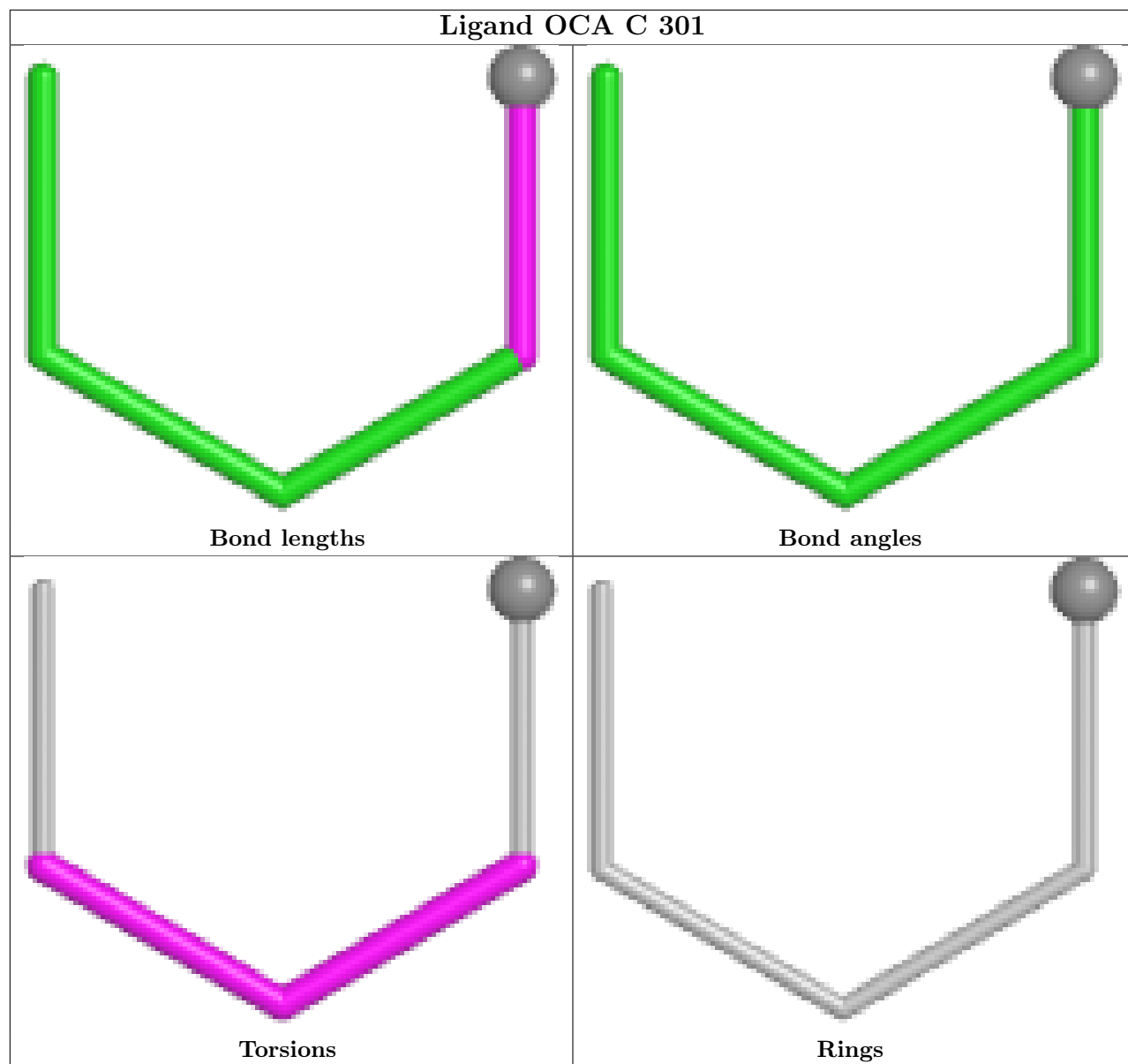
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

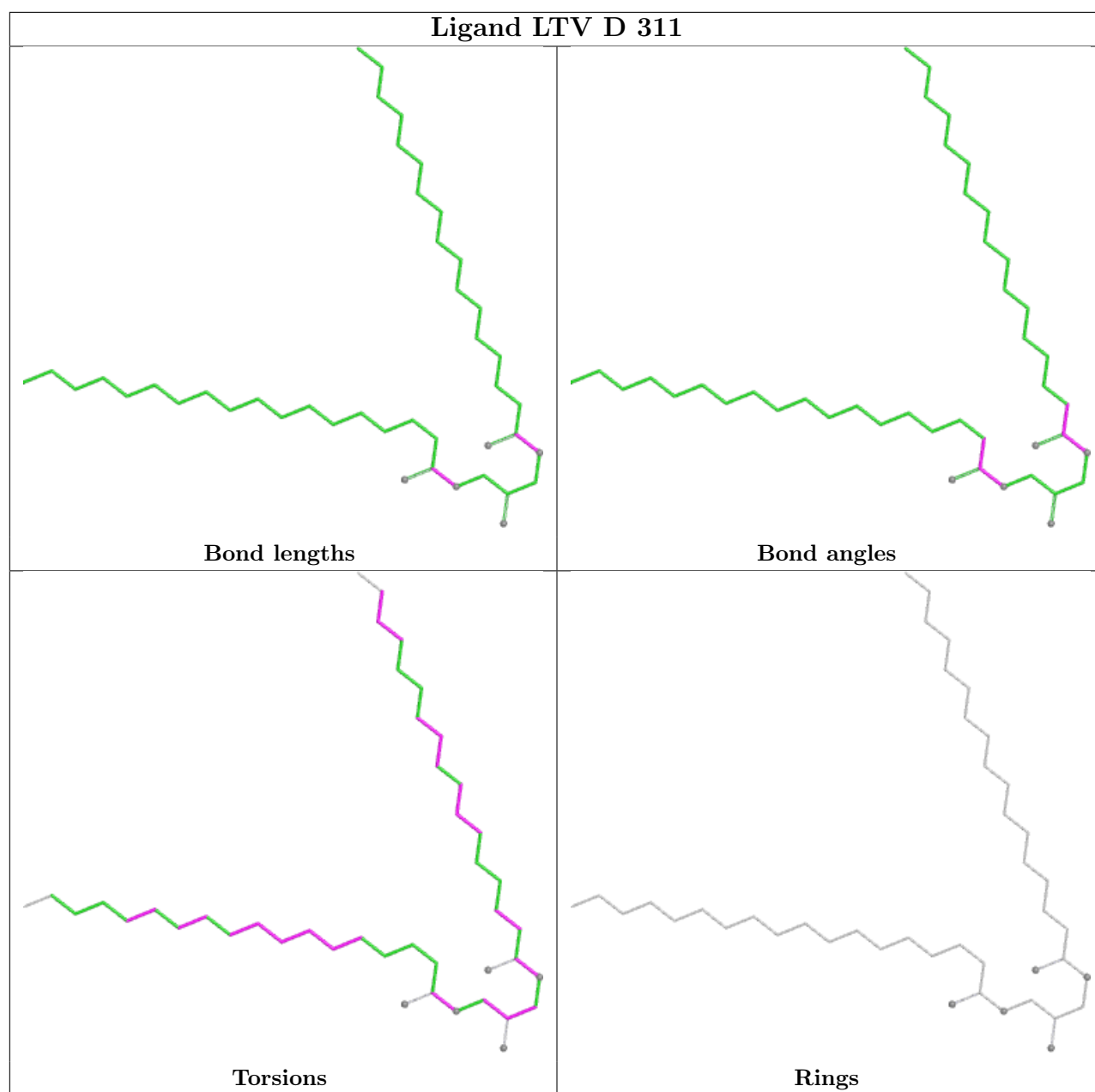


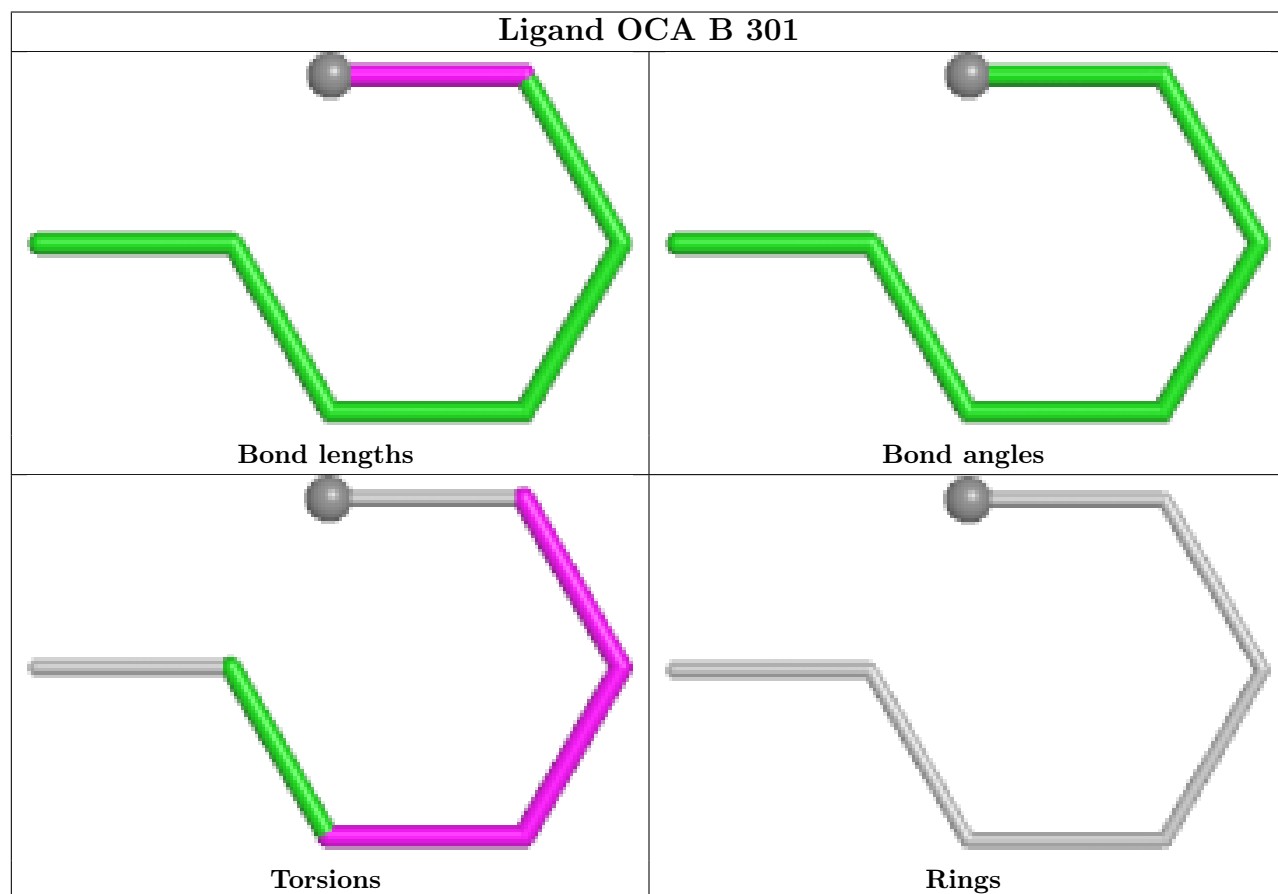
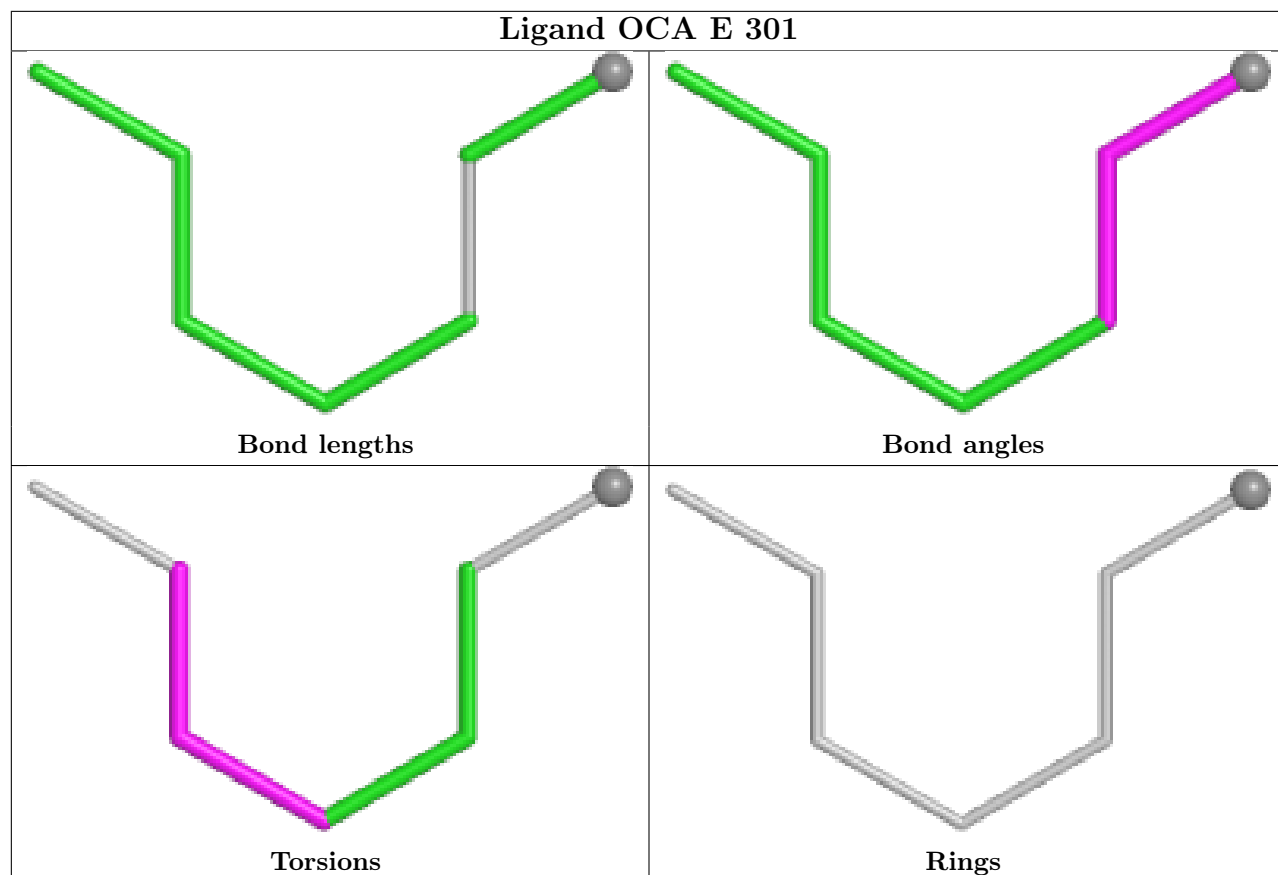


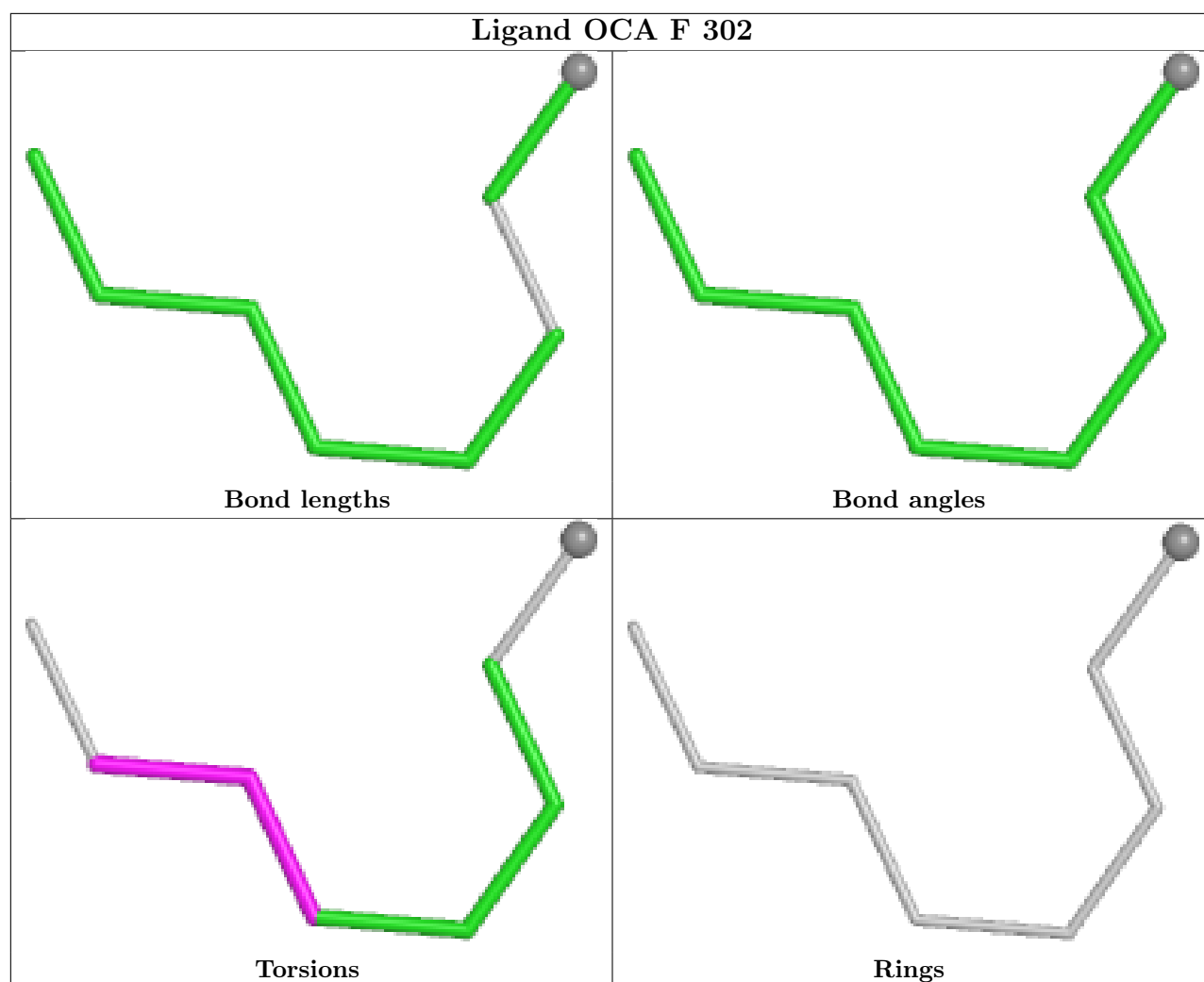


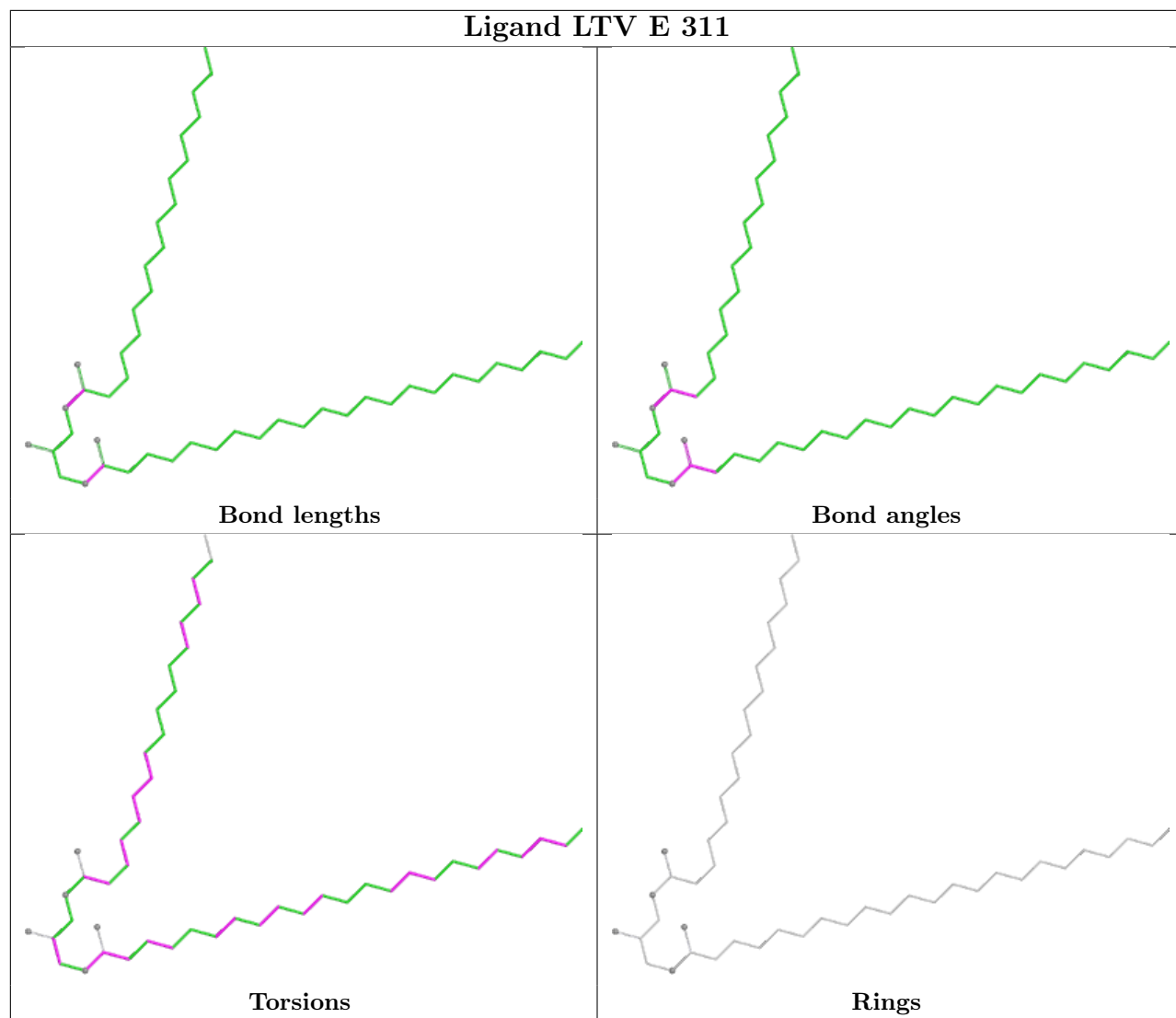


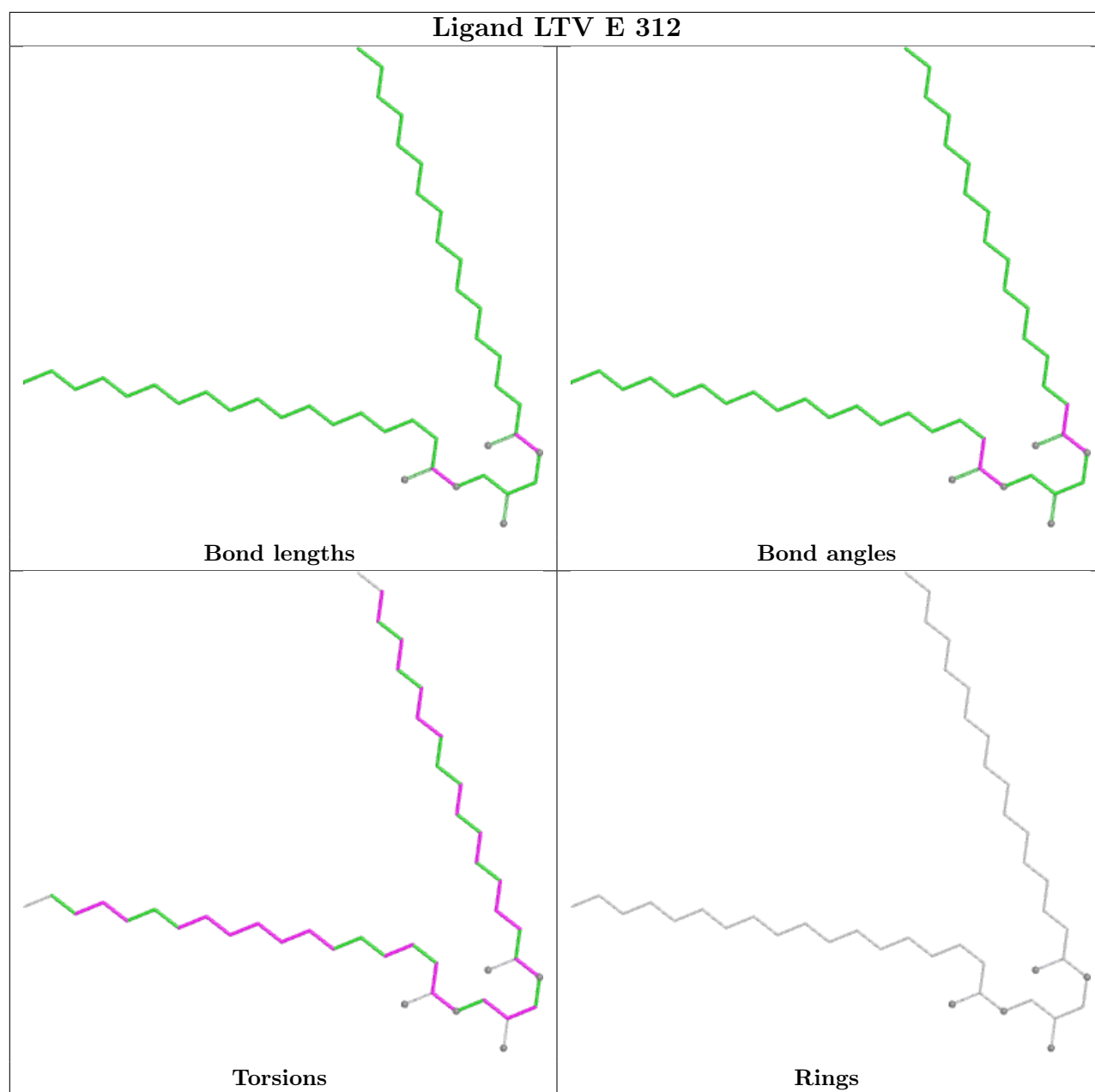












5.7 Other polymers [i](#)

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%)	-0.66	0	100 100	10, 24, 42, 57	11 (4%)
1	B	269/291 (92%)	-0.63	0	100 100	12, 25, 42, 62	7 (2%)
1	C	269/291 (92%)	-0.46	0	100 100	11, 29, 50, 61	13 (4%)
1	D	269/291 (92%)	-0.60	1 (0%)	88 91	12, 27, 45, 69	9 (3%)
1	E	269/291 (92%)	-0.38	0	100 100	12, 31, 48, 61	8 (2%)
1	F	269/291 (92%)	-0.70	0	100 100	11, 25, 41, 79	8 (2%)
All	All	1614/1746 (92%)	-0.57	1 (0%)	92 93	10, 27, 46, 79	56 (3%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	89	TRP	2.9

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
4	PEG	E	316	7/7	0.56	0.14	84,126,166,176	0
4	PEG	D	316	7/7	0.59	0.11	75,111,135,147	0
4	PEG	D	306	7/7	0.68	0.14	80,111,160,160	0
4	PEG	D	307	7/7	0.68	0.16	41,69,104,106	17
4	PEG	B	308	7/7	0.68	0.15	71,124,213,213	0
4	PEG	C	306	7/7	0.70	0.12	73,90,141,160	0
4	PEG	C	318	7/7	0.70	0.16	68,96,180,180	0
5	PG4	B	307	13/13	0.70	0.15	74,105,144,148	0
5	PG4	C	311	10/13	0.71	0.19	42,69,224,245	0
5	PG4	C	309	13/13	0.72	0.18	56,110,148,171	0
4	PEG	D	302	7/7	0.72	0.17	50,70,130,170	17
8	NAG	C	314	14/15	0.72	0.12	57,69,83,83	0
4	PEG	E	305	7/7	0.73	0.15	57,75,125,129	0
11	PG5	C	308	12/12	0.73	0.16	84,122,190,194	0
8	NAG	A	315	14/15	0.74	0.11	68,74,88,90	0
4	PEG	D	305	7/7	0.75	0.19	82,121,178,178	0
4	PEG	D	314	7/7	0.75	0.14	76,97,153,182	0
4	PEG	E	315	7/7	0.75	0.17	65,85,167,167	0
5	PG4	E	307	13/13	0.76	0.14	51,89,152,156	31
4	PEG	B	312	7/7	0.76	0.17	62,122,148,162	0
4	PEG	F	303	7/7	0.77	0.17	53,118,141,143	0
4	PEG	A	310	7/7	0.77	0.19	34,67,110,141	17
5	PG4	C	310	13/13	0.78	0.23	41,62,133,135	31
4	PEG	A	306	7/7	0.78	0.20	24,94,206,224	0
4	PEG	C	303	7/7	0.78	0.18	53,86,121,145	0
4	PEG	B	303	7/7	0.80	0.15	37,55,67,160	17
4	PEG	E	306	7/7	0.81	0.14	41,77,95,124	0
2	OCA	E	301	7/10	0.81	0.22	27,40,48,48	17
2	OCA	D	301	5/10	0.81	0.17	30,33,40,40	11
2	OCA	B	301	7/10	0.81	0.25	30,38,43,43	17
4	PEG	E	302	7/7	0.81	0.23	46,97,181,181	17
4	PEG	A	307	7/7	0.81	0.24	58,150,165,171	0
4	PEG	A	303	7/7	0.82	0.21	36,85,129,129	17
6	GOL	A	311	6/6	0.82	0.23	32,62,166,199	14
9	LTV	E	311	50/51	0.82	0.22	51,74,117,119	137
6	GOL	F	304	6/6	0.82	0.20	32,57,114,137	14
3	ACT	A	302	4/4	0.83	0.18	43,65,76,199	0
2	OCA	C	301	5/10	0.83	0.15	30,35,42,42	11
4	PEG	F	301	7/7	0.83	0.24	33,66,145,145	17
4	PEG	B	305	7/7	0.83	0.17	49,67,170,170	17
9	LTV	E	312	43/51	0.83	0.19	40,63,89,90	116
4	PEG	E	304	7/7	0.83	0.18	37,52,96,96	17
4	PEG	E	303	7/7	0.84	0.15	41,62,100,100	17

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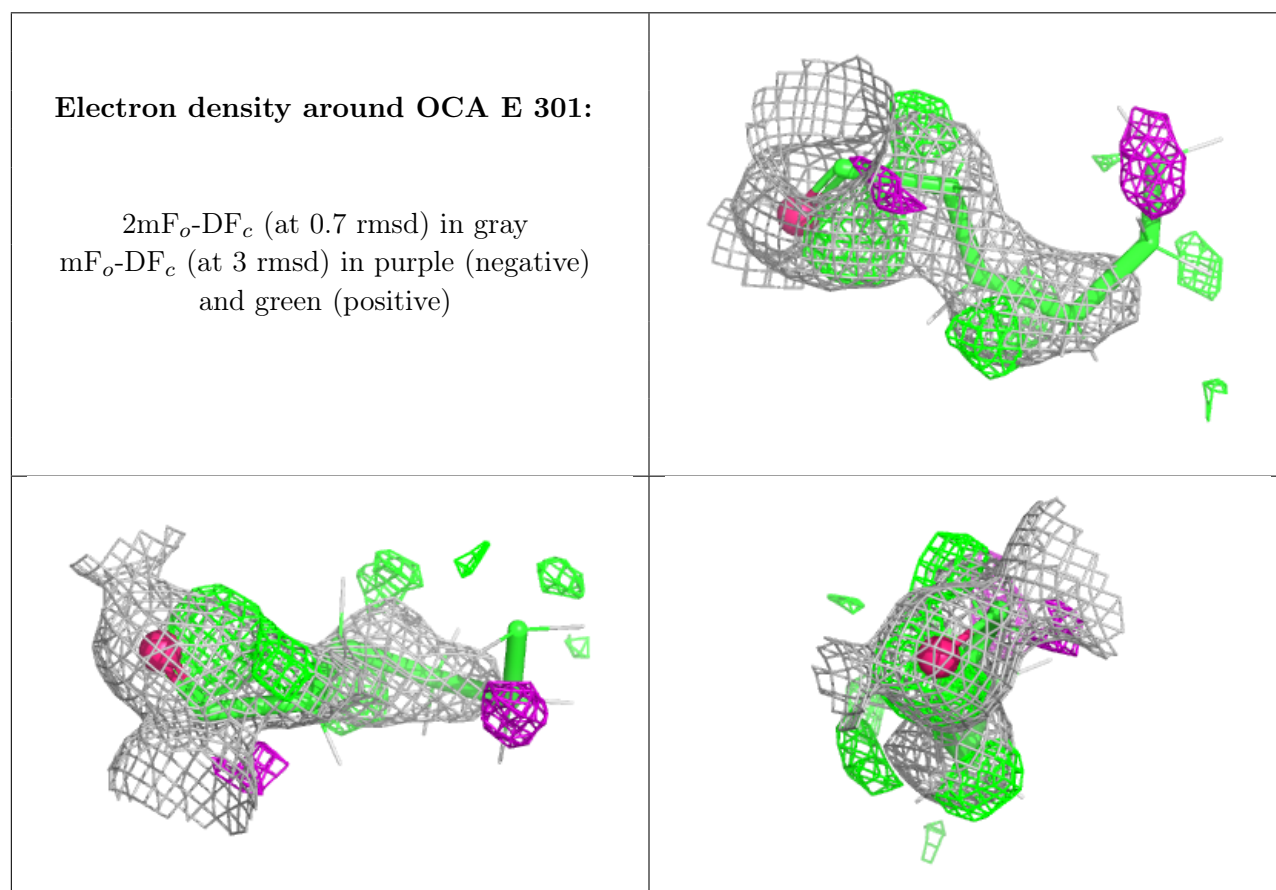
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	C	302	4/4	0.84	0.12	42,67,80,80	0
5	PG4	A	304	11/13	0.84	0.20	43,140,212,228	0
2	OCA	A	301	9/10	0.84	0.16	29,38,47,48	24
9	LTV	D	311	43/51	0.84	0.16	56,79,97,97	0
4	PEG	C	305	7/7	0.84	0.14	40,99,125,125	0
4	PEG	B	315	7/7	0.85	0.24	37,63,121,121	17
4	PEG	A	305	7/7	0.85	0.18	35,59,152,152	17
4	PEG	C	319	7/7	0.85	0.18	38,115,158,158	0
9	LTV	F	307	40/51	0.85	0.15	45,74,91,92	0
3	ACT	C	307	4/4	0.85	0.20	53,58,69,212	0
4	PEG	D	315	7/7	0.86	0.13	48,75,110,110	17
4	PEG	B	304	7/7	0.86	0.14	40,76,123,123	17
8	NAG	E	310	14/15	0.86	0.09	66,69,83,84	0
8	NAG	D	310	14/15	0.86	0.09	49,65,78,78	0
10	PO4	B	314	5/5	0.86	0.13	74,100,143,150	0
10	PO4	C	316	5/5	0.86	0.14	59,63,137,163	0
10	PO4	E	313	5/5	0.86	0.11	83,84,85,85	5
9	LTV	A	316	36/51	0.86	0.14	47,68,83,84	0
9	LTV	C	315	40/51	0.87	0.15	53,78,95,96	0
4	PEG	C	320	7/7	0.87	0.18	45,65,116,116	17
10	PO4	D	312	5/5	0.87	0.15	51,56,57,58	5
4	PEG	B	306	7/7	0.87	0.18	48,80,163,163	0
2	OCA	F	302	8/10	0.88	0.17	27,36,43,43	20
4	PEG	C	304	7/7	0.88	0.17	32,54,89,107	17
4	PEG	C	317	7/7	0.88	0.15	31,60,122,122	17
8	NAG	F	306	14/15	0.89	0.09	44,53,62,64	0
4	PEG	D	304	7/7	0.89	0.15	29,58,172,172	17
4	PEG	A	308	7/7	0.89	0.19	40,80,151,160	0
4	PEG	D	303	7/7	0.89	0.18	24,102,219,219	0
10	PO4	B	313	5/5	0.90	0.10	74,76,76,76	5
4	PEG	A	309	7/7	0.90	0.17	29,86,171,171	17
10	PO4	A	317	5/5	0.91	0.11	74,76,77,77	0
8	NAG	B	311	14/15	0.92	0.08	42,50,61,61	0
10	PO4	F	308	5/5	0.93	0.09	40,44,45,46	5
10	PO4	E	314	5/5	0.93	0.10	57,60,62,63	0
10	PO4	D	313	5/5	0.94	0.07	53,55,57,57	5
10	PO4	A	318	5/5	0.96	0.07	32,37,38,38	0
10	PO4	B	302	5/5	0.97	0.06	35,38,40,42	5
7	CA	C	312	1/1	0.97	0.10	47,47,47,47	1
7	CA	A	314	1/1	0.98	0.27	37,37,37,37	0
7	CA	A	313	1/1	0.98	0.10	29,29,29,29	1
7	CA	E	309	1/1	0.98	0.09	33,33,33,33	0

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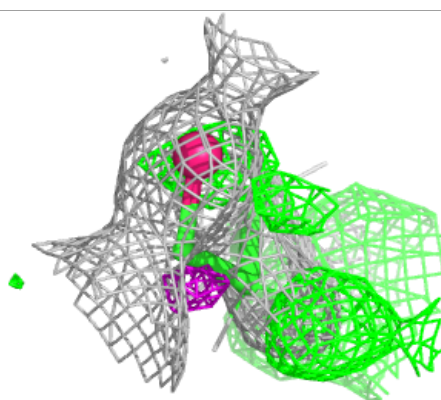
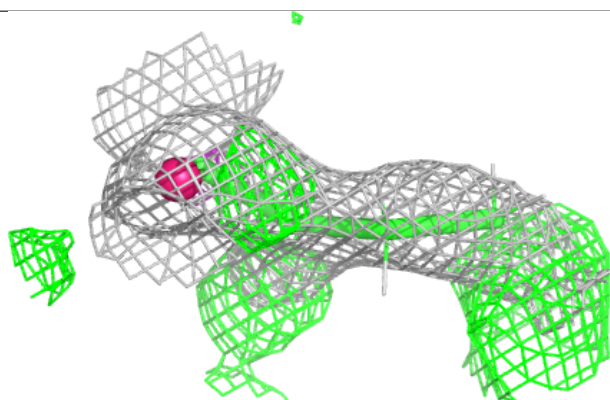
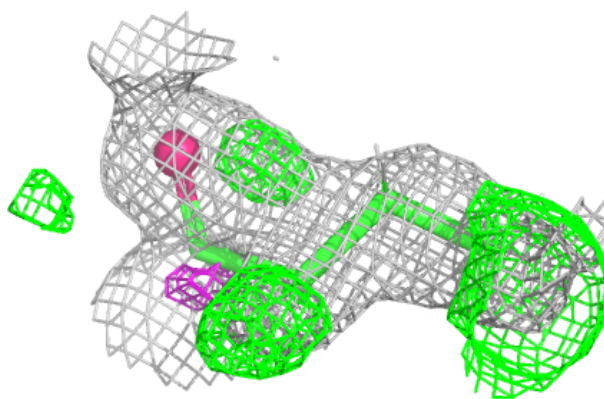
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	A	312	1/1	0.99	0.08	27,27,27,27	1
7	CA	C	313	1/1	0.99	0.05	26,26,26,26	0
7	CA	E	308	1/1	0.99	0.05	59,59,59,59	0
7	CA	B	310	1/1	0.99	0.06	26,26,26,26	0
7	CA	D	309	1/1	0.99	0.09	22,22,22,22	0
7	CA	F	305	1/1	0.99	0.05	35,35,35,35	1
7	CA	B	309	1/1	1.00	0.02	20,20,20,20	0
7	CA	D	308	1/1	1.00	0.09	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.

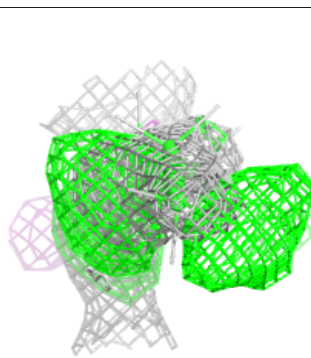
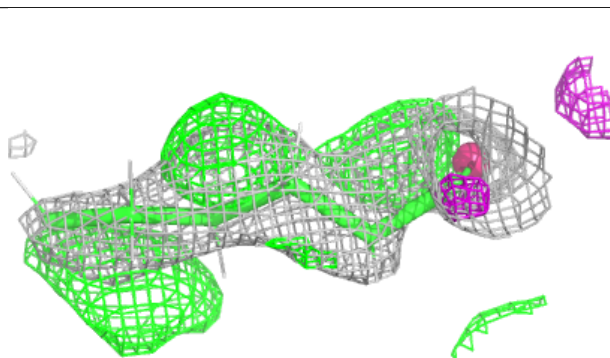
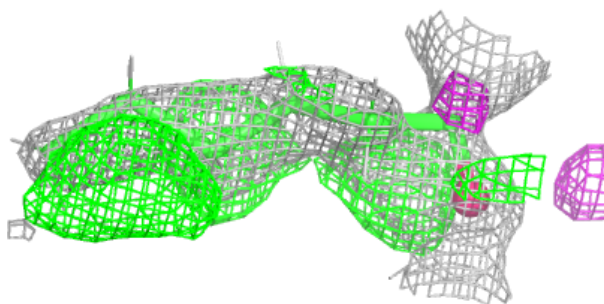


Electron density around OCA D 301:

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

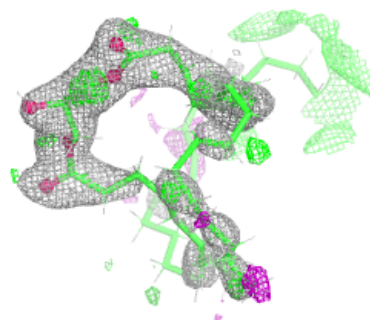
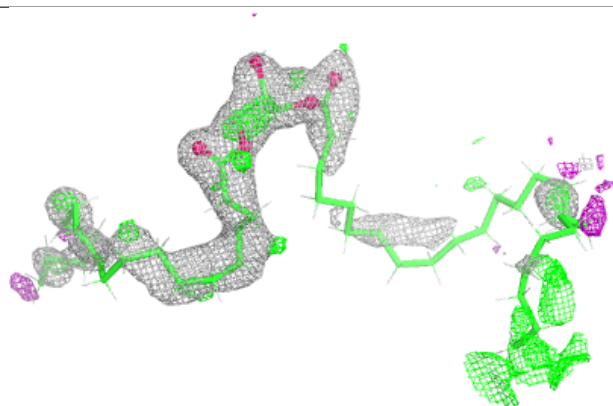
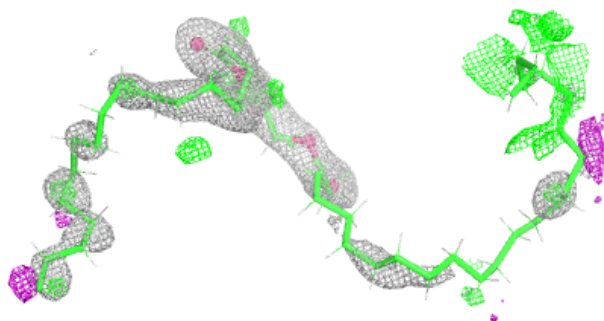
**Electron density around OCA B 301:**

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

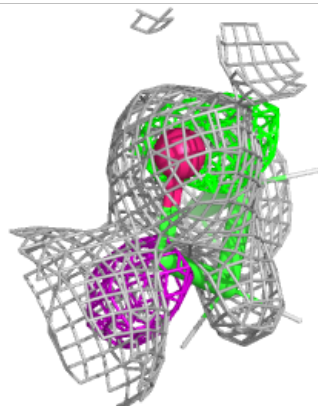
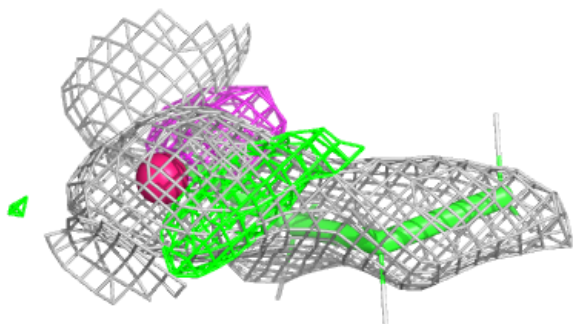
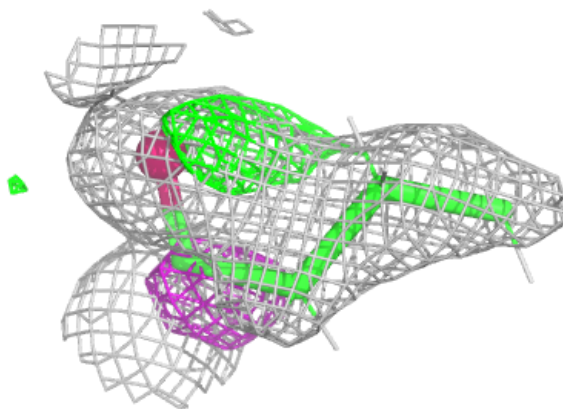


Electron density around LTV E 311:

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

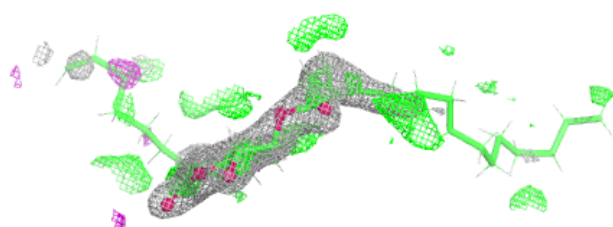
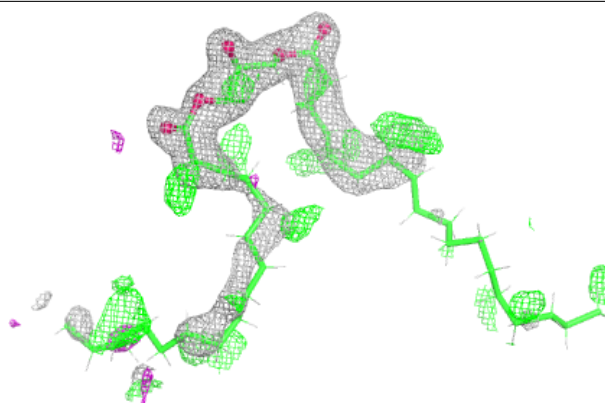
**Electron density around OCA C 301:**

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

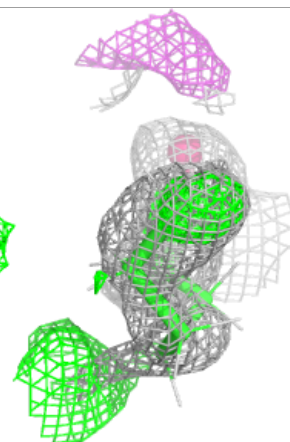
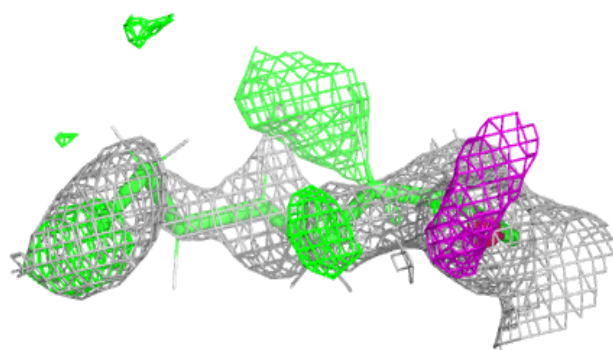
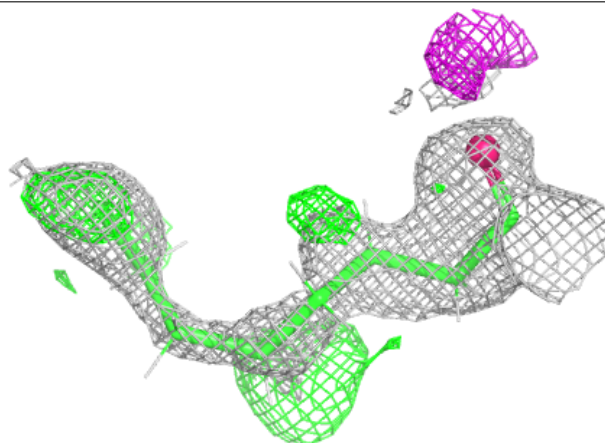


Electron density around LTV E 312:

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

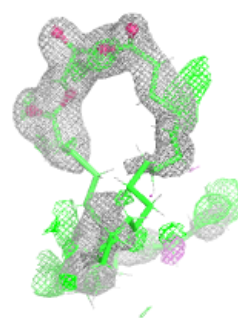
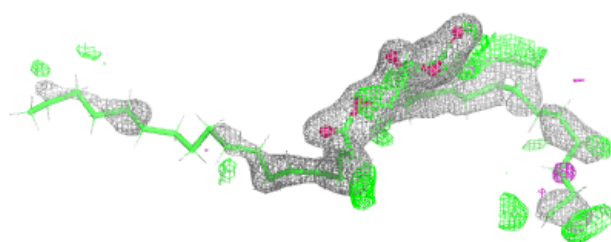
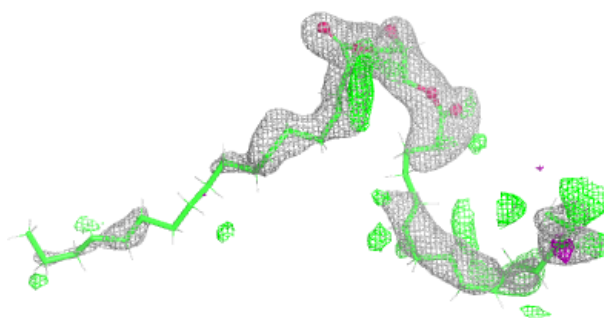
**Electron density around OCA A 301:**

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

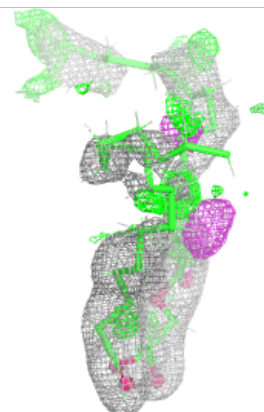
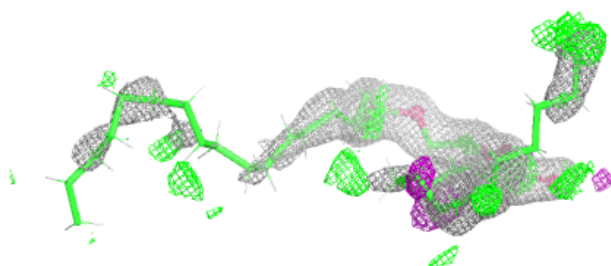
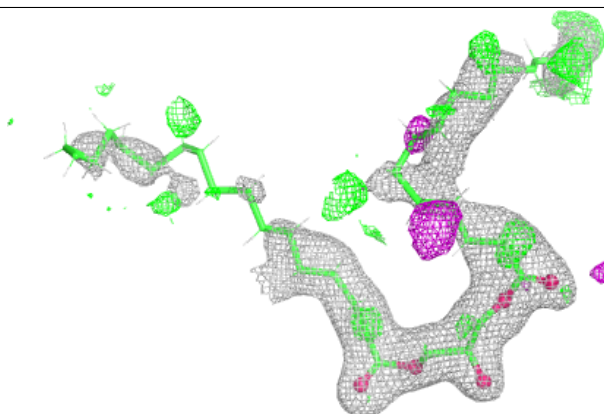


Electron density around LTV D 311:

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

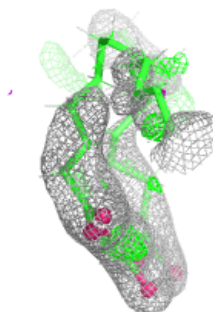
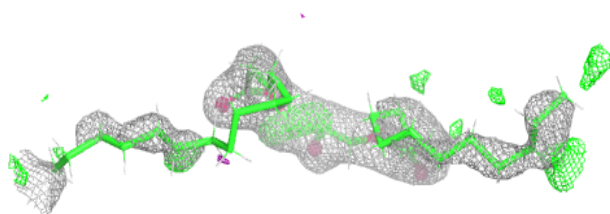
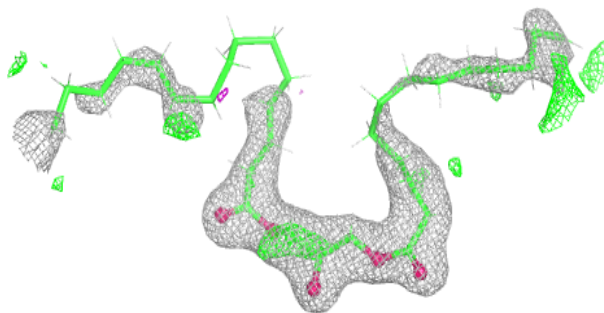
**Electron density around LTV F 307:**

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



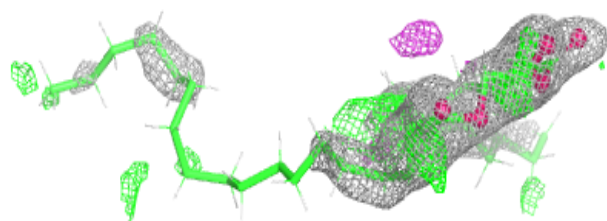
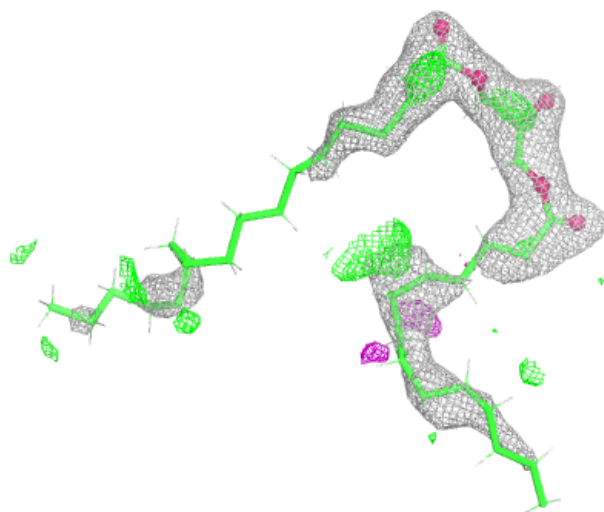
Electron density around LTV A 316:

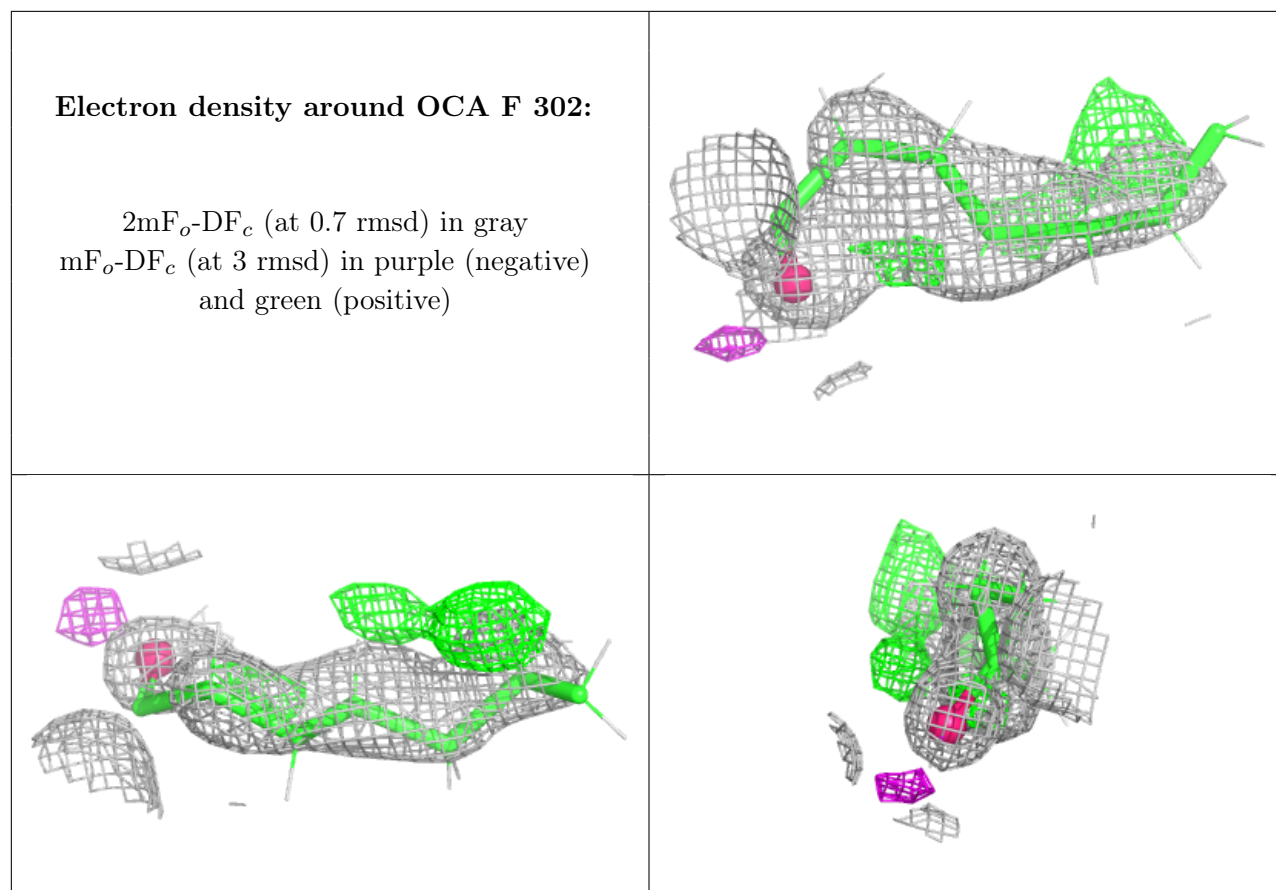
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LTV 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.