



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:27 AM UTC

PDB ID : 6OSZ / pdb_00006osz
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 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

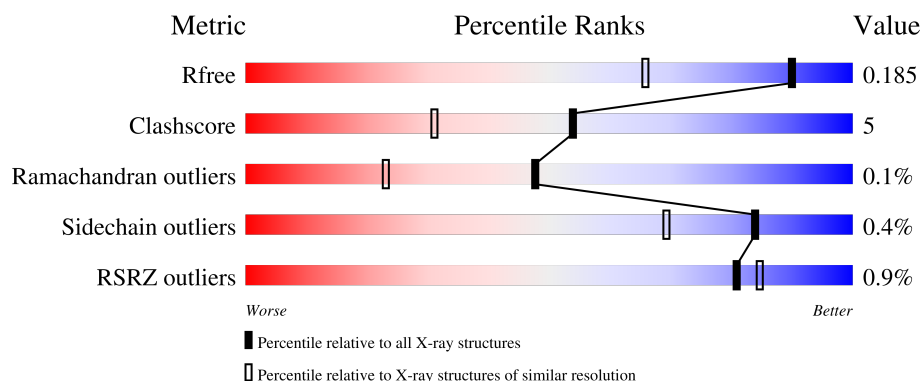
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	88% 5% 8%
1	B	291	85% 7% 8%
1	C	291	86% 6% 8%
1	D	291	88% . 8%
1	E	291	86% 6% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	291	

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	-
2	OCA	F	301	-	-	X	-

2 Entry composition [i](#)

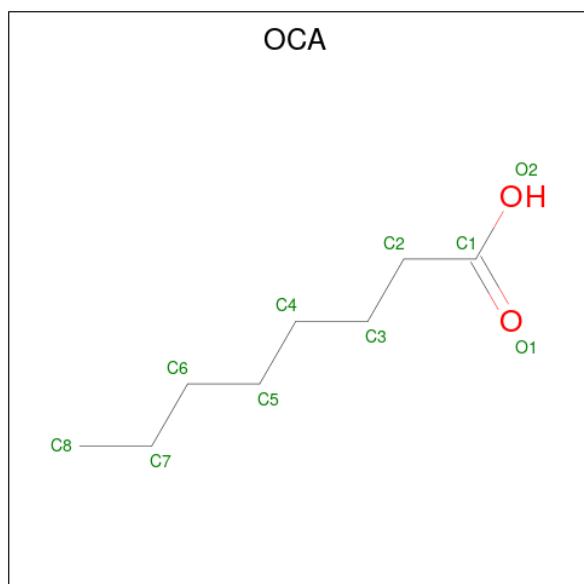
There are 7 unique types of molecules in this entry. The entry contains 27446 atoms, of which 12612 are hydrogens and 0 are deuteriums.

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.

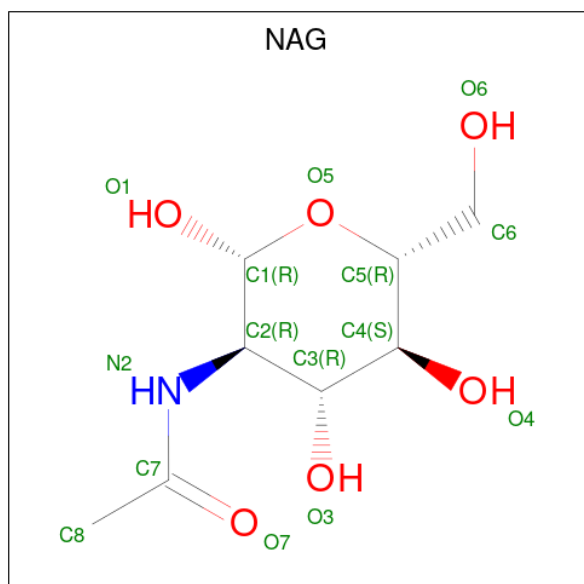
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	H	N	O	S	0	7	0
			4126	1329	2018	364	409	6			
1	B	269	Total	C	H	N	O	S	0	5	0
			4107	1327	2005	364	405	6			
1	C	269	Total	C	H	N	O	S	10	9	0
			4137	1332	2018	368	413	6			
1	E	269	Total	C	H	N	O	S	0	5	0
			4096	1321	1994	365	410	6			
1	D	269	Total	C	H	N	O	S	0	4	0
			4086	1317	1992	364	407	6			
1	F	269	Total	C	H	N	O	S	0	7	0
			4121	1332	2009	365	409	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
			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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



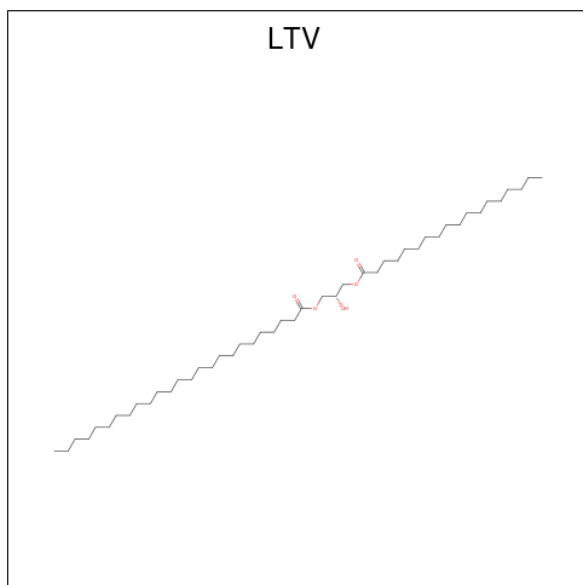
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 8	H 13	N 1	O 5	0	0
3	B	1	Total 27	C 8	H 13	N 1	O 5	0	0
3	C	1	Total 27	C 8	H 13	N 1	O 5	0	0
3	E	1	Total 27	C 8	H 13	N 1	O 5	0	0
3	D	1	Total 27	C 8	H 13	N 1	O 5	0	0

Continued on next page...

Continued from previous page...

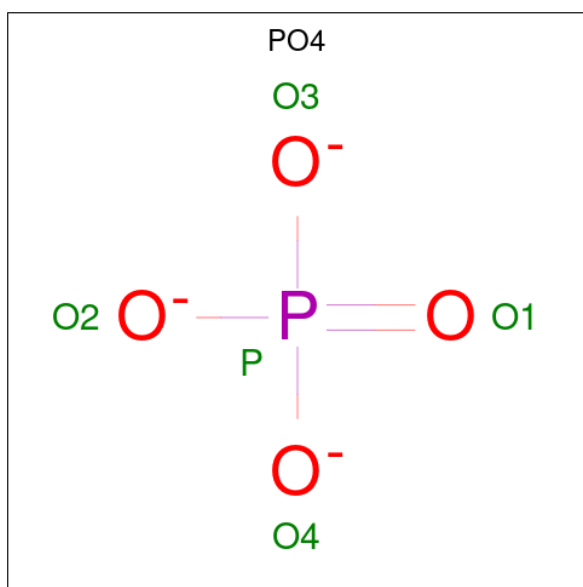
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	H	N	O	
			27	8	13	1	5	
							0	0

- Molecule 4 is 2-hydroxy-3-(octadecanoyloxy)propyl pentacosanoate (CCD ID: LTV) (formula: C₄₆H₉₀O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

Continued on next page...

Continued from previous page...

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

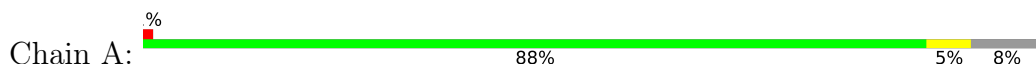
- Molecule 7 is water.

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

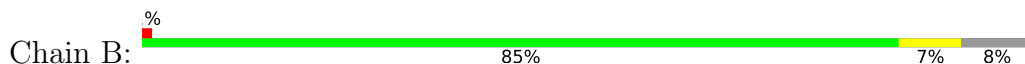
3 Residue-property plots [i](#)

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.

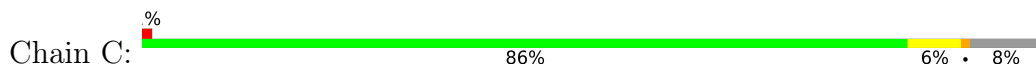
- Molecule 1: Lipase



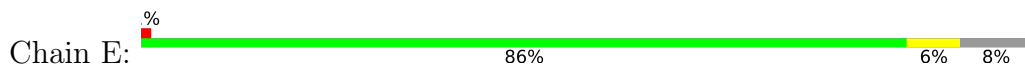
- Molecule 1: Lipase



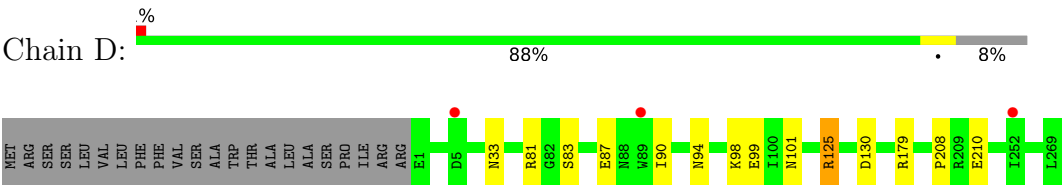
- Molecule 1: Lipase



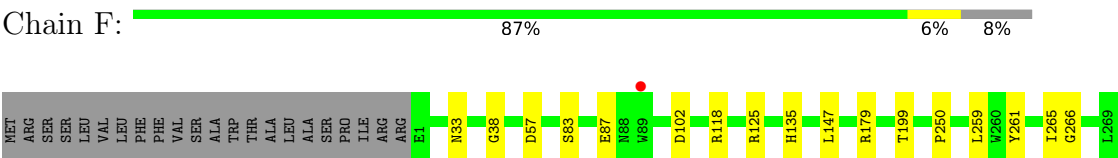
- Molecule 1: Lipase



● 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)	Xtriage
Refinement program	PHENIX 1.19rc7_4070	Depositor
R, R_{free}	0.149 , 0.185 0.149 , 0.185	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 , 46.3	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	27446	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2179	0.55	0/2964
1	B	0.26	0/2167	0.53	0/2950
1	C	0.25	0/2200	0.54	3/2991 (0.1%)
1	D	0.25	0/2156	0.49	0/2934
1	E	0.22	0/2166	0.48	0/2947
1	F	0.29	1/2188 (0.0%)	0.52	0/2978
All	All	0.26	1/13056 (0.0%)	0.52	3/17764 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	250	PRO	CA-CB	6.36	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ASN	CB-CG-ND2	6.00	125.41	116.40
1	C	33	ASN	CA-CB-CG	5.65	118.25	112.60
1	C	33	ASN	CB-CA-C	-5.19	100.78	109.65

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	20	1
1	C	2119	2018	2006	21	2
1	D	2094	1992	1993	19	0
1	E	2102	1994	1987	21	1
1	F	2112	2009	1995	19	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	4	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	124	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.

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)
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

The worst 5 of 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

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	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%)	30	11
All	All	1639/1746 (94%)	1592 (97%)	46 (3%)	1 (0%)	48	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	199	THR

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	224/239 (94%)	224 (100%)	0	100	100
1	C	228/239 (95%)	226 (99%)	2 (1%)	70	44
1	D	224/239 (94%)	223 (100%)	1 (0%)	84	69
1	E	225/239 (94%)	223 (99%)	2 (1%)	70	44
1	F	227/239 (95%)	227 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1355/1434 (94%)	1350 (100%)	5 (0%)	84	69

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	83	SER
1	C	215	HIS
1	E	223	LYS
1	E	239	GLU
1	D	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	11	ASN
1	D	33	ASN
1	F	71	ASN
1	F	11	ASN
1	F	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 oligosaccharides 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	305	-	4,4,4	0.97	0	6,6,6	0.46	0
5	PO4	F	305	-	4,4,4	0.94	0	6,6,6	0.40	0
5	PO4	A	305	-	4,4,4	0.94	0	6,6,6	0.73	0
4	LTV	D	304	-	50,50,50	0.85	3 (6%)	52,52,52	0.77	2 (3%)
2	OCA	B	301	1	8,8,9	1.14	1 (12%)	7,7,9	0.85	0
4	LTV	B	306	-	42,42,50	0.88	3 (7%)	44,44,52	0.87	2 (4%)
5	PO4	B	302	-	4,4,4	0.90	0	6,6,6	0.63	0
5	PO4	C	305	-	4,4,4	1.06	0	6,6,6	0.81	0
3	NAG	C	303	1	14,14,15	1.42	2 (14%)	17,19,21	1.01	2 (11%)
3	NAG	B	305	-	14,14,15	0.47	0	17,19,21	1.15	3 (17%)
4	LTV	E	304	-	50,50,50	0.82	3 (6%)	52,52,52	0.75	2 (3%)
5	PO4	B	307	-	4,4,4	0.95	0	6,6,6	0.50	0
5	PO4	E	305	-	4,4,4	0.98	0	6,6,6	0.39	0
4	LTV	F	304	-	41,41,50	0.89	3 (7%)	43,43,52	0.75	2 (4%)
2	OCA	D	301	1	7,8,9	0.48	0	6,7,9	1.22	1 (16%)
3	NAG	E	303	1	14,14,15	0.39	0	17,19,21	0.41	0
5	PO4	D	306	-	4,4,4	0.88	0	6,6,6	0.55	0
4	LTV	C	304	-	40,40,50	0.90	3 (7%)	42,42,52	0.79	2 (4%)
3	NAG	F	303	-	14,14,15	0.63	0	17,19,21	0.79	0
2	OCA	E	301	1	7,8,9	0.43	0	6,7,9	0.86	0
4	LTV	A	303	-	35,35,50	0.95	3 (8%)	37,37,52	0.83	2 (5%)
2	OCA	F	301	1	7,8,9	0.53	0	6,7,9	0.95	0
2	OCA	C	301	1	8,8,9	1.15	1 (12%)	7,7,9	1.40	2 (28%)
5	PO4	E	306	-	4,4,4	0.99	0	6,6,6	0.24	0
2	OCA	A	301	1	7,8,9	0.47	0	6,7,9	0.85	0
5	PO4	A	304	-	4,4,4	0.94	0	6,6,6	0.67	0
3	NAG	A	302	1	14,14,15	0.46	0	17,19,21	0.76	1 (5%)
3	NAG	D	303	-	14,14,15	0.56	0	17,19,21	0.81	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
2	OCA	D	301	1	-	1/6/6/7	-
3	NAG	E	303	1	-	2/6/23/26	0/1/1/1
2	OCA	B	301	1	-	2/6/6/7	-
4	LTV	A	303	-	-	24/36/36/51	-
2	OCA	F	301	1	-	3/6/6/7	-
4	LTV	B	306	-	-	22/43/43/51	-
2	OCA	C	301	1	-	2/6/6/7	-
4	LTV	C	304	-	-	23/41/41/51	-
3	NAG	C	303	1	-	0/6/23/26	0/1/1/1
3	NAG	B	305	-	-	0/6/23/26	0/1/1/1
4	LTV	E	304	-	-	21/51/51/51	-
4	LTV	D	304	-	-	24/51/51/51	-
3	NAG	F	303	-	-	2/6/23/26	0/1/1/1
2	OCA	A	301	1	-	3/6/6/7	-
4	LTV	F	304	-	-	23/42/42/51	-
2	OCA	E	301	1	-	1/6/6/7	-
3	NAG	A	302	1	-	0/6/23/26	0/1/1/1
3	NAG	D	303	-	-	1/6/23/26	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	NAG	C1-C2	4.47	1.58	1.52
2	B	301	OCA	O2-C1	-3.14	1.26	1.42
2	C	301	OCA	O2-C1	-3.06	1.26	1.42
4	D	304	LTV	O1-C17	2.86	1.41	1.33
3	C	303	NAG	O5-C1	2.71	1.48	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	306	LTV	O3-C21-C22	3.23	121.69	111.83
4	E	304	LTV	O3-C21-C22	2.98	120.93	111.83
4	C	304	LTV	O3-C21-C22	2.92	120.72	111.83
4	D	304	LTV	O3-C21-C22	2.80	120.37	111.83
4	D	304	LTV	O1-C17-C16	2.67	119.97	111.83

There are no chirality outliers.

5 of 154 torsion outliers are listed below:

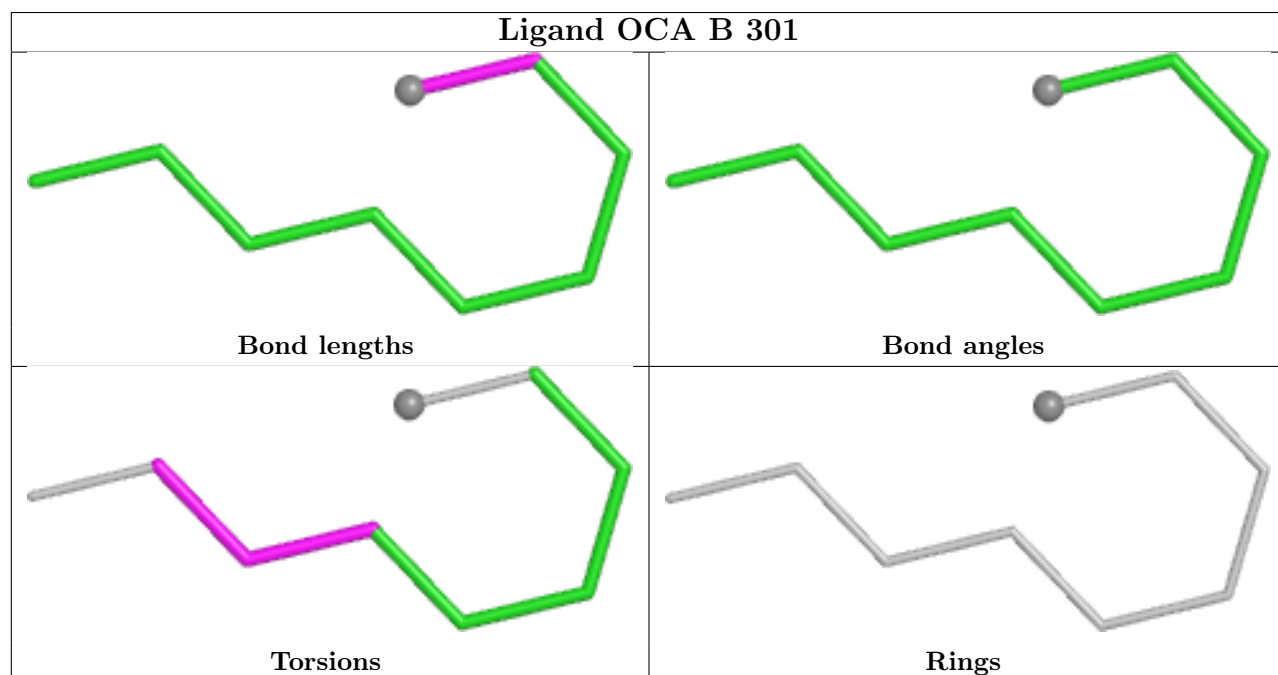
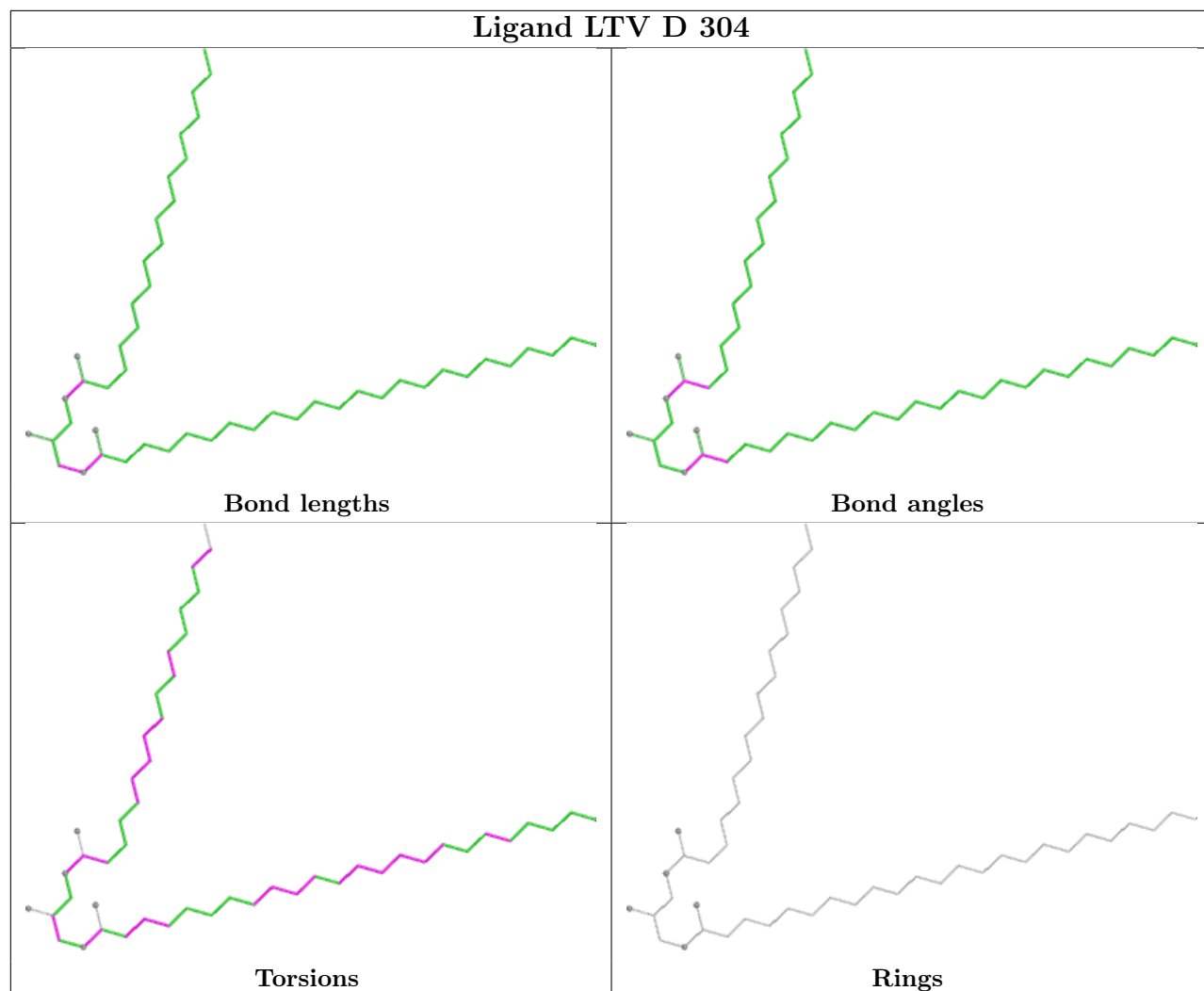
Mol	Chain	Res	Type	Atoms
4	A	303	LTV	O1-C18-C19-O2
4	B	306	LTV	O4-C21-O3-C20
4	B	306	LTV	C22-C21-O3-C20
4	B	306	LTV	O2-C19-C20-O3
4	B	306	LTV	C18-C19-C20-O3

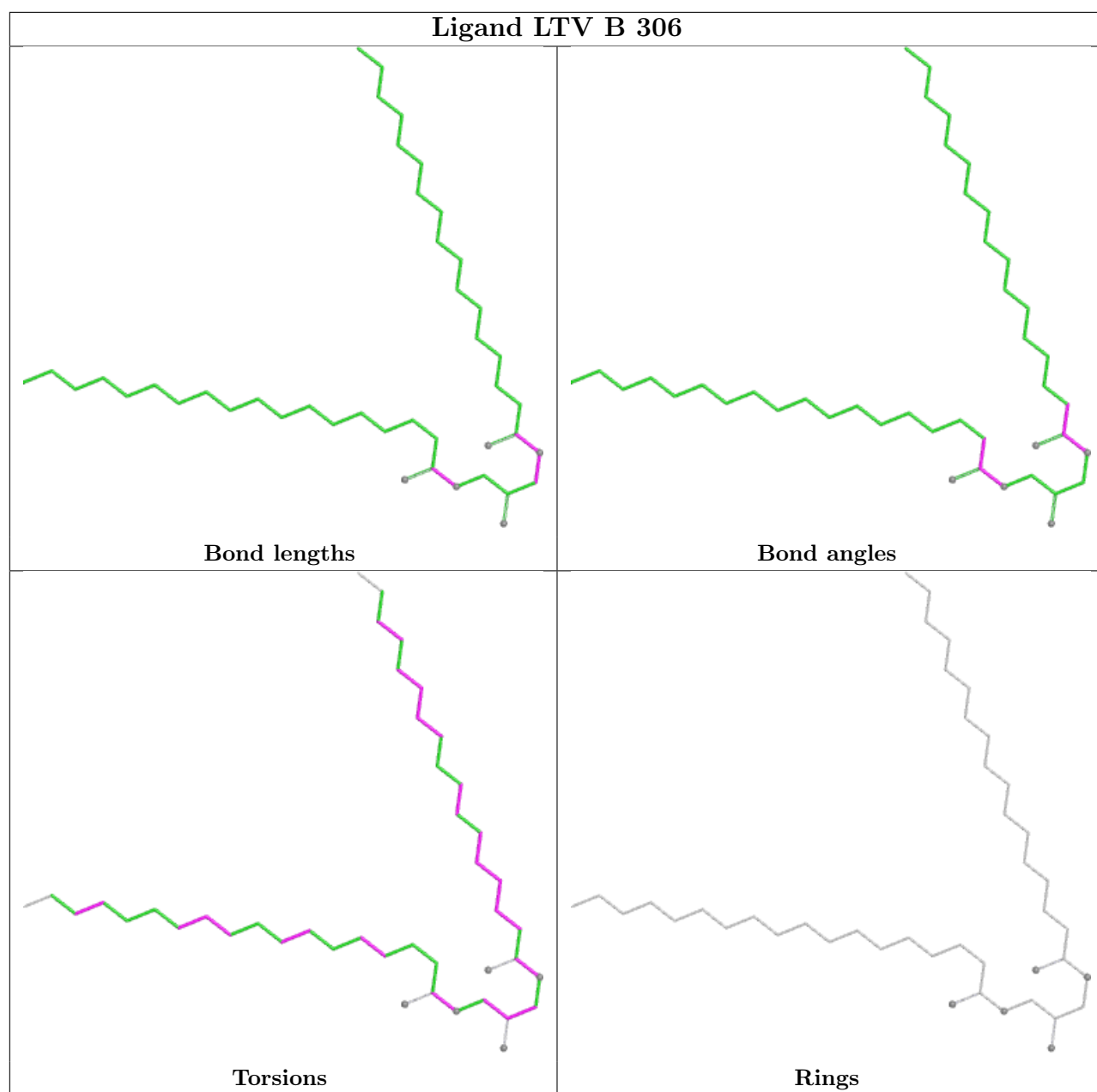
There are no ring outliers.

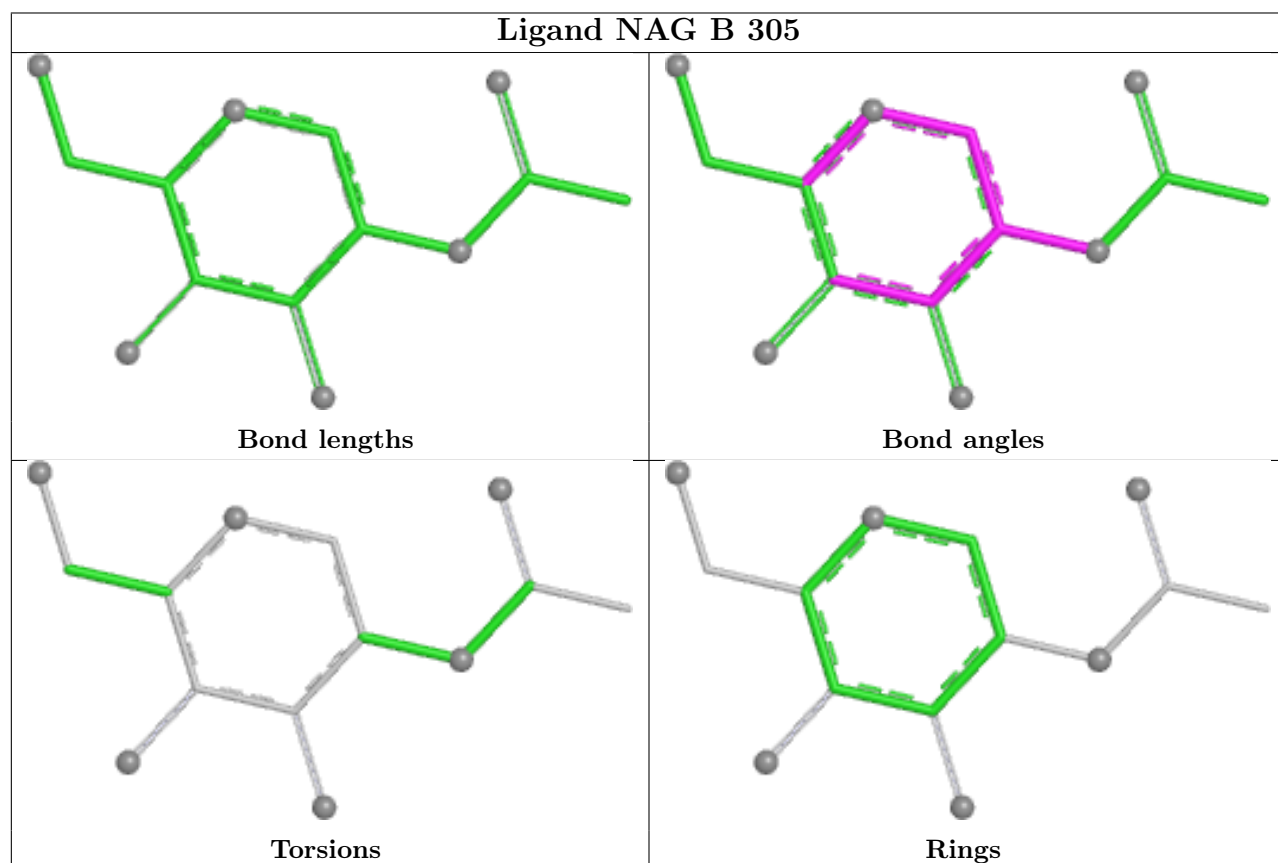
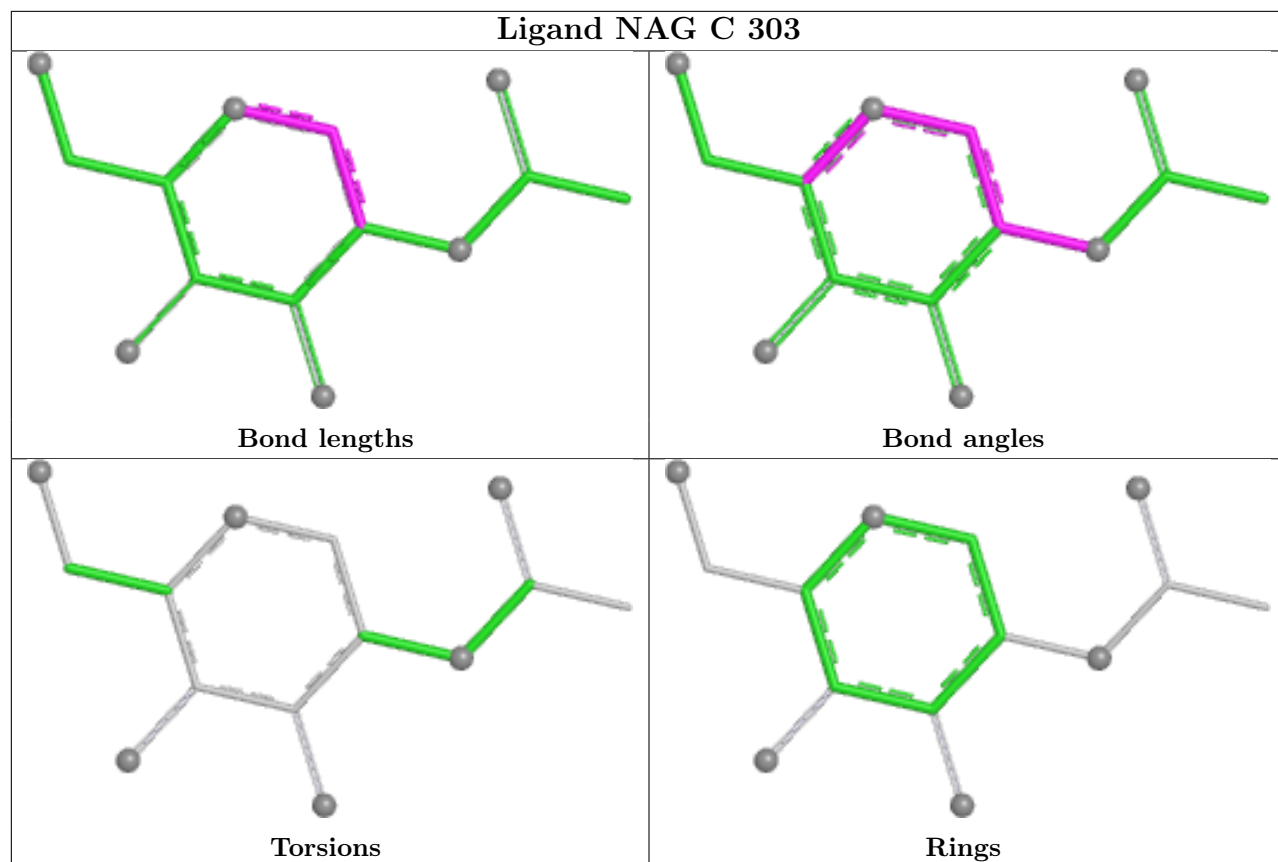
18 monomers are involved in 71 short contacts:

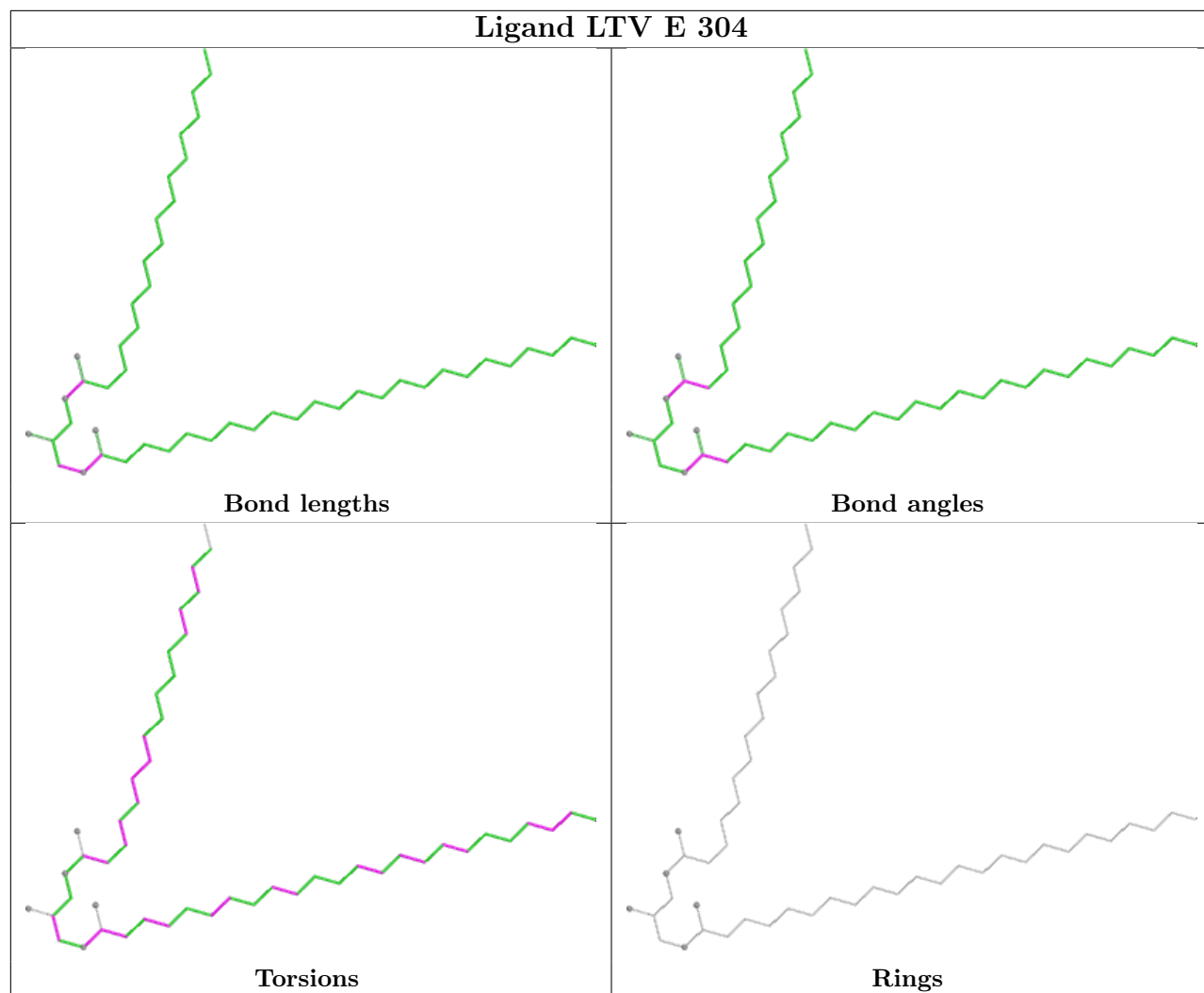
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	305	PO4	1	0
5	F	305	PO4	1	0
2	B	301	OCA	9	0
5	B	302	PO4	1	0
3	C	303	NAG	2	0
3	B	305	NAG	3	0
4	E	304	LTV	4	0
5	E	305	PO4	1	0
2	D	301	OCA	6	0
4	C	304	LTV	1	0
3	F	303	NAG	4	0
2	E	301	OCA	10	0
2	F	301	OCA	6	0
2	C	301	OCA	12	0
5	E	306	PO4	1	0
2	A	301	OCA	6	0
3	A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

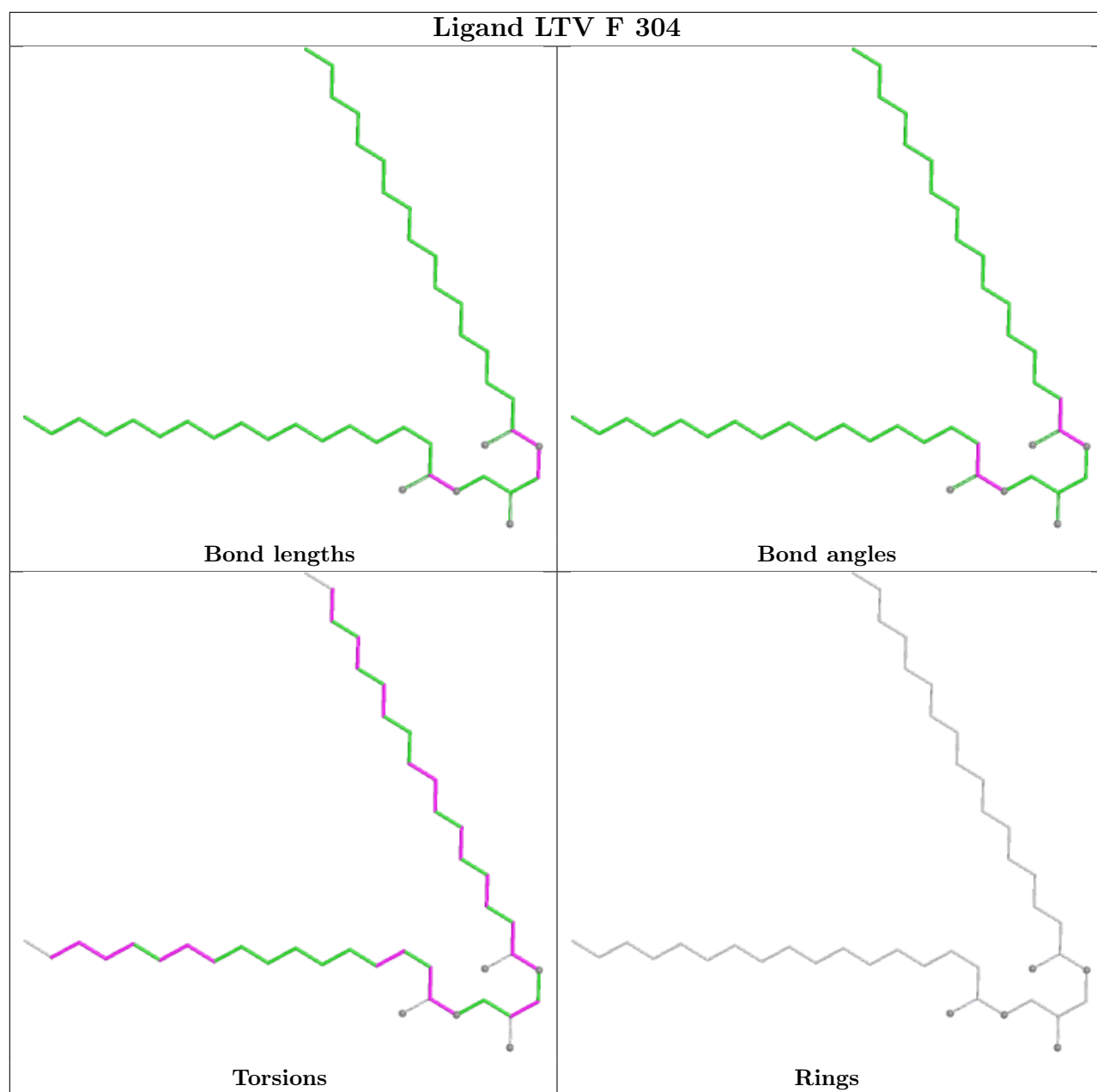
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











6.4 Ligands ⓘ

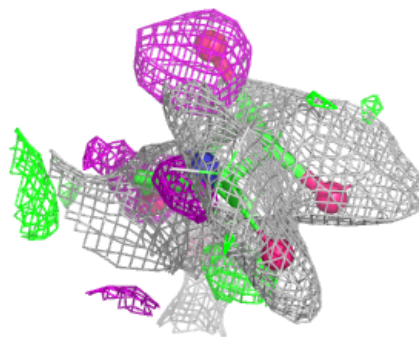
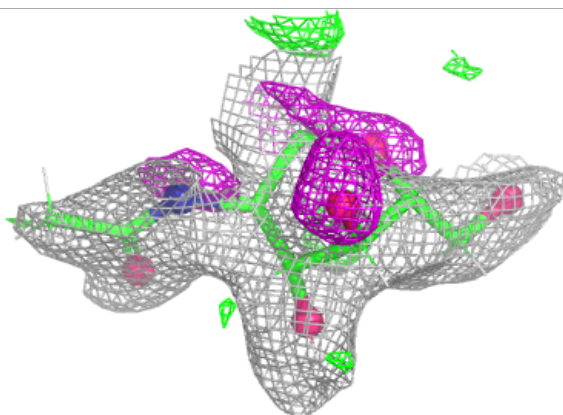
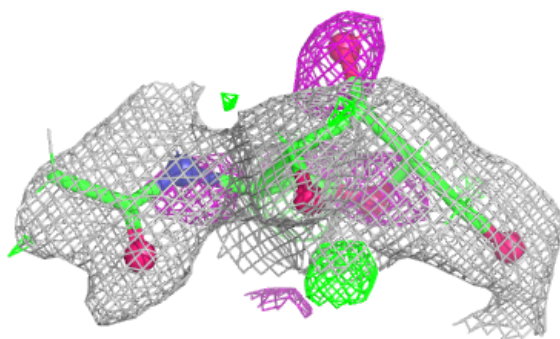
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	302	14/15	0.57	0.16	56,59,71,72	0
2	OCA	E	301	9/10	0.58	0.27	35,46,55,55	24
2	OCA	A	301	9/10	0.61	0.38	28,41,48,48	24
2	OCA	C	301	9/10	0.64	0.49	30,41,47,47	24
3	NAG	D	303	14/15	0.70	0.13	50,54,65,65	0
4	LTV	E	304	51/51	0.70	0.23	54,70,80,81	0
2	OCA	D	301	9/10	0.71	0.36	30,45,53,53	24
3	NAG	E	303	14/15	0.72	0.13	55,59,71,71	0
5	PO4	C	305	5/5	0.72	0.14	58,61,71,76	0
2	OCA	F	301	9/10	0.73	0.32	29,42,52,52	24
4	LTV	D	304	51/51	0.73	0.20	52,66,73,73	0
3	NAG	C	303	14/15	0.73	0.13	48,53,64,64	0
4	LTV	F	304	42/51	0.75	0.20	44,59,71,71	0
4	LTV	B	306	43/51	0.75	0.20	48,63,75,76	0
2	OCA	B	301	9/10	0.76	0.42	32,49,59,59	24
4	LTV	C	304	41/51	0.76	0.20	52,66,74,75	0
3	NAG	F	303	14/15	0.79	0.12	42,45,54,55	0
5	PO4	B	307	5/5	0.80	0.16	55,56,56,56	5
4	LTV	A	303	36/51	0.81	0.18	46,61,73,74	0
5	PO4	D	305	5/5	0.84	0.17	51,53,54,54	5
5	PO4	E	305	5/5	0.86	0.12	54,54,55,55	5
5	PO4	A	304	5/5	0.87	0.14	47,49,50,50	5
5	PO4	E	306	5/5	0.89	0.12	38,41,42,43	5
3	NAG	B	305	14/15	0.89	0.09	36,40,49,49	0
5	PO4	D	306	5/5	0.89	0.11	45,45,46,47	5
5	PO4	F	305	5/5	0.89	0.11	41,43,43,44	5
5	PO4	A	305	5/5	0.92	0.10	26,29,30,30	5
5	PO4	B	302	5/5	0.93	0.09	37,39,40,41	5
6	CA	B	304	1/1	0.96	0.13	52,52,52,52	0
6	CA	C	302	1/1	0.98	0.10	37,37,37,37	1
6	CA	B	303	1/1	0.99	0.02	20,20,20,20	0
6	CA	E	302	1/1	0.99	0.07	50,50,50,50	0

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

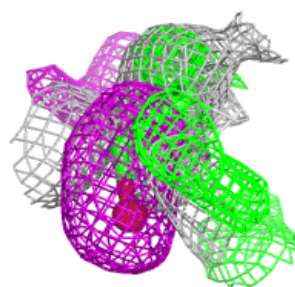
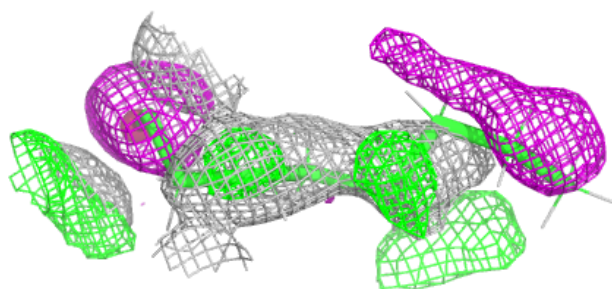
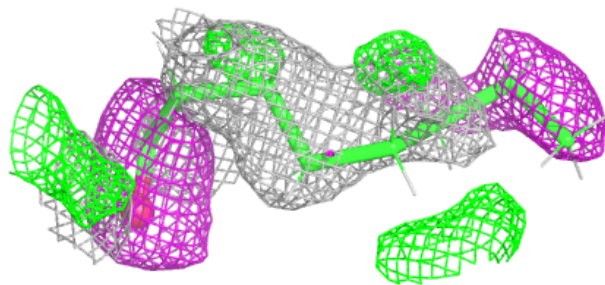
Electron density around NAG A 302:

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

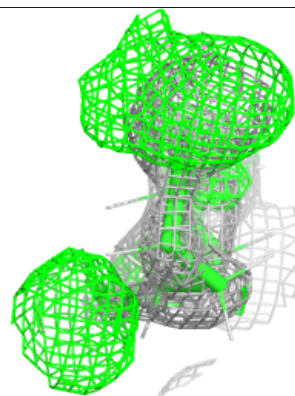
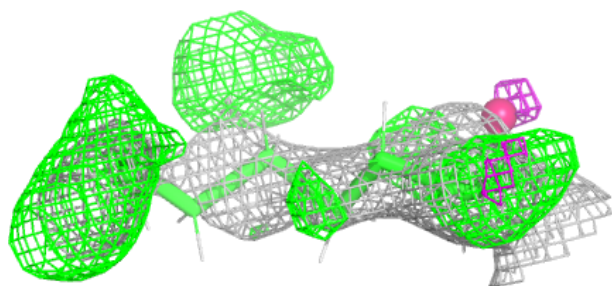
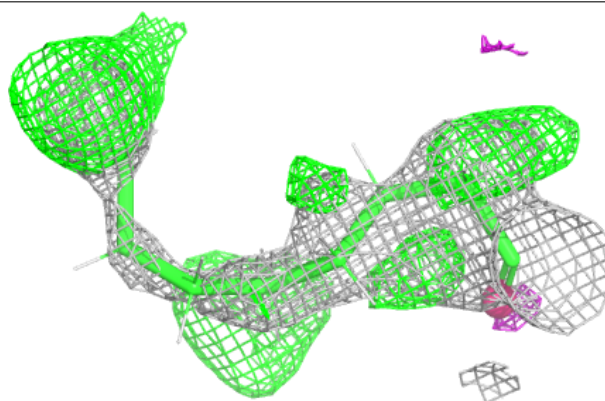


Electron density around OCA E 301:

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

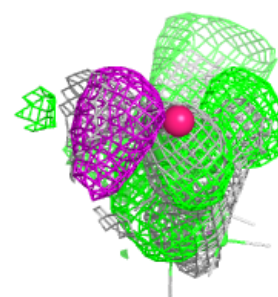
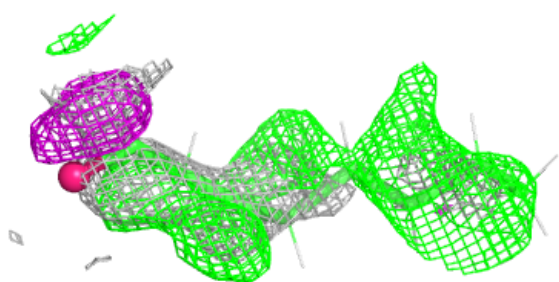
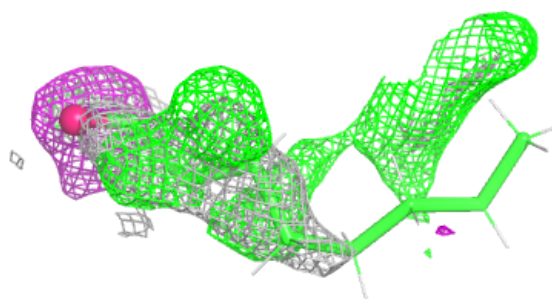
**Electron density around OCA A 301:**

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

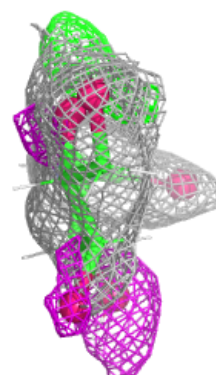
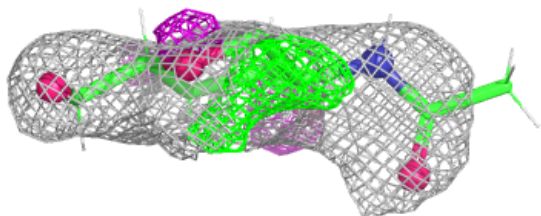
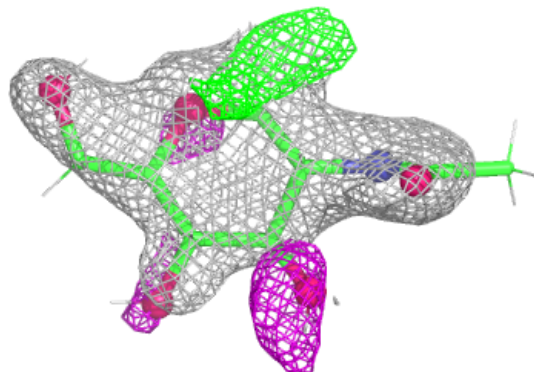


Electron density around OCA C 301:

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

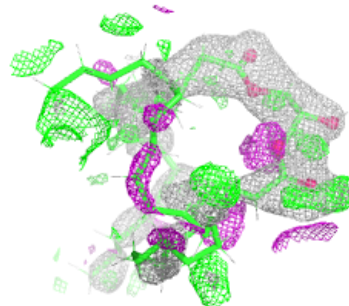
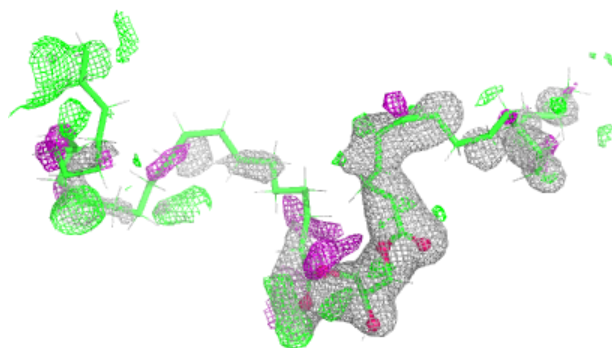
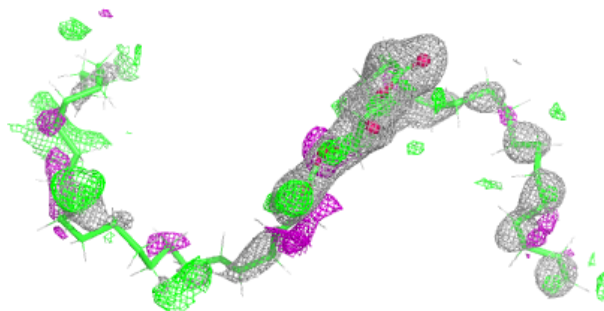
**Electron density around NAG D 303:**

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

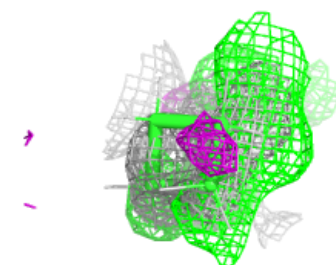
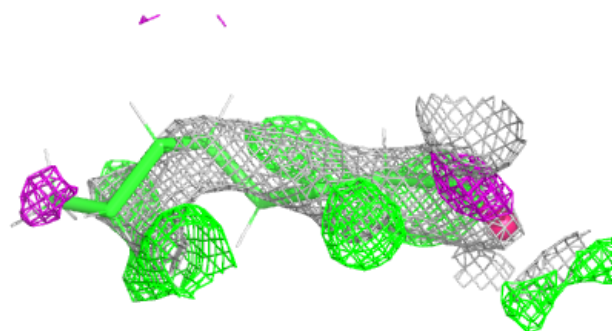
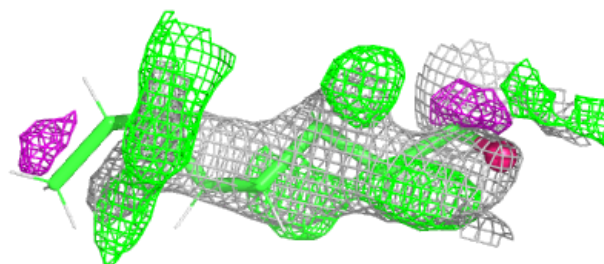


Electron density around LTV E 304:

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

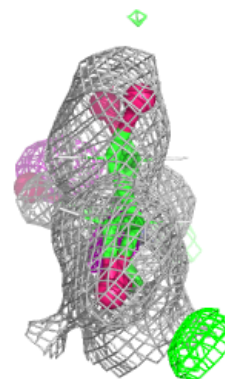
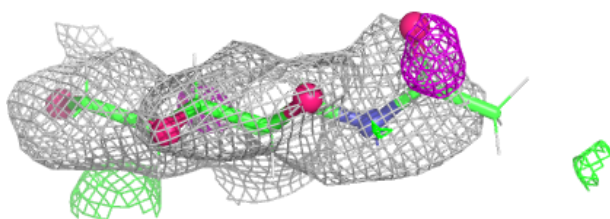
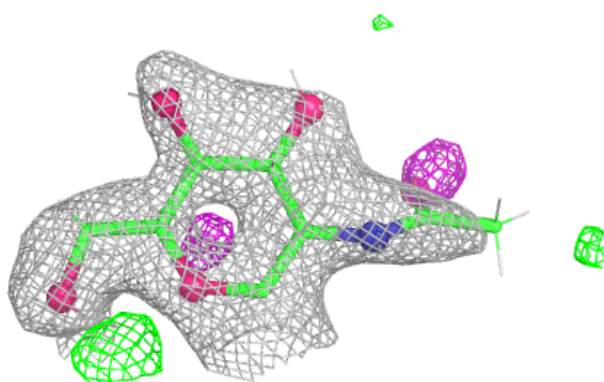
**Electron density around OCA D 301:**

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

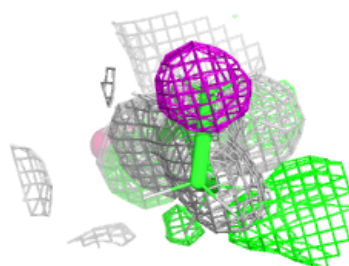
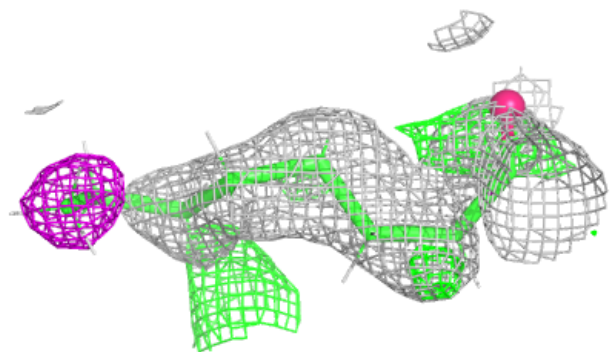
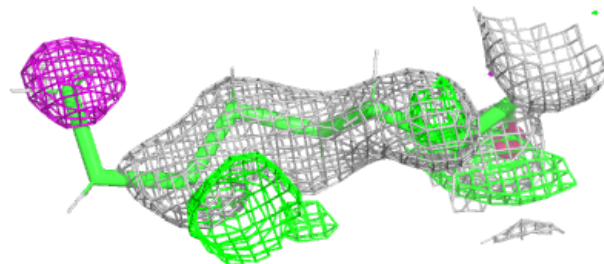


Electron density around NAG E 303:

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

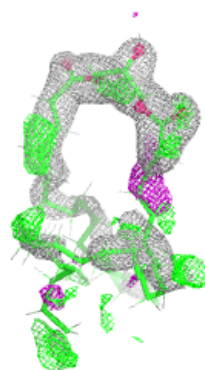
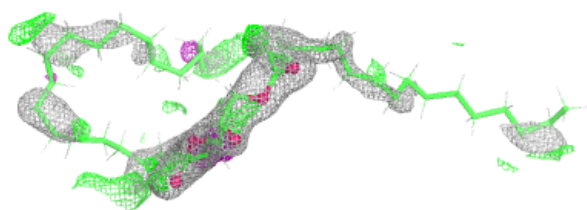
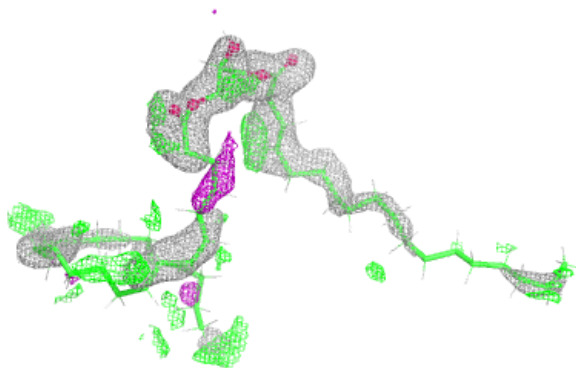
**Electron density around OCA F 301:**

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

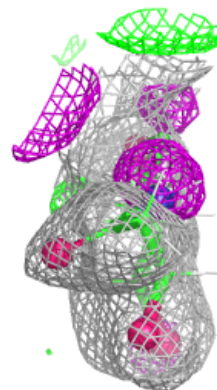
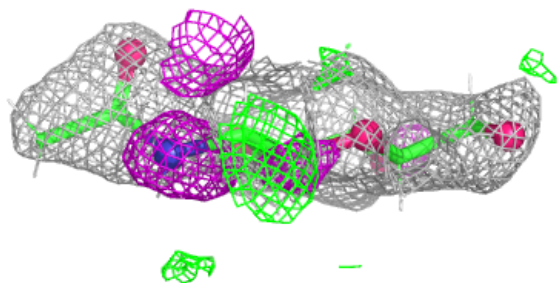
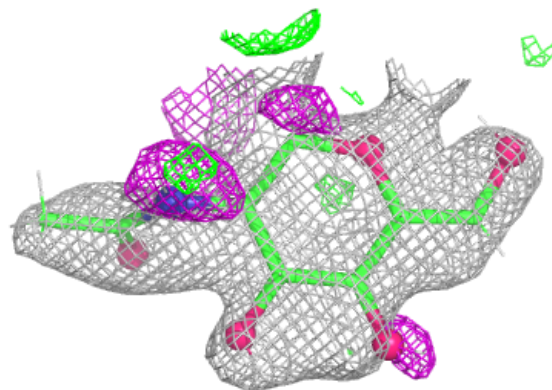


Electron density around LTV D 304:

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

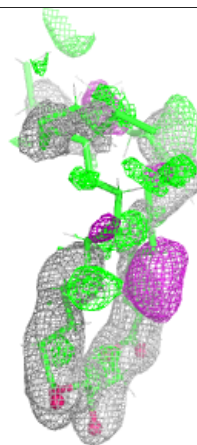
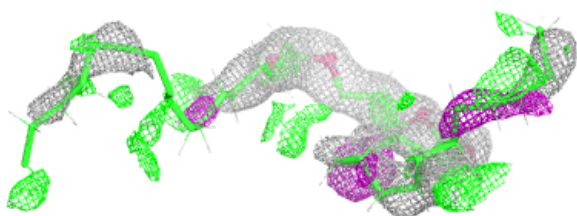
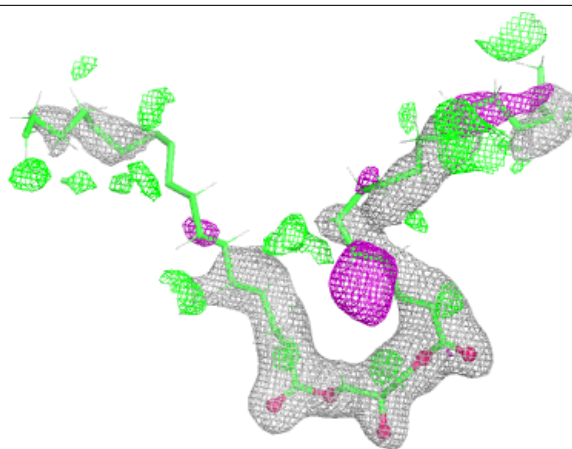
**Electron density around NAG C 303:**

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



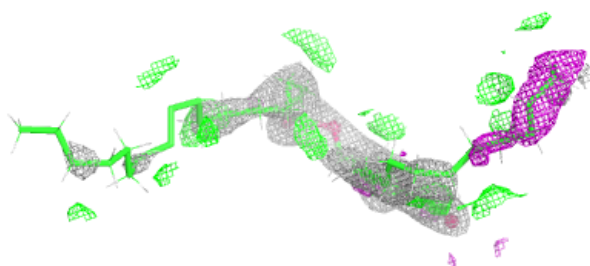
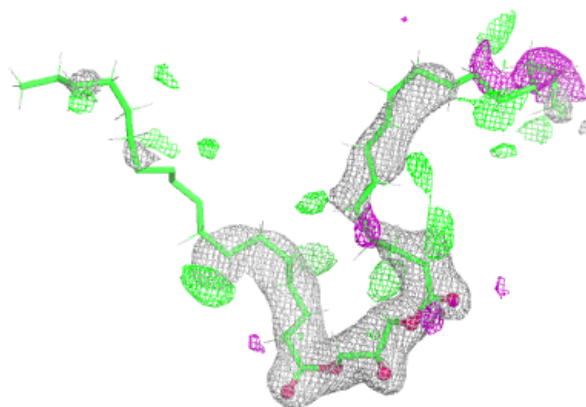
Electron density around LTV F 304:

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

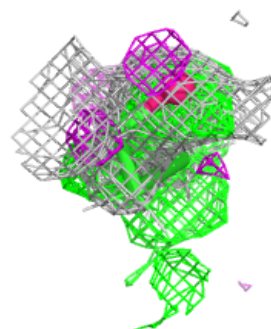
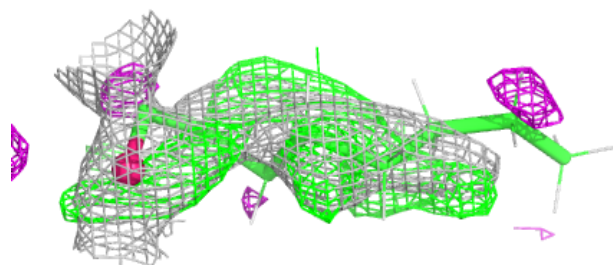
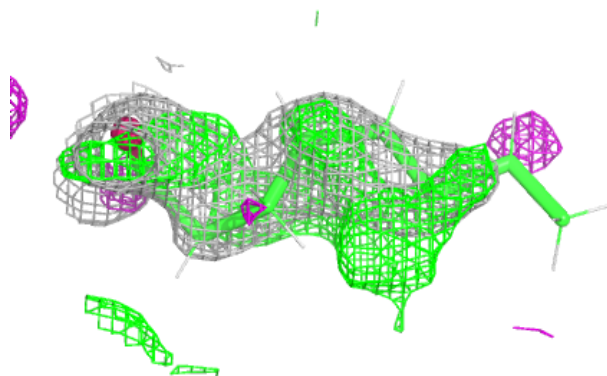


Electron density around LTV B 306:

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

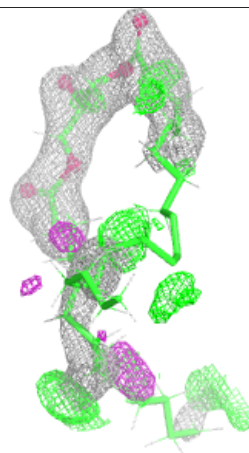
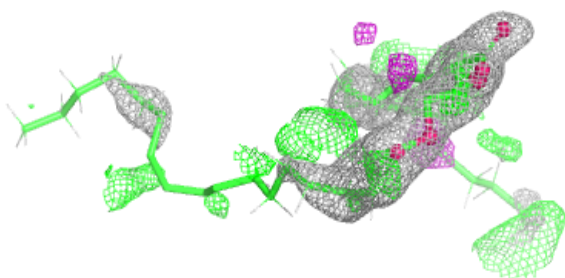
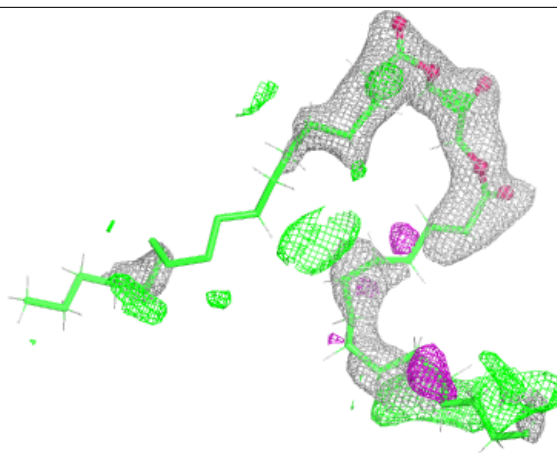
**Electron density around OCA B 301:**

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

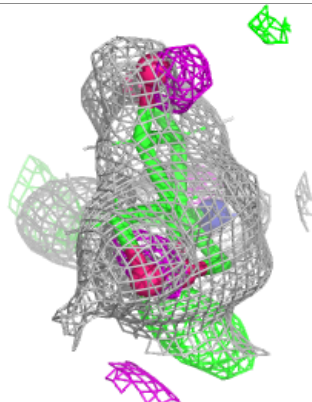
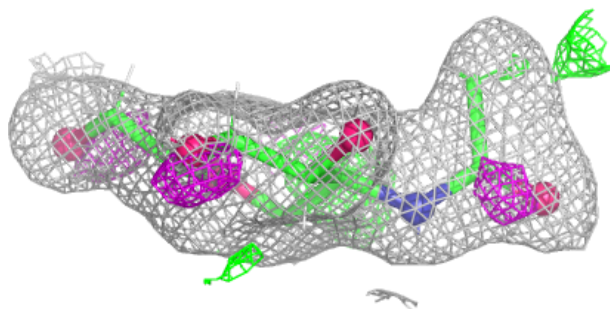
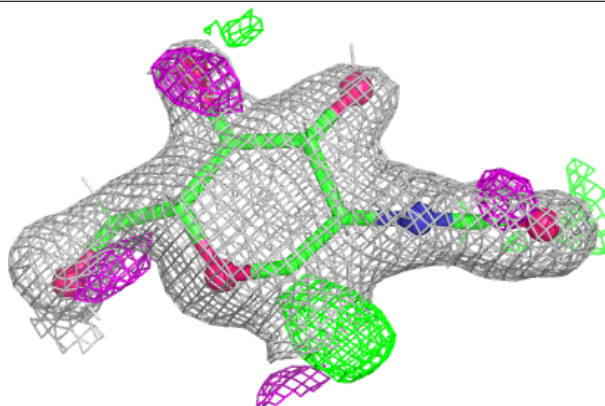


Electron density around LTV C 304:

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

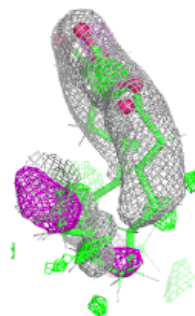
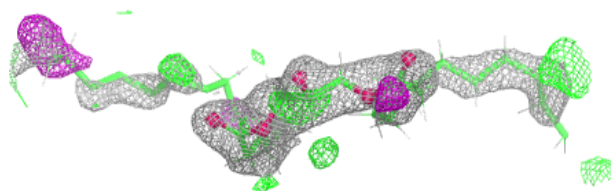
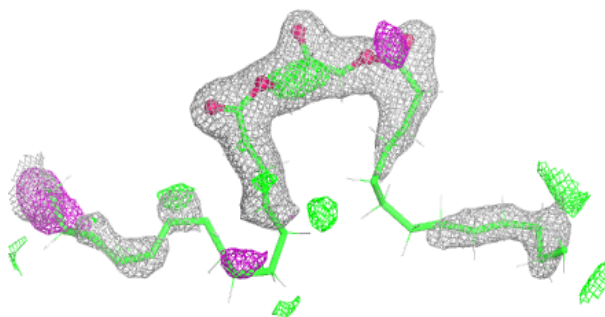
**Electron density around NAG F 303:**

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

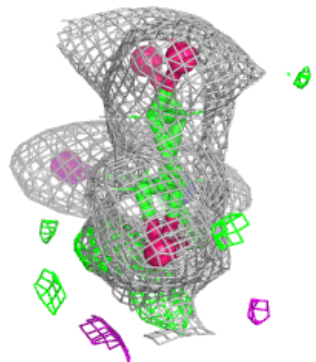
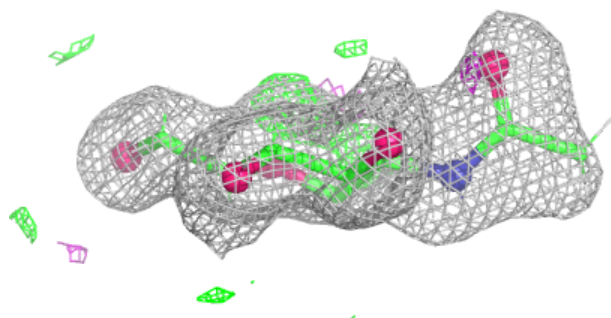
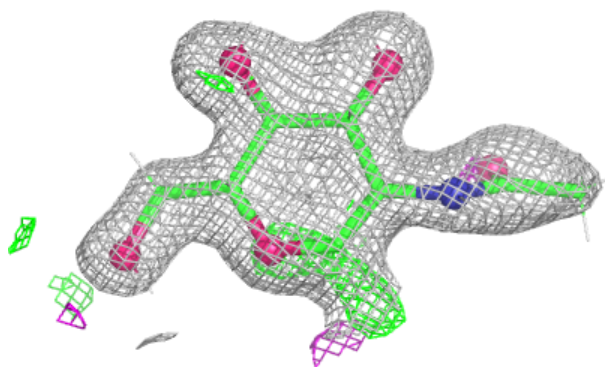


Electron density around LTV A 303:

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

**Electron density around NAG B 305:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.