



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 PM UTC

PDB ID : 4C00 / pdb_00004c00
Title : Crystal structure of TamA from E. coli
Authors : Gruss, F.; Zaehringer, F.; Jakob, R.P.; Burmann, B.M.; Hiller, S.; Maier, T.
Deposited on : 2013-07-30
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

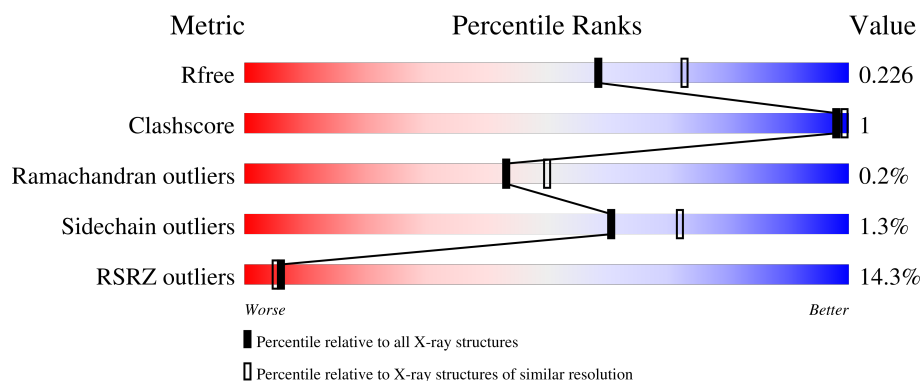
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	559	14% 94%

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
4	CL	A	801	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9926 atoms, of which 4883 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.

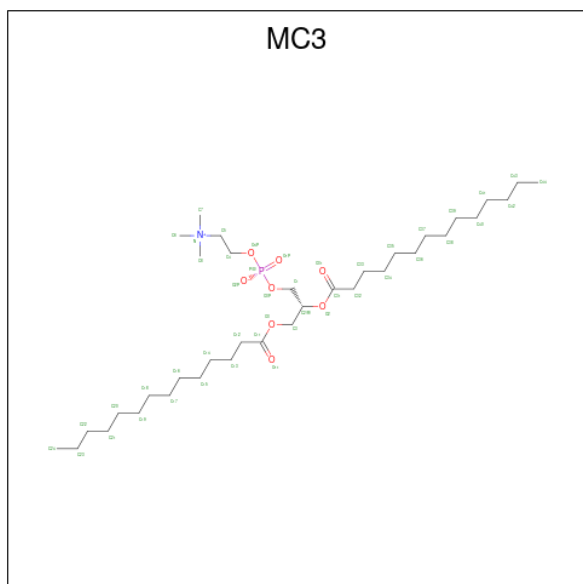
- Molecule 1 is a protein called TRANSLOCATION AND ASSEMBLY MODULE TAMA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	544	8695	2792	4306	760	832	5	0	10	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP P0ADE4
A	20	ILE	-	expression tag	UNP P0ADE4
A	21	GLN	-	expression tag	UNP P0ADE4

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: C₃₆H₇₂NO₈P).



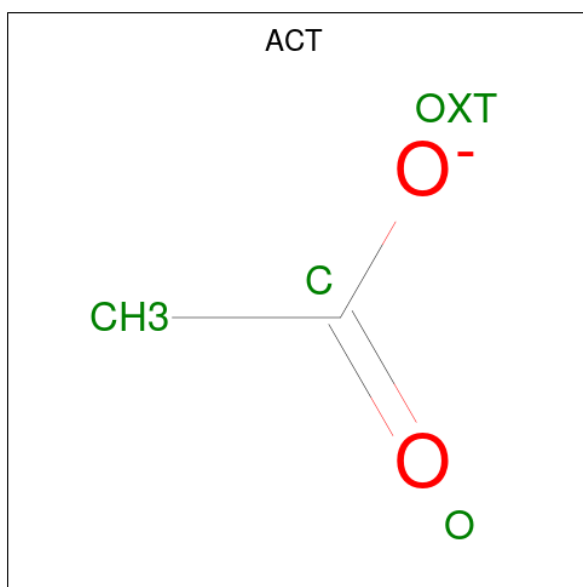
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	118	36	72	1	8	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H N O P 118 36 72 1 8 1	0	0
2	A	1	Total C H O P 99 31 59 8 1	0	0
2	A	1	Total C H 30 10 20	0	0
2	A	1	Total C H O P 15 4 5 5 1	0	0
2	A	1	Total C H O P 57 18 31 7 1	0	0
2	A	1	Total C H O P 21 6 7 7 1	0	0
2	A	1	Total C H O 95 31 59 5	0	0
2	A	1	Total C H O 25 9 14 2	0	0
2	A	1	Total C H O P 49 15 25 8 1	0	0
2	A	1	Total C H N O P 107 33 64 1 8 1	0	0
2	A	1	Total C H O P 58 18 31 8 1	0	0
2	A	1	Total C H N O P 71 21 40 1 8 1	0	0
2	A	1	Total C H O P 78 25 44 8 1	0	0
2	A	1	Total C H N O P 24 5 13 1 4 1	0	0
2	A	1	Total C H 23 8 15	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		

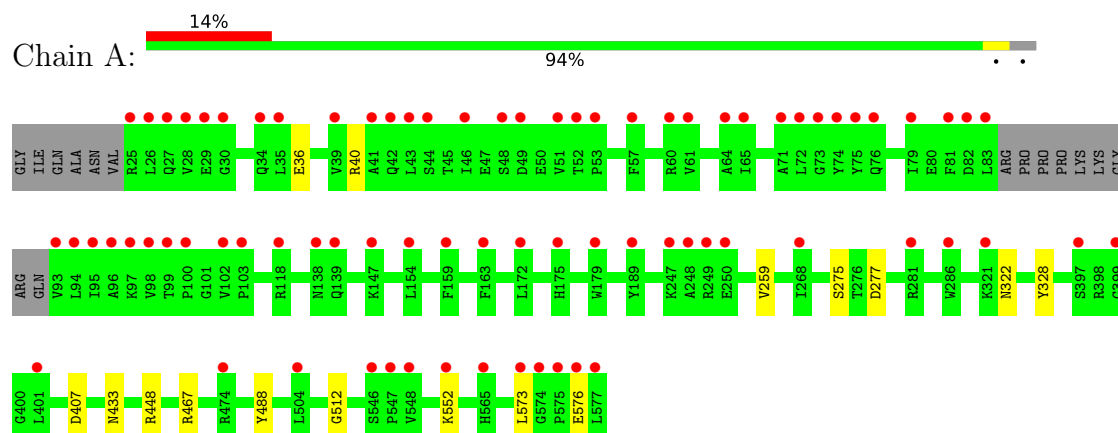
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total	O	0	0
			226	226		

3 Residue-property plots

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: TRANSLOCATION AND ASSEMBLY MODULE TAMA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.47Å 261.06Å 57.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.27 – 2.25 74.27 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.4 (74.27-2.25) 98.4 (74.27-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.217 0.206 , 0.226	Depositor DCC
R_{free} test set	1947 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9926	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: CL, ACT, MC3

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	0.28	0/4536	0.59	0/6145

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4389	4306	4260	7	0
2	A	417	571	537	1	0
3	A	8	6	6	0	0
4	A	3	0	0	2	0
5	A	226	0	0	1	0
All	All	5043	4883	4803	7	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (7) 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:A:488:TYR:OH	4:A:801:CL:CL	2.32	0.84
1:A:448[B]:ARG:NH2	5:A:2161:HOH:O	2.23	0.70
1:A:36:GLU:O	1:A:40:ARG:NH1	2.40	0.55
1:A:467:ARG:NH1	4:A:801:CL:CL	2.78	0.50
1:A:275:SER:OG	1:A:277:ASP:OD1	2.29	0.47
1:A:328:TYR:OH	2:A:615:MC3:O2P	2.22	0.46
1:A:448[A]:ARG:NH1	1:A:576:GLU:O	2.53	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	551/559 (99%)	525 (95%)	25 (4%)	1 (0%)	43 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	512	GLY

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	473/475 (100%)	465 (98%)	8 (2%)	53 65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	VAL
1	A	322	ASN
1	A	407	ASP
1	A	433	ASN
1	A	552[A]	LYS
1	A	552[B]	LYS
1	A	552[C]	LYS
1	A	573	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	184	ASN
1	A	193	HIS
1	A	227	ASN
1	A	366	ASN
1	A	376	GLN
1	A	409	GLN

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 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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
2	MC3	A	615	-	10,10,45	2.04	2 (20%)	15,15,53	1.61	2 (13%)
2	MC3	A	601	-	45,45,45	0.93	2 (4%)	51,53,53	0.77	2 (3%)
2	MC3	A	606	-	25,25,45	1.44	1 (4%)	27,29,53	1.51	4 (14%)
2	MC3	A	608	-	35,35,45	0.52	1 (2%)	37,37,53	0.86	3 (8%)
2	MC3	A	612	-	26,26,45	1.44	3 (11%)	29,31,53	1.76	7 (24%)
3	ACT	A	702	-	3,3,3	0.79	0	3,3,3	1.32	0
2	MC3	A	607	-	13,13,45	1.90	1 (7%)	15,17,53	2.33	5 (33%)
2	MC3	A	610	-	23,23,45	1.49	1 (4%)	26,28,53	2.11	7 (26%)
2	MC3	A	603	-	39,39,45	1.12	2 (5%)	42,44,53	1.32	4 (9%)
2	MC3	A	613	-	30,30,45	1.13	1 (3%)	36,38,53	0.91	2 (5%)
2	MC3	A	604	-	9,9,45	0.21	0	8,8,53	0.15	0
2	MC3	A	602	-	45,45,45	0.92	2 (4%)	51,53,53	0.81	3 (5%)
2	MC3	A	605	-	8,9,45	2.38	1 (12%)	8,12,53	2.29	2 (25%)
3	ACT	A	701	-	3,3,3	0.82	0	3,3,3	1.36	0
2	MC3	A	609	-	10,10,45	0.78	1 (10%)	11,11,53	0.86	1 (9%)
2	MC3	A	616	-	7,7,45	0.23	0	6,6,53	0.15	0
2	MC3	A	614	-	33,33,45	1.26	1 (3%)	36,38,53	1.48	5 (13%)
2	MC3	A	611	-	42,42,45	0.95	1 (2%)	48,50,53	0.97	4 (8%)

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	MC3	A	615	-	-	2/8/8/49	-
2	MC3	A	601	-	-	11/49/49/49	-
2	MC3	A	606	-	-	11/26/26/49	-
2	MC3	A	608	-	-	4/37/37/49	-
2	MC3	A	612	-	-	9/28/28/49	-
2	MC3	A	607	-	-	6/13/13/49	-
2	MC3	A	610	-	-	10/25/25/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	A	603	-	-	12/41/41/49	-
2	MC3	A	613	-	-	5/34/34/49	-
2	MC3	A	604	-	-	0/7/7/49	-
2	MC3	A	602	-	-	11/49/49/49	-
2	MC3	A	605	-	-	2/8/8/49	-
2	MC3	A	609	-	-	0/9/9/49	-
2	MC3	A	616	-	-	0/5/5/49	-
2	MC3	A	614	-	-	12/35/35/49	-
2	MC3	A	611	-	-	12/46/46/49	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	614	MC3	P-O4P	6.00	1.77	1.54
2	A	606	MC3	P-O4P	5.99	1.77	1.54
2	A	610	MC3	P-O4P	5.99	1.77	1.54
2	A	605	MC3	P-O4P	5.97	1.77	1.54
2	A	612	MC3	P-O4P	5.96	1.76	1.54
2	A	607	MC3	P-O4P	5.93	1.76	1.54
2	A	603	MC3	P-O4P	5.88	1.76	1.54
2	A	615	MC3	P-O4P	5.13	1.76	1.60
2	A	601	MC3	P-O4P	4.65	1.77	1.59
2	A	613	MC3	P-O4P	4.55	1.77	1.59
2	A	611	MC3	P-O4P	4.47	1.76	1.59
2	A	602	MC3	P-O4P	4.33	1.76	1.59
2	A	615	MC3	P-O3P	3.07	1.66	1.54
2	A	612	MC3	O3-C11	2.33	1.40	1.33
2	A	608	MC3	O3-C11	2.14	1.39	1.33
2	A	609	MC3	O2-C2	-2.13	1.42	1.47
2	A	612	MC3	O2-C2	-2.13	1.41	1.46
2	A	602	MC3	O4P-C4	-2.12	1.36	1.44
2	A	601	MC3	O2-C2	-2.09	1.41	1.46
2	A	603	MC3	P-O3P	2.04	1.66	1.60

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	610	MC3	C2-O2-C31	5.50	130.96	117.80
2	A	603	MC3	O2P-P-O1P	4.68	129.06	110.83
2	A	607	MC3	C2-O2-C31	4.67	126.10	117.85
2	A	605	MC3	O2P-P-O1P	4.62	128.85	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	614	MC3	O2P-P-O1P	4.59	128.71	110.83
2	A	606	MC3	O2P-P-O1P	4.59	128.71	110.83
2	A	610	MC3	O2P-P-O1P	4.58	128.68	110.83
2	A	607	MC3	O2P-P-O1P	4.56	128.59	110.83
2	A	612	MC3	O2P-P-O1P	4.54	128.52	110.83
2	A	615	MC3	O2P-P-O1P	4.50	128.36	110.83
2	A	615	MC3	O4P-P-O1P	-3.98	95.68	106.44
2	A	610	MC3	O4P-P-O1P	-3.91	95.61	110.83
2	A	607	MC3	O4P-P-O1P	-3.84	95.87	110.83
2	A	606	MC3	O4P-P-O1P	-3.84	95.89	110.83
2	A	605	MC3	O4P-P-O1P	-3.83	95.91	110.83
2	A	610	MC3	O2-C31-C32	3.70	119.48	111.48
2	A	614	MC3	O2-C31-C32	3.61	119.29	111.48
2	A	602	MC3	O2P-P-O1P	3.57	129.05	112.44
2	A	603	MC3	O4P-P-O2P	-3.47	94.80	107.80
2	A	601	MC3	O2P-P-O1P	3.47	128.57	112.44
2	A	611	MC3	O2P-P-O1P	3.46	128.53	112.44
2	A	612	MC3	C2-O2-C31	3.39	125.92	117.80
2	A	614	MC3	C2-O2-C31	3.38	125.89	117.80
2	A	613	MC3	O2P-P-O1P	3.34	127.97	112.44
2	A	610	MC3	O2-C31-O31	-3.33	115.91	123.70
2	A	612	MC3	O4P-P-O2P	-3.27	95.54	107.80
2	A	614	MC3	O4P-P-O2P	-3.23	95.68	107.80
2	A	607	MC3	O2-C31-C32	3.20	116.80	111.09
2	A	603	MC3	C2-O2-C31	3.15	125.35	117.80
2	A	611	MC3	O3-C11-O11	-3.04	116.02	123.63
2	A	612	MC3	O3-C11-C12	3.02	121.05	111.83
2	A	612	MC3	O3-C11-O11	-2.96	116.23	123.63
2	A	614	MC3	O2-C31-O31	-2.82	117.12	123.70
2	A	606	MC3	O3-C11-O11	-2.65	116.99	123.63
2	A	608	MC3	O3-C11-O11	-2.64	117.03	123.63
2	A	608	MC3	O3-C11-C12	2.56	119.63	111.83
2	A	602	MC3	O2P-P-O4P	-2.55	96.01	107.57
2	A	601	MC3	O2P-P-O4P	-2.54	96.07	107.57
2	A	613	MC3	O2P-P-O4P	-2.50	96.23	107.57
2	A	603	MC3	O2-C2-C1	2.37	116.85	108.34
2	A	611	MC3	O3-C11-C12	2.32	118.92	111.83
2	A	608	MC3	C3-O3-C11	2.32	125.61	117.12
2	A	612	MC3	C3-O3-C11	2.32	125.58	117.12
2	A	610	MC3	O3-C3-C2	2.31	115.07	108.40
2	A	607	MC3	O2-C31-O31	-2.27	118.61	122.99
2	A	610	MC3	O2-C2-C3	2.26	116.46	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	606	MC3	O3-C11-C12	2.22	118.62	111.83
2	A	612	MC3	O2-C2-C1	2.20	116.25	108.34
2	A	611	MC3	O2P-P-O4P	-2.20	97.61	107.57
2	A	602	MC3	O2-C2-C1	2.15	116.04	108.34
2	A	609	MC3	O2-C2-C1	2.02	112.52	107.13

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MC3	C1-O3P-P-O2P
2	A	602	MC3	C4-O4P-P-O1P
2	A	602	MC3	C4-O4P-P-O3P
2	A	605	MC3	C1-O3P-P-O2P
2	A	605	MC3	C1-O3P-P-O4P
2	A	606	MC3	C12-C11-O3-C3
2	A	606	MC3	O11-C11-O3-C3
2	A	606	MC3	C1-O3P-P-O2P
2	A	606	MC3	C1-O3P-P-O4P
2	A	608	MC3	C12-C11-O3-C3
2	A	608	MC3	O11-C11-O3-C3
2	A	610	MC3	C32-C31-O2-C2
2	A	610	MC3	O31-C31-O2-C2
2	A	610	MC3	C1-O3P-P-O2P
2	A	610	MC3	C1-O3P-P-O4P
2	A	611	MC3	C12-C11-O3-C3
2	A	611	MC3	O11-C11-O3-C3
2	A	612	MC3	C12-C11-O3-C3
2	A	612	MC3	O11-C11-O3-C3
2	A	612	MC3	C1-O3P-P-O1P
2	A	612	MC3	C1-O3P-P-O4P
2	A	614	MC3	C32-C31-O2-C2
2	A	614	MC3	O31-C31-O2-C2
2	A	607	MC3	C32-C31-O2-C2
2	A	607	MC3	O31-C31-O2-C2
2	A	608	MC3	C11-C12-C13-C14
2	A	611	MC3	C11-C12-C13-C14
2	A	614	MC3	C34-C35-C36-C37
2	A	601	MC3	C12-C13-C14-C15
2	A	613	MC3	C32-C33-C34-C35
2	A	612	MC3	C13-C14-C15-C16
2	A	602	MC3	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	A	603	MC3	C37-C38-C39-C40
2	A	606	MC3	C19-C20-C21-C22
2	A	602	MC3	C32-C33-C34-C35
2	A	601	MC3	C18-C19-C20-C21
2	A	614	MC3	C35-C36-C37-C38
2	A	603	MC3	C38-C39-C40-C41
2	A	603	MC3	C12-C13-C14-C15
2	A	606	MC3	O2-C2-C3-O3
2	A	612	MC3	C2-C1-O3P-P
2	A	611	MC3	C14-C15-C16-C17
2	A	611	MC3	C12-C13-C14-C15
2	A	607	MC3	O3P-C1-C2-C3
2	A	603	MC3	C33-C34-C35-C36
2	A	606	MC3	C1-C2-C3-O3
2	A	615	MC3	C4-O4P-P-O1P
2	A	603	MC3	C1-C2-O2-C31
2	A	610	MC3	C14-C15-C16-C17
2	A	610	MC3	C32-C33-C34-C35
2	A	614	MC3	C31-C32-C33-C34
2	A	613	MC3	C33-C34-C35-C36
2	A	606	MC3	C20-C21-C22-C23
2	A	606	MC3	C1-C2-O2-C31
2	A	606	MC3	C3-C2-O2-C31
2	A	603	MC3	C39-C40-C41-C42
2	A	602	MC3	C11-C12-C13-C14
2	A	614	MC3	C16-C17-C18-C19
2	A	601	MC3	C39-C40-C41-C42
2	A	613	MC3	C11-C12-C13-C14
2	A	602	MC3	C37-C38-C39-C40
2	A	603	MC3	C36-C37-C38-C39
2	A	614	MC3	O3-C11-C12-C13
2	A	607	MC3	O3P-C1-C2-O2
2	A	611	MC3	C1-C2-C3-O3
2	A	603	MC3	O2-C2-C3-O3
2	A	611	MC3	O2-C2-C3-O3
2	A	603	MC3	C15-C16-C17-C18
2	A	601	MC3	C34-C35-C36-C37
2	A	602	MC3	C15-C16-C17-C18
2	A	601	MC3	C36-C37-C38-C39
2	A	602	MC3	C4-O4P-P-O2P
2	A	601	MC3	C4-C5-N-C8
2	A	613	MC3	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	A	603	MC3	O3-C11-C12-C13
2	A	614	MC3	C12-C13-C14-C15
2	A	614	MC3	C33-C34-C35-C36
2	A	603	MC3	C13-C14-C15-C16
2	A	603	MC3	C34-C35-C36-C37
2	A	610	MC3	C1-C2-C3-O3
2	A	610	MC3	C3-C2-O2-C31
2	A	611	MC3	C13-C14-C15-C16
2	A	602	MC3	C39-C40-C41-C42
2	A	614	MC3	C32-C33-C34-C35
2	A	614	MC3	C15-C16-C17-C18
2	A	601	MC3	C4-C5-N-C7
2	A	613	MC3	O2-C31-C32-C33
2	A	611	MC3	C34-C35-C36-C37
2	A	610	MC3	C1-O3P-P-O1P
2	A	612	MC3	C1-O3P-P-O2P
2	A	615	MC3	C4-O4P-P-O3P
2	A	610	MC3	C31-C32-C33-C34
2	A	612	MC3	C1-C2-O2-C31
2	A	611	MC3	C15-C16-C17-C18
2	A	611	MC3	C39-C40-C41-C42
2	A	602	MC3	C5-C4-O4P-P
2	A	601	MC3	C4-C5-N-C6
2	A	607	MC3	C2-C3-O3-C11
2	A	601	MC3	O3-C11-C12-C13
2	A	611	MC3	C18-C19-C20-C21
2	A	614	MC3	O11-C11-C12-C13
2	A	607	MC3	C1-C2-O2-C31
2	A	602	MC3	C31-C32-C33-C34
2	A	606	MC3	C12-C13-C14-C15
2	A	601	MC3	O11-C11-C12-C13
2	A	612	MC3	O3-C11-C12-C13
2	A	608	MC3	O3-C11-C12-C13

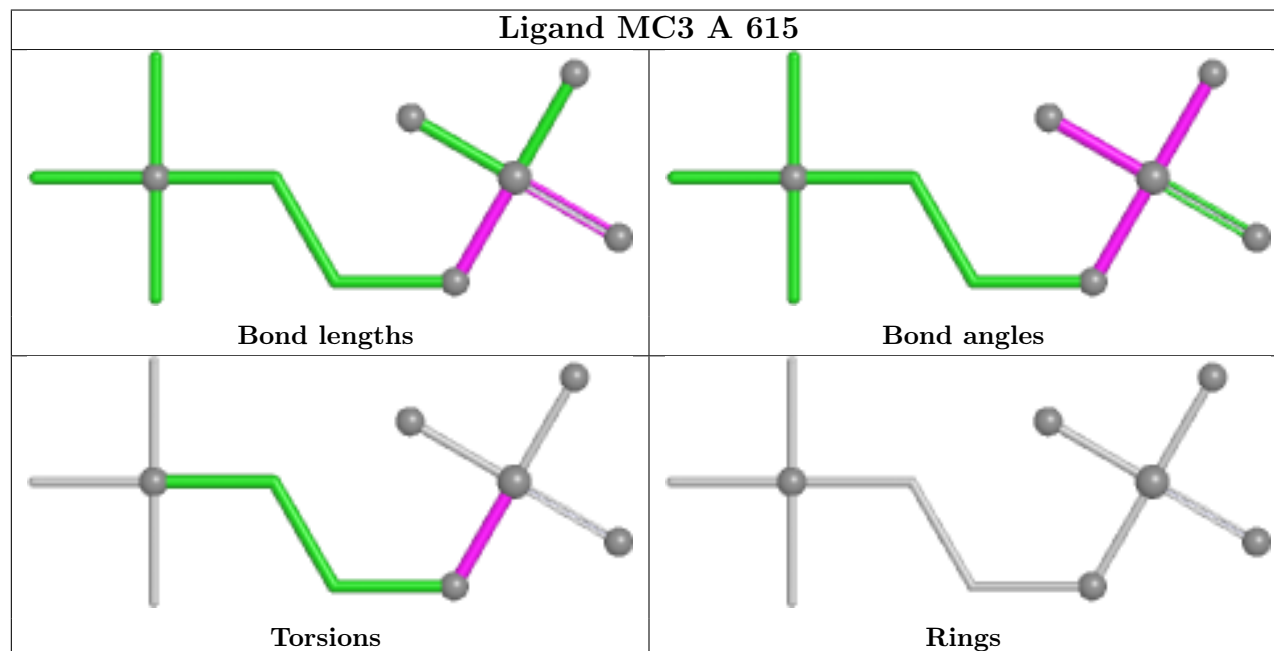
There are no ring outliers.

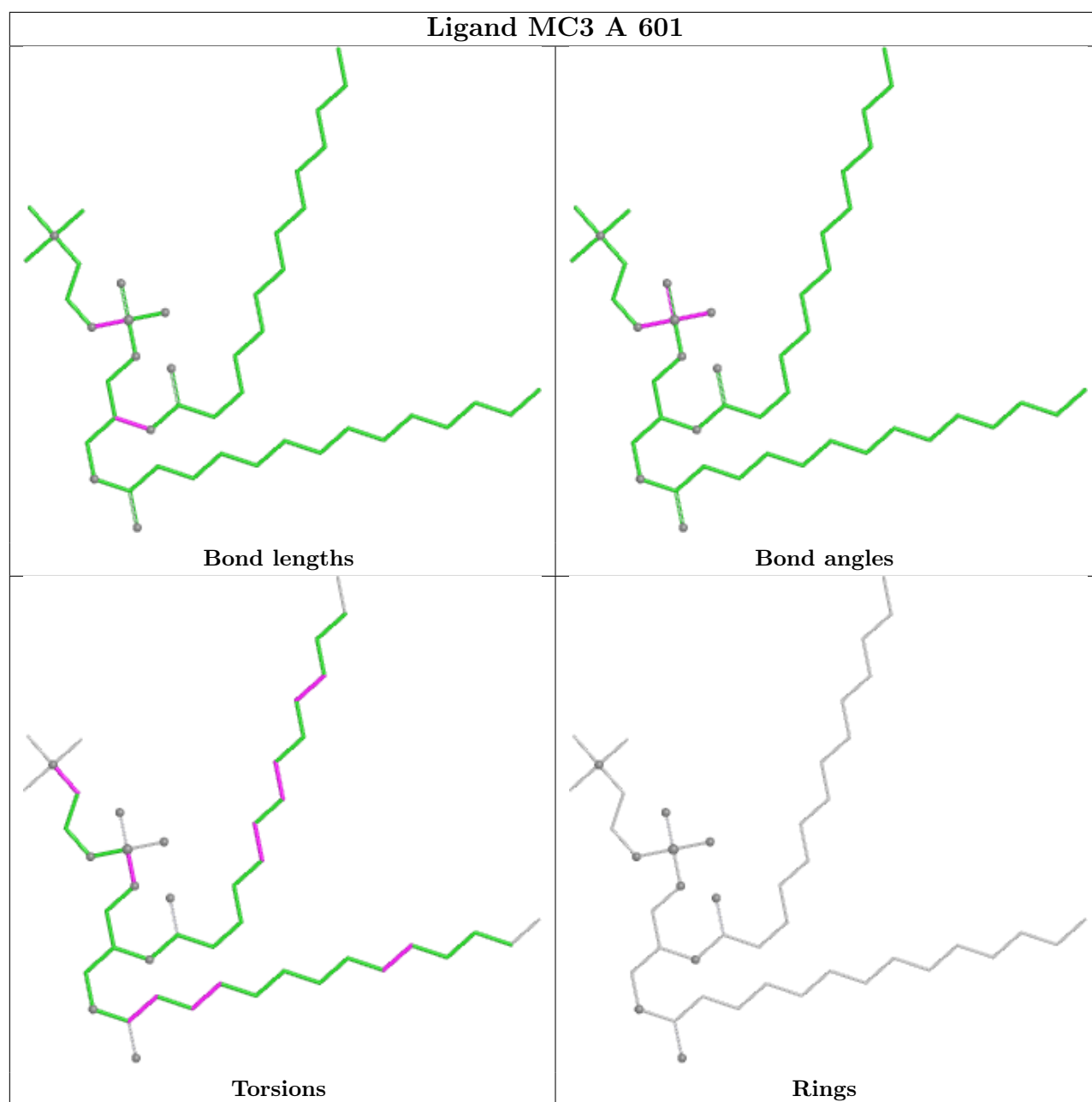
1 monomer is involved in 1 short contact:

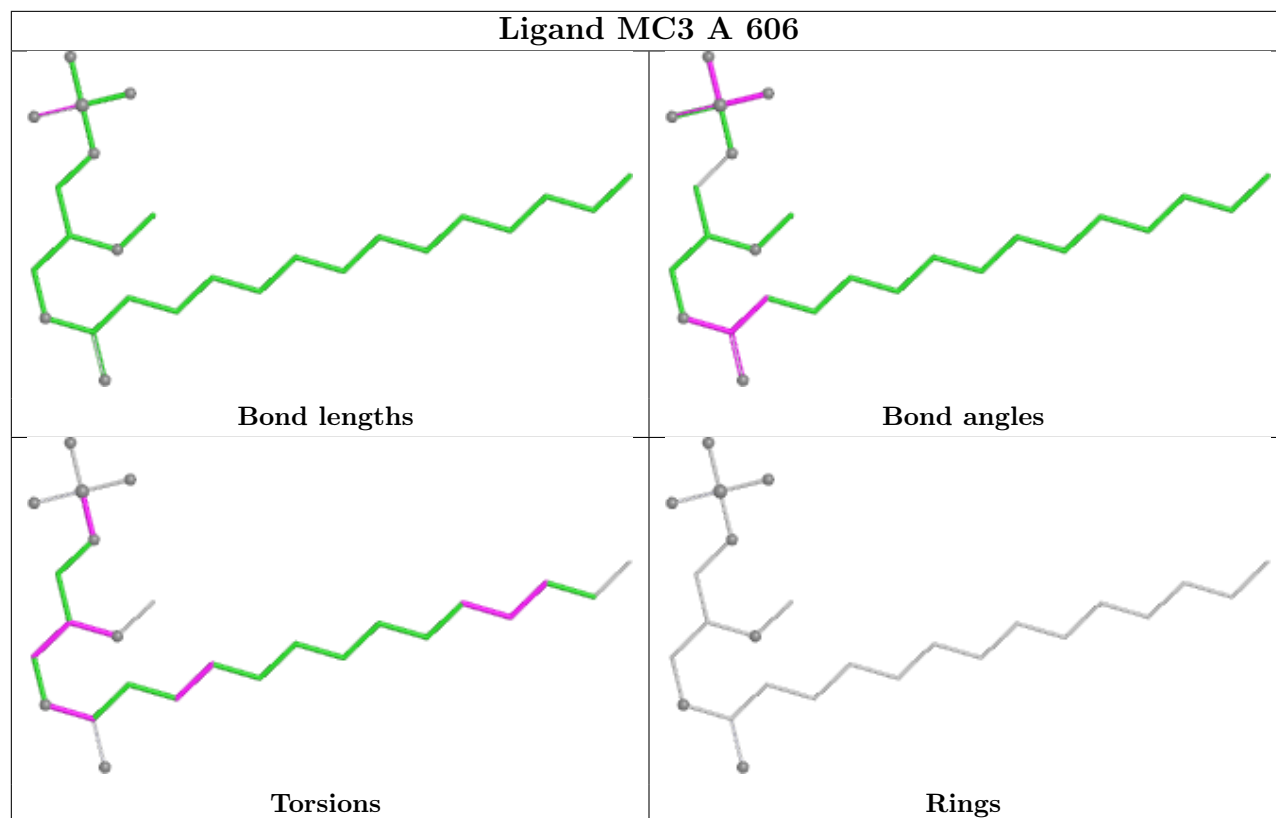
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	615	MC3	1	0

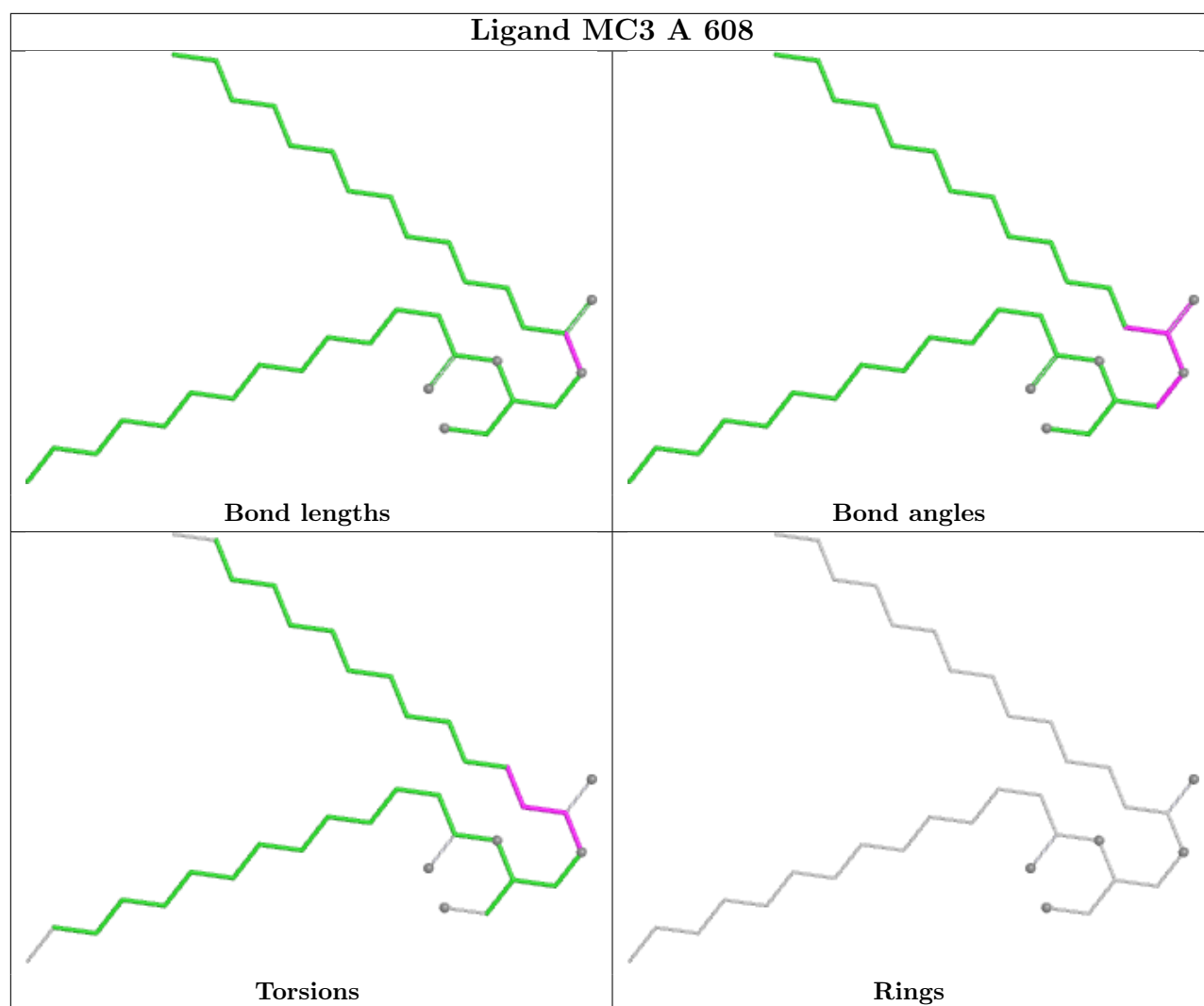
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

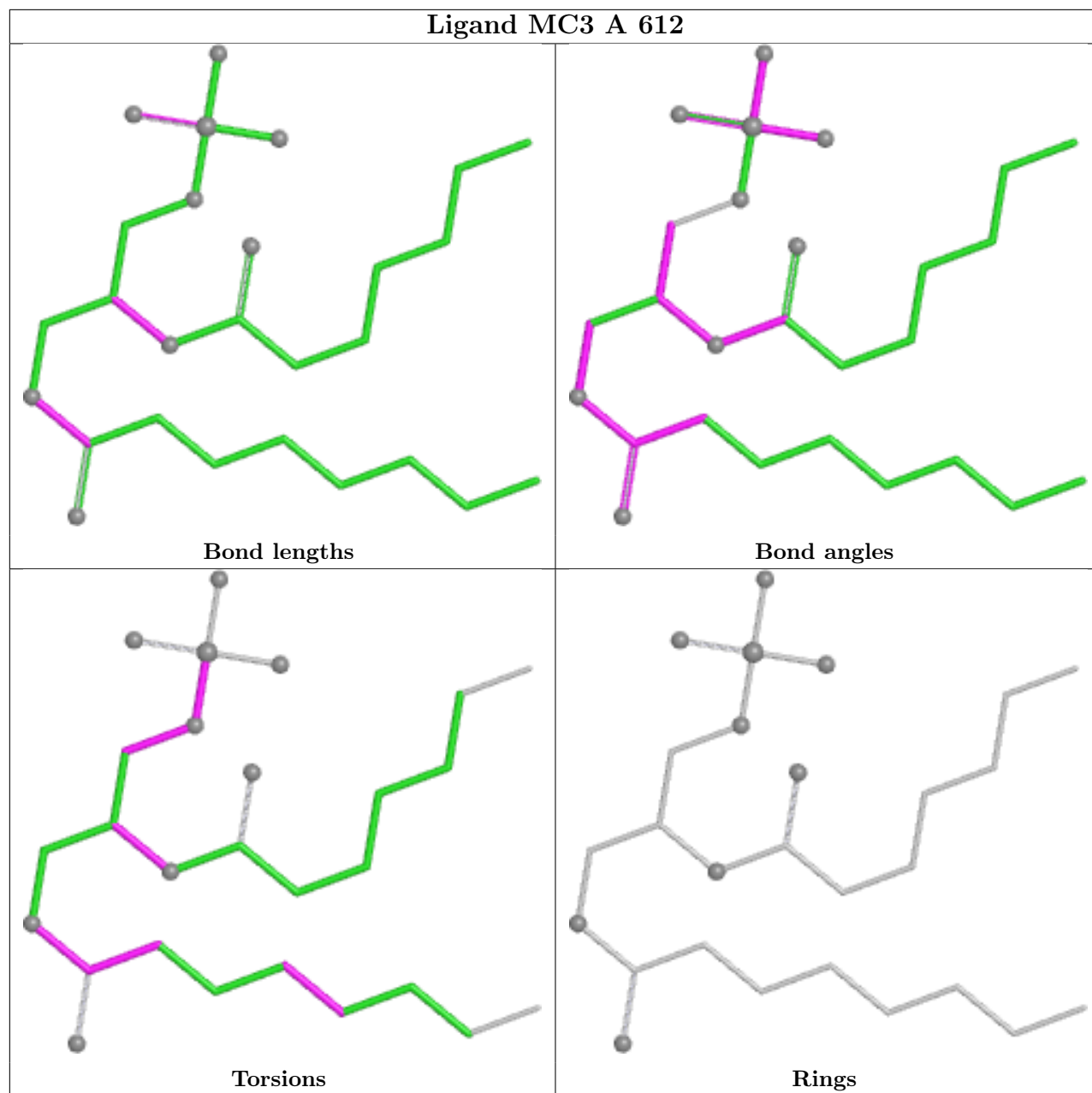
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

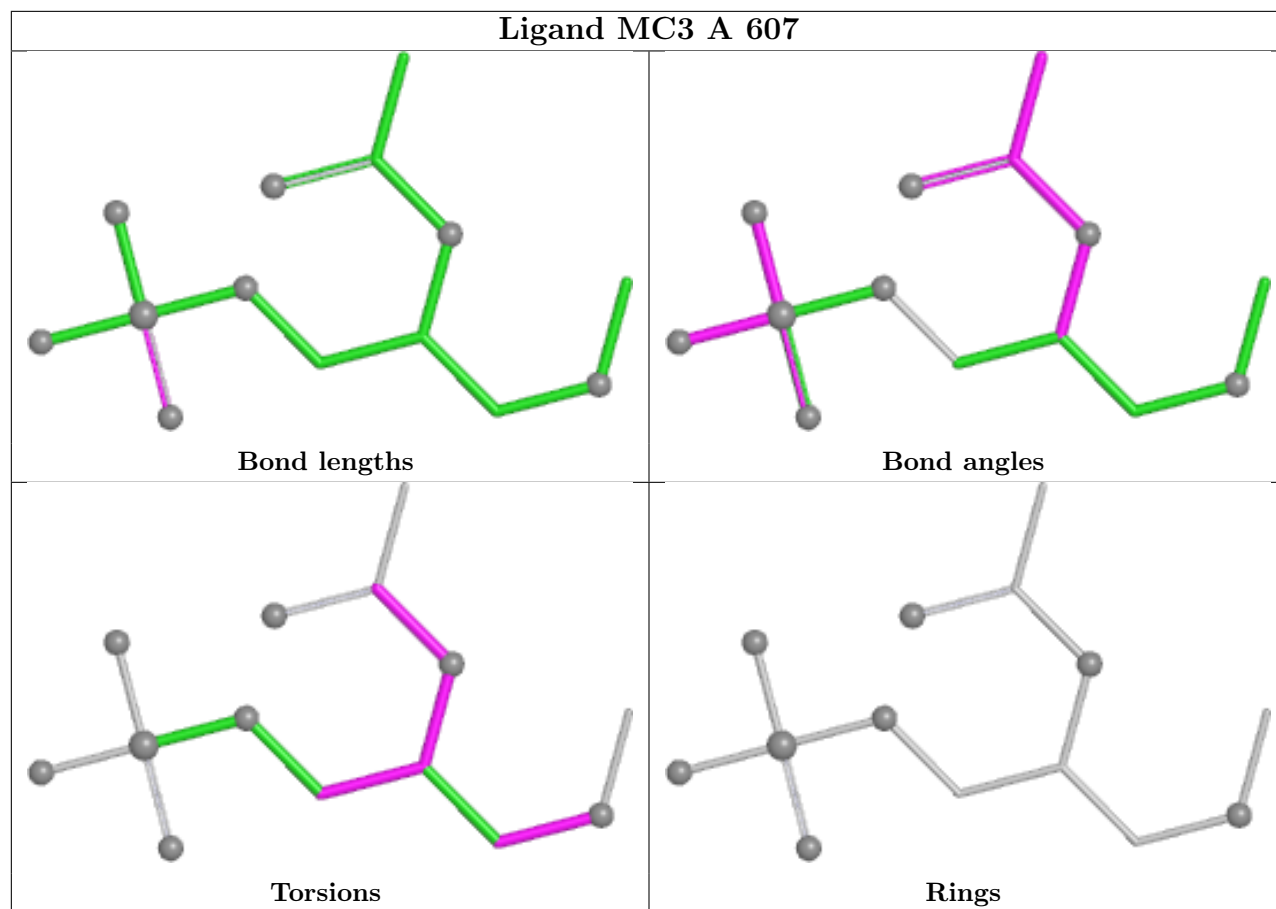


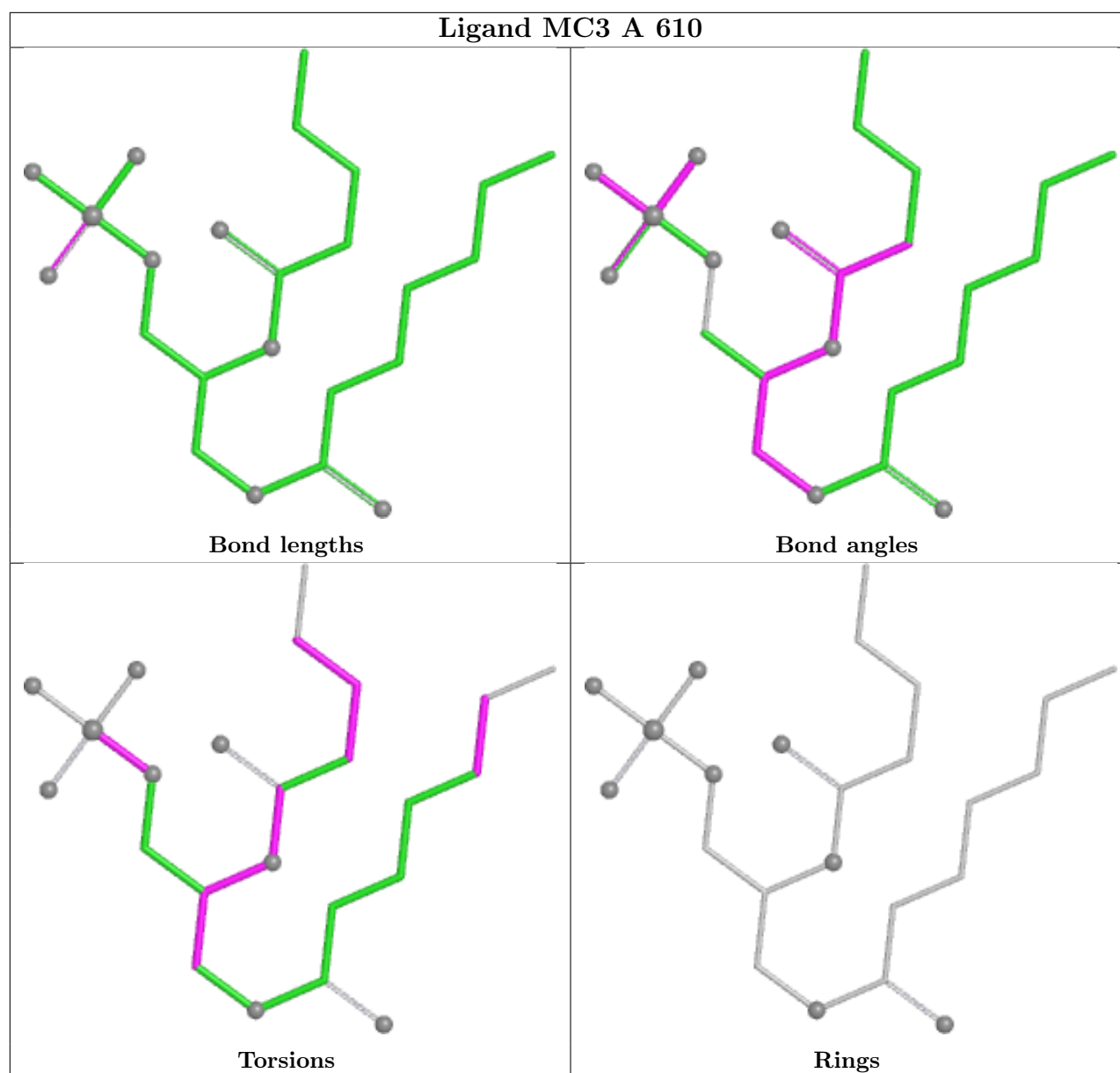


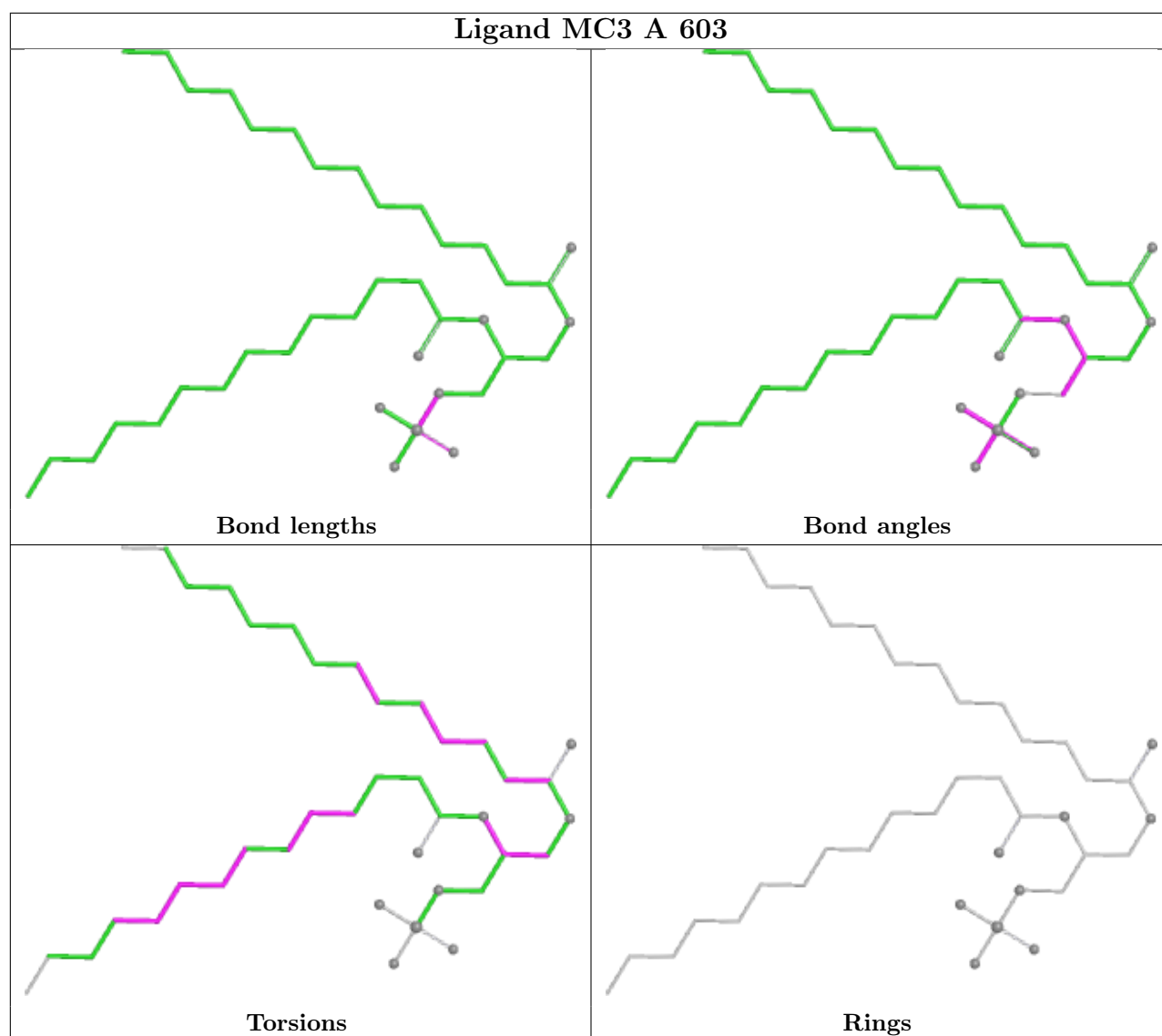


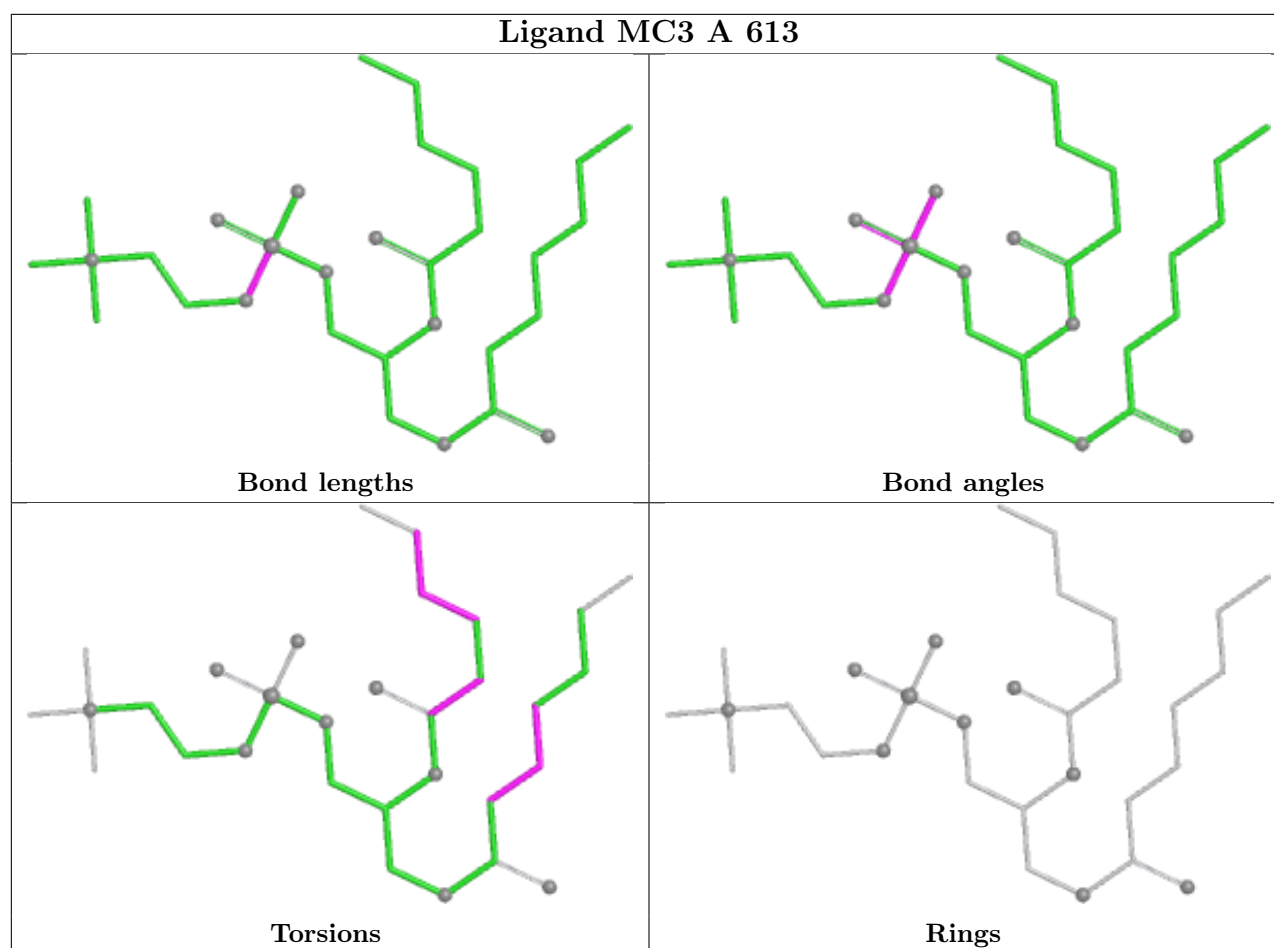


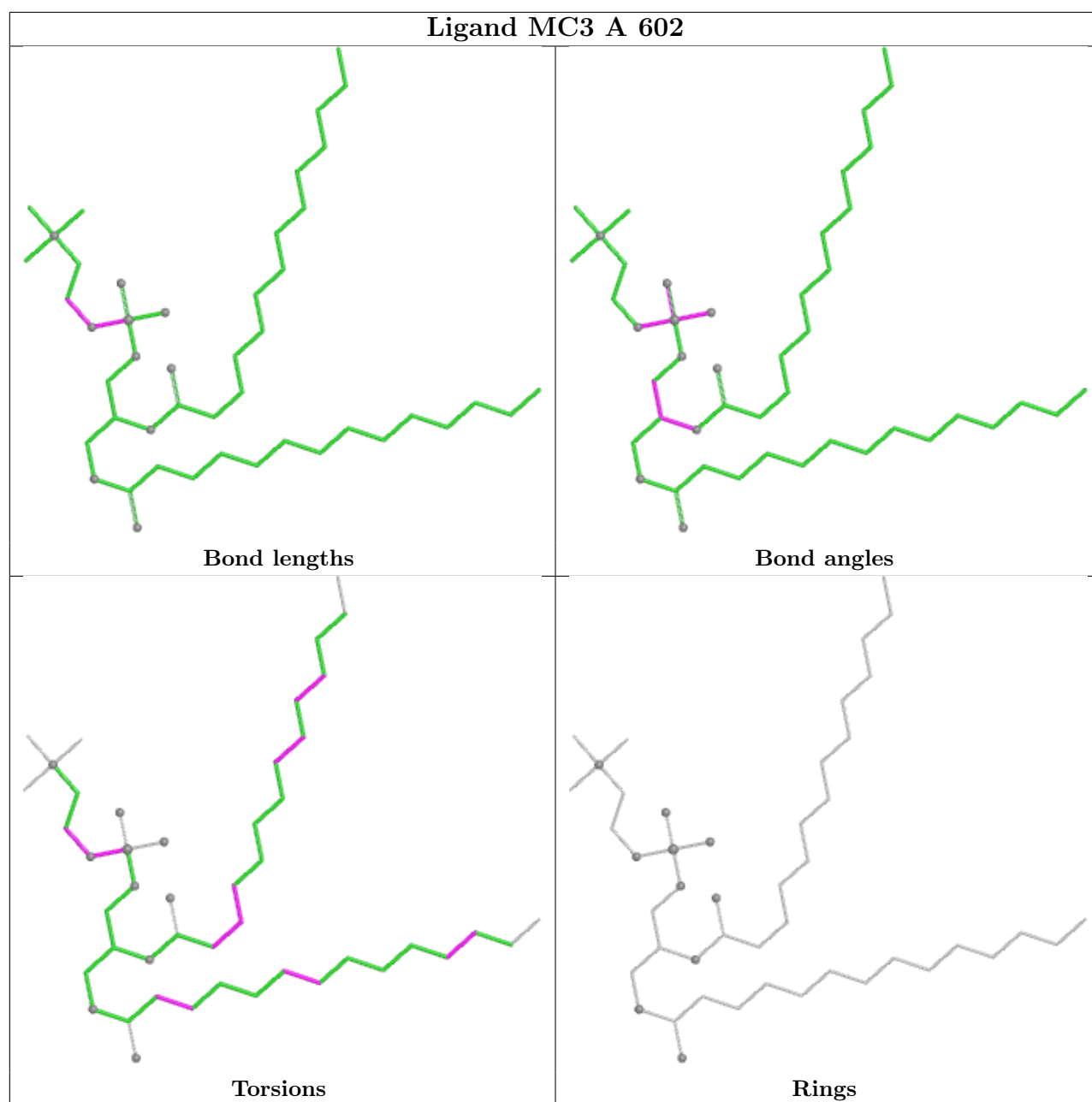


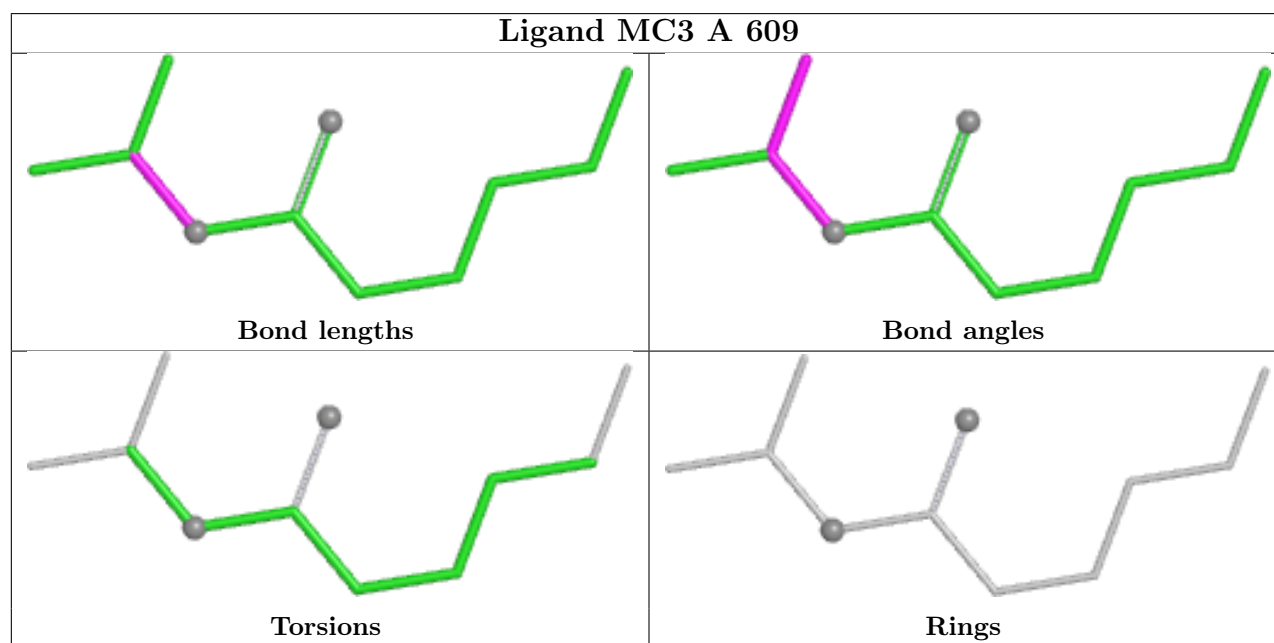
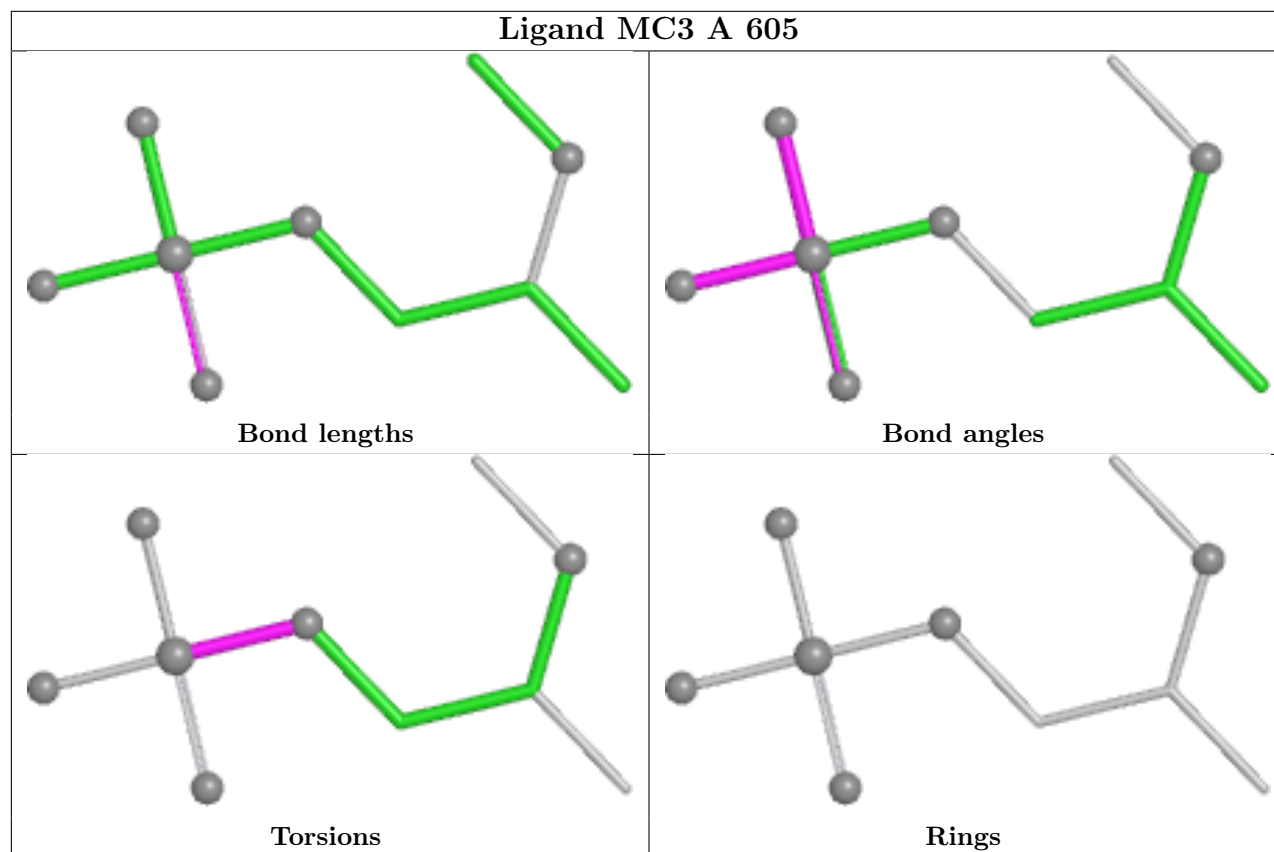


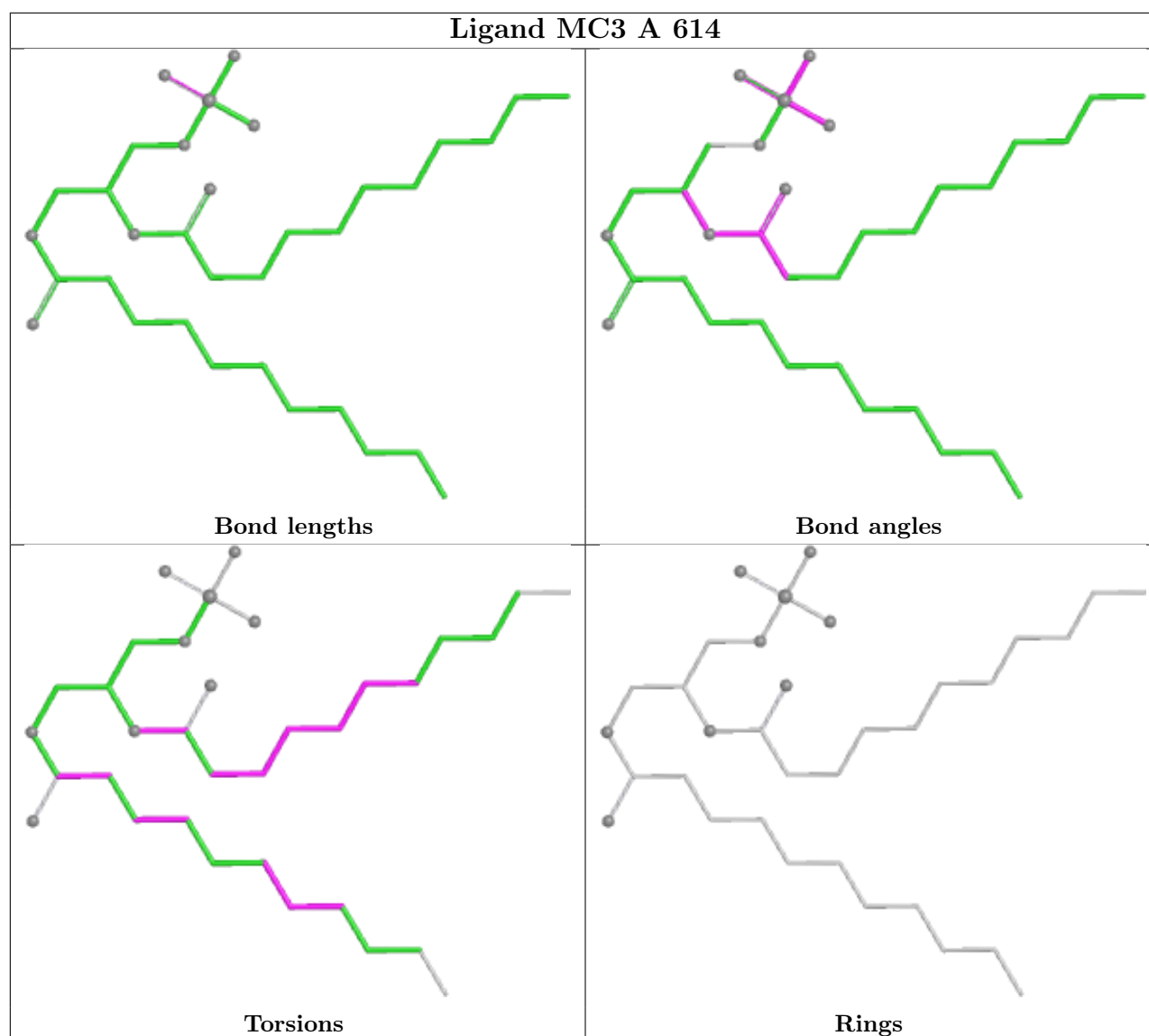


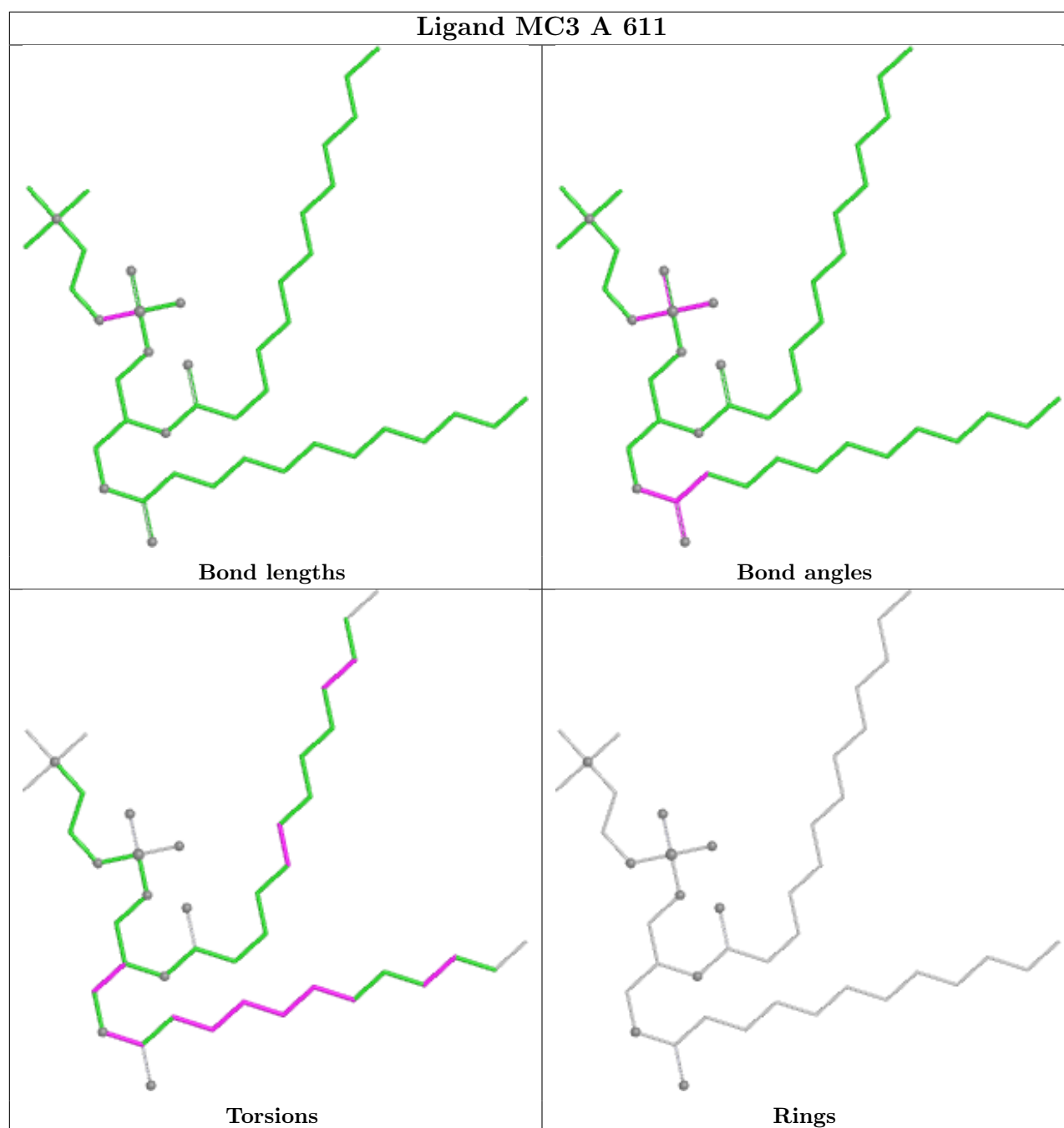












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	544/559 (97%)	0.76	78 (14%) 6 5	20, 61, 212, 263	5 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	LEU	9.5
1	A	575	PRO	8.1
1	A	93	VAL	7.8
1	A	548	VAL	6.9
1	A	57	PHE	6.1
1	A	26	LEU	5.8
1	A	574	GLY	5.4
1	A	95	ILE	5.2
1	A	576	GLU	5.1
1	A	43	LEU	5.0
1	A	573	LEU	4.6
1	A	28	VAL	4.4
1	A	94	LEU	4.3
1	A	39	VAL	4.3
1	A	46	ILE	4.3
1	A	51	VAL	4.3
1	A	65	ILE	4.2
1	A	53	PRO	4.2
1	A	565	HIS	4.1
1	A	61	VAL	3.9
1	A	401	LEU	3.8
1	A	98	VAL	3.7
1	A	44	SER	3.6
1	A	41	ALA	3.6
1	A	96	ALA	3.6
1	A	577	LEU	3.5
1	A	30	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	25	ARG	3.3
1	A	82	ASP	3.2
1	A	49	ASP	3.2
1	A	247	LYS	3.1
1	A	35	LEU	3.1
1	A	27	GLN	3.0
1	A	75	TYR	3.0
1	A	52	THR	3.0
1	A	74	TYR	3.0
1	A	97	LYS	2.9
1	A	547	PRO	2.8
1	A	139	GLN	2.8
1	A	72	LEU	2.8
1	A	71	ALA	2.8
1	A	552[A]	LYS	2.8
1	A	64	ALA	2.7
1	A	268	ILE	2.7
1	A	474	ARG	2.6
1	A	286	TRP	2.6
1	A	397	SER	2.6
1	A	99	THR	2.6
1	A	100	PRO	2.6
1	A	48	SER	2.6
1	A	189	TYR	2.6
1	A	76	GLN	2.5
1	A	29	GLU	2.5
1	A	81	PHE	2.5
1	A	138	ASN	2.5
1	A	163	PHE	2.4
1	A	321	LYS	2.4
1	A	546	SER	2.4
1	A	248	ALA	2.4
1	A	102	VAL	2.3
1	A	79	ILE	2.3
1	A	73	GLY	2.3
1	A	249	ARG	2.3
1	A	118	ARG	2.2
1	A	179	TRP	2.2
1	A	175	HIS	2.2
1	A	147	LYS	2.2
1	A	399	GLY	2.2
1	A	250	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	154	LEU	2.2
1	A	172	LEU	2.2
1	A	281	ARG	2.2
1	A	60	ARG	2.1
1	A	159	PHE	2.1
1	A	42	GLN	2.1
1	A	103	PRO	2.1
1	A	34	GLN	2.0
1	A	504	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

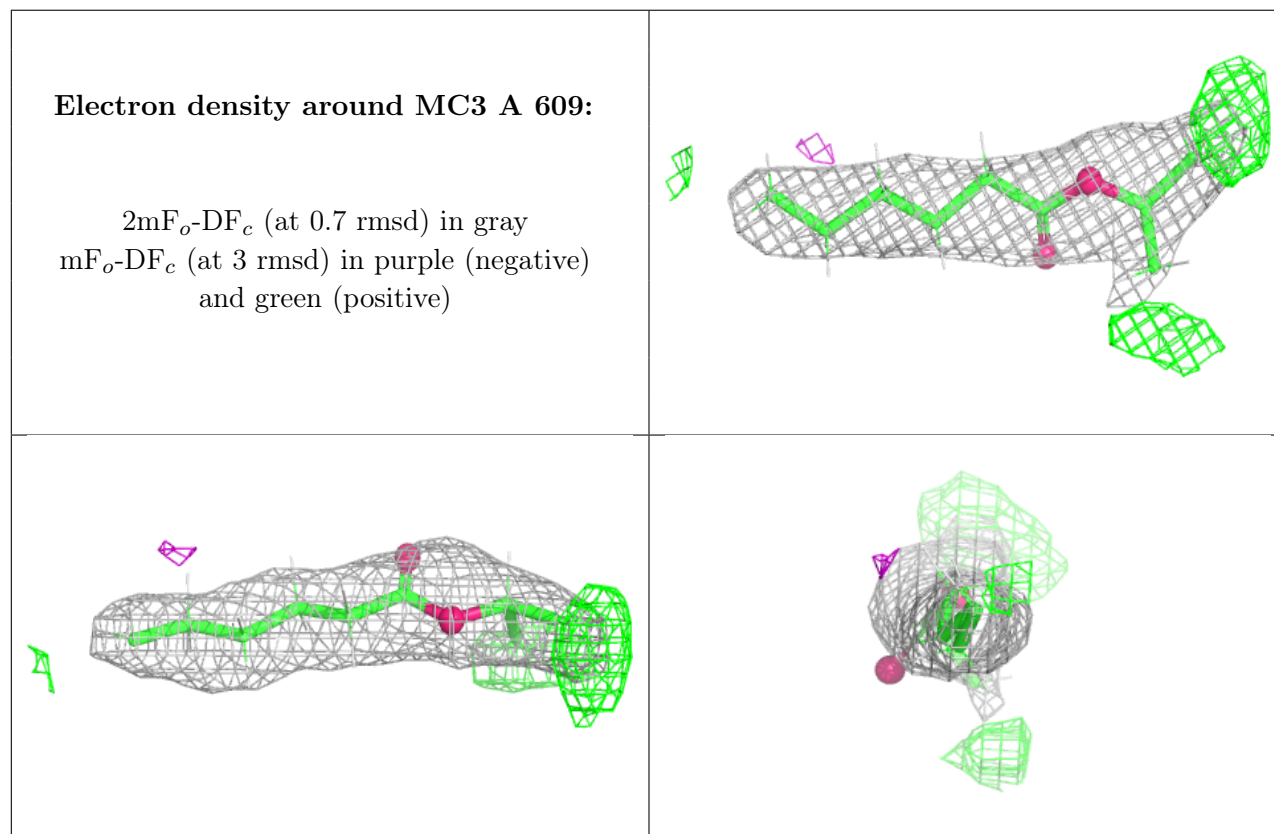
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MC3	A	609	11/46	0.69	0.31	51,92,120,129	0
2	MC3	A	605	10/46	0.70	0.23	91,130,154,154	0
2	MC3	A	607	14/46	0.72	0.25	83,121,140,210	0
2	MC3	A	612	27/46	0.73	0.27	52,102,144,355	0
2	MC3	A	614	34/46	0.74	0.33	71,104,157,508	0
2	MC3	A	610	24/46	0.75	0.22	64,112,141,148	0
2	MC3	A	616	8/46	0.78	0.30	62,80,99,99	0
2	MC3	A	606	26/46	0.79	0.20	48,80,119,129	0
2	MC3	A	603	40/46	0.80	0.28	41,71,124,507	0
2	MC3	A	604	10/46	0.82	0.25	50,73,98,100	0
2	MC3	A	608	36/46	0.84	0.22	60,85,140,168	0
2	MC3	A	602	46/46	0.84	0.21	55,84,141,144	0
3	ACT	A	702	4/4	0.86	0.17	49,59,62,67	0
2	MC3	A	615	11/46	0.88	0.20	58,94,123,123	0

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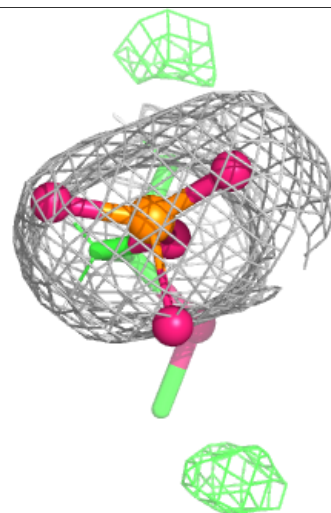
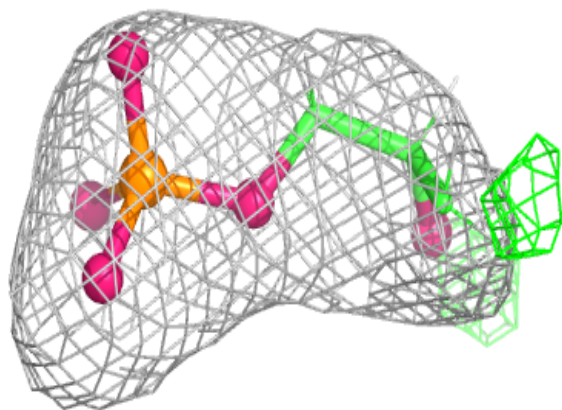
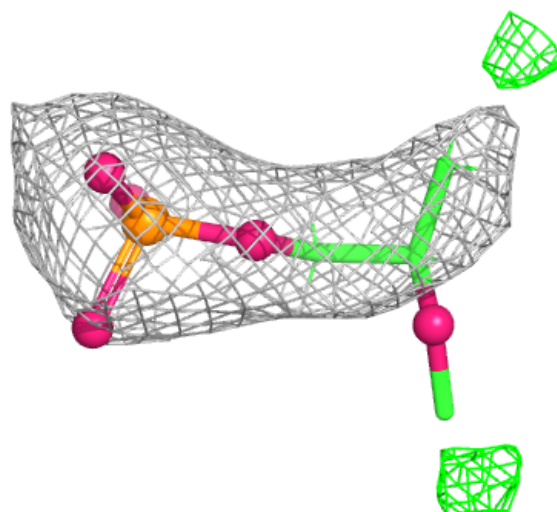
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MC3	A	611	43/46	0.92	0.16	40,74,130,141	0
2	MC3	A	601	46/46	0.92	0.16	44,69,102,106	0
4	CL	A	801	1/1	0.92	0.22	93,93,93,93	0
4	CL	A	803	1/1	0.94	0.15	86,86,86,86	0
3	ACT	A	701	4/4	0.95	0.10	54,56,65,65	0
2	MC3	A	613	31/46	0.95	0.15	44,74,102,115	0
4	CL	A	802	1/1	0.98	0.06	51,51,51,51	0

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



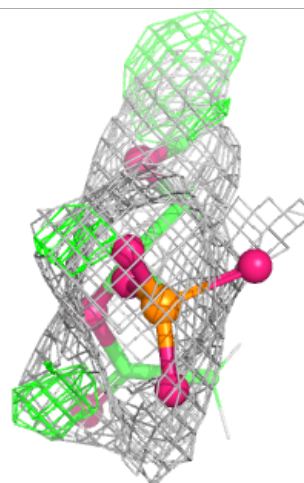
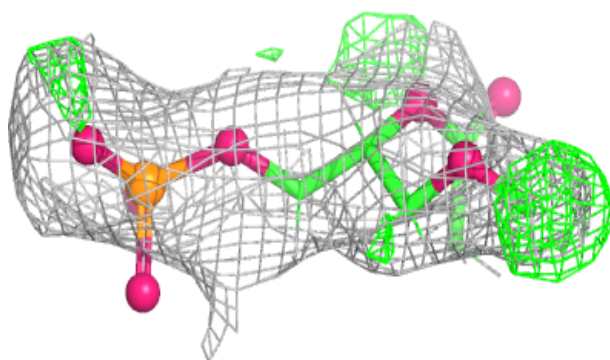
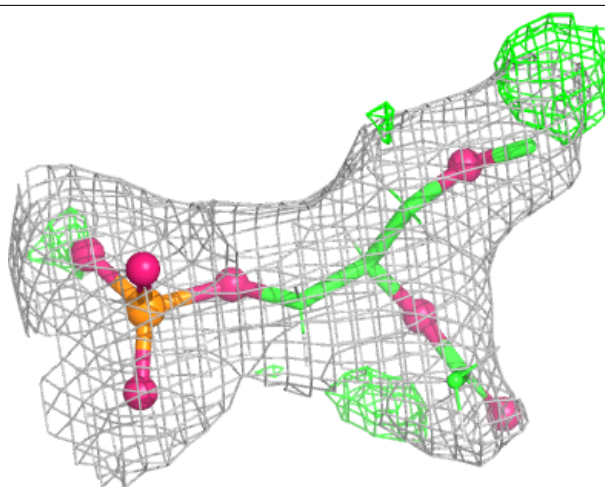
Electron density around MC3 A 605:

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



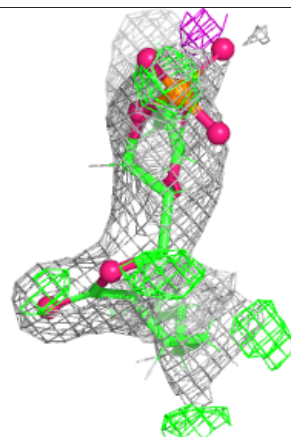
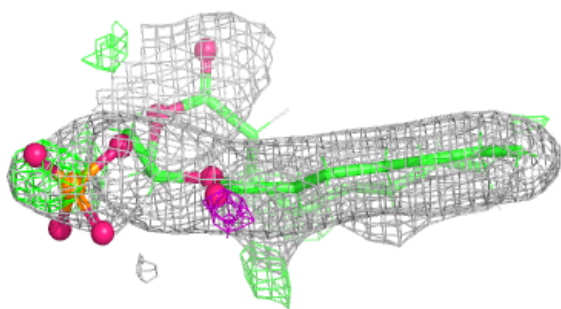
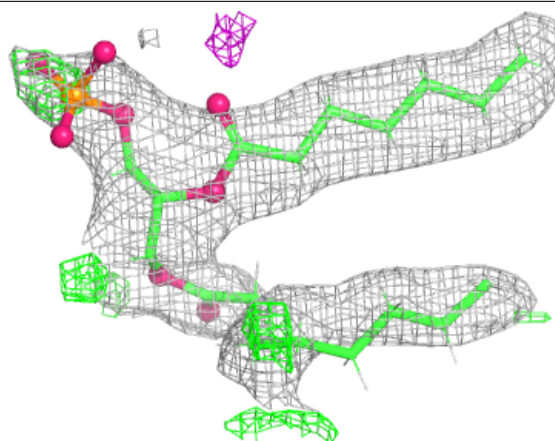
Electron density around MC3 A 607:

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



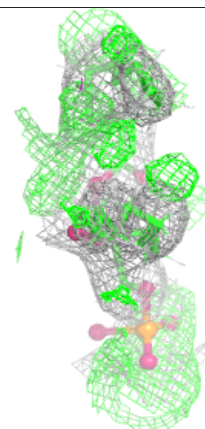
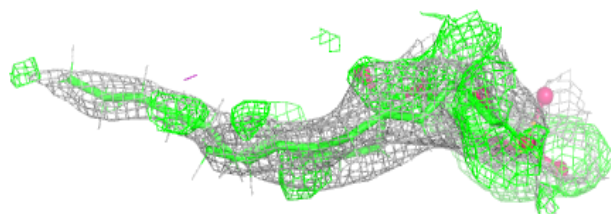
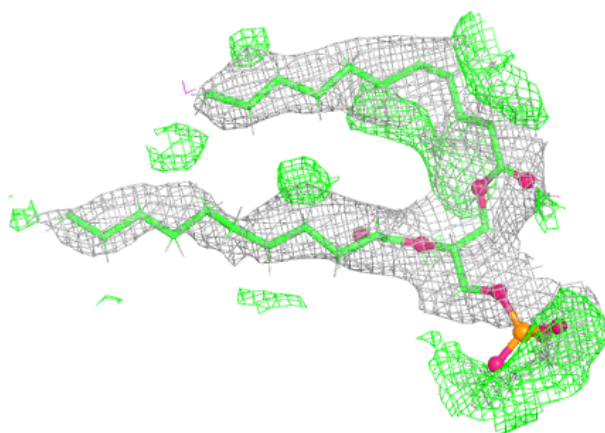
Electron density around MC3 A 612:

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



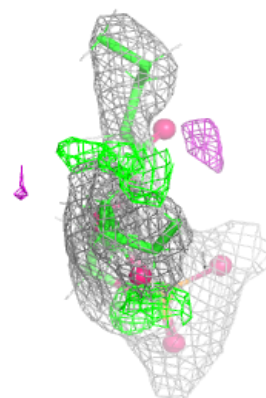
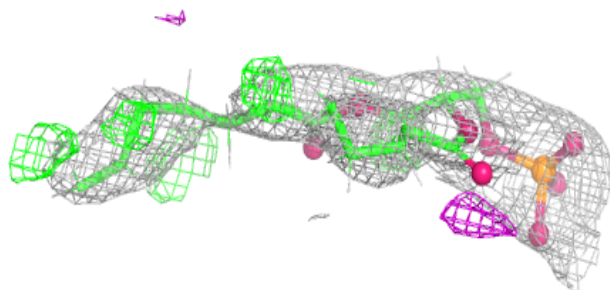
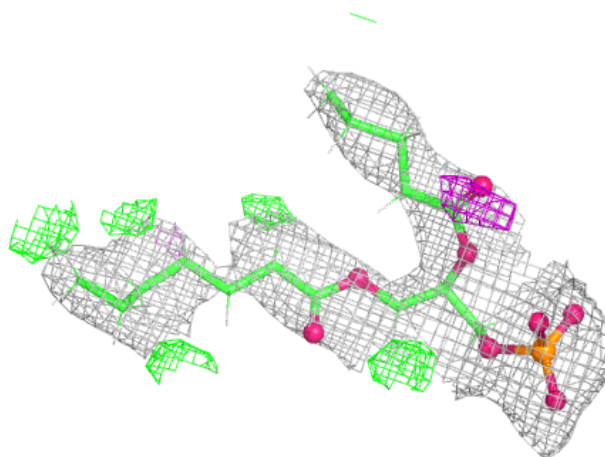
Electron density around MC3 A 614:

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



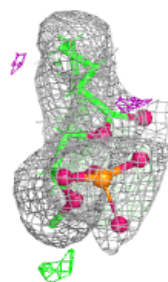
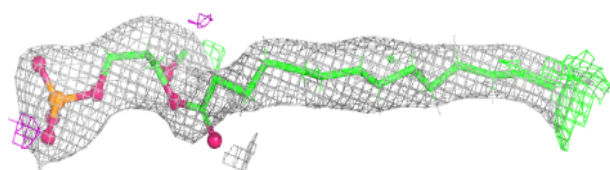
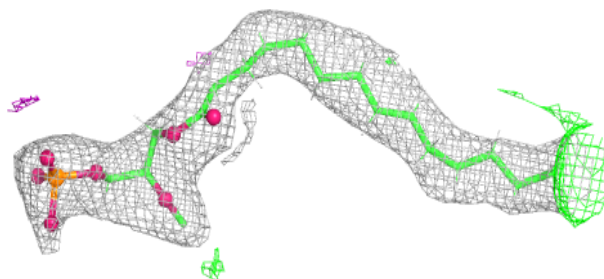
Electron density around MC3 A 610:

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

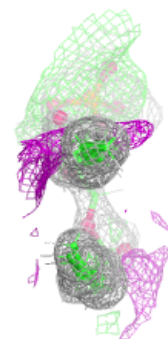
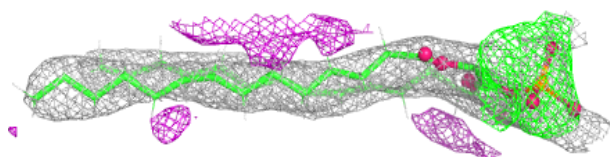
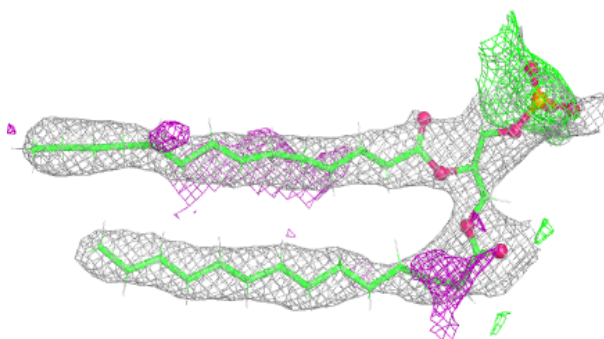


Electron density around MC3 A 606:

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

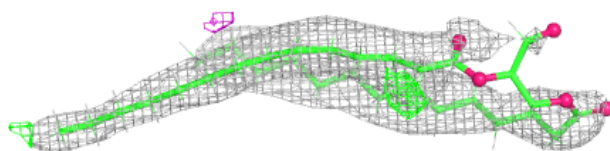
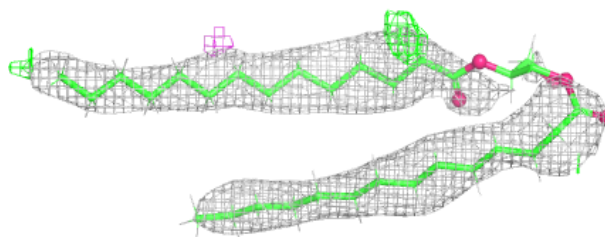
**Electron density around MC3 A 603:**

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

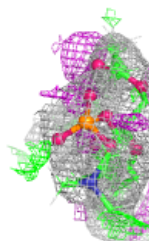
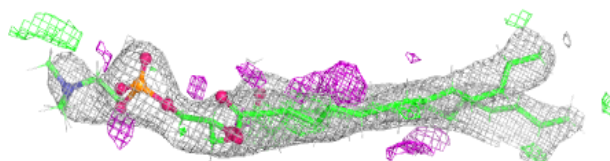
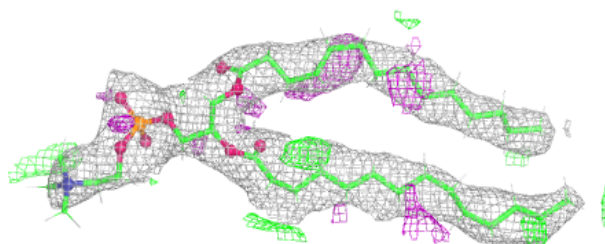


Electron density around MC3 A 608:

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

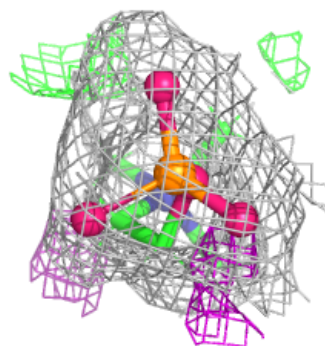
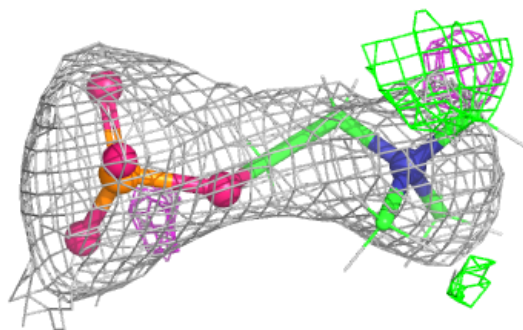
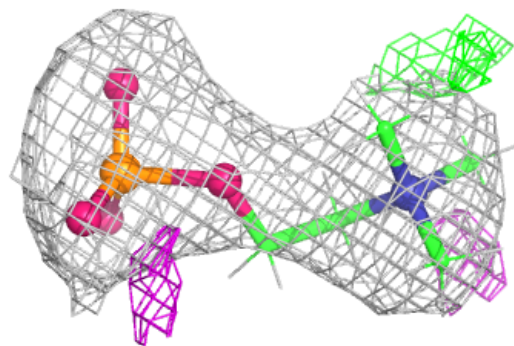
**Electron density around MC3 A 602:**

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

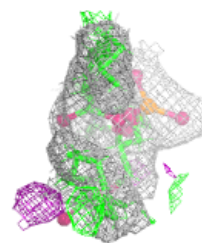
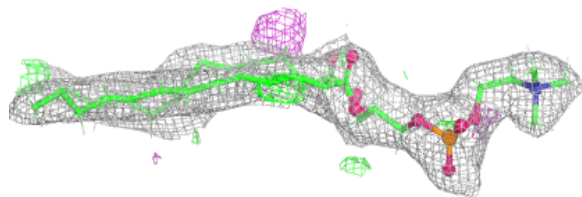
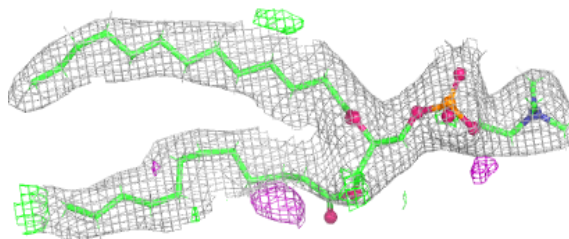


Electron density around MC3 A 615:

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

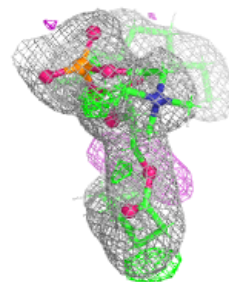
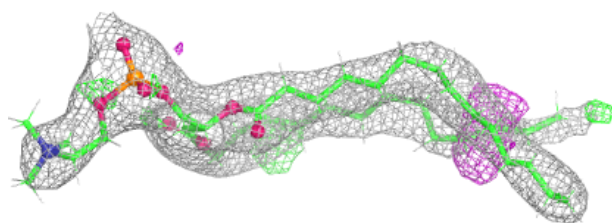
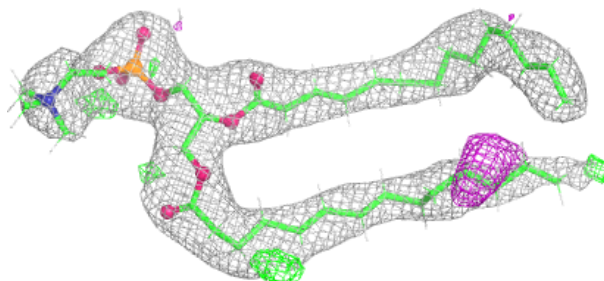
**Electron density around MC3 A 611:**

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

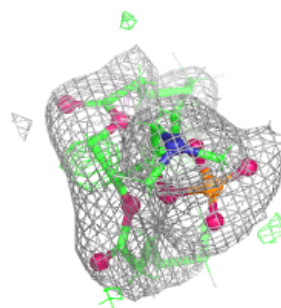
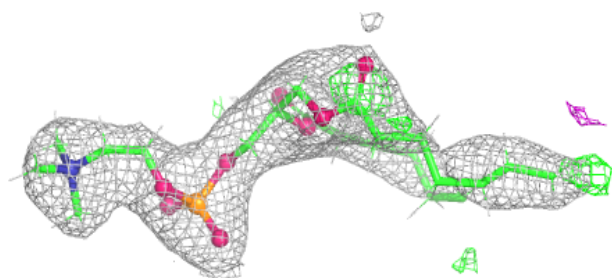
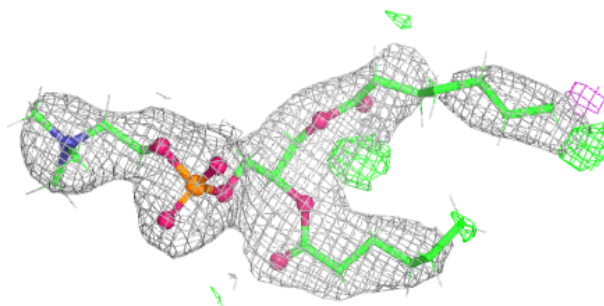


Electron density around MC3 A 601:

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

**Electron density around MC3 A 613:**

$2mF_o-DF_c$ (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.