



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:44 PM EDT

PDB ID : 2XTV  
Title : Structure of E.coli rhomboid protease GlpG, active site mutant, S201T, orthorhombic crystal form  
Authors : Vinothkumar, K.R.  
Deposited on : 2010-10-12  
Resolution : 1.70 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

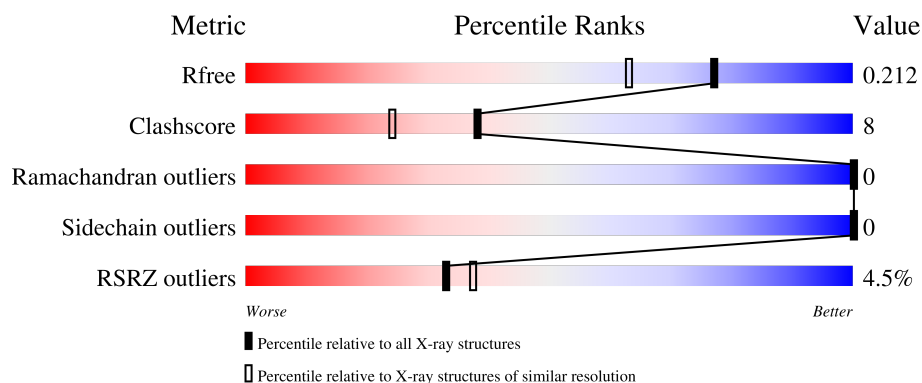
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	180	

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	MC3	A	504	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

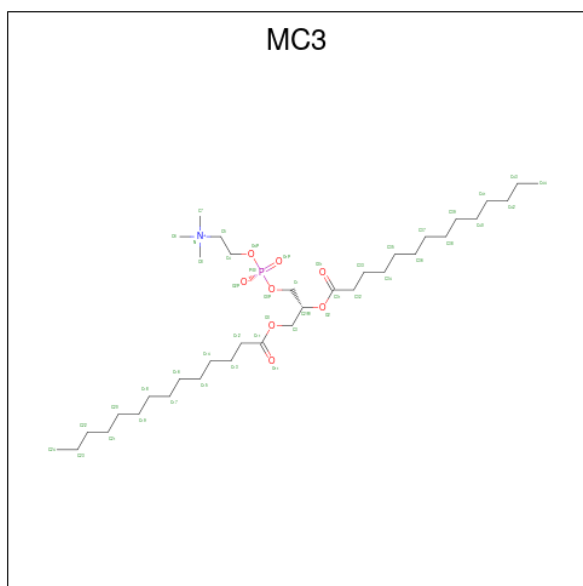
- Molecule 1 is a protein called RHOMBOID PROTEASE GLPG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	1	0
			1413	955	223	226	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	THR	SER	engineered mutation	UNP P09391

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula:  $C_{36}H_{72}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			34	24	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			46	36	1	8	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 40 31 8 1	0	0
2	A	1	Total C O 18 14 4	0	0
2	A	1	Total C O 27 22 5	0	0
2	A	1	Total C O 16 15 1	0	0
2	A	1	Total C O 17 14 3	0	0
2	A	1	Total C O 16 13 3	0	0
2	A	1	Total C O 20 17 3	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 15 14 1	0	0

- Molecule 3 is water.

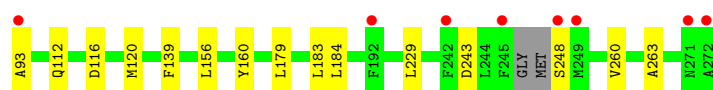
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	79	Total O 79 79	0	0

### 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: RHOMBOID PROTEASE GLPG

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.63Å 58.87Å 91.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.01 – 1.70 28.01 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (28.01-1.70) 95.0 (28.01-1.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.186 , 0.215 0.180 , 0.212	Depositor DCC
$R_{free}$ test set	1148 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 70.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.33	0/1464	0.47	0/1996

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

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	1413	0	1401	17	0
2	A	296	0	438	21	0
3	A	79	0	0	1	0
All	All	1788	0	1839	27	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 8.

All (27) 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:156:LEU:HD23	2:A:503:MC3:H171	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:HB2	2:A:502:MC3:H131	1.75	0.67
1:A:184:LEU:HD21	2:A:504:MC3:H332	1.83	0.60
1:A:156:LEU:CD2	2:A:503:MC3:H171	2.28	0.60
2:A:503:MC3:H243	2:A:511:MC3:H191	1.88	0.54
1:A:116:ASP:O	1:A:120:MET:HG3	2.08	0.54
1:A:93:ALA:HA	3:A:2029:HOH:O	2.07	0.53
2:A:502:MC3:O31	2:A:502:MC3:H12	2.08	0.53
1:A:179:LEU:HD11	2:A:509:MC3:H162	1.92	0.52
1:A:263:ALA:HA	2:A:501:MC3:H161	1.93	0.51
1:A:160:TYR:CZ	1:A:229:LEU:HD13	2.47	0.50
2:A:502:MC3:C31	2:A:502:MC3:O3	2.60	0.49
1:A:183:LEU:HD11	2:A:507:MC3:H342	1.94	0.49
2:A:505:MC3:H201	2:A:507:MC3:C41	2.43	0.48
1:A:243:ASP:OD1	1:A:248:SER:HA	2.15	0.47
1:A:139:PHE:CB	2:A:509:MC3:H222	2.45	0.47
1:A:112:GLN:HG3	2:A:511:MC3:H131	1.96	0.46
1:A:260:VAL:HA	2:A:504:MC3:H372	1.98	0.45
2:A:505:MC3:O31	2:A:505:MC3:H31	2.16	0.45
2:A:503:MC3:O31	2:A:503:MC3:C3	2.65	0.44
1:A:160:TYR:CE2	1:A:229:LEU:HD13	2.53	0.43
2:A:508:MC3:H321	2:A:508:MC3:H352	1.65	0.43
1:A:160:TYR:CZ	1:A:229:LEU:CD1	3.02	0.42
1:A:160:TYR:CD1	2:A:502:MC3:O11	2.73	0.42
2:A:501:MC3:H42	2:A:501:MC3:H62	1.77	0.42
2:A:502:MC3:H62	2:A:502:MC3:H42	1.85	0.40
2:A:503:MC3:H162	2:A:503:MC3:H191	1.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	175/180 (97%)	173 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	140/143 (98%)	140 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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	510	-	8,8,45	0.26	0	7,7,53	0.56	0
2	MC3	A	504	-	17,17,45	1.12	1 (5%)	18,18,53	1.52	2 (11%)
2	MC3	A	502	-	45,45,45	0.99	2 (4%)	51,53,53	1.05	3 (5%)
2	MC3	A	505	-	26,26,45	1.26	2 (7%)	28,28,53	1.23	3 (10%)
2	MC3	A	507	-	16,16,45	1.15	1 (6%)	16,16,53	1.07	1 (6%)
2	MC3	A	509	-	19,19,45	1.05	1 (5%)	20,20,53	0.94	1 (5%)
2	MC3	A	513	-	7,7,45	0.28	0	6,6,53	0.52	0
2	MC3	A	514	-	14,14,45	1.05	1 (7%)	13,13,53	0.72	0
2	MC3	A	512	-	15,15,45	1.21	1 (6%)	15,15,53	0.97	1 (6%)
2	MC3	A	501	-	33,33,45	1.18	3 (9%)	39,41,53	1.09	4 (10%)
2	MC3	A	506	-	15,15,45	0.32	0	14,14,53	0.92	1 (7%)
2	MC3	A	511	-	13,13,45	0.23	0	12,12,53	0.59	0
2	MC3	A	503	-	39,39,45	1.09	2 (5%)	42,44,53	1.31	4 (9%)
2	MC3	A	508	-	15,15,45	1.14	1 (6%)	15,15,53	1.09	1 (6%)

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	510	-	-	1/6/6/49	-
2	MC3	A	504	-	1/1/2/5	0/18/18/49	-
2	MC3	A	502	-	-	19/49/49/49	-
2	MC3	A	505	-	-	9/28/28/49	-
2	MC3	A	507	-	-	5/15/15/49	-
2	MC3	A	509	-	-	2/18/18/49	-
2	MC3	A	513	-	-	0/5/5/49	-
2	MC3	A	514	-	-	2/12/12/49	-
2	MC3	A	512	-	-	3/13/13/49	-
2	MC3	A	501	-	-	8/37/37/49	-
2	MC3	A	506	-	-	4/13/13/49	-
2	MC3	A	511	-	-	1/11/11/49	-
2	MC3	A	503	-	-	11/41/41/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	A	508	-	-	6/14/14/49	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	512	MC3	O3-C11	4.62	1.46	1.30
2	A	503	MC3	O2-C31	4.40	1.46	1.34
2	A	509	MC3	O3-C11	4.37	1.46	1.33
2	A	505	MC3	O3-C11	4.34	1.46	1.33
2	A	503	MC3	O3-C11	4.34	1.46	1.33
2	A	507	MC3	O2-C31	4.31	1.45	1.33
2	A	505	MC3	O2-C31	4.24	1.46	1.34
2	A	508	MC3	O2-C31	4.23	1.45	1.33
2	A	504	MC3	O2-C31	4.21	1.46	1.34
2	A	502	MC3	O2-C31	4.07	1.45	1.34
2	A	501	MC3	O3-C11	4.06	1.45	1.33
2	A	502	MC3	O3-C11	3.96	1.44	1.33
2	A	514	MC3	O3-C11	-3.83	1.22	1.42
2	A	501	MC3	O2-C31	3.55	1.44	1.34
2	A	501	MC3	O2-C2	-2.78	1.40	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	MC3	O2-C31-C32	4.80	121.86	111.48
2	A	504	MC3	O2-C31-C32	4.48	121.17	111.48
2	A	505	MC3	O2-C31-C32	3.87	119.86	111.48
2	A	502	MC3	O2-C31-C32	3.65	119.39	111.48
2	A	505	MC3	O3-C11-C12	3.07	121.20	111.83
2	A	509	MC3	O3-C11-C12	2.85	120.53	111.83
2	A	501	MC3	O2-C2-C1	-2.82	98.22	108.34
2	A	507	MC3	O2-C31-C32	2.80	120.37	111.83
2	A	501	MC3	O3-C11-C12	2.79	120.35	111.83
2	A	508	MC3	O2-C31-C32	2.66	119.95	111.83
2	A	503	MC3	O3-C11-C12	2.63	119.86	111.83
2	A	504	MC3	C3-C2-C1	-2.60	108.28	112.79
2	A	506	MC3	O3-C11-C12	2.54	119.77	109.79
2	A	502	MC3	O3-C11-C12	2.54	119.58	111.83
2	A	501	MC3	C3-C2-C1	-2.54	105.87	111.78
2	A	503	MC3	O2P-P-O1P	2.33	119.93	110.83
2	A	505	MC3	O3-C11-O11	-2.23	118.04	123.63
2	A	503	MC3	C33-C32-C31	-2.11	105.98	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	MC3	C4-C5-N	-2.10	109.09	115.82
2	A	501	MC3	O2P-P-O1P	2.04	121.95	112.44
2	A	512	MC3	O3-C11-C12	2.03	120.40	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	504	MC3	C2

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MC3	C1-O3P-P-O4P
2	A	502	MC3	O2-C2-C3-O3
2	A	502	MC3	C1-O3P-P-O1P
2	A	502	MC3	C1-O3P-P-O2P
2	A	502	MC3	C1-O3P-P-O4P
2	A	503	MC3	C12-C11-O3-C3
2	A	503	MC3	O11-C11-O3-C3
2	A	507	MC3	O2-C2-C3-O3
2	A	507	MC3	C2-C3-O3-C11
2	A	502	MC3	C31-C32-C33-C34
2	A	503	MC3	C11-C12-C13-C14
2	A	502	MC3	C11-C12-C13-C14
2	A	505	MC3	C32-C31-O2-C2
2	A	505	MC3	O31-C31-O2-C2
2	A	502	MC3	C12-C11-O3-C3
2	A	503	MC3	C32-C31-O2-C2
2	A	503	MC3	O31-C31-O2-C2
2	A	503	MC3	C3-C2-O2-C31
2	A	505	MC3	C3-C2-O2-C31
2	A	508	MC3	O3P-C1-C2-O2
2	A	509	MC3	C16-C17-C18-C19
2	A	510	MC3	C14-C15-C16-C17
2	A	502	MC3	O11-C11-O3-C3
2	A	514	MC3	C14-C15-C16-C17
2	A	501	MC3	C14-C15-C16-C17
2	A	503	MC3	C32-C33-C34-C35
2	A	508	MC3	C32-C33-C34-C35
2	A	507	MC3	C33-C34-C35-C36
2	A	501	MC3	C1-C2-C3-O3
2	A	505	MC3	C17-C18-C19-C20

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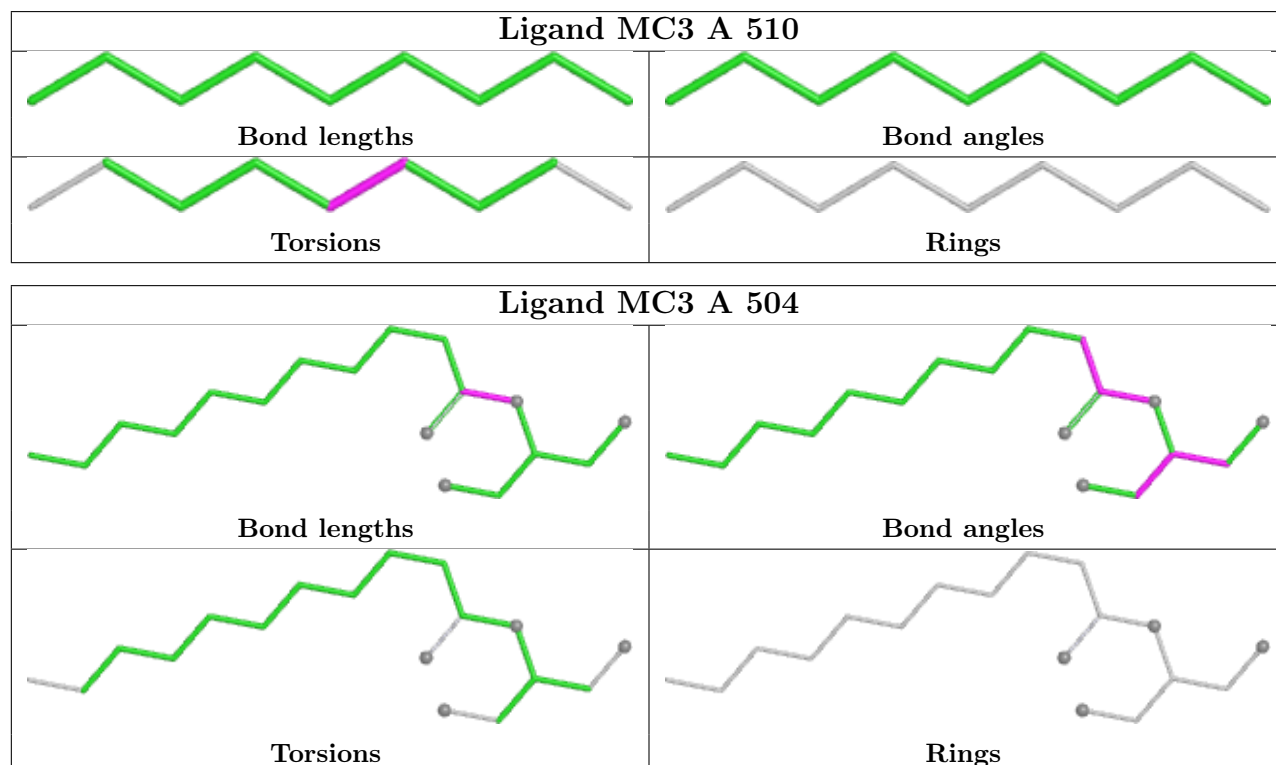
Mol	Chain	Res	Type	Atoms
2	A	506	MC3	C15-C16-C17-C18
2	A	507	MC3	C38-C39-C40-C41
2	A	512	MC3	C21-C22-C23-C24
2	A	502	MC3	C41-C42-C43-C44
2	A	501	MC3	C32-C31-O2-C2
2	A	505	MC3	O3P-C1-C2-C3
2	A	503	MC3	C14-C15-C16-C17
2	A	508	MC3	C34-C35-C36-C37
2	A	501	MC3	O31-C31-O2-C2
2	A	502	MC3	C1-C2-C3-O3
2	A	505	MC3	C13-C14-C15-C16
2	A	506	MC3	C14-C15-C16-C17
2	A	501	MC3	C1-O3P-P-O1P
2	A	502	MC3	C4-O4P-P-O1P
2	A	502	MC3	C4-O4P-P-O2P
2	A	502	MC3	C4-O4P-P-O3P
2	A	503	MC3	C18-C19-C20-C21
2	A	511	MC3	C11-C12-C13-C14
2	A	505	MC3	C12-C11-O3-C3
2	A	507	MC3	C34-C35-C36-C37
2	A	501	MC3	C33-C34-C35-C36
2	A	505	MC3	O11-C11-O3-C3
2	A	502	MC3	C38-C39-C40-C41
2	A	503	MC3	C17-C18-C19-C20
2	A	502	MC3	C32-C33-C34-C35
2	A	502	MC3	C1-C2-O2-C31
2	A	509	MC3	C14-C15-C16-C17
2	A	512	MC3	O11-C11-C12-C13
2	A	501	MC3	O2-C2-C3-O3
2	A	503	MC3	C20-C21-C22-C23
2	A	502	MC3	C2-C1-O3P-P
2	A	505	MC3	O3P-C1-C2-O2
2	A	512	MC3	O3-C11-C12-C13
2	A	506	MC3	C12-C13-C14-C15
2	A	506	MC3	C16-C17-C18-C19
2	A	508	MC3	C31-C32-C33-C34
2	A	502	MC3	O4P-C4-C5-N
2	A	502	MC3	C3-C2-O2-C31
2	A	508	MC3	O2-C31-C32-C33
2	A	514	MC3	C13-C14-C15-C16
2	A	508	MC3	O31-C31-C32-C33

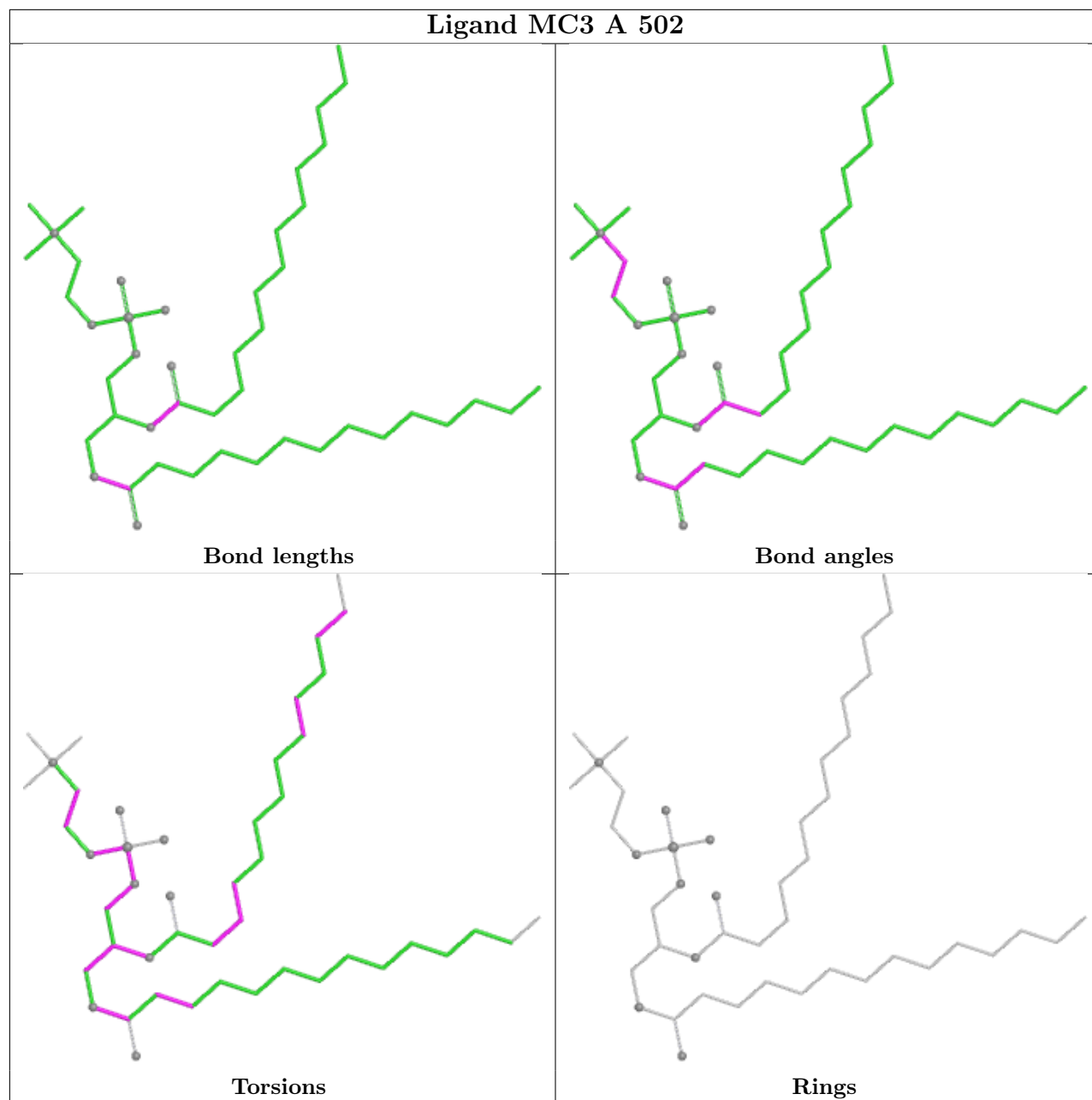
There are no ring outliers.

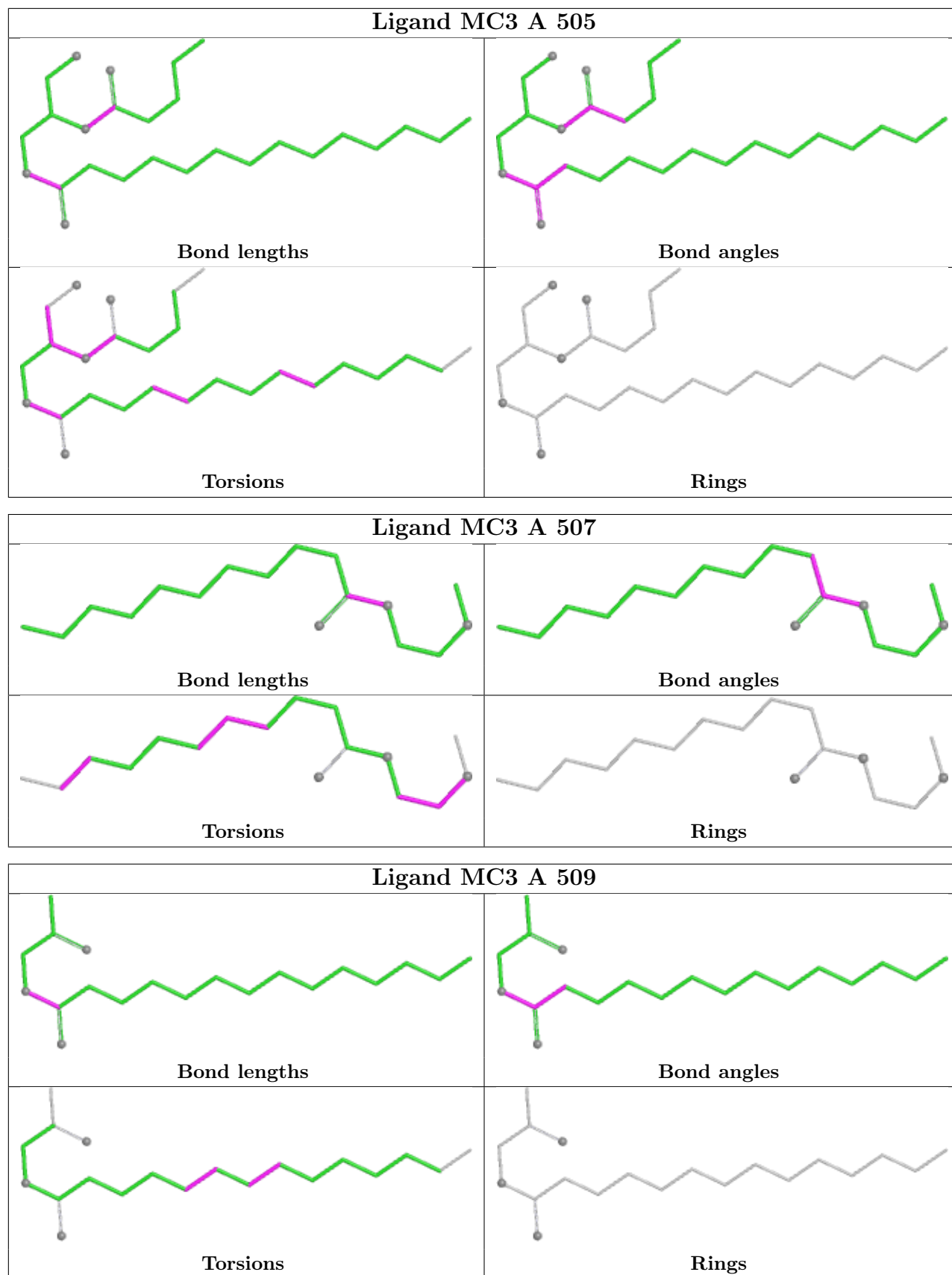
9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	MC3	2	0
2	A	502	MC3	5	0
2	A	505	MC3	2	0
2	A	507	MC3	2	0
2	A	509	MC3	2	0
2	A	501	MC3	2	0
2	A	511	MC3	2	0
2	A	503	MC3	5	0
2	A	508	MC3	1	0

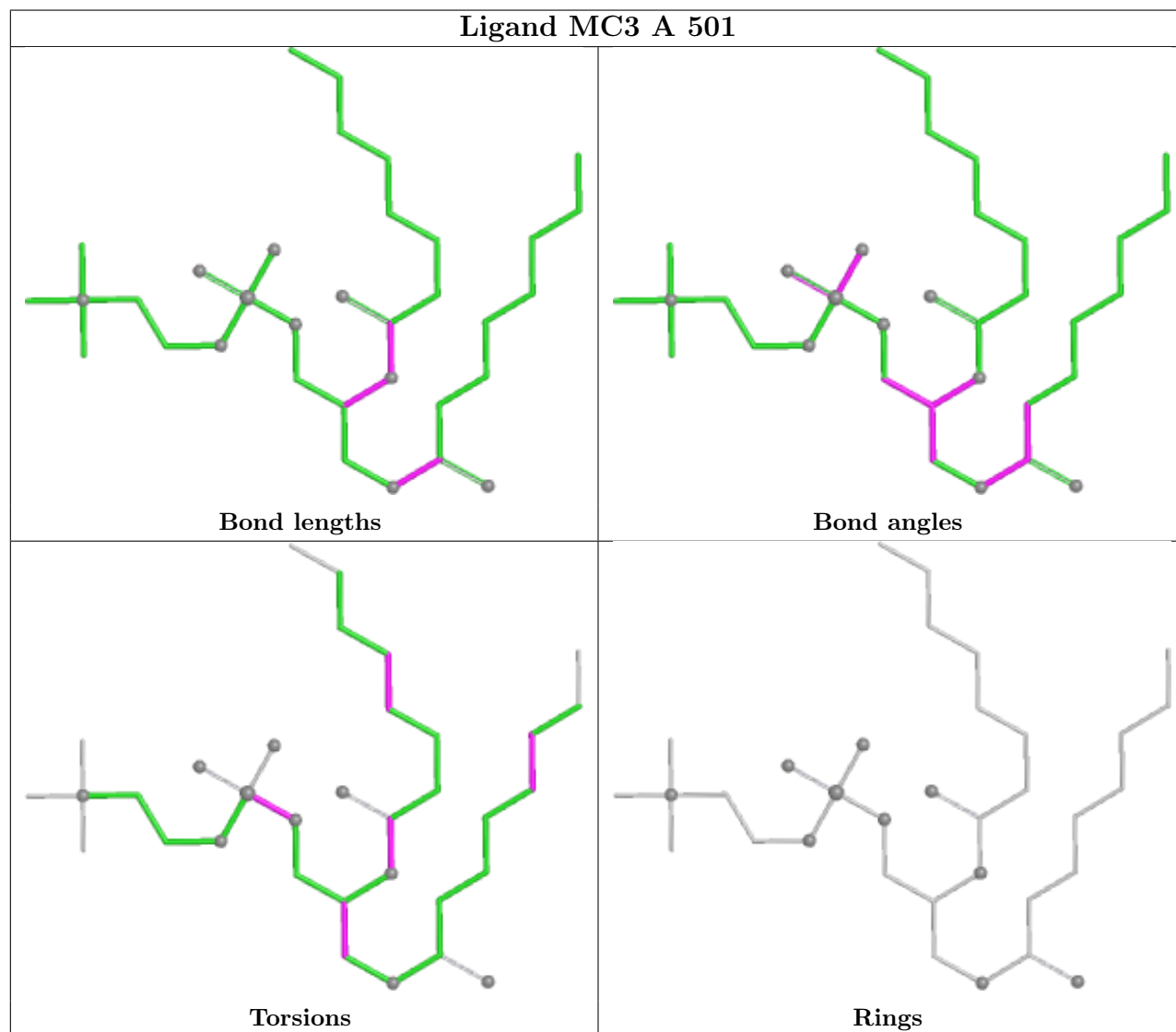
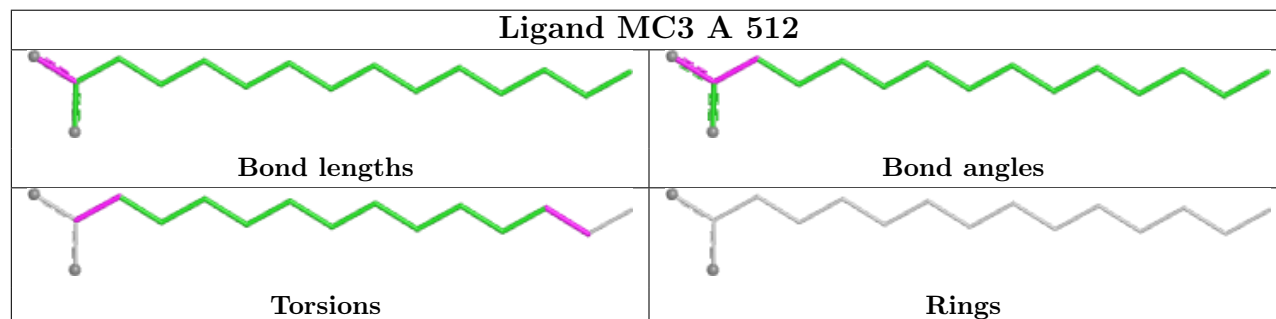
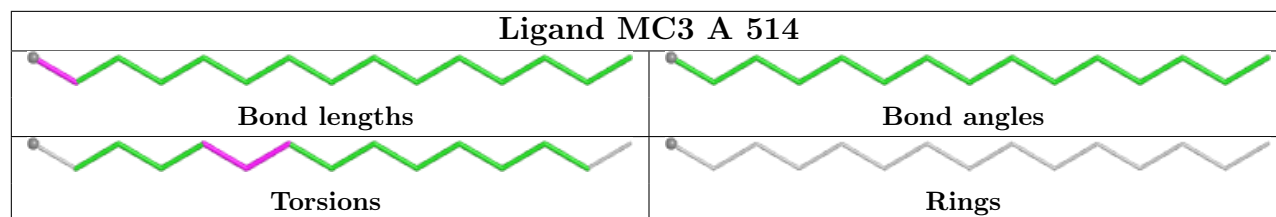
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

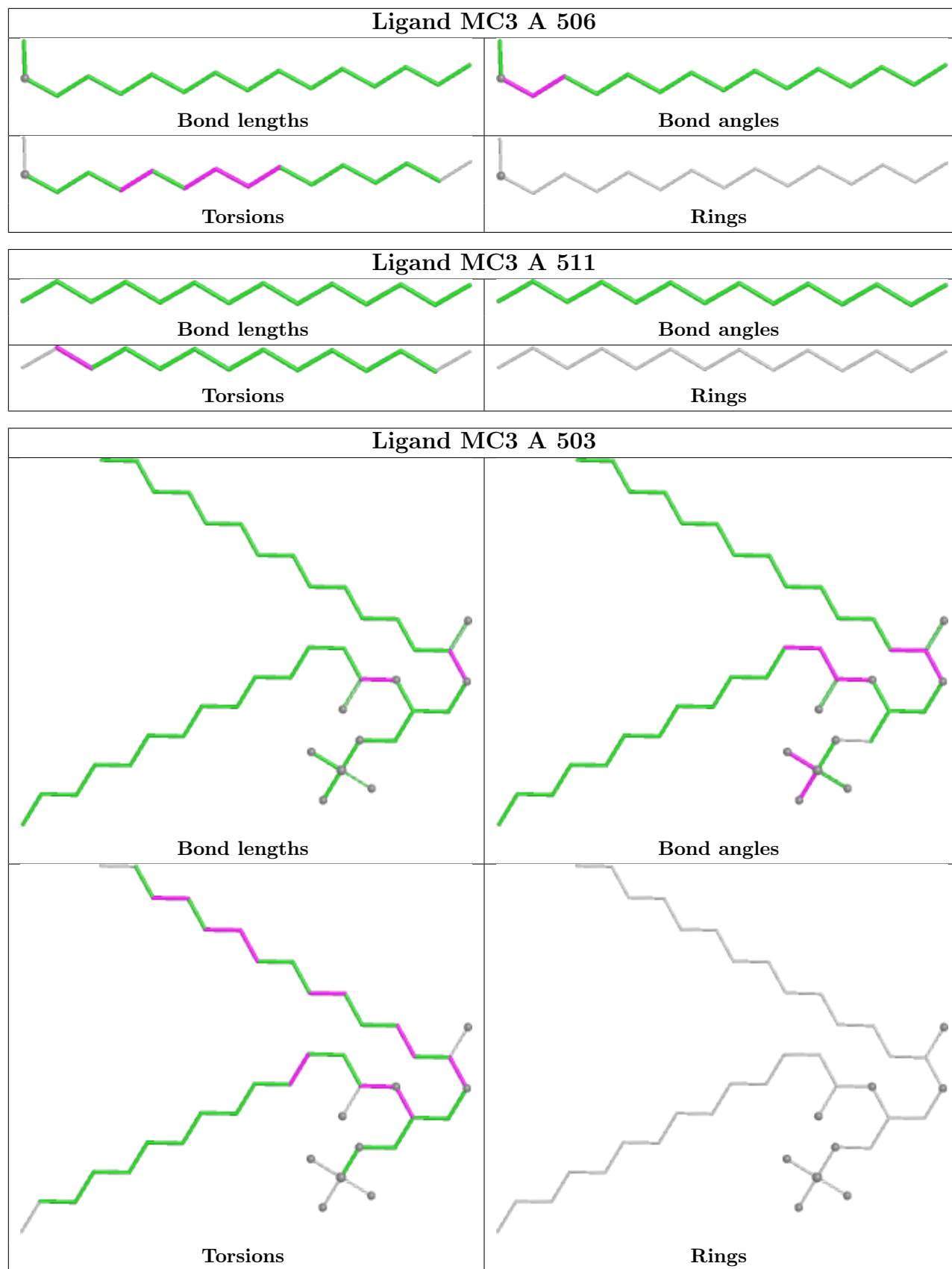


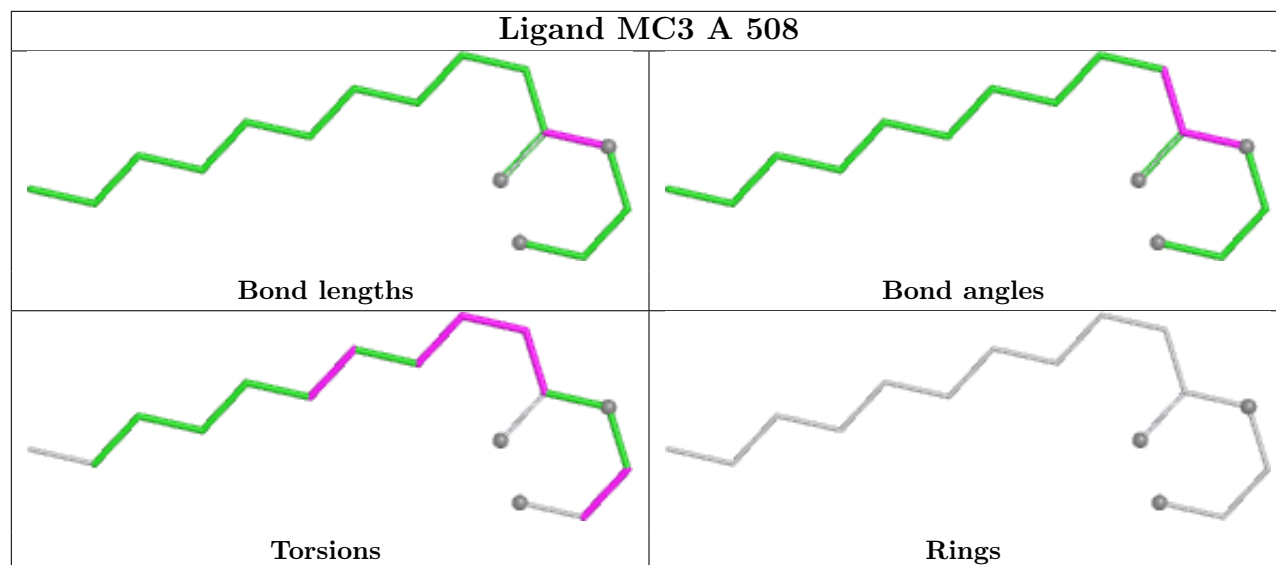












## 5.7 Other polymers [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	178/180 (98%)	0.03	8 (4%) 33 37	12, 18, 32, 44	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	PHE	6.4
1	A	93	ALA	5.8
1	A	249	MET	5.3
1	A	272	ALA	4.3
1	A	242	PHE	3.7
1	A	245	PHE	3.4
1	A	271	ASN	2.9
1	A	248	SER	2.5

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

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

### 6.3 Carbohydrates [i](#)

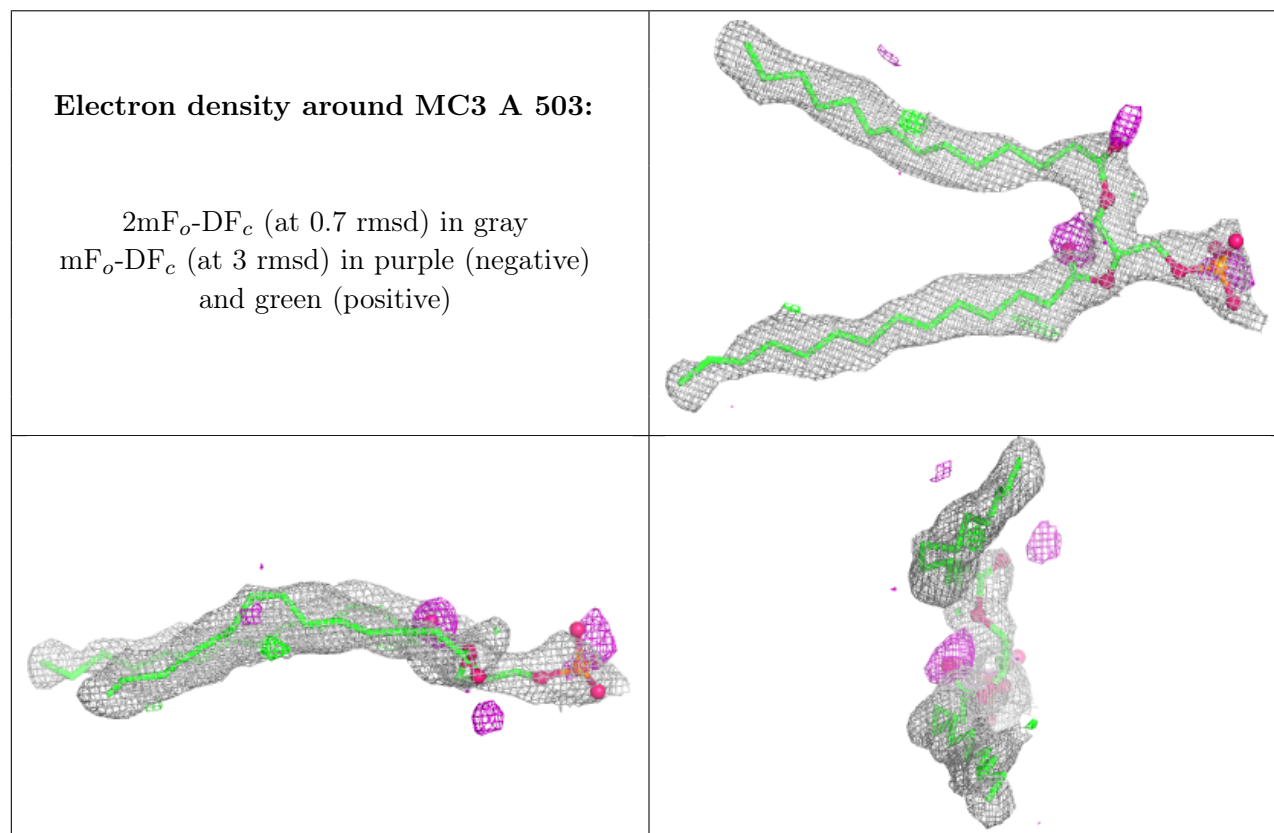
There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

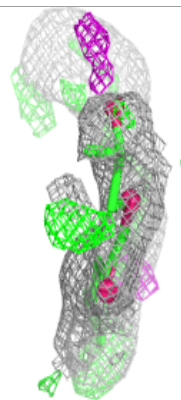
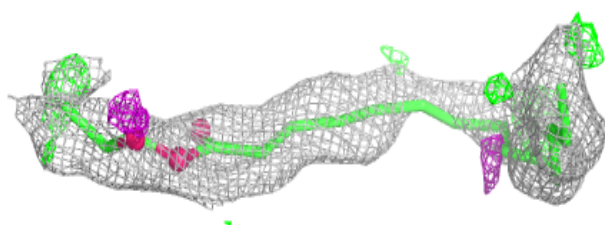
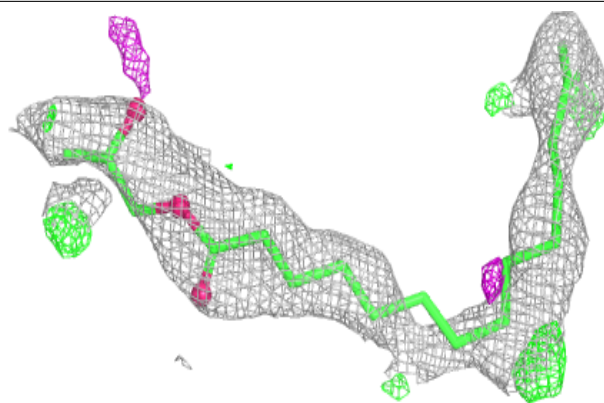
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MC3	A	503	40/46	0.55	0.23	31,40,61,71	0
2	MC3	A	509	20/46	0.55	0.29	27,44,53,57	0
2	MC3	A	502	46/46	0.63	0.20	23,40,55,63	0
2	MC3	A	505	27/46	0.64	0.30	33,46,55,55	0
2	MC3	A	510	9/46	0.71	0.17	31,39,44,46	0
2	MC3	A	508	16/46	0.72	0.26	38,47,52,54	0
2	MC3	A	504	18/46	0.73	0.23	40,45,51,55	0
2	MC3	A	514	15/46	0.76	0.24	31,42,48,52	0
2	MC3	A	511	14/46	0.78	0.21	36,43,52,59	0
2	MC3	A	513	8/46	0.79	0.14	41,42,49,51	0
2	MC3	A	512	16/46	0.80	0.18	33,39,57,61	0
2	MC3	A	507	17/46	0.81	0.21	36,40,46,48	0
2	MC3	A	506	16/46	0.83	0.17	33,38,46,47	0
2	MC3	A	501	34/46	0.94	0.13	17,34,46,48	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.

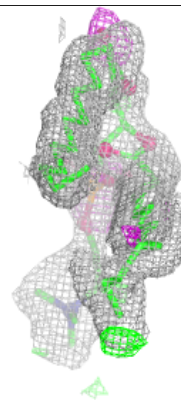
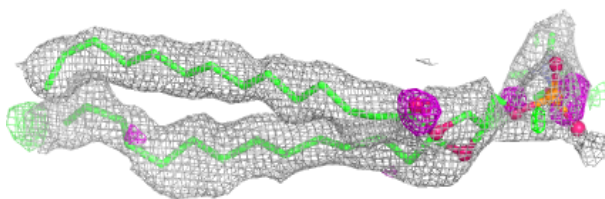
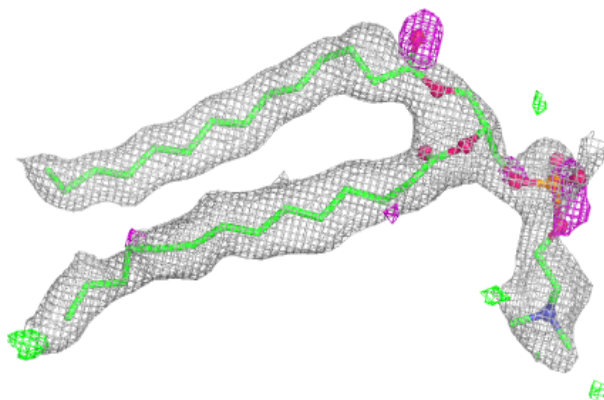


**Electron density around MC3 A 509:**

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

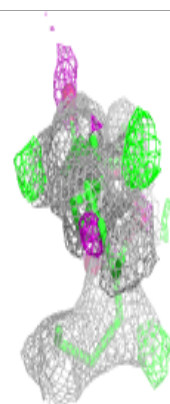
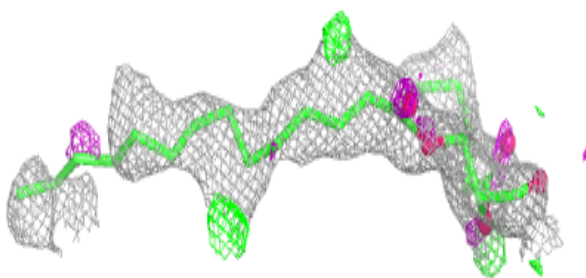
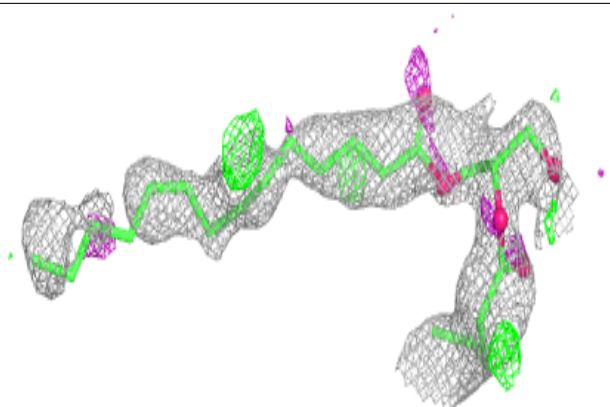
**Electron density around MC3 A 502:**

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

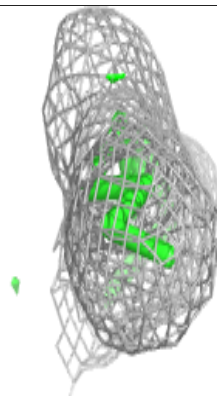
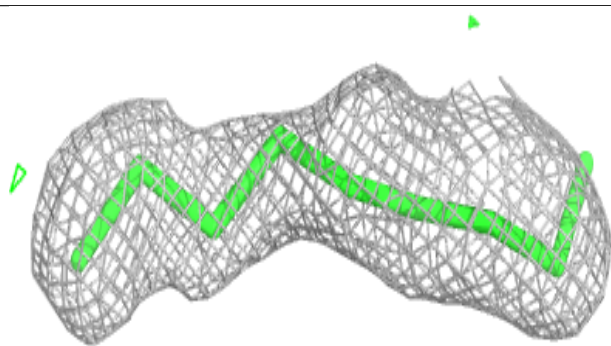
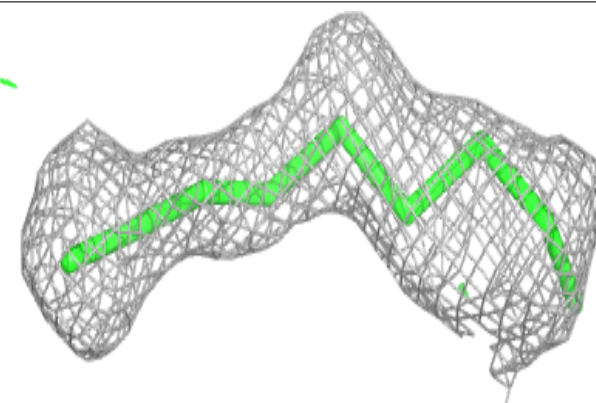


**Electron density around MC3 A 505:**

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

**Electron density around MC3 A 510:**

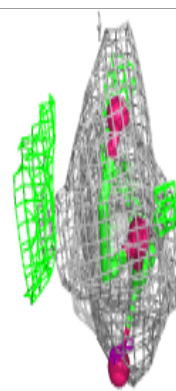
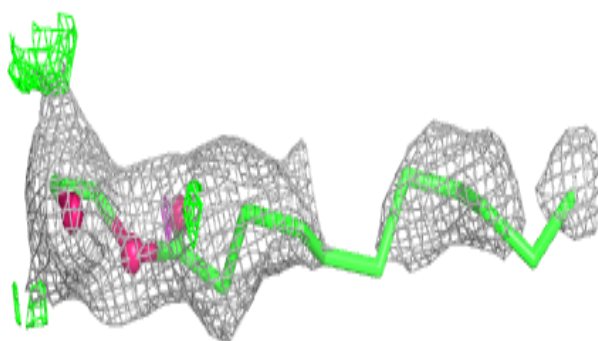
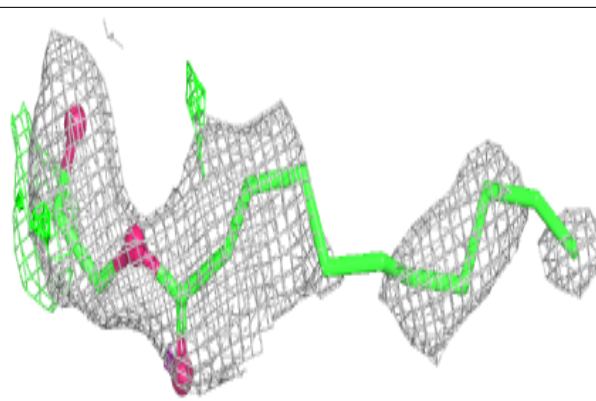
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



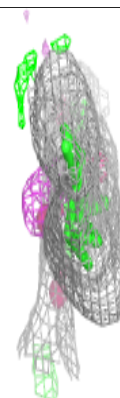
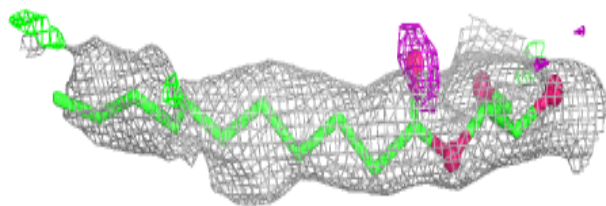
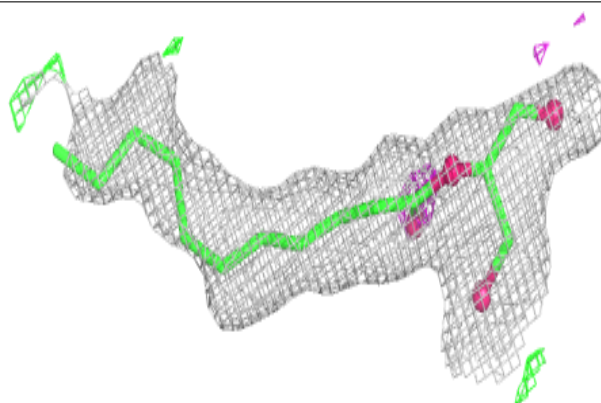


**Electron density around MC3 A 508:**

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

**Electron density around MC3 A 504:**

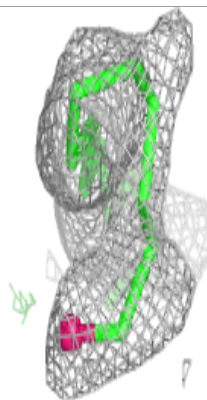
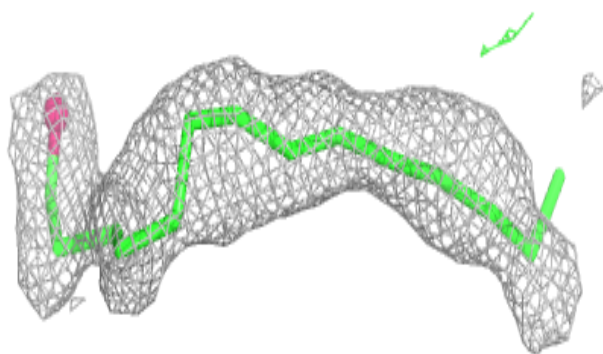
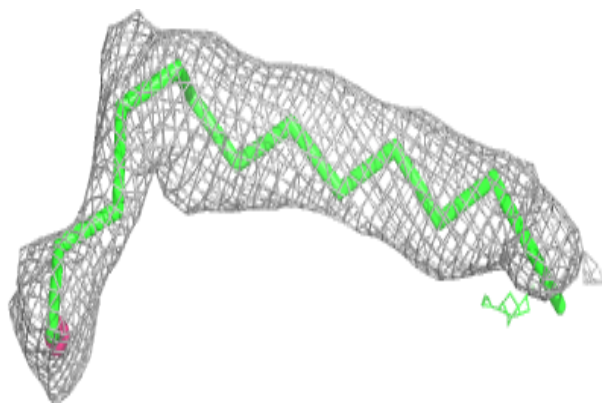
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



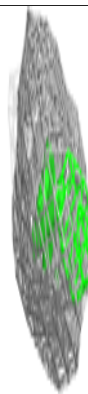
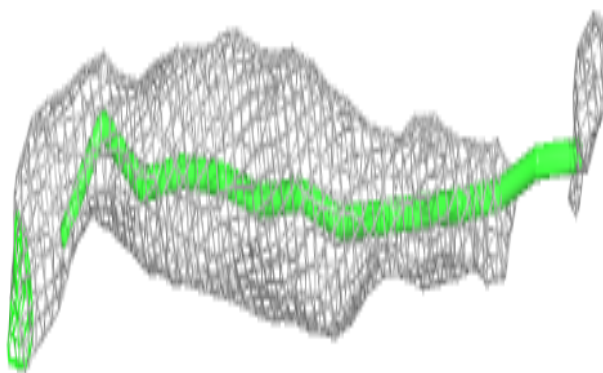
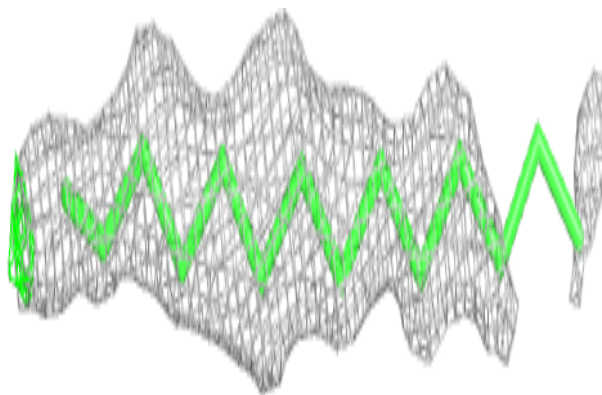


**Electron density around MC3 A 514:**

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

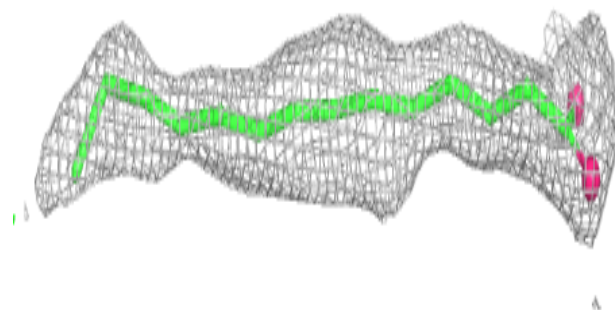
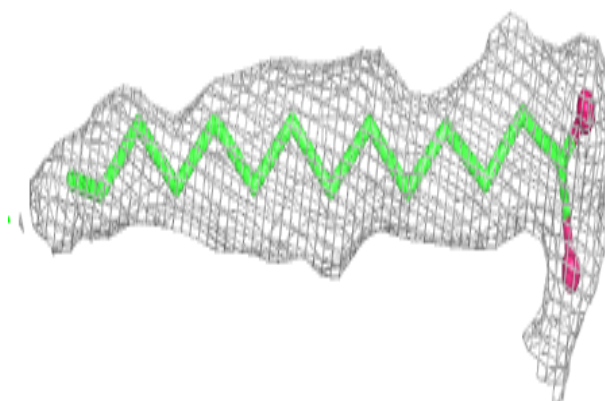
**Electron density around MC3 A 511:**

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

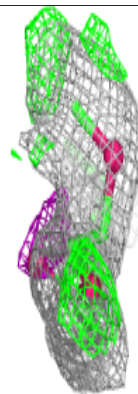
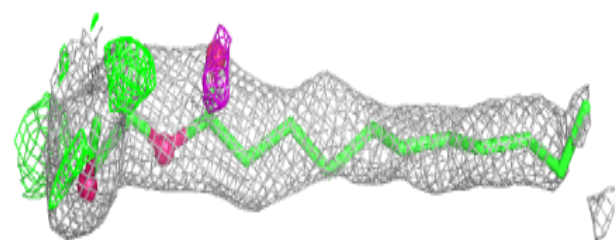
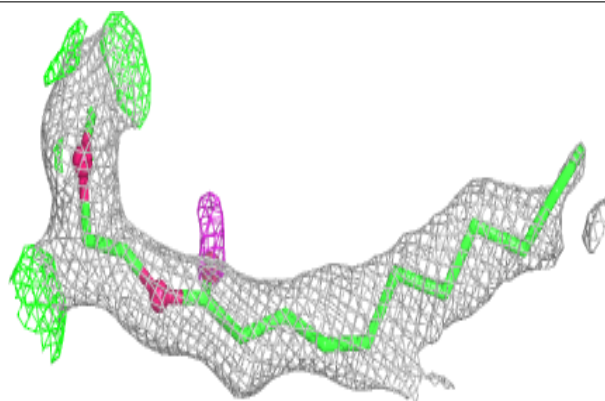


**Electron density around MC3 A 512:**

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

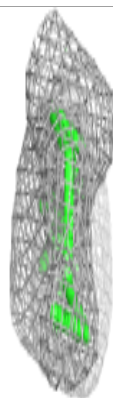
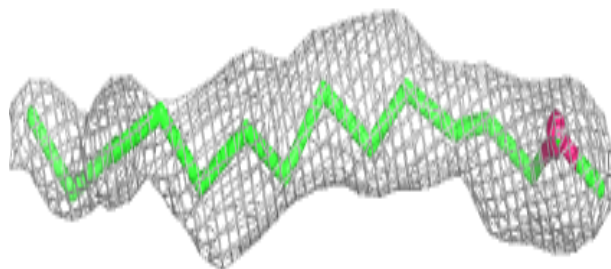
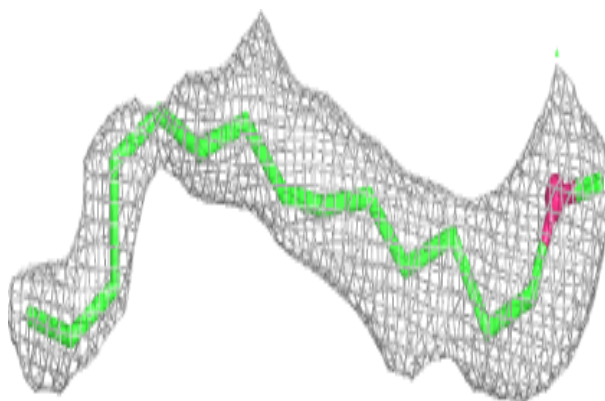
**Electron density around MC3 A 507:**

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

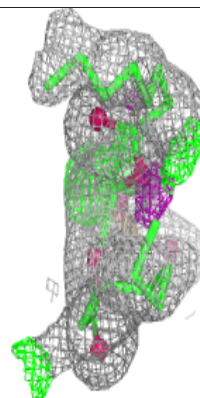
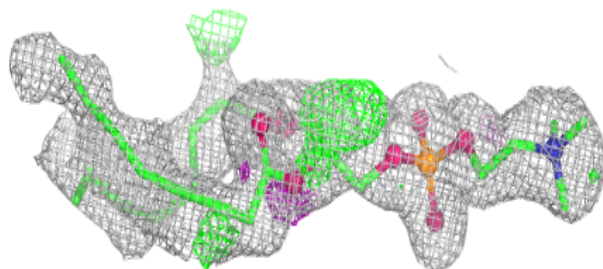
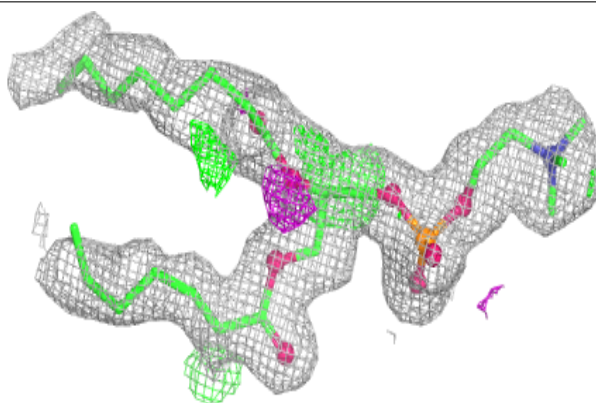


**Electron density around MC3 A 506:**

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

**Electron density around MC3 A 501:**

$2mF_o-DF_c$  (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.