



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:56 AM BST

PDB ID : 5MHF  
Title : Murine endoplasmic reticulum alpha-glucosidase I with N-9'-methoxynonyl-1-deoxynojirimycin  
Authors : Hill, J.C.; Caputo, A.T.; Roversi, P.; Zitzmann, N.  
Deposited on : 2016-11-24  
Resolution : 2.10 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

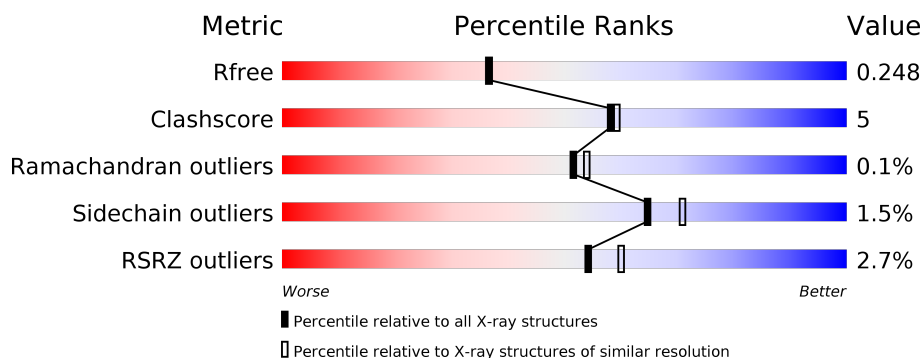
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.




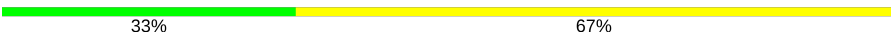
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	795	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	795	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>5%</div> </div> </div>
1	C	795	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>
1	D	795	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>• •</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	3	
3	H	3	

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
6	7PG	C	905	-	-	X	-
6	7PG	D	905	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26145 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 Mannosyl-oligosaccharide glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	2	0
			5975	3862	1051	1051	11			
1	B	752	Total	C	N	O	S	0	2	0
			5979	3864	1052	1052	11			
1	C	762	Total	C	N	O	S	0	2	0
			6051	3909	1063	1068	11			
1	D	767	Total	C	N	O	S	0	2	0
			6081	3925	1070	1075	11			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	GLU	-	expression tag	UNP Q80UM7
A	57	THR	-	expression tag	UNP Q80UM7
A	58	GLY	-	expression tag	UNP Q80UM7
A	835	ALA	-	expression tag	UNP Q80UM7
A	836	SER	-	expression tag	UNP Q80UM7
A	837	TRP	-	expression tag	UNP Q80UM7
A	838	SER	-	expression tag	UNP Q80UM7
A	839	HIS	-	expression tag	UNP Q80UM7
A	840	PRO	-	expression tag	UNP Q80UM7
A	841	GLN	-	expression tag	UNP Q80UM7
A	842	PHE	-	expression tag	UNP Q80UM7
A	843	GLU	-	expression tag	UNP Q80UM7
A	844	LYS	-	expression tag	UNP Q80UM7
A	845	HIS	-	expression tag	UNP Q80UM7
A	846	HIS	-	expression tag	UNP Q80UM7
A	847	HIS	-	expression tag	UNP Q80UM7
A	848	HIS	-	expression tag	UNP Q80UM7
A	849	HIS	-	expression tag	UNP Q80UM7
A	850	HIS	-	expression tag	UNP Q80UM7
B	56	GLU	-	expression tag	UNP Q80UM7
B	57	THR	-	expression tag	UNP Q80UM7

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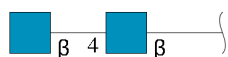
Chain	Residue	Modelled	Actual	Comment	Reference
B	58	GLY	-	expression tag	UNP Q80UM7
B	835	ALA	-	expression tag	UNP Q80UM7
B	836	SER	-	expression tag	UNP Q80UM7
B	837	TRP	-	expression tag	UNP Q80UM7
B	838	SER	-	expression tag	UNP Q80UM7
B	839	HIS	-	expression tag	UNP Q80UM7
B	840	PRO	-	expression tag	UNP Q80UM7
B	841	GLN	-	expression tag	UNP Q80UM7
B	842	PHE	-	expression tag	UNP Q80UM7
B	843	GLU	-	expression tag	UNP Q80UM7
B	844	LYS	-	expression tag	UNP Q80UM7
B	845	HIS	-	expression tag	UNP Q80UM7
B	846	HIS	-	expression tag	UNP Q80UM7
B	847	HIS	-	expression tag	UNP Q80UM7
B	848	HIS	-	expression tag	UNP Q80UM7
B	849	HIS	-	expression tag	UNP Q80UM7
B	850	HIS	-	expression tag	UNP Q80UM7
C	56	GLU	-	expression tag	UNP Q80UM7
C	57	THR	-	expression tag	UNP Q80UM7
C	58	GLY	-	expression tag	UNP Q80UM7
C	835	ALA	-	expression tag	UNP Q80UM7
C	836	SER	-	expression tag	UNP Q80UM7
C	837	TRP	-	expression tag	UNP Q80UM7
C	838	SER	-	expression tag	UNP Q80UM7
C	839	HIS	-	expression tag	UNP Q80UM7
C	840	PRO	-	expression tag	UNP Q80UM7
C	841	GLN	-	expression tag	UNP Q80UM7
C	842	PHE	-	expression tag	UNP Q80UM7
C	843	GLU	-	expression tag	UNP Q80UM7
C	844	LYS	-	expression tag	UNP Q80UM7
C	845	HIS	-	expression tag	UNP Q80UM7
C	846	HIS	-	expression tag	UNP Q80UM7
C	847	HIS	-	expression tag	UNP Q80UM7
C	848	HIS	-	expression tag	UNP Q80UM7
C	849	HIS	-	expression tag	UNP Q80UM7
C	850	HIS	-	expression tag	UNP Q80UM7
D	56	GLU	-	expression tag	UNP Q80UM7
D	57	THR	-	expression tag	UNP Q80UM7
D	58	GLY	-	expression tag	UNP Q80UM7
D	835	ALA	-	expression tag	UNP Q80UM7
D	836	SER	-	expression tag	UNP Q80UM7
D	837	TRP	-	expression tag	UNP Q80UM7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	838	SER	-	expression tag	UNP Q80UM7
D	839	HIS	-	expression tag	UNP Q80UM7
D	840	PRO	-	expression tag	UNP Q80UM7
D	841	GLN	-	expression tag	UNP Q80UM7
D	842	PHE	-	expression tag	UNP Q80UM7
D	843	GLU	-	expression tag	UNP Q80UM7
D	844	LYS	-	expression tag	UNP Q80UM7
D	845	HIS	-	expression tag	UNP Q80UM7
D	846	HIS	-	expression tag	UNP Q80UM7
D	847	HIS	-	expression tag	UNP Q80UM7
D	848	HIS	-	expression tag	UNP Q80UM7
D	849	HIS	-	expression tag	UNP Q80UM7
D	850	HIS	-	expression tag	UNP Q80UM7

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



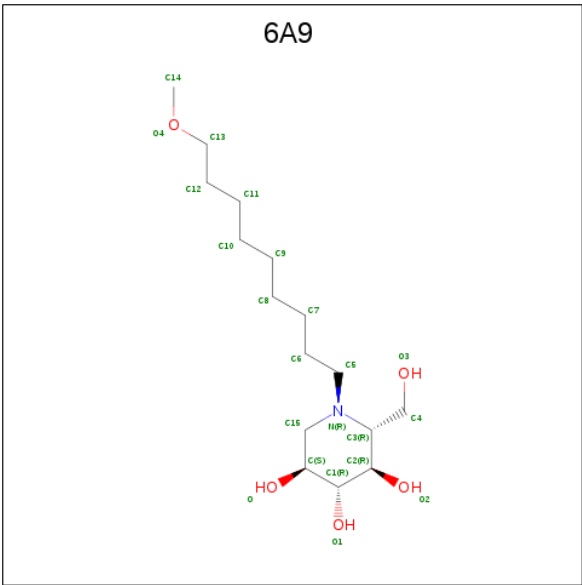
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



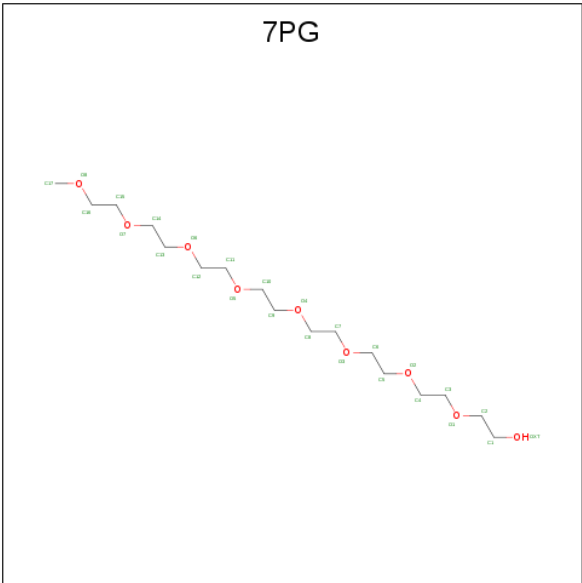
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total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

- Molecule 5 is N-9'-methoxynonyl-1-deoxynojirimycin (three-letter code: 6A9) (formula: C<sub>16</sub>H<sub>33</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			88	64	4	20		
5	B	1	Total	C	N	O	0	1
			88	64	4	20		
5	C	1	Total	C	N	O	0	1
			88	64	4	20		
5	D	1	Total	C	N	O	0	1
			88	64	4	20		

- Molecule 6 is 2,5,8,11,14,17,20,23-OCTAOXAPENTACOSAN-25-OL (three-letter code: 7PG) (formula: C<sub>17</sub>H<sub>36</sub>O<sub>9</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			24	16	8		
6	B	1	Total	C	O	0	0
			24	16	8		
6	C	1	Total	C	O	0	0
			22	15	7		
6	C	1	Total	C	O	0	0
			17	11	6		
6	D	1	Total	C	O	0	0
			22	15	7		
6	D	1	Total	C	O	0	0
			17	11	6		

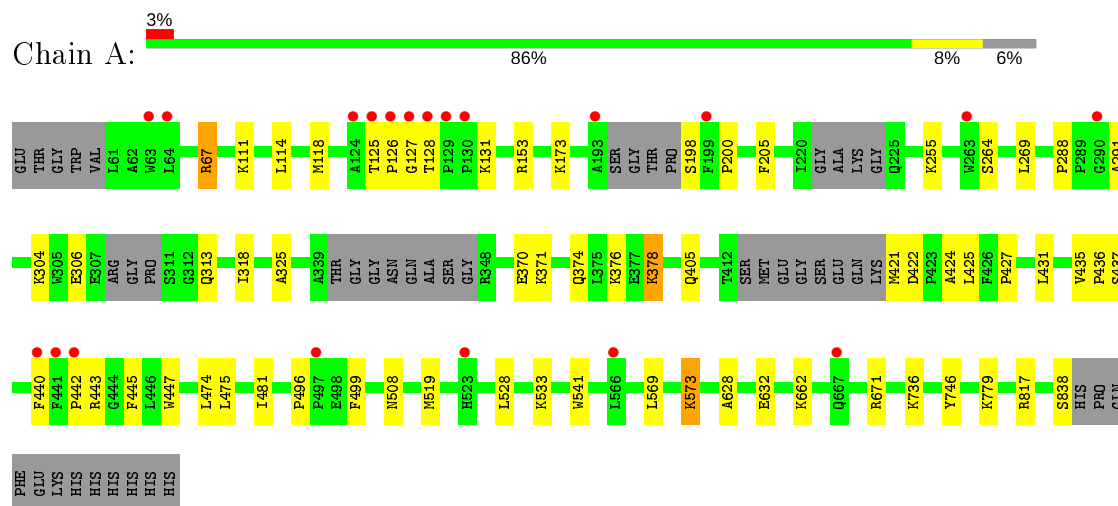
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	321	Total	O	0	0
			321	321		
7	B	359	Total	O	0	0
			359	359		
7	C	358	Total	O	0	0
			358	358		
7	D	349	Total	O	0	0
			349	349		

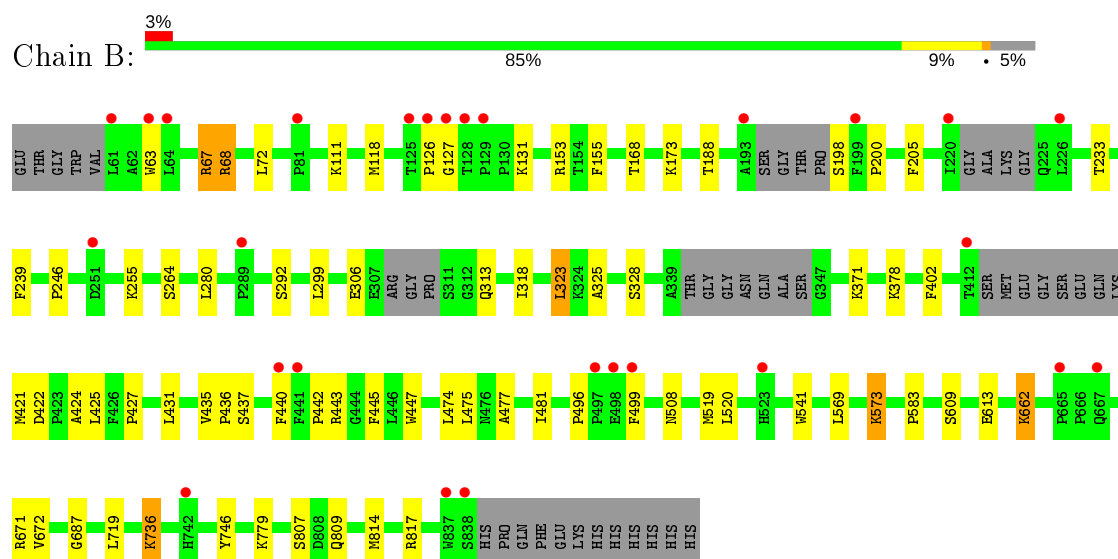
### 3 Residue-property plots

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.

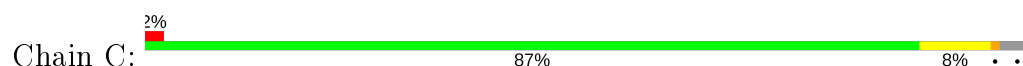
- Molecule 1: Mannosyl-oligosaccharide glucosidase

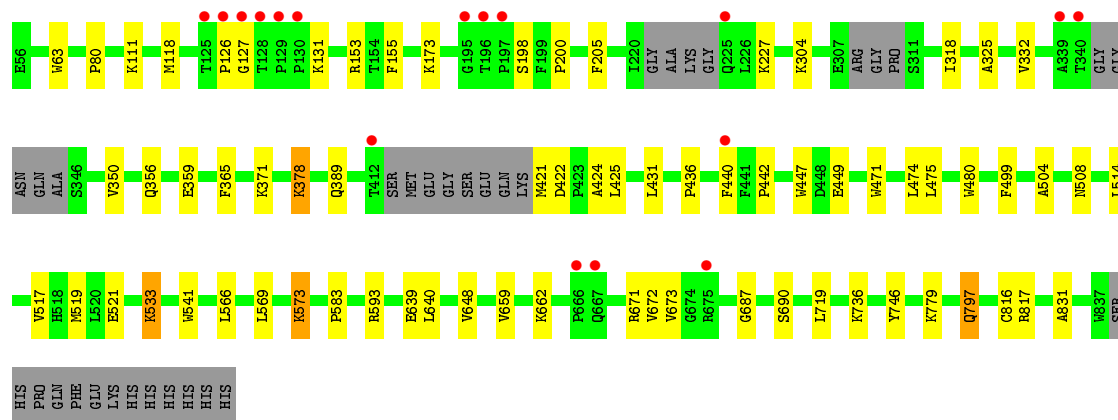


- Molecule 1: Mannosyl-oligosaccharide glucosidase

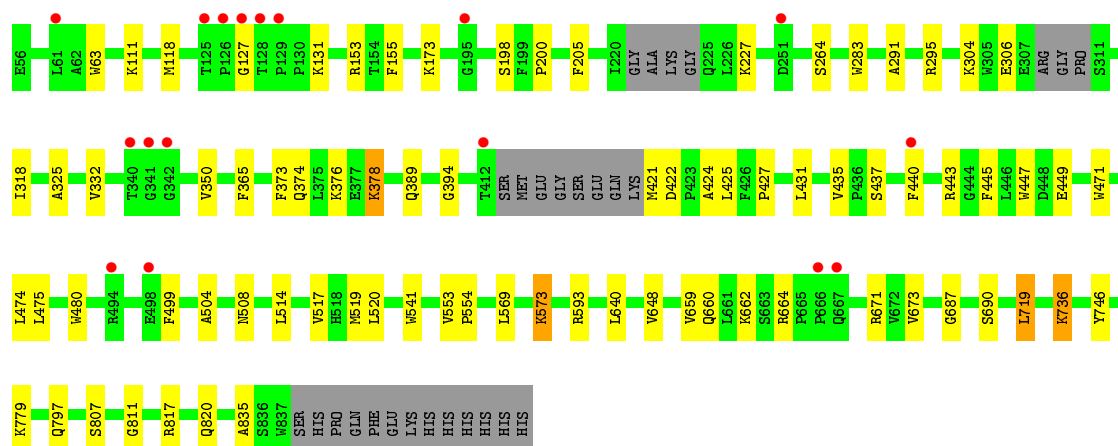
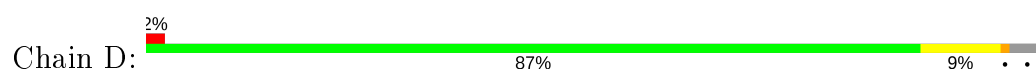


- Molecule 1: Mannosyl-oligosaccharide glucosidase





• Molecule 1: Mannosyl-oligosaccharide glucosidase



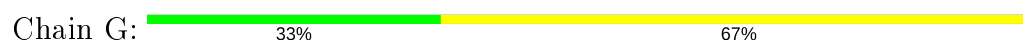
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  33% 67%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.01Å 130.92Å 135.37Å 90.00° 99.53° 90.00°	Depositor
Resolution (Å)	133.50 – 2.10 133.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (133.50-2.10) 99.4 (133.50-2.10)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.10Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.188 , 0.216 0.220 , 0.248	Depositor DCC
$R_{free}$ test set	10477 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtrriage
Anisotropy	0.522	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	26145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9185e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MLY, 6A9, SO4, SME, 7PG

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	0.52	0/6016	0.65	0/8222
1	B	0.51	0/6020	0.66	1/8227 (0.0%)
1	C	0.51	0/6096	0.65	0/8335
1	D	0.52	0/6127	0.66	0/8378
All	All	0.52	0/24259	0.66	1/33162 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	LEU	CB-CA-C	-5.20	100.33	110.20

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	5975	0	5848	49	0
1	B	5979	0	5851	66	0
1	C	6051	0	5916	52	0
1	D	6081	0	5942	64	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	39	0	34	0	0
3	H	39	0	34	0	0
4	A	15	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
5	A	88	0	0	1	0
5	B	88	0	0	0	0
5	C	88	0	0	0	0
5	D	88	0	0	0	0
6	A	24	0	31	6	0
6	B	24	0	31	14	0
6	C	39	0	46	31	0
6	D	39	0	46	36	0
7	A	321	0	0	4	0
7	B	359	0	0	2	0
7	C	358	0	0	3	0
7	D	349	0	0	3	0
All	All	26145	0	23829	233	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 5.

All (233) 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:C:436:PRO:HD2	1:C:440[B]:PHE:CZ	1.82	1.12
1:C:436:PRO:HD2	1:C:440[B]:PHE:CE2	1.99	0.98
6:A:907:7PG:H132	7:A:1162:HOH:O	1.64	0.98
6:B:906:7PG:H62	6:C:905:7PG:H62	1.46	0.97
1:A:425:LEU:H	6:D:905:7PG:H102	1.29	0.96
1:B:127:GLY:H	1:C:127:GLY:N	1.66	0.92
1:A:374:GLN:HB2	1:A:378:MLY:HH22	1.50	0.90
1:B:440[B]:PHE:CE2	1:B:445:PHE:HE1	1.89	0.90
1:B:127:GLY:H	1:C:127:GLY:H	0.93	0.88
1:A:127:GLY:H	1:D:127:GLY:H	1.17	0.88
1:C:422:ASP:OD2	6:C:905:7PG:H131	1.74	0.87
1:D:422:ASP:HB2	6:D:905:7PG:H151	1.58	0.86
1:B:127:GLY:N	1:C:127:GLY:H	1.72	0.86
1:C:436:PRO:HD2	1:C:440[B]:PHE:HZ	1.43	0.84
1:B:188:THR:HG22	1:B:328:SER:OG	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:907:7PG:H42	6:D:905:7PG:H61	1.62	0.81
1:B:662:MLY:HH13	1:B:672:VAL:HG11	1.64	0.80
1:A:573:MLY:HH22	7:A:1174:HOH:O	1.82	0.79
1:B:440[B]:PHE:HE2	1:B:445:PHE:HE1	1.28	0.78
1:D:427:PRO:HG3	6:D:905:7PG:H62	1.66	0.77
1:C:425:LEU:H	6:C:905:7PG:H71	1.49	0.76
1:C:797:GLN:HG2	7:C:1093:HOH:O	1.86	0.75
1:B:424:ALA:HA	6:C:905:7PG:H72	1.69	0.74
1:B:437:SER:O	1:B:440[B]:PHE:HD1	1.71	0.73
1:A:405:GLN:NE2	6:D:905:7PG:H141	2.06	0.71
1:B:569:LEU:O	1:B:671:ARG:HD3	1.90	0.71
1:A:427:PRO:HA	6:D:905:7PG:H152	1.72	0.70
6:B:906:7PG:H131	6:C:905:7PG:H141	1.74	0.70
1:B:425:LEU:H	6:C:905:7PG:H82	1.56	0.69
1:B:573:MLY:HH22	7:B:1109:HOH:O	1.92	0.69
1:C:422:ASP:HB2	6:C:905:7PG:H131	1.73	0.69
1:A:422:ASP:OD2	6:D:905:7PG:H42	1.94	0.68
1:C:659:VAL:HG12	1:C:673:VAL:HG12	1.76	0.68
1:A:440[B]:PHE:HE2	1:A:445:PHE:HE1	1.40	0.68
1:A:374:GLN:HB2	1:A:378:MLY:CH2	2.23	0.67
1:A:424:ALA:HA	6:D:905:7PG:H92	1.76	0.67
1:D:425:LEU:H	6:D:905:7PG:H101	1.58	0.67
1:B:425:LEU:HB2	6:C:905:7PG:H82	1.76	0.67
1:D:440[B]:PHE:HE2	1:D:445:PHE:HE1	1.43	0.66
1:B:280:LEU:HD23	1:B:299:LEU:HD12	1.77	0.66
6:B:906:7PG:C6	6:C:905:7PG:H62	2.24	0.66
1:D:437:SER:O	1:D:440[B]:PHE:CD1	2.49	0.66
1:D:283:TRP:CE3	1:D:295:ARG:HG2	2.32	0.65
1:D:425:LEU:HB2	6:D:905:7PG:H91	1.78	0.65
1:A:440[B]:PHE:HE2	1:A:445:PHE:CE1	2.15	0.65
1:B:67:ARG:HH21	6:B:906:7PG:H112	1.63	0.64
1:B:609:SER:O	1:B:613:GLU:HG2	1.98	0.64
1:A:440[B]:PHE:CE2	1:A:445:PHE:HE1	2.15	0.64
1:B:425:LEU:H	6:C:905:7PG:C8	2.10	0.64
1:D:427:PRO:HB3	6:D:905:7PG:H41	1.80	0.64
1:D:422:ASP:CB	6:D:905:7PG:H151	2.28	0.63
1:D:573:MLY:HH22	7:D:1217:HOH:O	1.99	0.63
1:C:425:LEU:H	6:C:905:7PG:C7	2.11	0.62
1:C:573:MLY:HH22	7:C:1217:HOH:O	1.99	0.61
1:B:440[B]:PHE:CE2	1:B:445:PHE:CE1	2.80	0.61
1:D:427:PRO:HA	6:D:905:7PG:H51	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440[B]:PHE:CE2	1:D:445:PHE:HE1	2.18	0.60
1:A:67:ARG:HH21	6:A:907:7PG:H101	1.65	0.60
1:A:425:LEU:O	6:D:905:7PG:H112	2.02	0.60
1:B:118:MET:HB2	1:B:205:PHE:HB2	1.83	0.59
1:C:378:MLY:HE3	1:C:831:ALA:O	2.02	0.59
1:A:628:ALA:O	1:A:632:GLU:HG2	2.03	0.59
6:B:906:7PG:H132	7:B:1195:HOH:O	2.02	0.59
1:B:168:THR:HB	1:B:188:THR:OG1	2.03	0.58
1:D:374:GLN:HB2	1:D:378:MLY:HH22	1.84	0.58
1:A:118:MET:HB2	1:A:205:PHE:HB2	1.86	0.58
1:B:814:MET:HE1	1:D:291:ALA:HA	1.85	0.58
1:A:569:LEU:O	1:A:671:ARG:HD3	2.04	0.57
1:A:153:ARG:O	1:A:173:LYS:HE2	2.04	0.57
5:A:903[D]:6A9:C14	7:A:1299:HOH:O	2.52	0.57
1:B:424:ALA:CA	6:C:905:7PG:H72	2.33	0.57
1:B:427:PRO:HA	6:C:905:7PG:O6	2.05	0.57
1:A:125:THR:O	1:A:128:THR:O	2.23	0.57
1:D:648:VAL:HG21	1:D:690:SER:HB3	1.86	0.57
1:C:424:ALA:HA	6:C:905:7PG:H81	1.87	0.56
1:D:264:SER:HB3	1:D:306:GLU:HB3	1.86	0.56
1:C:118:MET:HB2	1:C:205:PHE:HB2	1.87	0.56
1:C:569:LEU:O	1:C:671:ARG:HD3	2.05	0.56
1:D:435:VAL:HB	1:D:440[B]:PHE:CZ	2.41	0.56
1:A:475:LEU:HD23	1:A:481:ILE:HG13	1.87	0.56
1:D:662:MLY:HD3	1:D:664:ARG:HE	1.71	0.56
1:C:514:LEU:O	1:C:517:VAL:HG22	2.06	0.55
1:C:422:ASP:CB	6:C:905:7PG:H131	2.36	0.55
1:B:435:VAL:HB	1:B:440[B]:PHE:HE1	1.70	0.55
1:B:440[B]:PHE:CE2	1:B:443:ARG:HB2	2.41	0.55
1:B:153:ARG:O	1:B:173:LYS:HE3	2.07	0.55
1:D:153:ARG:O	1:D:173:LYS:HE3	2.06	0.55
1:D:514:LEU:O	1:D:517:VAL:HG22	2.07	0.55
1:B:246:PRO:HG3	1:B:323:LEU:HD11	1.89	0.55
1:A:437:SER:O	1:A:440[B]:PHE:CD1	2.59	0.55
1:D:118:MET:HB2	1:D:205:PHE:HB2	1.88	0.54
1:D:554:PRO:O	6:D:906:7PG:H152	2.07	0.54
1:C:153:ARG:O	1:C:173:LYS:HE3	2.07	0.54
1:D:332:VAL:HG21	1:D:350:VAL:HG12	1.88	0.54
1:D:440[B]:PHE:HE2	1:D:445:PHE:CE1	2.24	0.54
6:B:906:7PG:C13	6:C:905:7PG:H141	2.38	0.54
1:D:640:LEU:HD21	6:D:906:7PG:H141	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LEU:CD1	6:B:906:7PG:H162	2.38	0.54
1:B:569:LEU:O	1:B:671:ARG:CD	2.56	0.53
1:A:126:PRO:C	1:A:128:THR:H	2.10	0.53
1:B:126:PRO:HB3	1:C:126:PRO:HB2	1.89	0.53
1:C:356:GLN:HA	1:C:359:GLU:HG2	1.90	0.53
1:A:127:GLY:H	1:D:127:GLY:N	1.95	0.53
1:C:422:ASP:HB2	6:C:905:7PG:C13	2.38	0.53
1:A:405:GLN:HE21	6:D:905:7PG:H141	1.74	0.53
1:A:436:PRO:HD2	1:A:440[B]:PHE:CE2	2.44	0.53
1:B:475:LEU:HD23	1:B:481:ILE:HG13	1.89	0.53
6:B:906:7PG:H92	6:C:905:7PG:H91	1.92	0.52
1:A:313:GLN:HG2	1:D:499:PHE:CZ	2.44	0.52
1:D:569:LEU:O	1:D:671:ARG:HD3	2.09	0.52
1:A:427:PRO:HA	6:D:905:7PG:C15	2.38	0.52
1:B:475:LEU:HD21	1:B:541:TRP:HB2	1.92	0.52
6:B:906:7PG:H81	6:C:905:7PG:C9	2.39	0.52
1:D:425:LEU:H	6:D:905:7PG:C10	2.22	0.52
1:B:425:LEU:H	6:C:905:7PG:C7	2.23	0.52
1:A:205:PHE:HB3	1:A:318:ILE:HD11	1.93	0.51
1:B:807:SER:HB2	1:B:814:MET:CE	2.41	0.51
1:C:475:LEU:HD21	1:C:541:TRP:HB2	1.93	0.51
1:D:687:GLY:HA2	1:D:719:LEU:HD11	1.92	0.50
1:D:425:LEU:O	6:D:905:7PG:C7	2.60	0.50
1:D:427:PRO:CB	6:D:905:7PG:H41	2.42	0.50
1:B:807:SER:HB2	1:B:814:MET:HE3	1.93	0.50
1:B:200:PRO:HD2	1:B:325:ALA:HB3	1.94	0.50
1:B:422:ASP:HB2	6:C:905:7PG:H22	1.94	0.50
1:D:475:LEU:HD21	1:D:541:TRP:HB2	1.93	0.50
1:D:554:PRO:O	6:D:906:7PG:C15	2.60	0.50
1:B:437:SER:O	1:B:440[B]:PHE:CD1	2.59	0.49
1:B:440[B]:PHE:HE2	1:B:443:ARG:HB2	1.77	0.49
1:B:807:SER:HA	1:B:814:MET:HE3	1.95	0.49
1:C:436:PRO:CD	1:C:440[B]:PHE:HZ	2.22	0.49
1:A:435:VAL:HB	1:A:440[B]:PHE:CZ	2.48	0.48
1:C:640:LEU:CD2	6:C:906:7PG:H122	2.42	0.48
1:D:374:GLN:OE1	1:D:378:MLY:HH23	2.14	0.48
1:A:427:PRO:HG3	6:A:907:7PG:H131	1.94	0.48
1:B:72:LEU:HD11	6:B:906:7PG:H162	1.96	0.48
6:A:907:7PG:C4	6:D:905:7PG:H61	2.38	0.48
1:B:313:GLN:HG2	1:C:499:PHE:CE2	2.49	0.47
1:D:424:ALA:HA	6:D:905:7PG:H101	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:553:VAL:HG21	6:D:906:7PG:H122	1.97	0.47
1:C:640:LEU:HD23	6:C:906:7PG:H122	1.97	0.47
1:C:566:LEU:HB2	1:C:569:LEU:HD12	1.97	0.47
1:B:205:PHE:HB3	1:B:318:ILE:HD11	1.96	0.47
1:D:373:PHE:O	1:D:378:MLY:HH22	2.15	0.47
1:C:648:VAL:HG21	1:C:690:SER:HB3	1.97	0.47
1:C:440[A]:PHE:HE1	1:C:816[A]:CYS:HG	1.62	0.47
1:B:264:SER:HB3	1:B:306:GLU:HB3	1.97	0.47
1:C:365:PHE:HE1	1:C:389:GLN:HG3	1.79	0.47
1:B:63:TRP:HZ3	6:B:906:7PG:H52	1.79	0.46
1:C:422:ASP:CG	6:C:905:7PG:H131	2.32	0.46
1:A:370:GLU:OE1	1:A:376:MLY:HB2	2.14	0.46
1:D:807:SER:O	1:D:811:GLY:HA2	2.16	0.46
1:B:63:TRP:CZ3	6:B:906:7PG:H52	2.50	0.46
1:C:378:MLY:HH22	1:C:831:ALA:O	2.16	0.46
1:C:662:MLY:HH13	1:C:672:VAL:HG11	1.97	0.46
1:D:435:VAL:HB	1:D:440[B]:PHE:CE1	2.51	0.46
1:A:114:LEU:HD13	1:A:269:LEU:HD21	1.97	0.46
1:A:425:LEU:HB2	6:D:905:7PG:H111	1.98	0.45
1:A:427:PRO:CA	6:D:905:7PG:H152	2.44	0.45
1:D:425:LEU:O	6:D:905:7PG:H72	2.17	0.45
1:A:424:ALA:CA	6:D:905:7PG:H92	2.45	0.45
1:D:200:PRO:HD2	1:D:325:ALA:HB3	1.98	0.45
1:C:200:PRO:HD2	1:C:325:ALA:HB3	1.99	0.44
1:B:402:PHE:CE1	1:B:442:PRO:HB2	2.53	0.44
1:B:814:MET:HE1	1:D:291:ALA:CA	2.46	0.44
1:B:424:ALA:CB	6:C:905:7PG:H61	2.47	0.44
1:B:436:PRO:HD2	1:B:440[B]:PHE:CZ	2.52	0.44
1:B:736:MLY:HH11	1:B:809:GLN:OE1	2.17	0.44
1:D:736:MLY:HG2	7:D:1025:HOH:O	2.16	0.44
1:D:427:PRO:CA	6:D:905:7PG:H51	2.48	0.44
1:B:427:PRO:HB3	6:B:906:7PG:H161	1.99	0.44
1:B:67:ARG:HE	6:B:906:7PG:H102	1.83	0.44
1:B:687:GLY:HA2	1:B:719:LEU:HD11	2.00	0.44
1:B:280:LEU:HD23	1:B:299:LEU:CD1	2.47	0.43
1:B:440[B]:PHE:HZ	1:B:443:ARG:O	2.00	0.43
1:C:205:PHE:HB3	1:C:318:ILE:HD11	2.00	0.43
1:C:431:LEU:HD13	1:C:474:LEU:HD11	2.00	0.43
1:D:424:ALA:CA	6:D:905:7PG:H101	2.48	0.43
1:D:517:VAL:HG23	1:D:835:ALA:HB1	2.00	0.43
1:D:648:VAL:CG2	1:D:690:SER:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:LEU:HD13	1:D:474:LEU:HD11	2.00	0.43
1:A:440[B]:PHE:HZ	1:A:443:ARG:O	2.01	0.43
1:B:431:LEU:HD13	1:B:474:LEU:HD11	2.01	0.43
1:D:659:VAL:HG12	1:D:673:VAL:HG22	2.00	0.43
1:A:200:PRO:HD2	1:A:325:ALA:HB3	2.01	0.43
1:C:687:GLY:HA2	1:C:719:LEU:HD11	2.00	0.43
1:A:264:SER:HB3	1:A:306:GLU:HB3	2.01	0.42
1:D:422:ASP:HB2	6:D:905:7PG:C15	2.38	0.42
1:A:288:PRO:HG2	1:A:291:ALA:HB3	2.01	0.42
1:B:440[B]:PHE:HE2	1:B:445:PHE:CE1	2.19	0.42
1:B:280:LEU:CD2	1:B:299:LEU:CD1	2.96	0.42
1:D:480:TRP:CE2	1:D:504:ALA:HA	2.55	0.42
1:C:449:GLU:HG2	1:C:471:TRP:NE1	2.35	0.42
1:D:593:ARG:NH1	6:D:906:7PG:H112	2.34	0.42
1:A:496:PRO:HG2	1:A:499:PHE:CD1	2.55	0.42
1:C:639:GLU:O	6:C:906:7PG:H102	2.20	0.42
1:C:424:ALA:CA	6:C:905:7PG:H81	2.48	0.42
1:A:440[B]:PHE:CE2	1:A:445:PHE:CE1	2.98	0.42
1:C:436:PRO:CD	1:C:440[B]:PHE:CZ	2.77	0.42
1:C:521:GLU:HG3	7:C:1101:HOH:O	2.19	0.42
1:C:80:PRO:HA	1:C:533:MLY:CH1	2.49	0.42
1:B:807:SER:CA	1:B:814:MET:HE3	2.50	0.41
1:D:205:PHE:HB3	1:D:318:ILE:HD11	2.02	0.41
1:D:449:GLU:HG2	1:D:471:TRP:NE1	2.35	0.41
1:A:528:LEU:HD13	1:A:528:LEU:HA	1.96	0.41
1:C:593:ARG:NH1	6:C:906:7PG:H112	2.34	0.41
1:A:425:LEU:O	6:D:905:7PG:C11	2.68	0.41
1:B:422:ASP:HB2	6:C:905:7PG:C2	2.49	0.41
1:D:440[B]:PHE:HZ	1:D:443:ARG:O	2.03	0.41
6:C:905:7PG:H102	6:C:905:7PG:H121	1.64	0.41
1:A:431:LEU:HD13	1:A:474:LEU:HD11	2.02	0.41
1:B:68:ARG:HG2	1:B:477:ALA:HB3	2.02	0.41
1:C:480:TRP:CE2	1:C:504:ALA:HA	2.56	0.41
1:D:365:PHE:HE1	1:D:389:GLN:HG3	1.84	0.41
1:B:736:MLY:HH11	1:B:809:GLN:CD	2.41	0.41
1:C:332:VAL:HG21	1:C:350:VAL:HG12	2.01	0.41
1:D:425:LEU:N	6:D:905:7PG:H101	2.30	0.41
1:A:475:LEU:HD21	1:A:541:TRP:HB2	2.03	0.41
1:A:838:SER:HB3	7:A:1133:HOH:O	2.20	0.41
1:B:233:THR:HG23	1:B:239:PHE:HE2	1.86	0.41
1:D:394:GLY:HA3	1:D:820:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PRO:CG	6:A:907:7PG:H131	2.51	0.41
1:B:496:PRO:HG2	1:B:499:PHE:CD1	2.55	0.40
1:D:553:VAL:HG21	6:D:906:7PG:C12	2.51	0.40
1:D:659:VAL:HG22	7:D:1182:HOH:O	2.20	0.40
1:C:378:MLY:HH22	1:C:831:ALA:HB1	2.03	0.40
1:B:425:LEU:CB	6:C:905:7PG:H82	2.48	0.40
1:D:520:LEU:HA	1:D:520:LEU:HD12	1.86	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	727/795 (91%)	701 (96%)	25 (3%)	1 (0%)	51	54
1	B	728/795 (92%)	707 (97%)	21 (3%)	0	100	100
1	C	740/795 (93%)	719 (97%)	20 (3%)	1 (0%)	51	54
1	D	747/795 (94%)	726 (97%)	21 (3%)	0	100	100
All	All	2942/3180 (92%)	2853 (97%)	87 (3%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	442	PRO
1	A	442	PRO

### 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	611/642 (95%)	604 (99%)	7 (1%)	73	79
1	B	611/642 (95%)	599 (98%)	12 (2%)	55	60
1	C	619/642 (96%)	610 (98%)	9 (2%)	65	71
1	D	621/642 (97%)	611 (98%)	10 (2%)	62	69
All	All	2462/2568 (96%)	2424 (98%)	38 (2%)	65	71

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	198	SER
1	A	255	LYS
1	A	447	TRP
1	A	508	ASN
1	A	746	TYR
1	A	817	ARG
1	B	67	ARG
1	B	68	ARG
1	B	155	PHE
1	B	198	SER
1	B	255	LYS
1	B	292	SER
1	B	447	TRP
1	B	508	ASN
1	B	520	LEU
1	B	583	PRO
1	B	746	TYR
1	B	817	ARG
1	C	63	TRP
1	C	155	PHE
1	C	198	SER
1	C	447	TRP
1	C	508	ASN
1	C	583	PRO
1	C	746	TYR
1	C	797	GLN
1	C	817	ARG
1	D	63	TRP
1	D	155	PHE

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Mol	Chain	Res	Type
1	D	198	SER
1	D	447	TRP
1	D	508	ASN
1	D	660	GLN
1	D	719	LEU
1	D	746	TYR
1	D	797	GLN
1	D	817	ARG

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

Mol	Chain	Res	Type
1	A	405	GLN
1	C	667	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

60 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	MLY	B	131	1	9,10,11	1.00	0	6,11,13	1.85	1 (16%)
1	MLY	C	304	1	9,10,11	1.24	0	6,11,13	1.75	1 (16%)
1	MLY	A	376	1	9,10,11	0.87	0	6,11,13	0.68	0
1	MLY	A	304	1	9,10,11	1.29	1 (11%)	6,11,13	2.10	4 (66%)
1	SME	A	519	1	7,8,9	3.15	2 (28%)	4,9,11	1.10	0
1	MLY	C	779	1	9,10,11	1.06	1 (11%)	6,11,13	1.62	1 (16%)
1	SME	C	519	1	7,8,9	1.78	1 (14%)	4,9,11	2.59	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	736	1	9,10,11	1.29	1 (11%)	6,11,13	1.79	2 (33%)
1	MLY	C	662	1	9,10,11	1.14	0	6,11,13	1.12	0
1	MLY	C	131	1	9,10,11	0.98	0	6,11,13	2.01	1 (16%)
1	MLY	B	111	1	9,10,11	1.23	2 (22%)	6,11,13	1.96	3 (50%)
1	MLY	B	227	1	9,10,11	0.93	0	6,11,13	0.88	0
1	MLY	A	366	1	9,10,11	0.78	0	6,11,13	1.10	0
1	MLY	A	378	1	9,10,11	0.67	0	6,11,13	5.11	5 (83%)
1	MLY	C	533	1	9,10,11	1.40	2 (22%)	6,11,13	1.84	2 (33%)
1	MLY	C	371	1	9,10,11	1.17	0	6,11,13	1.79	3 (50%)
1	MLY	A	662	1	9,10,11	1.02	0	6,11,13	1.31	1 (16%)
1	SME	D	421	1	7,8,9	1.62	2 (28%)	4,9,11	1.75	1 (25%)
1	MLY	D	304	1	9,10,11	1.15	1 (11%)	6,11,13	1.47	2 (33%)
1	MLY	B	662	1	9,10,11	1.07	0	6,11,13	1.45	1 (16%)
1	MLY	A	779	1	9,10,11	1.00	0	6,11,13	1.76	2 (33%)
1	MLY	B	378	1	9,10,11	0.69	0	6,11,13	1.58	1 (16%)
1	MLY	D	111	1	9,10,11	1.05	1 (11%)	6,11,13	2.04	3 (50%)
1	MLY	B	533	1	9,10,11	0.69	0	6,11,13	0.85	0
1	SME	C	421	1	7,8,9	1.57	2 (28%)	4,9,11	1.85	2 (50%)
1	MLY	D	376	1	9,10,11	1.17	1 (11%)	6,11,13	0.92	0
1	MLY	B	366	1	9,10,11	0.85	0	6,11,13	1.14	0
1	MLY	A	227	1	9,10,11	1.09	0	6,11,13	0.81	0
1	MLY	D	371	1	9,10,11	0.84	0	6,11,13	1.30	0
1	MLY	B	304	1	9,10,11	1.11	0	6,11,13	0.67	0
1	MLY	D	131	1	9,10,11	1.09	1 (11%)	6,11,13	1.90	2 (33%)
1	MLY	A	533	1	9,10,11	0.80	0	6,11,13	1.53	2 (33%)
1	MLY	B	371	1	9,10,11	1.07	1 (11%)	6,11,13	1.32	1 (16%)
1	MLY	B	573	1	9,10,11	0.95	0	6,11,13	2.18	1 (16%)
1	MLY	A	573	1	9,10,11	1.02	0	6,11,13	2.43	1 (16%)
1	MLY	B	779	1	9,10,11	0.91	0	6,11,13	1.64	2 (33%)
1	SME	B	519	1	7,8,9	1.73	2 (28%)	4,9,11	2.03	1 (25%)
1	MLY	C	736	1	9,10,11	1.95	1 (11%)	6,11,13	0.96	0
1	MLY	D	736	1	9,10,11	1.27	1 (11%)	6,11,13	2.06	4 (66%)
1	MLY	D	533	1	9,10,11	0.70	0	6,11,13	1.17	0
1	MLY	A	371	1	9,10,11	1.06	1 (11%)	6,11,13	2.00	3 (50%)
1	MLY	D	378	1	9,10,11	0.81	0	6,11,13	2.99	1 (16%)
1	MLY	D	227	1	9,10,11	0.94	0	6,11,13	1.32	1 (16%)
1	MLY	C	366	1	9,10,11	0.94	0	6,11,13	1.08	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SME	B	421	1	7,8,9	1.21	1 (14%)	4,9,11	2.15	2 (50%)
1	MLY	A	111	1	9,10,11	0.92	0	6,11,13	1.48	1 (16%)
1	MLY	C	376	1	9,10,11	0.95	0	6,11,13	1.15	0
1	MLY	D	662	1	9,10,11	0.90	0	6,11,13	0.91	0
1	MLY	B	736	1	9,10,11	0.92	0	6,11,13	2.89	3 (50%)
1	MLY	D	573	1	9,10,11	0.96	0	6,11,13	1.81	1 (16%)
1	MLY	C	573	1	9,10,11	1.02	0	6,11,13	1.77	1 (16%)
1	SME	A	421	1	7,8,9	1.17	1 (14%)	4,9,11	2.13	3 (75%)
1	MLY	C	227	1	9,10,11	1.31	2 (22%)	6,11,13	1.86	3 (50%)
1	MLY	D	779	1	9,10,11	1.16	1 (11%)	6,11,13	1.51	1 (16%)
1	MLY	B	376	1	9,10,11	0.73	0	6,11,13	1.12	0
1	MLY	A	131	1	9,10,11	0.86	0	6,11,13	1.49	1 (16%)
1	MLY	C	378	1	9,10,11	0.77	0	6,11,13	2.36	3 (50%)
1	MLY	C	111	1	9,10,11	0.90	0	6,11,13	1.83	2 (33%)
1	MLY	D	366	1	9,10,11	0.95	0	6,11,13	1.01	0
1	SME	D	519	1	7,8,9	2.01	1 (14%)	4,9,11	3.24	3 (75%)

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
1	MLY	B	131	1	-	1/8/9/11	-
1	MLY	C	304	1	-	3/8/9/11	-
1	MLY	A	376	1	-	6/8/9/11	-
1	MLY	A	304	1	-	4/8/9/11	-
1	SME	A	519	1	-	2/6/7/9	-
1	MLY	C	779	1	-	5/8/9/11	-
1	SME	C	519	1	-	2/6/7/9	-
1	MLY	A	736	1	-	2/8/9/11	-
1	MLY	C	662	1	-	1/8/9/11	-
1	MLY	C	131	1	-	1/8/9/11	-
1	MLY	B	111	1	-	2/8/9/11	-
1	MLY	B	227	1	-	1/8/9/11	-
1	MLY	A	366	1	-	3/8/9/11	-
1	MLY	A	378	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	C	533	1	-	6/8/9/11	-
1	MLY	C	371	1	-	3/8/9/11	-
1	MLY	A	662	1	-	2/8/9/11	-
1	SME	D	421	1	-	2/6/7/9	-
1	MLY	D	304	1	-	5/8/9/11	-
1	MLY	B	662	1	-	3/8/9/11	-
1	MLY	A	779	1	-	3/8/9/11	-
1	MLY	B	378	1	-	4/8/9/11	-
1	MLY	D	111	1	-	2/8/9/11	-
1	MLY	B	533	1	-	5/8/9/11	-
1	SME	C	421	1	-	2/6/7/9	-
1	MLY	D	376	1	-	3/8/9/11	-
1	MLY	B	366	1	-	3/8/9/11	-
1	MLY	A	227	1	-	2/8/9/11	-
1	MLY	D	371	1	-	3/8/9/11	-
1	MLY	B	304	1	-	4/8/9/11	-
1	MLY	D	131	1	-	3/8/9/11	-
1	MLY	A	533	1	-	4/8/9/11	-
1	MLY	B	371	1	-	4/8/9/11	-
1	MLY	B	573	1	-	0/8/9/11	-
1	MLY	A	573	1	-	0/8/9/11	-
1	MLY	B	779	1	-	2/8/9/11	-
1	SME	B	519	1	-	0/6/7/9	-
1	MLY	C	736	1	-	4/8/9/11	-
1	MLY	D	736	1	-	5/8/9/11	-
1	MLY	D	533	1	-	5/8/9/11	-
1	MLY	A	371	1	-	3/8/9/11	-
1	MLY	D	378	1	-	2/8/9/11	-
1	MLY	D	227	1	-	4/8/9/11	-
1	MLY	C	366	1	-	3/8/9/11	-
1	SME	B	421	1	-	3/6/7/9	-
1	MLY	A	111	1	-	1/8/9/11	-
1	MLY	C	376	1	-	2/8/9/11	-
1	MLY	D	662	1	-	5/8/9/11	-
1	MLY	B	736	1	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	573	1	-	0/8/9/11	-
1	MLY	C	573	1	-	0/8/9/11	-
1	SME	A	421	1	-	3/6/7/9	-
1	MLY	C	227	1	-	3/8/9/11	-
1	MLY	D	779	1	-	3/8/9/11	-
1	MLY	B	376	1	-	3/8/9/11	-
1	MLY	A	131	1	-	3/8/9/11	-
1	MLY	C	378	1	-	2/8/9/11	-
1	MLY	C	111	1	-	2/8/9/11	-
1	MLY	D	366	1	-	3/8/9/11	-
1	SME	D	519	1	-	1/6/7/9	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	SME	OE-S	-6.64	1.32	1.50
1	C	736	MLY	CB-CA	5.07	1.60	1.53
1	A	519	SME	CB-CA	-4.90	1.47	1.53
1	D	519	SME	OE-S	-4.79	1.37	1.50
1	C	519	SME	OE-S	-4.11	1.39	1.50
1	B	519	SME	OE-S	-3.35	1.41	1.50
1	C	421	SME	OE-S	-3.27	1.41	1.50
1	A	736	MLY	CB-CA	3.17	1.57	1.53
1	D	421	SME	OE-S	-2.95	1.42	1.50
1	B	519	SME	CB-CA	-2.89	1.49	1.53
1	D	421	SME	CB-CA	-2.69	1.50	1.53
1	A	421	SME	OE-S	-2.63	1.43	1.50
1	C	533	MLY	CH2-NZ	2.62	1.54	1.46
1	D	131	MLY	CB-CA	-2.60	1.50	1.53
1	C	533	MLY	CH1-NZ	-2.54	1.38	1.46
1	A	371	MLY	CH1-NZ	2.52	1.53	1.46
1	B	421	SME	OE-S	-2.51	1.43	1.50
1	C	227	MLY	CH1-NZ	2.51	1.53	1.46
1	D	779	MLY	CH2-NZ	2.37	1.53	1.46
1	B	371	MLY	CB-CA	-2.21	1.50	1.53
1	D	736	MLY	CB-CA	2.21	1.56	1.53
1	C	227	MLY	CH2-NZ	2.19	1.52	1.46
1	C	779	MLY	CH2-NZ	2.19	1.52	1.46
1	B	111	MLY	CE-NZ	2.17	1.54	1.46
1	A	304	MLY	CB-CA	2.14	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	421	SME	CB-CA	-2.09	1.50	1.53
1	D	111	MLY	CE-NZ	2.08	1.53	1.46
1	B	111	MLY	CH2-NZ	2.07	1.52	1.46
1	D	376	MLY	CD-CE	2.04	1.60	1.51
1	D	304	MLY	CB-CA	2.03	1.56	1.53

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	MLY	CH2-NZ-CH1	-10.65	82.20	109.73
1	D	378	MLY	CH2-NZ-CH1	-6.86	92.00	109.73
1	A	573	MLY	CH2-NZ-CH1	-5.55	95.39	109.73
1	B	736	MLY	CH2-NZ-CH1	-5.14	96.44	109.73
1	B	573	MLY	CH2-NZ-CH1	-5.06	96.66	109.73
1	D	519	SME	OE-S-CE	5.04	116.45	106.25
1	C	519	SME	OE-S-CE	4.37	115.09	106.25
1	C	131	MLY	CD-CG-CB	-4.26	98.57	113.62
1	D	573	MLY	CH2-NZ-CH1	-4.17	98.96	109.73
1	C	573	MLY	CH2-NZ-CH1	-4.08	99.19	109.73
1	C	378	MLY	CH2-NZ-CE	4.02	126.66	110.74
1	B	519	SME	OE-S-CE	-3.88	98.40	106.25
1	C	304	MLY	CH2-NZ-CH1	-3.83	99.82	109.73
1	B	131	MLY	CD-CG-CB	-3.81	100.15	113.62
1	A	378	MLY	CH2-NZ-CE	-3.74	95.92	110.74
1	A	378	MLY	CD-CE-NZ	-3.50	104.32	113.79
1	C	378	MLY	CD-CE-NZ	3.46	123.14	113.79
1	B	111	MLY	CH2-NZ-CE	3.45	124.39	110.74
1	C	533	MLY	CH2-NZ-CE	3.38	124.13	110.74
1	A	378	MLY	CH1-NZ-CE	3.31	123.85	110.74
1	D	131	MLY	CD-CG-CB	-3.29	101.98	113.62
1	B	736	MLY	CD-CG-CB	-3.24	102.15	113.62
1	D	111	MLY	CH2-NZ-CE	3.20	123.43	110.74
1	D	131	MLY	CD-CE-NZ	-3.15	105.25	113.79
1	A	779	MLY	CH2-NZ-CE	3.15	123.20	110.74
1	C	779	MLY	CD-CG-CB	-3.04	102.86	113.62
1	D	519	SME	OE-S-CG	2.98	114.24	106.03
1	B	736	MLY	CH1-NZ-CE	-2.89	99.28	110.74
1	A	371	MLY	CH2-NZ-CE	-2.84	99.48	110.74
1	C	371	MLY	CD-CG-CB	-2.83	103.62	113.62
1	C	227	MLY	CD-CG-CB	-2.81	103.67	113.62
1	D	736	MLY	CD-CE-NZ	2.81	121.38	113.79
1	B	421	SME	CE-S-CG	2.78	104.04	97.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	MLY	CD-CG-CB	-2.75	103.91	113.62
1	A	779	MLY	CD-CG-CB	-2.72	104.00	113.62
1	D	111	MLY	CD-CG-CB	-2.71	104.04	113.62
1	B	662	MLY	CH2-NZ-CH1	-2.66	102.86	109.73
1	A	304	MLY	CD-CG-CB	-2.66	104.22	113.62
1	D	111	MLY	CD-CE-NZ	2.58	120.78	113.79
1	B	371	MLY	CD-CG-CB	-2.56	104.56	113.62
1	D	519	SME	CE-S-CG	-2.55	91.92	97.71
1	B	421	SME	OE-S-CG	2.52	112.98	106.03
1	A	421	SME	OE-S-CG	2.51	112.94	106.03
1	A	736	MLY	CD-CG-CB	-2.51	104.76	113.62
1	B	378	MLY	CH2-NZ-CH1	-2.49	103.28	109.73
1	A	304	MLY	CH2-NZ-CH1	-2.49	103.30	109.73
1	A	371	MLY	CD-CG-CB	-2.47	104.89	113.62
1	A	304	MLY	CH2-NZ-CE	2.47	120.52	110.74
1	D	421	SME	OE-S-CG	2.45	112.77	106.03
1	B	779	MLY	CD-CG-CB	-2.43	105.04	113.62
1	A	131	MLY	CH2-NZ-CE	-2.42	101.14	110.74
1	A	533	MLY	CD-CE-NZ	-2.41	107.27	113.79
1	A	662	MLY	CD-CG-CB	-2.40	105.14	113.62
1	A	421	SME	OE-S-CE	2.38	111.07	106.25
1	D	779	MLY	CD-CG-CB	-2.38	105.20	113.62
1	D	736	MLY	CH2-NZ-CH1	-2.37	103.60	109.73
1	C	111	MLY	CD-CE-NZ	2.36	120.17	113.79
1	B	111	MLY	CD-CG-CB	-2.31	105.45	113.62
1	D	227	MLY	CD-CE-NZ	-2.30	107.57	113.79
1	B	779	MLY	CH2-NZ-CE	2.27	119.75	110.74
1	C	421	SME	OE-S-CG	2.27	112.29	106.03
1	D	736	MLY	CH1-NZ-CE	-2.25	101.81	110.74
1	D	304	MLY	CD-CG-CB	-2.24	105.71	113.62
1	A	111	MLY	CD-CG-CB	-2.23	105.75	113.62
1	A	736	MLY	CG-CD-CE	-2.20	103.05	113.21
1	A	421	SME	CE-S-CG	2.20	102.72	97.71
1	C	533	MLY	CG-CD-CE	2.19	123.32	113.21
1	A	371	MLY	CG-CD-CE	-2.17	103.21	113.21
1	A	533	MLY	CD-CG-CB	-2.16	105.99	113.62
1	C	227	MLY	CH2-NZ-CH1	2.13	115.24	109.73
1	C	378	MLY	CD-CG-CB	-2.12	106.12	113.62
1	C	421	SME	CE-S-CG	2.11	102.51	97.71
1	A	378	MLY	CD-CG-CB	-2.10	106.19	113.62
1	B	111	MLY	CD-CE-NZ	2.10	119.46	113.79
1	C	371	MLY	CD-CE-NZ	2.09	119.44	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	MLY	CD-CE-NZ	2.08	119.42	113.79
1	D	304	MLY	CH2-NZ-CH1	-2.07	104.37	109.73
1	D	736	MLY	CD-CG-CB	-2.06	106.35	113.62
1	C	371	MLY	CH1-NZ-CE	-2.03	102.70	110.74
1	C	227	MLY	CH2-NZ-CE	2.01	118.70	110.74

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	376	MLY	N-CA-CB-CG
1	A	376	MLY	C-CA-CB-CG
1	A	304	MLY	N-CA-CB-CG
1	A	519	SME	CB-CG-S-OE
1	C	779	MLY	N-CA-CB-CG
1	C	533	MLY	N-CA-CB-CG
1	C	533	MLY	C-CA-CB-CG
1	C	371	MLY	C-CA-CB-CG
1	A	662	MLY	C-CA-CB-CG
1	D	421	SME	O-C-CA-CB
1	D	304	MLY	N-CA-CB-CG
1	B	662	MLY	O-C-CA-CB
1	B	533	MLY	N-CA-CB-CG
1	B	533	MLY	C-CA-CB-CG
1	C	421	SME	O-C-CA-CB
1	A	533	MLY	N-CA-CB-CG
1	A	533	MLY	C-CA-CB-CG
1	B	371	MLY	C-CA-CB-CG
1	C	736	MLY	N-CA-CB-CG
1	C	736	MLY	C-CA-CB-CG
1	D	736	MLY	C-CA-CB-CG
1	D	736	MLY	O-C-CA-CB
1	D	533	MLY	N-CA-CB-CG
1	D	533	MLY	C-CA-CB-CG
1	A	371	MLY	C-CA-CB-CG
1	C	376	MLY	N-CA-CB-CG
1	C	376	MLY	C-CA-CB-CG
1	D	662	MLY	N-CA-CB-CG
1	D	662	MLY	C-CA-CB-CG
1	B	736	MLY	O-C-CA-CB
1	B	376	MLY	O-C-CA-CB
1	B	376	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	C	304	MLY	CD-CE-NZ-CH1
1	A	376	MLY	CD-CE-NZ-CH2
1	B	111	MLY	CD-CE-NZ-CH1
1	B	111	MLY	CD-CE-NZ-CH2
1	B	662	MLY	CD-CE-NZ-CH1
1	B	662	MLY	CD-CE-NZ-CH2
1	B	378	MLY	CD-CE-NZ-CH1
1	B	378	MLY	CD-CE-NZ-CH2
1	D	111	MLY	CD-CE-NZ-CH1
1	B	533	MLY	CD-CE-NZ-CH1
1	B	304	MLY	CD-CE-NZ-CH2
1	D	131	MLY	CD-CE-NZ-CH1
1	A	533	MLY	CD-CE-NZ-CH1
1	A	533	MLY	CD-CE-NZ-CH2
1	B	371	MLY	CD-CE-NZ-CH1
1	B	371	MLY	CD-CE-NZ-CH2
1	D	533	MLY	CD-CE-NZ-CH1
1	D	533	MLY	CD-CE-NZ-CH2
1	D	378	MLY	CD-CE-NZ-CH2
1	D	227	MLY	CD-CE-NZ-CH1
1	D	227	MLY	CD-CE-NZ-CH2
1	D	662	MLY	CD-CE-NZ-CH1
1	D	662	MLY	CD-CE-NZ-CH2
1	C	227	MLY	CD-CE-NZ-CH1
1	A	131	MLY	CD-CE-NZ-CH1
1	A	131	MLY	CD-CE-NZ-CH2
1	A	779	MLY	CG-CD-CE-NZ
1	A	376	MLY	CG-CD-CE-NZ
1	D	376	MLY	CG-CD-CE-NZ
1	B	131	MLY	CG-CD-CE-NZ
1	C	131	MLY	CG-CD-CE-NZ
1	C	378	MLY	CG-CD-CE-NZ
1	D	779	MLY	CG-CD-CE-NZ
1	B	533	MLY	CG-CD-CE-NZ
1	A	378	MLY	CG-CD-CE-NZ
1	D	371	MLY	CG-CD-CE-NZ
1	B	779	MLY	CG-CD-CE-NZ
1	C	779	MLY	CG-CD-CE-NZ
1	D	736	MLY	CG-CD-CE-NZ
1	A	376	MLY	CD-CE-NZ-CH1
1	A	378	MLY	CD-CE-NZ-CH2
1	C	533	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	B	533	MLY	CD-CE-NZ-CH2
1	D	131	MLY	CD-CE-NZ-CH2
1	C	371	MLY	CG-CD-CE-NZ
1	C	533	MLY	CG-CD-CE-NZ
1	D	227	MLY	CA-CB-CG-CD
1	D	111	MLY	CD-CE-NZ-CH2
1	C	227	MLY	CD-CE-NZ-CH2
1	D	371	MLY	CA-CB-CG-CD
1	B	304	MLY	CD-CE-NZ-CH1
1	D	304	MLY	CA-CB-CG-CD
1	A	366	MLY	CD-CE-NZ-CH2
1	A	779	MLY	CD-CE-NZ-CH2
1	B	366	MLY	CD-CE-NZ-CH2
1	C	111	MLY	CD-CE-NZ-CH2
1	A	304	MLY	CA-CB-CG-CD
1	D	662	MLY	CA-CB-CG-CD
1	D	779	MLY	CA-CB-CG-CD
1	A	366	MLY	CE-CD-CG-CB
1	D	736	MLY	CE-CD-CG-CB
1	C	366	MLY	CE-CD-CG-CB
1	D	366	MLY	CE-CD-CG-CB
1	C	366	MLY	CD-CE-NZ-CH2
1	B	366	MLY	CE-CD-CG-CB
1	B	779	MLY	CE-CD-CG-CB
1	C	371	MLY	CE-CD-CG-CB
1	B	227	MLY	CE-CD-CG-CB
1	C	779	MLY	CA-CB-CG-CD
1	A	519	SME	CB-CG-S-CE
1	C	519	SME	CB-CG-S-CE
1	A	227	MLY	CE-CD-CG-CB
1	A	662	MLY	CA-CB-CG-CD
1	B	304	MLY	CE-CD-CG-CB
1	D	371	MLY	CE-CD-CG-CB
1	C	304	MLY	CE-CD-CG-CB
1	B	376	MLY	CA-CB-CG-CD
1	D	366	MLY	CD-CE-NZ-CH2
1	D	779	MLY	CE-CD-CG-CB
1	D	376	MLY	CE-CD-CG-CB
1	C	779	MLY	CE-CD-CG-CB
1	C	304	MLY	CA-CB-CG-CD
1	C	533	MLY	CA-CB-CG-CD
1	A	304	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	C	779	MLY	C-CA-CB-CG
1	D	304	MLY	C-CA-CB-CG
1	D	378	MLY	CD-CE-NZ-CH1
1	C	533	MLY	CE-CD-CG-CB
1	A	376	MLY	CE-CD-CG-CB
1	B	304	MLY	CA-CB-CG-CD
1	B	378	MLY	CG-CD-CE-NZ
1	B	736	MLY	CG-CD-CE-NZ
1	C	519	SME	CB-CG-S-OE
1	B	421	SME	CB-CG-S-OE
1	C	662	MLY	CE-CD-CG-CB
1	C	736	MLY	CD-CE-NZ-CH1
1	A	371	MLY	CD-CE-NZ-CH1
1	B	371	MLY	CE-CD-CG-CB
1	C	378	MLY	CE-CD-CG-CB
1	D	227	MLY	CE-CD-CG-CB
1	B	378	MLY	CE-CD-CG-CB
1	B	421	SME	CB-CG-S-CE
1	A	736	MLY	CG-CD-CE-NZ
1	A	227	MLY	CD-CE-NZ-CH2
1	D	131	MLY	CE-CD-CG-CB
1	D	304	MLY	CG-CD-CE-NZ
1	A	131	MLY	CE-CD-CG-CB
1	D	421	SME	CA-CB-CG-S
1	C	421	SME	CA-CB-CG-S
1	D	376	MLY	N-CA-CB-CG
1	B	421	SME	CA-CB-CG-S
1	A	421	SME	CA-CB-CG-S
1	A	366	MLY	C-CA-CB-CG
1	B	366	MLY	C-CA-CB-CG
1	D	366	MLY	C-CA-CB-CG
1	A	304	MLY	CD-CE-NZ-CH2
1	A	421	SME	CB-CG-S-CE
1	A	421	SME	CB-CG-S-OE
1	D	304	MLY	CD-CE-NZ-CH2
1	D	736	MLY	CD-CE-NZ-CH2
1	C	736	MLY	CE-CD-CG-CB
1	C	366	MLY	C-CA-CB-CG
1	A	779	MLY	CA-CB-CG-CD
1	A	371	MLY	CE-CD-CG-CB
1	D	533	MLY	CA-CB-CG-CD
1	C	111	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	D	519	SME	N-CA-CB-CG
1	A	736	MLY	CE-CD-CG-CB
1	C	227	MLY	CE-CD-CG-CB
1	A	111	MLY	CE-CD-CG-CB

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	376	MLY	1	0
1	C	662	MLY	1	0
1	A	378	MLY	2	0
1	C	533	MLY	1	0
1	B	662	MLY	1	0
1	B	573	MLY	1	0
1	A	573	MLY	1	0
1	D	736	MLY	1	0
1	D	378	MLY	3	0
1	D	662	MLY	1	0
1	B	736	MLY	2	0
1	D	573	MLY	1	0
1	C	573	MLY	1	0
1	C	378	MLY	3	0

## 5.5 Carbohydrates ⓘ

10 monosaccharides 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	NAG	E	1	1,2	14,14,15	0.30	0	17,19,21	0.54	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.87	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.30	0	17,19,21	0.51	0
2	NAG	F	2	2	14,14,15	0.31	0	17,19,21	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	G	1	1,3	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	G	2	3	14,14,15	0.39	0	17,19,21	1.25	1 (5%)
3	BMA	G	3	3	11,11,12	0.61	0	15,15,17	1.25	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.31	0	17,19,21	0.50	0
3	NAG	H	2	3	14,14,15	0.41	0	17,19,21	1.55	3 (17%)
3	BMA	H	3	3	11,11,12	0.63	0	15,15,17	1.28	2 (13%)

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	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	O5-C1-C2	-4.55	104.11	111.29
3	G	2	NAG	O5-C1-C2	-3.91	105.11	111.29
3	G	3	BMA	C1-C2-C3	3.58	114.07	109.67
3	H	3	BMA	C1-C2-C3	3.27	113.68	109.67
2	E	2	NAG	O5-C1-C2	-2.79	106.88	111.29
2	F	2	NAG	O5-C1-C2	-2.73	106.97	111.29
3	H	3	BMA	C1-O5-C5	-2.40	108.94	112.19
3	H	2	NAG	C1-O5-C5	2.37	115.40	112.19
3	H	2	NAG	O4-C4-C3	-2.04	105.64	110.35

There are no chirality outliers.

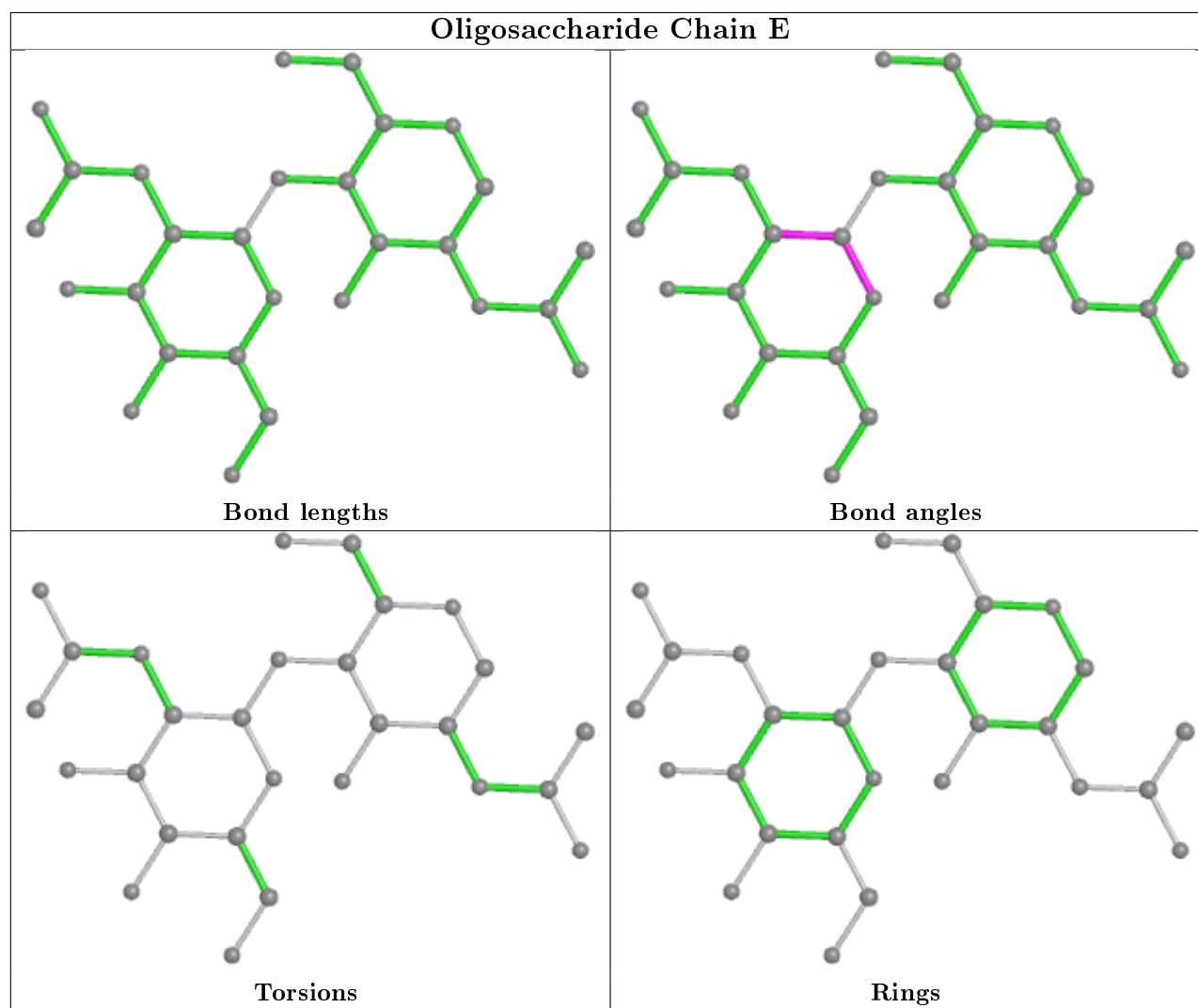
All (6) torsion outliers are listed below:

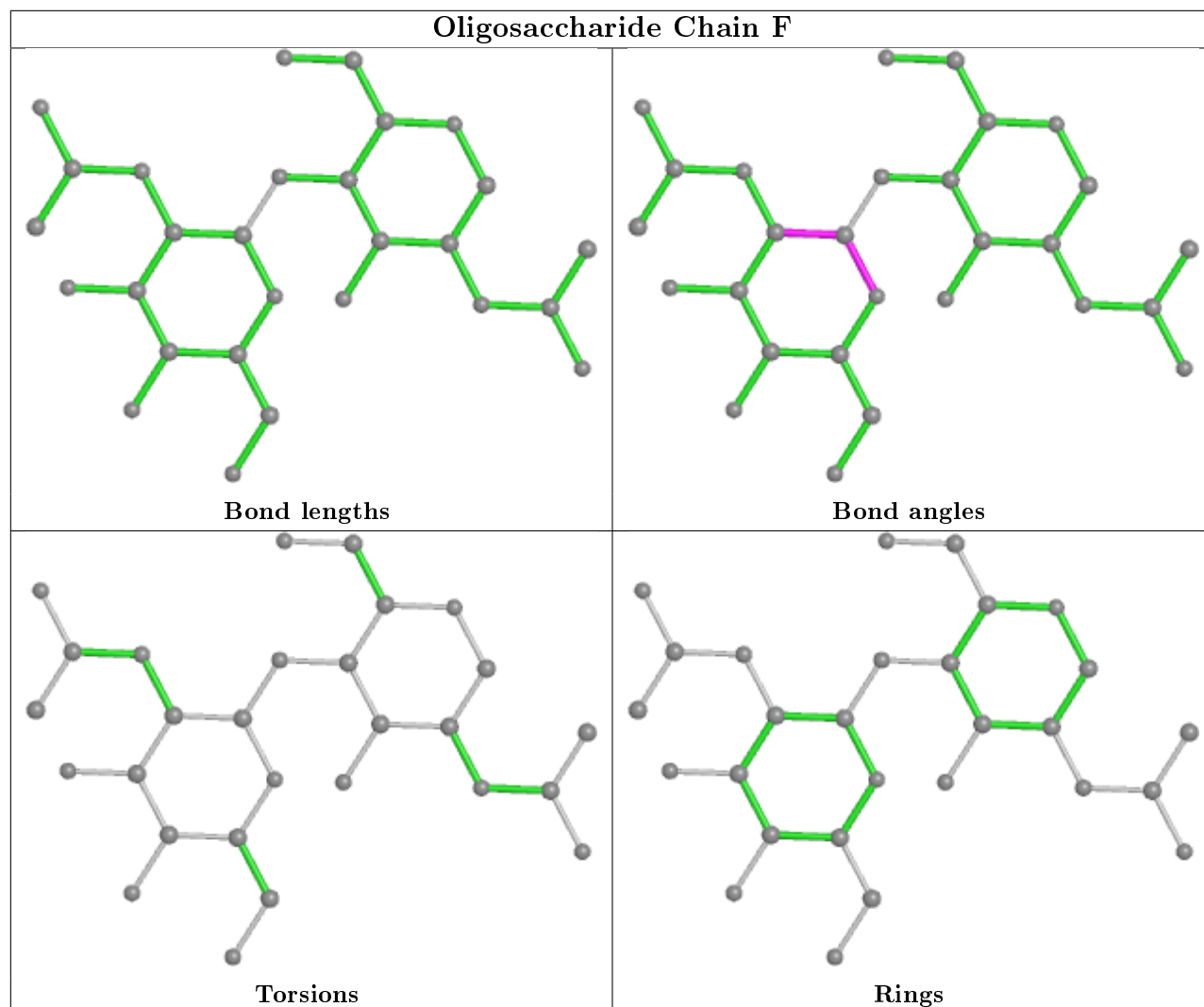
Mol	Chain	Res	Type	Atoms
3	H	3	BMA	C4-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6

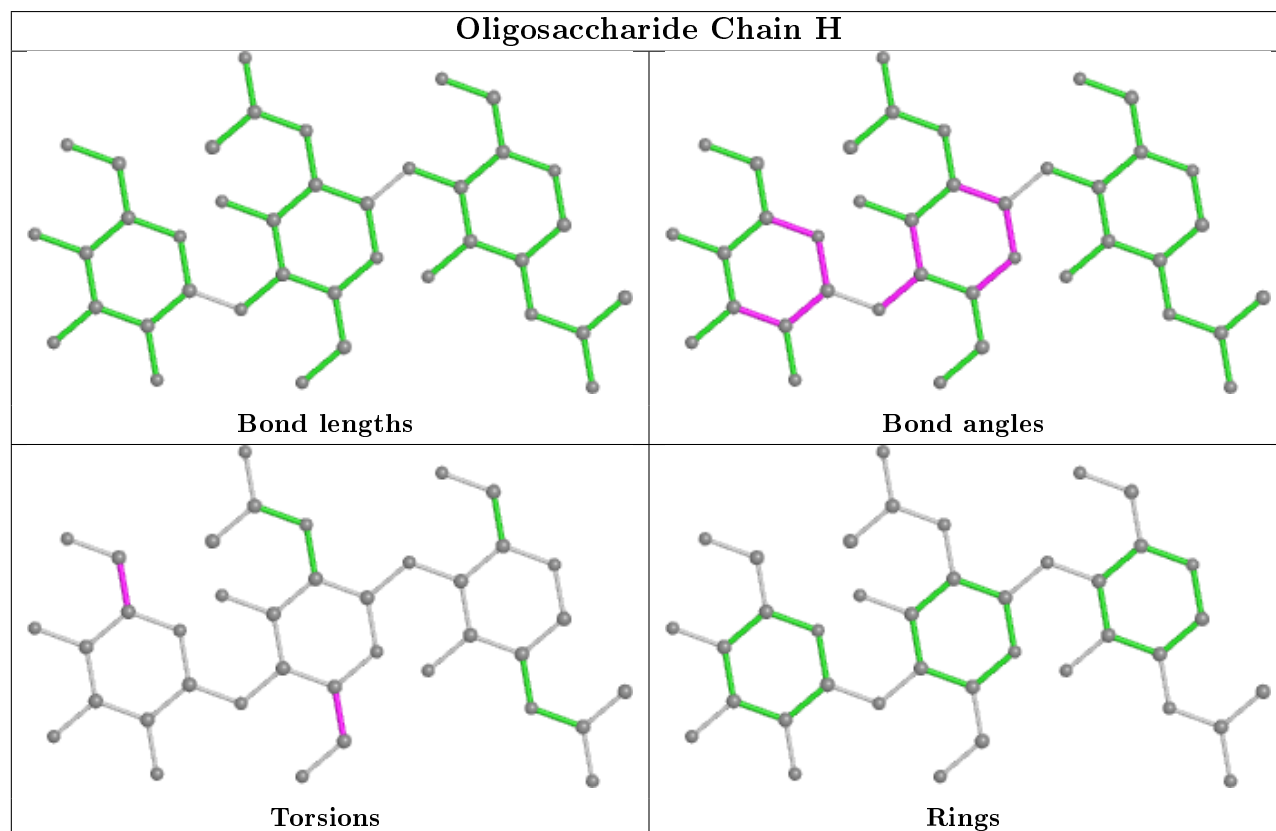
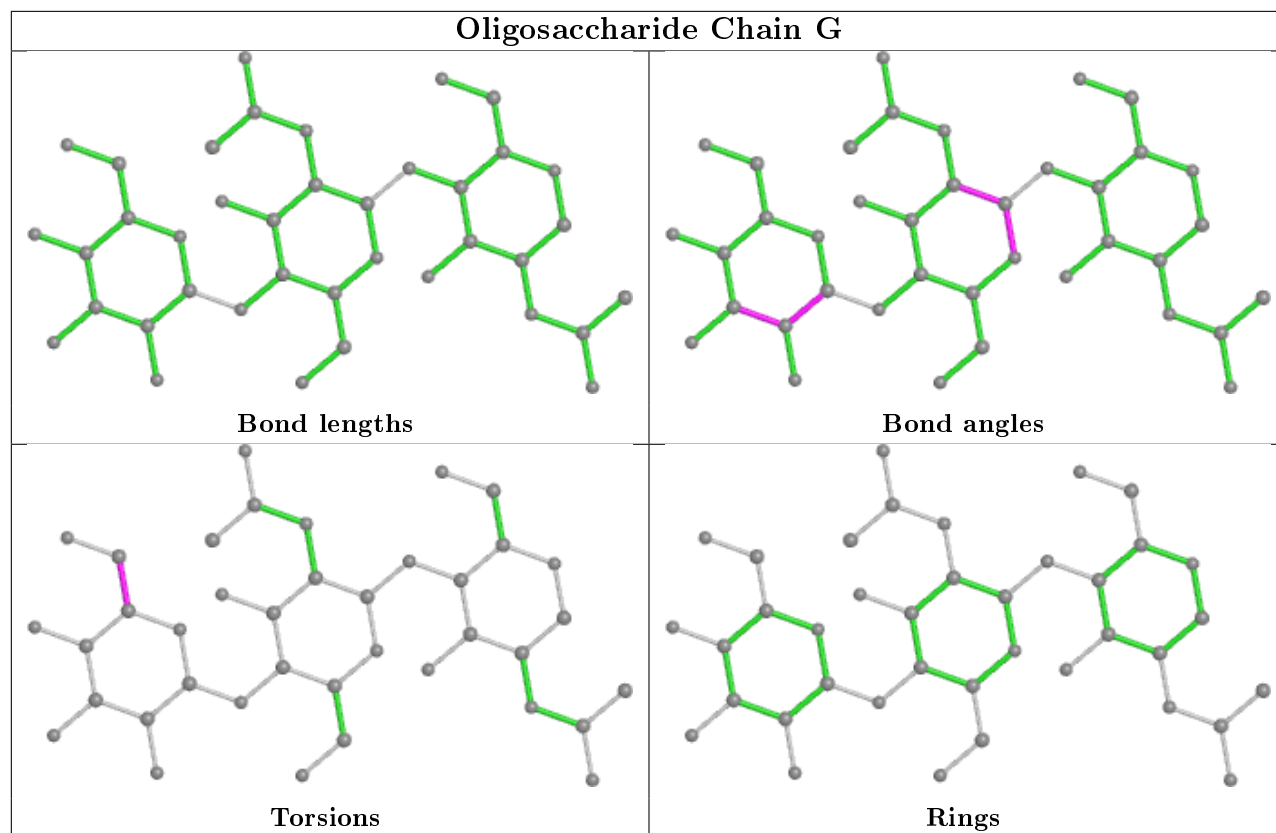
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry

34 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
5	6A9	B	903[D]	-	22,22,22	0.29	0	25,27,27	0.95	3 (12%)
6	7PG	C	906	-	16,16,25	0.27	0	15,15,24	0.45	0
4	SO4	C	903	-	4,4,4	0.14	0	6,6,6	0.07	0
5	6A9	D	904[D]	-	22,22,22	0.30	0	25,27,27	0.94	3 (12%)
4	SO4	D	903	-	4,4,4	0.12	0	6,6,6	0.10	0
4	SO4	C	901	-	4,4,4	0.28	0	6,6,6	0.28	0
6	7PG	D	905	-	21,21,25	0.26	0	20,20,24	0.49	0
4	SO4	A	906	-	4,4,4	0.19	0	6,6,6	0.11	0
4	SO4	D	902	-	4,4,4	0.28	0	6,6,6	0.19	0
4	SO4	D	901	-	4,4,4	0.36	0	6,6,6	0.31	0
4	SO4	A	901	-	4,4,4	0.26	0	6,6,6	0.18	0
5	6A9	D	904[B]	-	22,22,22	0.34	0	25,27,27	1.09	3 (12%)
6	7PG	B	906	-	23,23,25	0.18	0	22,22,24	0.43	0
5	6A9	C	904[A]	-	22,22,22	0.31	0	25,27,27	0.93	3 (12%)
5	6A9	D	904[C]	-	22,22,22	0.29	0	25,27,27	0.95	2 (8%)
5	6A9	D	904[A]	-	22,22,22	0.32	0	25,27,27	0.93	2 (8%)
5	6A9	C	904[C]	-	22,22,22	0.30	0	25,27,27	0.94	2 (8%)
5	6A9	C	904[B]	-	22,22,22	0.34	0	25,27,27	1.07	3 (12%)
5	6A9	C	904[D]	-	22,22,22	0.28	0	25,27,27	0.92	3 (12%)
6	7PG	D	906	-	16,16,25	0.31	0	15,15,24	0.64	0
6	7PG	C	905	-	21,21,25	0.35	0	20,20,24	0.51	0
5	6A9	A	903[A]	-	22,22,22	0.33	0	25,27,27	0.94	2 (8%)
4	SO4	B	907	-	4,4,4	0.27	0	6,6,6	0.14	0
5	6A9	A	903[B]	-	22,22,22	0.35	0	25,27,27	1.09	3 (12%)
5	6A9	B	903[C]	-	22,22,22	0.31	0	25,27,27	0.95	2 (8%)
5	6A9	A	903[C]	-	22,22,22	0.30	0	25,27,27	0.95	2 (8%)
5	6A9	B	903[B]	-	22,22,22	0.34	0	25,27,27	1.09	3 (12%)
5	6A9	A	903[D]	-	22,22,22	0.32	0	25,27,27	0.96	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	6A9	B	903[A]	-	22,22,22	0.33	0	25,27,27	0.95	3 (12%)
4	SO4	B	901	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	C	902	-	4,4,4	0.25	0	6,6,6	0.18	0
6	7PG	A	907	-	23,23,25	0.23	0	22,22,24	0.41	0
4	SO4	B	902	-	4,4,4	0.27	0	6,6,6	0.22	0
4	SO4	A	902	-	4,4,4	0.33	0	6,6,6	0.17	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
5	6A9	B	903[D]	-	-	6/13/33/33	0/1/1/1
6	7PG	C	906	-	-	8/14/14/23	-
6	7PG	B	906	-	-	13/21/21/23	-
6	7PG	D	905	-	-	12/19/19/23	-
5	6A9	D	904[D]	-	-	6/13/33/33	0/1/1/1
5	6A9	D	904[B]	-	-	5/13/33/33	0/1/1/1
5	6A9	D	904[C]	-	-	5/13/33/33	0/1/1/1
5	6A9	C	904[A]	-	-	4/13/33/33	0/1/1/1
5	6A9	D	904[A]	-	-	4/13/33/33	0/1/1/1
5	6A9	C	904[C]	-	-	5/13/33/33	0/1/1/1
5	6A9	C	904[B]	-	-	5/13/33/33	0/1/1/1
5	6A9	C	904[D]	-	-	6/13/33/33	0/1/1/1
6	7PG	D	906	-	-	10/14/14/23	-
5	6A9	A	903[A]	-	-	4/13/33/33	0/1/1/1
5	6A9	A	903[B]	-	-	5/13/33/33	0/1/1/1
5	6A9	B	903[C]	-	-	5/13/33/33	0/1/1/1
5	6A9	A	903[C]	-	-	5/13/33/33	0/1/1/1
5	6A9	B	903[B]	-	-	5/13/33/33	0/1/1/1
5	6A9	A	903[D]	-	-	6/13/33/33	0/1/1/1
5	6A9	B	903[A]	-	-	4/13/33/33	0/1/1/1
6	7PG	A	907	-	-	16/21/21/23	-
6	7PG	C	905	-	-	13/19/19/23	-

There are no bond length outliers.



All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	904[B]	6A9	C4-C3-C2	-3.71	107.21	112.90
5	B	903[B]	6A9	C4-C3-C2	-3.70	107.23	112.90
5	A	903[B]	6A9	C4-C3-C2	-3.70	107.23	112.90
5	C	904[B]	6A9	C4-C3-C2	-3.63	107.34	112.90
5	B	903[C]	6A9	C4-C3-C2	-3.59	107.40	112.90
5	D	904[C]	6A9	C4-C3-C2	-3.58	107.42	112.90
5	A	903[C]	6A9	C4-C3-C2	-3.58	107.42	112.90
5	C	904[C]	6A9	C4-C3-C2	-3.51	107.53	112.90
5	D	904[D]	6A9	C4-C3-C2	-3.23	107.95	112.90
5	B	903[D]	6A9	C4-C3-C2	-3.22	107.97	112.90
5	A	903[D]	6A9	C4-C3-C2	-3.21	107.98	112.90
5	B	903[A]	6A9	C4-C3-C2	-3.13	108.10	112.90
5	C	904[D]	6A9	C4-C3-C2	-3.11	108.14	112.90
5	D	904[A]	6A9	C4-C3-C2	-3.07	108.19	112.90
5	A	903[A]	6A9	C4-C3-C2	-3.06	108.22	112.90
5	C	904[A]	6A9	C4-C3-C2	-3.02	108.27	112.90
5	A	903[A]	6A9	C6-C5-N	2.49	120.69	113.88
5	A	903[B]	6A9	C6-C5-N	2.47	120.63	113.88
5	D	904[B]	6A9	C6-C5-N	2.45	120.57	113.88
5	B	903[B]	6A9	C6-C5-N	2.43	120.52	113.88
5	B	903[A]	6A9	C6-C5-N	2.43	120.51	113.88
5	D	904[A]	6A9	C6-C5-N	2.43	120.51	113.88
5	C	904[A]	6A9	C6-C5-N	2.42	120.48	113.88
5	C	904[B]	6A9	C6-C5-N	2.41	120.47	113.88
5	A	903[D]	6A9	C6-C5-N	2.32	120.21	113.88
5	C	904[D]	6A9	C6-C5-N	2.27	120.09	113.88
5	B	903[D]	6A9	C6-C5-N	2.27	120.08	113.88
5	D	904[D]	6A9	C6-C5-N	2.26	120.04	113.88
5	B	903[C]	6A9	C15-N-C3	2.18	114.74	109.69
5	B	903[B]	6A9	C15-N-C3	2.15	114.68	109.69
5	C	904[C]	6A9	C15-N-C3	2.15	114.68	109.69
5	C	904[B]	6A9	C15-N-C3	2.14	114.66	109.69
5	D	904[B]	6A9	C15-N-C3	2.13	114.63	109.69
5	A	903[B]	6A9	C15-N-C3	2.12	114.60	109.69
5	D	904[C]	6A9	C15-N-C3	2.12	114.59	109.69
5	A	903[C]	6A9	C15-N-C3	2.08	114.51	109.69
5	B	903[D]	6A9	C15-N-C3	2.08	114.50	109.69
5	B	903[A]	6A9	C15-N-C3	2.07	114.50	109.69
5	C	904[A]	6A9	C15-N-C3	2.02	114.36	109.69
5	D	904[D]	6A9	C15-N-C3	2.01	114.36	109.69
5	C	904[D]	6A9	C15-N-C3	2.01	114.35	109.69

There are no chirality outliers.

All (152) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	903[D]	6A9	C6-C5-N-C3
5	D	904[D]	6A9	C6-C5-N-C3
5	D	904[B]	6A9	C6-C5-N-C3
5	C	904[A]	6A9	C6-C5-N-C3
5	D	904[A]	6A9	C6-C5-N-C3
5	C	904[B]	6A9	C6-C5-N-C3
5	C	904[D]	6A9	C6-C5-N-C3
5	A	903[A]	6A9	C6-C5-N-C3
5	A	903[B]	6A9	C6-C5-N-C3
5	B	903[B]	6A9	C6-C5-N-C3
5	B	903[A]	6A9	C6-C5-N-C3
6	C	905	7PG	C14-C13-O6-C12
6	C	905	7PG	C3-C4-O2-C5
6	C	905	7PG	C10-C9-O4-C8
5	D	904[B]	6A9	C11-C12-C13-O4
5	B	903[B]	6A9	C11-C12-C13-O4
5	A	903[B]	6A9	C11-C12-C13-O4
5	C	904[B]	6A9	C11-C12-C13-O4
6	C	905	7PG	O6-C13-C14-O7
6	D	905	7PG	O6-C13-C14-O7
6	C	905	7PG	O2-C5-C6-O3
6	D	905	7PG	O5-C11-C12-O6
6	C	905	7PG	O1-C3-C4-O2
6	D	905	7PG	O3-C7-C8-O4
5	B	903[C]	6A9	N-C5-C6-C7
6	C	906	7PG	O3-C7-C8-O4
5	D	904[C]	6A9	N-C5-C6-C7
5	C	904[C]	6A9	N-C5-C6-C7
6	D	906	7PG	O3-C7-C8-O4
5	A	903[C]	6A9	N-C5-C6-C7
6	C	905	7PG	C12-C11-O5-C10
6	B	906	7PG	O5-C10-C9-O4
5	B	903[D]	6A9	N-C5-C6-C7
5	D	904[D]	6A9	N-C5-C6-C7
6	C	905	7PG	O5-C10-C9-O4
5	C	904[D]	6A9	N-C5-C6-C7
5	A	903[D]	6A9	N-C5-C6-C7
5	D	904[C]	6A9	C7-C8-C9-C10
5	C	904[C]	6A9	C7-C8-C9-C10
5	A	903[C]	6A9	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	B	903[C]	6A9	C7-C8-C9-C10
5	B	903[A]	6A9	N-C5-C6-C7
5	A	903[A]	6A9	N-C5-C6-C7
5	D	904[A]	6A9	N-C5-C6-C7
5	C	904[A]	6A9	N-C5-C6-C7
6	A	907	7PG	O3-C7-C8-O4
6	D	906	7PG	O5-C10-C9-O4
6	B	906	7PG	O3-C7-C8-O4
5	B	903[D]	6A9	C9-C10-C11-C12
5	D	904[D]	6A9	C9-C10-C11-C12
5	D	904[D]	6A9	C7-C8-C9-C10
5	C	904[B]	6A9	C7-C8-C9-C10
5	A	903[B]	6A9	C7-C8-C9-C10
5	B	903[B]	6A9	C7-C8-C9-C10
5	A	903[D]	6A9	C9-C10-C11-C12
5	B	903[D]	6A9	C7-C8-C9-C10
5	D	904[B]	6A9	C7-C8-C9-C10
5	A	903[D]	6A9	C7-C8-C9-C10
5	C	904[D]	6A9	C9-C10-C11-C12
5	C	904[D]	6A9	C7-C8-C9-C10
5	C	904[B]	6A9	C10-C11-C12-C13
5	A	903[B]	6A9	C10-C11-C12-C13
5	D	904[B]	6A9	C10-C11-C12-C13
5	C	904[D]	6A9	C11-C12-C13-O4
5	B	903[B]	6A9	C10-C11-C12-C13
6	C	906	7PG	O5-C10-C9-O4
5	A	903[D]	6A9	C11-C12-C13-O4
6	D	905	7PG	C16-C15-O7-C14
5	D	904[D]	6A9	C11-C12-C13-O4
5	B	903[D]	6A9	C11-C12-C13-O4
6	A	907	7PG	O5-C10-C9-O4
5	B	903[A]	6A9	C6-C7-C8-C9
5	C	904[A]	6A9	C6-C7-C8-C9
5	A	903[A]	6A9	C6-C7-C8-C9
5	D	904[A]	6A9	C6-C7-C8-C9
6	D	906	7PG	C16-C15-O7-C14
5	D	904[B]	6A9	C9-C10-C11-C12
5	C	904[B]	6A9	C9-C10-C11-C12
5	B	903[B]	6A9	C9-C10-C11-C12
5	A	903[B]	6A9	C9-C10-C11-C12
6	D	906	7PG	O7-C15-C16-O8
6	D	905	7PG	C11-C12-O6-C13

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Mol	Chain	Res	Type	Atoms
6	D	906	7PG	C7-C8-O4-C9
6	D	905	7PG	C12-C11-O5-C10
6	C	906	7PG	C14-C13-O6-C12
6	C	906	7PG	C7-C8-O4-C9
6	D	906	7PG	C9-C10-O5-C11
6	A	907	7PG	C9-C10-O5-C11
6	B	906	7PG	C3-C4-O2-C5
6	C	906	7PG	C9-C10-O5-C11
6	D	905	7PG	C6-C5-O2-C4
6	D	906	7PG	C14-C13-O6-C12
6	A	907	7PG	C15-C16-O8-C17
6	A	907	7PG	C5-C6-O3-C7
6	A	907	7PG	C16-C15-O7-C14
6	B	906	7PG	C5-C6-O3-C7
6	A	907	7PG	C10-C9-O4-C8
6	C	905	7PG	C8-C7-O3-C6
6	A	907	7PG	C6-C5-O2-C4
5	D	904[C]	6A9	C6-C5-N-C15
5	D	904[C]	6A9	C6-C5-N-C3
5	C	904[A]	6A9	C6-C5-N-C15
5	D	904[A]	6A9	C6-C5-N-C15
5	C	904[C]	6A9	C6-C5-N-C15
5	C	904[C]	6A9	C6-C5-N-C3
5	A	903[A]	6A9	C6-C5-N-C15
5	B	903[C]	6A9	C6-C5-N-C15
5	B	903[C]	6A9	C6-C5-N-C3
5	A	903[C]	6A9	C6-C5-N-C15
5	A	903[C]	6A9	C6-C5-N-C3
5	A	903[D]	6A9	C6-C5-N-C3
5	B	903[A]	6A9	C6-C5-N-C15
6	A	907	7PG	O7-C15-C16-O8
5	B	903[D]	6A9	C12-C13-O4-C14
5	D	904[D]	6A9	C12-C13-O4-C14
5	C	904[D]	6A9	C12-C13-O4-C14
5	A	903[D]	6A9	C12-C13-O4-C14
6	A	907	7PG	O2-C5-C6-O3
6	D	905	7PG	O5-C10-C9-O4
6	C	905	7PG	C9-C10-O5-C11
6	C	905	7PG	C5-C6-O3-C7
6	D	905	7PG	C7-C8-O4-C9
6	A	907	7PG	C3-C4-O2-C5
6	C	906	7PG	C13-C14-O7-C15

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Mol	Chain	Res	Type	Atoms
6	C	905	7PG	C4-C3-O1-C2
6	B	906	7PG	C11-C12-O6-C13
6	A	907	7PG	C11-C12-O6-C13
6	D	906	7PG	O6-C13-C14-O7
6	A	907	7PG	C7-C8-O4-C9
6	D	905	7PG	C5-C6-O3-C7
6	D	906	7PG	C8-C7-O3-C6
6	C	906	7PG	O6-C13-C14-O7
6	C	906	7PG	C8-C7-O3-C6
6	B	906	7PG	C15-C16-O8-C17
6	B	906	7PG	C8-C7-O3-C6
5	B	903[C]	6A9	C10-C11-C12-C13
5	D	904[C]	6A9	C10-C11-C12-C13
5	C	904[C]	6A9	C10-C11-C12-C13
5	A	903[C]	6A9	C10-C11-C12-C13
6	D	905	7PG	O2-C5-C6-O3
6	D	906	7PG	O5-C11-C12-O6
6	B	906	7PG	C10-C9-O4-C8
6	B	906	7PG	O2-C5-C6-O3
6	B	906	7PG	O7-C15-C16-O8
6	A	907	7PG	O1-C3-C4-O2
6	C	905	7PG	O5-C11-C12-O6
6	B	906	7PG	C6-C5-O2-C4
6	D	905	7PG	C3-C4-O2-C5
6	B	906	7PG	O6-C13-C14-O7
6	A	907	7PG	O6-C13-C14-O7
6	B	906	7PG	O1-C3-C4-O2
6	A	907	7PG	C14-C13-O6-C12

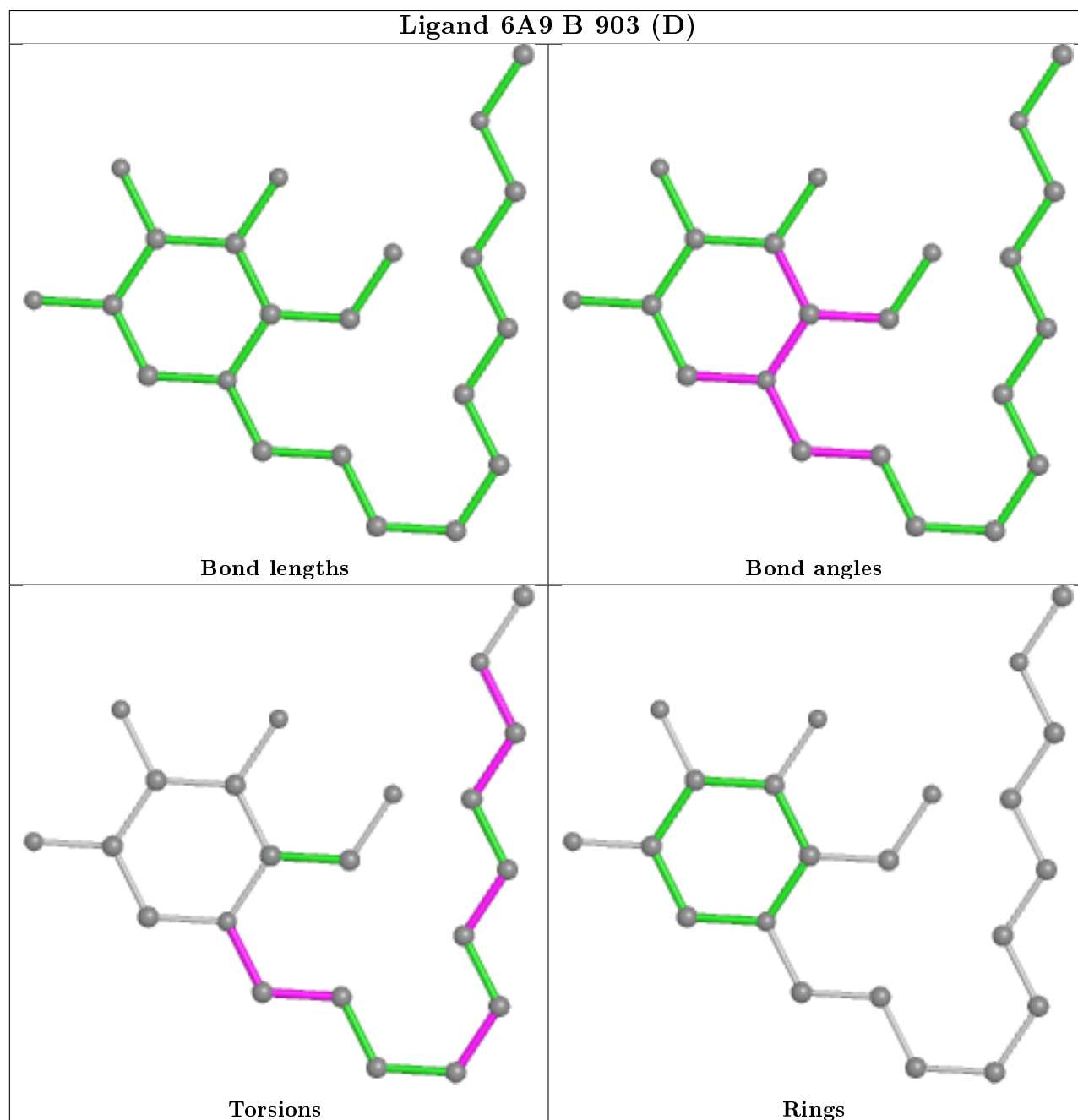
There are no ring outliers.

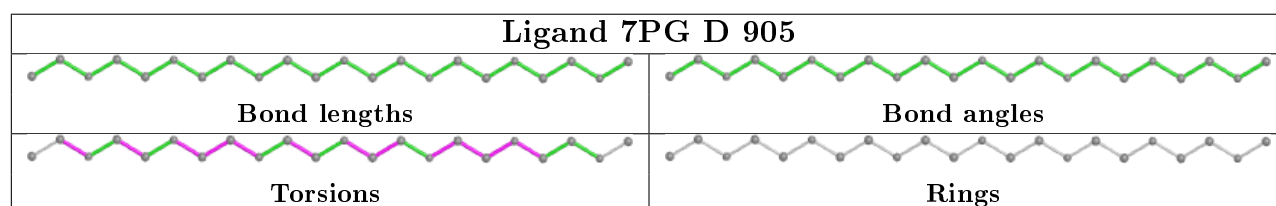
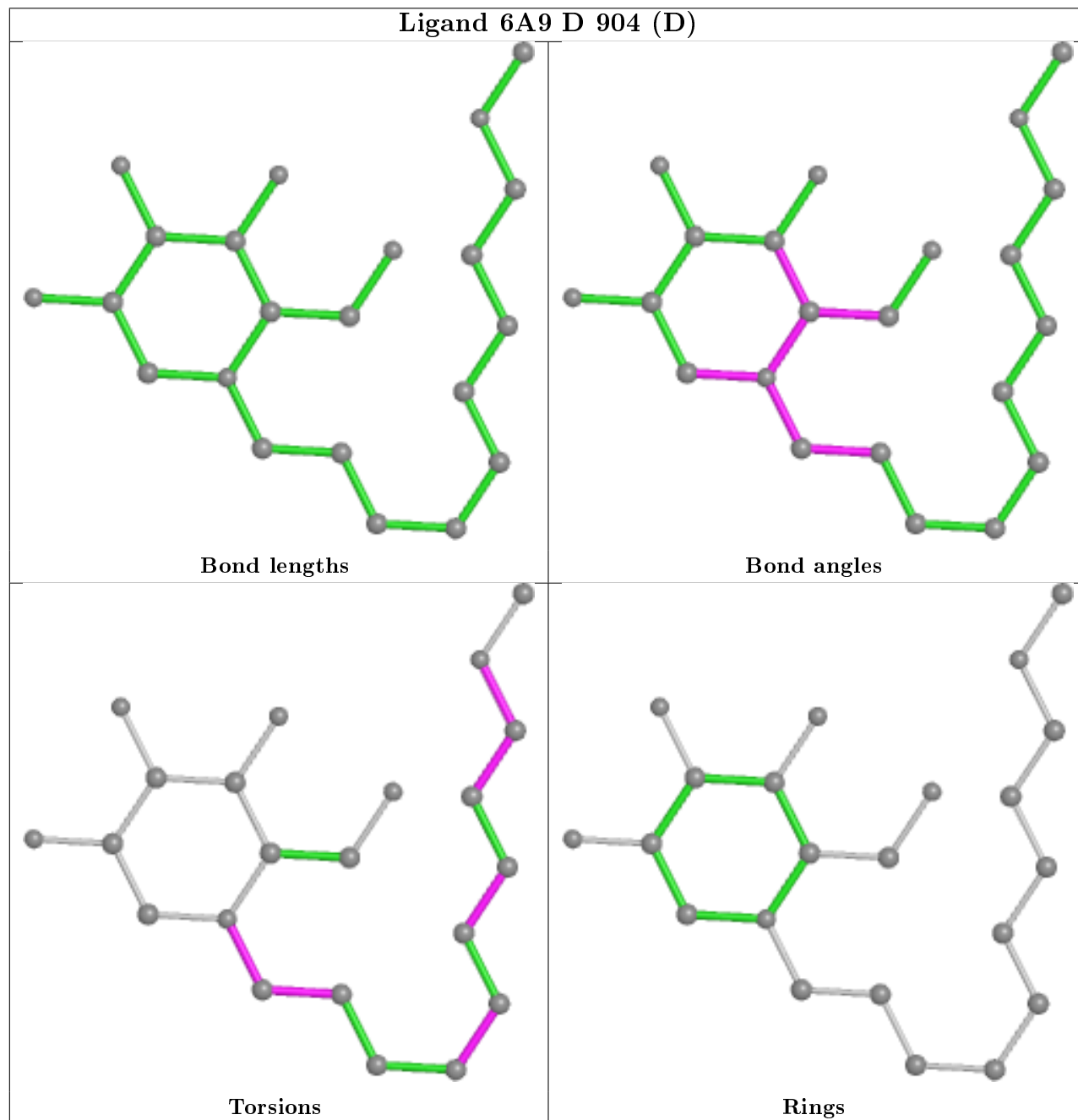
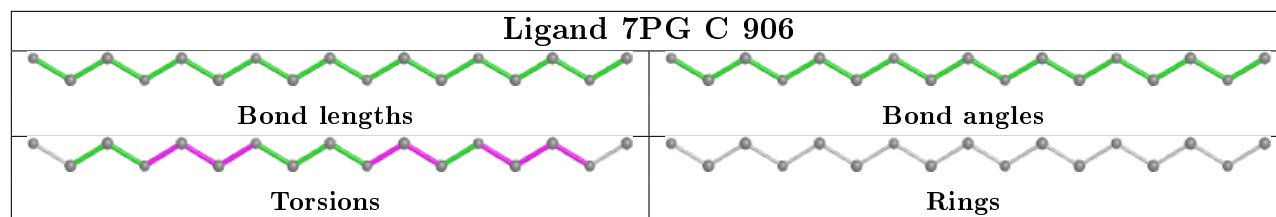
7 monomers are involved in 80 short contacts:

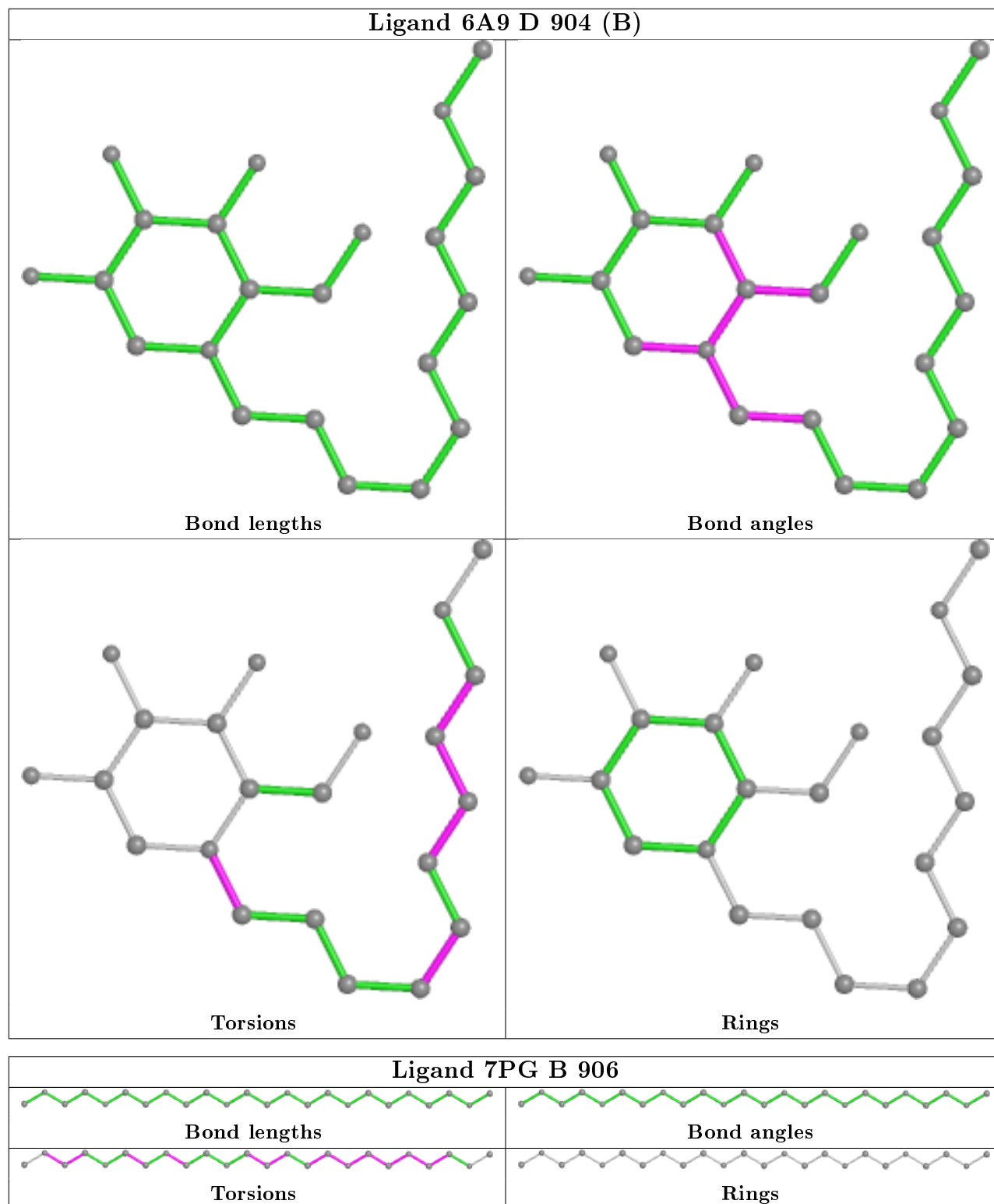
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	906	7PG	4	0
6	D	905	7PG	30	0
6	B	906	7PG	14	0
6	D	906	7PG	6	0
6	C	905	7PG	27	0
5	A	903[D]	6A9	1	0
6	A	907	7PG	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

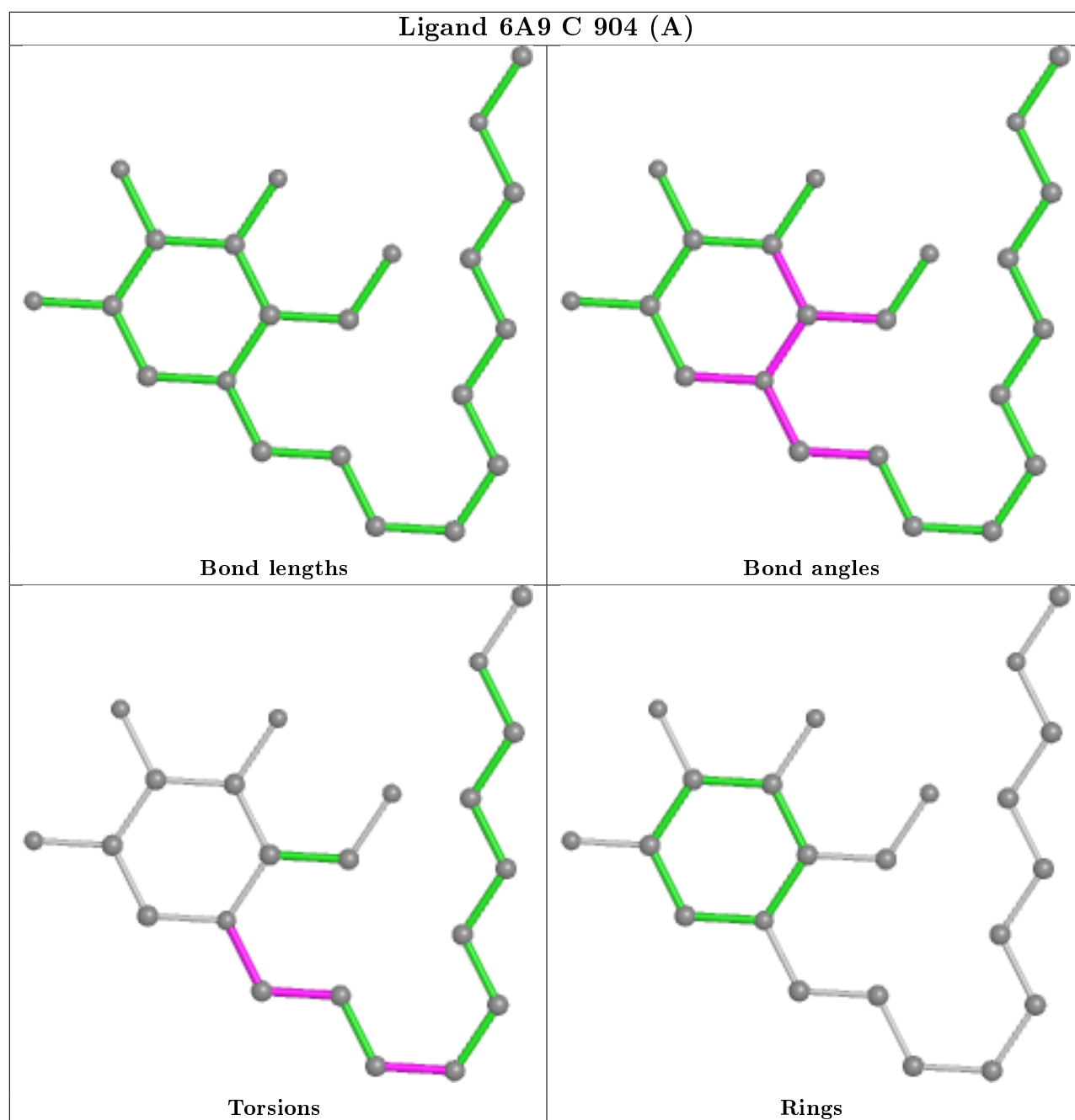
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



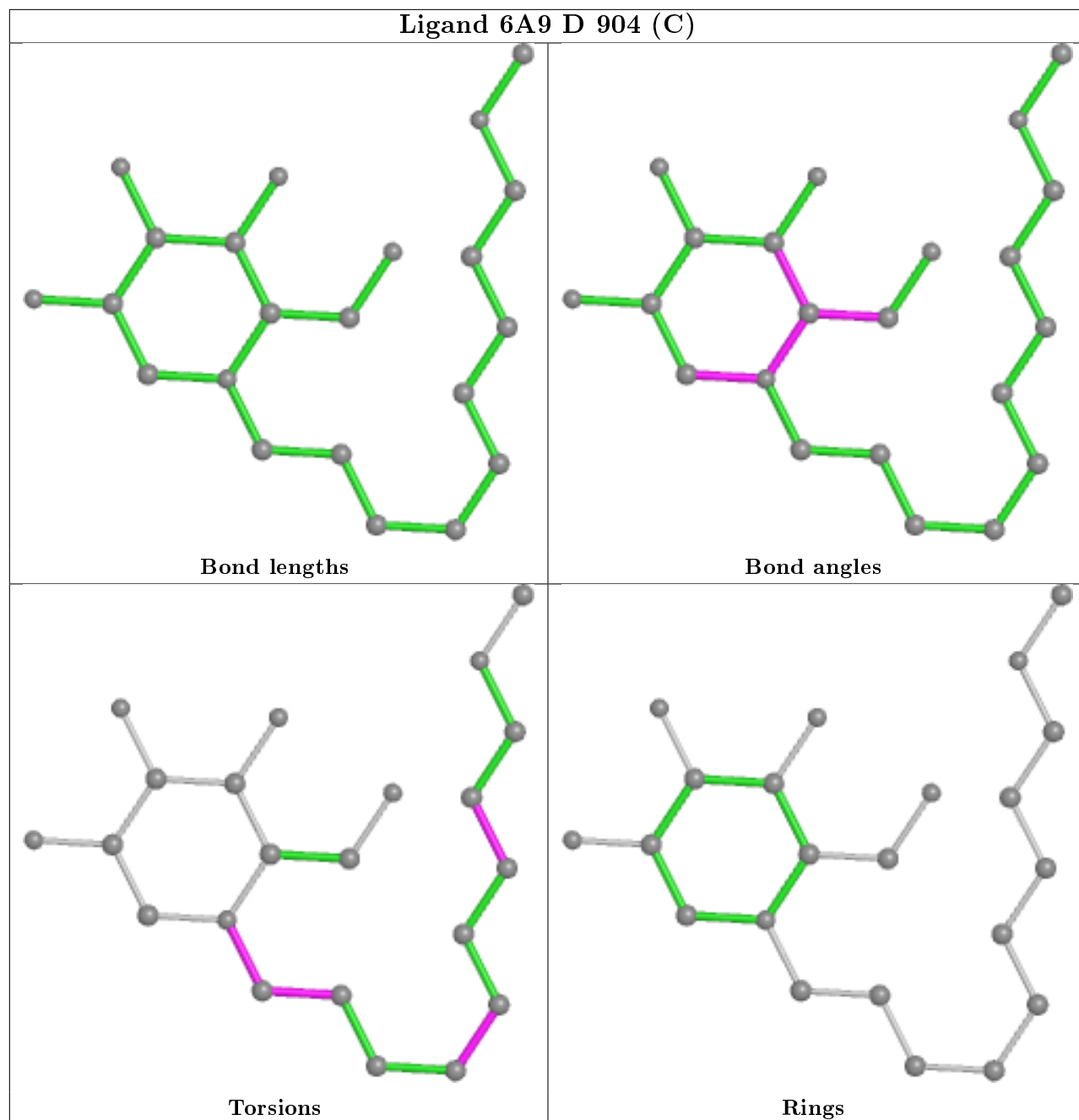


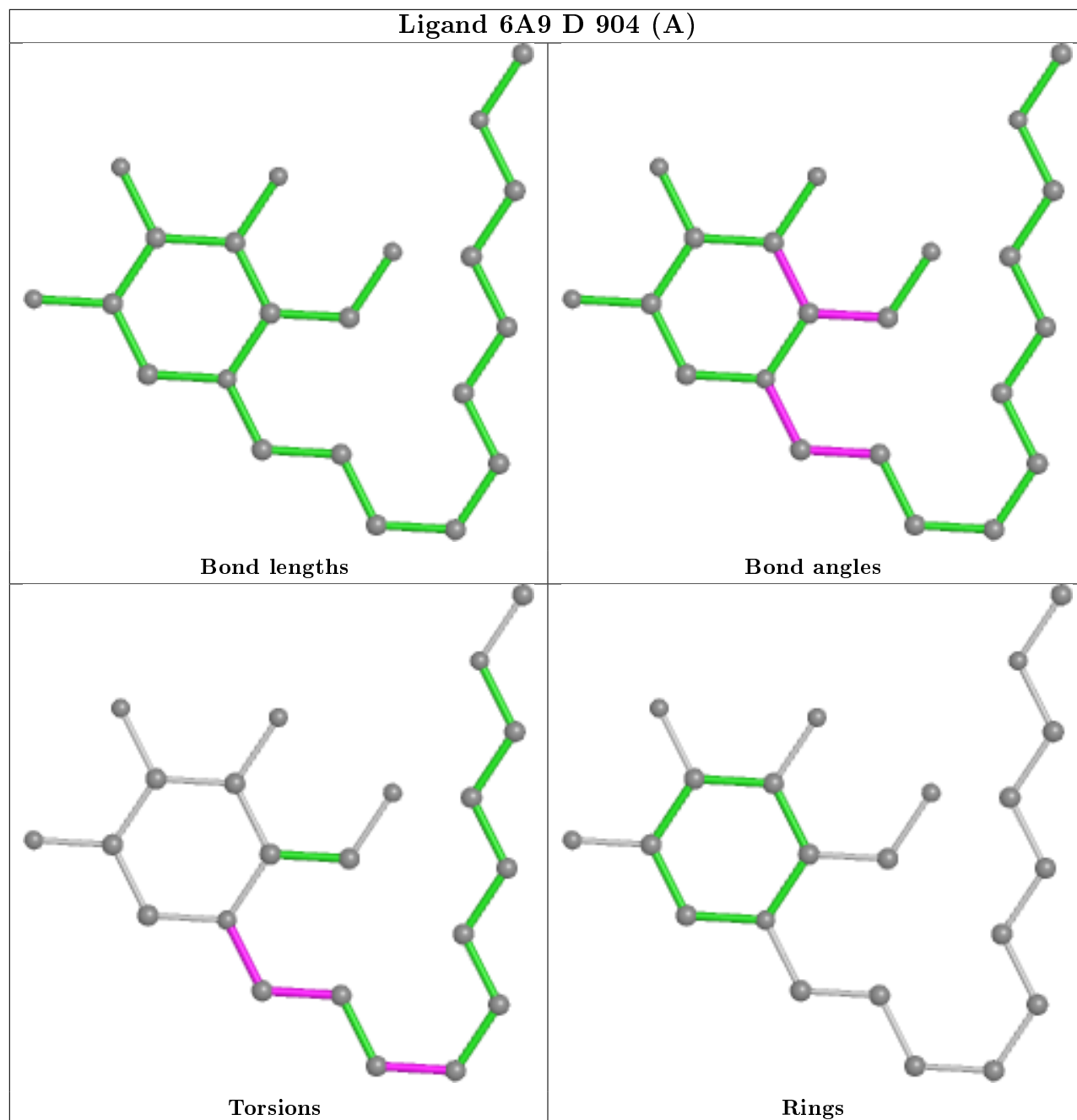


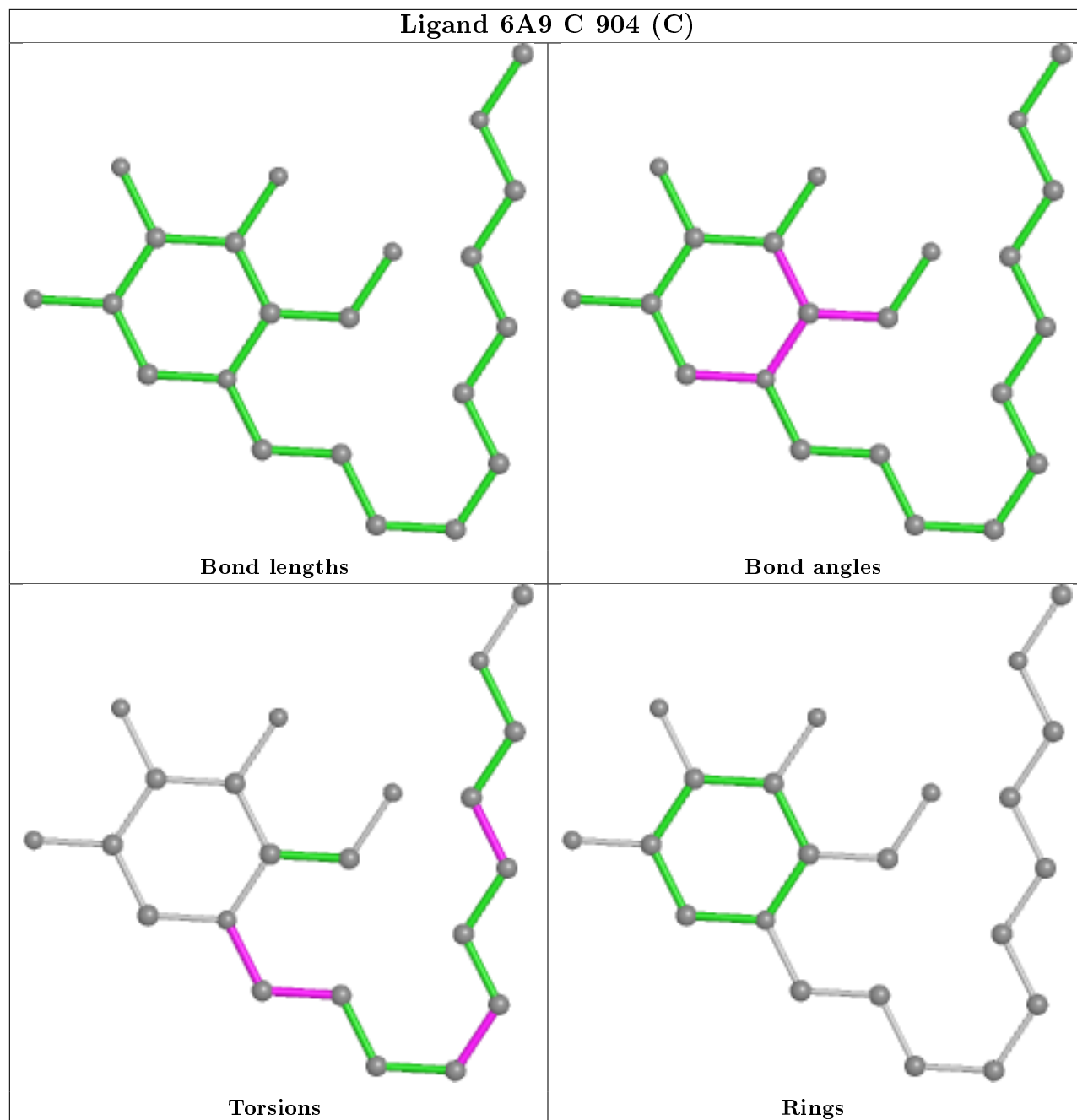


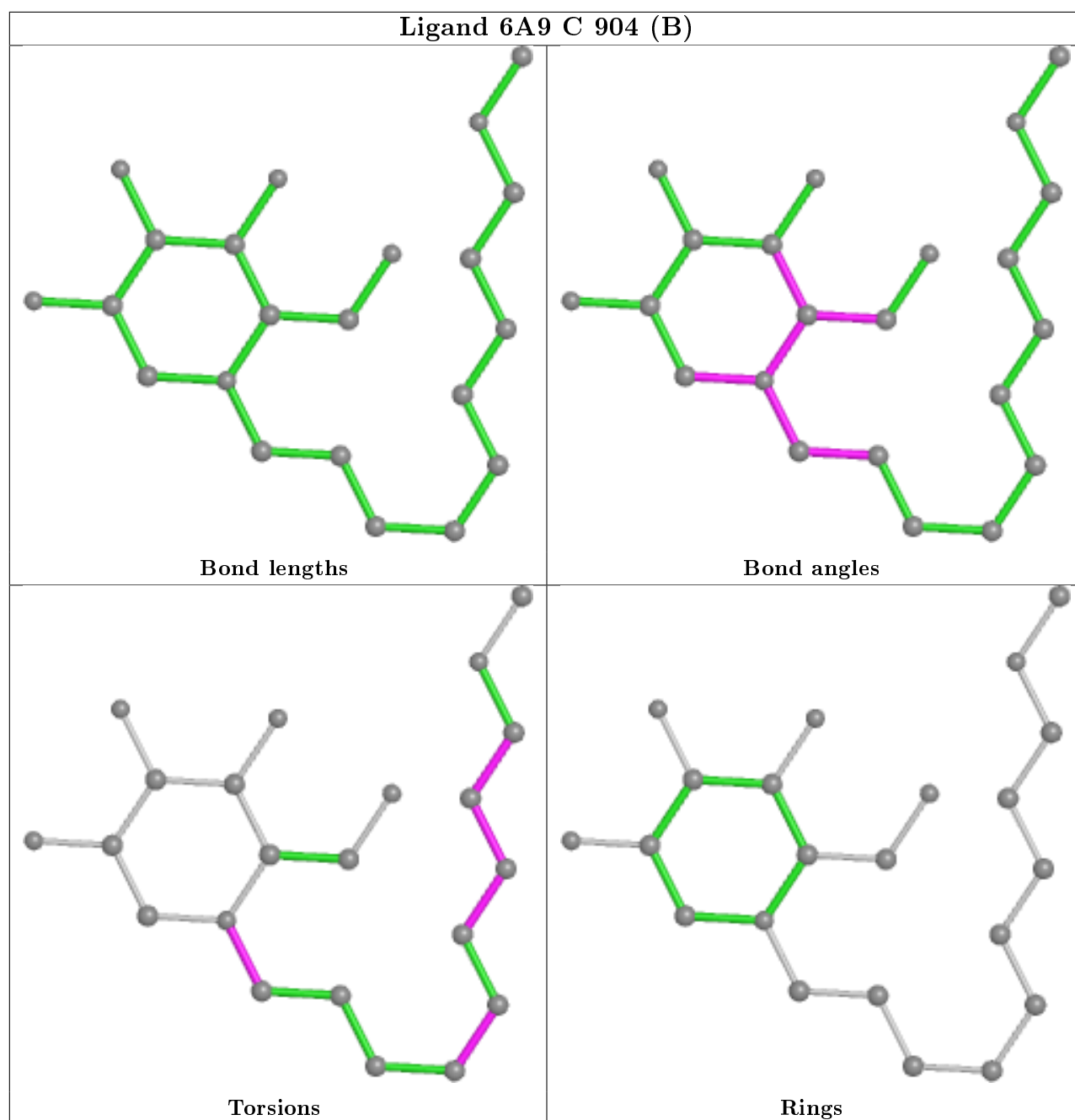


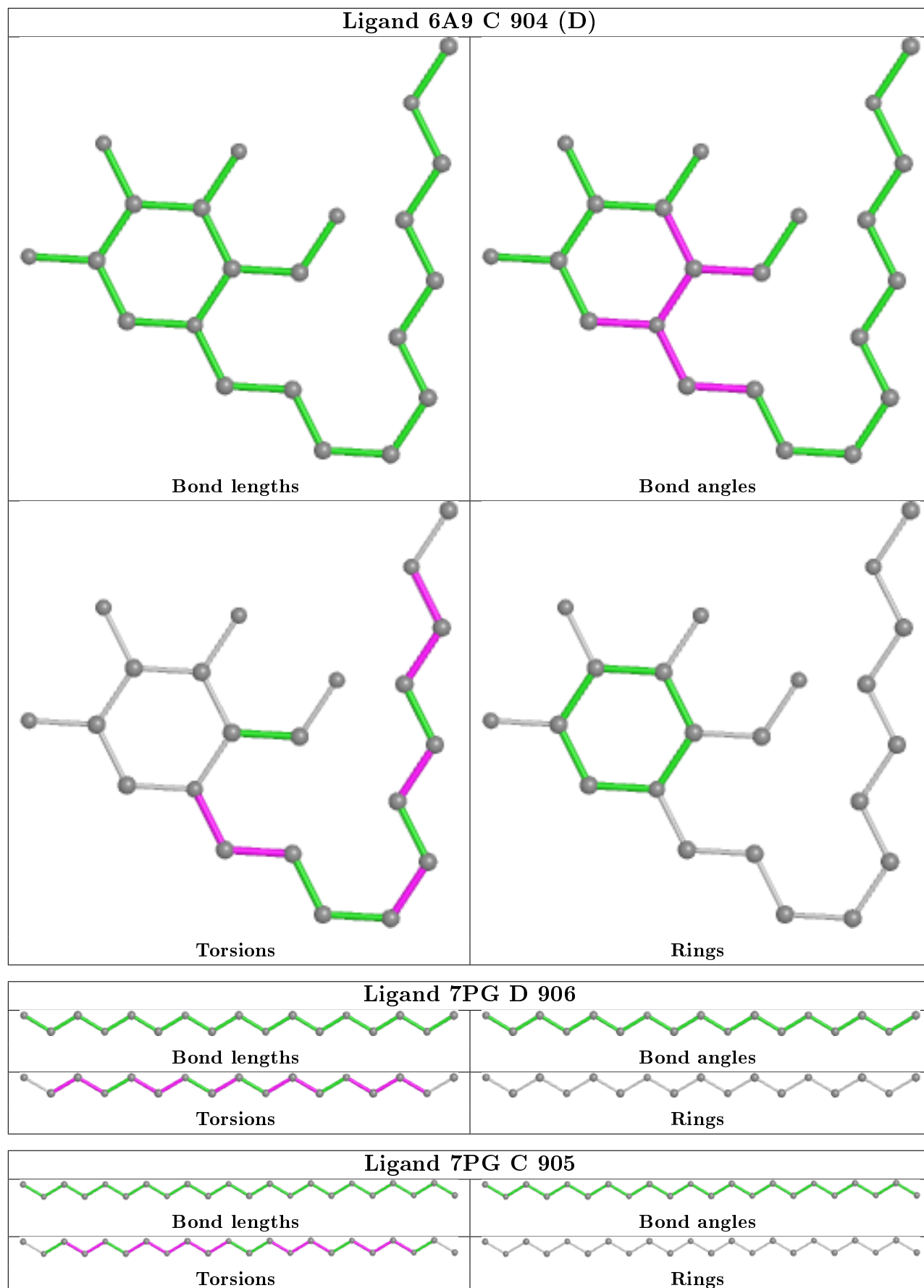
## Ligand 6A9 D 904 (C)



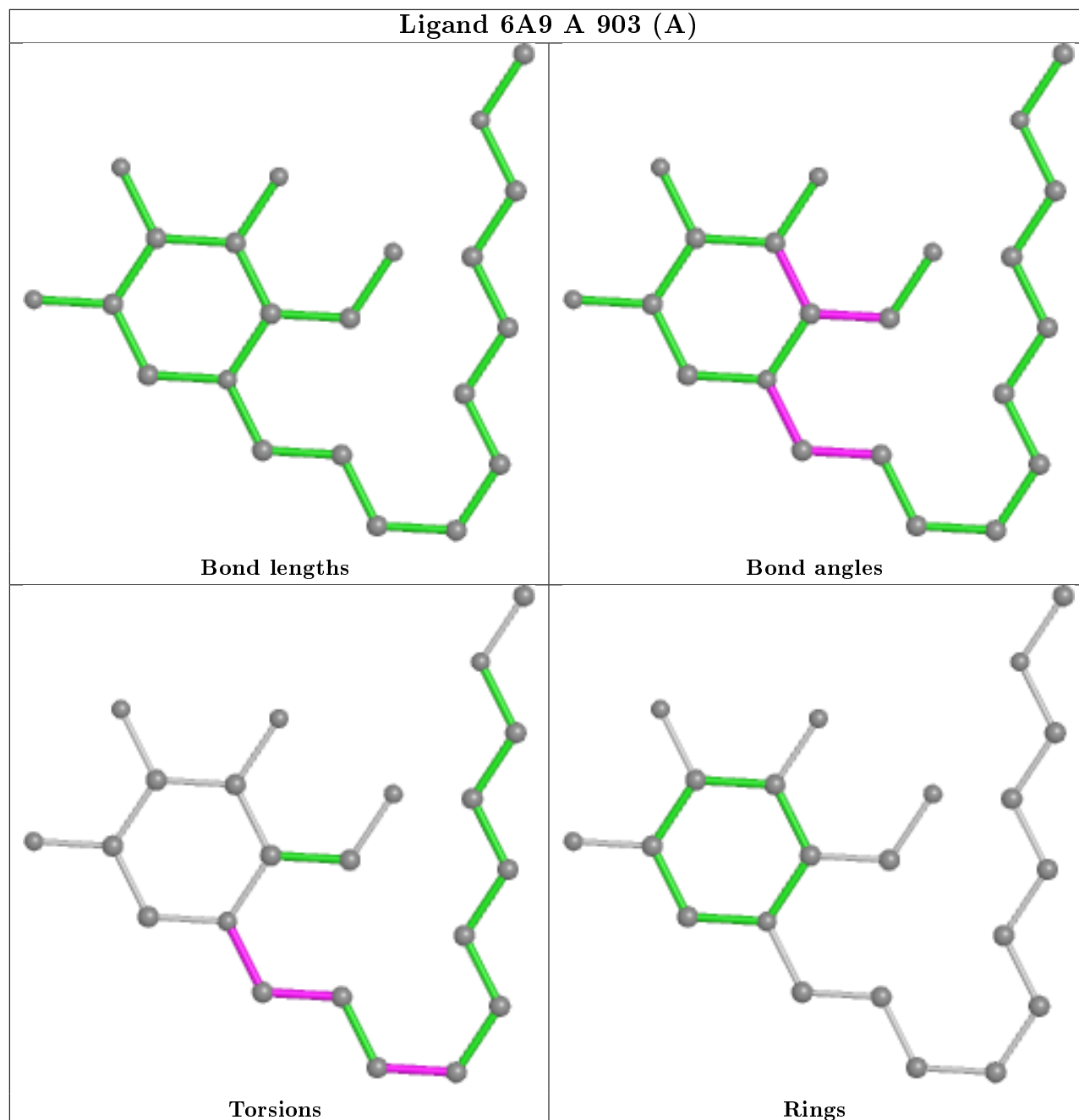




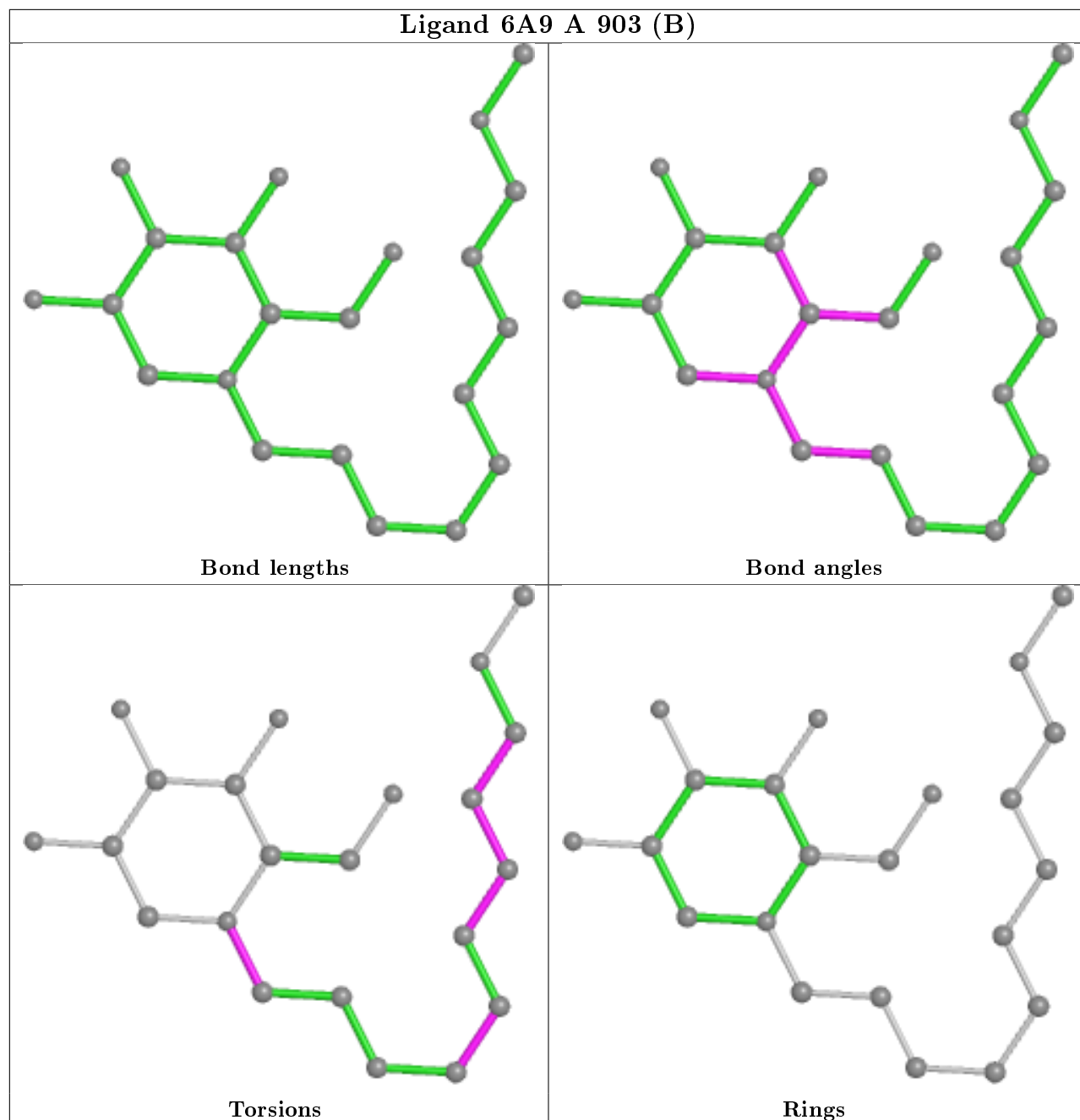




## Ligand 6A9 A 903 (A)

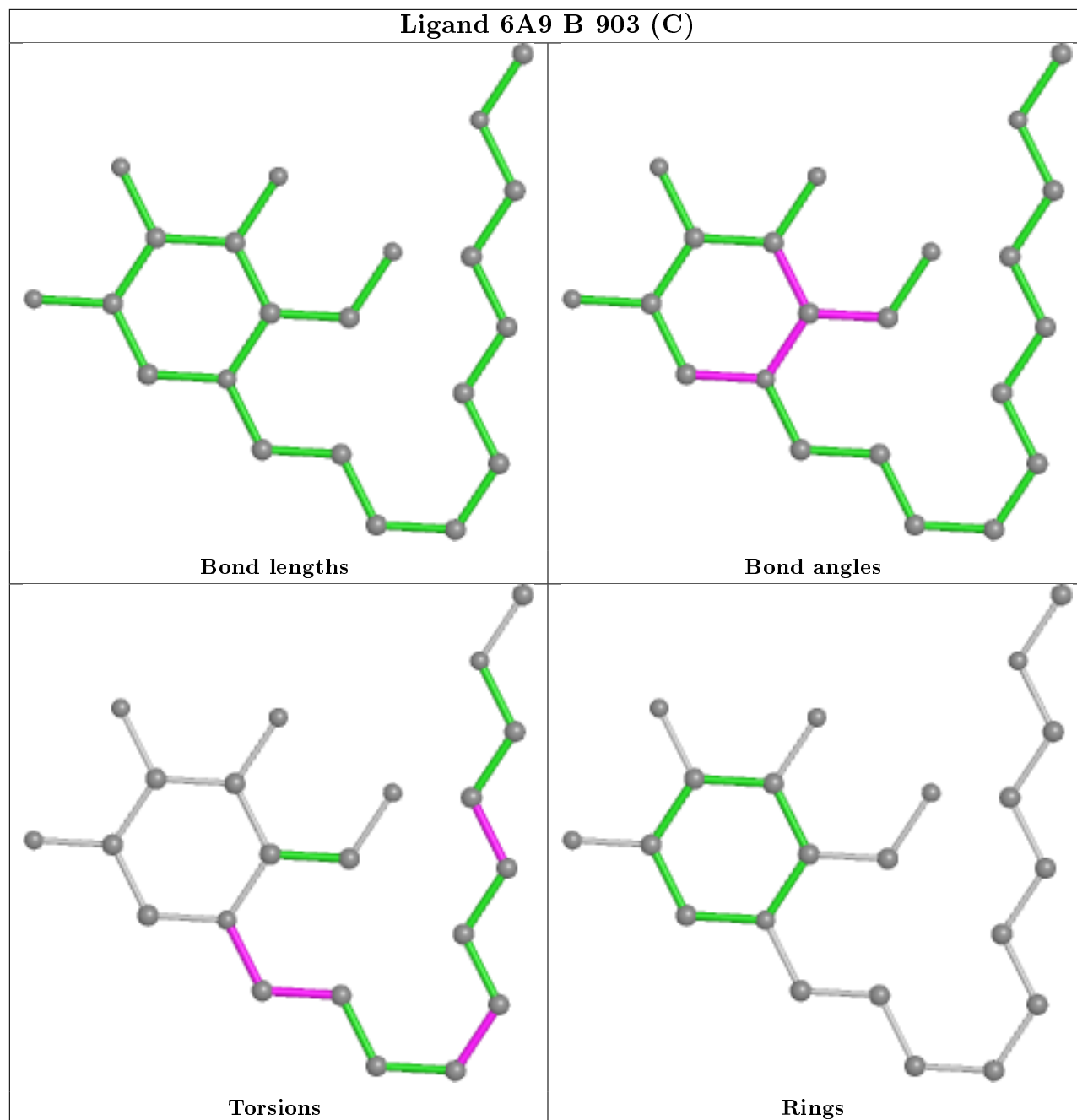


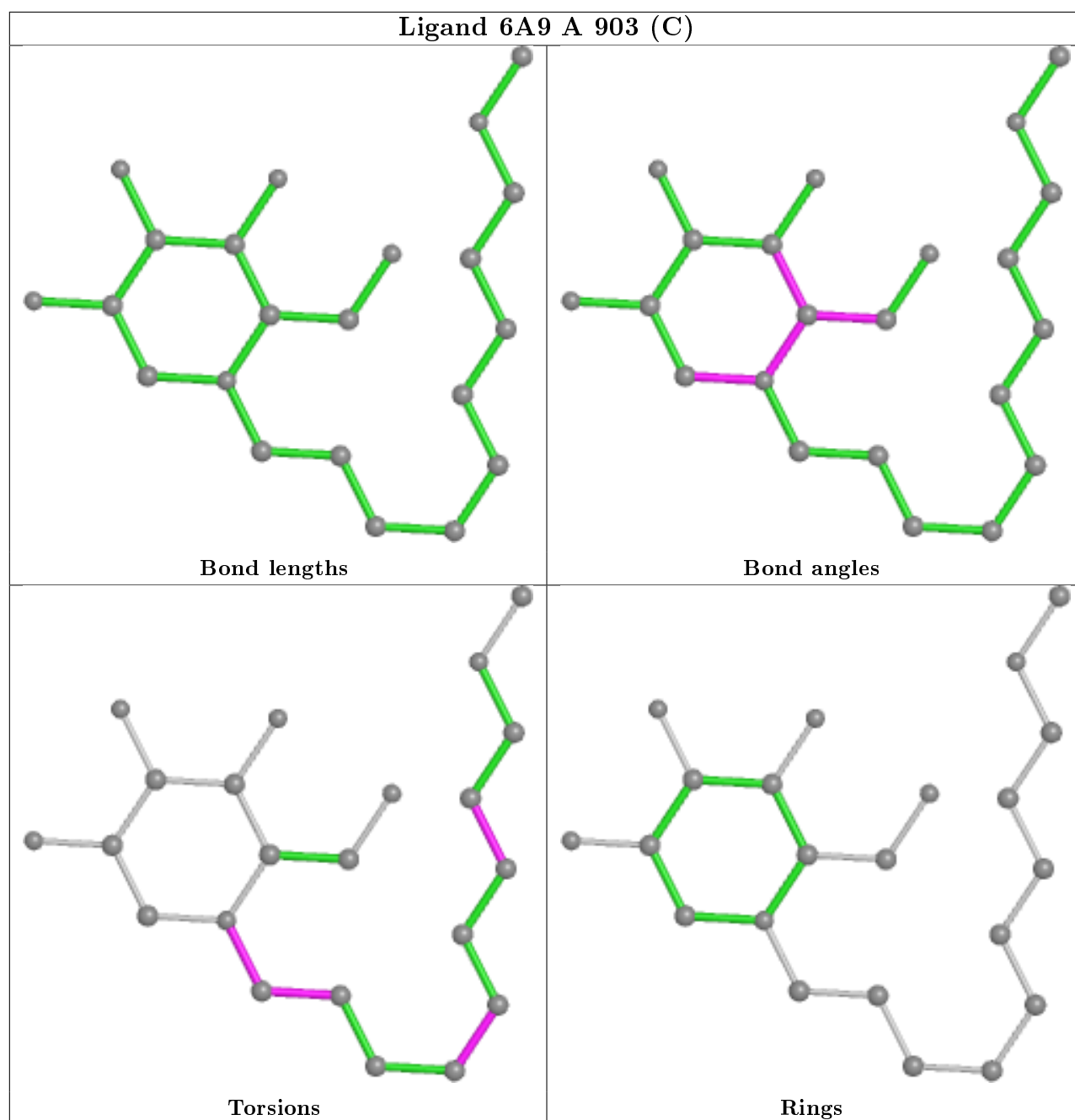
## Ligand 6A9 A 903 (B)



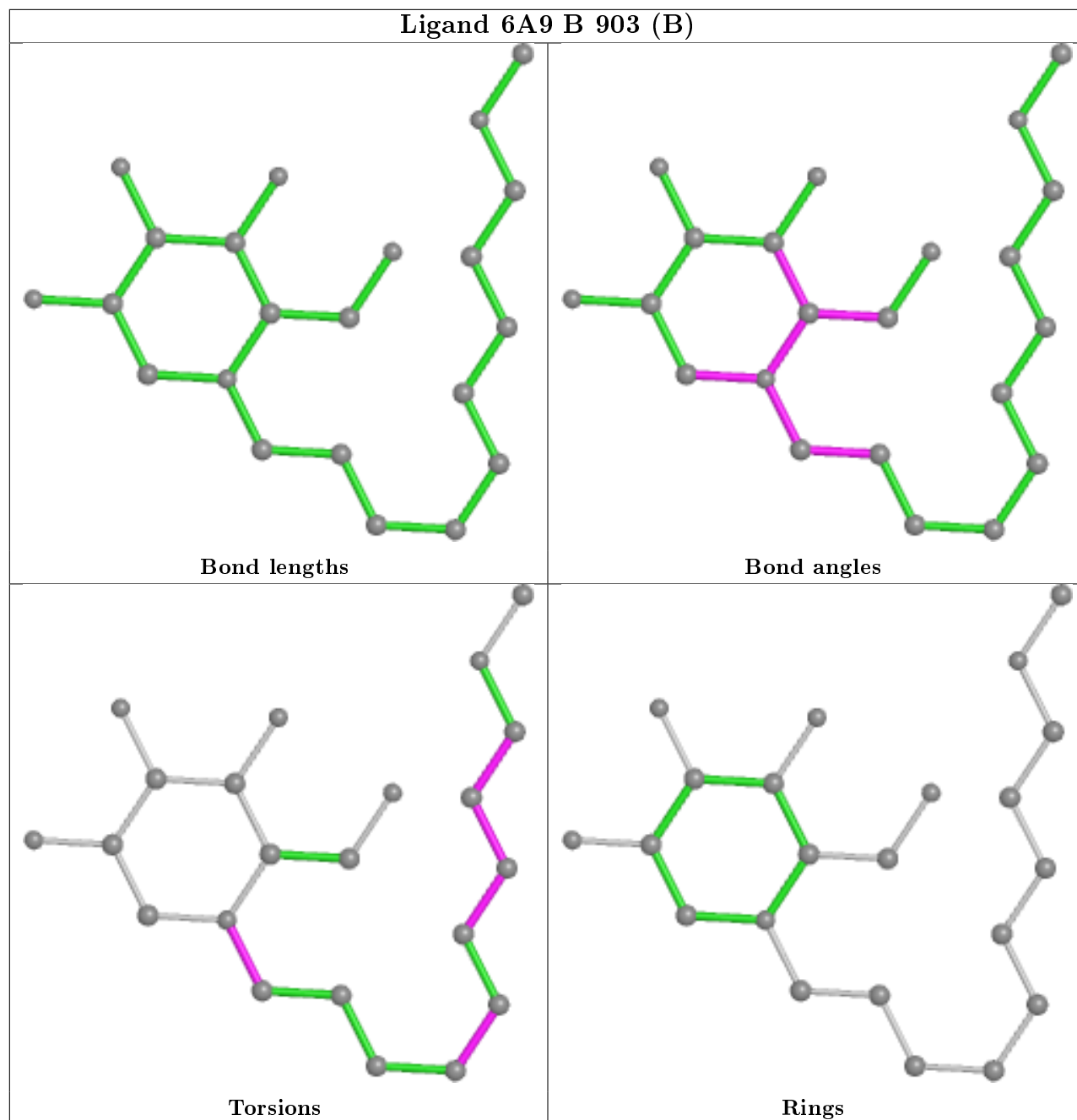


## Ligand 6A9 B 903 (C)

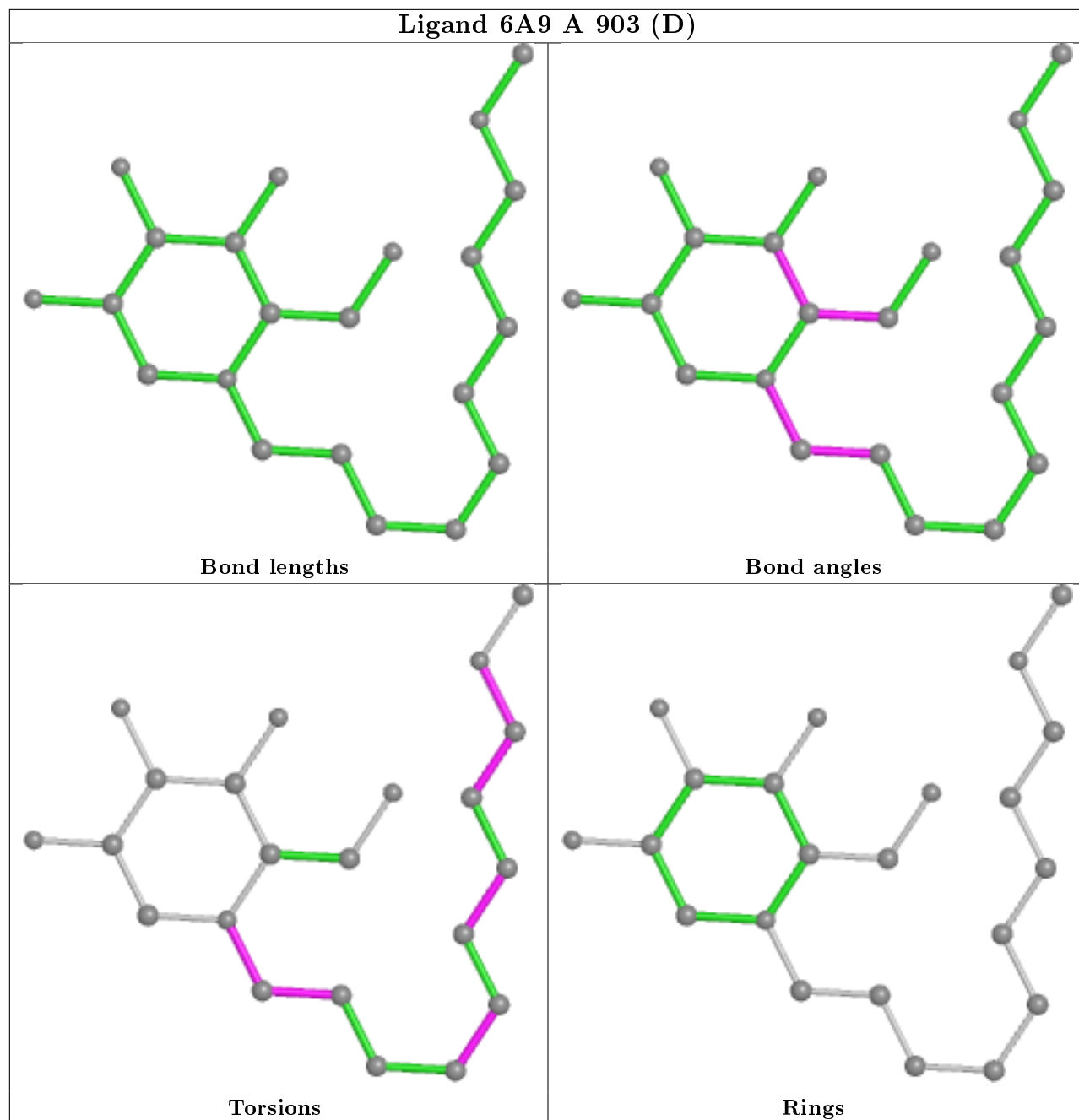


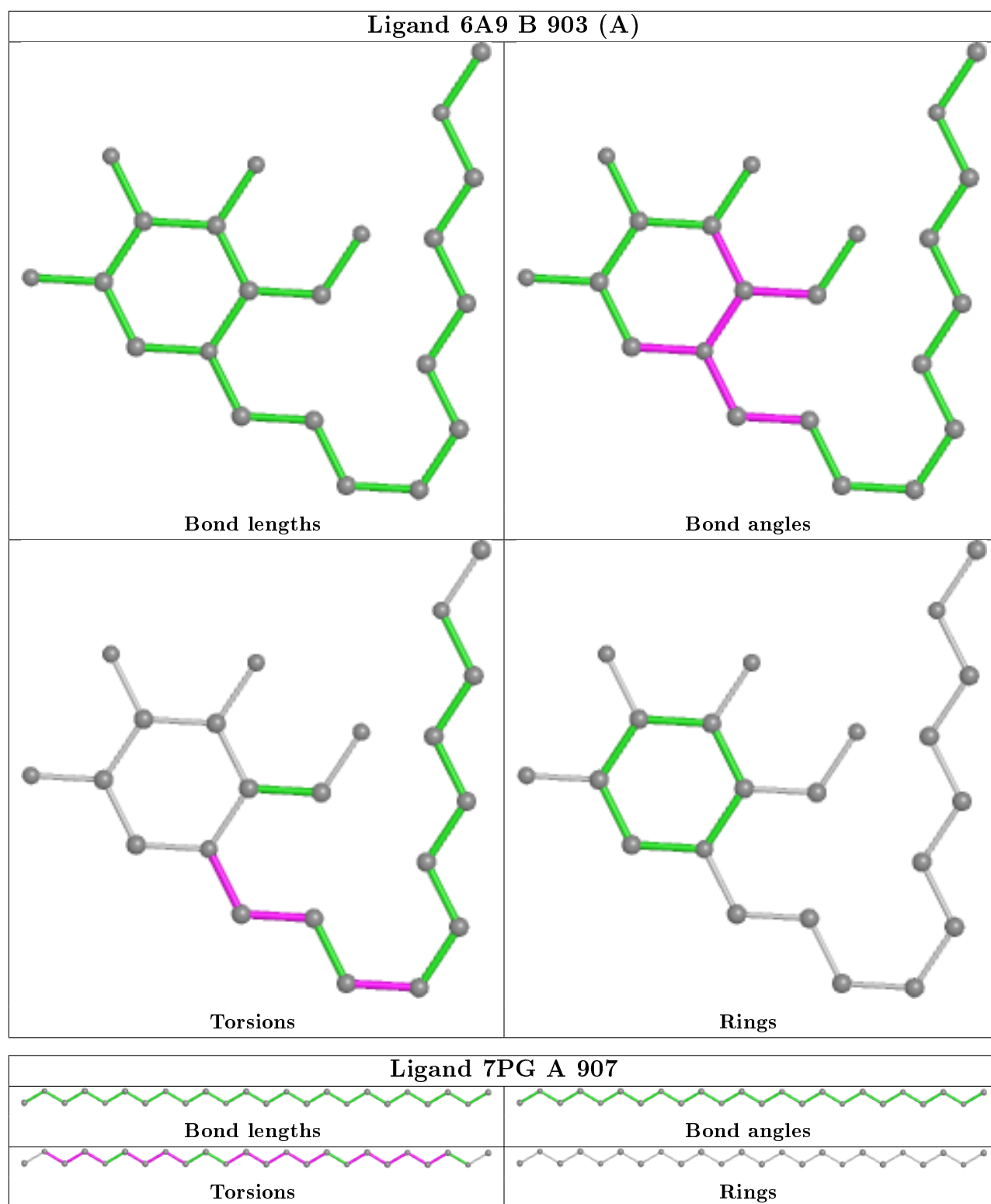


## Ligand 6A9 B 903 (B)



## Ligand 6A9 A 903 (D)





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	736/795 (92%)	-0.03	20 (2%) 54 60	19, 37, 75, 109	0
1	B	737/795 (92%)	0.04	27 (3%) 41 48	22, 41, 73, 105	0
1	C	747/795 (93%)	-0.04	17 (2%) 60 65	24, 41, 73, 113	0
1	D	752/795 (94%)	-0.02	17 (2%) 60 65	22, 40, 74, 107	0
All	All	2972/3180 (93%)	-0.01	81 (2%) 54 60	19, 40, 74, 113	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	GLY	6.1
1	B	125	THR	6.0
1	D	129	PRO	5.8
1	A	128	THR	5.4
1	C	197	PRO	5.1
1	D	127	GLY	5.0
1	B	497	PRO	4.9
1	C	666	PRO	4.8
1	B	667	GLN	4.5
1	C	195	GLY	4.4
1	A	667	GLN	4.2
1	A	126	PRO	4.1
1	B	199	PHE	4.0
1	A	125	THR	3.9
1	A	64	LEU	3.8
1	D	341	GLY	3.8
1	B	64	LEU	3.8
1	D	126	PRO	3.8
1	D	128	THR	3.7
1	C	129	PRO	3.7
1	D	125	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	289	PRO	3.6
1	B	127	GLY	3.6
1	D	666	PRO	3.6
1	C	667	GLN	3.4
1	B	61	LEU	3.4
1	D	412	THR	3.3
1	B	440[A]	PHE	3.3
1	D	440[A]	PHE	3.2
1	B	63	TRP	3.2
1	B	226	LEU	3.2
1	C	128	THR	3.2
1	B	128	THR	3.0
1	A	523	HIS	3.0
1	B	251	ASP	2.9
1	A	199	PHE	2.9
1	B	126	PRO	2.9
1	C	127	GLY	2.8
1	B	837	TRP	2.7
1	C	675	ARG	2.7
1	A	193	ALA	2.7
1	C	125	THR	2.6
1	B	129	PRO	2.6
1	D	340	THR	2.6
1	A	441	PHE	2.6
1	A	440[A]	PHE	2.5
1	B	838	SER	2.5
1	A	63	TRP	2.5
1	C	339	ALA	2.5
1	C	440[A]	PHE	2.5
1	B	441	PHE	2.5
1	B	220	ILE	2.4
1	B	193	ALA	2.4
1	C	196	THR	2.4
1	B	742	HIS	2.4
1	D	61	LEU	2.4
1	B	498	GLU	2.4
1	D	251	ASP	2.4
1	B	499	PHE	2.3
1	A	442	PRO	2.3
1	A	129	PRO	2.3
1	A	130	PRO	2.3
1	B	523	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	665	PRO	2.3
1	D	494	ARG	2.3
1	D	667	GLN	2.3
1	A	124	ALA	2.3
1	C	340	THR	2.3
1	B	81	PRO	2.2
1	C	126	PRO	2.2
1	D	342	GLY	2.1
1	D	498	GLU	2.1
1	A	263	TRP	2.1
1	A	290	GLY	2.1
1	A	566	LEU	2.1
1	C	130	PRO	2.0
1	B	412	THR	2.0
1	A	497	PRO	2.0
1	C	412	THR	2.0
1	D	195	GLY	2.0
1	C	225	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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(Å <sup>2</sup> )	Q<0.9
1	MLY	B	662	11/12	0.79	0.22	66,77,81,82	0
1	MLY	C	662	11/12	0.80	0.24	72,82,85,86	0
1	MLY	B	227	11/12	0.81	0.22	58,63,73,74	0
1	MLY	D	662	11/12	0.81	0.13	60,69,72,72	0
1	SME	D	421	9/10	0.84	0.19	41,44,61,64	0
1	SME	B	421	9/10	0.85	0.20	56,62,75,80	0
1	MLY	C	304	11/12	0.86	0.23	52,59,68,70	0
1	MLY	B	304	11/12	0.86	0.20	57,61,70,71	0
1	MLY	C	227	11/12	0.86	0.21	49,53,64,66	0
1	MLY	C	366	11/12	0.87	0.25	57,63,71,72	0
1	SME	C	421	9/10	0.87	0.20	42,49,66,70	0
1	MLY	C	376	11/12	0.87	0.32	65,73,77,80	0
1	MLY	A	227	11/12	0.87	0.20	66,68,78,79	0
1	MLY	A	304	11/12	0.87	0.23	64,69,78,80	0
1	MLY	A	131	11/12	0.87	0.24	54,65,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	C	371	11/12	0.88	0.18	57,61,73,76	0
1	MLY	B	371	11/12	0.88	0.23	50,55,72,75	0
1	MLY	C	131	11/12	0.88	0.26	42,58,69,70	0
1	MLY	D	304	11/12	0.88	0.20	52,59,69,70	0
1	MLY	A	376	11/12	0.89	0.20	44,53,67,68	0
1	SME	A	421	9/10	0.89	0.19	53,59,71,76	0
1	MLY	A	662	11/12	0.89	0.18	55,65,71,73	0
1	MLY	D	376	11/12	0.89	0.24	52,57,62,62	0
1	MLY	C	736	11/12	0.90	0.16	37,45,56,59	0
1	MLY	B	111	11/12	0.90	0.18	38,40,57,58	0
1	MLY	C	378	11/12	0.90	0.22	70,71,74,74	0
1	MLY	B	378	11/12	0.91	0.17	54,55,59,61	0
1	MLY	D	533	11/12	0.91	0.20	40,45,60,61	0
1	MLY	D	378	11/12	0.91	0.16	57,59,63,64	0
1	MLY	D	227	11/12	0.91	0.17	53,58,69,70	0
1	MLY	B	736	11/12	0.92	0.13	39,44,55,55	0
1	MLY	D	371	11/12	0.92	0.19	57,61,76,76	0
1	MLY	C	533	11/12	0.92	0.18	42,45,57,58	0
1	MLY	B	376	11/12	0.92	0.20	55,62,71,71	0
1	MLY	D	131	11/12	0.92	0.25	51,64,73,75	0
1	MLY	A	366	11/12	0.92	0.16	41,46,58,60	0
1	MLY	A	371	11/12	0.93	0.18	40,46,63,64	0
1	MLY	A	573	11/12	0.93	0.17	25,29,44,45	0
1	MLY	B	779	11/12	0.93	0.12	47,52,65,66	0
1	SME	A	519	9/10	0.93	0.15	37,45,51,55	0
1	MLY	D	736	11/12	0.93	0.18	34,43,58,60	0
1	MLY	A	111	11/12	0.93	0.17	35,39,53,54	0
1	MLY	A	378	11/12	0.93	0.18	47,49,52,55	0
1	MLY	D	366	11/12	0.93	0.17	46,51,57,58	0
1	MLY	D	111	11/12	0.94	0.12	35,39,48,49	0
1	MLY	B	533	11/12	0.94	0.14	40,45,61,62	0
1	MLY	A	533	11/12	0.94	0.16	36,40,59,60	0
1	MLY	B	131	11/12	0.94	0.20	47,56,66,67	0
1	MLY	D	779	11/12	0.95	0.17	41,47,59,60	0
1	MLY	C	779	11/12	0.95	0.13	49,55,66,68	0
1	MLY	C	573	11/12	0.95	0.15	28,31,43,44	0
1	MLY	B	573	11/12	0.95	0.20	31,34,50,50	0
1	MLY	C	111	11/12	0.95	0.19	34,39,52,54	0
1	MLY	A	736	11/12	0.95	0.12	28,35,46,47	0
1	SME	D	519	9/10	0.95	0.12	46,53,58,61	0
1	MLY	B	366	11/12	0.96	0.14	45,50,63,65	0
1	SME	B	519	9/10	0.96	0.13	39,48,53,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	779	11/12	0.96	0.10	37,42,54,55	0
1	SME	C	519	9/10	0.96	0.10	47,53,58,61	0
1	MLY	D	573	11/12	0.97	0.15	27,29,40,42	0

### 6.3 Carbohydrates

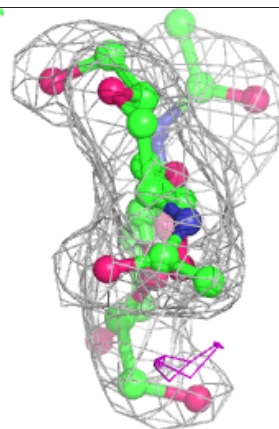
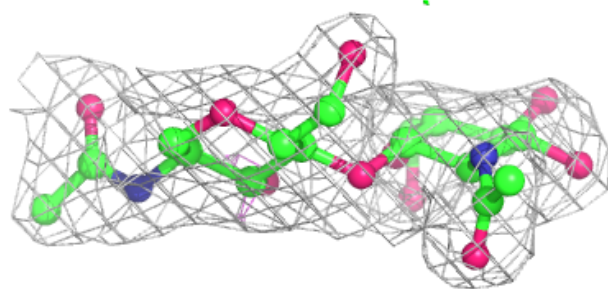
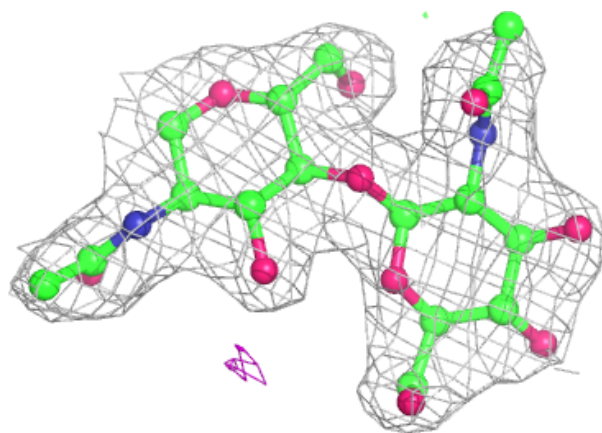
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	BMA	H	3	11/12	0.72	0.23	99,103,107,107	0
2	NAG	F	2	14/15	0.83	0.21	81,87,92,92	0
3	NAG	H	2	14/15	0.83	0.17	72,77,87,93	0
3	BMA	G	3	11/12	0.83	0.15	104,109,112,112	0
3	NAG	G	2	14/15	0.86	0.15	78,84,93,98	0
2	NAG	E	2	14/15	0.93	0.14	57,62,67,70	0
3	NAG	G	1	14/15	0.95	0.10	48,54,60,70	0
2	NAG	F	1	14/15	0.96	0.08	48,55,64,73	0
3	NAG	H	1	14/15	0.97	0.09	41,47,56,65	0
2	NAG	E	1	14/15	0.97	0.09	35,39,45,51	0

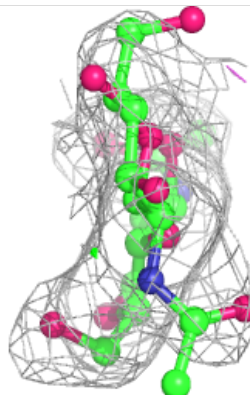
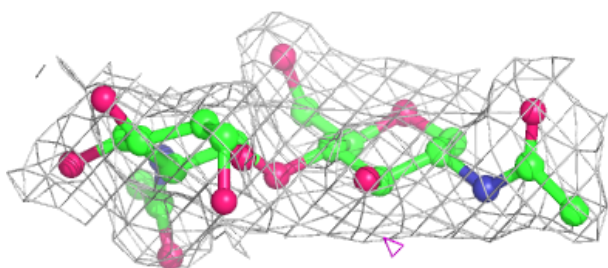
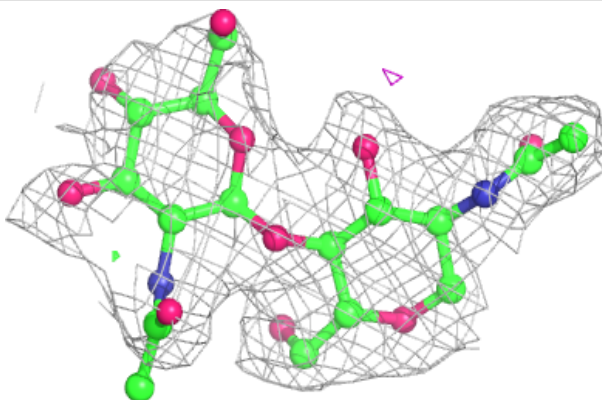
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain E:**

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

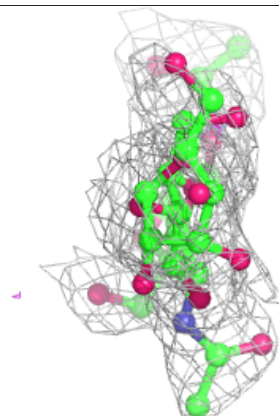
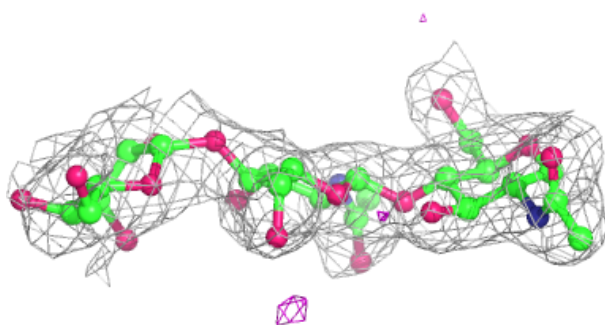
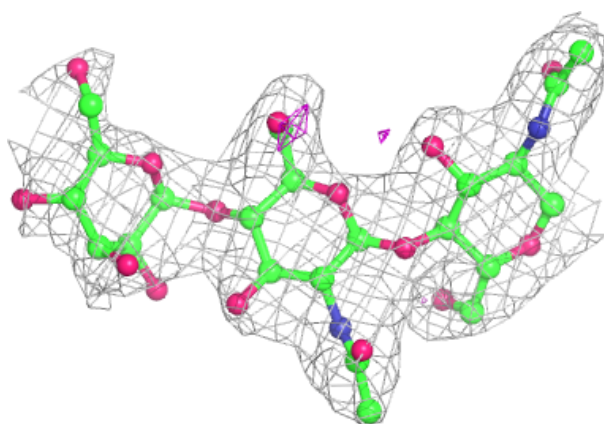
**Electron density around Chain F:**

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

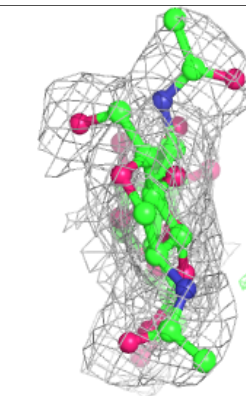
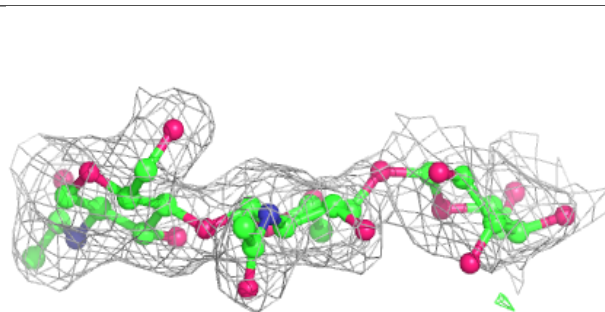
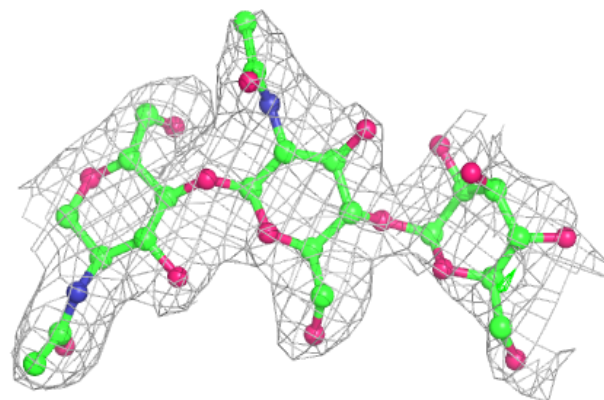


**Electron density around Chain G:**

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

**Electron density around Chain H:**

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



## 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, 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.

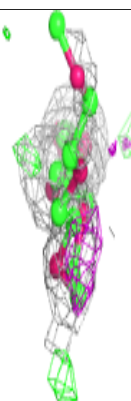
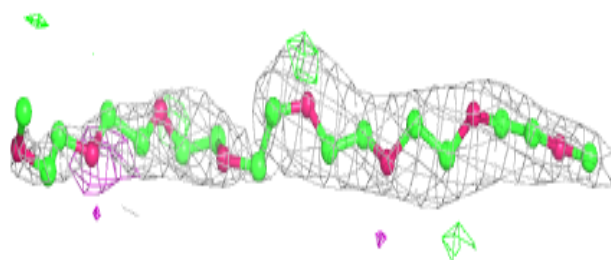
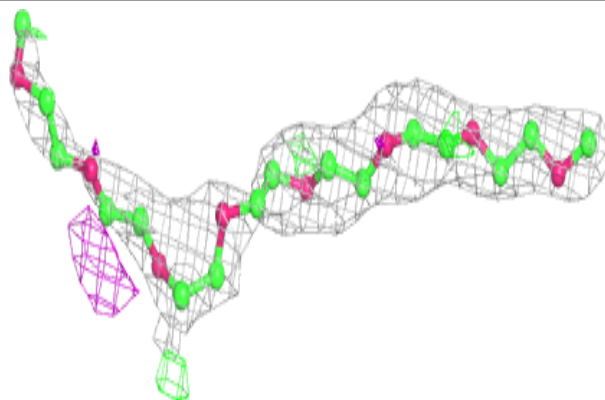
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	7PG	B	906	24/26	0.74	0.27	88,97,105,107	0
6	7PG	C	906	17/26	0.76	0.39	59,64,80,80	0
6	7PG	A	907	24/26	0.79	0.28	74,82,88,90	0
4	SO4	C	903	5/5	0.82	0.22	166,167,168,170	0
4	SO4	D	903	5/5	0.84	0.20	143,145,145,146	0
6	7PG	C	905	22/26	0.85	0.38	23,28,36,40	22
6	7PG	D	905	22/26	0.86	0.33	16,24,31,36	22
6	7PG	D	906	17/26	0.87	0.31	45,54,67,68	0
5	6A9	B	903[D]	22/22	0.90	0.29	12,14,21,24	22
5	6A9	B	903[C]	22/22	0.90	0.29	14,17,29,32	22
5	6A9	B	903[B]	22/22	0.90	0.29	36,41,45,46	22
5	6A9	B	903[A]	22/22	0.90	0.29	24,30,43,43	22
5	6A9	C	904[C]	22/22	0.91	0.26	27,28,30,30	22
5	6A9	C	904[B]	22/22	0.91	0.26	38,40,41,41	22
5	6A9	C	904[D]	22/22	0.91	0.26	13,16,25,26	22
5	6A9	C	904[A]	22/22	0.91	0.26	24,30,35,36	22
5	6A9	A	903[C]	22/22	0.92	0.28	25,27,35,37	22
5	6A9	A	903[B]	22/22	0.92	0.28	40,42,48,49	22
5	6A9	A	903[D]	22/22	0.92	0.28	9,11,15,17	22
5	6A9	A	903[A]	22/22	0.92	0.28	15,22,45,46	22
5	6A9	D	904[B]	22/22	0.93	0.24	33,38,41,42	22
5	6A9	D	904[C]	22/22	0.93	0.24	24,29,30,31	22
5	6A9	D	904[D]	22/22	0.93	0.24	11,15,27,31	22
5	6A9	D	904[A]	22/22	0.93	0.24	13,25,34,35	22
4	SO4	A	901	5/5	0.94	0.14	83,84,86,86	0
4	SO4	B	907	5/5	0.94	0.13	99,100,101,102	0
4	SO4	A	906	5/5	0.94	0.12	93,94,95,96	0
4	SO4	C	902	5/5	0.95	0.15	83,84,85,85	0
4	SO4	B	901	5/5	0.95	0.13	77,80,80,82	0
4	SO4	D	902	5/5	0.96	0.12	77,78,79,80	0
4	SO4	B	902	5/5	0.97	0.12	71,71,73,75	0
4	SO4	A	902	5/5	0.97	0.16	60,62,66,67	0
4	SO4	D	901	5/5	0.98	0.09	47,48,54,56	0
4	SO4	C	901	5/5	0.98	0.09	49,49,52,52	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.

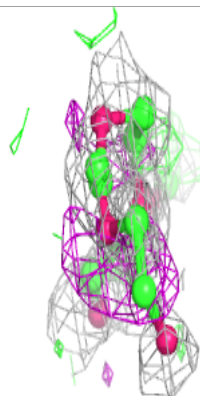
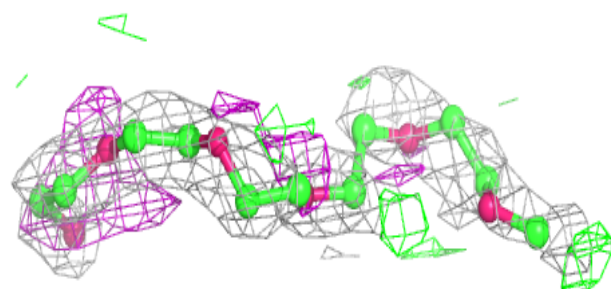
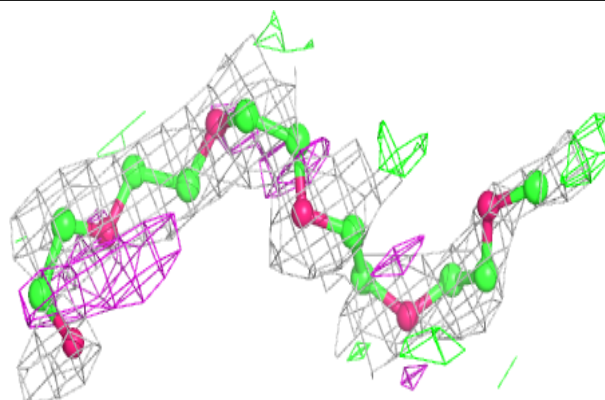
**Electron density around 7PG B 906:**

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



**Electron density around 7PG C 906:**

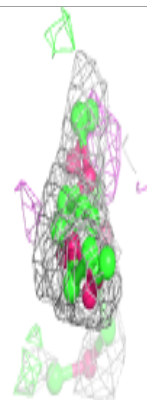
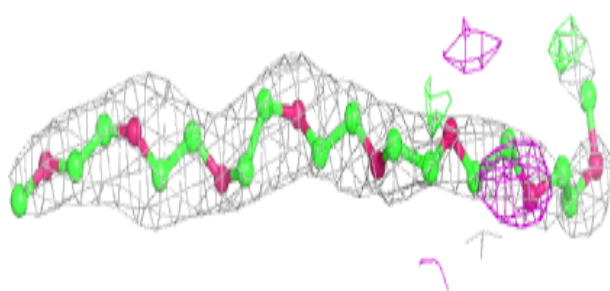
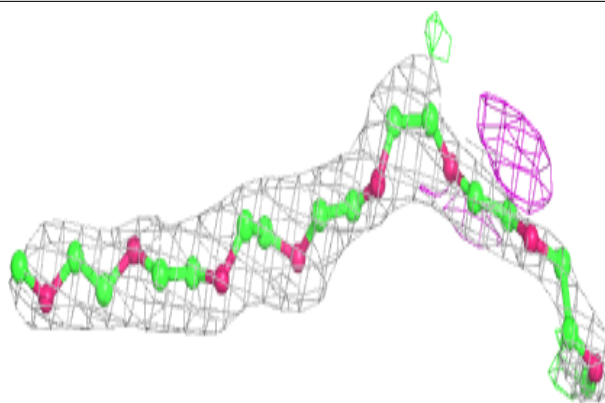
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



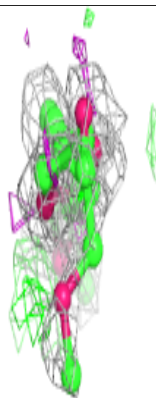
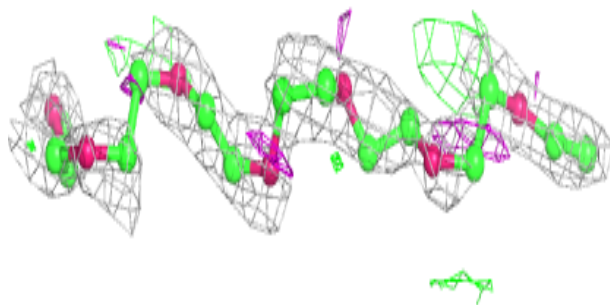
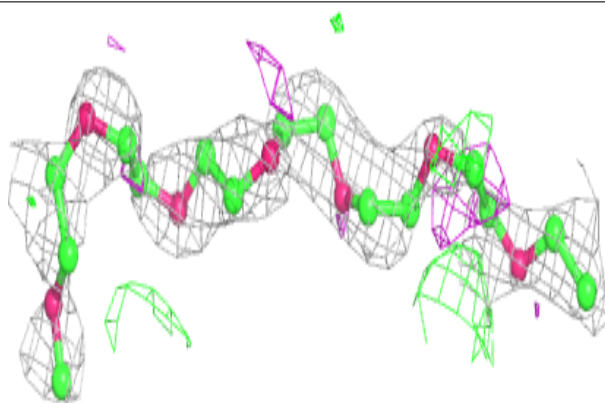


**Electron density around 7PG A 907:**

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

**Electron density around 7PG C 905:**

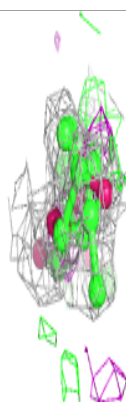
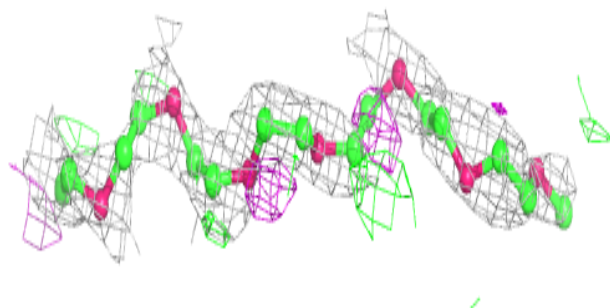
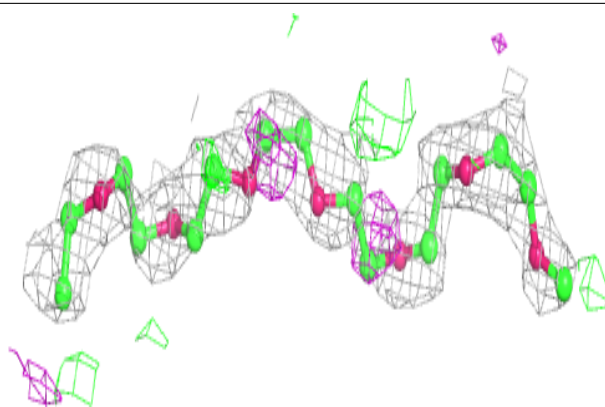
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



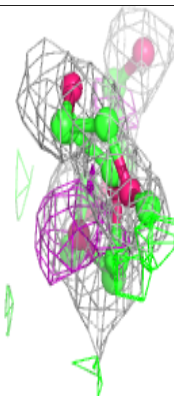
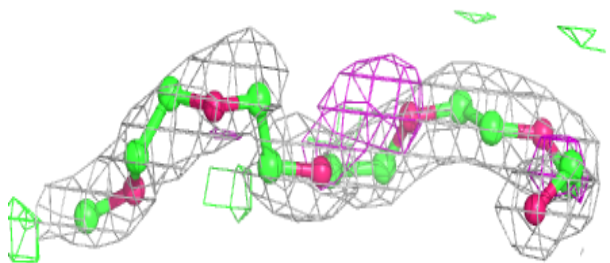
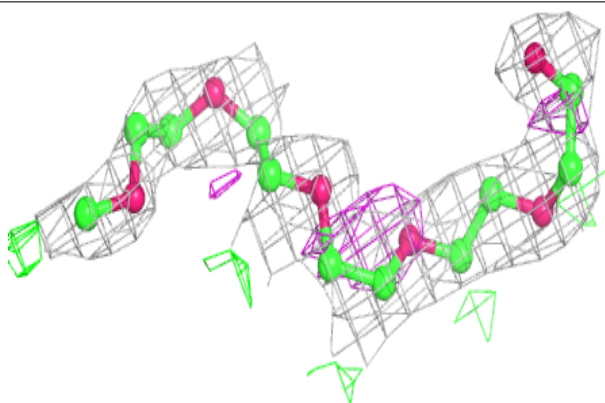


**Electron density around 7PG D 905:**

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

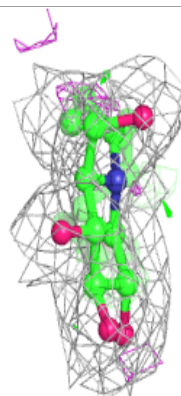
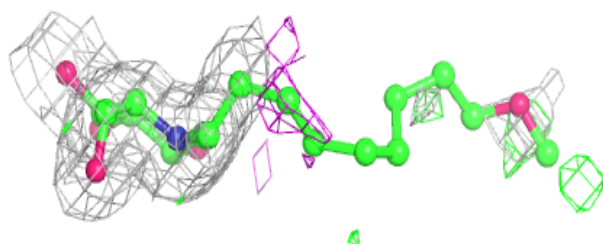
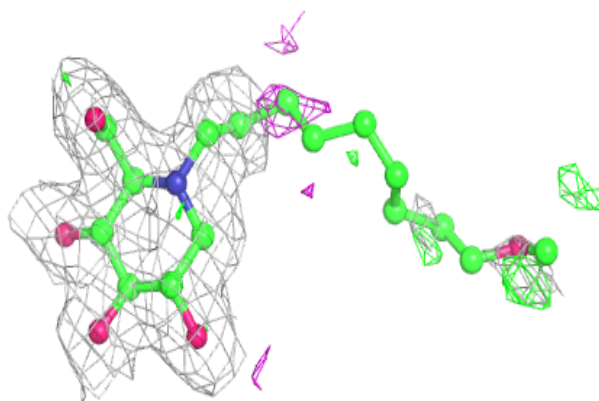
**Electron density around 7PG D 906:**

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and green (positive)

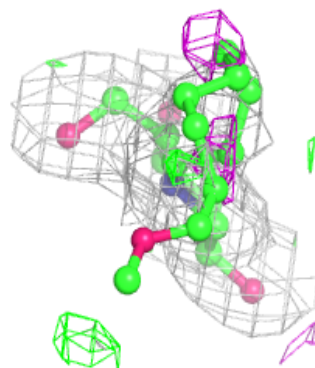
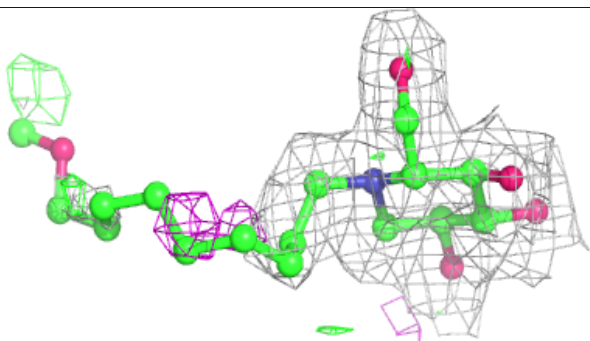
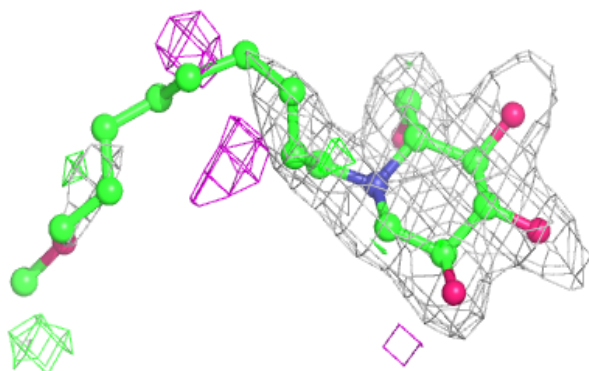


**Electron density around 6A9 B 903 (D):**

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

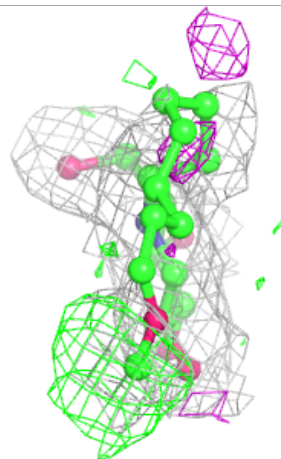
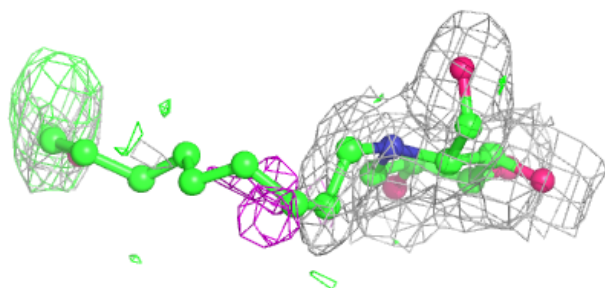
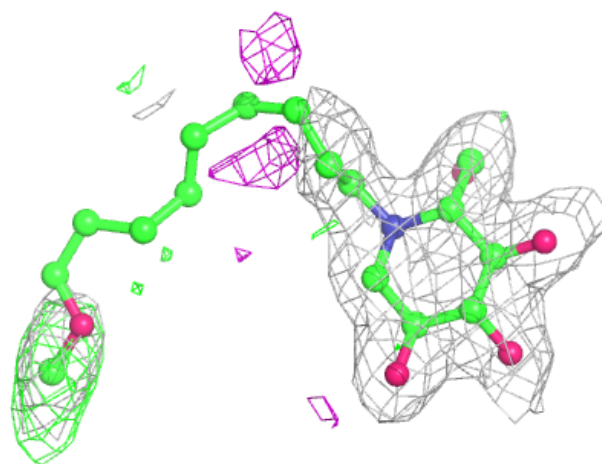
**Electron density around 6A9 B 903 (C):**

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



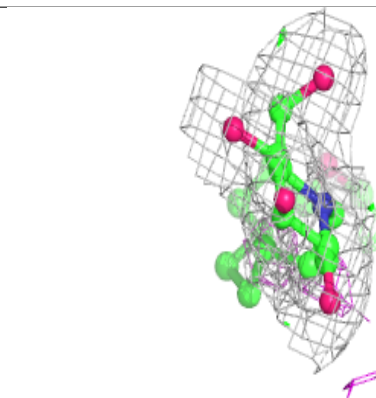
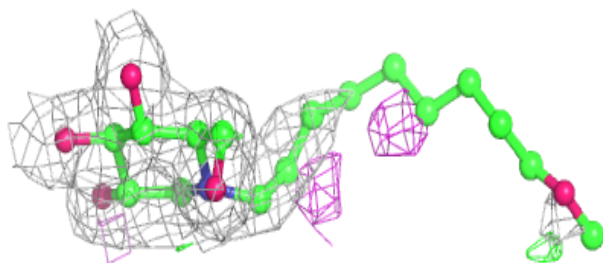
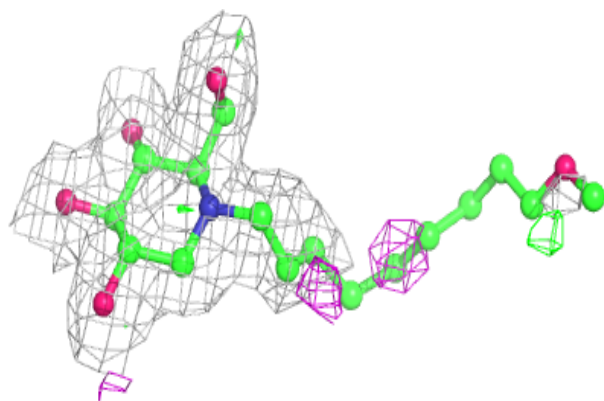
**Electron density around 6A9 B 903 (B):**

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

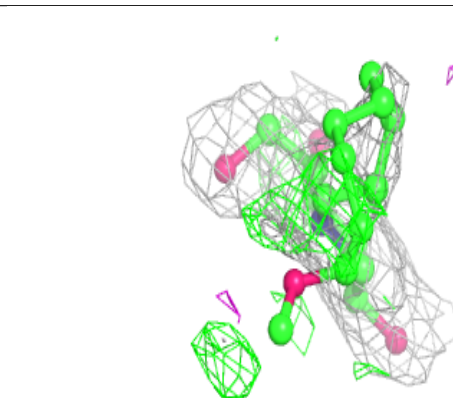
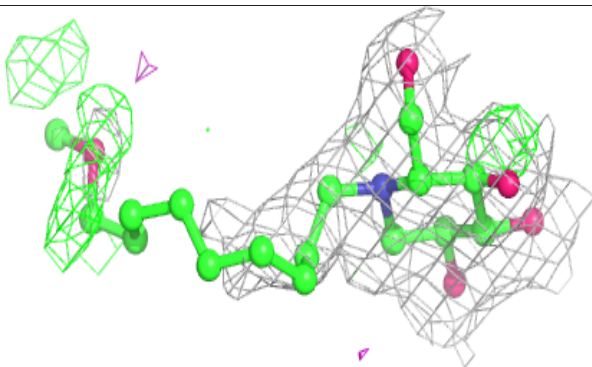
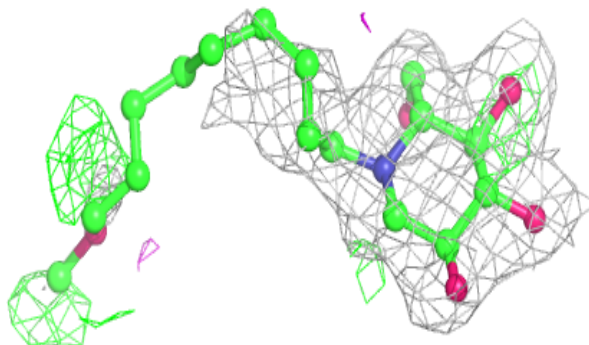


**Electron density around 6A9 B 903 (A):**

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

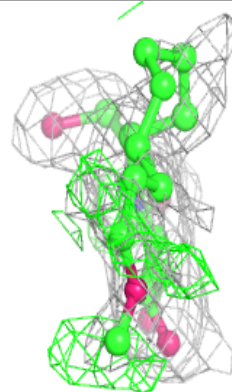
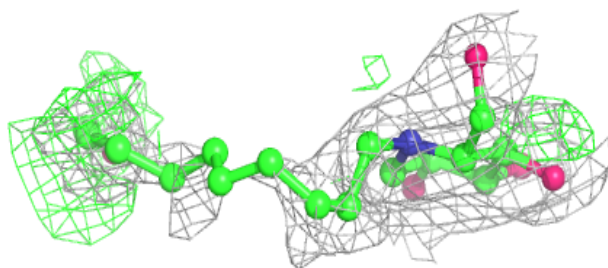
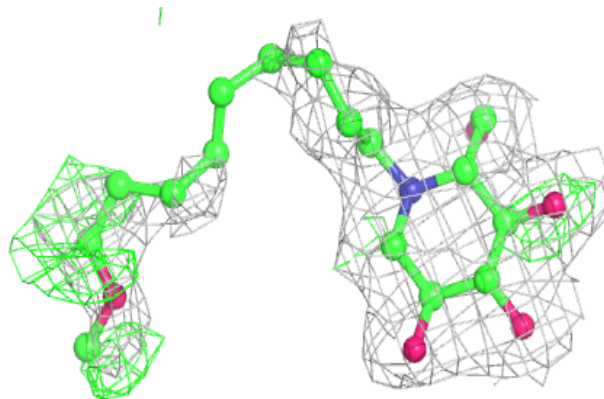
**Electron density around 6A9 C 904 (C):**

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

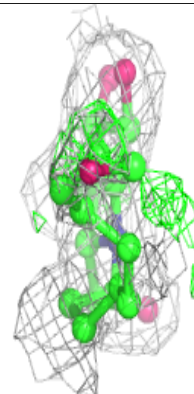
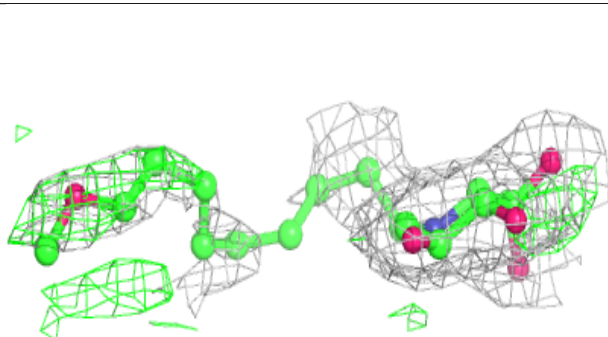
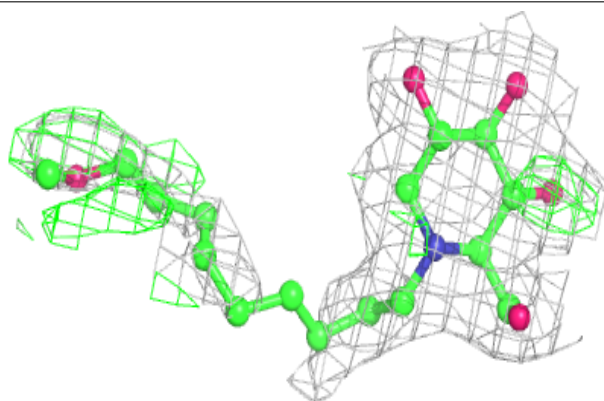


**Electron density around 6A9 C 904 (B):**

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

**Electron density around 6A9 C 904 (D):**

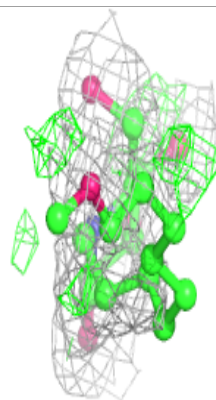
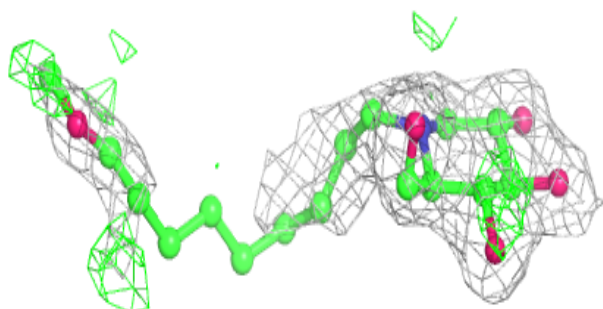
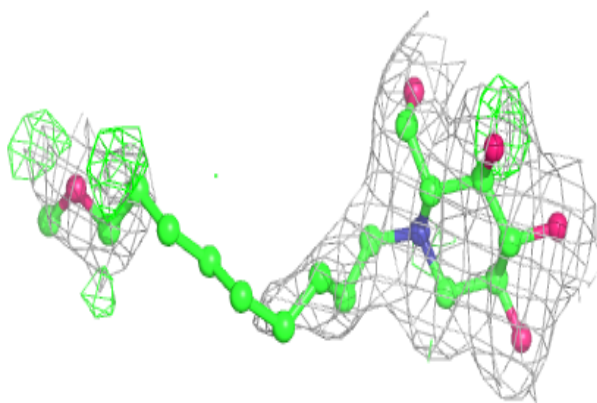
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



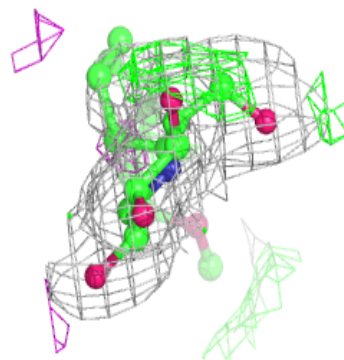
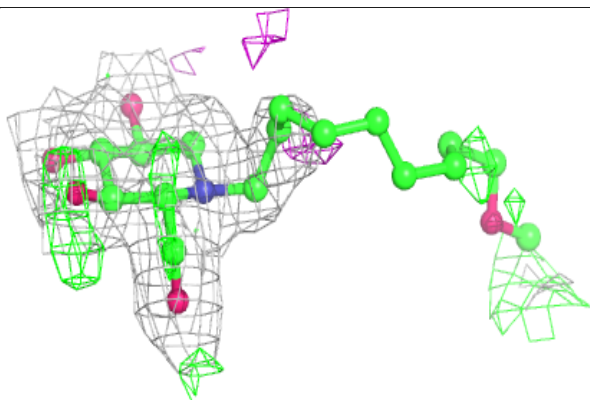
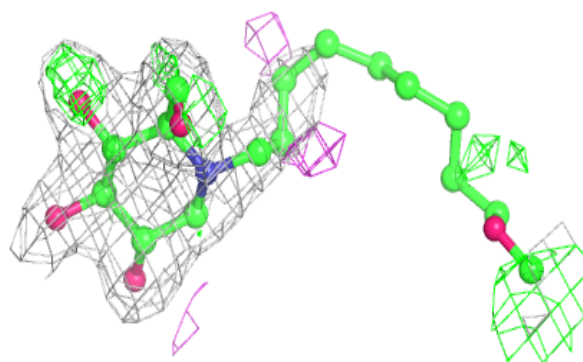


**Electron density around 6A9 C 904 (A):**

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

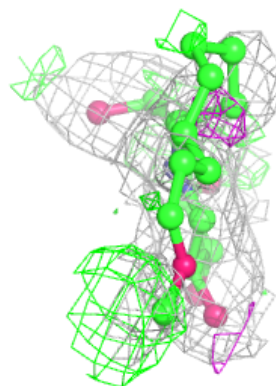
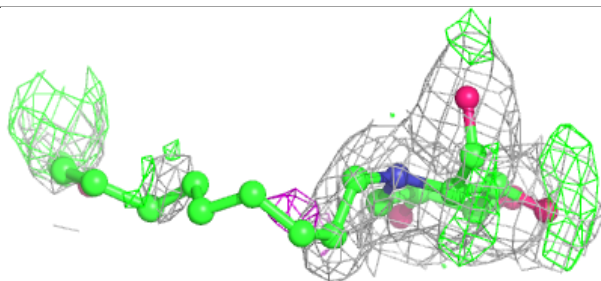
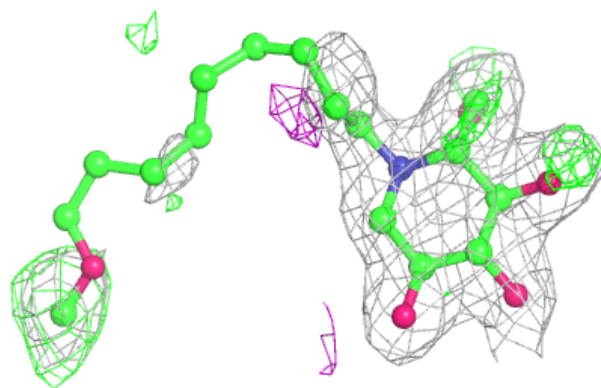
**Electron density around 6A9 A 903 (C):**

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

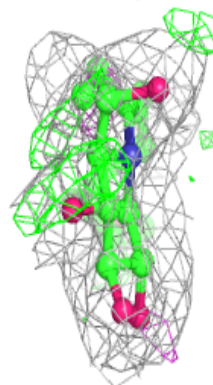
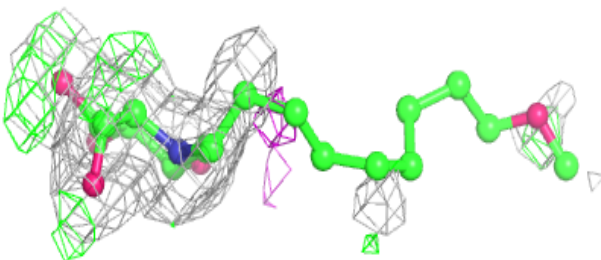
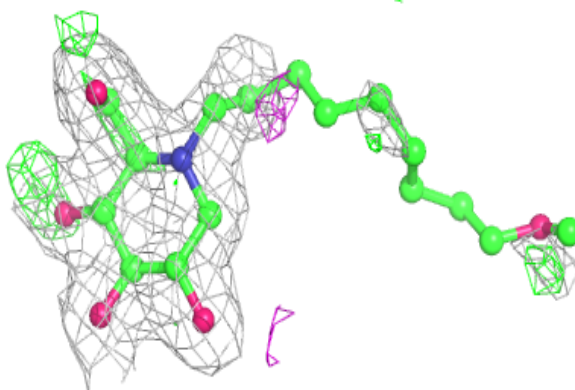


**Electron density around 6A9 A 903 (B):**

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

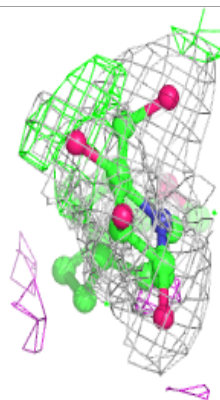
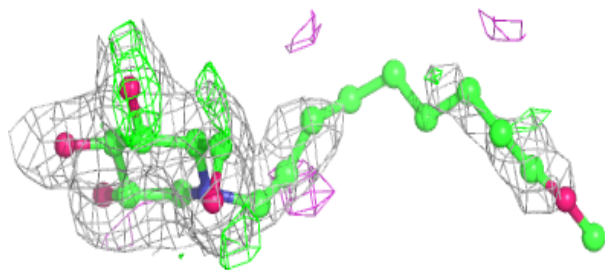
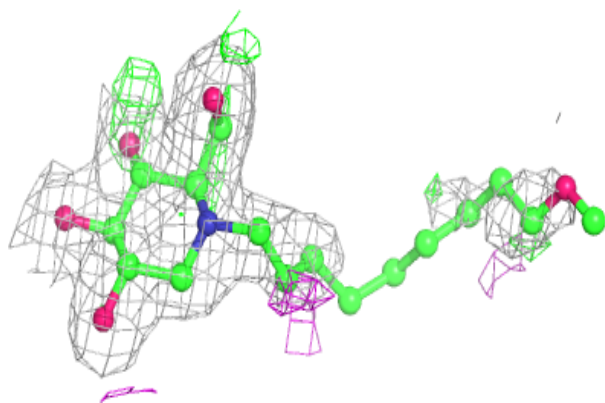
**Electron density around 6A9 A 903 (D):**

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

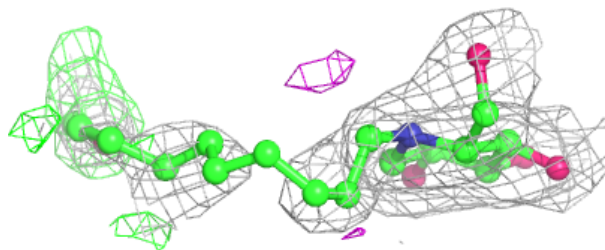
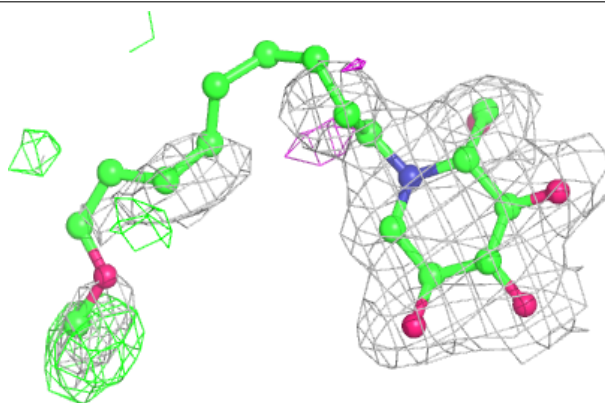


**Electron density around 6A9 A 903 (A):**

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

**Electron density around 6A9 D 904 (B):**

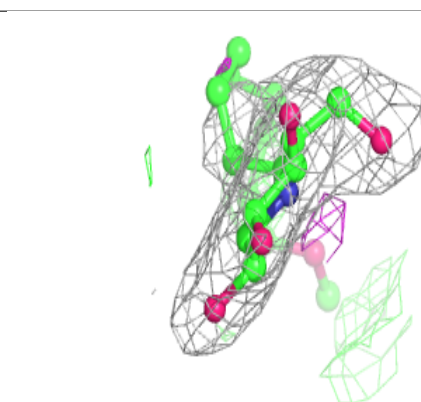
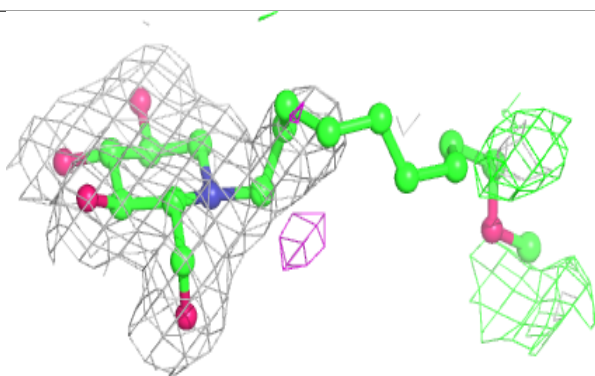
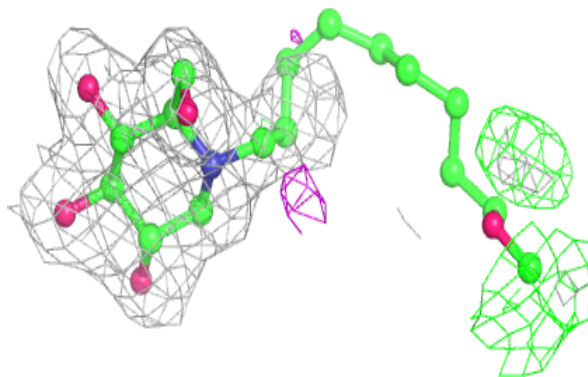
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



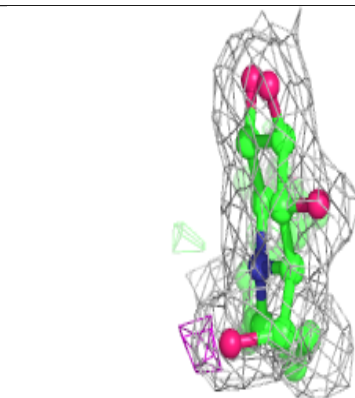
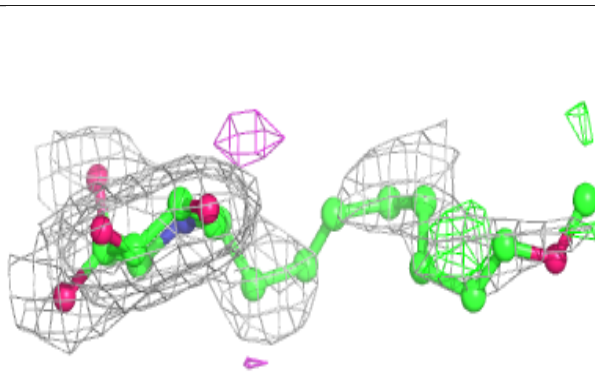
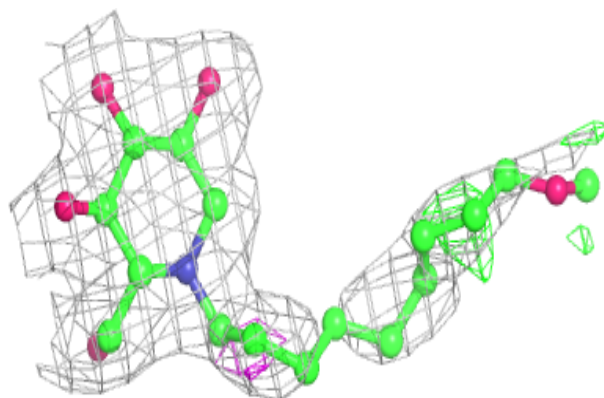


**Electron density around 6A9 D 904 (C):**

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

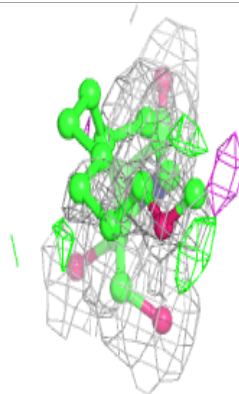
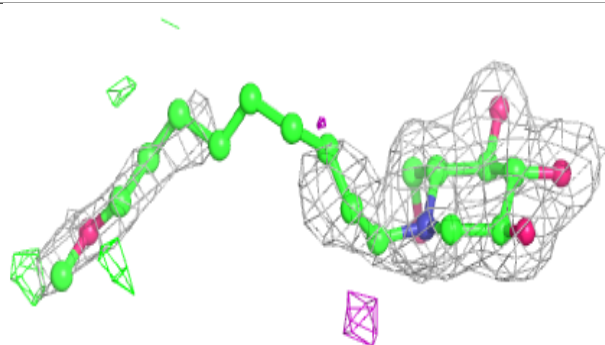
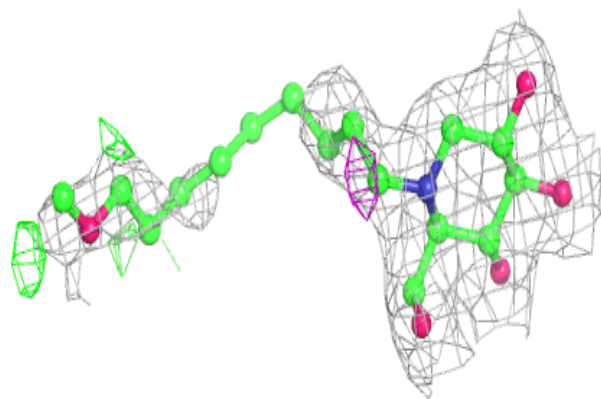
**Electron density around 6A9 D 904 (D):**

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



**Electron density around 6A9 D 904 (A):**

$2mF_o-DF_c$  (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.