



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:42 am GMT

PDB ID : 6H03  
EMDB ID : EMD-0106  
Title : OPEN CONFORMATION OF THE MEMBRANE ATTACK COMPLEX  
Authors : Menny, A.; Serna, M.; Boyd, C.M.; Gardner, S.; Joseph, A.P.; Topf, M.;  
Bubeck, D.  
Deposited on : 2018-07-06  
Resolution : 5.60 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

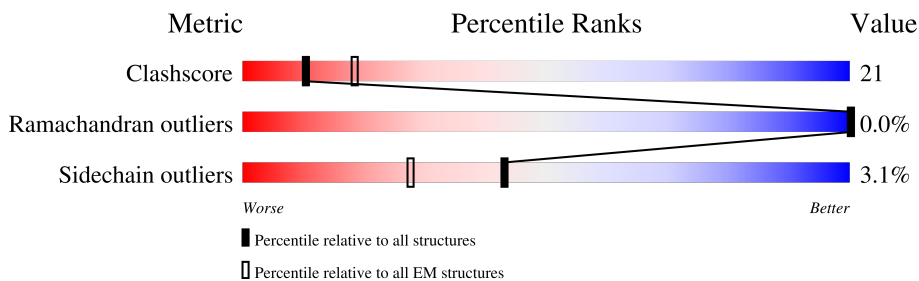
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1580	43% (Poor fit) 59% (0 outliers), 17% (1 outlier), 23% (2+ outliers)
2	C	537	10% (Poor fit) 74% (0 outliers), 21% (1 outlier)
3	D	821	25% (Poor fit) 63% (0 outliers), 16% (1 outlier), 20% (2+ outliers)
4	E	182	27% (Poor fit) 74% (0 outliers), 17% (1 outlier), 9% (2+ outliers)
5	F	554	12% (Poor fit) 66% (0 outliers), 25% (1 outlier), 8% (2+ outliers)
6	B	913	35% (Poor fit) 59% (0 outliers), 16% (1 outlier), 24% (2+ outliers)
7	G	538	14% (Poor fit) 58% (0 outliers), 33% (1 outlier), 7% (2+ outliers)
7	H	538	6% (Poor fit) 56% (0 outliers), 36% (1 outlier), 7% (2+ outliers)

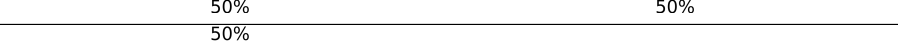
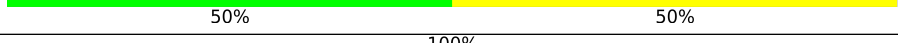
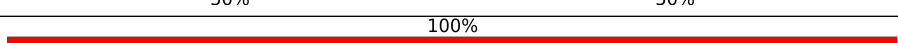
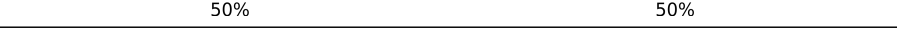
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Mol	Chain	Length	Quality of chain
7	I	538	 6% 56% 36% 7%
7	J	538	 6% 55% 36% 7%
7	K	538	 6% 56% 36% 7%
7	L	538	 5% 53% 39% 7%
7	M	538	 5% 54% 37% 7%
7	N	538	 8% 55% 36% 7%
7	O	538	 6% 54% 38% 7%
7	P	538	 8% 53% 39% 7%
7	Q	538	 7% 54% 37% 7%
7	R	538	 9% 53% 39% 7%
7	S	538	 12% 53% 39% 7%
7	T	538	 17% 53% 38% 7%
7	U	538	 21% 53% 38% 7%
7	V	538	 32% 51% 40% 7%
7	W	538	 51% 51% 41% 7%
7	X	538	 82% 56% 36% 7%
8	Y	3	 100%
9	Z	2	 50% 50%
9	a	2	 100%
9	b	2	 50% 50%
9	c	2	 50% 50%
9	d	2	 50% 50%
9	e	2	 50% 50%
9	f	2	 50% 50%
9	g	2	 50% 50%

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Mol	Chain	Length	Quality of chain
9	h	2	50% 
9	i	2	50% 
9	j	2	50% 
9	k	2	50% 
9	l	2	50% 
9	m	2	50% 
9	n	2	50% 
9	o	2	100% 
9	p	2	100% 
9	q	2	100% 
9	r	2	100% 
9	s	2	100% 

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 102310 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Complement C5, Complement C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1223	9686	6226	1594	1839	27	0	0

- Molecule 2 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	513	4119	2576	729	780	34	0	0

- Molecule 3 is a protein called Complement component C7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	657	5129	3190	896	1001	42	0	0

- Molecule 4 is a protein called Complement component C8 gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	165	1295	828	224	239	4	0	0

- Molecule 5 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	511	4017	2492	701	787	37	0	0

- Molecule 6 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	690	5427	3367	952	1058	50	0	0

- Molecule 7 is a protein called Complement component C9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	P	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	H	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	I	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	J	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	K	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	L	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	M	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	N	501	Total 3973	C 2486	N 690	O 766	S 31	0	0
7	O	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	Q	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	R	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	S	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	T	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	U	501	Total 3977	C 2488	N 691	O 767	S 31	0	0
7	V	501	Total 3951	C 2474	N 686	O 760	S 31	0	0
7	W	501	Total 3941	C 2466	N 682	O 762	S 31	0	0
7	X	501	Total 3977	C 2488	N 691	O 767	S 31	0	0

- Molecule 8 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				AltConf	Trace
			Total	C	N	O		
8	Y	3	39	22	2	15	0	0

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



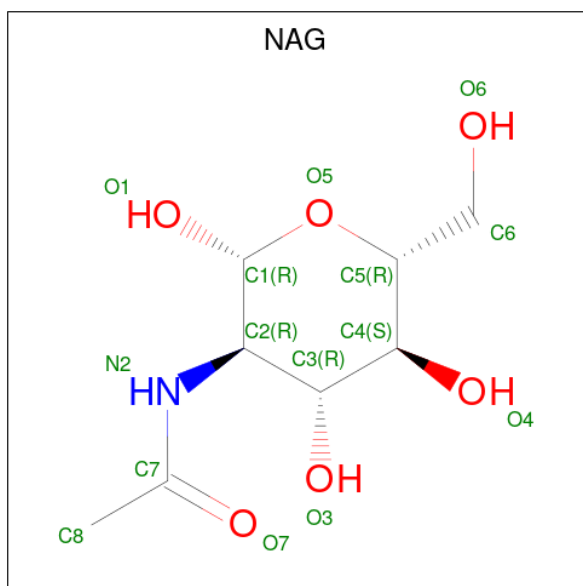
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Z	2	28	16	2	10	0	0
9	a	2	28	16	2	10	0	0
9	b	2	28	16	2	10	0	0
9	c	2	28	16	2	10	0	0
9	d	2	28	16	2	10	0	0
9	e	2	28	16	2	10	0	0
9	f	2	28	16	2	10	0	0
9	g	2	28	16	2	10	0	0
9	h	2	28	16	2	10	0	0
9	i	2	28	16	2	10	0	0
9	j	2	28	16	2	10	0	0
9	k	2	28	16	2	10	0	0
9	l	2	28	16	2	10	0	0
9	m	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	n	2	Total 28	C 16	N 2	O 10	0	0
9	o	2	Total 28	C 16	N 2	O 10	0	0
9	p	2	Total 28	C 16	N 2	O 10	0	0
9	q	2	Total 28	C 16	N 2	O 10	0	0
9	r	2	Total 28	C 16	N 2	O 10	0	0
9	s	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	F	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 28	C 16	N 2	O 10	0
10	G	1	Total 28	C 16	N 2	O 10	0
10	P	1	Total 28	C 16	N 2	O 10	0
10	P	1	Total 28	C 16	N 2	O 10	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	H	1	28	16	2	10	0
10	H	1	28	16	2	10	0
10	I	1	28	16	2	10	0
10	I	1	28	16	2	10	0
10	J	1	28	16	2	10	0
10	J	1	28	16	2	10	0
10	K	1	28	16	2	10	0
10	K	1	28	16	2	10	0
10	L	1	28	16	2	10	0
10	L	1	28	16	2	10	0
10	M	1	28	16	2	10	0
10	M	1	28	16	2	10	0
10	N	1	28	16	2	10	0
10	N	1	28	16	2	10	0
10	O	1	28	16	2	10	0
10	O	1	28	16	2	10	0
10	Q	1	28	16	2	10	0
10	Q	1	28	16	2	10	0
10	R	1	28	16	2	10	0
10	R	1	28	16	2	10	0
10	S	1	28	16	2	10	0

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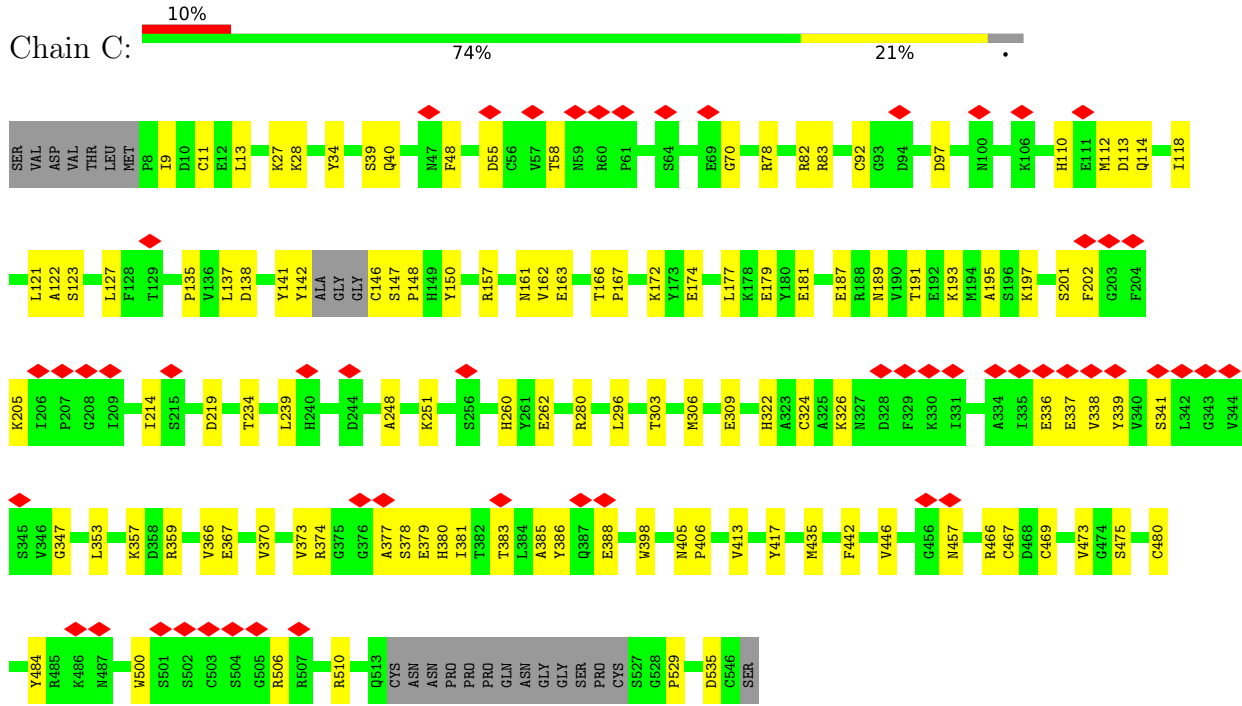
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	S	1	Total 28	C 16	N 2	O 10	0
10	T	1	Total 28	C 16	N 2	O 10	0
10	T	1	Total 28	C 16	N 2	O 10	0
10	U	1	Total 28	C 16	N 2	O 10	0
10	U	1	Total 28	C 16	N 2	O 10	0
10	V	1	Total 28	C 16	N 2	O 10	0
10	V	1	Total 28	C 16	N 2	O 10	0
10	W	1	Total 28	C 16	N 2	O 10	0
10	W	1	Total 28	C 16	N 2	O 10	0
10	X	1	Total 28	C 16	N 2	O 10	0
10	X	1	Total 28	C 16	N 2	O 10	0

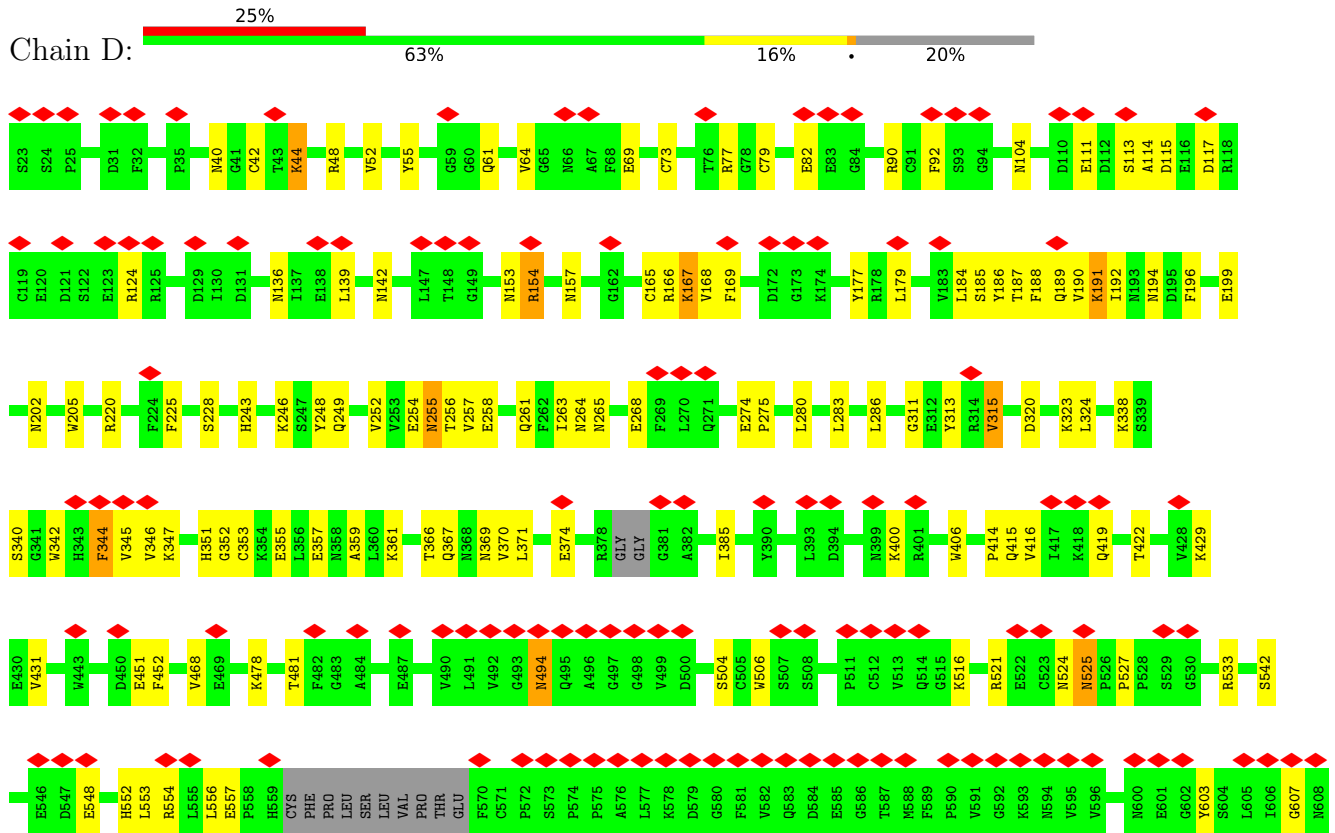


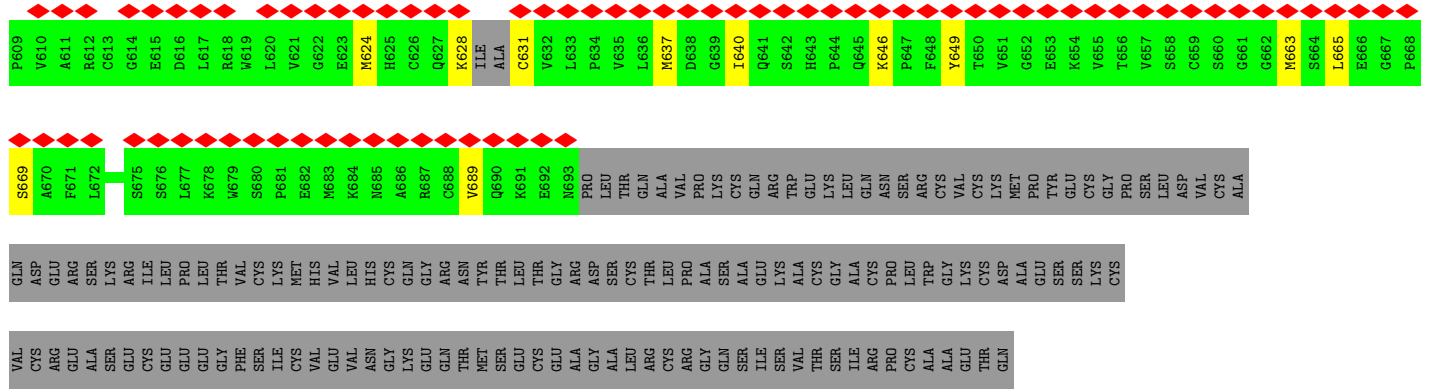


• Molecule 2: Complement component C8 beta chain

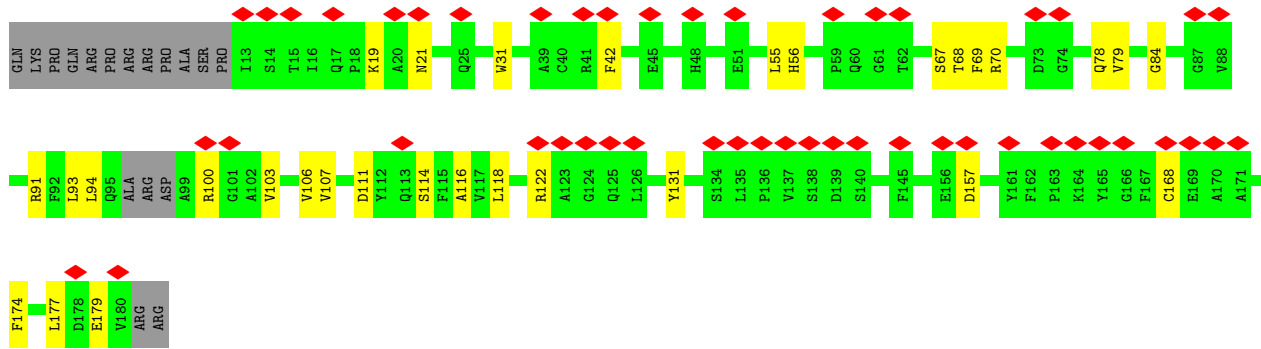
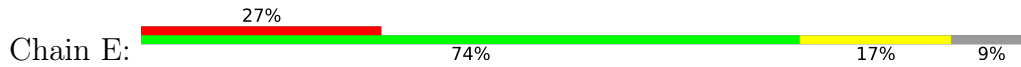


• Molecule 3: Complement component C7

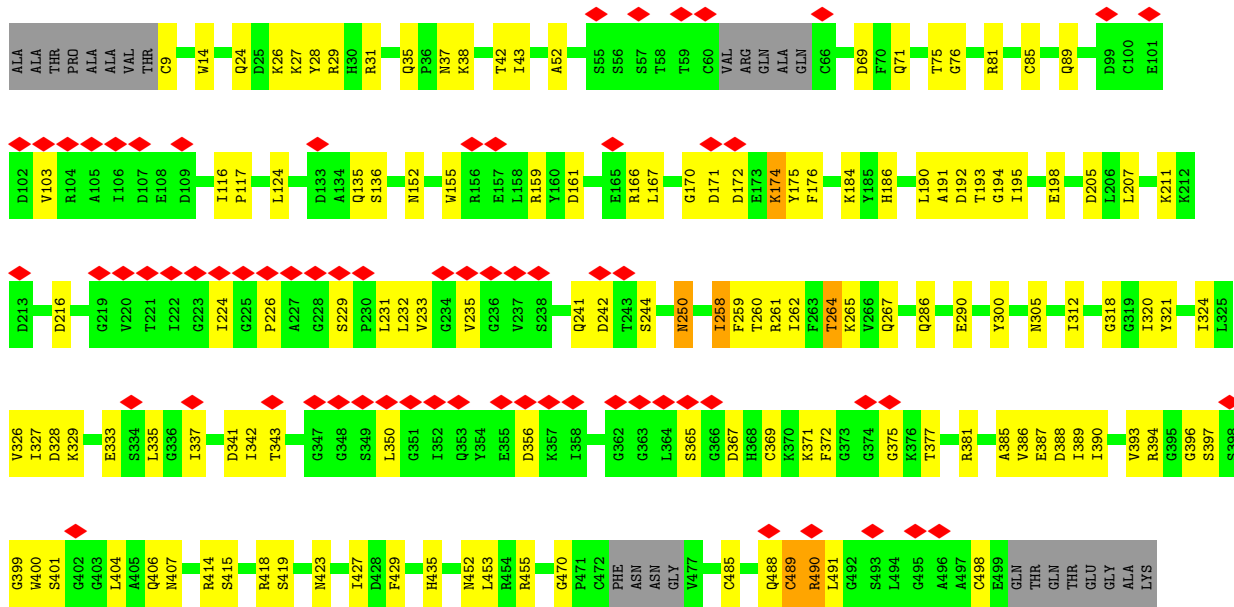




• Molecule 4: Complement component C8 gamma chain

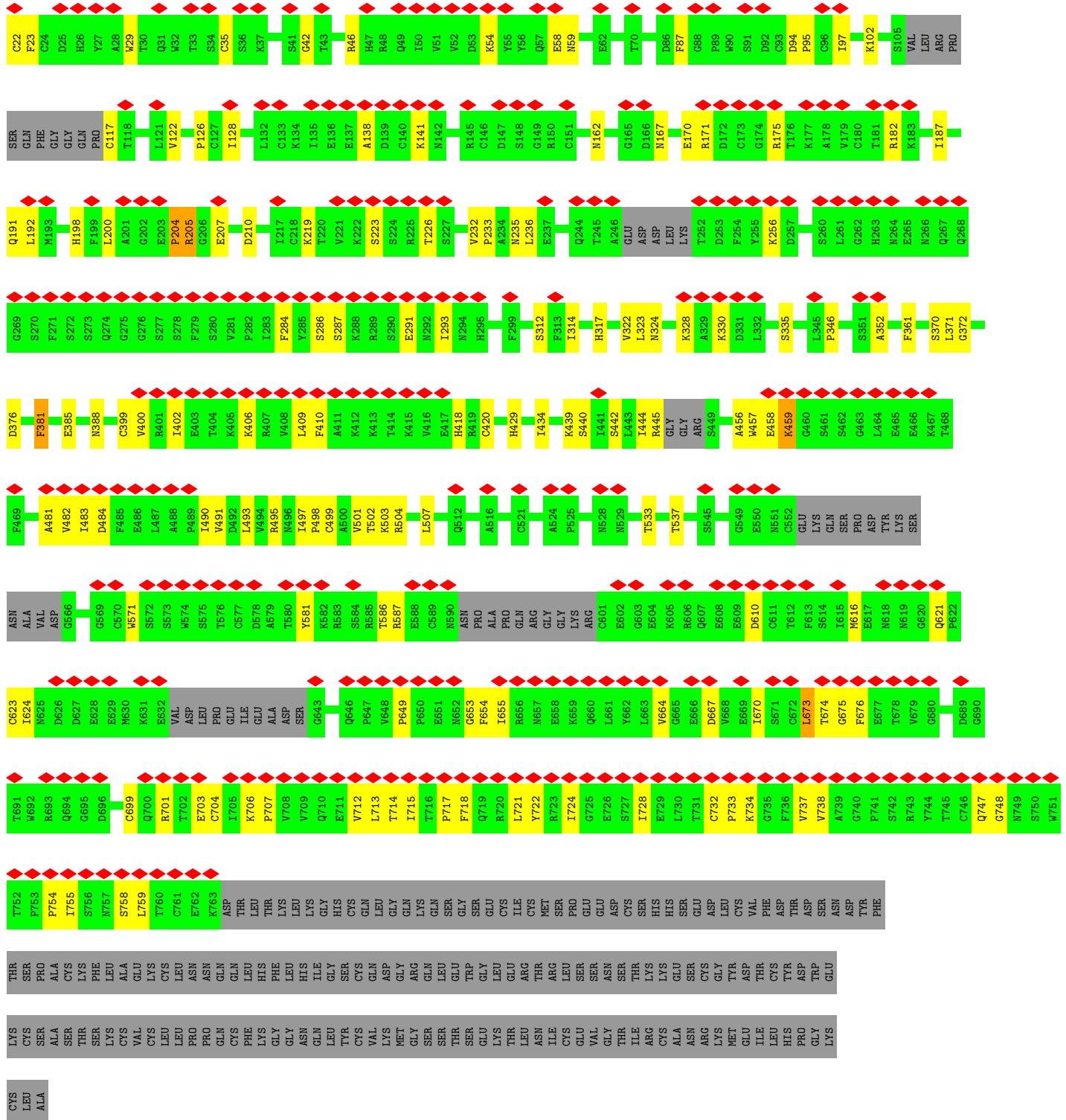


• Molecule 5: Complement component C8 alpha chain

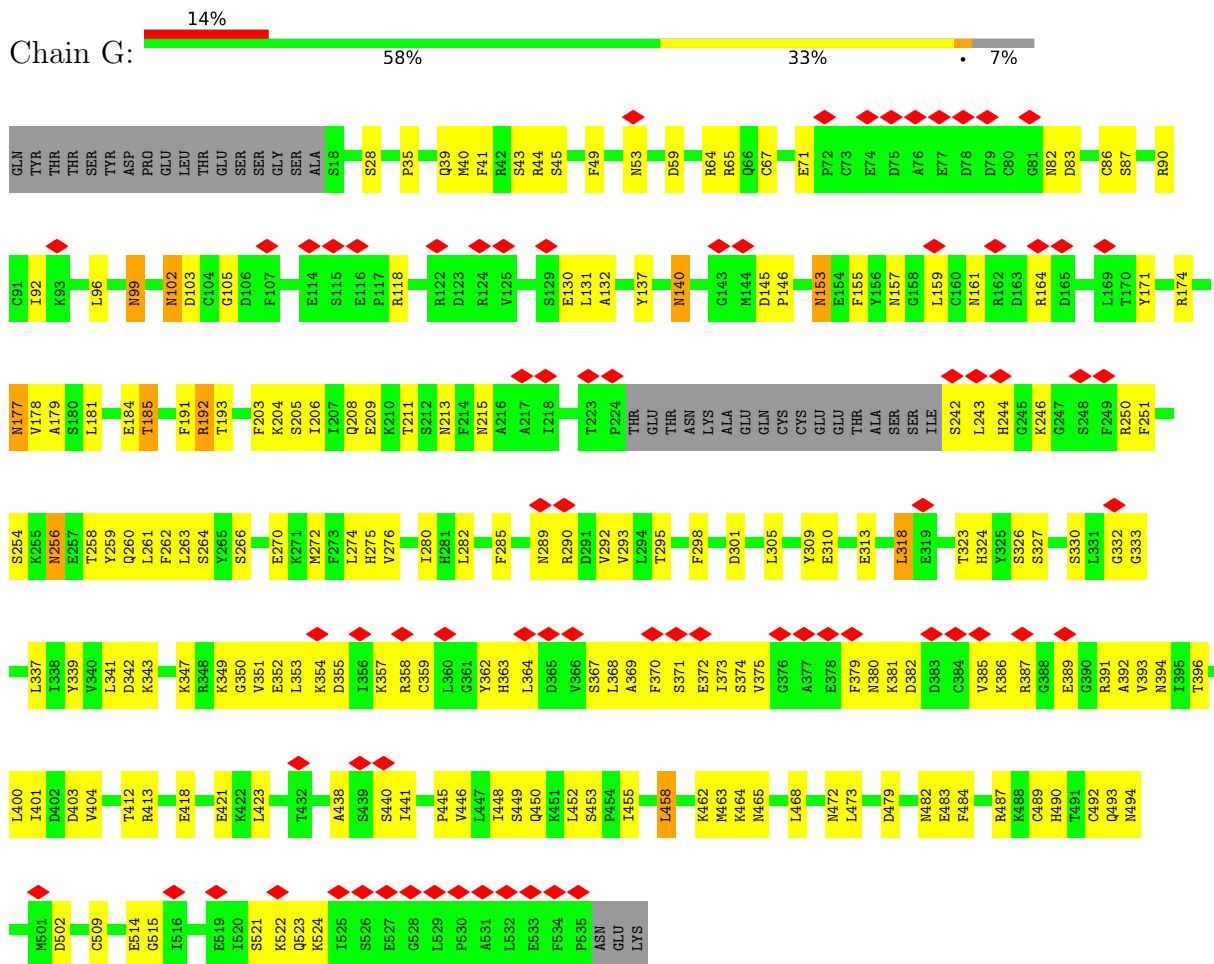




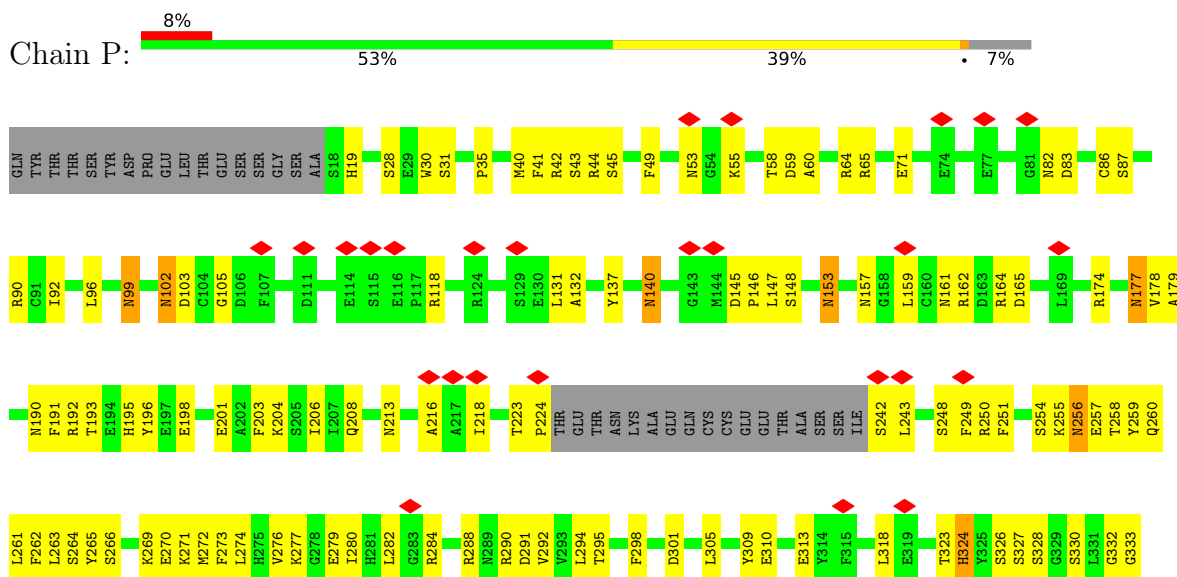
• Molecule 6: Complement component C6



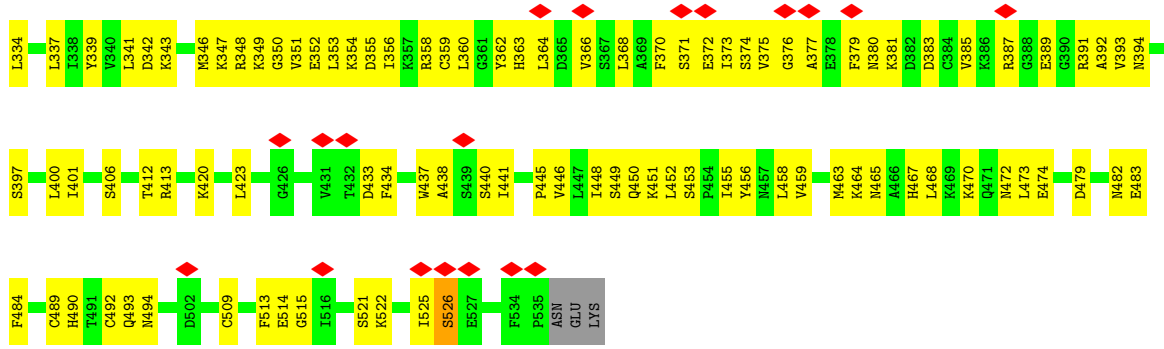
- Molecule 7: Complement component C9



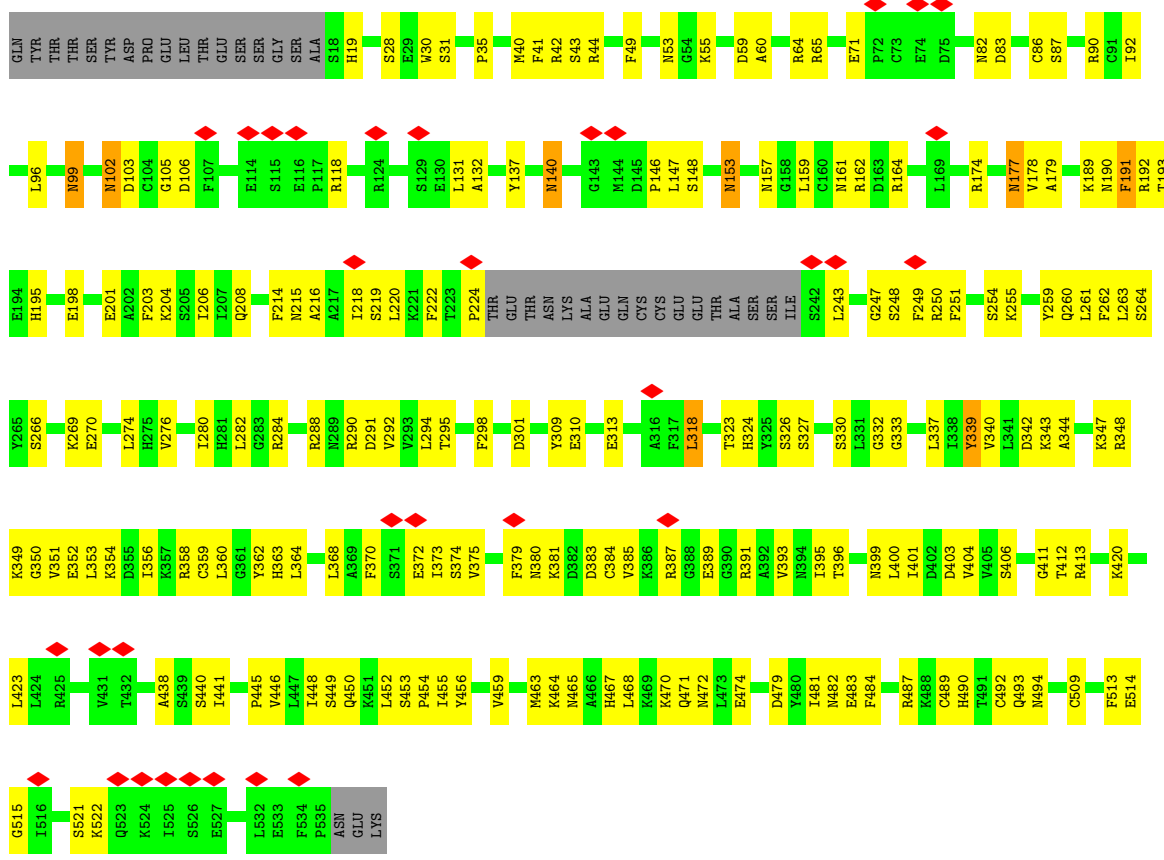
- Molecule 7: Complement component C9





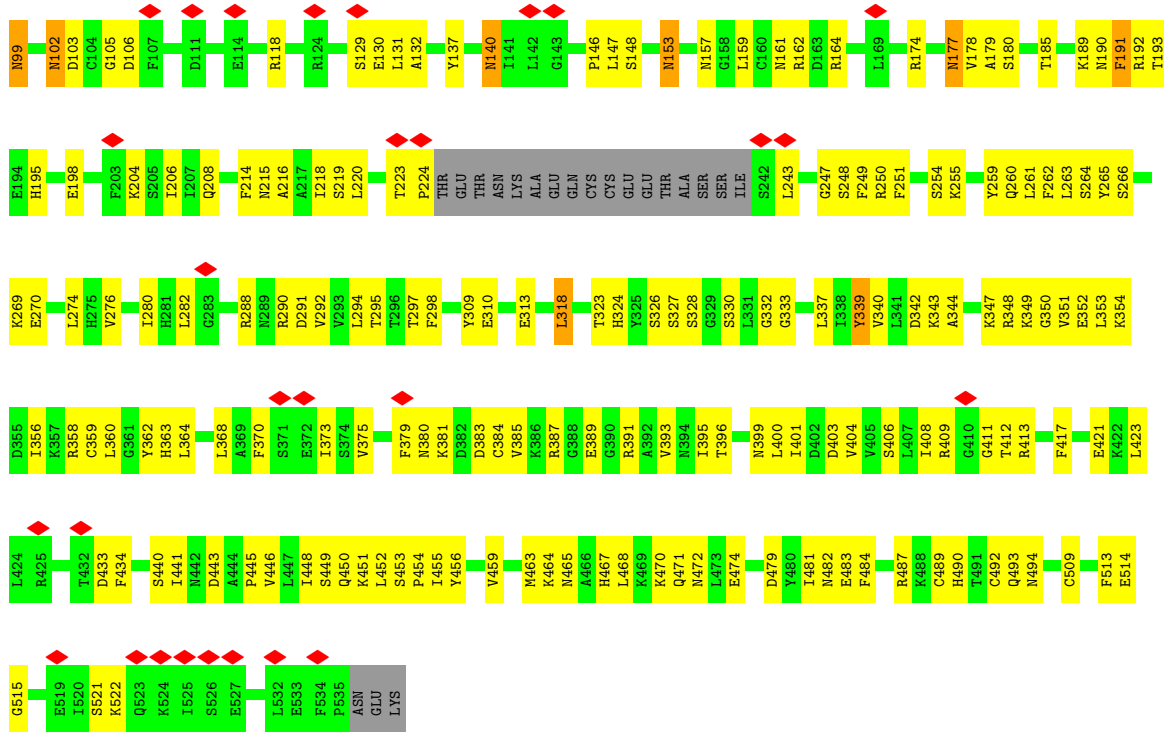


• Molecule 7: Complement component C9

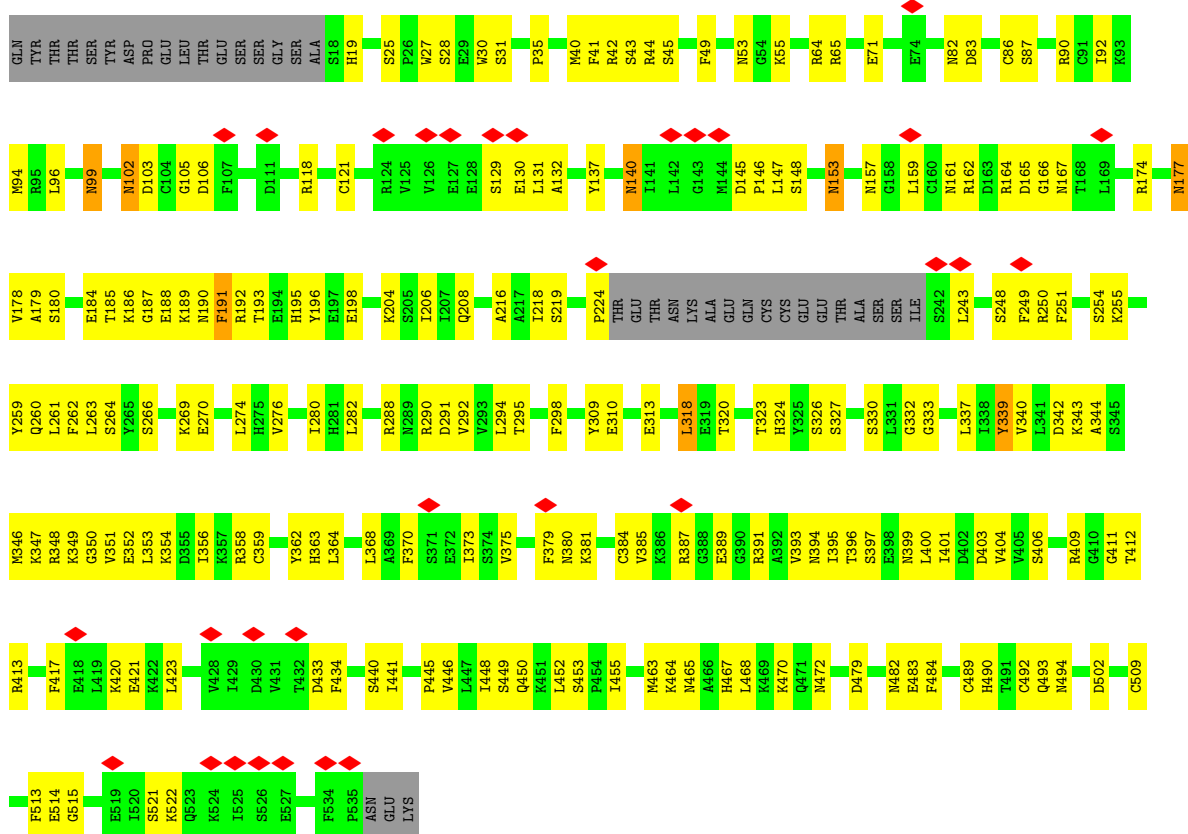


• Molecule 7: Complement component C9

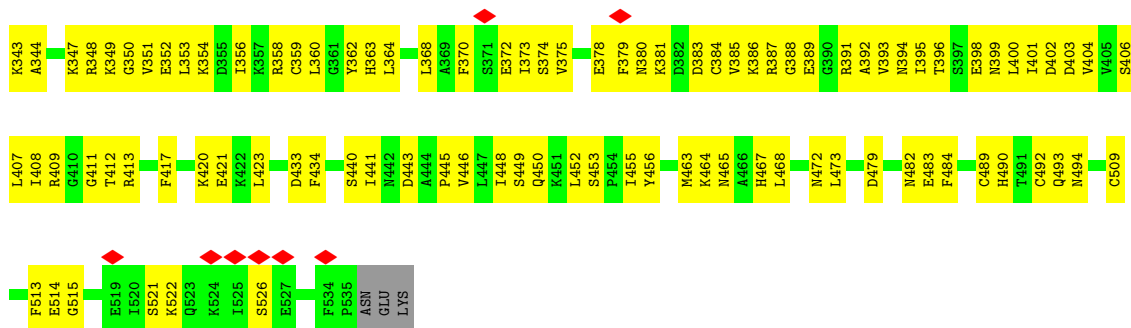




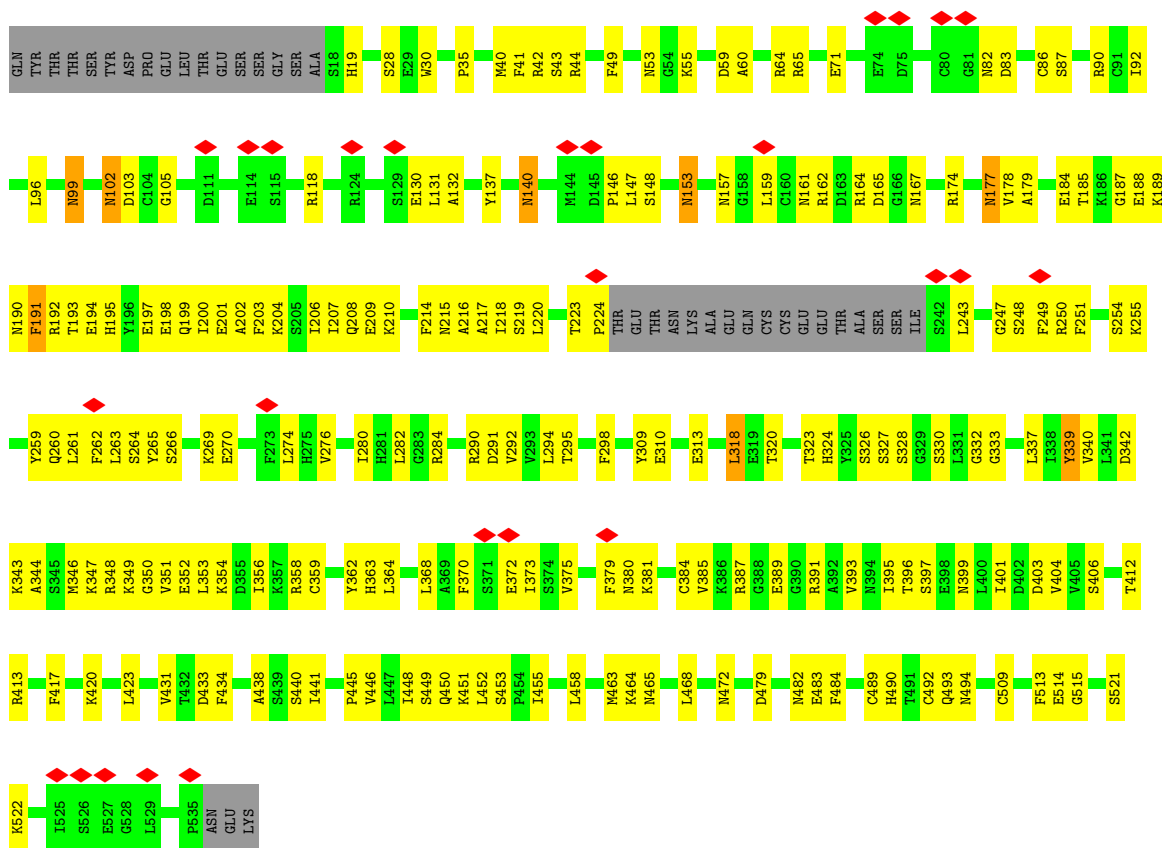
• Molecule 7: Complement component C9



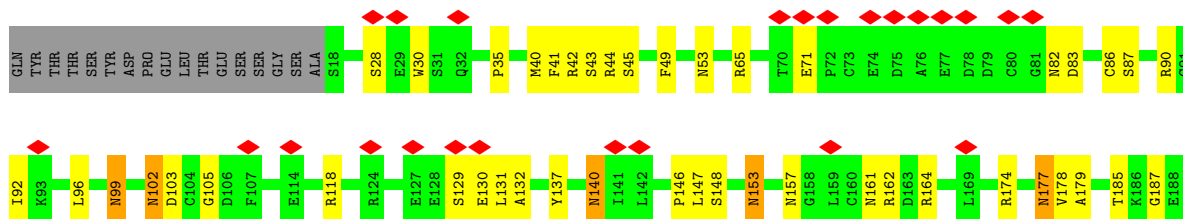


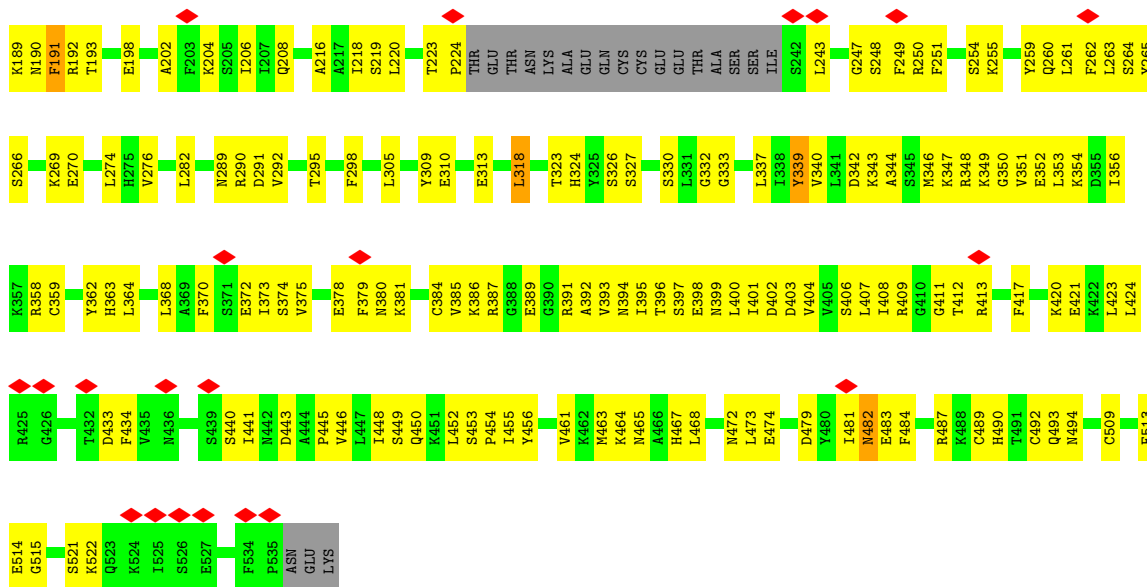


• Molecule 7: Complement component C9

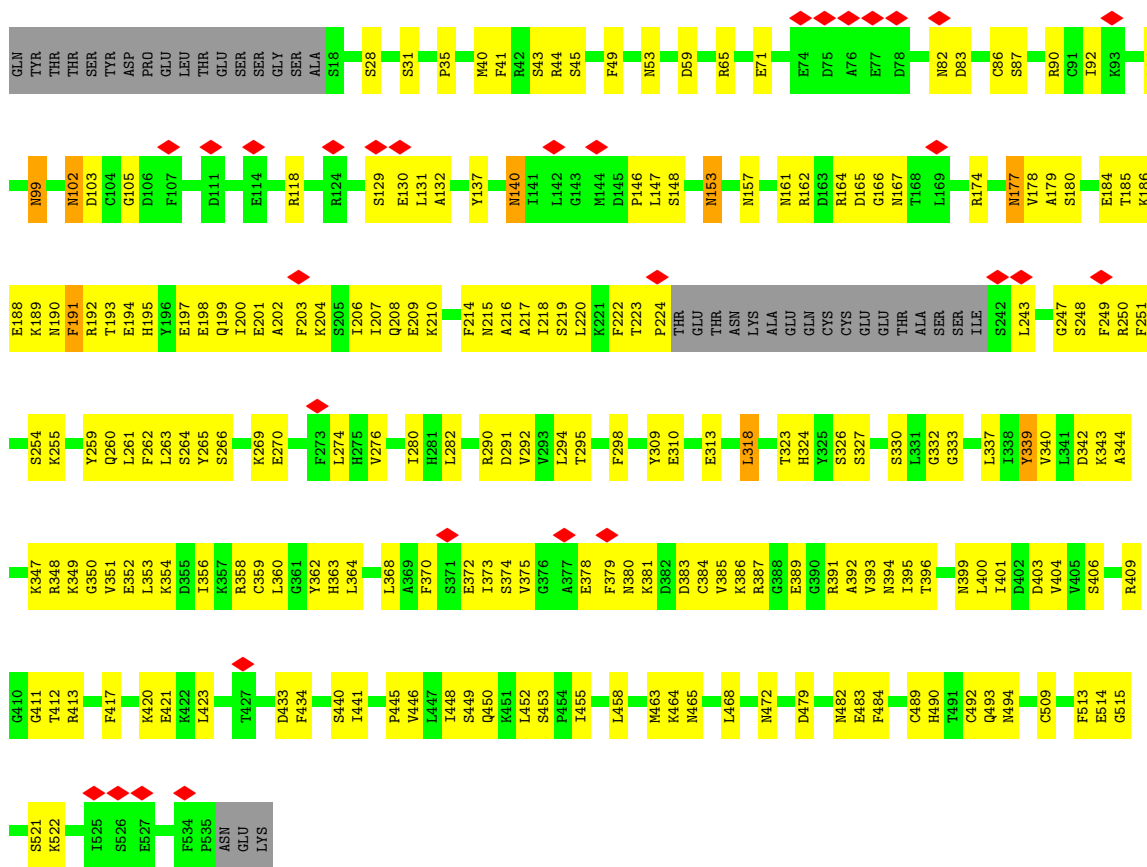


• Molecule 7: Complement component C9



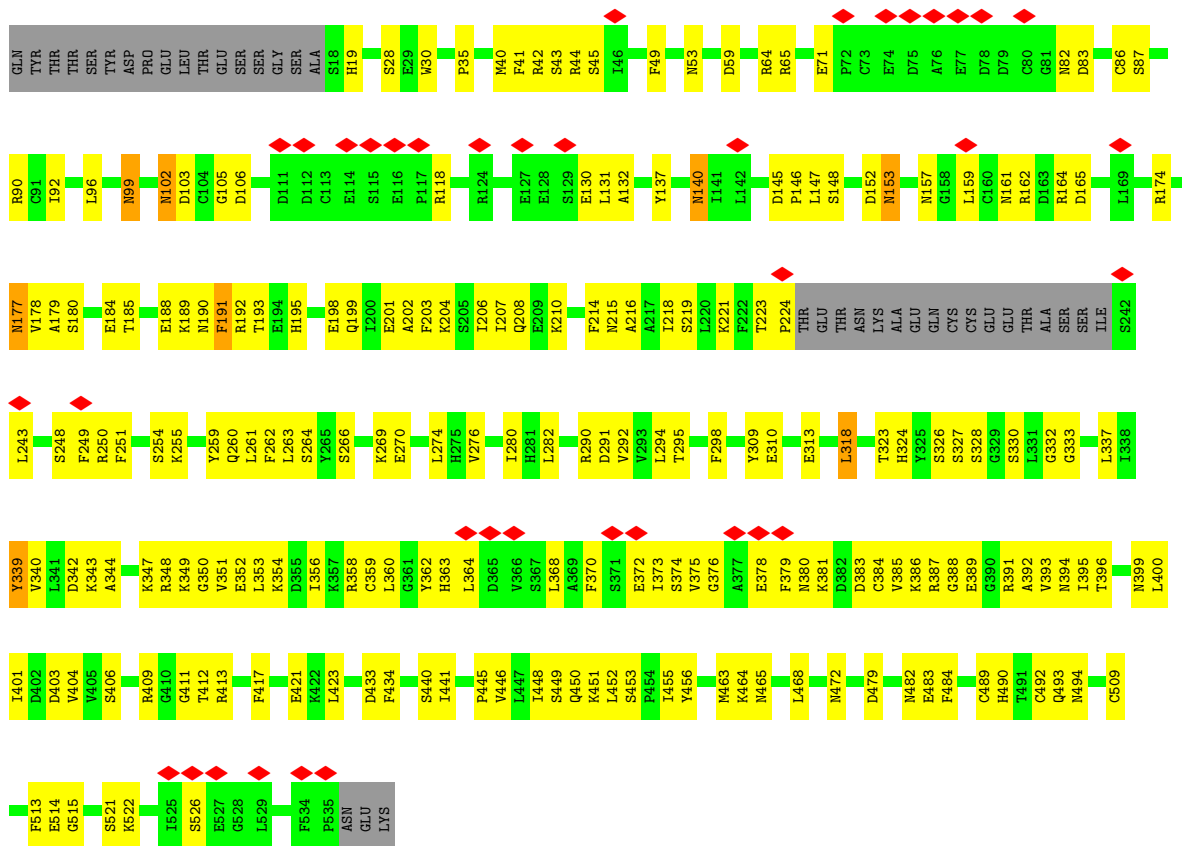


• Molecule 7: Complement component C9

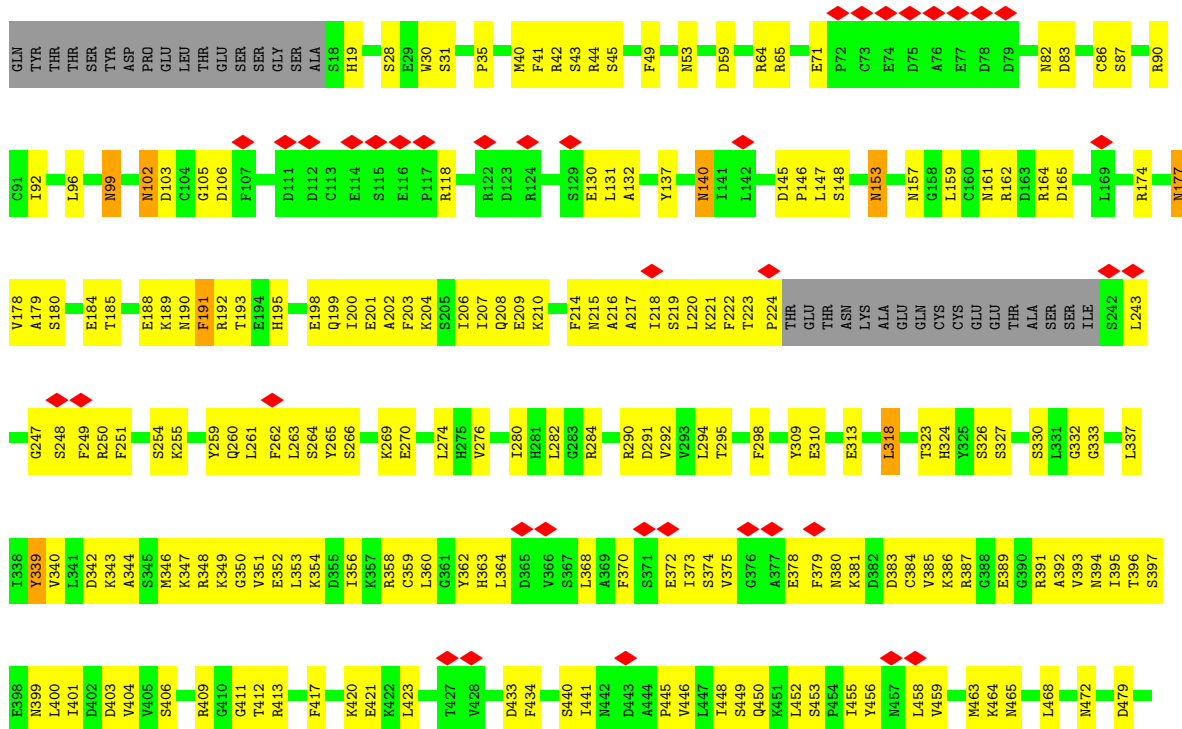


• Molecule 7: Complement component C9



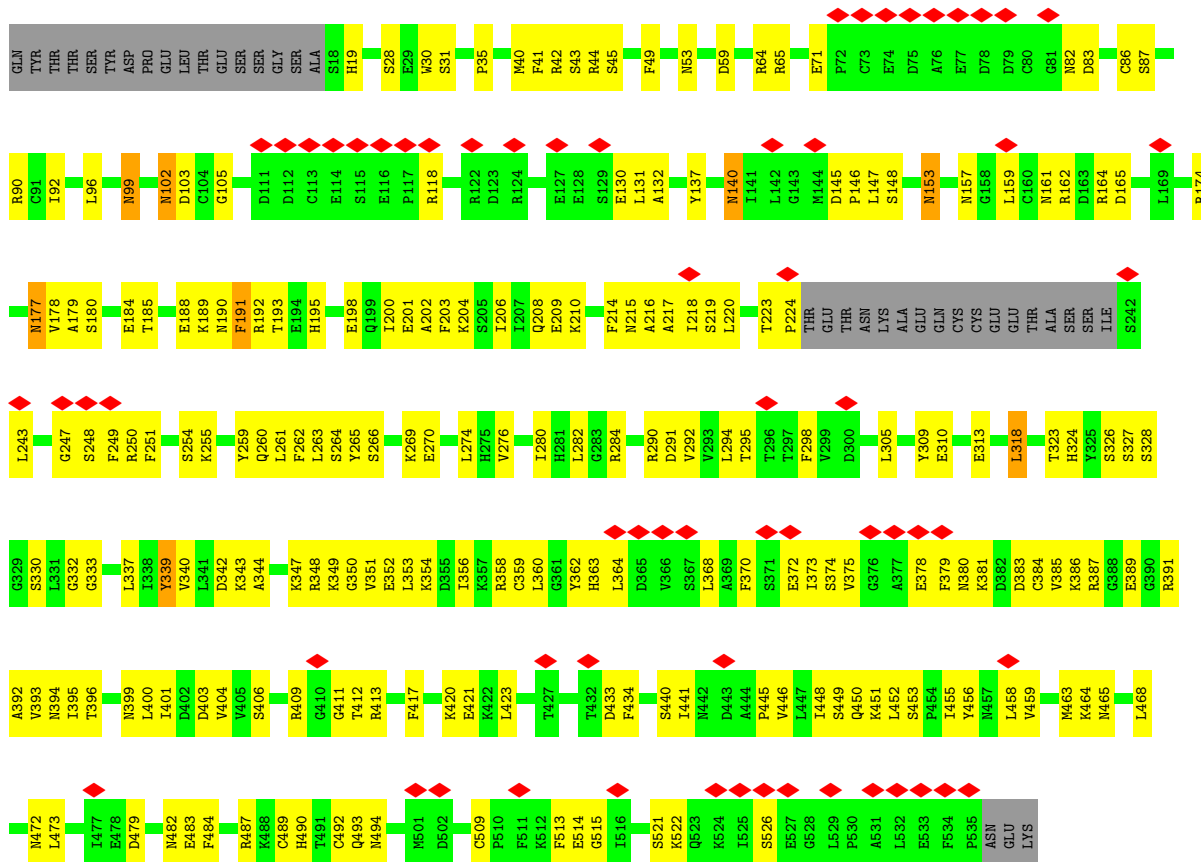


• Molecule 7: Complement component C9

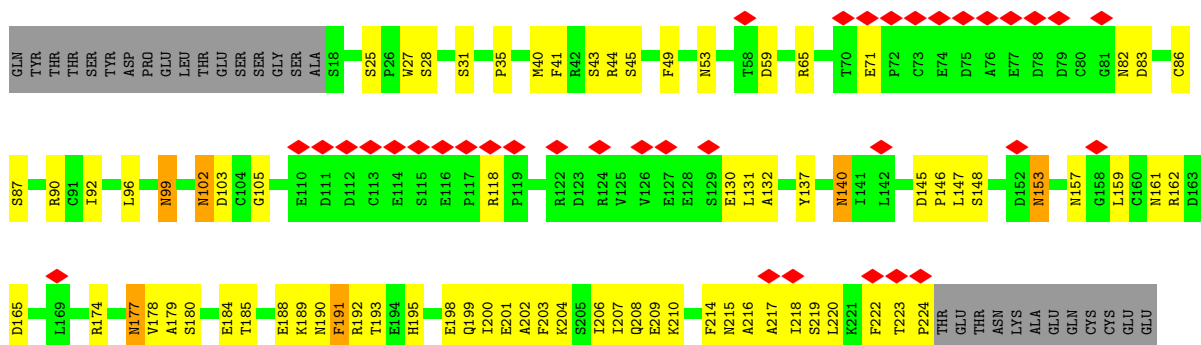


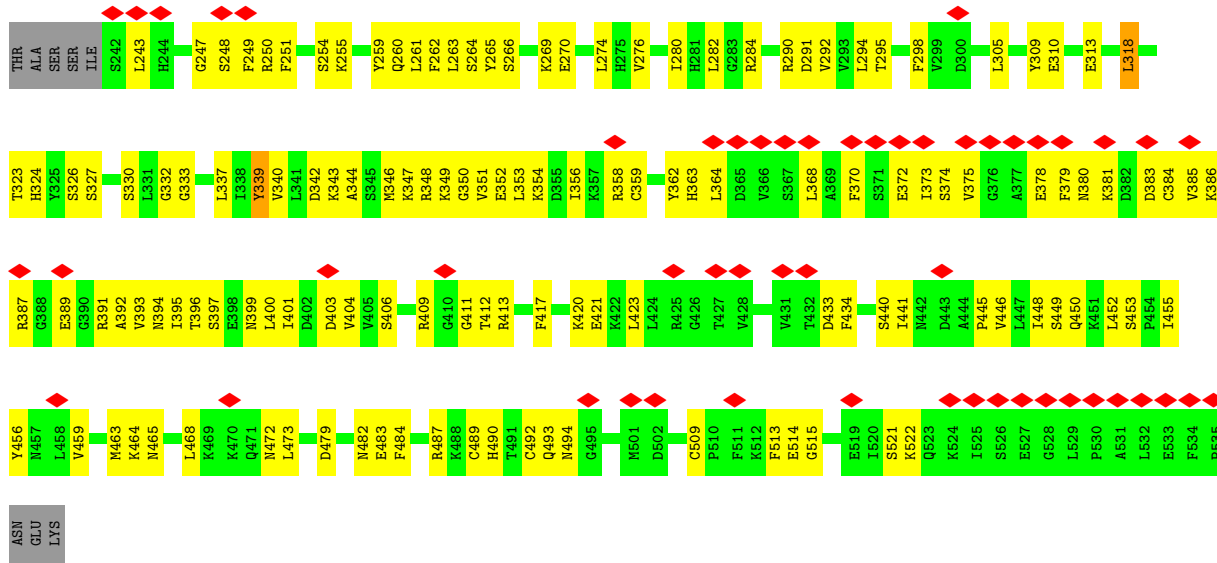


• Molecule 7: Complement component C9

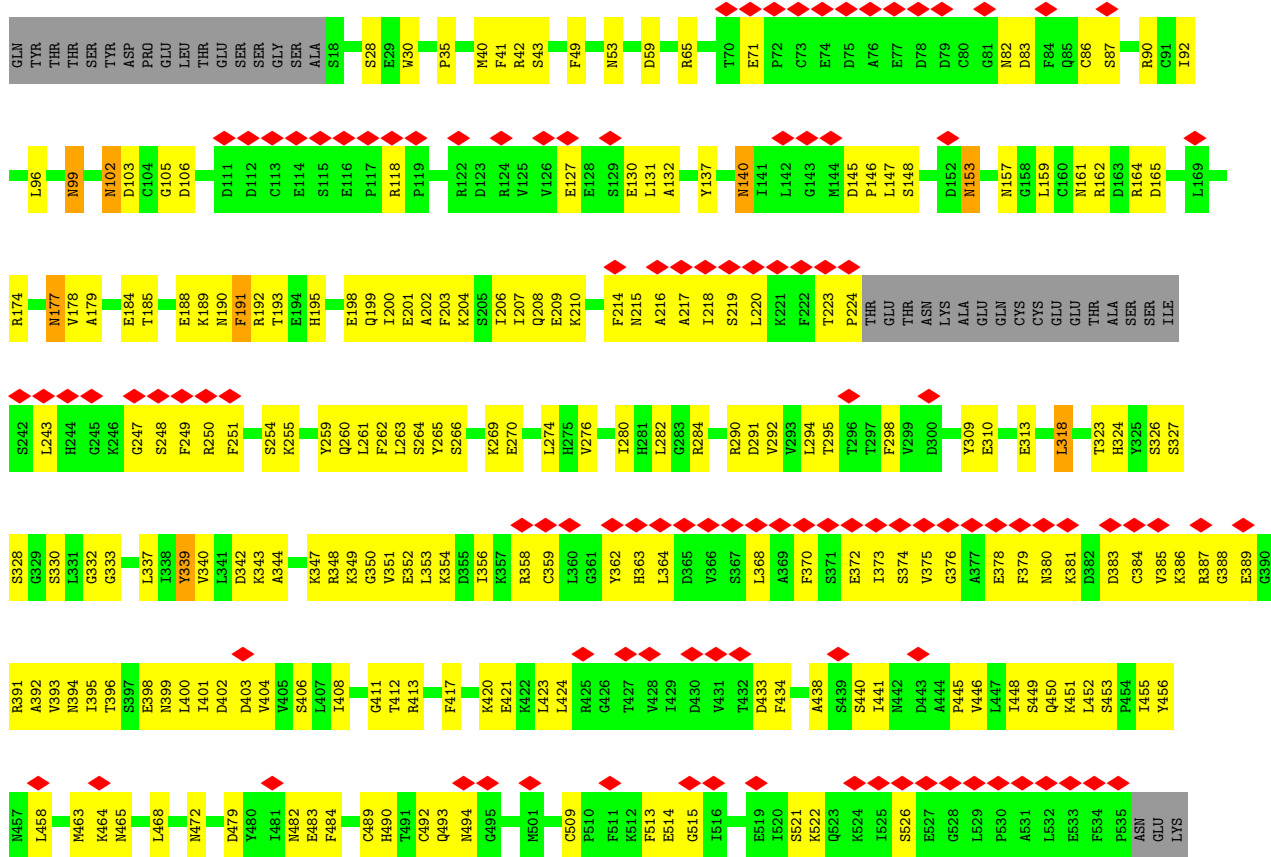


• Molecule 7: Complement component C9





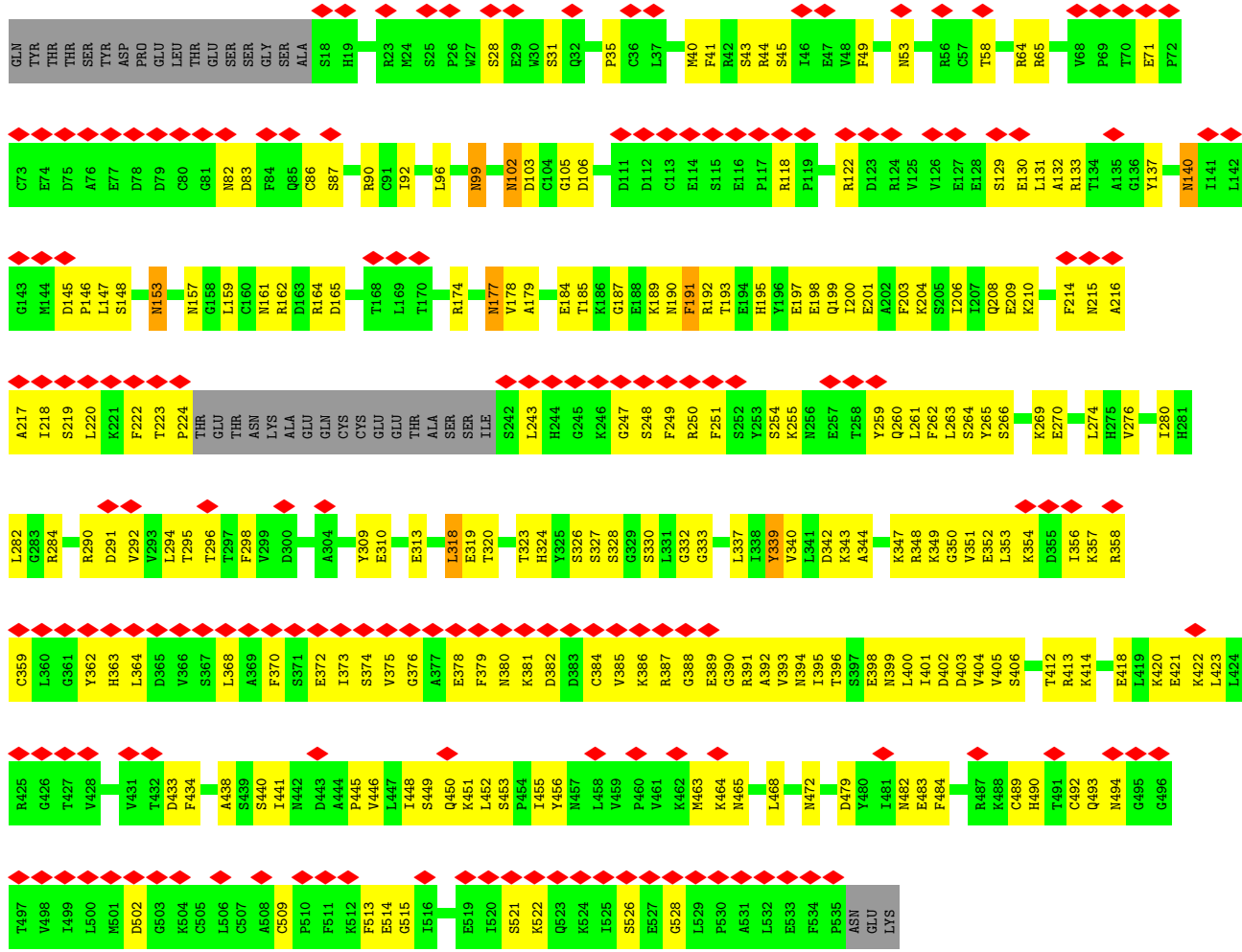
• Molecule 7: Complement component C9



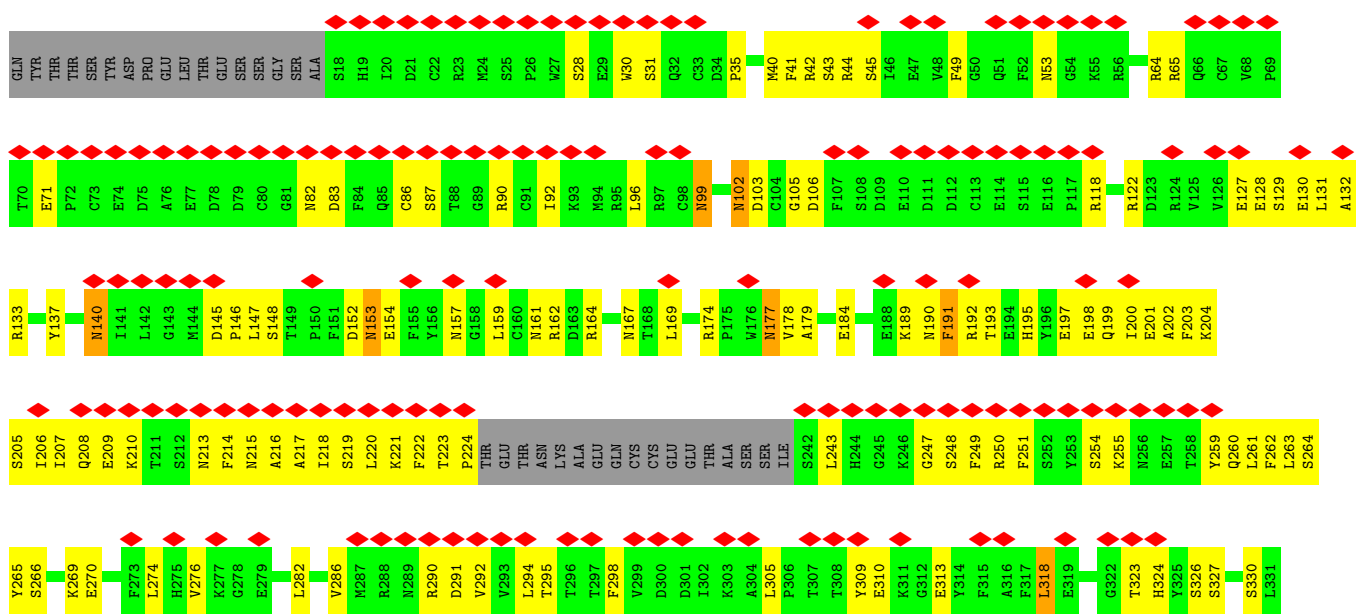
• Molecule 7: Complement component C9





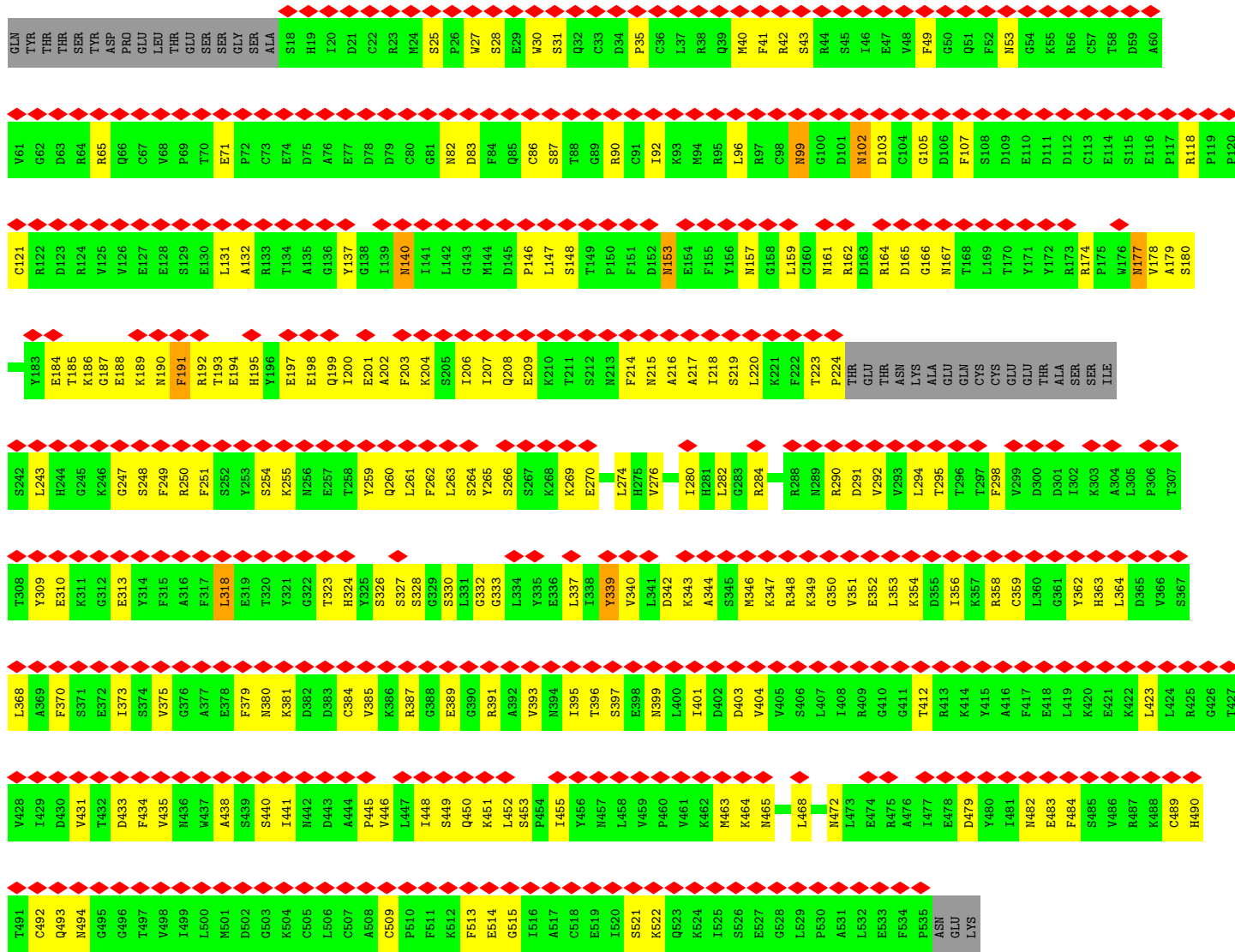
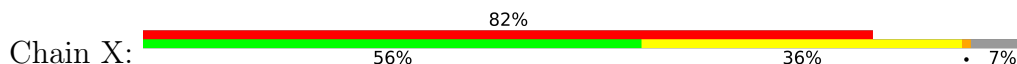


• Molecule 7: Complement component C9





● Molecule 7: Complement component C9



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%  
100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%  
50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%  
50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50%  
50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  50%  
50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50%  
50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81968	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	498.24, 498.24, 498.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.384, 1.384, 1.384	Depositor

## 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

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	0.24	0/9902	0.44	1/13446 (0.0%)
2	C	0.24	0/4211	0.42	0/5677
3	D	0.25	0/5254	0.44	0/7104
4	E	0.24	0/1323	0.41	0/1794
5	F	0.25	0/4096	0.42	0/5509
6	B	0.25	0/5540	0.42	0/7476
7	G	0.25	0/4054	0.43	0/5458
7	H	0.25	0/4054	0.43	0/5458
7	I	0.25	0/4054	0.43	0/5458
7	J	0.25	0/4054	0.43	0/5458
7	K	0.25	0/4054	0.43	0/5458
7	L	0.25	0/4054	0.43	0/5458
7	M	0.25	0/4054	0.43	0/5458
7	N	0.26	0/4050	0.43	0/5453
7	O	0.25	0/4054	0.43	0/5458
7	P	0.25	0/4054	0.43	0/5458
7	Q	0.25	0/4054	0.43	0/5458
7	R	0.25	0/4054	0.43	0/5458
7	S	0.25	0/4054	0.43	0/5458
7	T	0.26	0/4054	0.43	0/5458
7	U	0.26	0/4054	0.43	0/5458
7	V	0.25	0/4028	0.43	0/5427
7	W	0.26	0/4017	0.43	0/5412
7	X	0.25	0/4054	0.43	0/5458
All	All	0.25	0/103231	0.43	1/139168 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.



Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	D	0	1
5	F	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	61	ASP	C-N-CA	5.28	134.89	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	SER	Peptide
3	D	557	GLU	Peptide
5	F	488	GLN	Peptide

## 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	9686	0	9674	179	0
2	C	4119	0	3949	77	0
3	D	5129	0	4822	119	0
4	E	1295	0	1259	20	0
5	F	4017	0	3796	120	0
6	B	5427	0	5152	116	0
7	G	3977	0	3841	181	0
7	H	3977	0	3839	214	0
7	I	3977	0	3839	254	0
7	J	3977	0	3839	256	0
7	K	3977	0	3838	222	0
7	L	3977	0	3839	272	0
7	M	3977	0	3836	293	0
7	N	3973	0	3833	316	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	3977	0	3839	296	0
7	P	3977	0	3841	212	0
7	Q	3977	0	3839	244	0
7	R	3977	0	3839	249	0
7	S	3977	0	3839	239	0
7	T	3977	0	3839	242	0
7	U	3977	0	3839	276	0
7	V	3951	0	3799	414	0
7	W	3941	0	3782	495	0
7	X	3977	0	3839	306	0
8	Y	39	0	31	0	0
9	Z	28	0	25	2	0
9	a	28	0	25	0	0
9	b	28	0	25	0	0
9	c	28	0	25	0	0
9	d	28	0	25	0	0
9	e	28	0	25	0	0
9	f	28	0	25	0	0
9	g	28	0	25	0	0
9	h	28	0	25	0	0
9	i	28	0	25	0	0
9	j	28	0	25	0	0
9	k	28	0	25	0	0
9	l	28	0	25	0	0
9	m	28	0	25	0	0
9	n	28	0	25	0	0
9	o	28	0	25	0	0
9	p	28	0	25	0	0
9	q	28	0	25	0	0
9	r	28	0	25	0	0
9	s	28	0	25	0	0
10	F	14	0	13	1	0
10	G	28	0	26	0	0
10	H	28	0	26	0	0
10	I	28	0	26	0	0
10	J	28	0	26	0	0
10	K	28	0	26	0	0
10	L	28	0	26	0	0
10	M	28	0	26	0	0
10	N	28	0	26	0	0
10	O	28	0	26	0	0
10	P	28	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Q	28	0	26	0	0
10	R	28	0	26	0	0
10	S	28	0	26	0	0
10	T	28	0	26	0	0
10	U	28	0	26	0	0
10	V	28	0	26	0	0
10	W	28	0	26	0	0
10	X	28	0	26	0	0
All	All	102310	0	98663	4218	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 21.

The worst 5 of 4218 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:225:PHE:CD1	3:D:342:TRP:HB2	1.32	1.62
3:D:225:PHE:CE1	3:D:342:TRP:HB2	1.32	1.61
7:V:58:THR:HG21	7:W:452:LEU:CB	1.21	1.60
7:W:421:GLU:CB	7:X:434:PHE:HD2	1.17	1.58
7:V:58:THR:CG2	7:W:452:LEU:HB3	1.17	1.56

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 PDB entries followed by that with respect to all EM entries.

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	1211/1580 (77%)	1144 (94%)	67 (6%)	0	100	100
2	C	505/537 (94%)	482 (95%)	23 (5%)	0	100	100
3	D	649/821 (79%)	590 (91%)	58 (9%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	161/182 (88%)	160 (99%)	1 (1%)	0	100	100
5	F	499/554 (90%)	474 (95%)	23 (5%)	2 (0%)	34	72
6	B	676/913 (74%)	645 (95%)	30 (4%)	1 (0%)	51	85
7	G	497/538 (92%)	460 (93%)	37 (7%)	0	100	100
7	H	497/538 (92%)	460 (93%)	37 (7%)	0	100	100
7	I	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	J	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	K	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	L	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	M	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	N	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	O	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	P	497/538 (92%)	454 (91%)	42 (8%)	1 (0%)	47	81
7	Q	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	R	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	S	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	T	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
7	U	497/538 (92%)	460 (93%)	37 (7%)	0	100	100
7	V	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	W	497/538 (92%)	459 (92%)	38 (8%)	0	100	100
7	X	497/538 (92%)	458 (92%)	39 (8%)	0	100	100
All	All	12647/14271 (89%)	11747 (93%)	895 (7%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	P	526	SER
3	D	344	PHE
5	F	226	PRO
5	F	489	CYS
6	B	204	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 PDB entries followed by that with respect to all EM entries.

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	1083/1403 (77%)	1066 (98%)	17 (2%)	62	79
2	C	453/473 (96%)	446 (98%)	7 (2%)	65	80
3	D	571/714 (80%)	558 (98%)	13 (2%)	50	70
4	E	134/149 (90%)	132 (98%)	2 (2%)	65	80
5	F	437/466 (94%)	426 (98%)	11 (2%)	47	68
6	B	610/810 (75%)	603 (99%)	7 (1%)	73	84
7	G	440/477 (92%)	423 (96%)	17 (4%)	32	57
7	H	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	I	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	J	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	K	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	L	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	M	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	N	439/477 (92%)	423 (96%)	16 (4%)	35	59
7	O	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	P	440/477 (92%)	423 (96%)	17 (4%)	32	57
7	Q	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	R	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	S	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	T	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	U	440/477 (92%)	424 (96%)	16 (4%)	35	59
7	V	434/477 (91%)	418 (96%)	16 (4%)	34	58
7	W	433/477 (91%)	417 (96%)	16 (4%)	34	58
7	X	440/477 (92%)	424 (96%)	16 (4%)	35	59
All	All	11194/12601 (89%)	10847 (97%)	347 (3%)	43	62

5 of 347 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	Q	482	ASN
7	U	102	ASN
7	R	102	ASN
7	S	191	PHE
7	V	82	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 323 such sidechains are listed below:

Mol	Chain	Res	Type
7	S	82	ASN
7	V	380	ASN
7	S	177	ASN
7	U	99	ASN
7	W	177	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

43 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	$\# Z  > 2$
8	NAG	Y	1	2,8	14,14,15	0.33	0	17,19,21	0.42	0
8	NAG	Y	2	8	14,14,15	0.31	0	17,19,21	0.62	0
8	BMA	Y	3	8	11,11,12	0.58	0	15,15,17	0.84	0
9	NAG	Z	1	3,9	14,14,15	0.57	0	17,19,21	1.69	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	Z	2	9	14,14,15	0.42	0	17,19,21	0.52	0
9	NAG	a	1	9,6	14,14,15	0.52	0	17,19,21	1.16	1 (5%)
9	NAG	a	2	9	14,14,15	0.38	0	17,19,21	0.49	0
9	NAG	b	1	7,9	14,14,15	0.51	0	17,19,21	1.34	1 (5%)
9	NAG	b	2	9	14,14,15	0.50	0	17,19,21	0.52	0
9	NAG	c	1	7,9	14,14,15	0.56	0	17,19,21	0.94	1 (5%)
9	NAG	c	2	9	14,14,15	0.55	0	17,19,21	0.54	0
9	NAG	d	1	7,9	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
9	NAG	d	2	9	14,14,15	0.54	0	17,19,21	0.53	0
9	NAG	e	1	7,9	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
9	NAG	e	2	9	14,14,15	0.53	0	17,19,21	0.53	0
9	NAG	f	1	7,9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
9	NAG	f	2	9	14,14,15	0.56	0	17,19,21	0.51	0
9	NAG	g	1	7,9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
9	NAG	g	2	9	14,14,15	0.56	0	17,19,21	0.53	0
9	NAG	h	1	7,9	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
9	NAG	h	2	9	14,14,15	0.57	0	17,19,21	0.53	0
9	NAG	i	1	7,9	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
9	NAG	i	2	9	14,14,15	0.56	0	17,19,21	0.53	0
9	NAG	j	1	7,9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
9	NAG	j	2	9	14,14,15	0.55	0	17,19,21	0.52	0
9	NAG	k	1	7,9	14,14,15	0.52	0	17,19,21	0.89	1 (5%)
9	NAG	k	2	9	14,14,15	0.54	0	17,19,21	0.53	0
9	NAG	l	1	7,9	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
9	NAG	l	2	9	14,14,15	0.55	0	17,19,21	0.54	0
9	NAG	m	1	7,9	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
9	NAG	m	2	9	14,14,15	0.55	0	17,19,21	0.53	0
9	NAG	n	1	7,9	14,14,15	0.54	0	17,19,21	0.88	1 (5%)
9	NAG	n	2	9	14,14,15	0.55	0	17,19,21	0.53	0
9	NAG	o	1	7,9	14,14,15	0.53	0	17,19,21	0.90	1 (5%)
9	NAG	o	2	9	14,14,15	0.56	0	17,19,21	0.54	0
9	NAG	p	1	7,9	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
9	NAG	p	2	9	14,14,15	0.56	0	17,19,21	0.53	0
9	NAG	q	1	7,9	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
9	NAG	q	2	9	14,14,15	0.56	0	17,19,21	0.53	0
9	NAG	r	1	7,9	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
9	NAG	r	2	9	14,14,15	0.55	0	17,19,21	0.53	0
9	NAG	s	1	7,9	14,14,15	0.53	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	s	2	9	14,14,15	0.56	0	17,19,21	0.53	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
8	NAG	Y	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	3,9	-	5/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	3/6/23/26	0/1/1/1
9	NAG	a	1	9,6	-	3/6/23/26	0/1/1/1
9	NAG	a	2	9	-	2/6/23/26	0/1/1/1
9	NAG	b	1	7,9	-	5/6/23/26	0/1/1/1
9	NAG	b	2	9	-	0/6/23/26	0/1/1/1
9	NAG	c	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	c	2	9	-	2/6/23/26	0/1/1/1
9	NAG	d	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	d	2	9	-	2/6/23/26	0/1/1/1
9	NAG	e	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	e	2	9	-	2/6/23/26	0/1/1/1
9	NAG	f	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	f	2	9	-	2/6/23/26	0/1/1/1
9	NAG	g	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	g	2	9	-	2/6/23/26	0/1/1/1
9	NAG	h	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	h	2	9	-	2/6/23/26	0/1/1/1
9	NAG	i	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	i	2	9	-	2/6/23/26	0/1/1/1
9	NAG	j	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	j	2	9	-	2/6/23/26	0/1/1/1
9	NAG	k	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	k	2	9	-	2/6/23/26	0/1/1/1
9	NAG	l	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	l	2	9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	m	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	m	2	9	-	2/6/23/26	0/1/1/1
9	NAG	n	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	n	2	9	-	2/6/23/26	0/1/1/1
9	NAG	o	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	o	2	9	-	2/6/23/26	0/1/1/1
9	NAG	p	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	p	2	9	-	2/6/23/26	0/1/1/1
9	NAG	q	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	q	2	9	-	2/6/23/26	0/1/1/1
9	NAG	r	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	r	2	9	-	2/6/23/26	0/1/1/1
9	NAG	s	1	7,9	-	3/6/23/26	0/1/1/1
9	NAG	s	2	9	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Z	1	NAG	C2-N2-C7	4.57	129.41	122.90
9	b	1	NAG	C2-N2-C7	4.26	128.96	122.90
9	c	1	NAG	C1-O5-C5	2.94	116.18	112.19
9	o	1	NAG	C1-O5-C5	2.86	116.06	112.19
9	l	1	NAG	C1-O5-C5	2.83	116.02	112.19

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

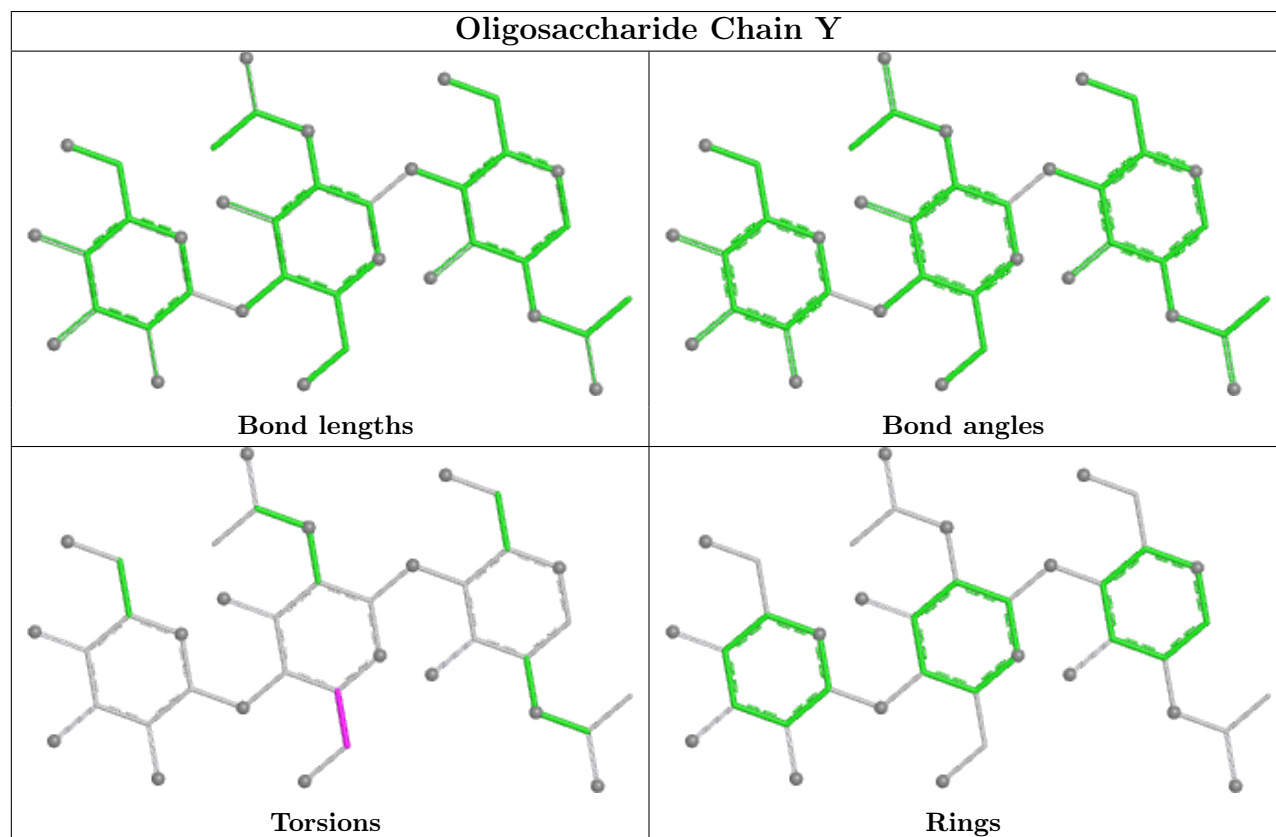
Mol	Chain	Res	Type	Atoms
8	Y	2	NAG	C4-C5-C6-O6
9	c	1	NAG	O5-C5-C6-O6
9	Z	1	NAG	C4-C5-C6-O6
9	Z	1	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6

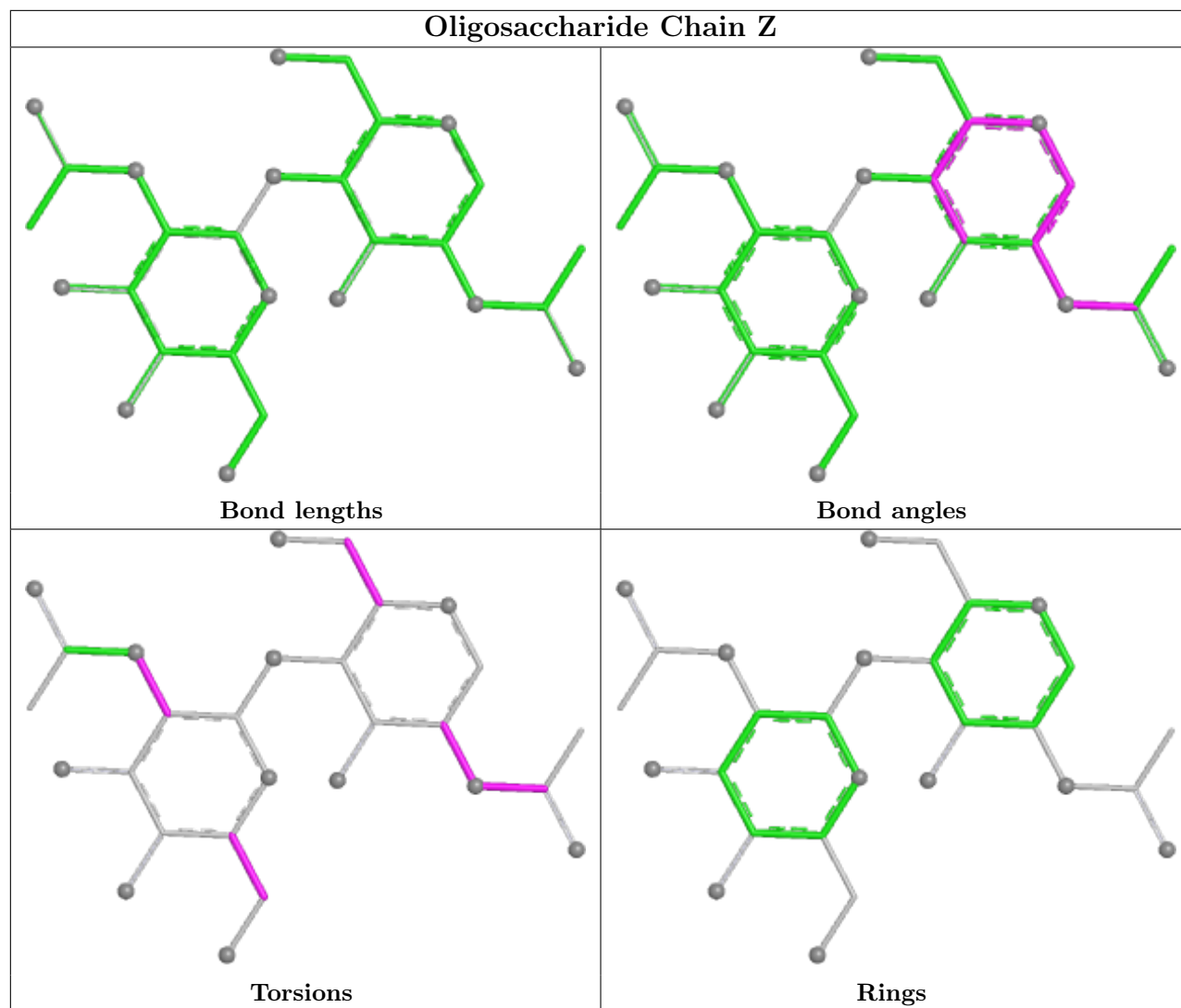
There are no ring outliers.

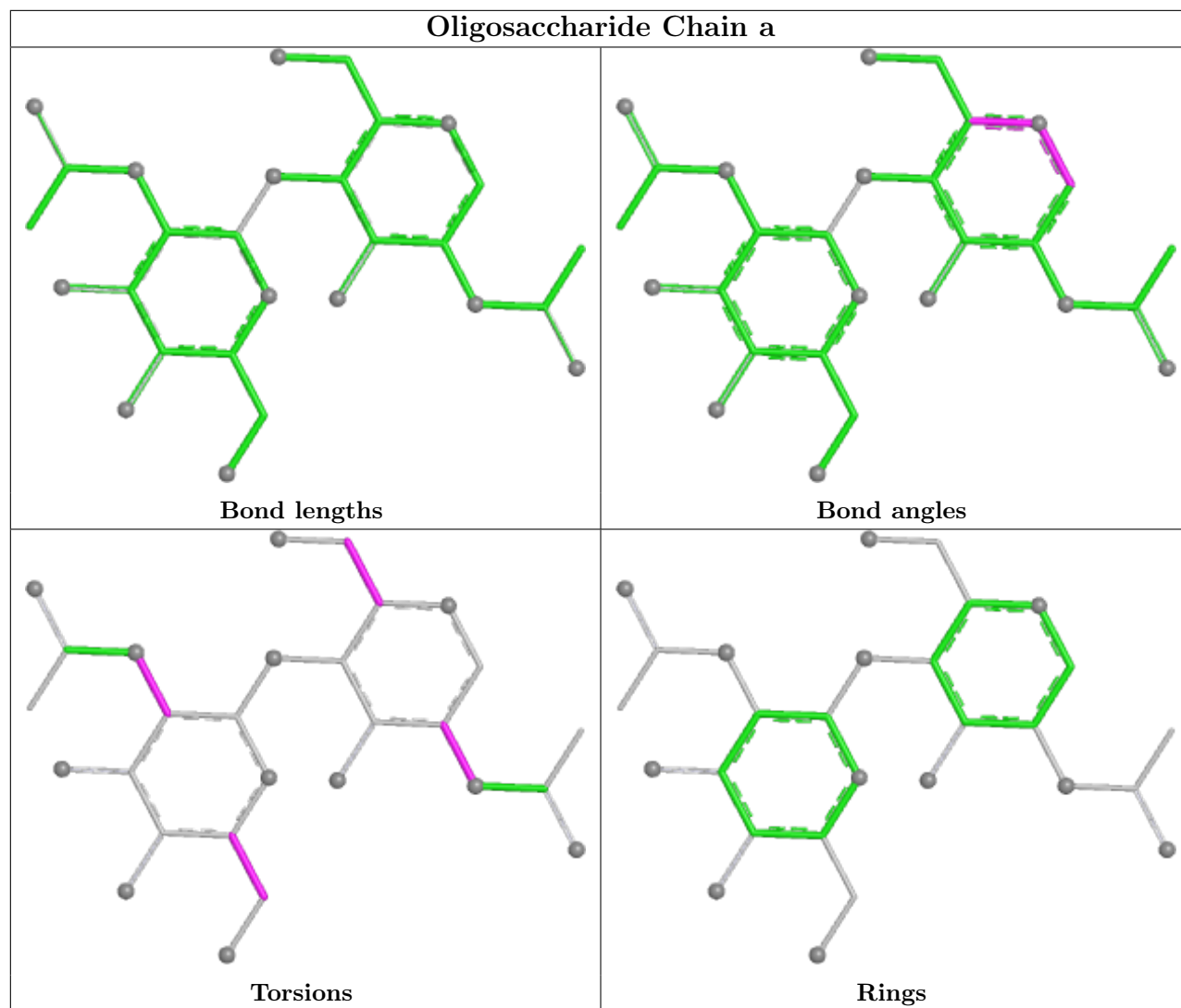
2 monomers are involved in 2 short contacts:

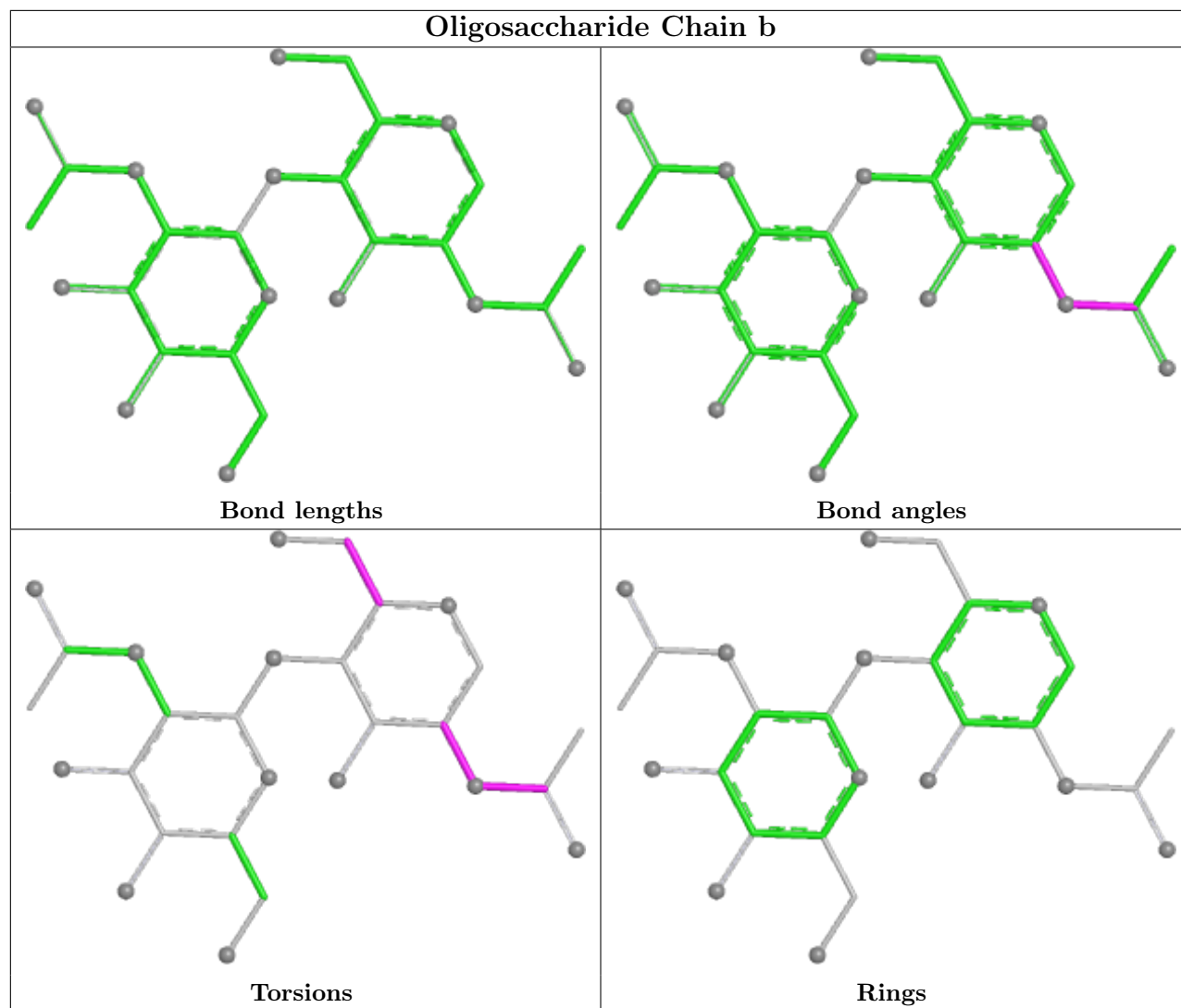
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Z	1	NAG	2	0
9	Z	2	NAG	1	0

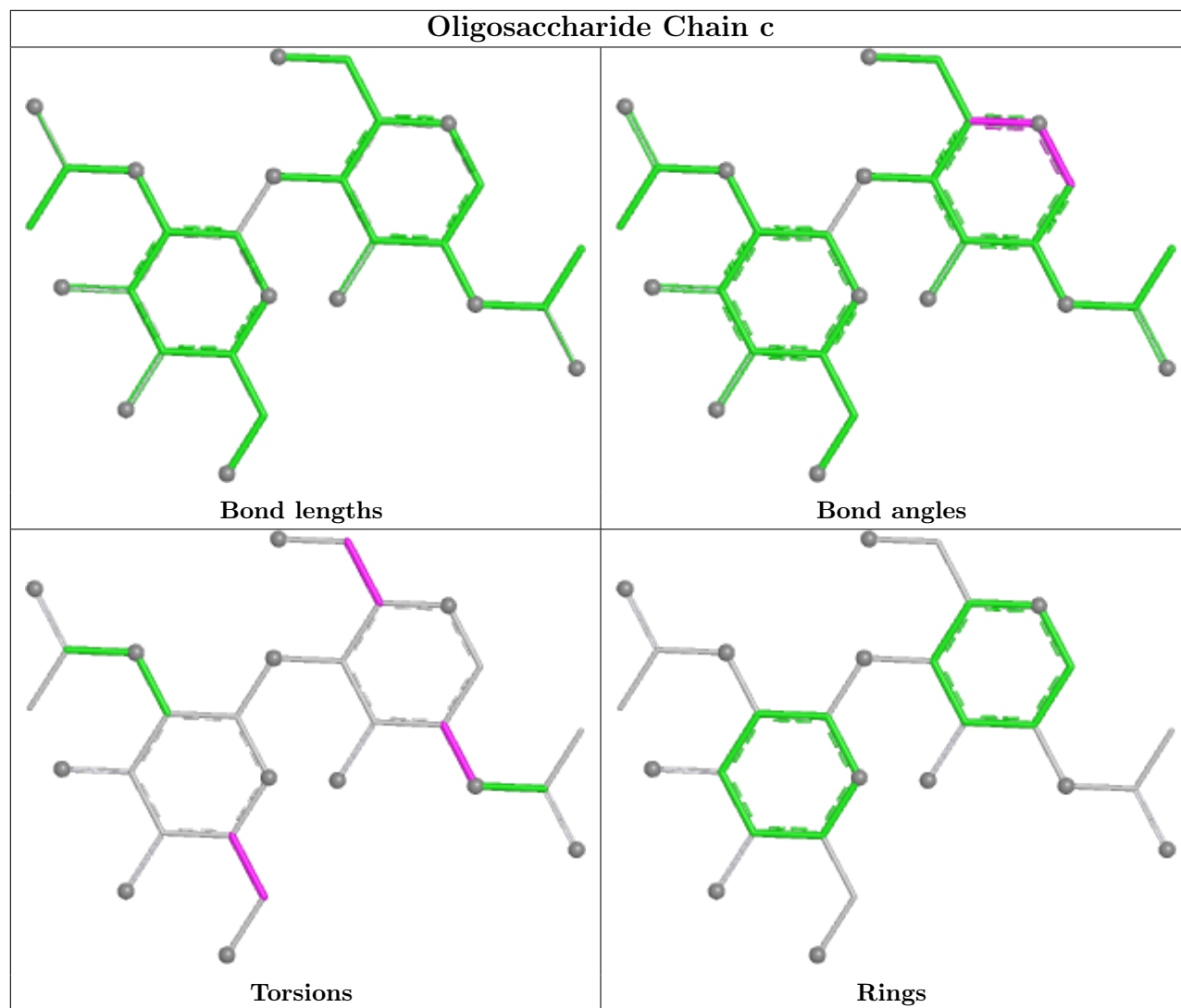
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

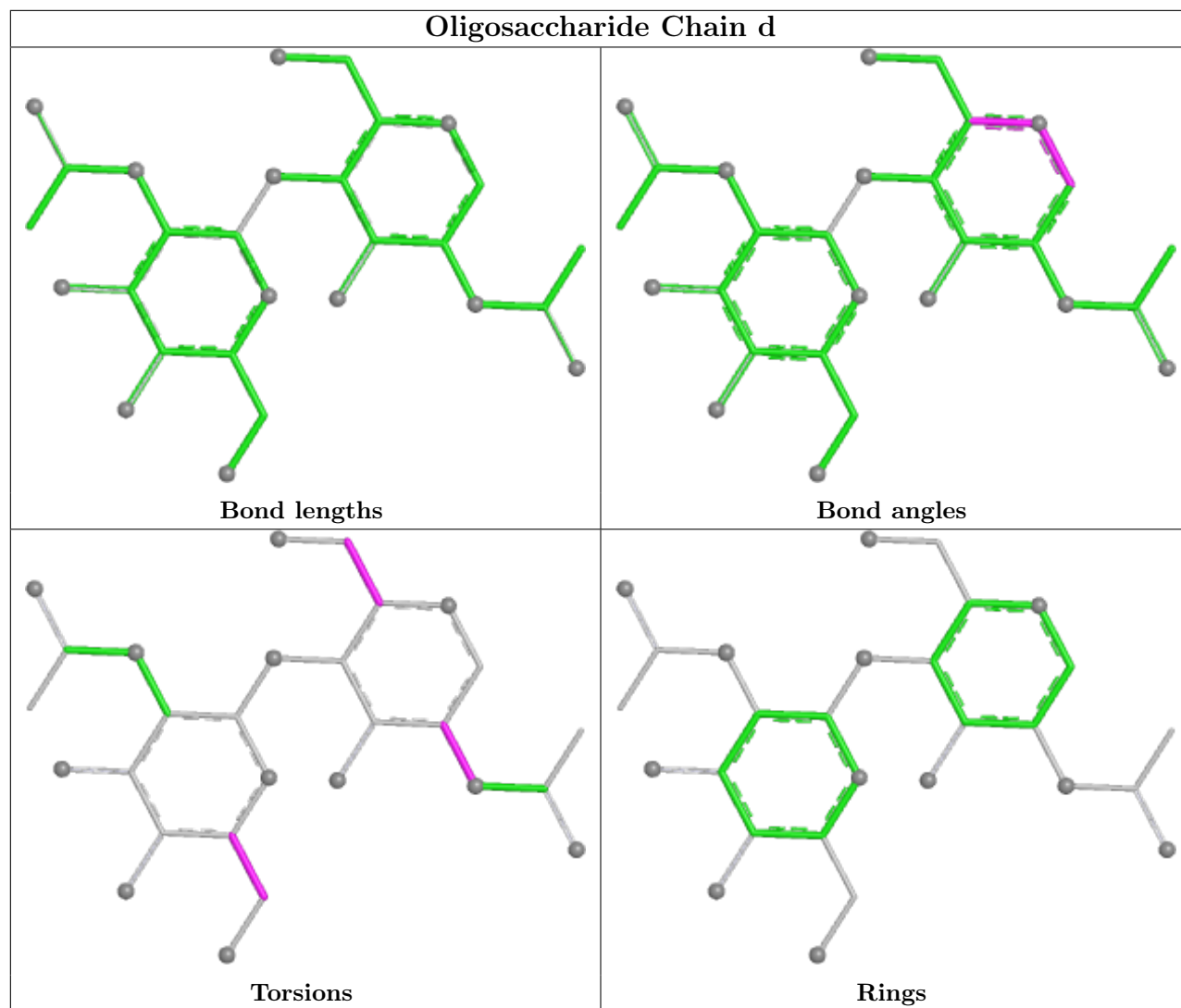


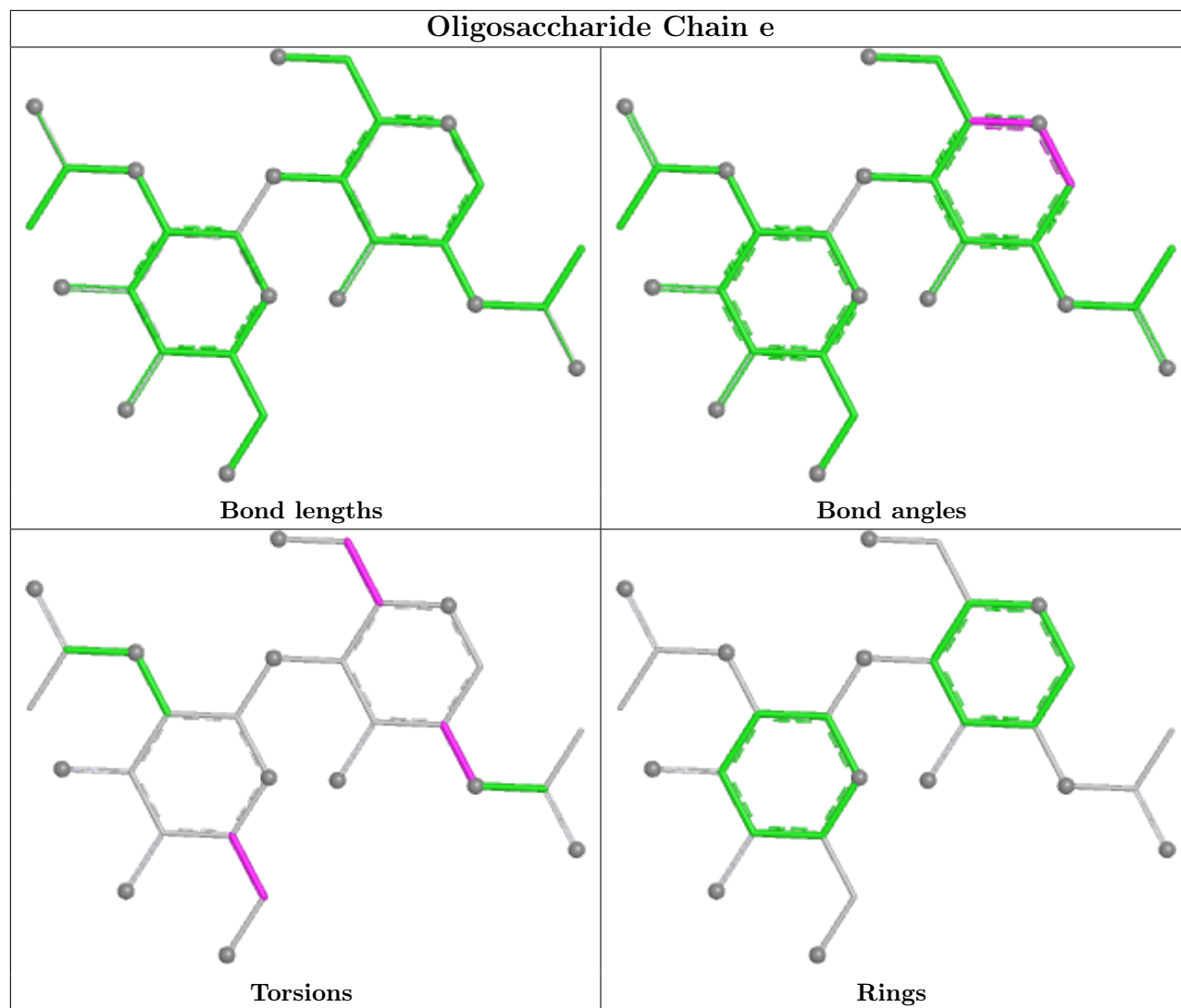




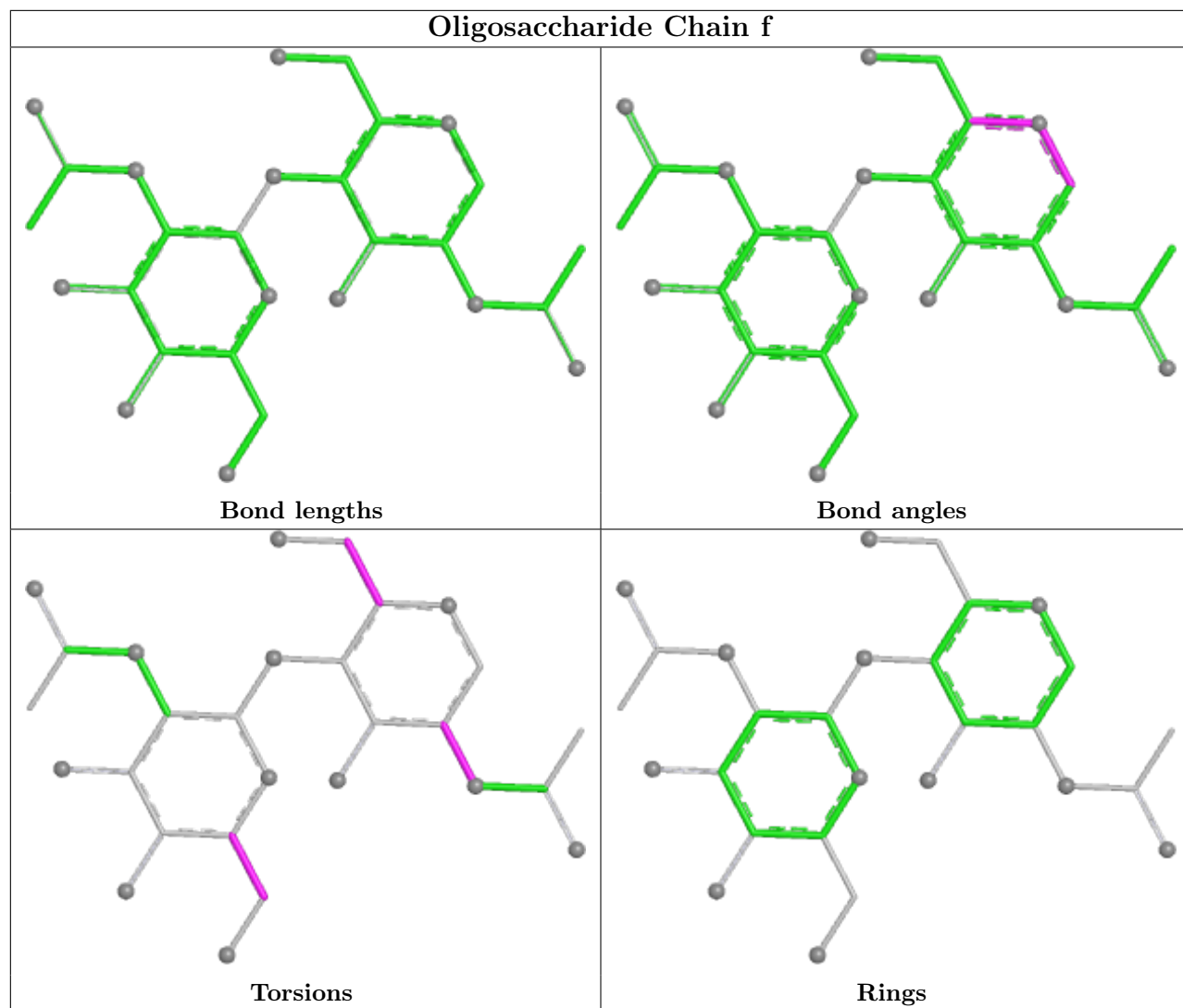


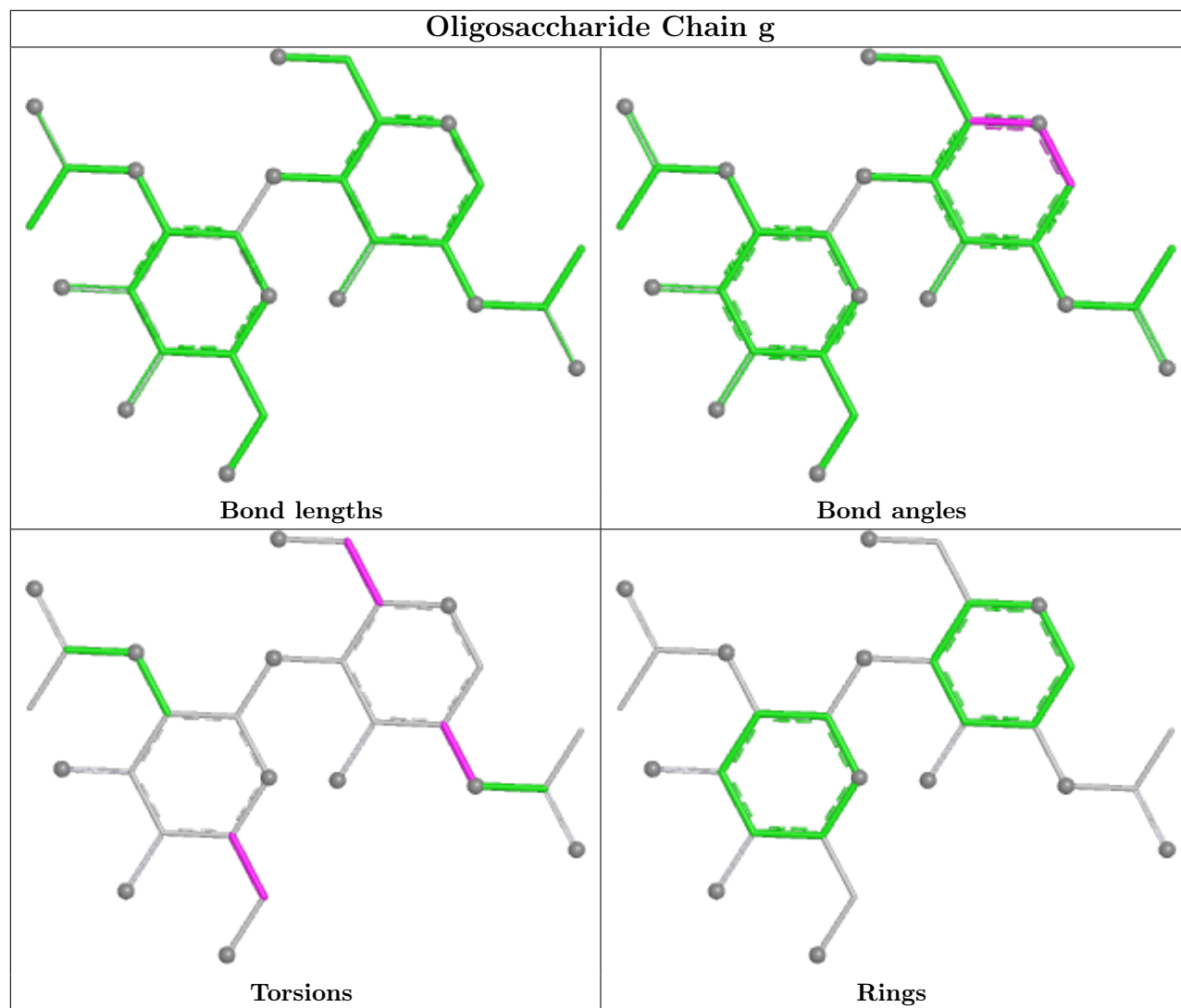


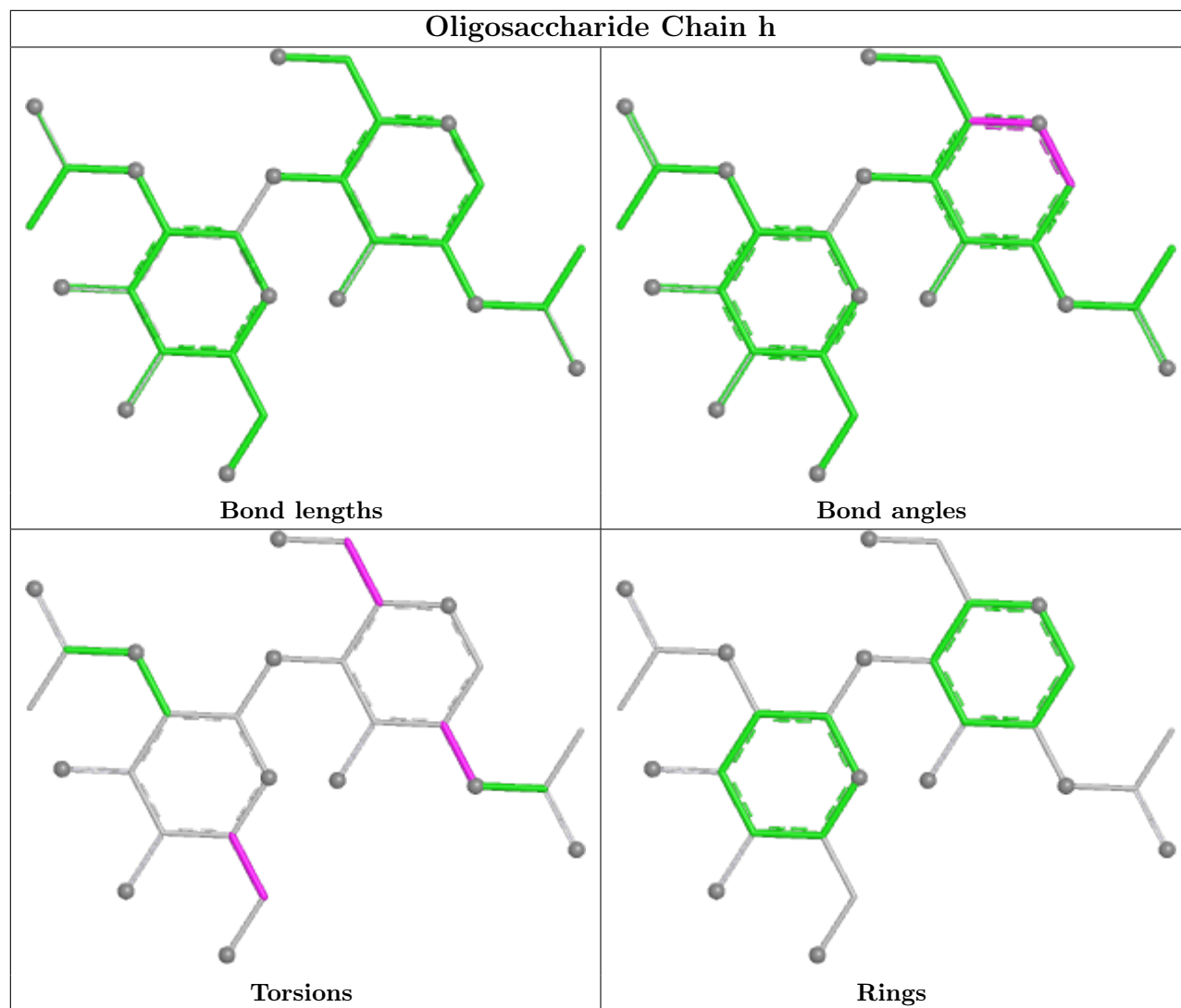


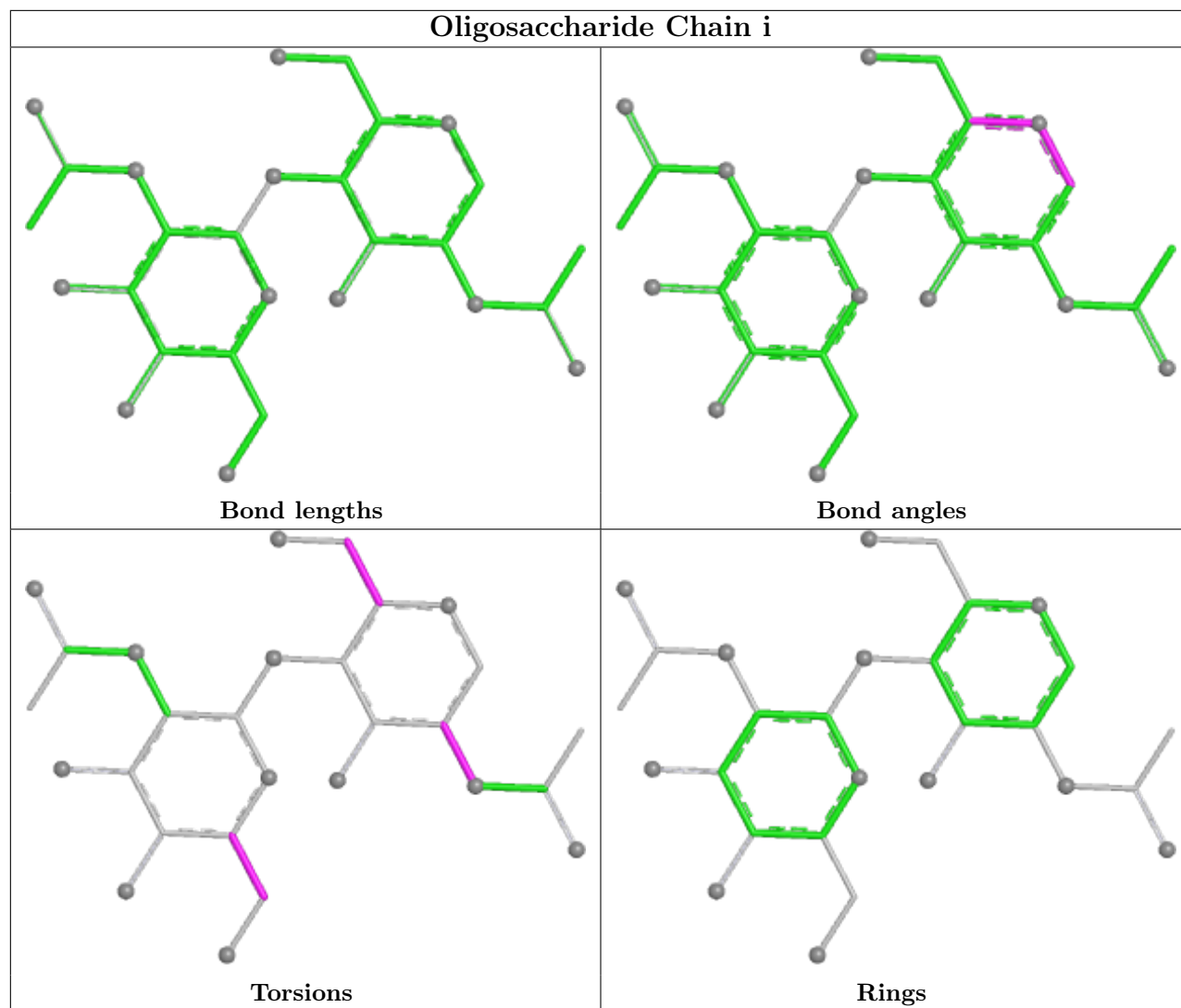


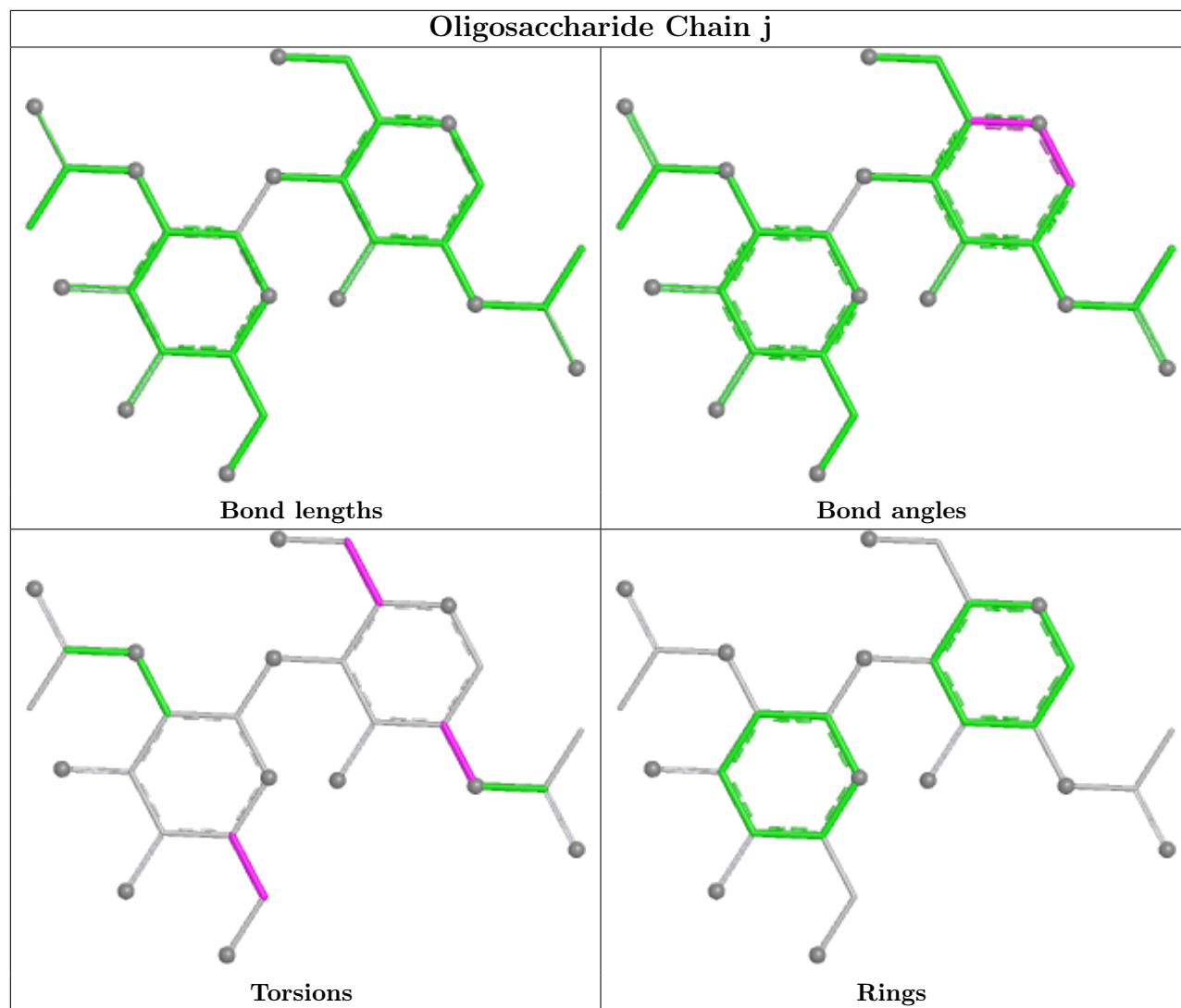


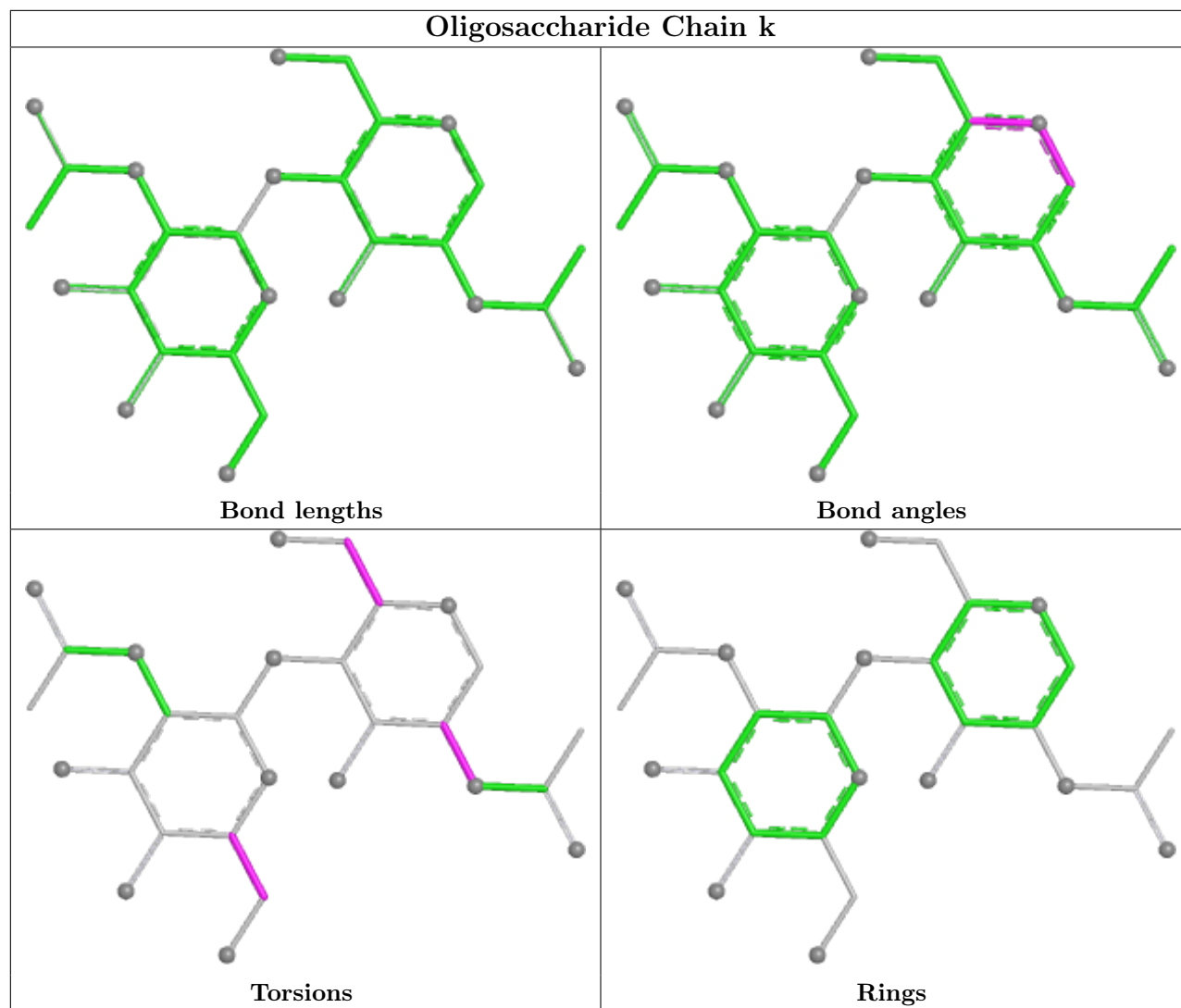


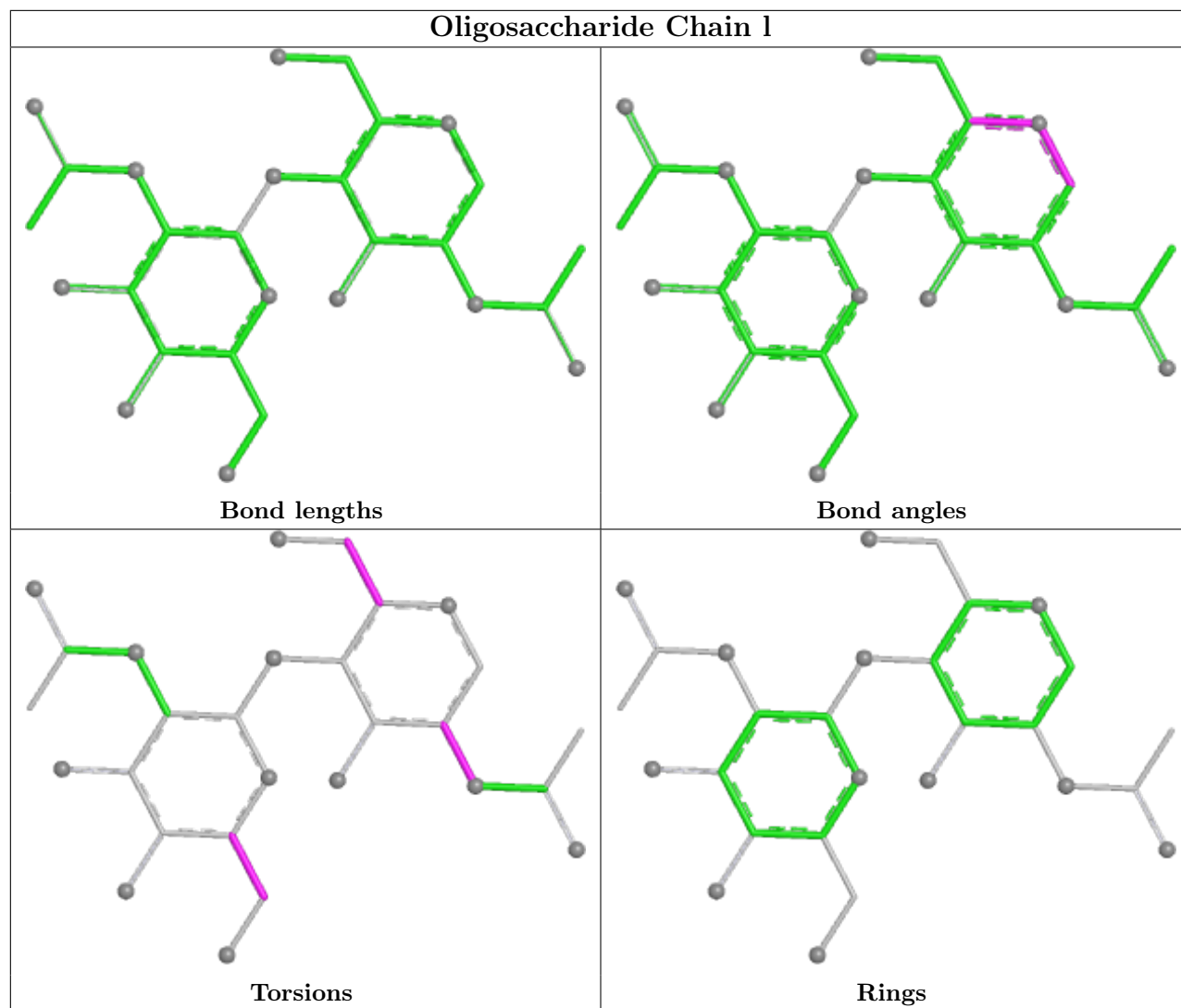


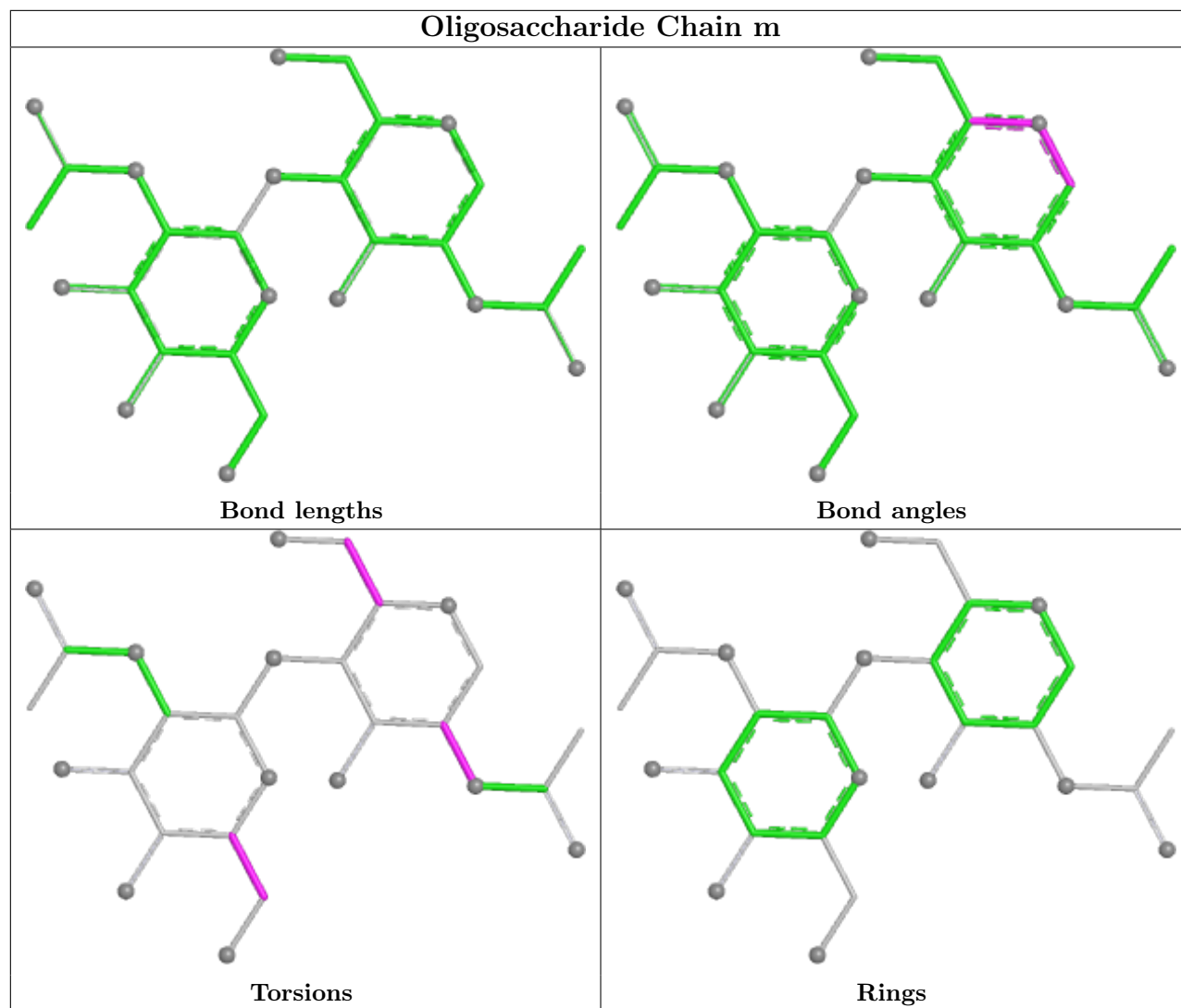




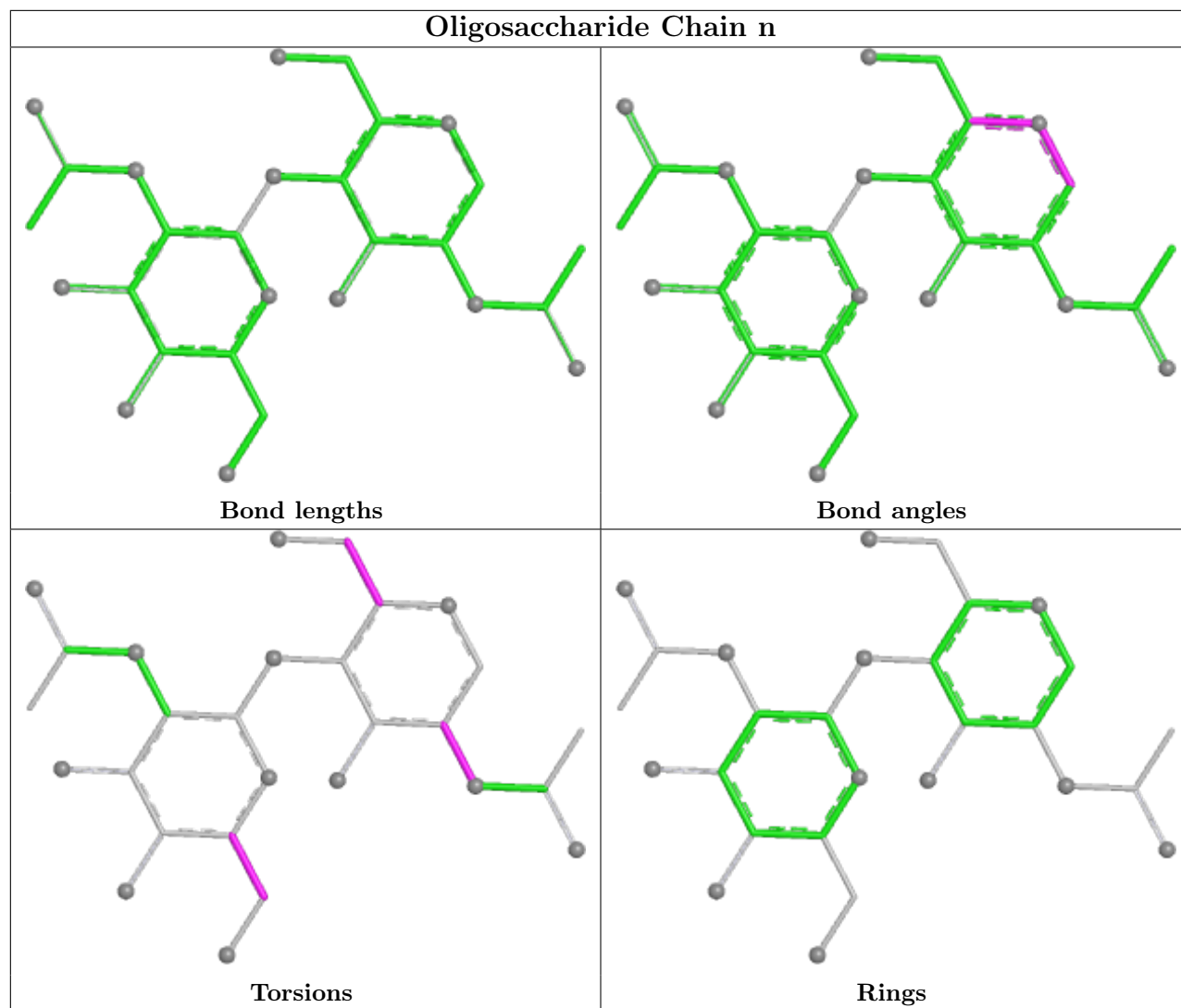


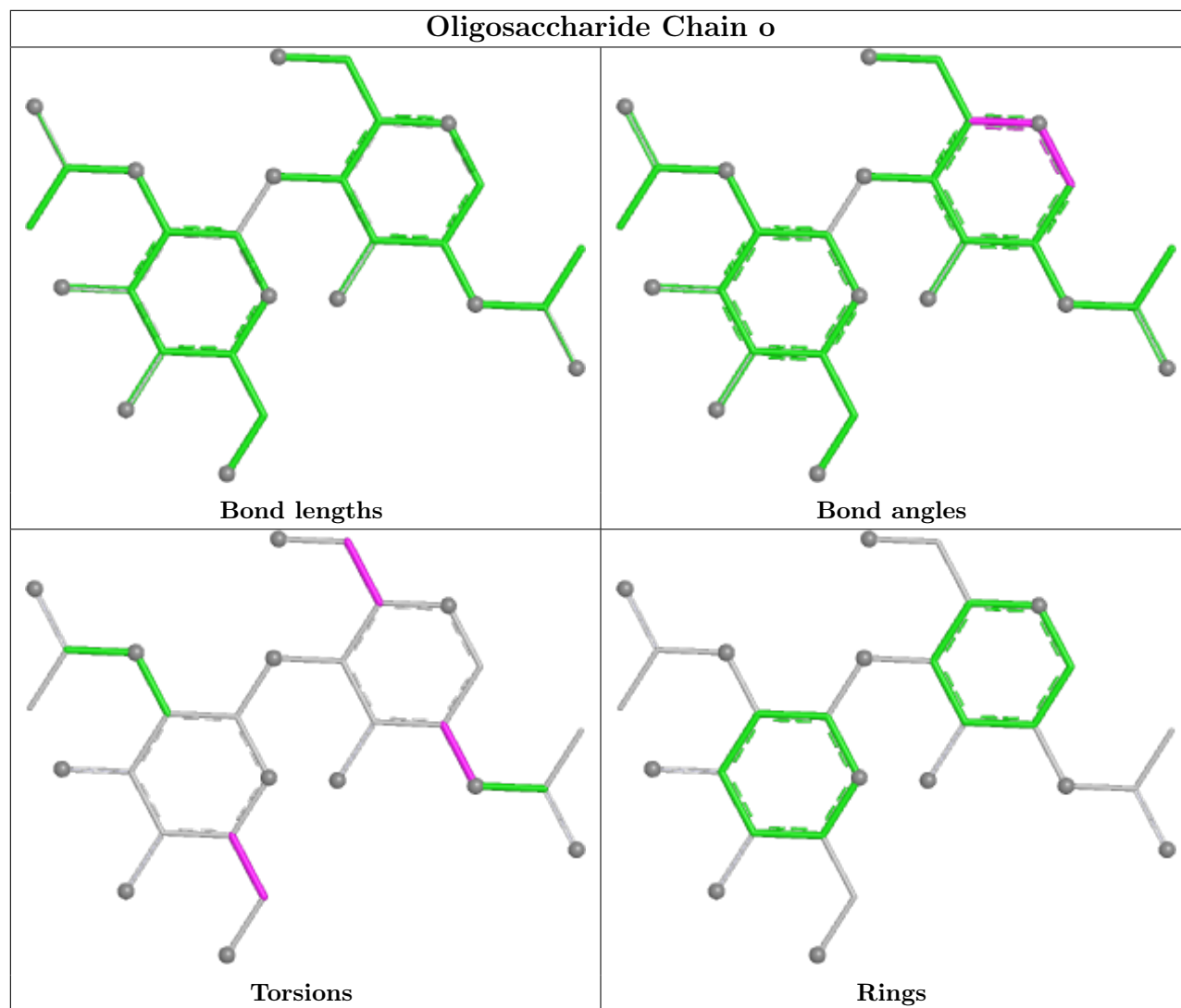


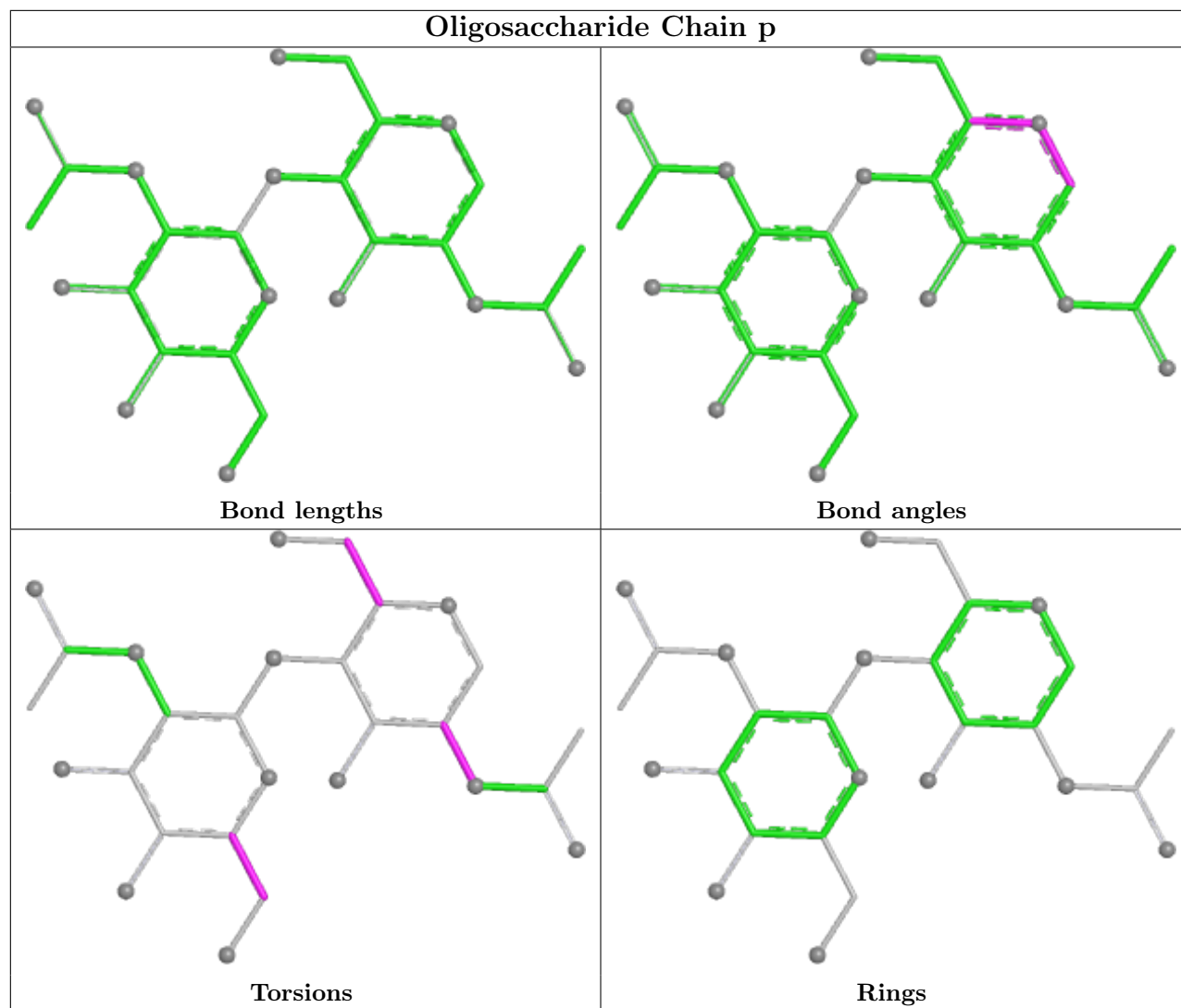


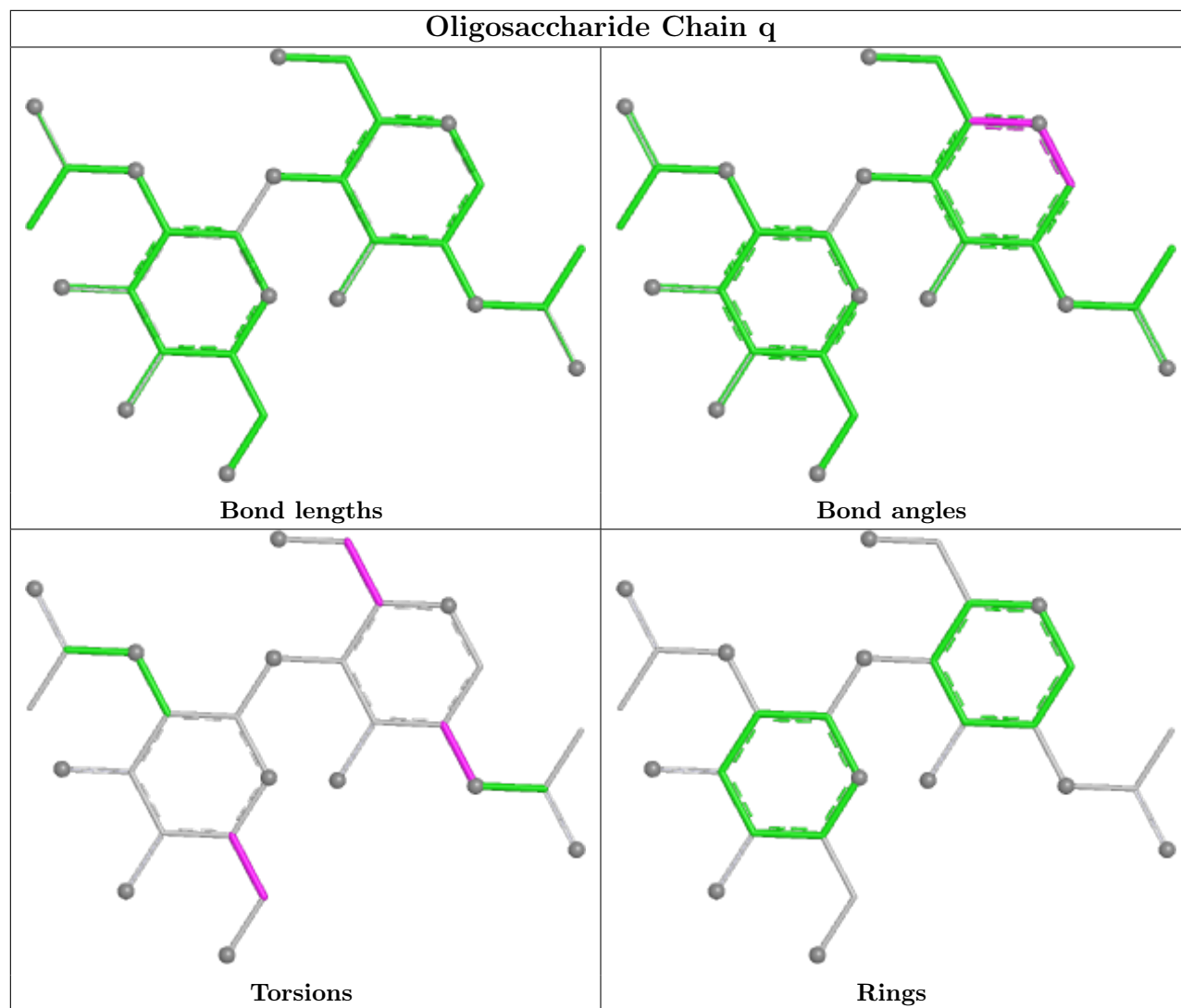


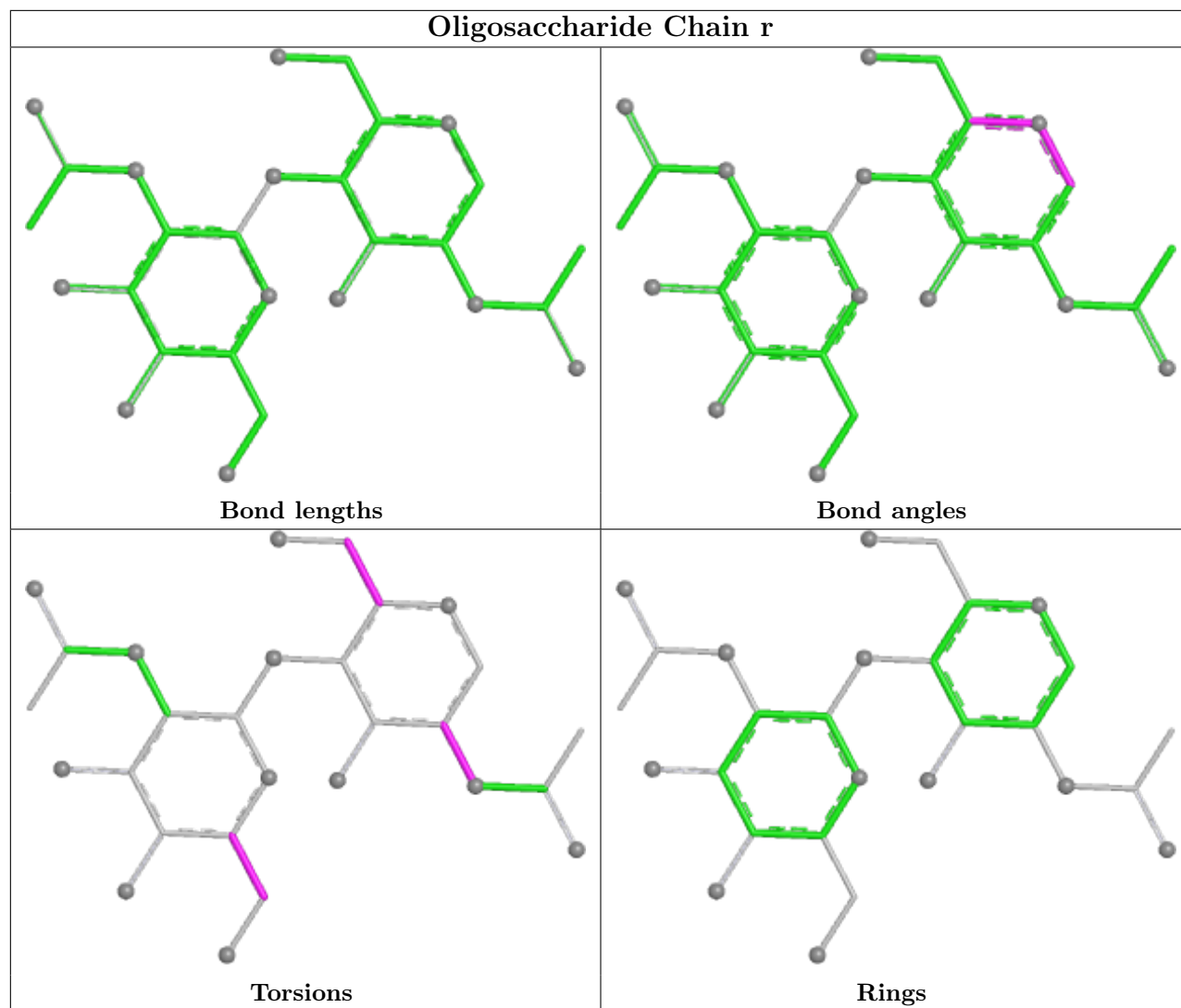


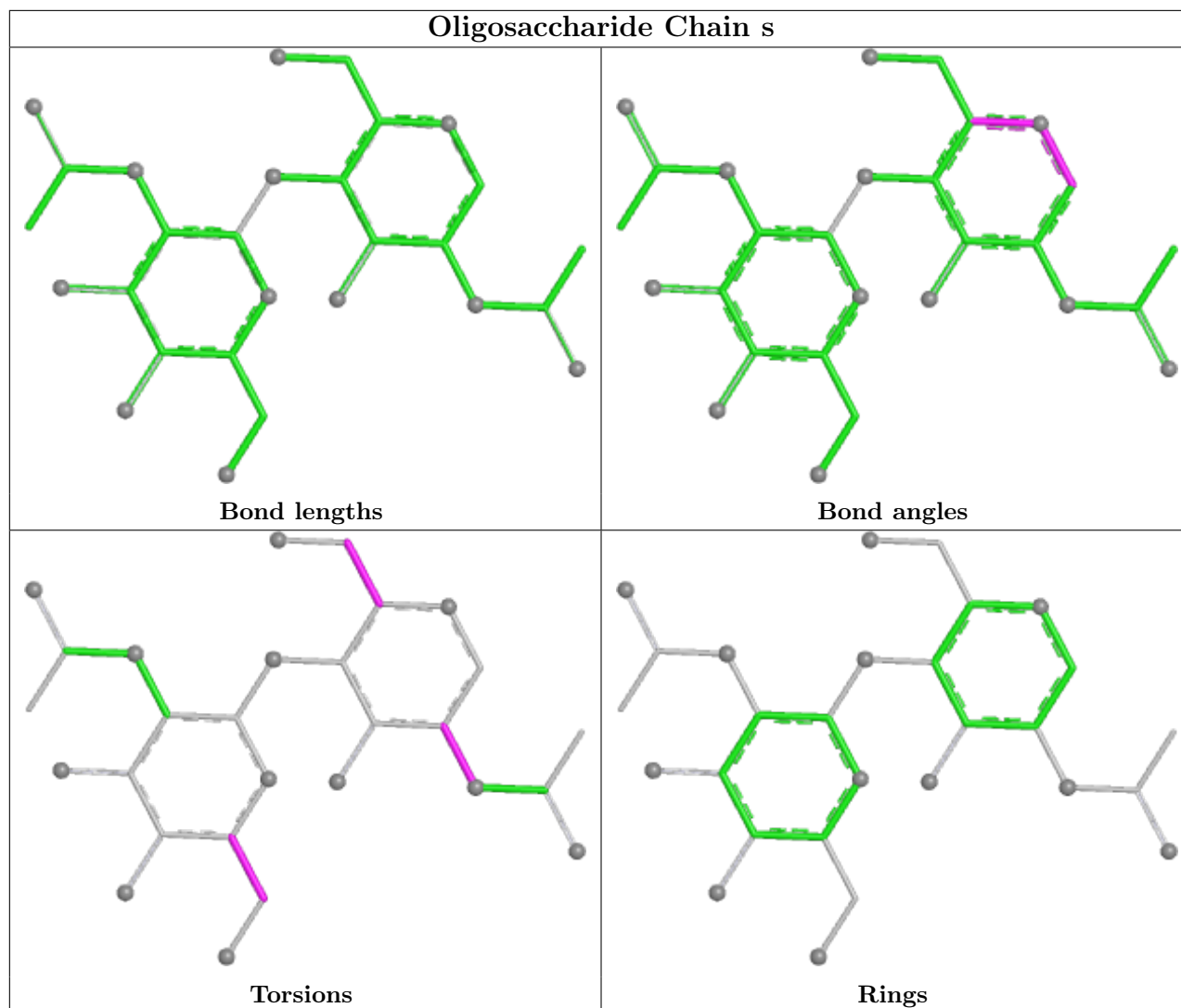












## 5.6 Ligand geometry [i](#)

37 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	$\# Z  > 2$
10	NAG	F	601	5	14,14,15	0.33	0	17,19,21	0.52	0
10	NAG	M	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	T	603	7	14,14,15	0.24	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	U	603	7	14,14,15	0.25	0	17,19,21	0.34	0
10	NAG	R	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	H	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	V	604	7	14,14,15	0.51	0	17,19,21	1.26	1 (5%)
10	NAG	U	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	X	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	M	603	7	14,14,15	0.23	0	17,19,21	0.36	0
10	NAG	O	604	7	14,14,15	0.52	0	17,19,21	1.26	1 (5%)
10	NAG	T	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	V	603	7	14,14,15	0.23	0	17,19,21	0.36	0
10	NAG	W	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	R	603	7	14,14,15	0.23	0	17,19,21	0.35	0
10	NAG	N	603	7	14,14,15	0.23	0	17,19,21	0.35	0
10	NAG	S	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	W	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	O	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	P	603	7	14,14,15	0.54	0	17,19,21	1.24	1 (5%)
10	NAG	K	603	7	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	L	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	Q	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	L	603	7	14,14,15	0.23	0	17,19,21	0.35	0
10	NAG	Q	603	7	14,14,15	0.22	0	17,19,21	0.35	0
10	NAG	J	603	7	14,14,15	0.23	0	17,19,21	0.34	0
10	NAG	S	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	J	604	7	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
10	NAG	N	604	7	14,14,15	0.50	0	17,19,21	1.26	1 (5%)
10	NAG	P	604	7	14,14,15	0.46	0	17,19,21	0.60	0
10	NAG	H	603	7	14,14,15	0.23	0	17,19,21	0.35	0
10	NAG	X	604	7	14,14,15	0.51	0	17,19,21	1.26	1 (5%)
10	NAG	K	604	7	14,14,15	0.52	0	17,19,21	1.26	1 (5%)
10	NAG	G	604	7	14,14,15	0.32	0	17,19,21	0.51	0
10	NAG	I	603	7	14,14,15	0.25	0	17,19,21	0.34	0
10	NAG	I	604	7	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
10	NAG	G	603	7	14,14,15	0.29	0	17,19,21	0.35	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
10	NAG	F	601	5	-	2/6/23/26	0/1/1/1
10	NAG	M	604	7	-	3/6/23/26	0/1/1/1
10	NAG	T	603	7	-	2/6/23/26	0/1/1/1
10	NAG	U	603	7	-	2/6/23/26	0/1/1/1
10	NAG	R	604	7	-	3/6/23/26	0/1/1/1
10	NAG	H	604	7	-	3/6/23/26	0/1/1/1
10	NAG	V	604	7	-	3/6/23/26	0/1/1/1
10	NAG	U	604	7	-	3/6/23/26	0/1/1/1
10	NAG	X	603	7	-	2/6/23/26	0/1/1/1
10	NAG	M	603	7	-	2/6/23/26	0/1/1/1
10	NAG	O	604	7	-	3/6/23/26	0/1/1/1
10	NAG	T	604	7	-	3/6/23/26	0/1/1/1
10	NAG	V	603	7	-	2/6/23/26	0/1/1/1
10	NAG	W	603	7	-	2/6/23/26	0/1/1/1
10	NAG	R	603	7	-	2/6/23/26	0/1/1/1
10	NAG	N	603	7	-	2/6/23/26	0/1/1/1
10	NAG	S	603	7	-	2/6/23/26	0/1/1/1
10	NAG	W	604	7	-	3/6/23/26	0/1/1/1
10	NAG	O	603	7	-	2/6/23/26	0/1/1/1
10	NAG	P	603	7	-	5/6/23/26	0/1/1/1
10	NAG	K	603	7	-	2/6/23/26	0/1/1/1
10	NAG	L	604	7	-	3/6/23/26	0/1/1/1
10	NAG	Q	604	7	-	3/6/23/26	0/1/1/1
10	NAG	L	603	7	-	2/6/23/26	0/1/1/1
10	NAG	Q	603	7	-	2/6/23/26	0/1/1/1
10	NAG	J	603	7	-	2/6/23/26	0/1/1/1
10	NAG	S	604	7	-	3/6/23/26	0/1/1/1
10	NAG	J	604	7	-	3/6/23/26	0/1/1/1
10	NAG	N	604	7	-	3/6/23/26	0/1/1/1
10	NAG	P	604	7	-	0/6/23/26	0/1/1/1
10	NAG	H	603	7	-	2/6/23/26	0/1/1/1
10	NAG	X	604	7	-	3/6/23/26	0/1/1/1
10	NAG	K	604	7	-	3/6/23/26	0/1/1/1
10	NAG	G	604	7	-	2/6/23/26	0/1/1/1
10	NAG	I	603	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	I	604	7	-	3/6/23/26	0/1/1/1
10	NAG	G	603	7	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	604	NAG	C2-N2-C7	4.27	128.99	122.90
10	P	603	NAG	C2-N2-C7	4.27	128.98	122.90
10	I	604	NAG	C2-N2-C7	4.26	128.98	122.90
10	W	604	NAG	C2-N2-C7	4.26	128.97	122.90
10	J	604	NAG	C2-N2-C7	4.26	128.97	122.90

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	603	NAG	C4-C5-C6-O6
10	I	603	NAG	C4-C5-C6-O6
10	J	603	NAG	C4-C5-C6-O6
10	K	603	NAG	C4-C5-C6-O6
10	L	603	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	601	NAG	1	0
10	P	603	NAG	1	0
10	P	604	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

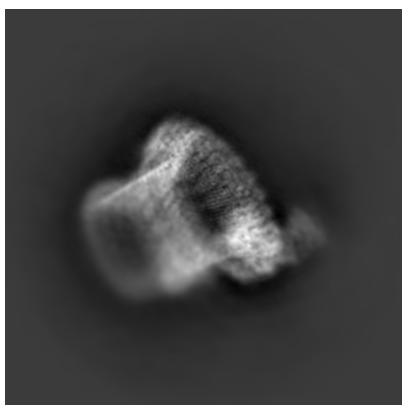
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0106. These allow visual inspection of the internal detail of the map and identification of artifacts.

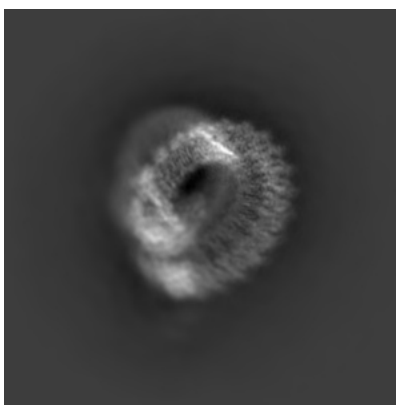
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

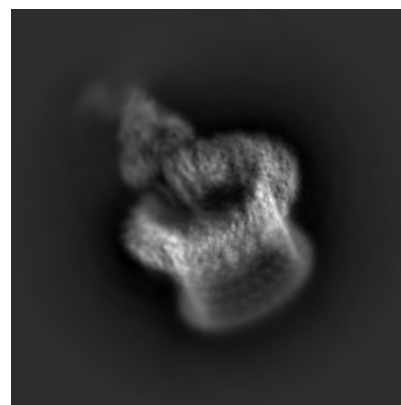
#### 6.1.1 Primary map



X



Y

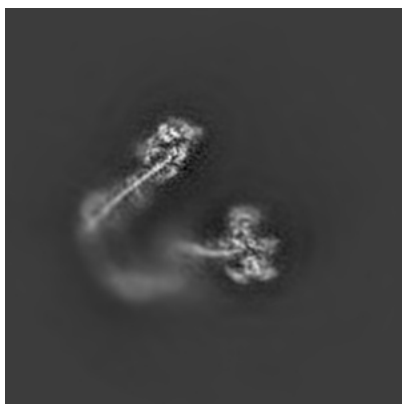


Z

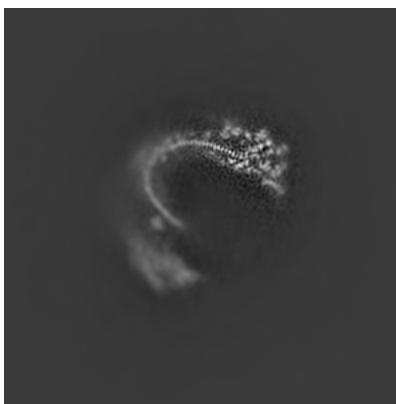
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

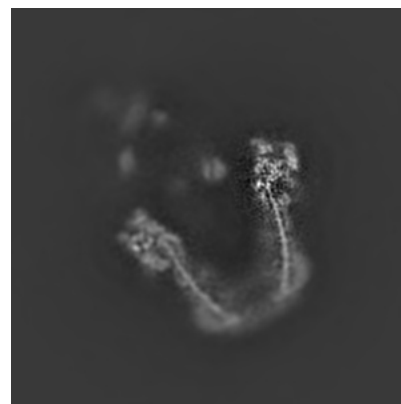
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

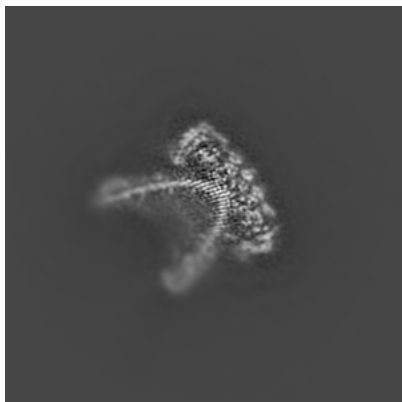


Z Index: 180

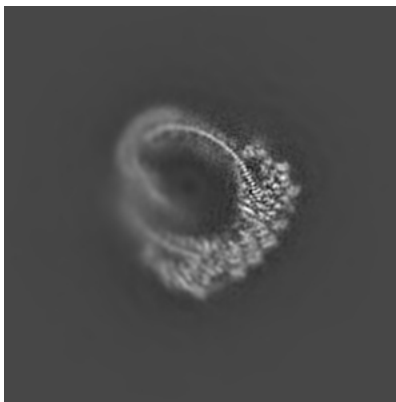
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

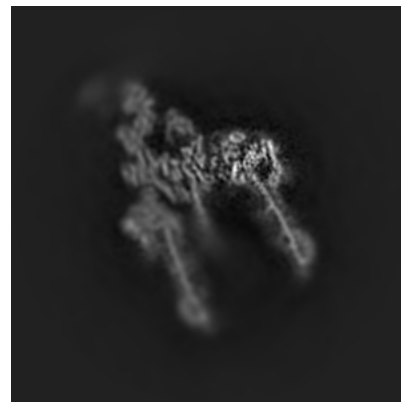
### 6.3.1 Primary map



X Index: 232



Y Index: 153

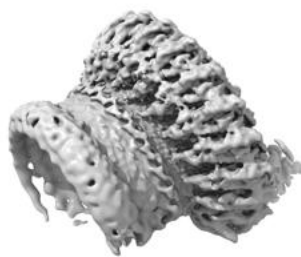


Z Index: 152

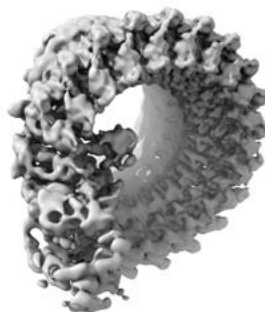
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

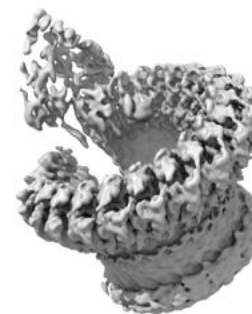
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

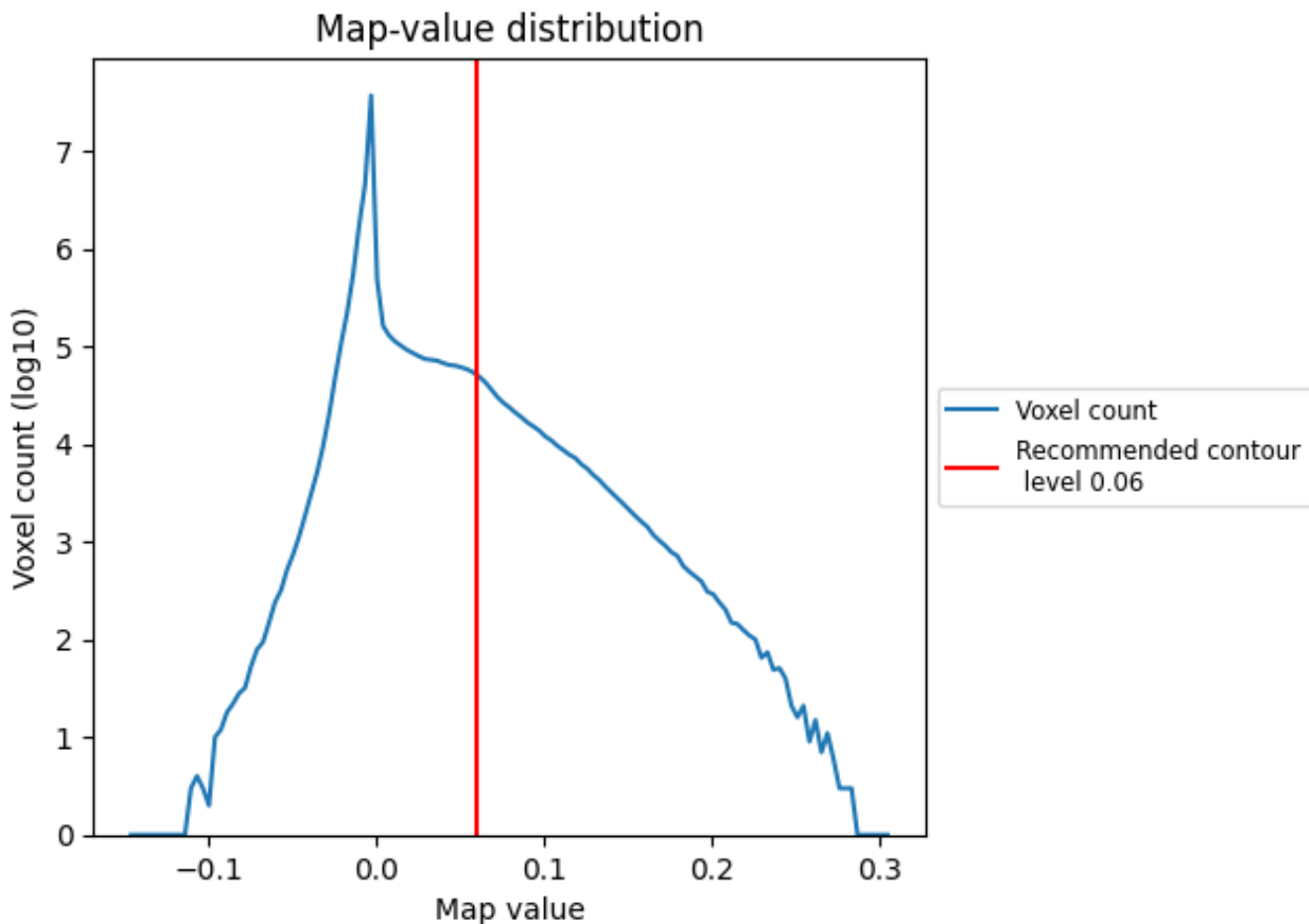
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

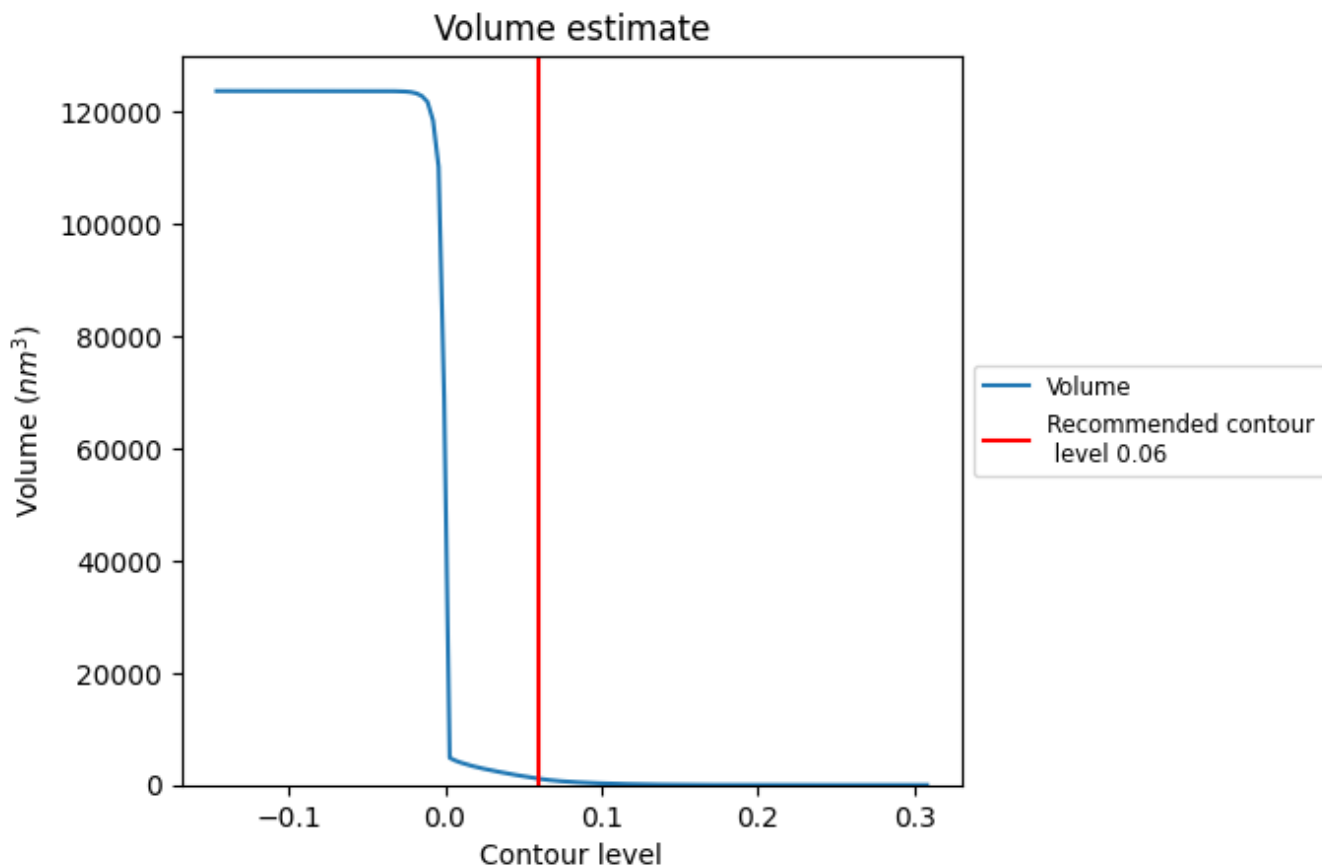
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

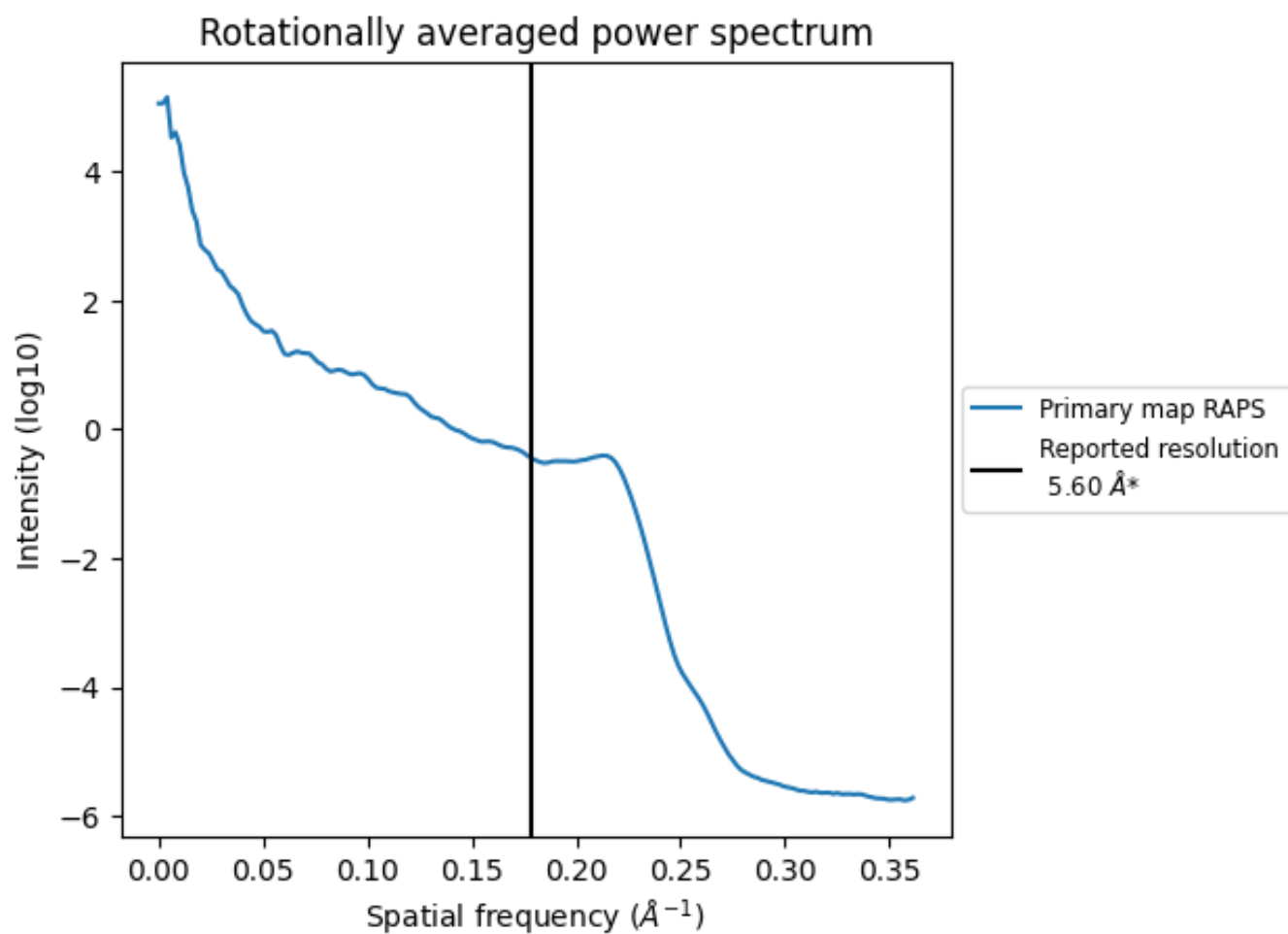
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1116 nm<sup>3</sup>; this corresponds to an approximate mass of 1008 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i



\*Reported resolution corresponds to spatial frequency of 0.179 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

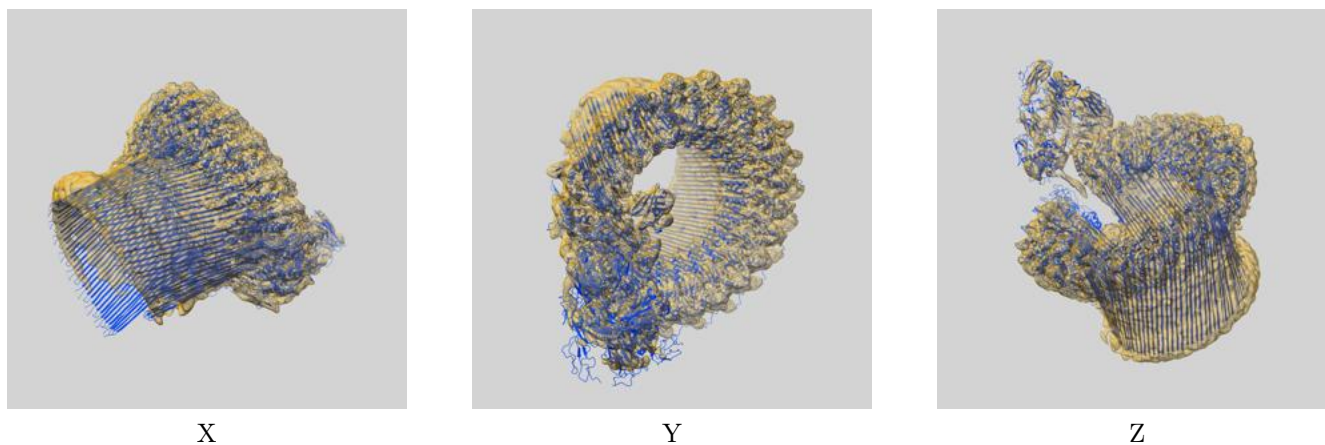
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

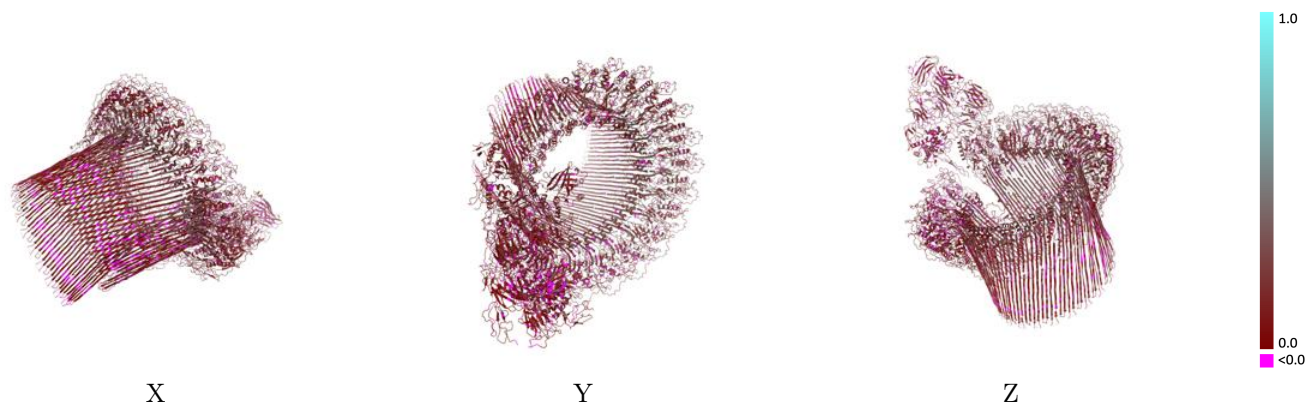
This section contains information regarding the fit between EMDB map EMD-0106 and PDB model 6H03. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



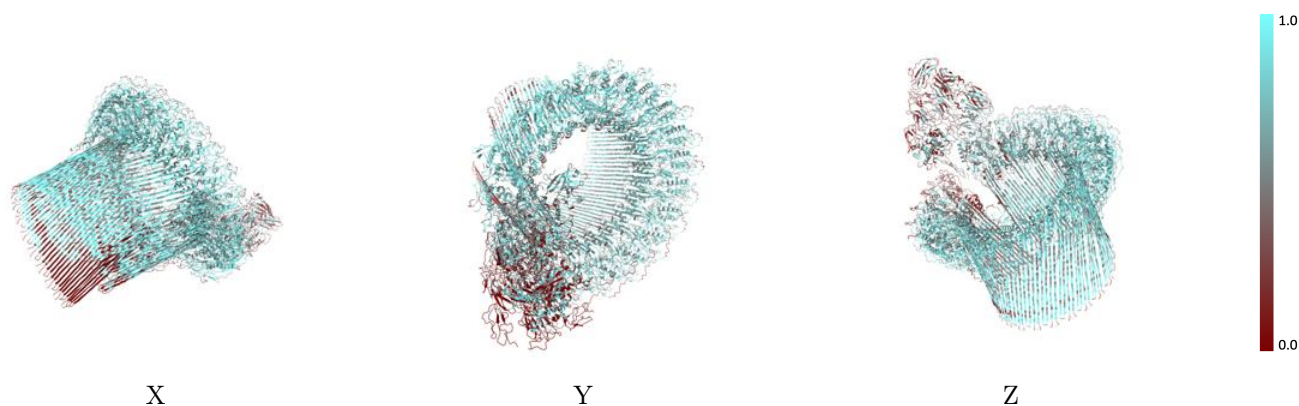
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



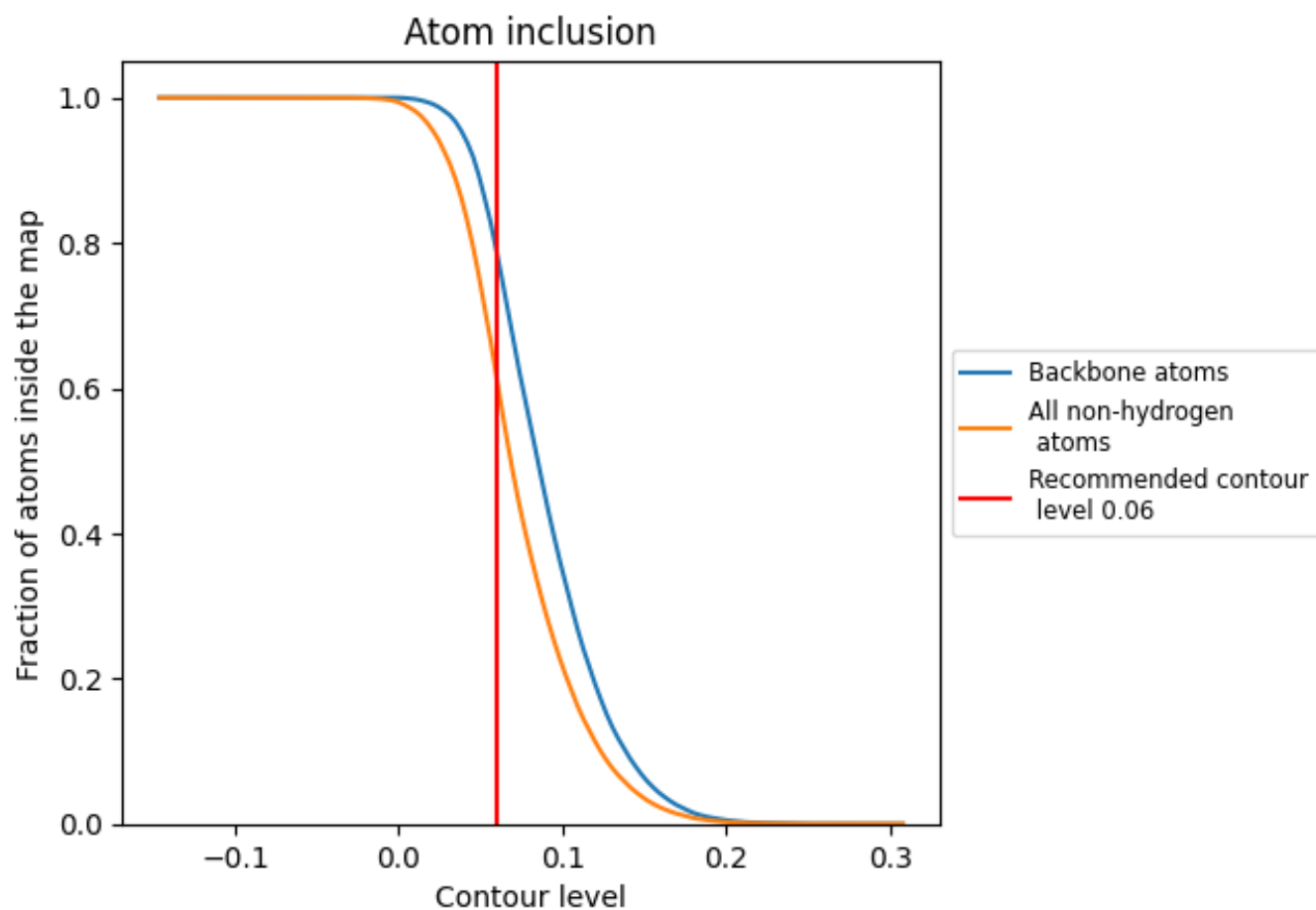
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6135	 0.1560
A	 0.3697	 0.1050
B	 0.4417	 0.1270
C	 0.6998	 0.1720
D	 0.5538	 0.1350
E	 0.5508	 0.1650
F	 0.7093	 0.1630
G	 0.6896	 0.1610
H	 0.7483	 0.1980
I	 0.7466	 0.1930
J	 0.7404	 0.1980
K	 0.7430	 0.2070
L	 0.7455	 0.2070
M	 0.7511	 0.2170
N	 0.7248	 0.1850
O	 0.7417	 0.2020
P	 0.7333	 0.1810
Q	 0.7289	 0.1870
R	 0.7172	 0.1620
S	 0.6924	 0.1550
T	 0.6506	 0.1280
U	 0.6248	 0.1280
V	 0.5419	 0.1170
W	 0.3947	 0.0780
X	 0.1108	 0.0670
Y	 0.1282	 0.1780
Z	 0.0000	 0.0820
a	 0.0000	 -0.0210
b	 0.3929	 0.2130
c	 0.4286	 0.2220
d	 0.3929	 0.1300
e	 0.3571	 0.1020
f	 0.4643	 0.2440
g	 0.3929	 0.2000
h	 0.6071	 0.1970



*Continued on next page...*

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Chain	Atom inclusion	Q-score
i	 0.5000	 0.1720
j	 0.6071	 0.1800
k	 0.4286	 0.2100
l	 0.4286	 0.2300
m	 0.5714	 0.2100
n	 0.2500	 0.1690
o	 0.1786	 0.1800
p	 0.1786	 0.0630
q	 0.1429	 0.0170
r	 0.0357	 0.0560
s	 0.0000	 0.0610