



## wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 11:56 am GMT

PDB ID : 6H04  
EMDB ID : EMD-0107  
Title : Closed 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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

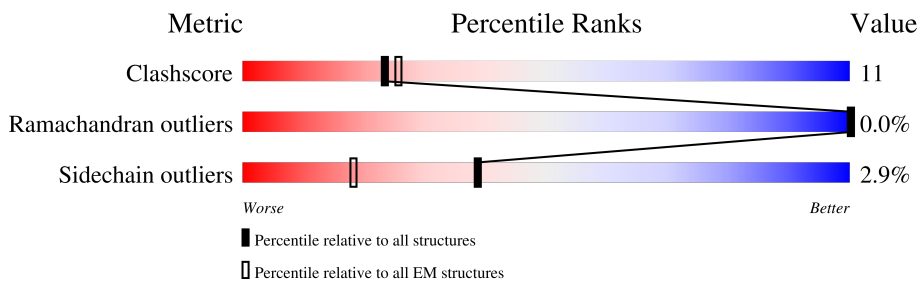
# 1 Overall quality at a glance i

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	G	538	
1	H	538	
1	I	538	
1	J	538	
1	K	538	
1	L	538	
1	M	538	
1	N	538	




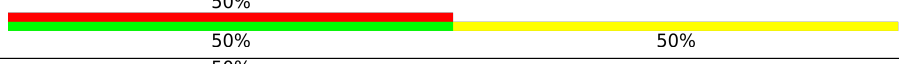
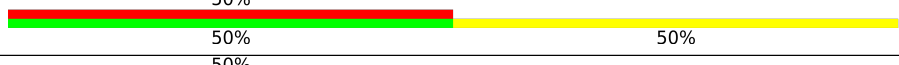
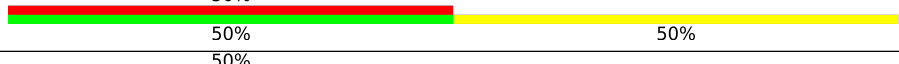
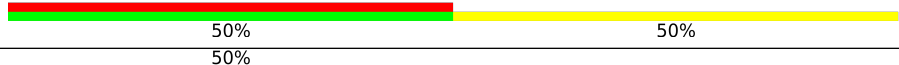



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Mol	Chain	Length	Quality of chain
1	O	538	63% 30% 7%
1	P	538	63% 30% 7%
1	Q	538	61% 32% 7%
1	R	538	62% 31% 7%
1	S	538	63% 29% 7%
1	T	538	65% 27% 7%
1	U	538	66% 27% 7%
1	V	538	66% 26% 7%
1	W	538	67% 25% 7%
1	X	538	70% 22% 7%
2	A	1580	61% 16% 23%
3	C	537	83% 12% 5%
4	D	821	69% 11% 20%
5	E	182	76% 14% 9%
6	F	554	71% 20% 8%
7	B	913	63% 13% 25%
8	Y	2	50% 50%
8	Z	2	50% 50%
8	a	2	50% 50%
8	b	2	50% 50%
8	c	2	50% 50%
8	d	2	50% 50%
8	e	2	50% 50%
8	f	2	50% 50%
8	g	2	50% 50%

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Mol	Chain	Length	Quality of chain
8	h	2	
8	i	2	
8	j	2	
8	k	2	
8	l	2	
8	m	2	
8	n	2	
8	o	2	
8	p	2	
8	q	2	

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 97178 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 component C9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	501	3785	2363	670	721	31	0	0
1	M	501	3785	2363	670	721	31	0	0
1	N	501	3785	2363	670	721	31	0	0
1	O	501	3785	2363	670	721	31	0	0
1	Q	501	3785	2363	670	721	31	0	0
1	R	501	3785	2363	670	721	31	0	0
1	S	501	3785	2363	670	721	31	0	0
1	T	501	3785	2363	670	721	31	0	0
1	U	501	3785	2363	670	721	31	0	0
1	V	501	3785	2363	670	721	31	0	0
1	W	501	3785	2363	670	721	31	0	0
1	X	501	3785	2363	670	721	31	0	0
1	P	501	3785	2363	670	721	31	0	0
1	H	501	3785	2363	670	721	31	0	0
1	I	501	3785	2363	670	721	31	0	0
1	J	501	3785	2363	670	721	31	0	0
1	K	501	3785	2363	670	721	31	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	501	3770	2352	668	720	30	0	0

- Molecule 2 is a protein called Complement C5, Complement C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	1219	9497	6097	1572	1801	27	0	0

- Molecule 3 is a protein called Complement component C8 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	513	3752	2345	664	713	30	0	0

- Molecule 4 is a protein called Complement component C7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	660	4578	2844	825	867	42	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	165	1286	823	223	236	4	0	0

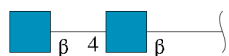
- Molecule 6 is a protein called Complement component C8 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	510	3758	2331	660	730	37	0	0

- Molecule 7 is a protein called Complement component C6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	688	5128	3174	918	990	46	0	0

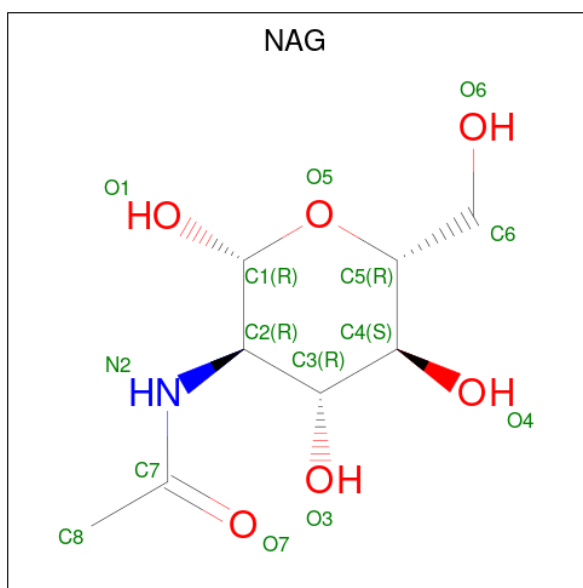
- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 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	
9	L	1	Total 14	8	1	5	0
9	L	1	Total 14	8	1	5	0
9	M	1	Total 14	8	1	5	0
9	M	1	Total 14	8	1	5	0
9	N	1	Total 14	8	1	5	0
9	N	1	Total 14	8	1	5	0
9	O	1	Total 14	8	1	5	0
9	O	1	Total 14	8	1	5	0
9	Q	1	Total 14	8	1	5	0
9	Q	1	Total 14	8	1	5	0
9	R	1	Total 14	8	1	5	0
9	R	1	Total 14	8	1	5	0
9	S	1	Total 14	8	1	5	0

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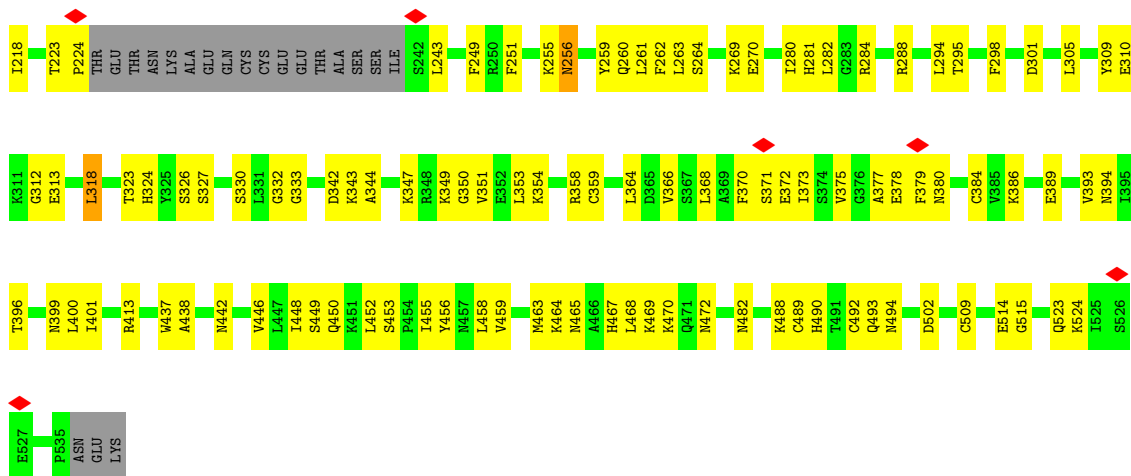
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	S	1	Total 14	8	1	5	0
9	T	1	Total 14	8	1	5	0
9	T	1	Total 14	8	1	5	0
9	U	1	Total 14	8	1	5	0
9	U	1	Total 14	8	1	5	0
9	V	1	Total 14	8	1	5	0
9	V	1	Total 14	8	1	5	0
9	W	1	Total 14	8	1	5	0
9	W	1	Total 14	8	1	5	0
9	X	1	Total 14	8	1	5	0
9	X	1	Total 14	8	1	5	0
9	P	1	Total 14	8	1	5	0
9	P	1	Total 14	8	1	5	0
9	H	1	Total 14	8	1	5	0
9	H	1	Total 14	8	1	5	0
9	I	1	Total 14	8	1	5	0
9	I	1	Total 14	8	1	5	0
9	J	1	Total 14	8	1	5	0
9	J	1	Total 14	8	1	5	0
9	K	1	Total 14	8	1	5	0
9	K	1	Total 14	8	1	5	0

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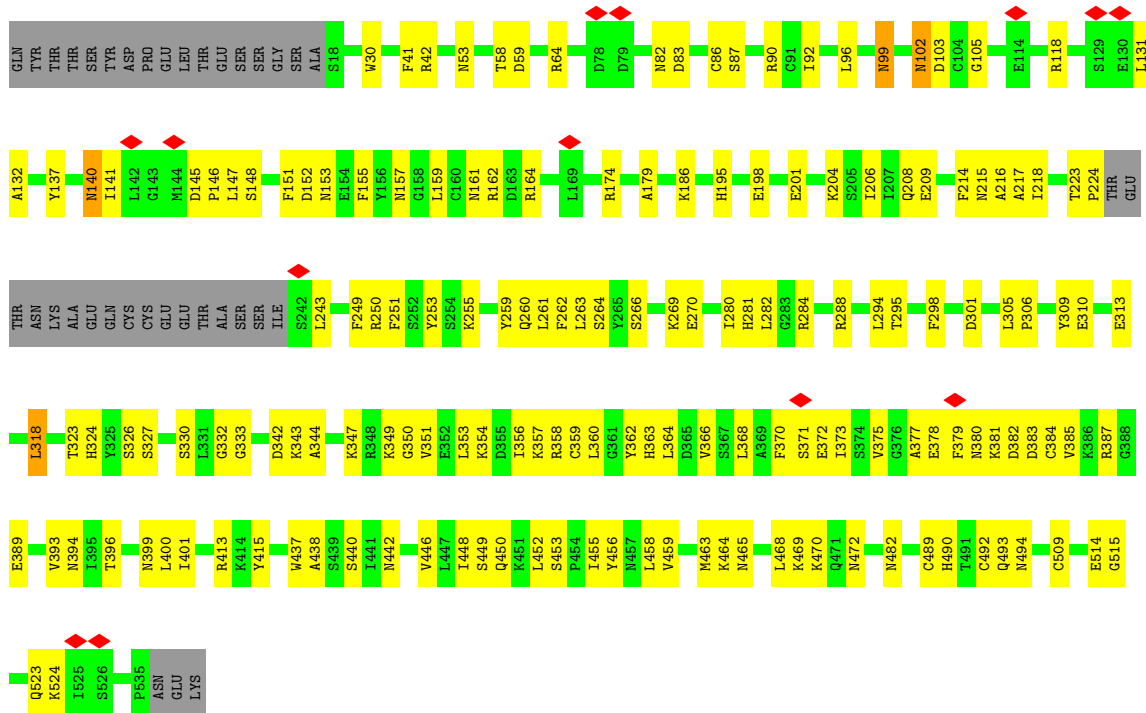
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	G	1	Total 14	8	1	5	0
9	G	1	Total 14	8	1	5	0
9	D	1	Total 14	8	1	5	0
9	B	1	Total 14	8	1	5	0

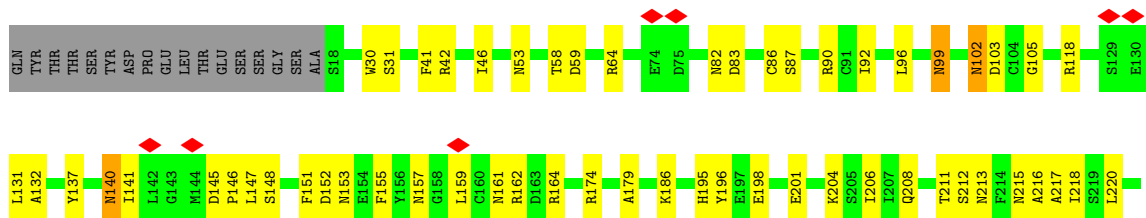


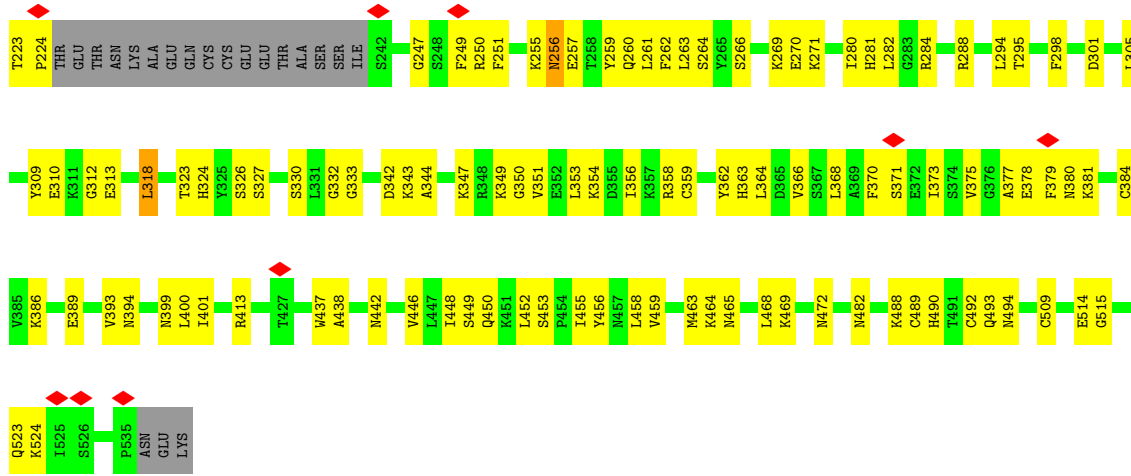


• Molecule 1: Complement component C9

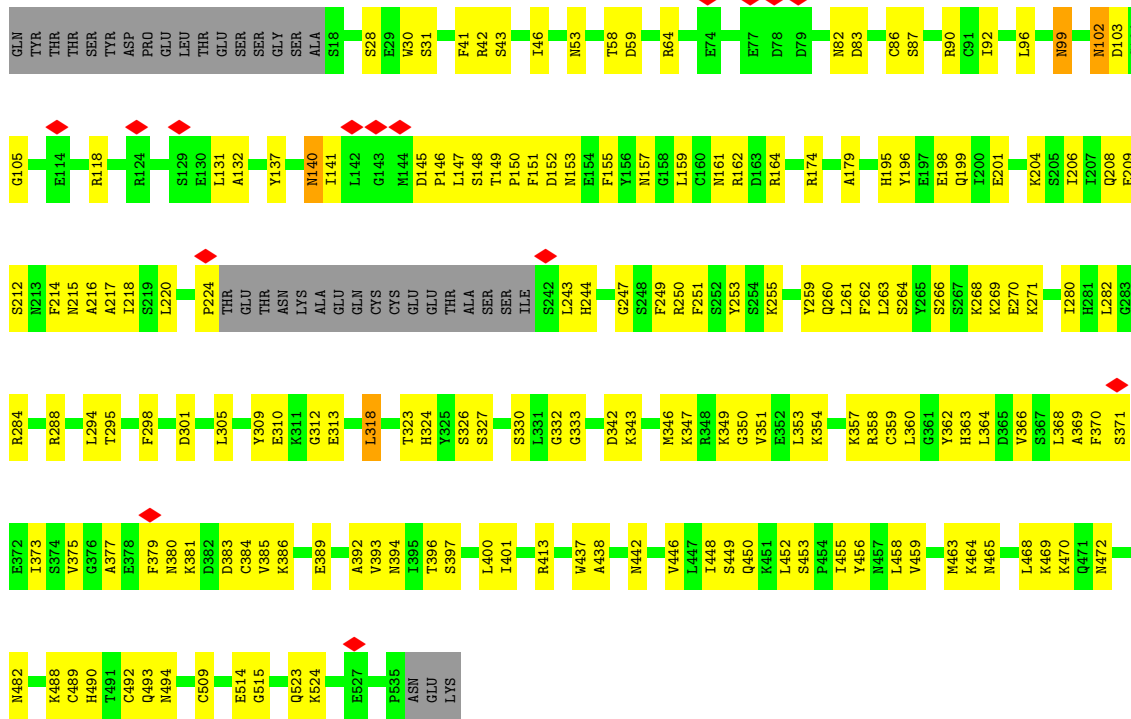


• Molecule 1: Complement component C9



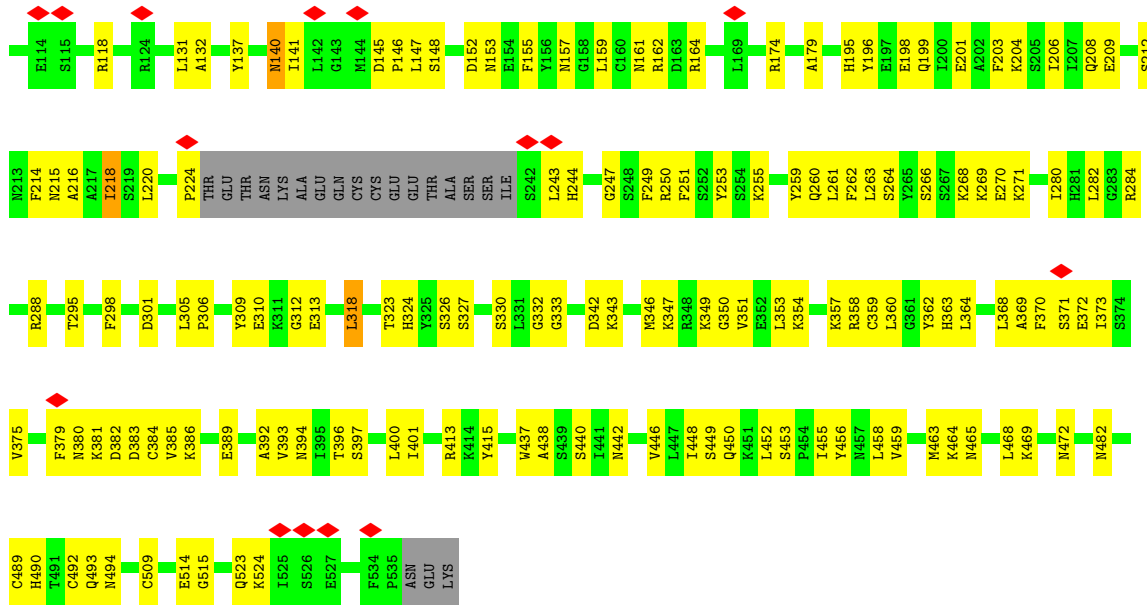


• Molecule 1: Complement component C9

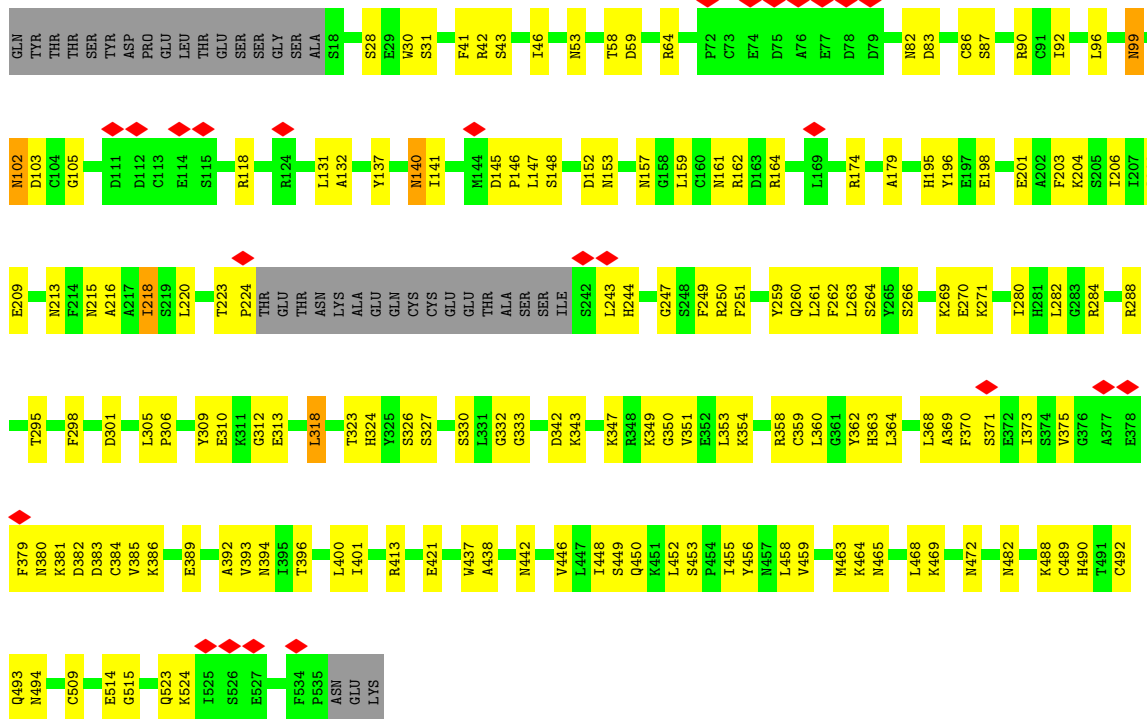


• Molecule 1: Complement component C9



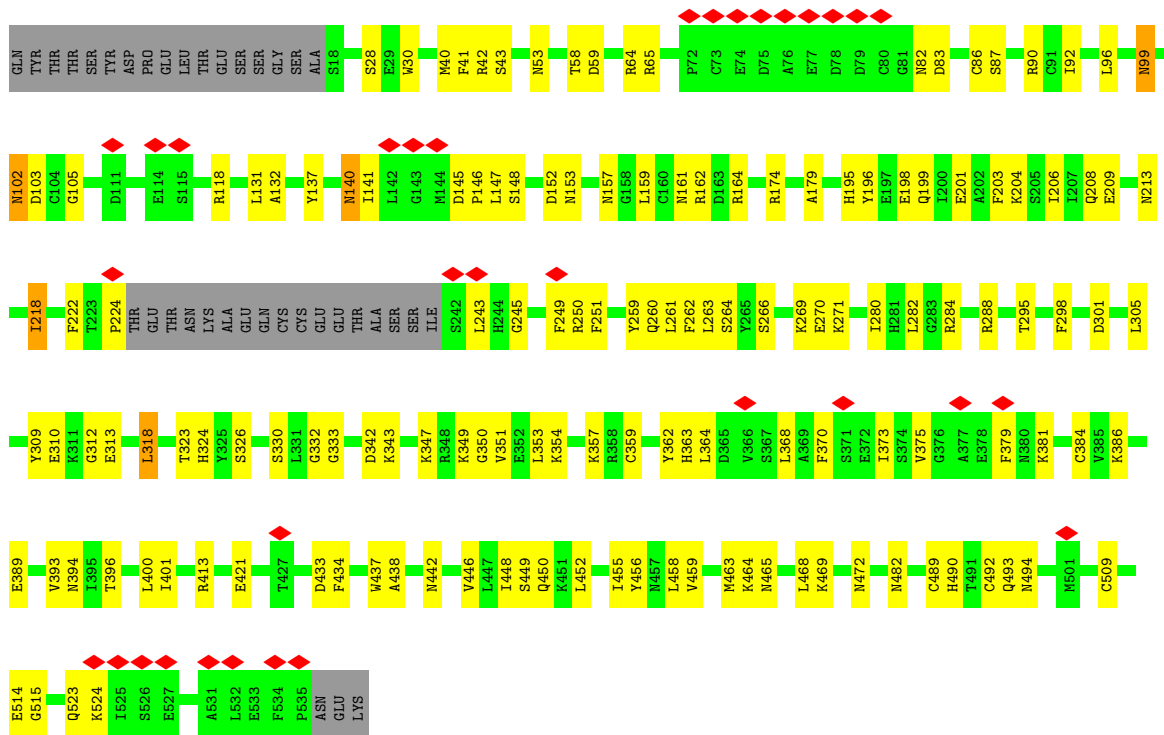


• Molecule 1: Complement component C9

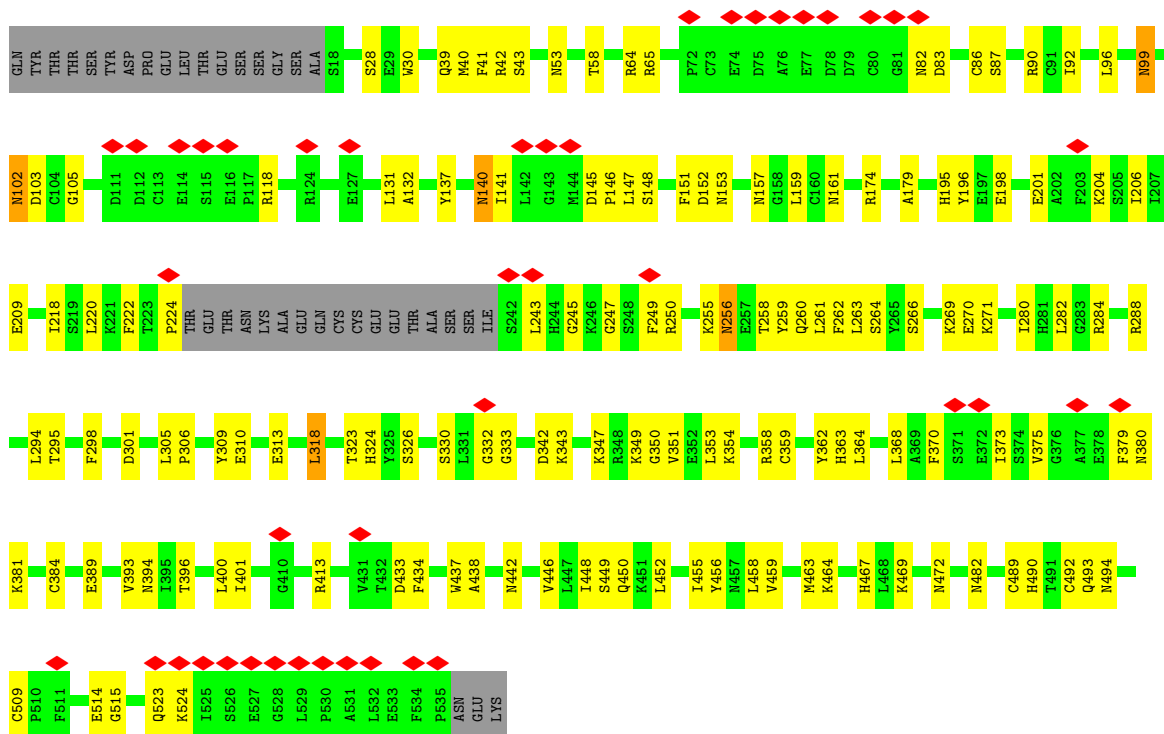


• Molecule 1: Complement component C9

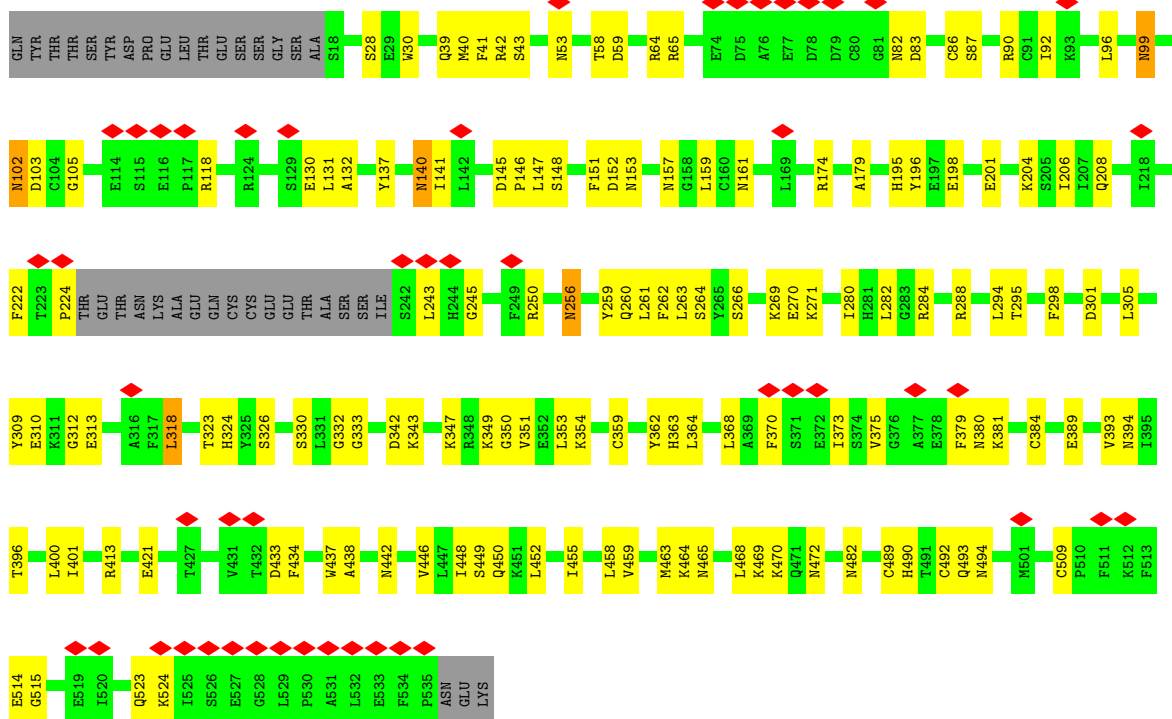




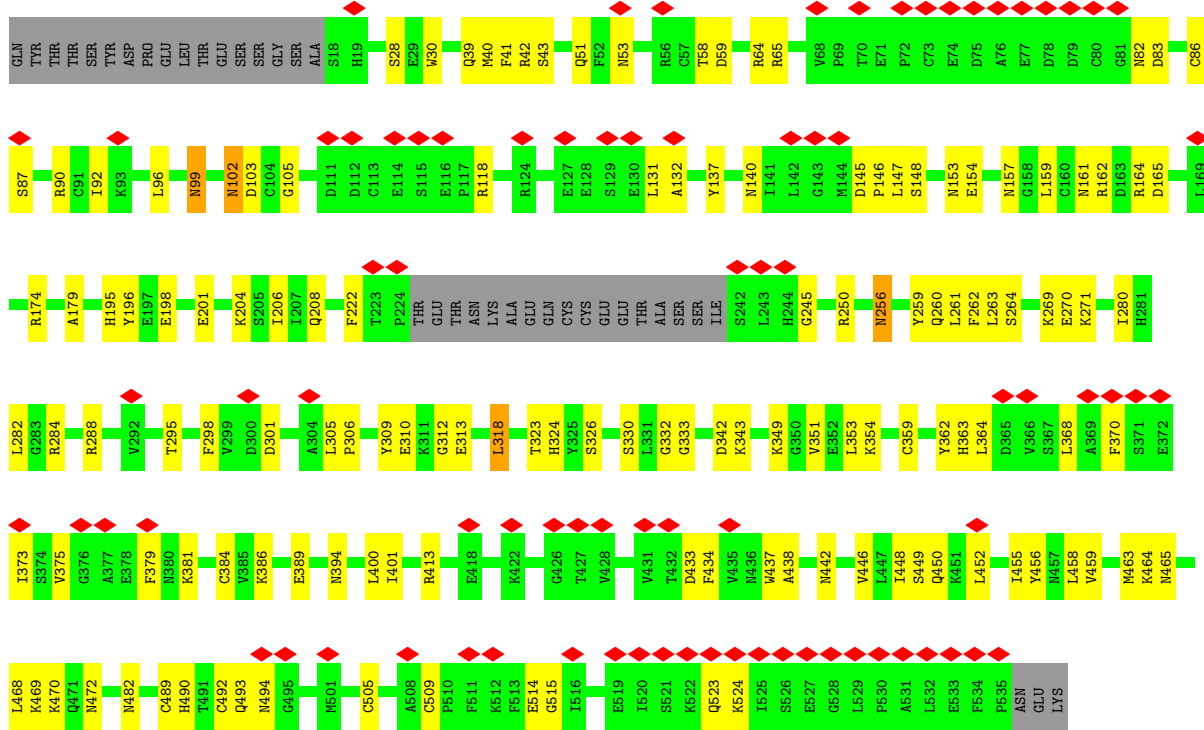
• Molecule 1: Complement component C9



• Molecule 1: Complement component C9



● Molecule 1: Complement component C9

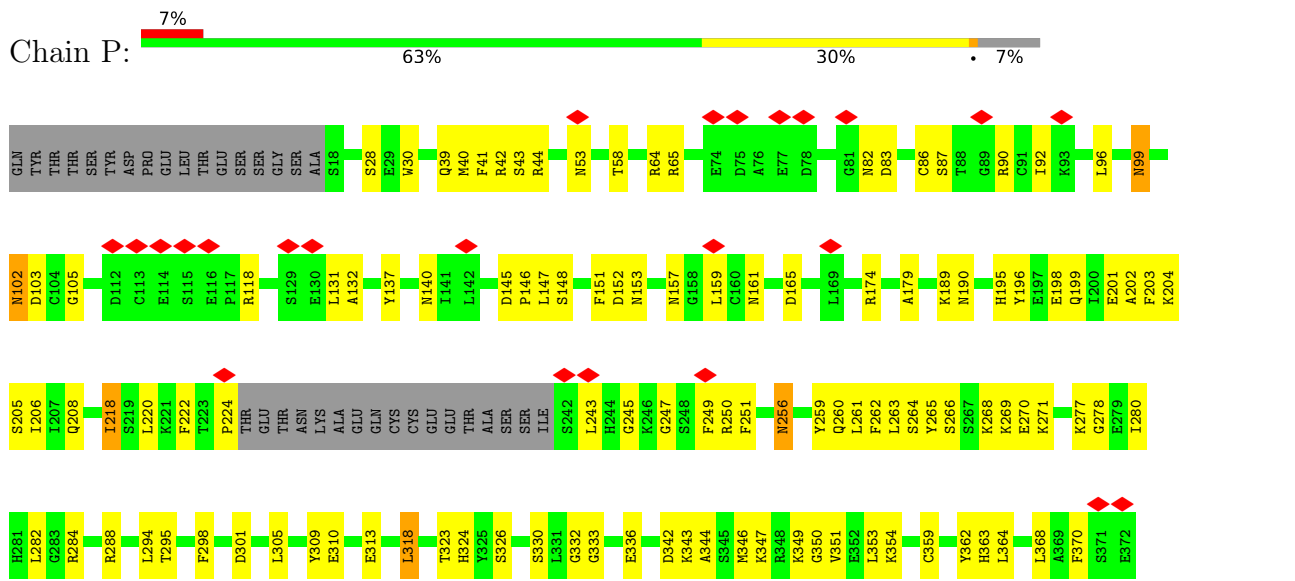


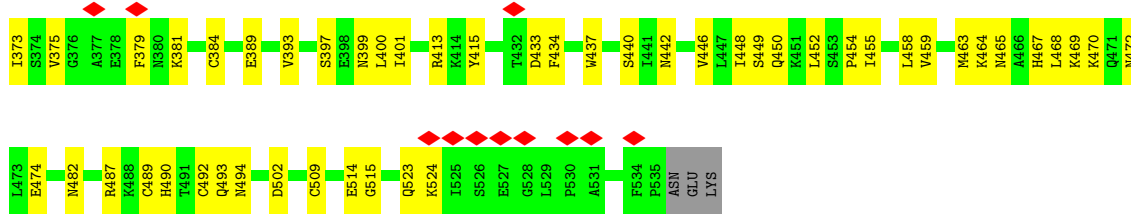


• Molecule 1: Complement component C9

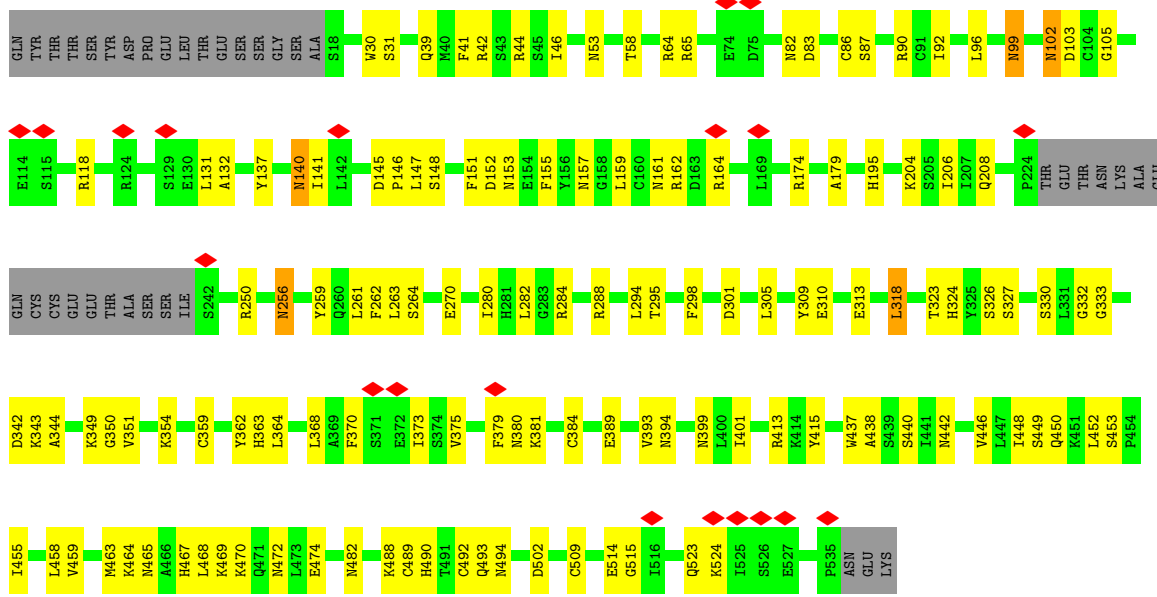


• Molecule 1: Complement component C9

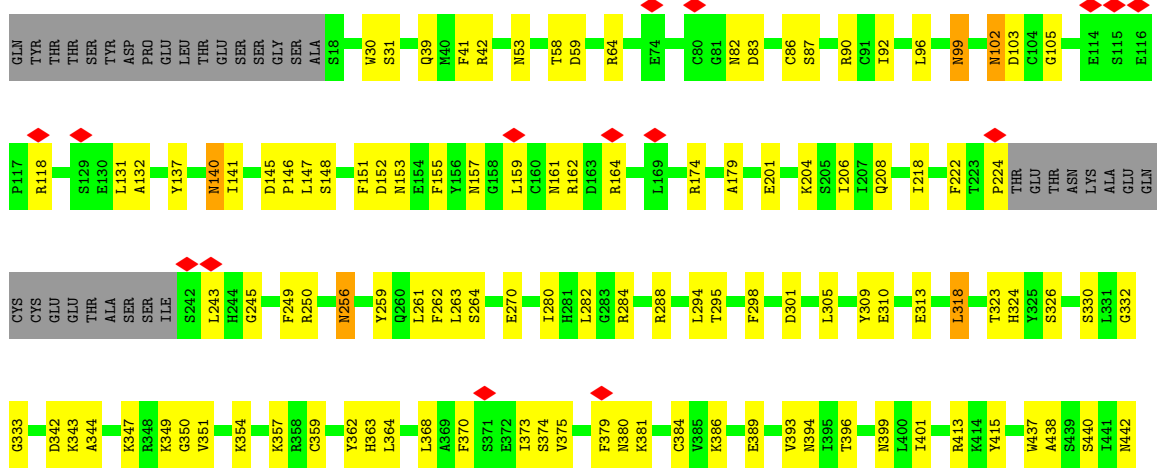




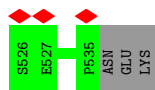
• Molecule 1: Complement component C9



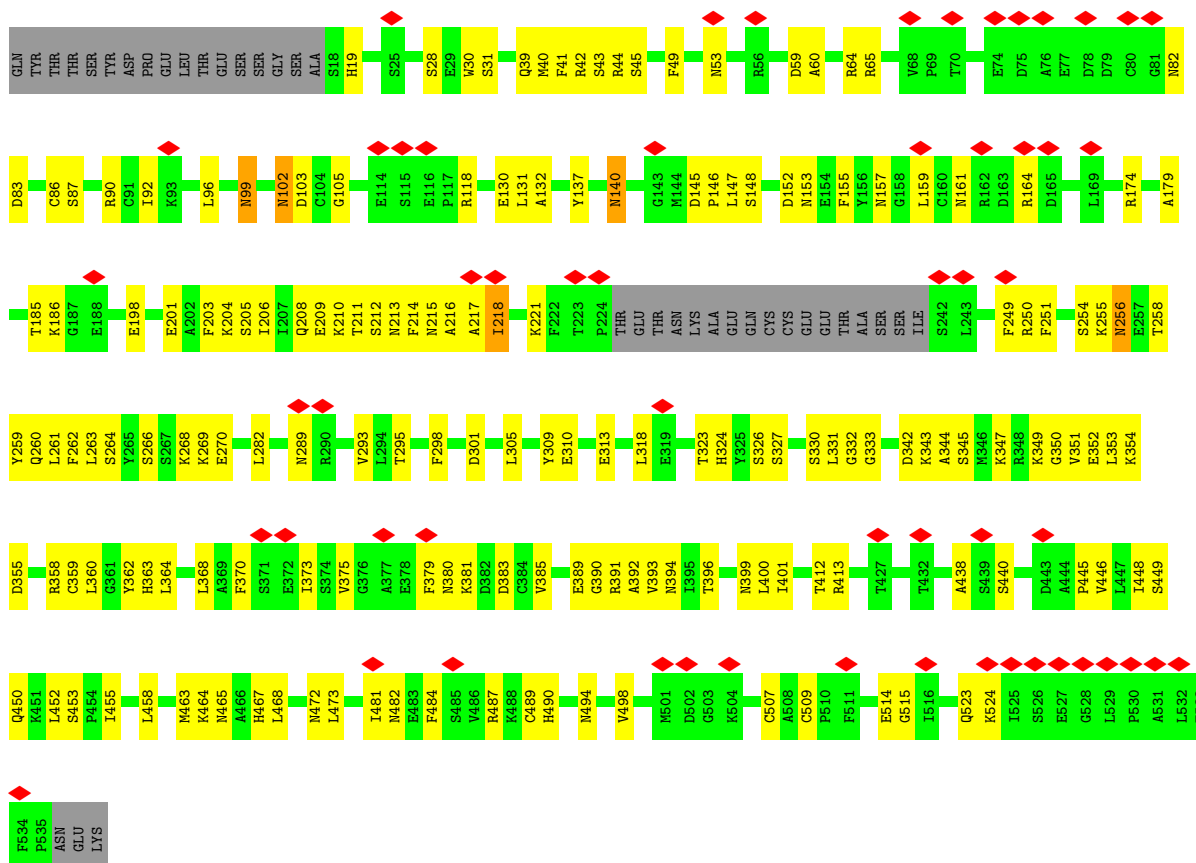
• Molecule 1: Complement component C9



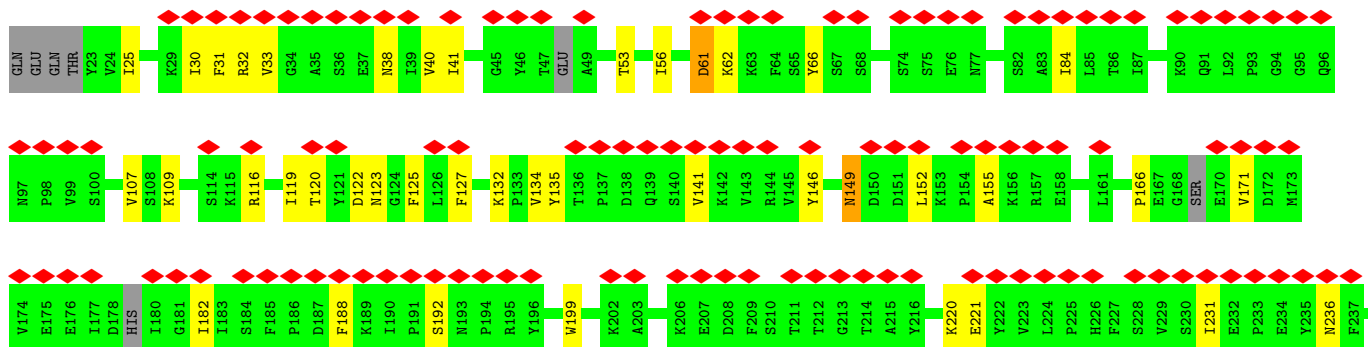


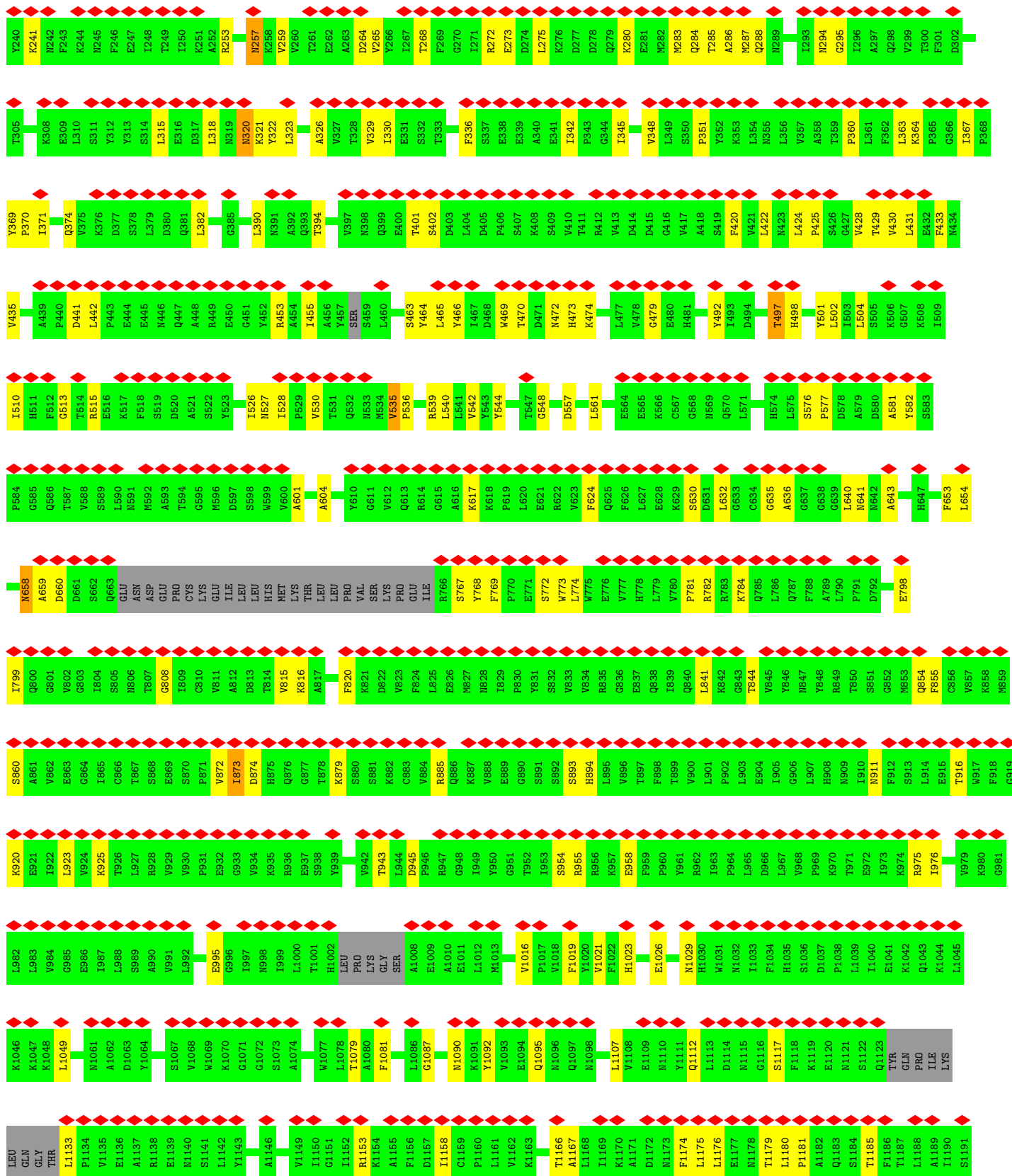


• Molecule 1: Complement component C9

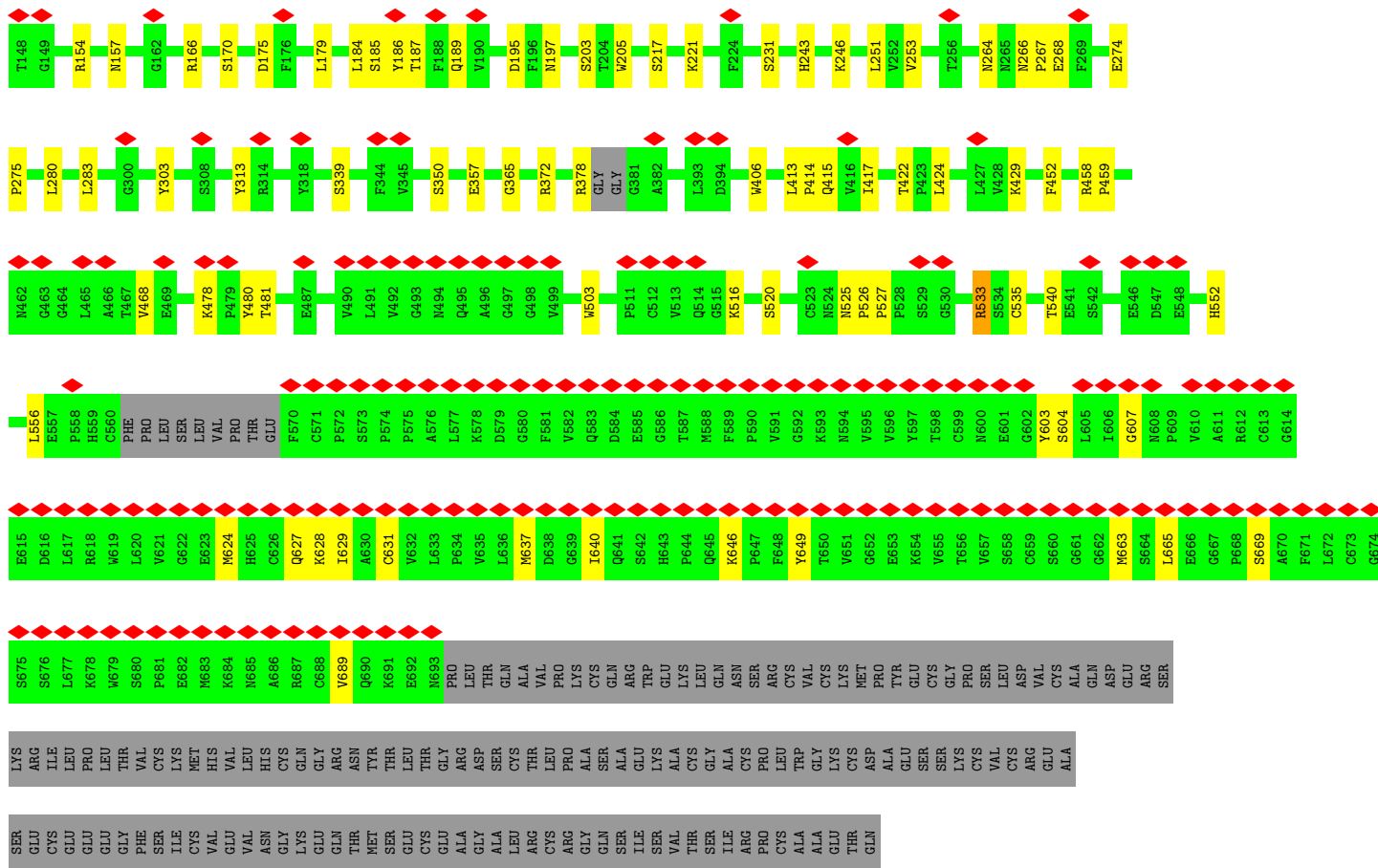


• Molecule 2: Complement C5, Complement C5

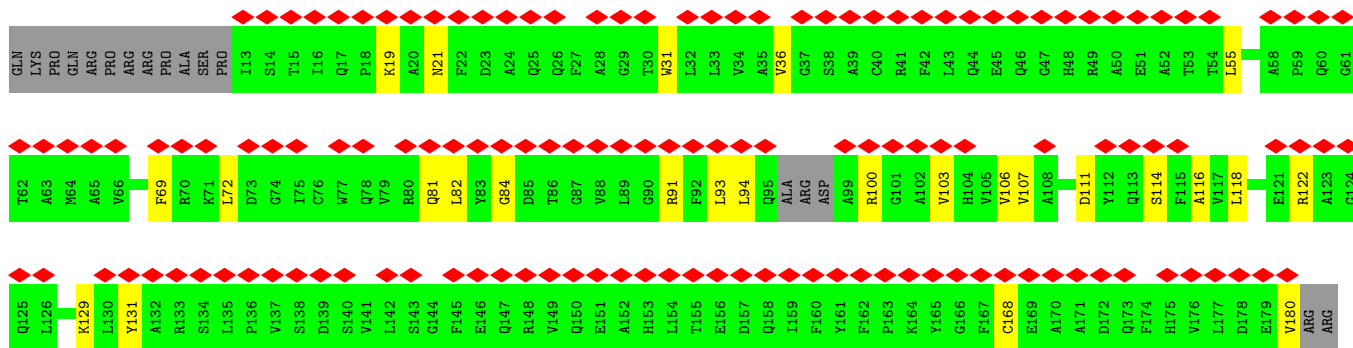
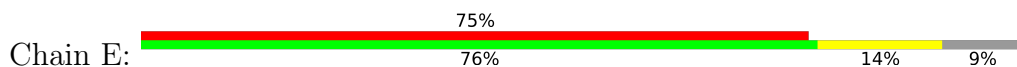








• Molecule 5: Complement component C8 gamma chain



• Molecule 6: Complement component C8 alpha chain







GLY SER CYS GLN ASP MET GLY ARG GLN LEU THR TRP GLY LEU GLU ARG THR ASN GLY THR LYS LYS GLU CYS TYR ASP THR CYS TYR ASP TRP GLY LYS CYS SER ALA THR SER LYS VAL CYS LEU LEU PRO GLN CYS PHE LYS GLY ASN GLN

LEU TYR VAL LYS MET GLY SER THR SER GLY THR LEU ASN THR CYS GLU VAL GLY THR ILE ARG CYS ALA ASN ARG LYS MET GLU ILE LEU HIS PRO GLY LYS CYS LEU ALA

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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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





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



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucofuranose-(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	53167	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	0.342	Depositor
Minimum map value	-0.153	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:  
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	G	0.23	0/3839	0.42	0/5181
1	H	0.23	0/3856	0.42	0/5203
1	I	0.23	0/3856	0.42	0/5203
1	J	0.24	0/3856	0.42	0/5203
1	K	0.23	0/3856	0.42	0/5203
1	L	0.23	0/3856	0.42	0/5203
1	M	0.23	0/3856	0.42	0/5203
1	N	0.23	0/3856	0.42	0/5203
1	O	0.23	0/3856	0.42	0/5203
1	P	0.23	0/3856	0.42	0/5203
1	Q	0.23	0/3856	0.42	0/5203
1	R	0.23	0/3856	0.42	0/5203
1	S	0.23	0/3856	0.42	0/5203
1	T	0.23	0/3856	0.42	0/5203
1	U	0.24	0/3856	0.42	0/5203
1	V	0.23	0/3856	0.42	0/5203
1	W	0.23	0/3856	0.42	0/5203
1	X	0.24	0/3856	0.42	0/5203
2	A	0.24	0/9707	0.44	1/13191 (0.0%)
3	C	0.23	0/3831	0.42	0/5203
4	D	0.24	0/4687	0.42	0/6362
5	E	0.24	0/1314	0.41	0/1782
6	F	0.23	0/3830	0.41	0/5157
7	B	0.24	0/5231	0.41	0/7085
All	All	0.23	0/97991	0.42	1/132412 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	61	ASP	C-N-CA	5.24	134.81	121.70

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	G	3770	0	3478	129	0
1	H	3785	0	3495	87	0
1	I	3785	0	3495	91	0
1	J	3785	0	3495	92	0
1	K	3785	0	3495	98	0
1	L	3785	0	3495	109	0
1	M	3785	0	3495	111	0
1	N	3785	0	3495	113	0
1	O	3785	0	3495	111	0
1	P	3785	0	3495	105	0
1	Q	3785	0	3495	113	0
1	R	3785	0	3495	112	0
1	S	3785	0	3495	110	0
1	T	3785	0	3495	96	0
1	U	3785	0	3495	93	0
1	V	3785	0	3495	90	0
1	W	3785	0	3495	88	0
1	X	3785	0	3495	73	0
2	A	9497	0	9310	160	0
3	C	3752	0	3289	42	0
4	D	4578	0	3862	55	0
5	E	1286	0	1244	15	0
6	F	3758	0	3313	90	0
7	B	5128	0	4610	71	0
8	Y	28	0	25	2	0
8	Z	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	a	28	0	25	0	0
8	b	28	0	25	0	0
8	c	28	0	25	0	0
8	d	28	0	25	0	0
8	e	28	0	25	0	0
8	f	28	0	25	0	0
8	g	28	0	25	0	0
8	h	28	0	25	0	0
8	i	28	0	25	0	0
8	j	28	0	25	0	0
8	k	28	0	25	0	0
8	l	28	0	25	0	0
8	m	28	0	25	0	0
8	n	28	0	25	0	0
8	o	28	0	25	0	0
8	p	28	0	25	0	0
8	q	28	0	25	0	0
9	B	14	0	13	1	0
9	D	14	0	13	1	0
9	G	28	0	26	2	0
9	H	28	0	26	2	0
9	I	28	0	26	3	0
9	J	28	0	26	2	0
9	K	28	0	26	2	0
9	L	28	0	26	2	0
9	M	28	0	26	2	0
9	N	28	0	26	2	0
9	O	28	0	26	1	0
9	P	28	0	26	1	0
9	Q	28	0	26	2	0
9	R	28	0	26	2	0
9	S	28	0	26	1	0
9	T	28	0	26	3	0
9	U	28	0	26	3	0
9	V	28	0	26	2	0
9	W	28	0	26	2	0
9	X	28	0	26	4	0
All	All	97178	0	89490	1978	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 11.

The worst 5 of 1978 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:O:250:ARG:HB2	1:O:363:HIS:HB3	1.60	0.82
1:G:326:SER:HB3	1:G:450:GLN:HE21	1.44	0.81
1:Q:250:ARG:HB2	1:Q:363:HIS:HB3	1.63	0.81
6:F:490:ARG:H	6:F:498:CYS:HB2	1.45	0.81
1:S:326:SER:HB3	1:S:450:GLN:HE21	1.46	0.81

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	G	493/538 (92%)	455 (92%)	38 (8%)	0	100	100
1	H	493/538 (92%)	461 (94%)	32 (6%)	0	100	100
1	I	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	J	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	K	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	L	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	M	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
1	N	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	O	493/538 (92%)	459 (93%)	34 (7%)	0	100	100
1	P	493/538 (92%)	462 (94%)	31 (6%)	0	100	100
1	Q	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	R	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	S	493/538 (92%)	459 (93%)	34 (7%)	0	100	100
1	T	493/538 (92%)	461 (94%)	32 (6%)	0	100	100
1	U	493/538 (92%)	460 (93%)	33 (7%)	0	100	100
1	V	493/538 (92%)	460 (93%)	33 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	493/538 (92%)	458 (93%)	35 (7%)	0	100	100
1	X	493/538 (92%)	457 (93%)	36 (7%)	0	100	100
2	A	1201/1580 (76%)	1136 (95%)	65 (5%)	0	100	100
3	C	501/537 (93%)	481 (96%)	20 (4%)	0	100	100
4	D	648/821 (79%)	603 (93%)	45 (7%)	0	100	100
5	E	161/182 (88%)	160 (99%)	1 (1%)	0	100	100
6	F	492/554 (89%)	472 (96%)	20 (4%)	0	100	100
7	B	668/913 (73%)	642 (96%)	25 (4%)	1 (0%)	48	83
All	All	12545/14271 (88%)	11746 (94%)	798 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	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	G	382/477 (80%)	366 (96%)	16 (4%)	25	46
1	H	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	I	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	J	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	K	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	L	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	M	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	N	385/477 (81%)	372 (97%)	13 (3%)	32	51
1	O	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	P	385/477 (81%)	370 (96%)	15 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	385/477 (81%)	372 (97%)	13 (3%)	32	51
1	R	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	S	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	T	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	U	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	V	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	W	385/477 (81%)	371 (96%)	14 (4%)	30	50
1	X	385/477 (81%)	372 (97%)	13 (3%)	32	51
2	A	1030/1403 (73%)	1012 (98%)	18 (2%)	56	71
3	C	357/473 (76%)	355 (99%)	2 (1%)	84	88
4	D	411/714 (58%)	409 (100%)	2 (0%)	86	89
5	E	131/149 (88%)	129 (98%)	2 (2%)	60	74
6	F	363/466 (78%)	358 (99%)	5 (1%)	62	75
7	B	522/810 (64%)	518 (99%)	4 (1%)	79	84
All	All	9741/12601 (77%)	9456 (97%)	285 (3%)	39	56

5 of 285 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	318	LEU
1	G	99	ASN
2	A	528	ILE
1	T	82	ASN
1	S	494	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 238 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	161	ASN
4	D	282	HIS
1	H	53	ASN
4	D	157	ASN
7	B	100	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

38 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	8,1	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
8	NAG	Y	2	8	14,14,15	0.55	0	17,19,21	0.51	0
8	NAG	Z	1	8,1	14,14,15	0.54	0	17,19,21	0.90	1 (5%)
8	NAG	Z	2	8	14,14,15	0.56	0	17,19,21	0.52	0
8	NAG	a	1	8,1	14,14,15	0.51	0	17,19,21	0.89	1 (5%)
8	NAG	a	2	8	14,14,15	0.56	0	17,19,21	0.53	0
8	NAG	b	1	8,1	14,14,15	0.62	0	17,19,21	0.95	1 (5%)
8	NAG	b	2	8	14,14,15	0.56	0	17,19,21	0.52	0
8	NAG	c	1	8,1	14,14,15	0.61	0	17,19,21	0.96	1 (5%)
8	NAG	c	2	8	14,14,15	0.54	0	17,19,21	0.52	0
8	NAG	d	1	8,1	14,14,15	0.61	0	17,19,21	0.95	1 (5%)
8	NAG	d	2	8	14,14,15	0.53	0	17,19,21	0.54	0
8	NAG	e	1	8,1	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
8	NAG	e	2	8	14,14,15	0.56	0	17,19,21	0.53	0
8	NAG	f	1	8,1	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
8	NAG	f	2	8	14,14,15	0.55	0	17,19,21	0.53	0
8	NAG	g	1	8,1	14,14,15	0.56	0	17,19,21	0.90	1 (5%)
8	NAG	g	2	8	14,14,15	0.54	0	17,19,21	0.53	0
8	NAG	h	1	8,1	14,14,15	0.55	0	17,19,21	0.90	1 (5%)
8	NAG	h	2	8	14,14,15	0.54	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	i	1	8,1	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
8	NAG	i	2	8	14,14,15	0.55	0	17,19,21	0.52	0
8	NAG	j	1	8,1	14,14,15	0.53	0	17,19,21	0.88	1 (5%)
8	NAG	j	2	8	14,14,15	0.51	0	17,19,21	0.53	0
8	NAG	k	1	8,1	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
8	NAG	k	2	8	14,14,15	0.55	0	17,19,21	0.52	0
8	NAG	l	1	8,1	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
8	NAG	l	2	8	14,14,15	0.56	0	17,19,21	0.52	0
8	NAG	m	1	8,1	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
8	NAG	m	2	8	14,14,15	0.56	0	17,19,21	0.52	0
8	NAG	n	1	8,1	14,14,15	0.52	0	17,19,21	0.89	1 (5%)
8	NAG	n	2	8	14,14,15	0.55	0	17,19,21	0.52	0
8	NAG	o	1	8,1	14,14,15	0.53	0	17,19,21	0.89	1 (5%)
8	NAG	o	2	8	14,14,15	0.55	0	17,19,21	0.54	0
8	NAG	p	1	8,1	14,14,15	0.76	1 (7%)	17,19,21	1.04	1 (5%)
8	NAG	p	2	8	14,14,15	0.60	0	17,19,21	0.51	0
8	NAG	q	1	3,8	14,14,15	0.55	0	17,19,21	1.33	2 (11%)
8	NAG	q	2	8	14,14,15	0.27	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
8	NAG	Y	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	NAG	Z	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	2/6/23/26	0/1/1/1
8	NAG	a	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	NAG	c	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	c	2	8	-	2/6/23/26	0/1/1/1
8	NAG	d	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	NAG	e	1	8,1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	NAG	f	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	NAG	g	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
8	NAG	h	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	h	2	8	-	2/6/23/26	0/1/1/1
8	NAG	i	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	i	2	8	-	2/6/23/26	0/1/1/1
8	NAG	j	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	j	2	8	-	2/6/23/26	0/1/1/1
8	NAG	k	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
8	NAG	l	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	l	2	8	-	2/6/23/26	0/1/1/1
8	NAG	m	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	m	2	8	-	2/6/23/26	0/1/1/1
8	NAG	n	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	n	2	8	-	2/6/23/26	0/1/1/1
8	NAG	o	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	o	2	8	-	2/6/23/26	0/1/1/1
8	NAG	p	1	8,1	-	3/6/23/26	0/1/1/1
8	NAG	p	2	8	-	2/6/23/26	0/1/1/1
8	NAG	q	1	3,8	-	5/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	p	1	NAG	C1-C2	2.02	1.55	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	q	1	NAG	C2-N2-C7	4.34	129.09	122.90
8	p	1	NAG	C1-O5-C5	3.44	116.86	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	c	1	NAG	C1-O5-C5	3.06	116.34	112.19
8	d	1	NAG	C1-O5-C5	3.01	116.27	112.19
8	b	1	NAG	C1-O5-C5	3.00	116.26	112.19

There are no chirality outliers.

5 of 97 torsion outliers are listed below:

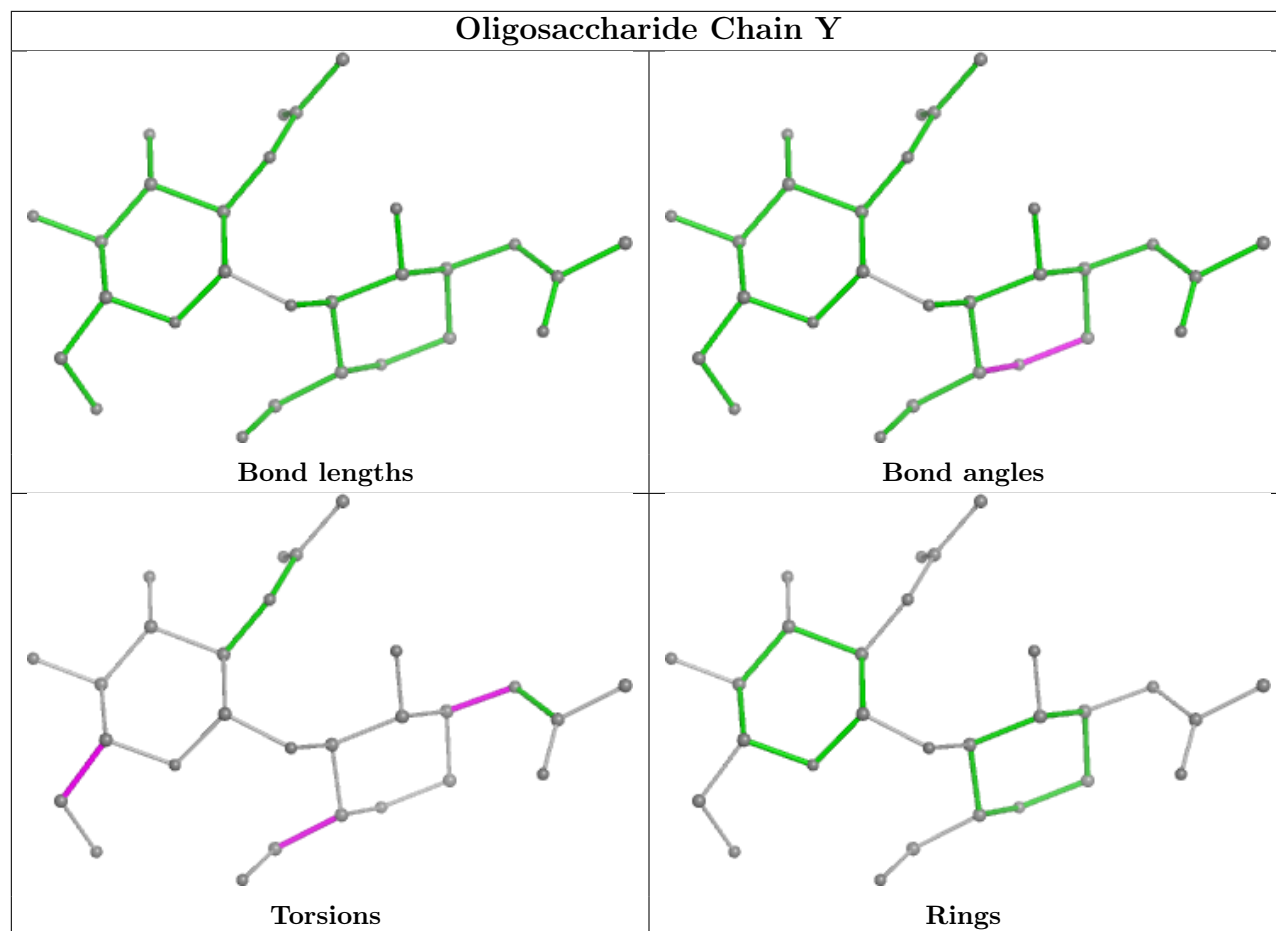
Mol	Chain	Res	Type	Atoms
8	p	2	NAG	O5-C5-C6-O6
8	q	2	NAG	O5-C5-C6-O6
8	h	1	NAG	O5-C5-C6-O6
8	p	1	NAG	O5-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6

There are no ring outliers.

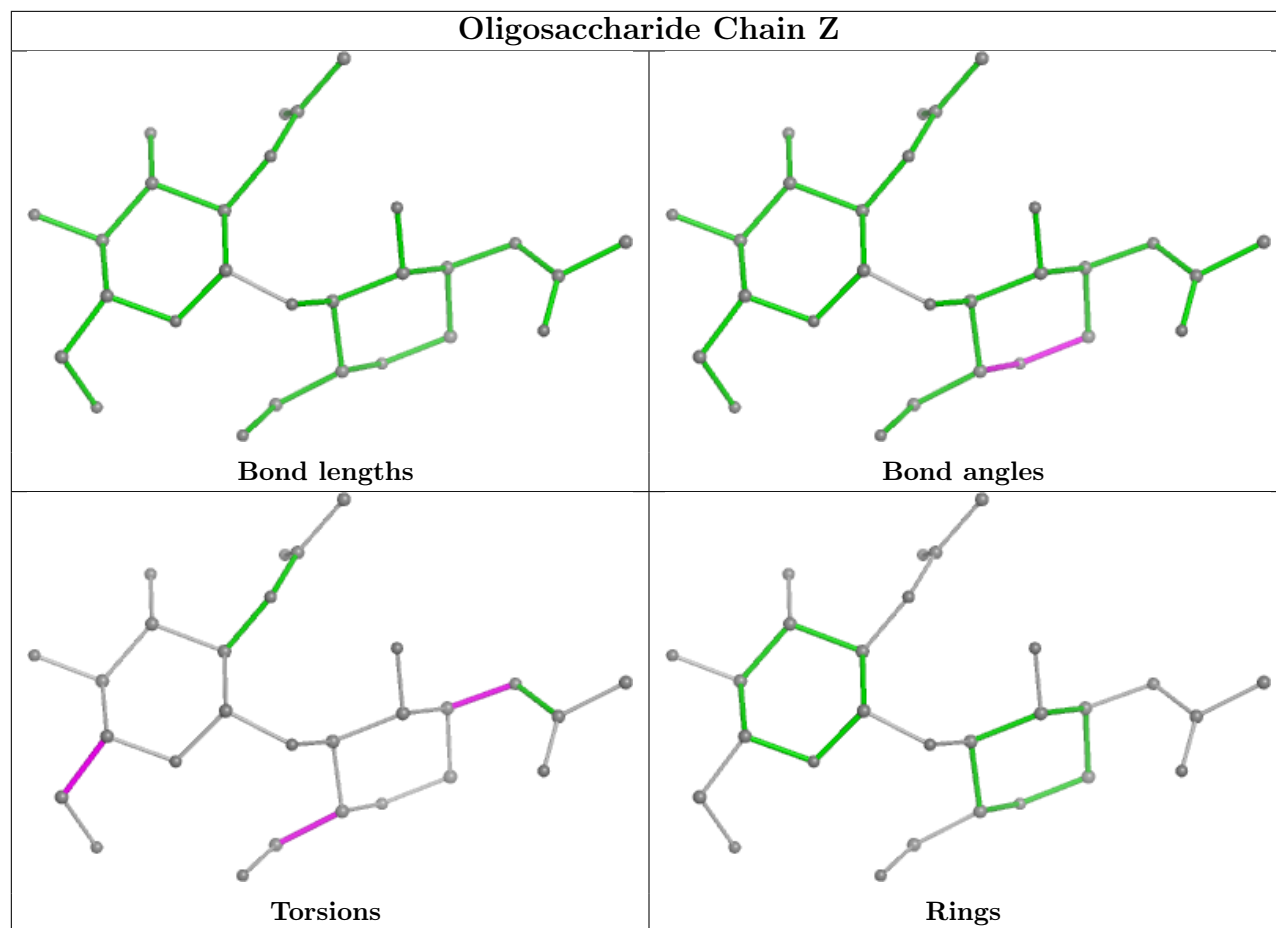
4 monomers are involved in 4 short contacts:

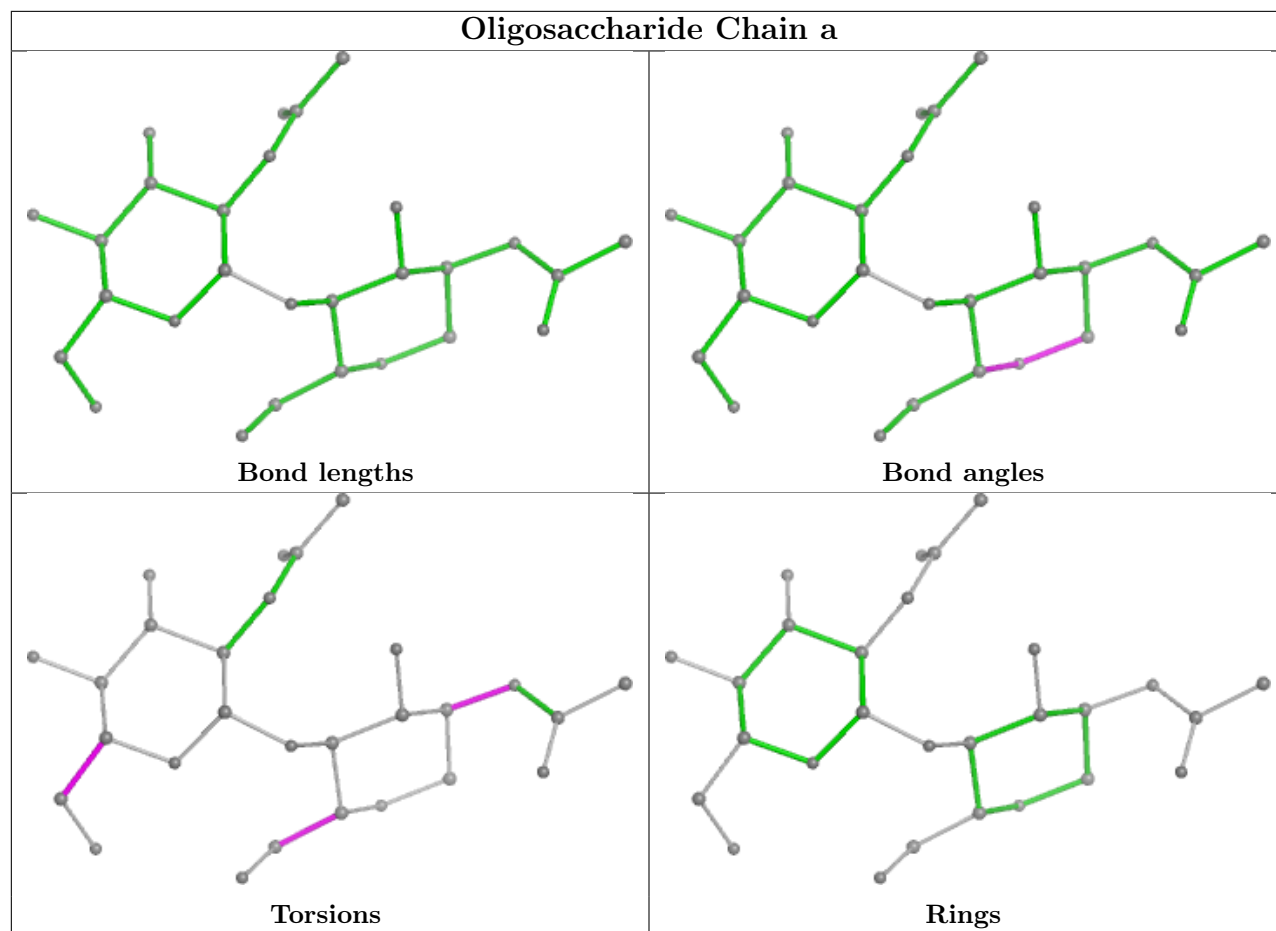
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Y	2	NAG	1	0
8	Z	1	NAG	2	0
8	Y	1	NAG	2	0
8	Z	2	NAG	1	0

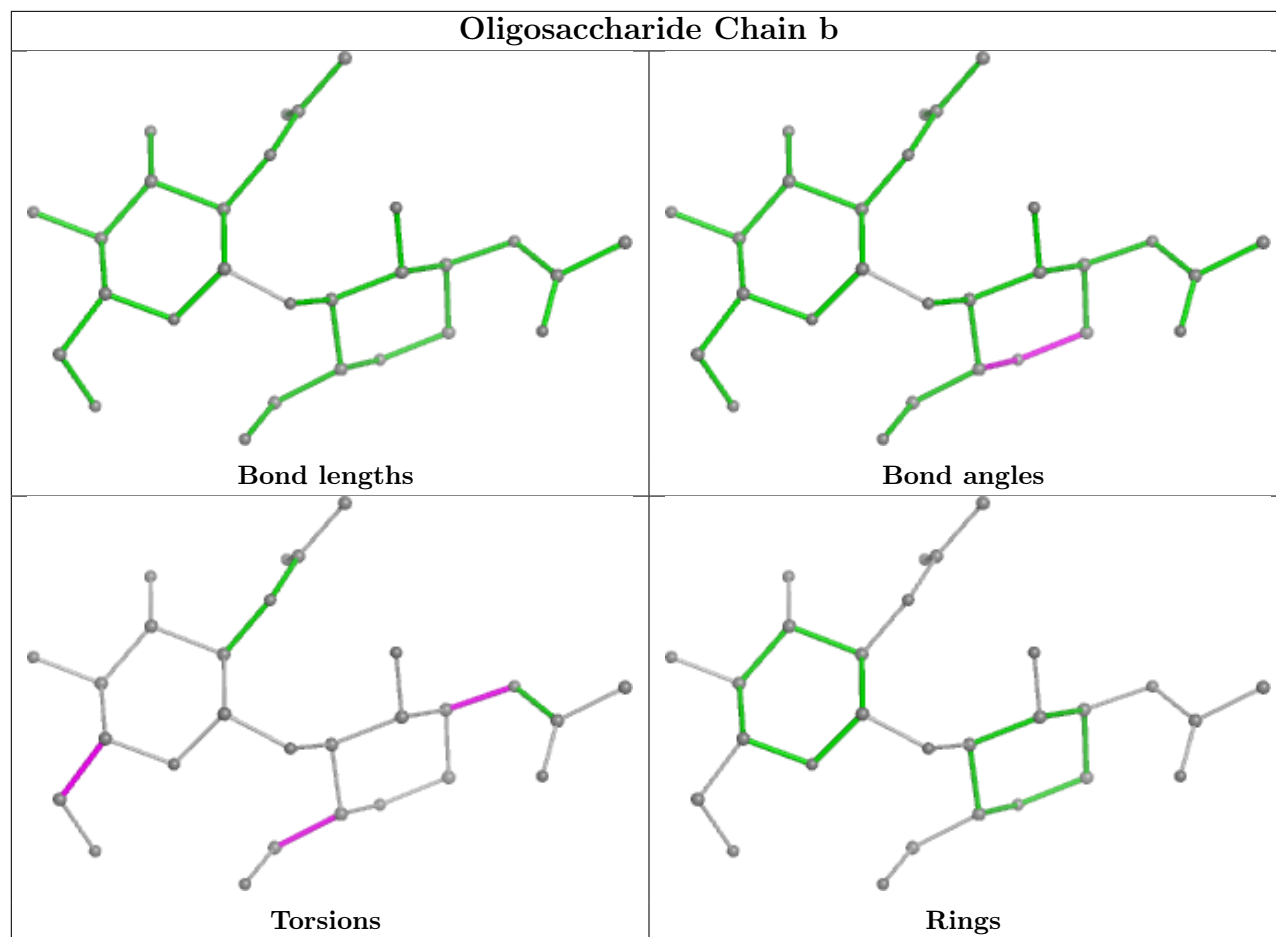
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

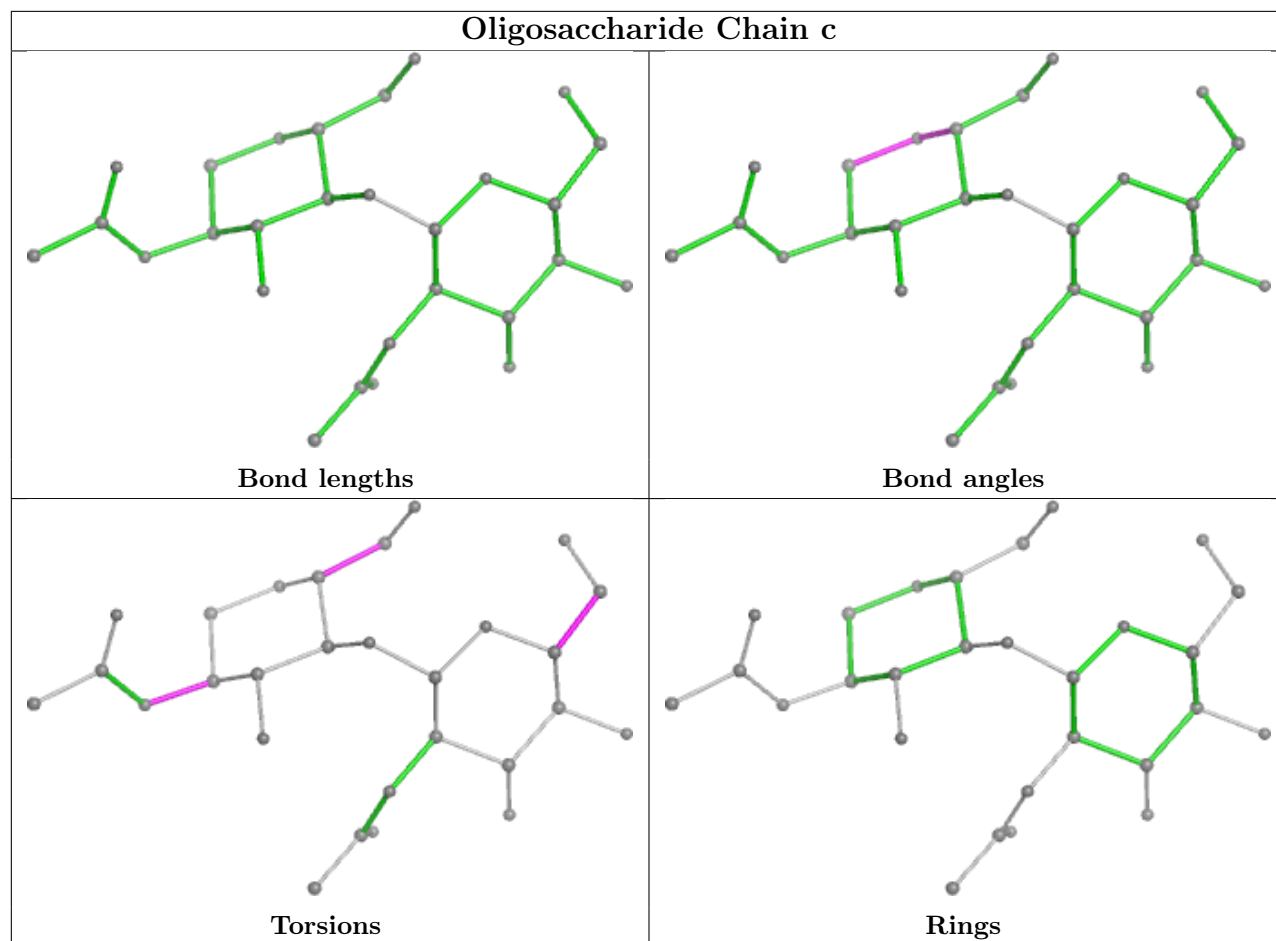


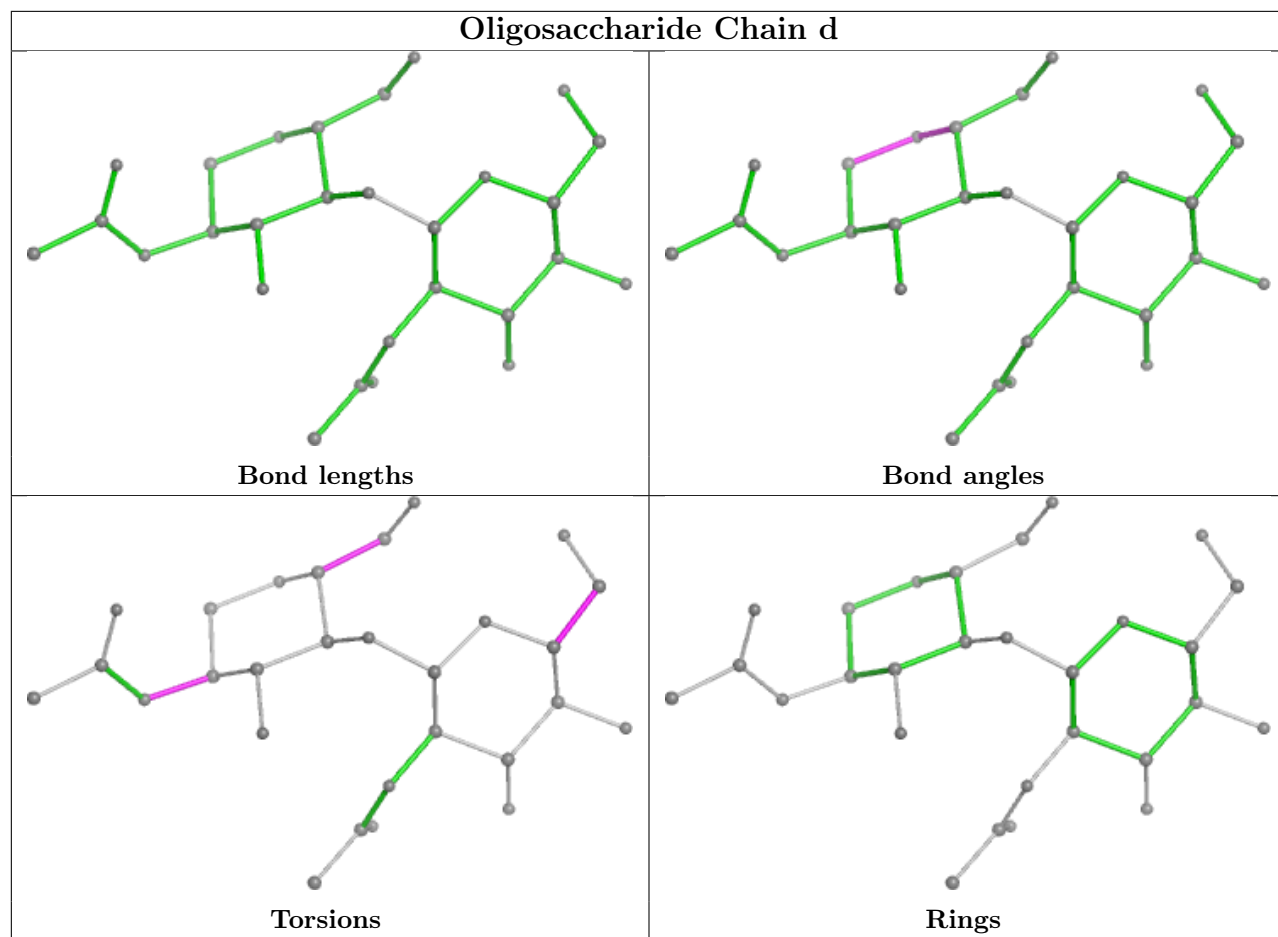


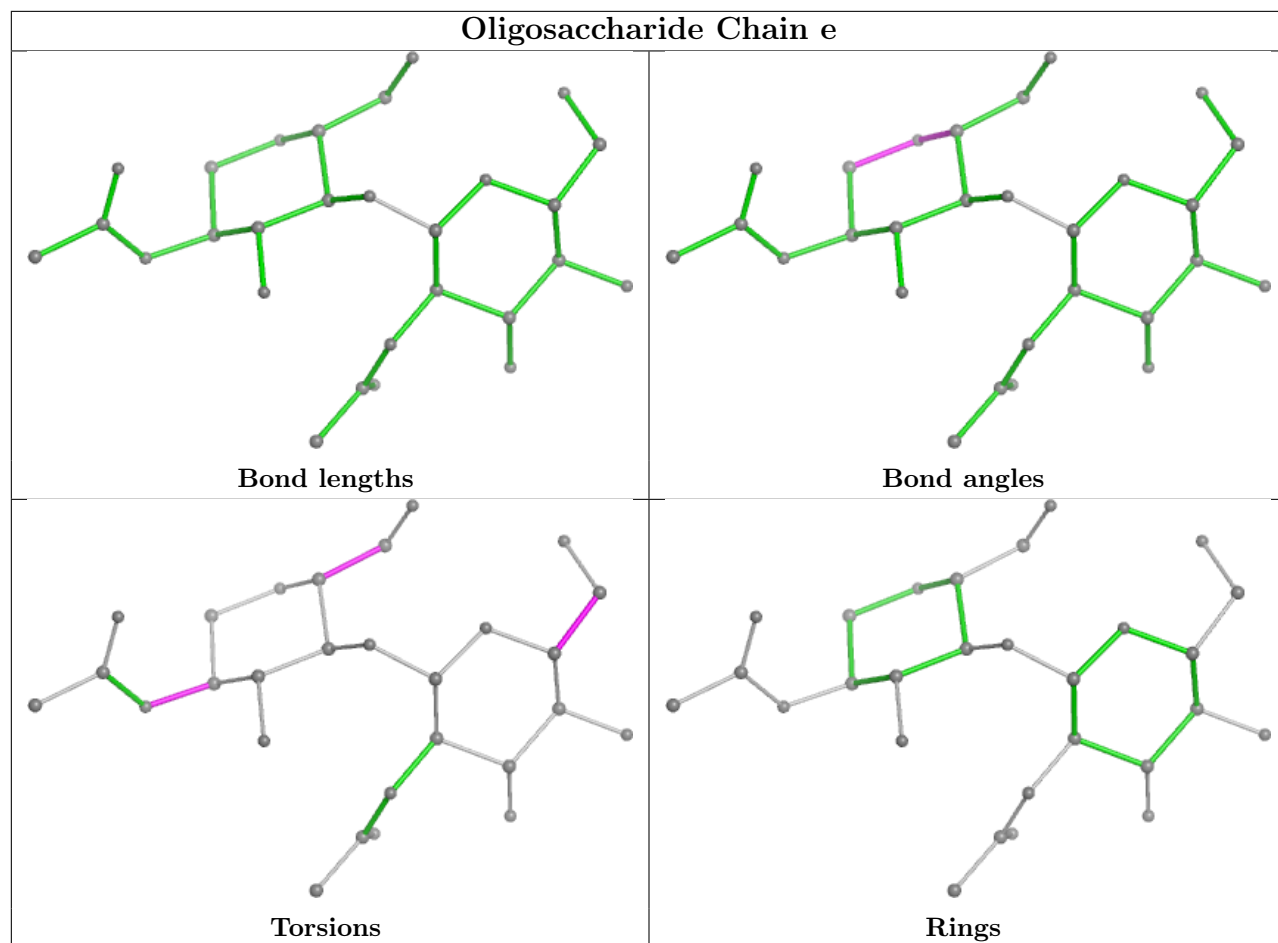


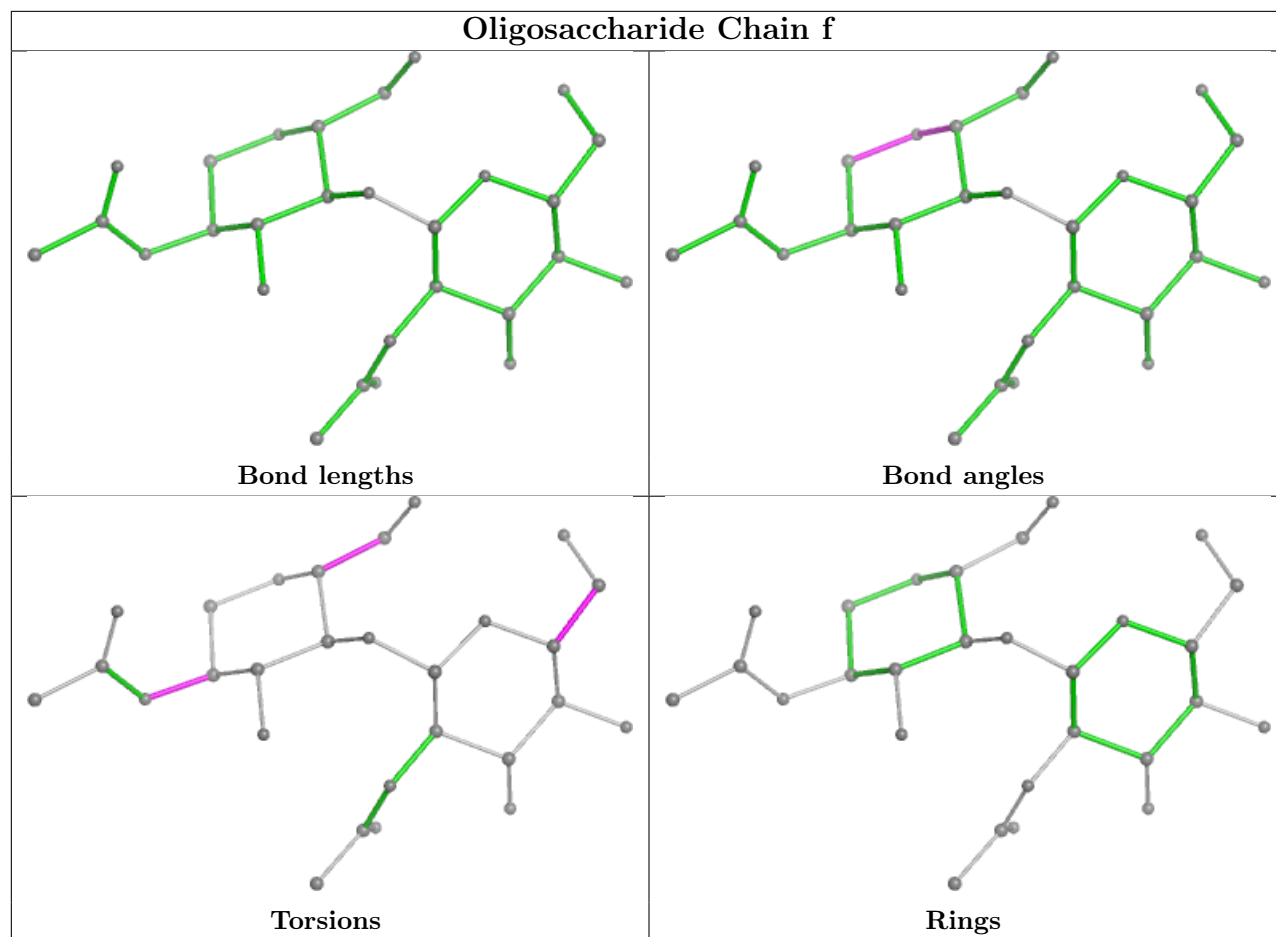


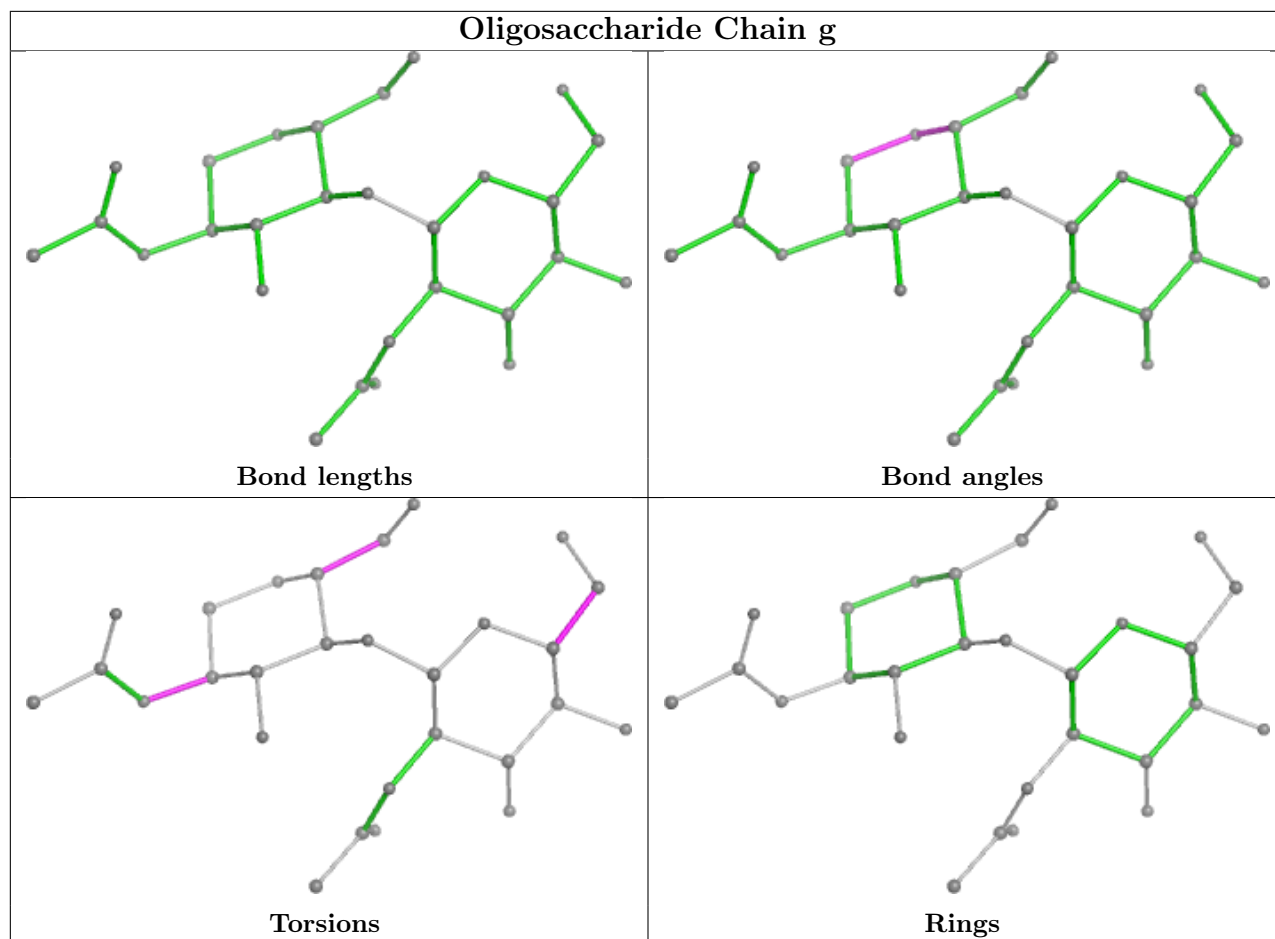




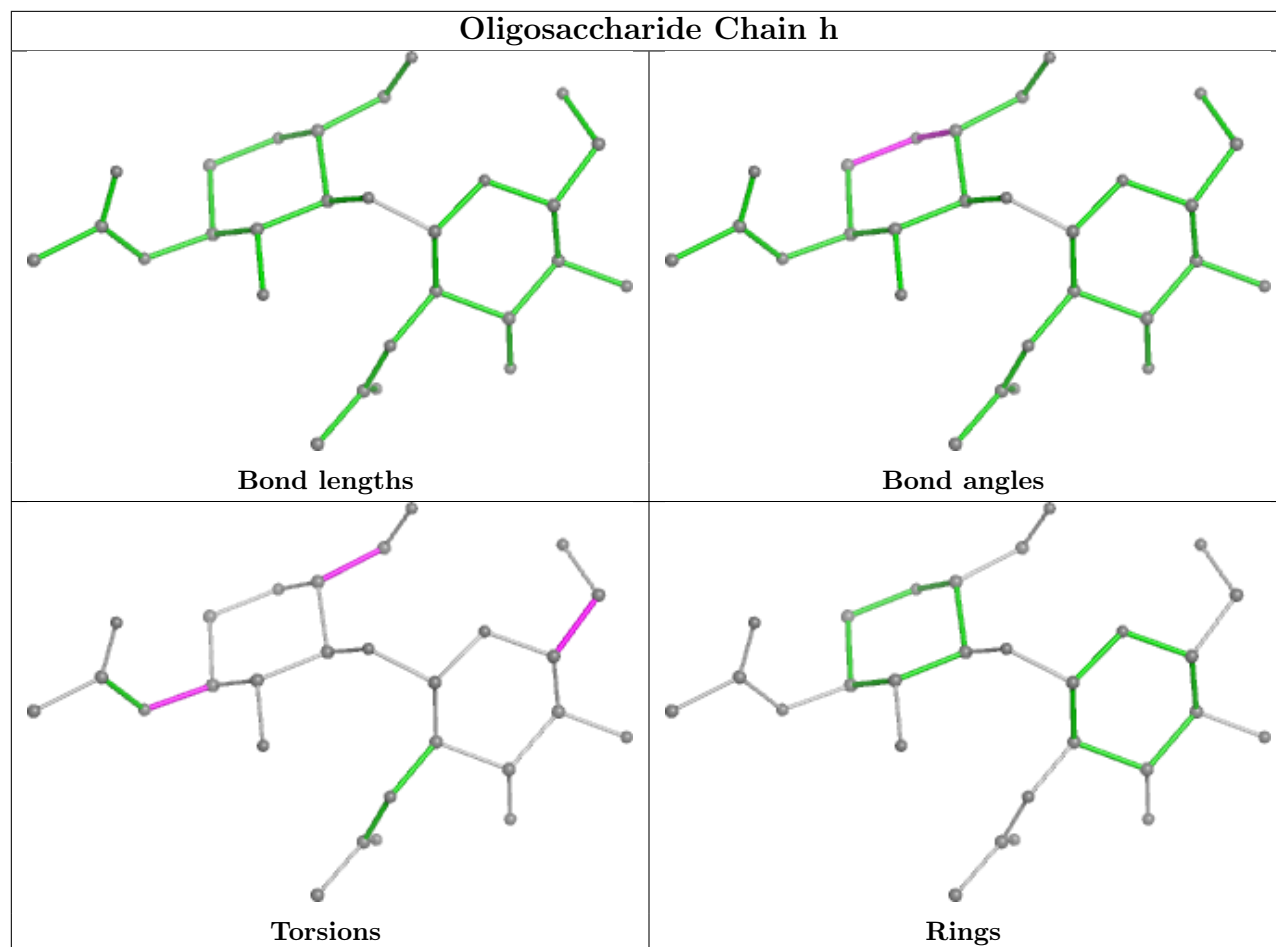


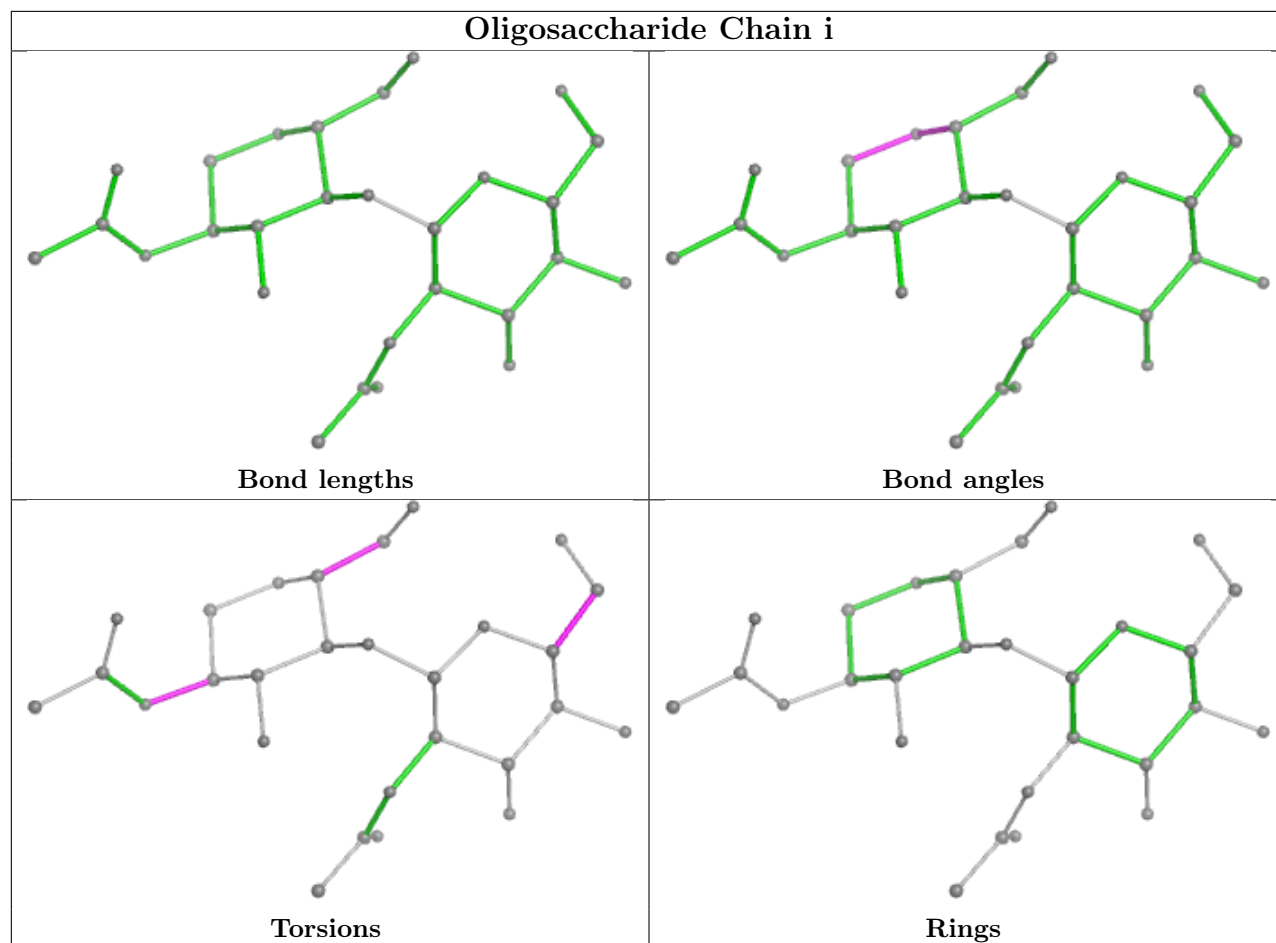


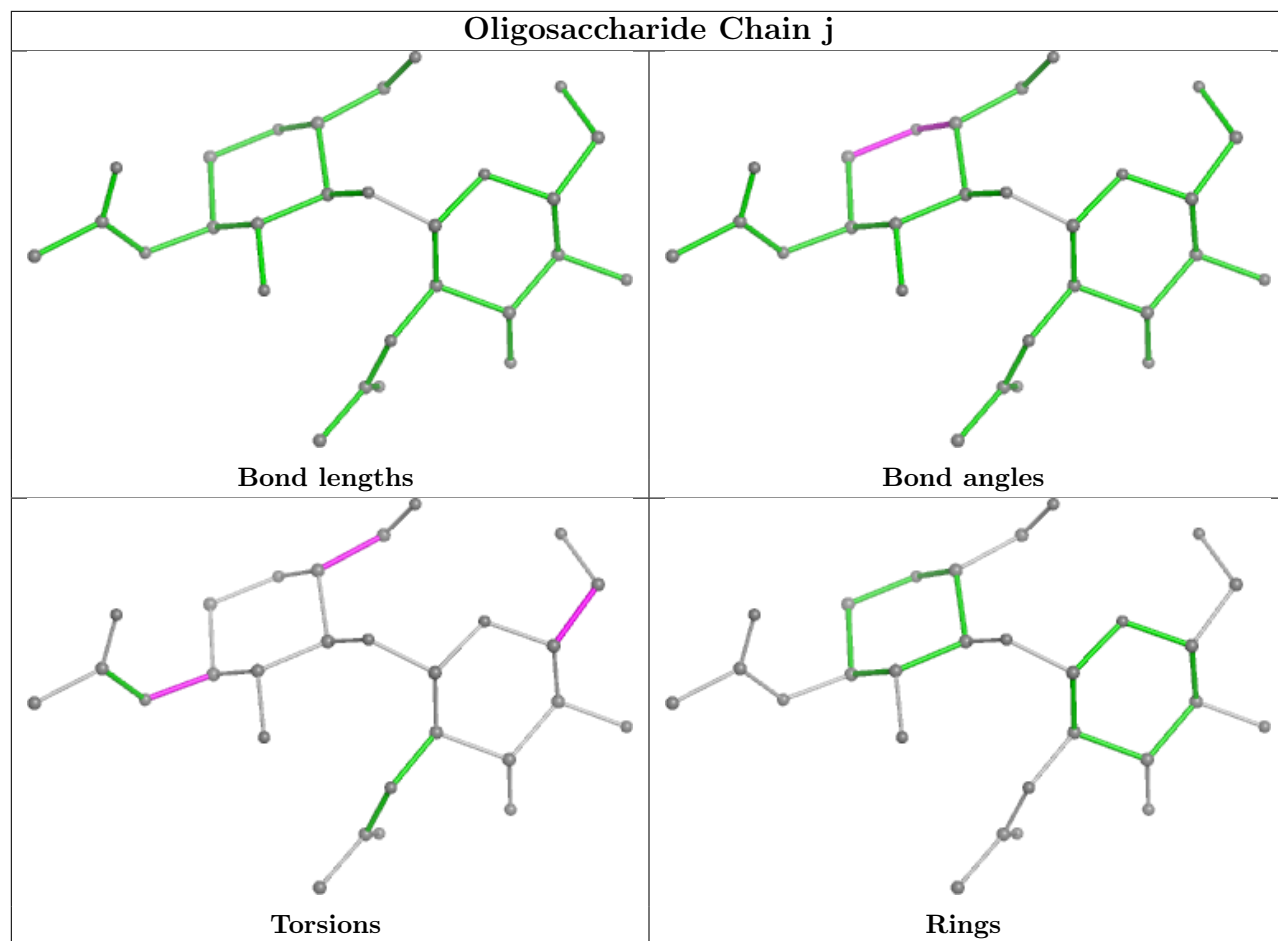


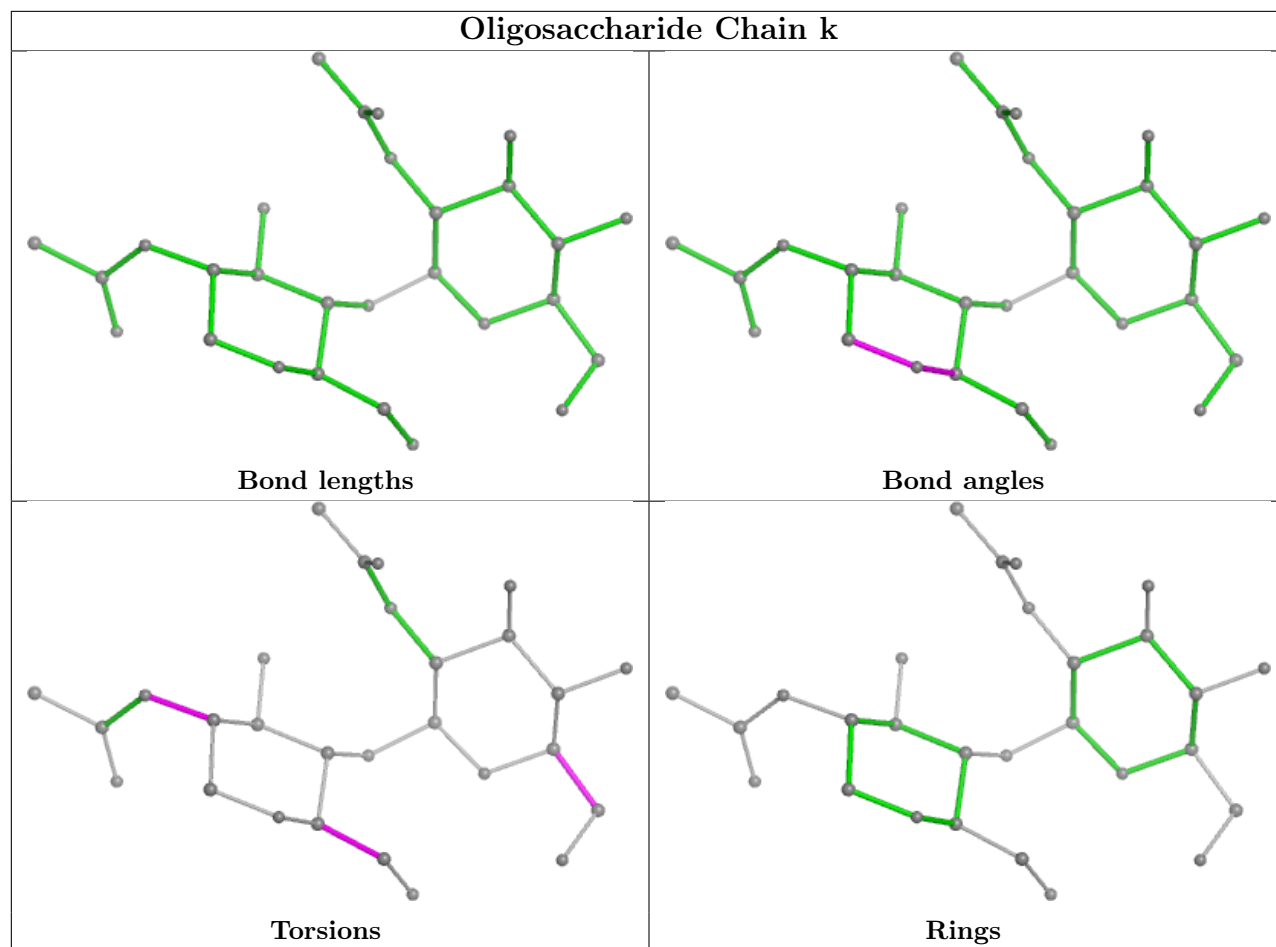


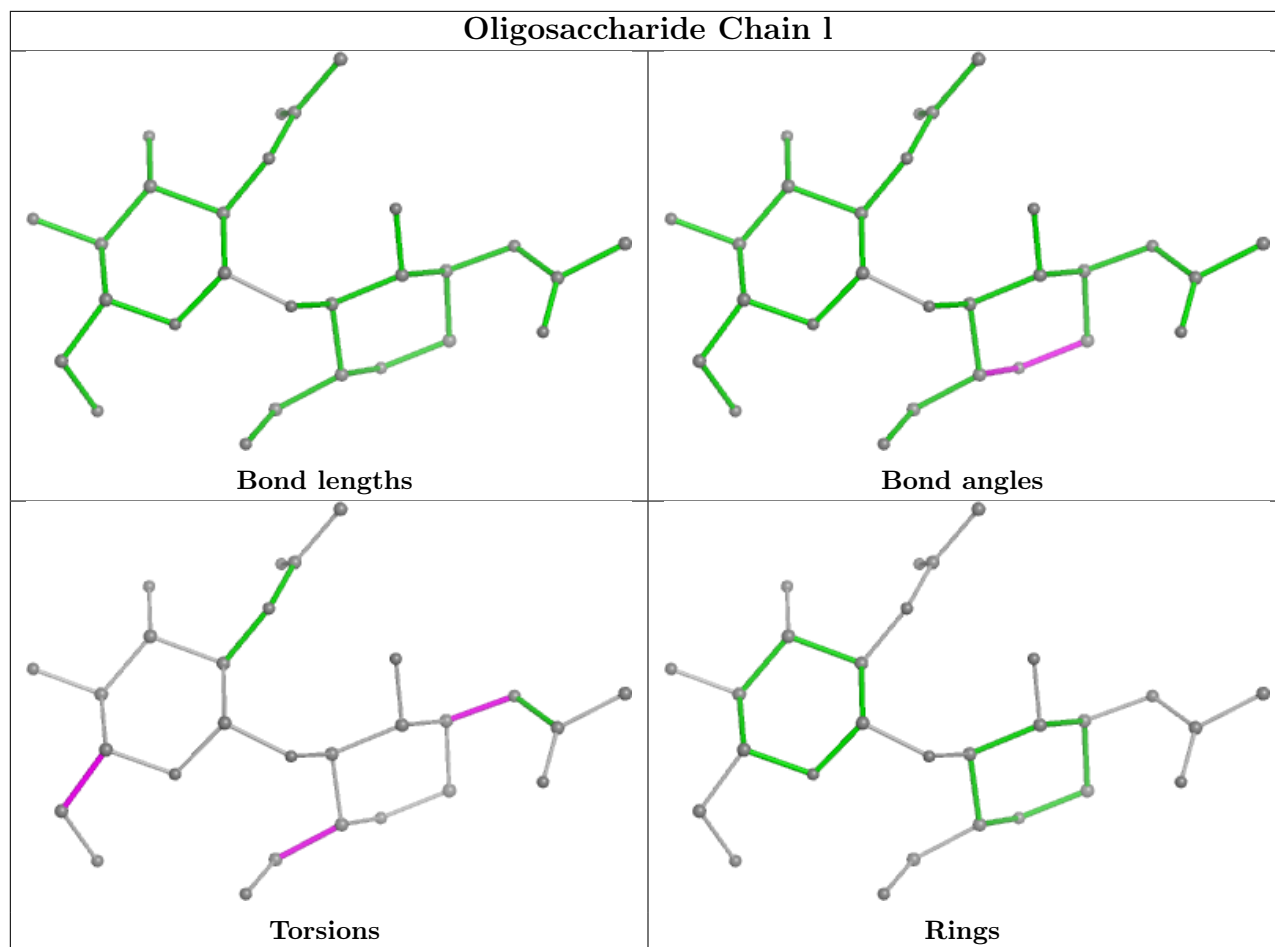


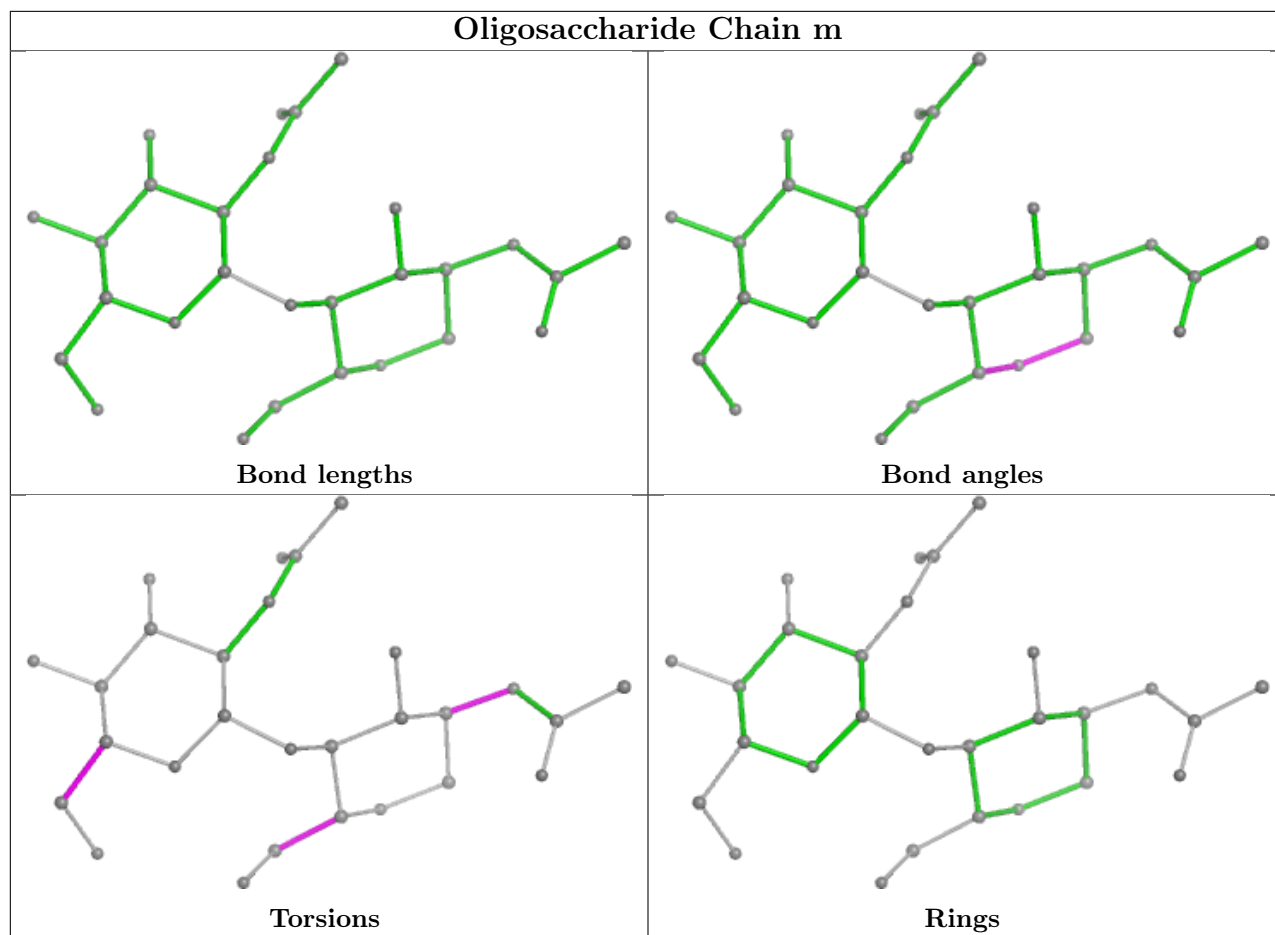


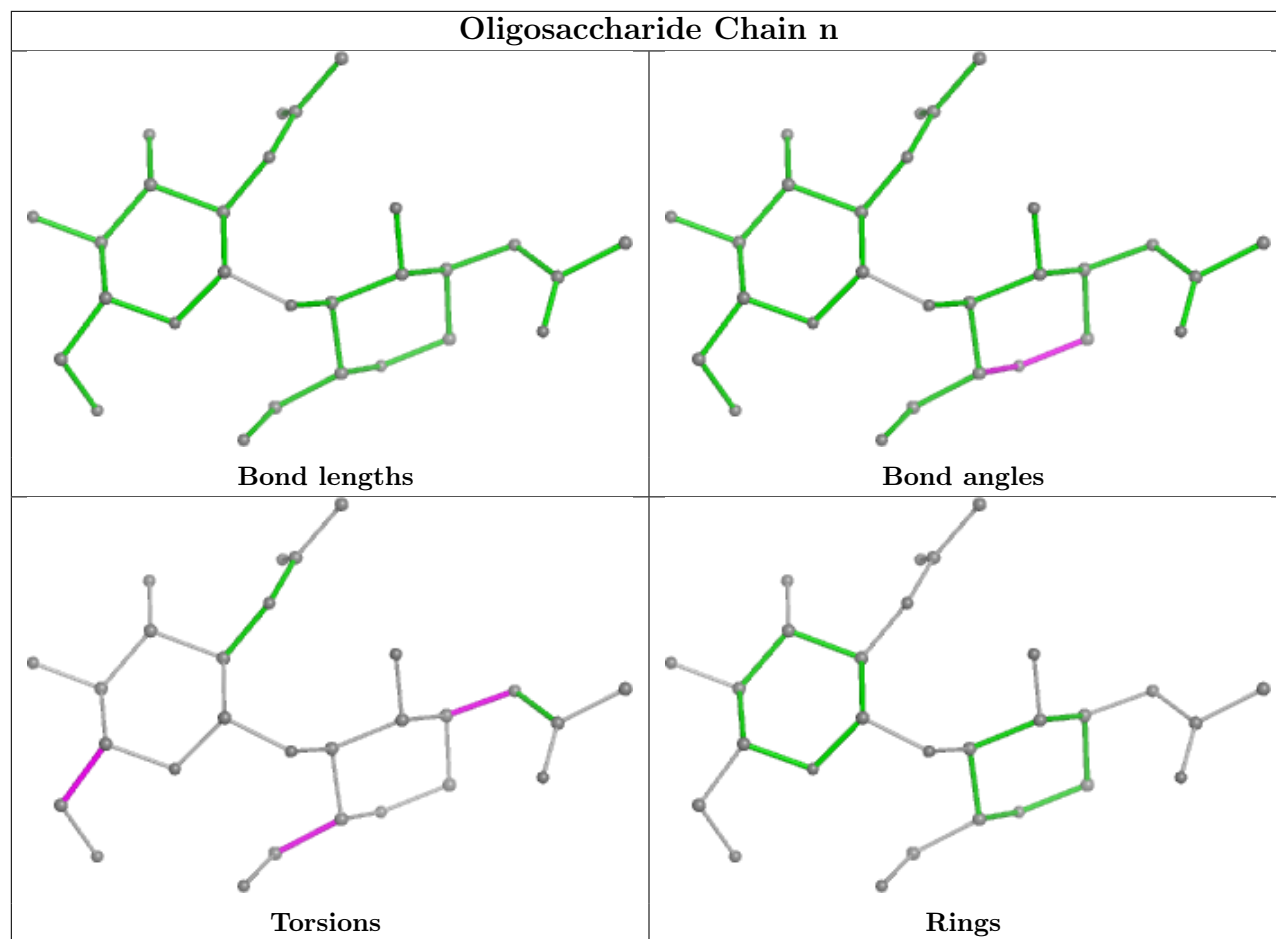


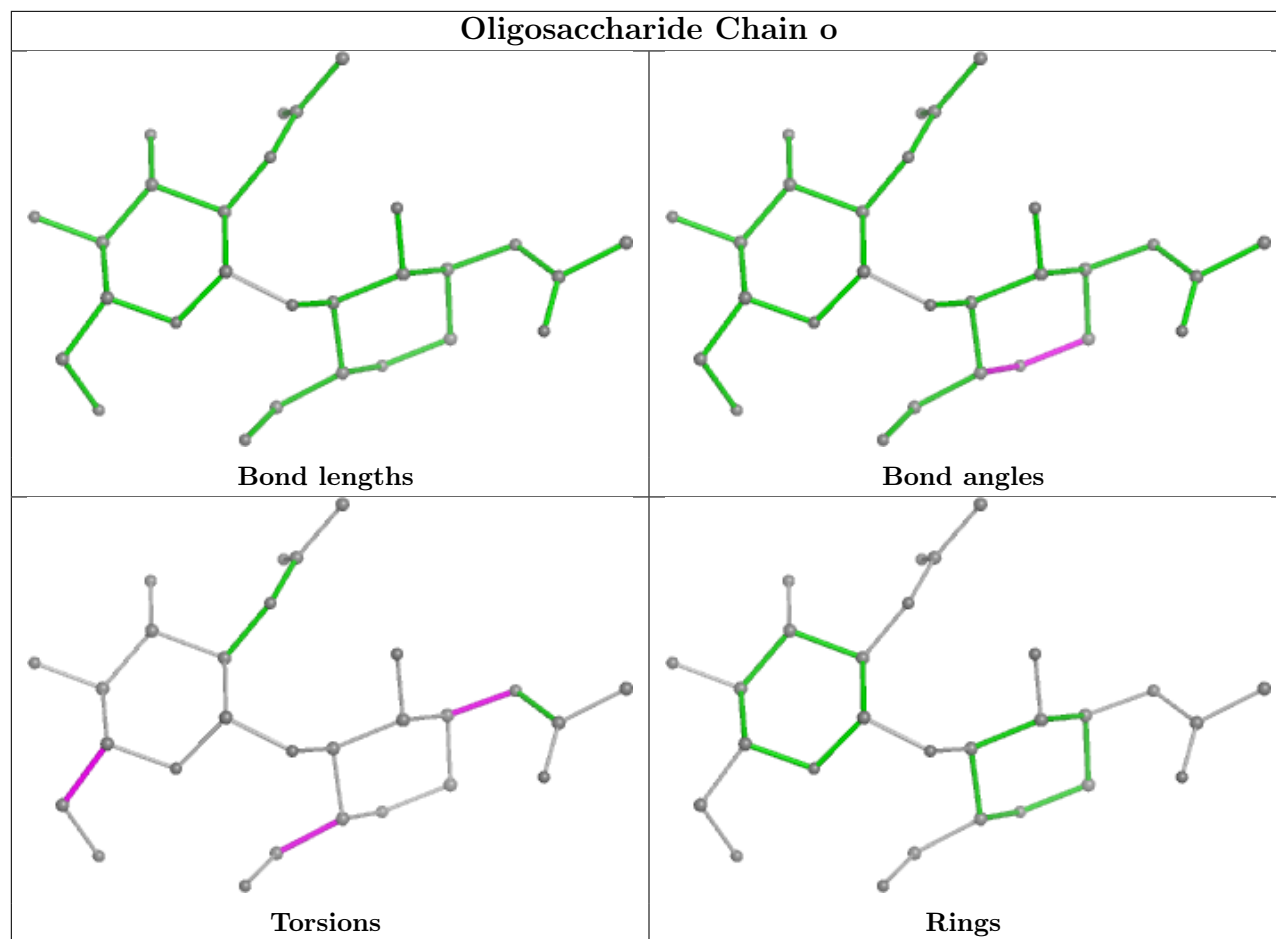




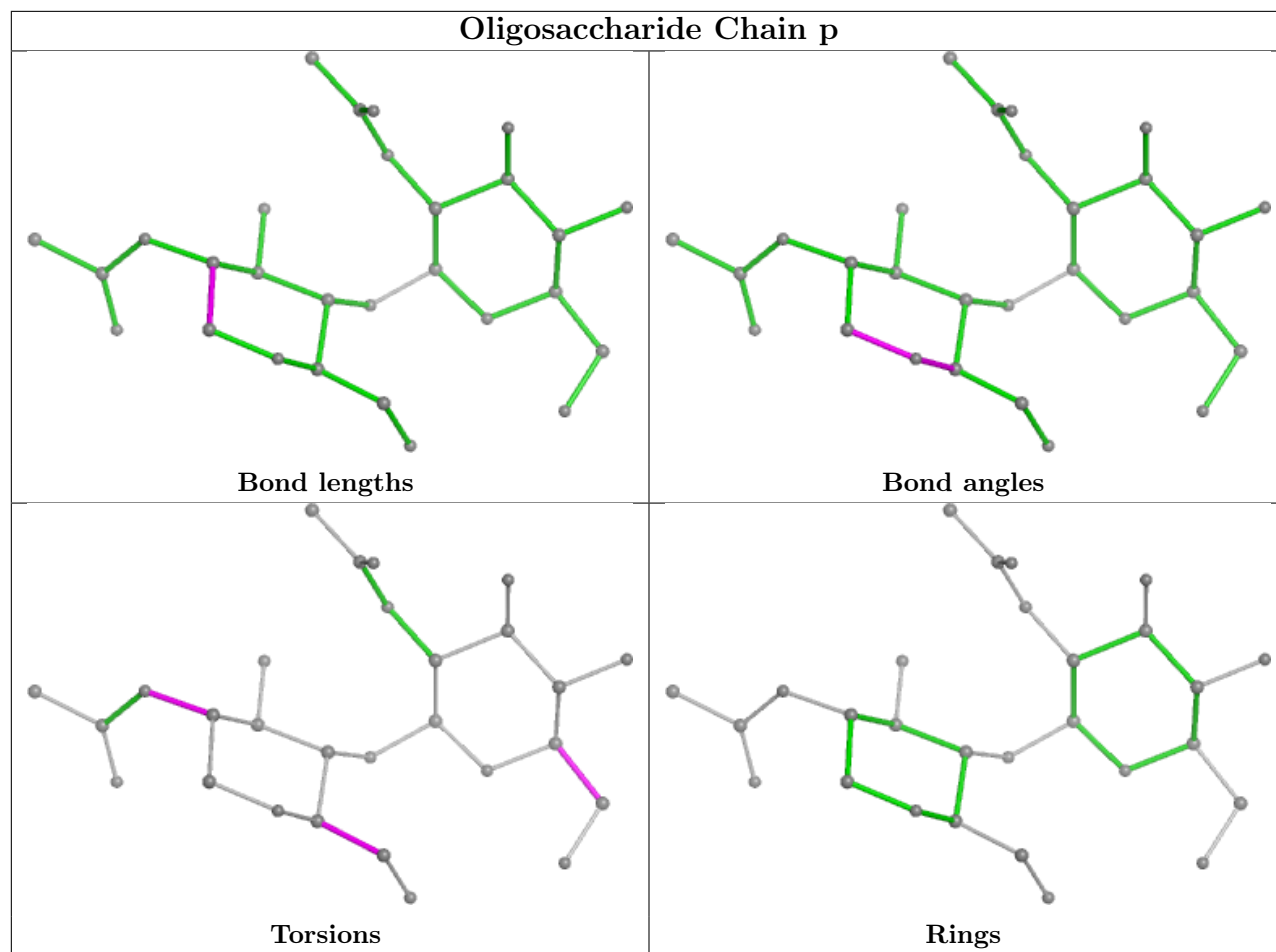


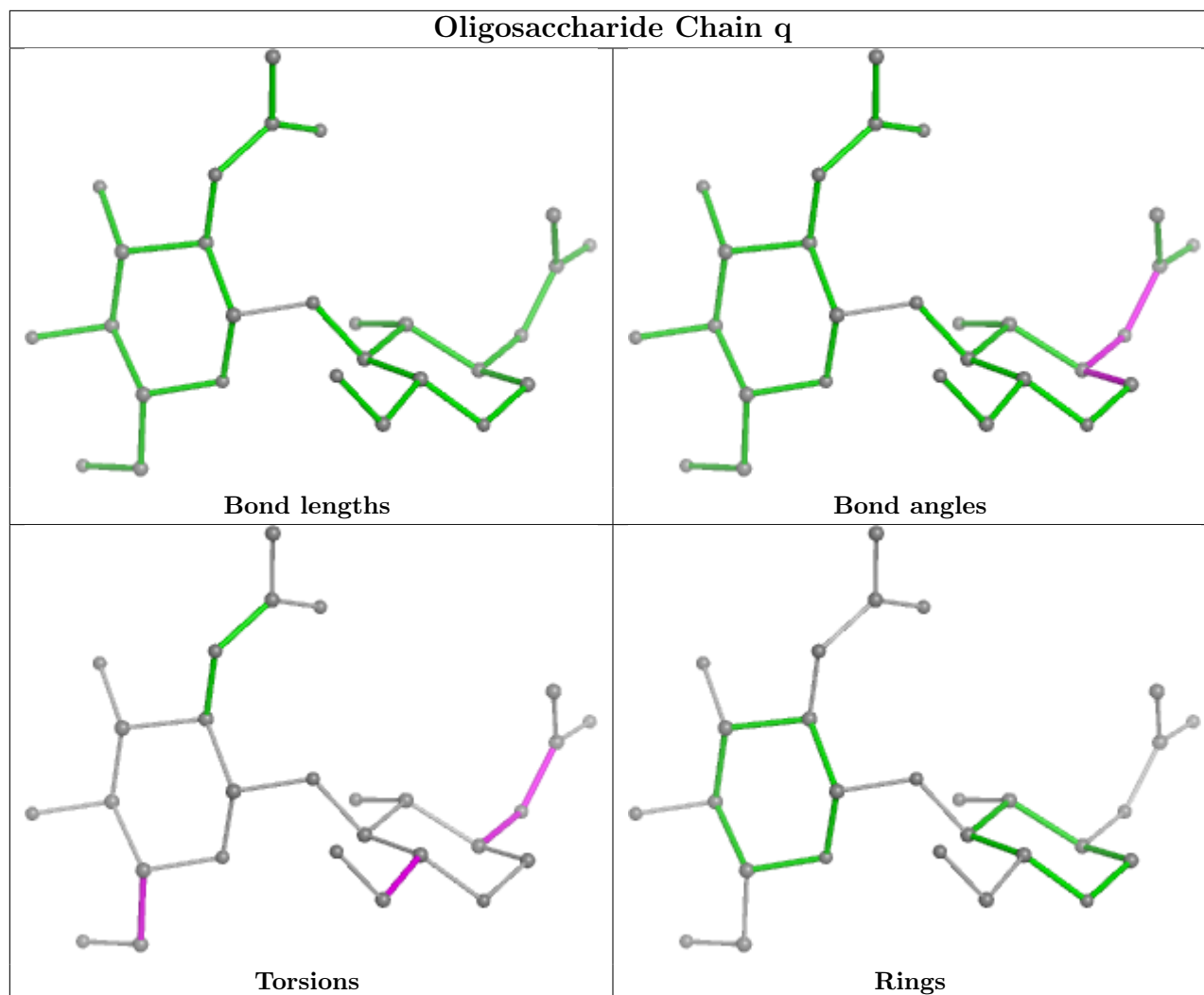












## 5.6 Ligand geometry [i](#)

38 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	$\# Z  > 2$
9	NAG	O	603	1	14,14,15	0.30	0	17,19,21	0.47	0
9	NAG	W	603	1	14,14,15	0.27	0	17,19,21	0.42	0
9	NAG	B	1001	7	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
9	NAG	J	603	1	14,14,15	0.55	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	U	603	1	14,14,15	0.57	0	17,19,21	0.42	0
9	NAG	K	604	1	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
9	NAG	U	604	1	14,14,15	0.53	0	17,19,21	1.23	1 (5%)
9	NAG	O	604	1	14,14,15	0.56	0	17,19,21	1.28	1 (5%)
9	NAG	X	603	1	14,14,15	0.69	0	17,19,21	0.43	0
9	NAG	Q	604	1	14,14,15	0.58	0	17,19,21	1.28	1 (5%)
9	NAG	T	604	1	14,14,15	0.52	0	17,19,21	1.22	1 (5%)
9	NAG	P	603	1	14,14,15	0.39	0	17,19,21	0.45	0
9	NAG	V	603	1	14,14,15	0.27	0	17,19,21	0.46	0
9	NAG	R	604	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
9	NAG	D	901	4	14,14,15	0.36	0	17,19,21	0.46	0
9	NAG	L	604	1	14,14,15	0.53	0	17,19,21	1.27	1 (5%)
9	NAG	W	604	1	14,14,15	0.51	0	17,19,21	1.23	1 (5%)
9	NAG	H	604	1	14,14,15	0.51	0	17,19,21	1.25	1 (5%)
9	NAG	M	604	1	14,14,15	0.56	0	17,19,21	1.27	1 (5%)
9	NAG	R	603	1	14,14,15	0.20	0	17,19,21	0.41	0
9	NAG	S	604	1	14,14,15	0.55	0	17,19,21	1.28	1 (5%)
9	NAG	P	604	1	14,14,15	0.51	0	17,19,21	1.22	1 (5%)
9	NAG	X	604	1	14,14,15	0.53	0	17,19,21	1.25	1 (5%)
9	NAG	N	604	1	14,14,15	0.64	1 (7%)	17,19,21	1.29	2 (11%)
9	NAG	L	603	1	14,14,15	0.32	0	17,19,21	0.48	0
9	NAG	I	604	1	14,14,15	0.50	0	17,19,21	1.24	1 (5%)
9	NAG	J	604	1	14,14,15	0.53	0	17,19,21	1.22	1 (5%)
9	NAG	M	603	1	14,14,15	0.28	0	17,19,21	0.45	0
9	NAG	Q	603	1	14,14,15	0.22	0	17,19,21	0.42	0
9	NAG	V	604	1	14,14,15	0.50	0	17,19,21	1.23	1 (5%)
9	NAG	T	603	1	14,14,15	0.24	0	17,19,21	0.35	0
9	NAG	G	603	1	14,14,15	0.51	0	17,19,21	0.64	0
9	NAG	K	603	1	14,14,15	0.29	0	17,19,21	0.43	0
9	NAG	N	603	1	14,14,15	0.24	0	17,19,21	0.36	0
9	NAG	I	603	1	14,14,15	0.32	0	17,19,21	0.45	0
9	NAG	S	603	1	14,14,15	0.22	0	17,19,21	0.37	0
9	NAG	G	604	1	14,14,15	0.54	0	17,19,21	1.29	1 (5%)
9	NAG	H	603	1	14,14,15	0.32	0	17,19,21	0.45	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
9	NAG	O	603	1	-	0/6/23/26	0/1/1/1
9	NAG	W	603	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1001	7	-	4/6/23/26	0/1/1/1
9	NAG	J	603	1	-	2/6/23/26	0/1/1/1
9	NAG	U	603	1	-	2/6/23/26	0/1/1/1
9	NAG	K	604	1	-	5/6/23/26	0/1/1/1
9	NAG	U	604	1	-	5/6/23/26	0/1/1/1
9	NAG	O	604	1	-	3/6/23/26	0/1/1/1
9	NAG	X	603	1	-	3/6/23/26	0/1/1/1
9	NAG	Q	604	1	-	3/6/23/26	0/1/1/1
9	NAG	T	604	1	-	4/6/23/26	0/1/1/1
9	NAG	P	603	1	-	0/6/23/26	0/1/1/1
9	NAG	V	603	1	-	0/6/23/26	0/1/1/1
9	NAG	R	604	1	-	3/6/23/26	0/1/1/1
9	NAG	D	901	4	-	4/6/23/26	0/1/1/1
9	NAG	L	604	1	-	5/6/23/26	0/1/1/1
9	NAG	W	604	1	-	5/6/23/26	0/1/1/1
9	NAG	H	604	1	-	5/6/23/26	0/1/1/1
9	NAG	M	604	1	-	5/6/23/26	0/1/1/1
9	NAG	R	603	1	-	2/6/23/26	0/1/1/1
9	NAG	S	604	1	-	3/6/23/26	0/1/1/1
9	NAG	P	604	1	-	5/6/23/26	0/1/1/1
9	NAG	X	604	1	-	5/6/23/26	0/1/1/1
9	NAG	N	604	1	-	3/6/23/26	0/1/1/1
9	NAG	L	603	1	-	1/6/23/26	0/1/1/1
9	NAG	I	604	1	-	5/6/23/26	0/1/1/1
9	NAG	J	604	1	-	5/6/23/26	0/1/1/1
9	NAG	M	603	1	-	0/6/23/26	0/1/1/1
9	NAG	Q	603	1	-	2/6/23/26	0/1/1/1
9	NAG	V	604	1	-	5/6/23/26	0/1/1/1
9	NAG	T	603	1	-	2/6/23/26	0/1/1/1
9	NAG	G	603	1	-	0/6/23/26	0/1/1/1
9	NAG	K	603	1	-	1/6/23/26	0/1/1/1
9	NAG	N	603	1	-	2/6/23/26	0/1/1/1
9	NAG	I	603	1	-	0/6/23/26	0/1/1/1
9	NAG	S	603	1	-	2/6/23/26	0/1/1/1
9	NAG	G	604	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	H	603	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	N	604	NAG	C1-C2	2.11	1.55	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	604	NAG	C2-N2-C7	4.32	129.05	122.90
9	U	604	NAG	C2-N2-C7	4.31	129.04	122.90
9	H	604	NAG	C2-N2-C7	4.30	129.03	122.90
9	W	604	NAG	C2-N2-C7	4.29	129.01	122.90
9	P	604	NAG	C2-N2-C7	4.28	129.00	122.90

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	S	603	NAG	C4-C5-C6-O6
9	N	603	NAG	C4-C5-C6-O6
9	Q	603	NAG	C4-C5-C6-O6
9	T	603	NAG	C4-C5-C6-O6
9	R	603	NAG	C4-C5-C6-O6

There are no ring outliers.

34 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	603	NAG	1	0
9	B	1001	NAG	1	0
9	J	603	NAG	1	0
9	U	603	NAG	2	0
9	K	604	NAG	1	0
9	U	604	NAG	1	0
9	O	604	NAG	1	0
9	X	603	NAG	3	0
9	Q	604	NAG	1	0
9	T	604	NAG	2	0
9	V	603	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	604	NAG	1	0
9	D	901	NAG	1	0
9	L	604	NAG	1	0
9	W	604	NAG	1	0
9	H	604	NAG	1	0
9	M	604	NAG	1	0
9	R	603	NAG	1	0
9	S	604	NAG	1	0
9	P	604	NAG	1	0
9	X	604	NAG	1	0
9	N	604	NAG	1	0
9	L	603	NAG	1	0
9	I	604	NAG	1	0
9	J	604	NAG	1	0
9	M	603	NAG	1	0
9	Q	603	NAG	1	0
9	V	604	NAG	1	0
9	T	603	NAG	1	0
9	K	603	NAG	1	0
9	N	603	NAG	1	0
9	I	603	NAG	2	0
9	G	604	NAG	2	0
9	H	603	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	3
6	F	3
1	G	2
1	X	2
1	W	2
1	T	2
1	U	2
1	V	2

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Mol	Chain	Number of breaks
1	P	2
1	H	2
1	M	2
1	Q	2
1	O	2
1	R	2
1	N	2
1	S	2
1	J	2
1	K	2
1	L	2
7	B	2
1	I	2
3	C	2

The worst 5 of 46 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	370:PHE	C	371:SER	N	7.60
1	X	370:PHE	C	371:SER	N	7.54
1	W	370:PHE	C	371:SER	N	7.35
1	T	370:PHE	C	371:SER	N	7.33
1	U	370:PHE	C	371:SER	N	7.32

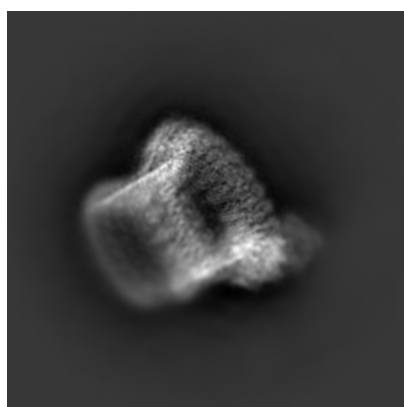
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0107. These allow visual inspection of the internal detail of the map and identification of artifacts.

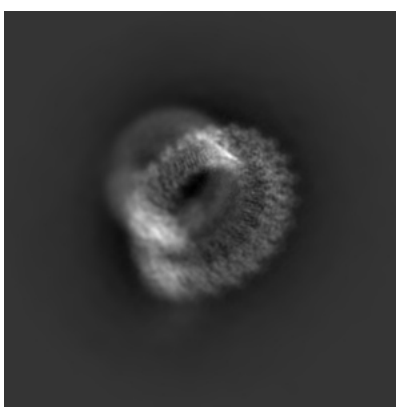
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

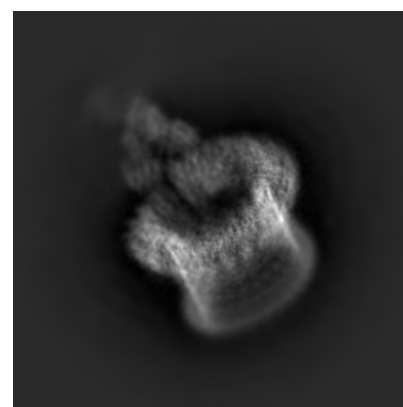
#### 6.1.1 Primary map



X



Y



Z

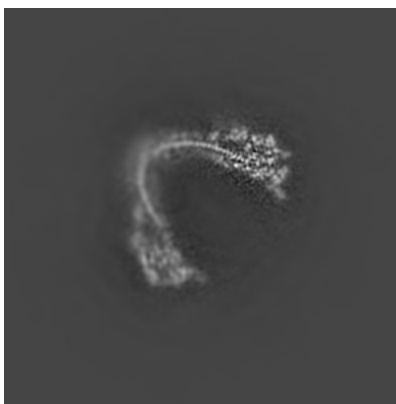
The images above show the map projected in three orthogonal directions.

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

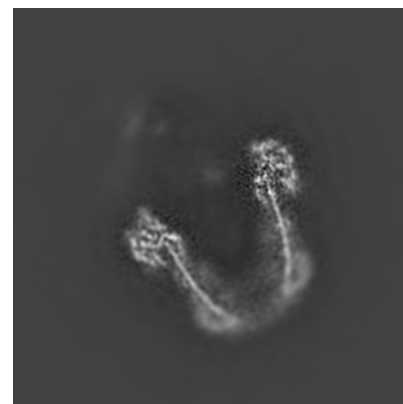
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



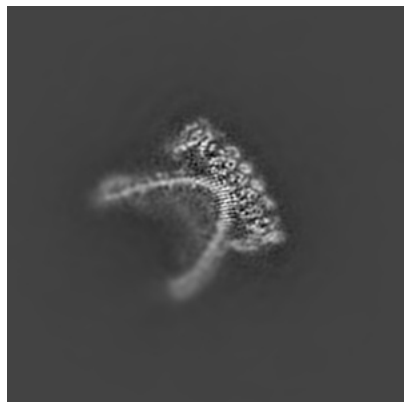
Z Index: 180



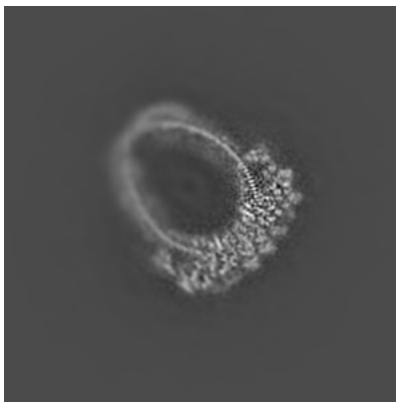
The images above show central slices of the map in three orthogonal directions.

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

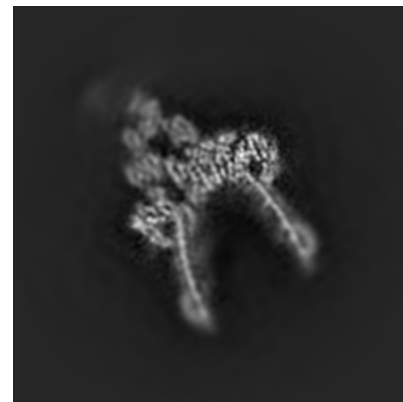
### 6.3.1 Primary map



X Index: 230



Y Index: 150

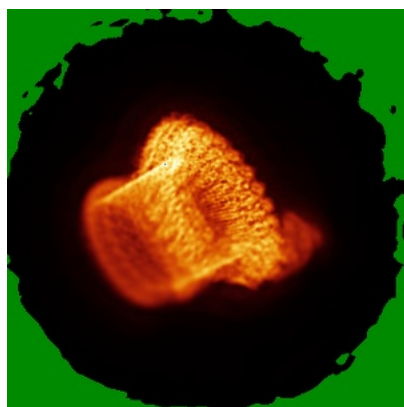


Z Index: 145

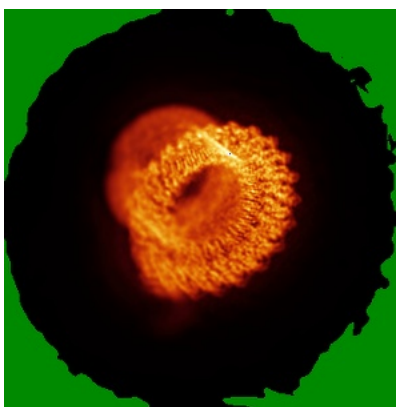
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

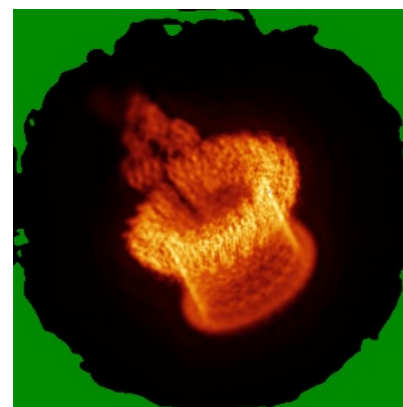
### 6.4.1 Primary map



X



Y

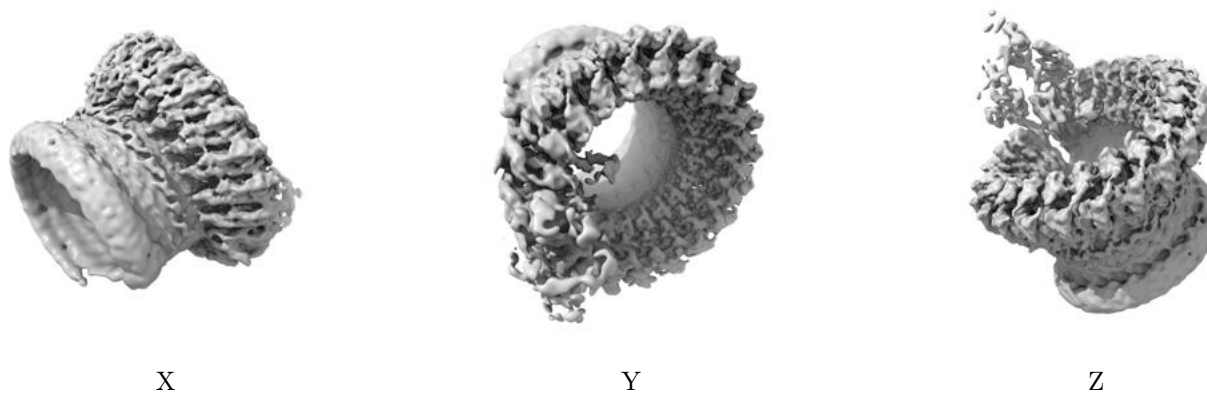


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



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.

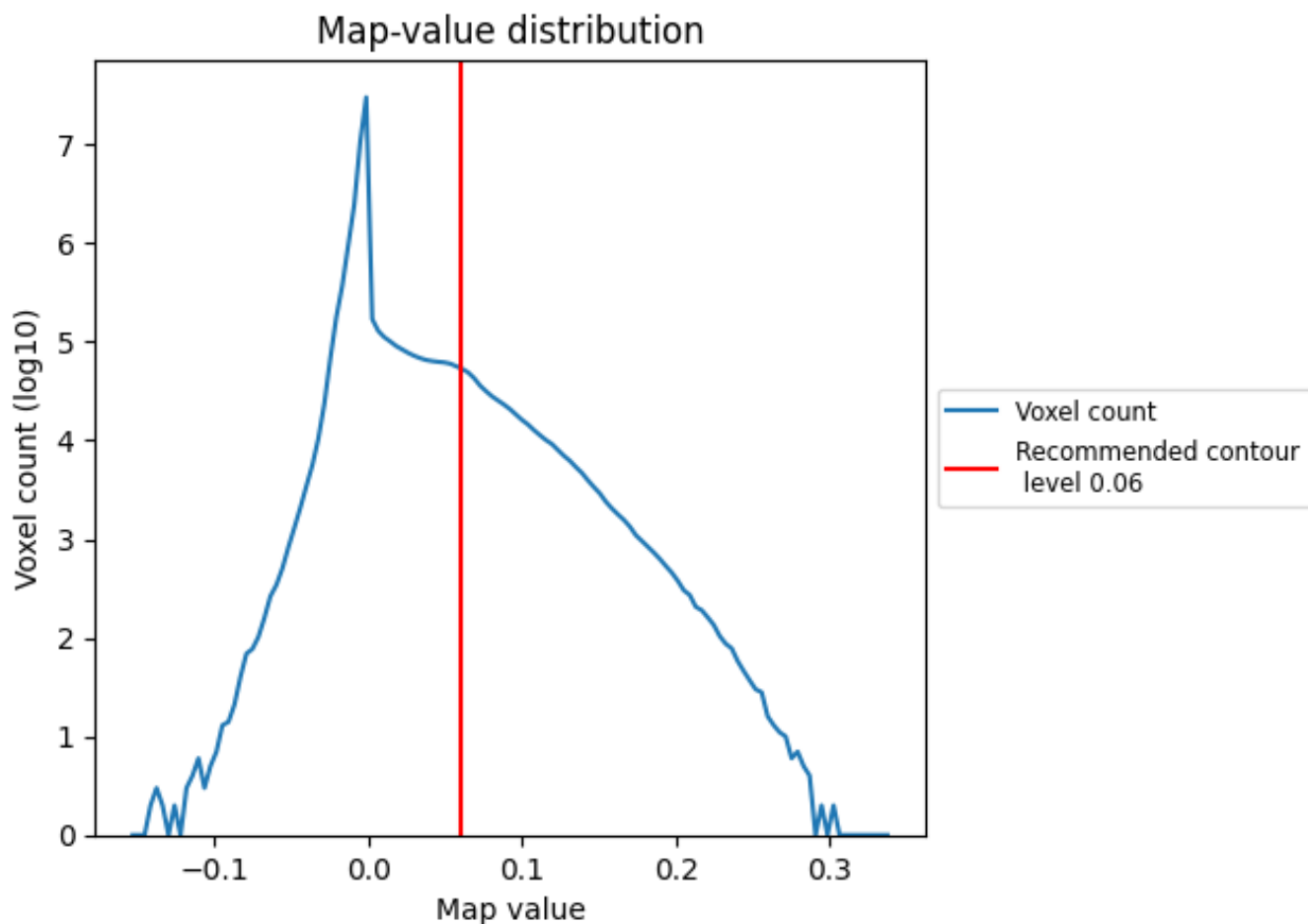
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

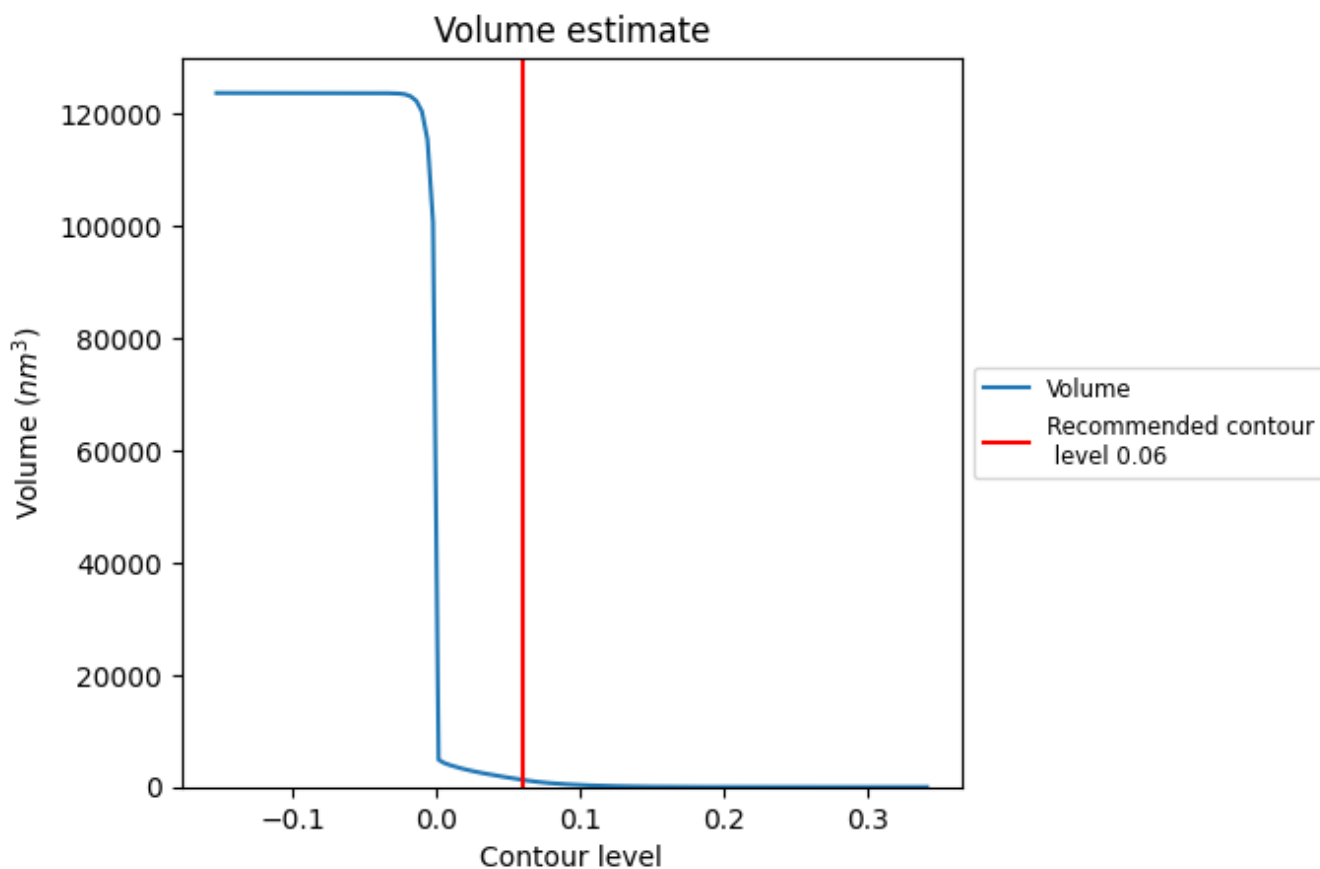
This section contains the results of statistical analysis of the map.

### 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.

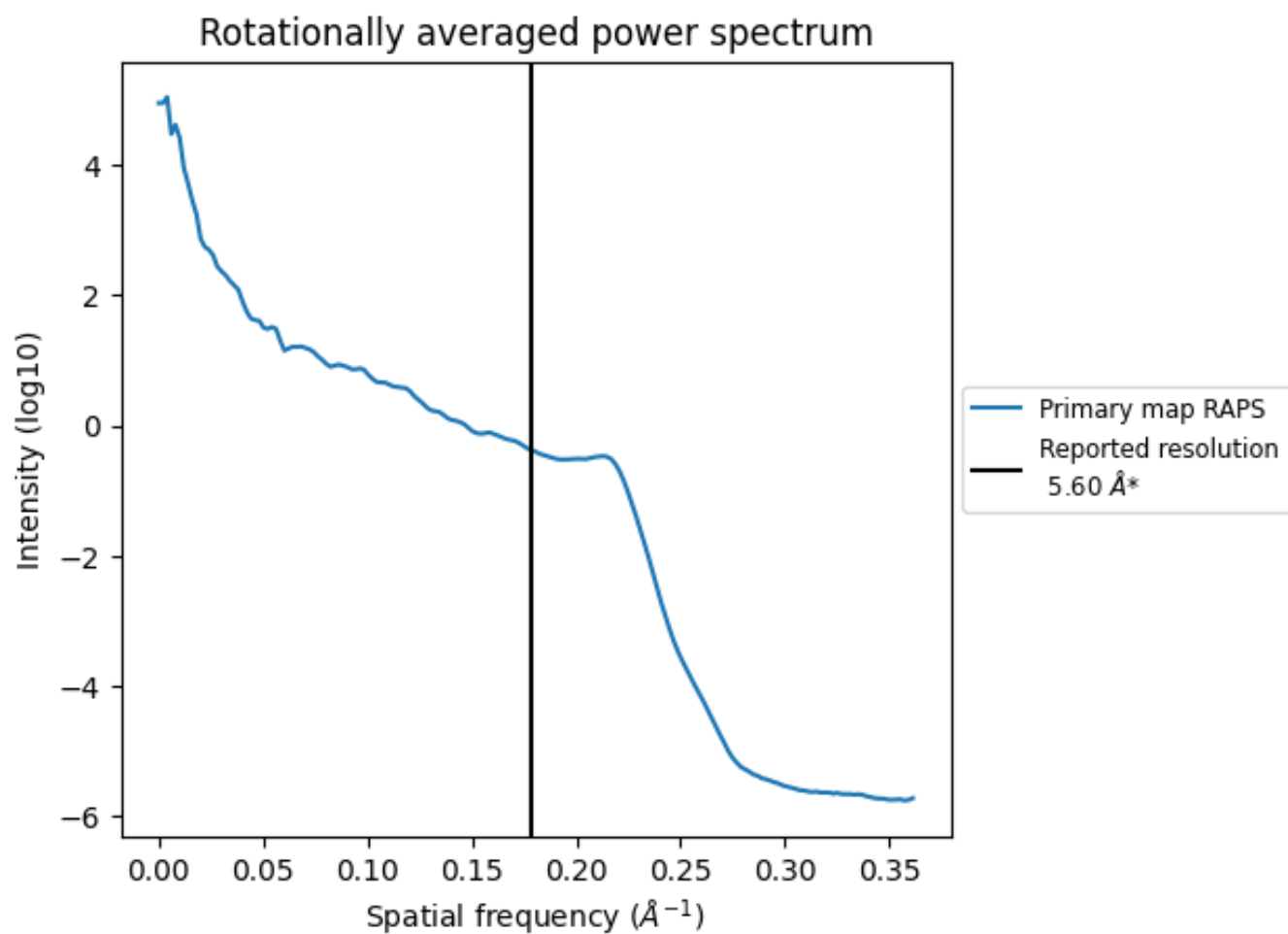
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1262 nm<sup>3</sup>; this corresponds to an approximate mass of 1140 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  $0.179 \text{\AA}^{-1}$

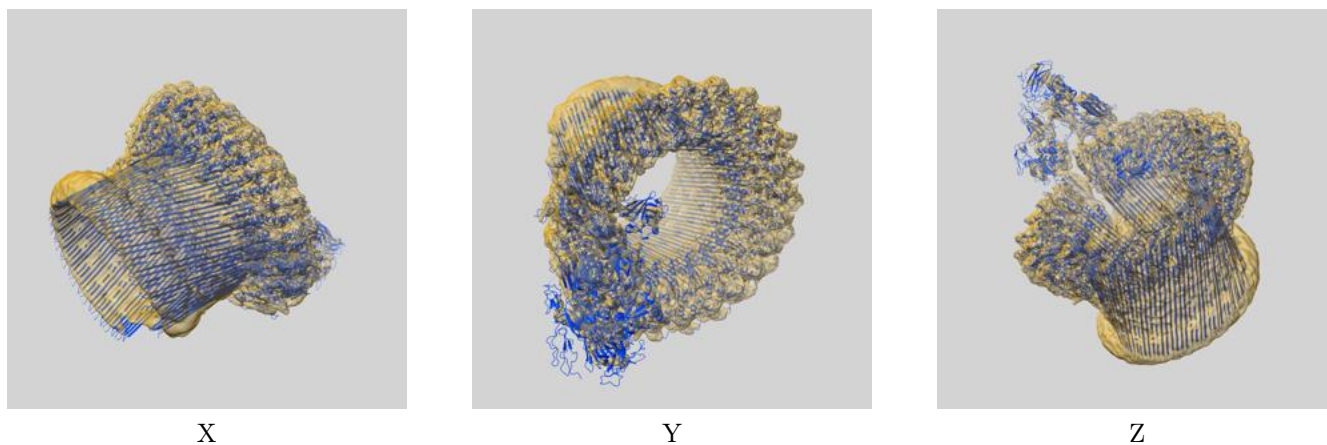
## 8 Fourier-Shell correlation

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

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

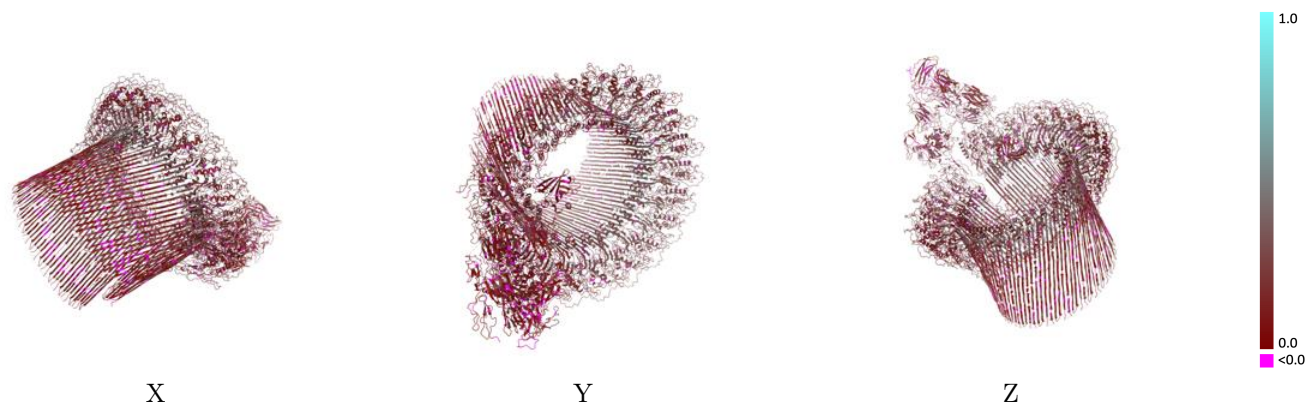
This section contains information regarding the fit between EMDB map EMD-0107 and PDB model 6H04. Per-residue inclusion information can be found in section 3 on page 11.

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



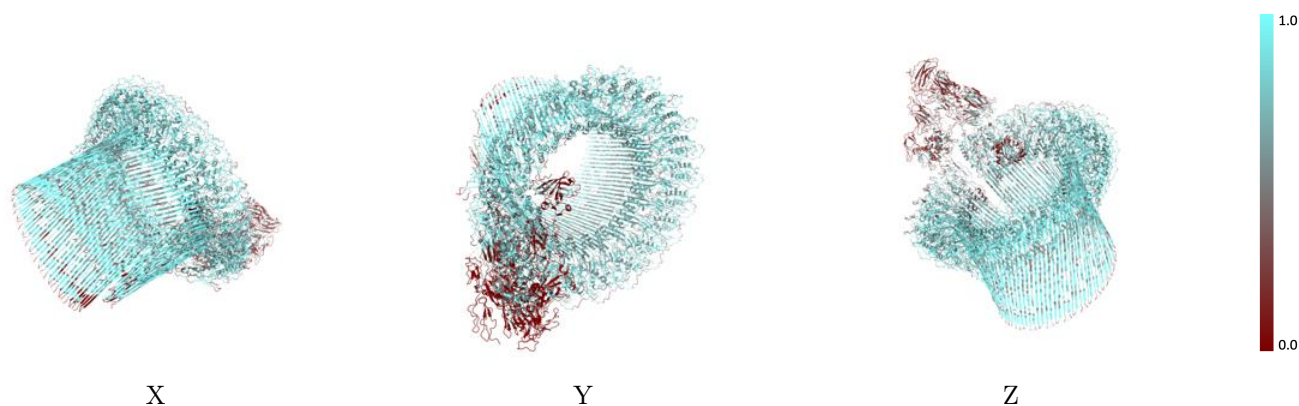
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

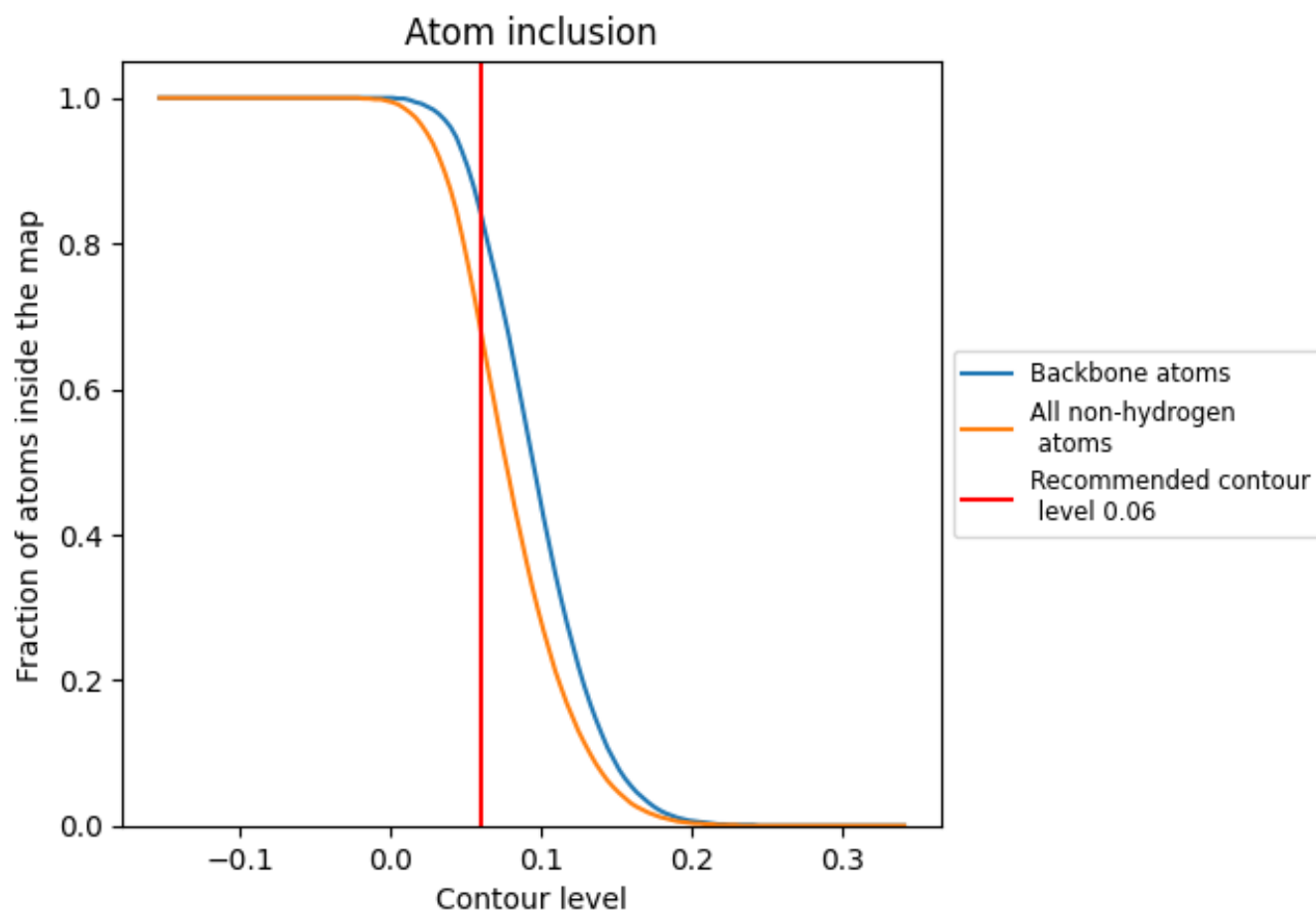
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 84% of all backbone atoms, 68% 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	 0.6820	 0.1790
A	 0.2710	 0.1130
B	 0.5610	 0.1380
C	 0.7160	 0.1580
D	 0.5950	 0.1530
E	 0.1680	 0.1100
F	 0.7440	 0.1520
G	 0.7370	 0.1560
H	 0.7850	 0.2120
I	 0.7800	 0.2110
J	 0.7840	 0.2210
K	 0.7810	 0.2180
L	 0.7900	 0.2300
M	 0.7900	 0.2270
N	 0.7930	 0.2280
O	 0.7860	 0.2230
P	 0.7740	 0.1990
Q	 0.7860	 0.2160
R	 0.7790	 0.2030
S	 0.7710	 0.1950
T	 0.7570	 0.1770
U	 0.7460	 0.1670
V	 0.7420	 0.1650
W	 0.7040	 0.1530
X	 0.5960	 0.1360
Y	 0.6070	 0.2400
Z	 0.5710	 0.1570
a	 0.5710	 0.1930
b	 0.4640	 0.2000
c	 0.3570	 0.1650
d	 0.3930	 0.2230
e	 0.3570	 0.1810
f	 0.2140	 0.1620
g	 0.2500	 0.1420
h	 0.2140	 0.0800



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Chain	Atom inclusion	Q-score
i	 0.3210	 0.0700
j	 0.3210	 0.1070
k	 0.4640	 0.1910
l	 0.3930	 0.2410
m	 0.5360	 0.2910
n	 0.4290	 0.2080
o	 0.3570	 0.1580
p	 0.4290	 0.2220
q	 0.2860	 0.1200