



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2025 – 09:52 PM JST

PDB ID : 7WG7 / pdb_00007wg7
EMDB ID : EMD-32479
Title : Acidic Omicron Spike Trimer
Authors : Cui, Z.
Deposited on : 2021-12-28
Resolution : 4.00 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

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>.

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

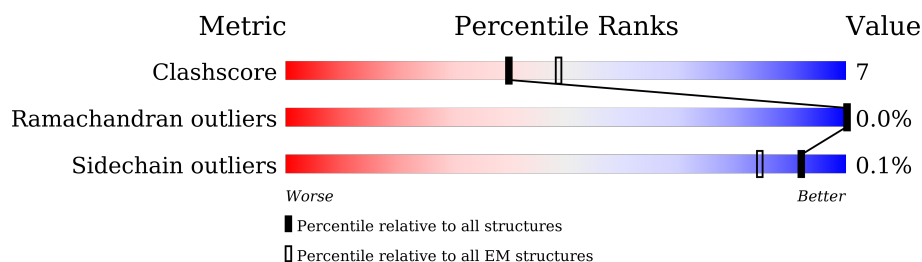
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



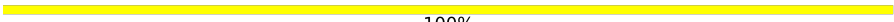

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	1270	<div> <div>5%</div> <div>70%</div> <div>16%</div> <div>14%</div> </div>
1	B	1270	<div> <div>8%</div> <div>71%</div> <div>15%</div> <div>14%</div> </div>
1	C	1270	<div> <div>17%</div> <div>71%</div> <div>17%</div> <div>12%</div> </div>
2	D	2	<div> <div>100%</div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>100%</div> <div>50%</div> </div>
2	F	2	<div> <div>100%</div> </div>
2	G	2	<div> <div>50%</div> <div>100%</div> </div>
2	H	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	K	2	 100%
2	L	2	 50% 50%
2	M	2	 100%
2	N	2	 50% 50%
2	P	2	 50% 100%
2	Q	2	 50% 50%
2	R	2	 100%
2	S	2	 50% 100%
2	T	2	 100%
3	I	3	 33% 67% 33%
3	J	3	 33% 33% 67%
3	O	3	 100%
3	U	3	 67% 33%
3	V	3	 33% 67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27041 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		
1	A	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		
1	C	1117	Total	C	N	O	S	0	0
			8770	5611	1462	1657	40		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	208	ILE	-	insertion	UNP P0DTC2
B	209	VAL	-	insertion	UNP P0DTC2
B	210	ARG	ASN	conflict	UNP P0DTC2
B	211	GLU	LEU	conflict	UNP P0DTC2
B	212	PRO	VAL	conflict	UNP P0DTC2
B	213	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	208	ILE	-	insertion	UNP P0DTC2
A	209	VAL	-	insertion	UNP P0DTC2
A	210	ARG	ASN	conflict	UNP P0DTC2
A	211	GLU	LEU	conflict	UNP P0DTC2
A	212	PRO	VAL	conflict	UNP P0DTC2
A	213	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
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A	446	SER	GLY	variant	UNP P0DTC2
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A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	208	ILE	-	insertion	UNP P0DTC2
C	209	VAL	-	insertion	UNP P0DTC2
C	210	ARG	ASN	conflict	UNP P0DTC2
C	211	GLU	LEU	conflict	UNP P0DTC2
C	212	PRO	VAL	conflict	UNP P0DTC2
C	213	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	685	ALA	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2

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



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

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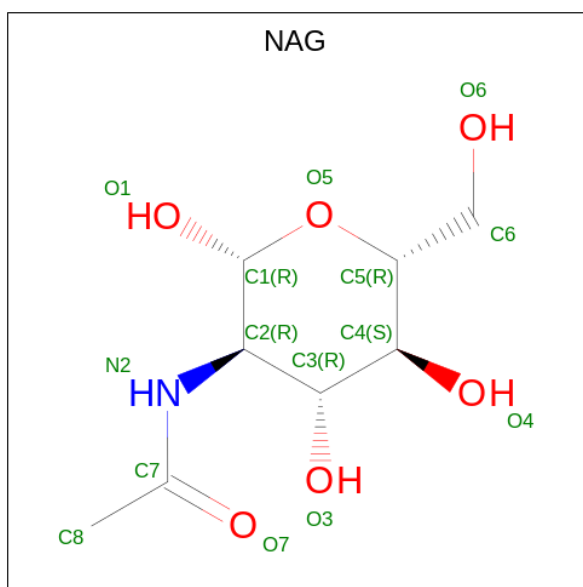
Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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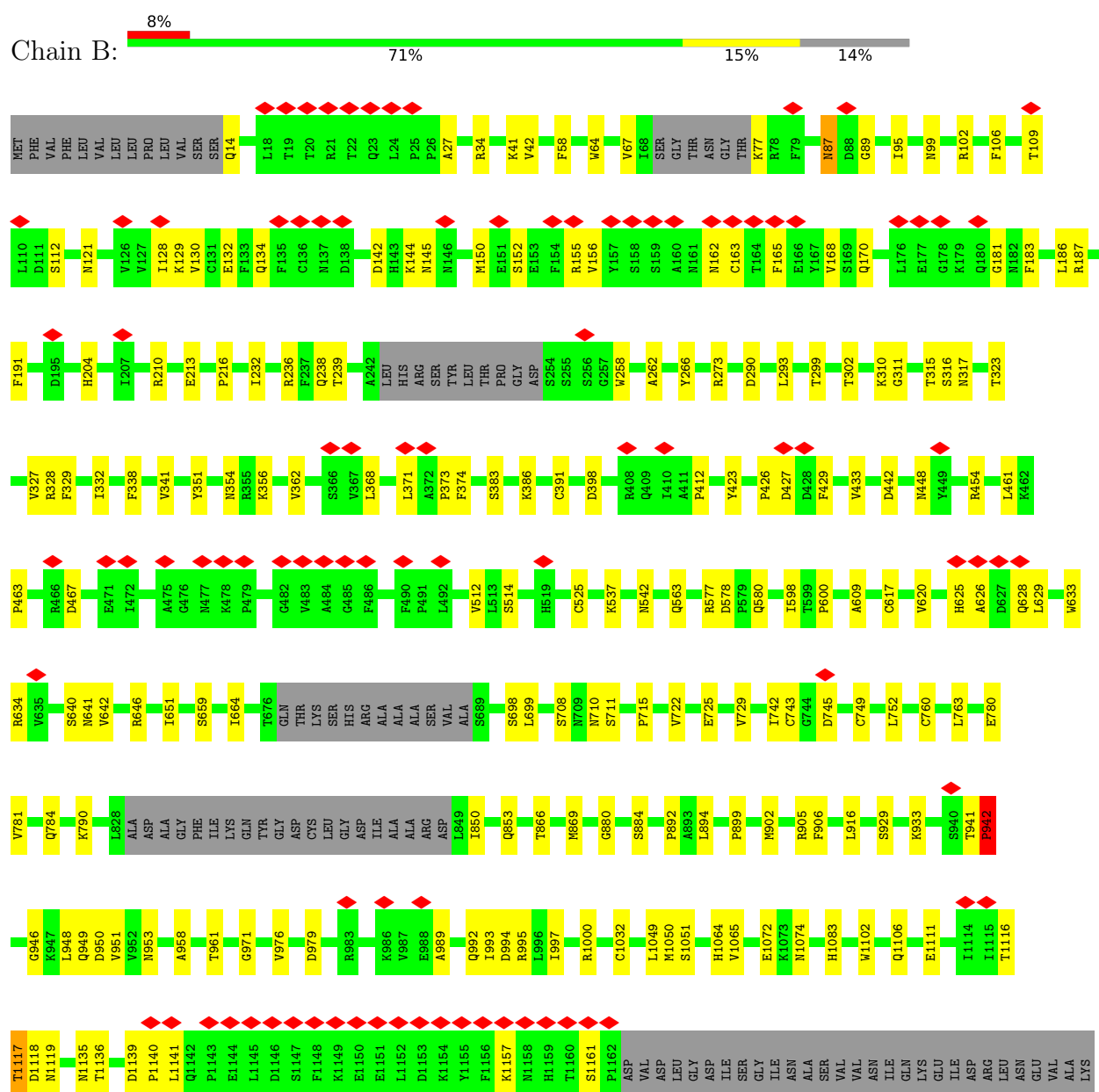
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein



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

● Molecule 1: Spike glycoprotein



LEU	LEU	VAL	PHE	E661	P521	T376	L241	L118
ILE	ASP	ASP	ILE	C662	A522	F377	A242	I119
ALA	LEU	GLY	LYS	D663	T523	K378	LEU	N125
VAL	ASP	VAL	GLN	I664	V524	C391	HIS	V126
MET	ASP	VAL	TYR	P665	C525	S399	ARG	I127
VAL	SER	VAL	GLY	I666	S530	S399	SER	I128
THR	GLY	VAL	CYS	A672	T531	R403	TYR	
ILE	LEU	VAL	GLY	T676	N532	I410	THR	E132
LEU	ASP	ALA	ASP	GLN	V534	T415	PRO	F133
ALA	SER	ALA	ILE	THR	ASP	G416	GLY	Q134
VAL	ALA	ALA	ALA	LYS	K537	P412	ASP	F135
VAL	VAL	ALA	ALA	SER	N542	T415	ASP	C136
THR	ASN	ARG	ARG	HIS	K547	G416	S254	N137
SER	GLN	ASP	L849	ARG	K557	L425	S255	C15
CYS	LYS	LYS	LYS	ALA	Q563	P426	G257	V16
CYS	GLU	ASP	ALA	ALA	Q564	D427	W258	N17
ILE	ASP	SER	SER	VAL	Q580	D428	T259	L18
ASP	ARG	ALA	ALA	ALA	Q580	F429	A260	T19
LEU	ASN	S884	S884	S689	Q580	V433	V267	T20
LYS	GLY	P892	P892	Y695	I584	S438	R273	T22
GLY	ASN	P899	P899	T696	L585	M439	K278	Q23
LEU	GLY	A924	A924	M697	T588	S443	Y279	P26
ASN	ASN	N928	N928	S698	I598	L452	N280	A27
CYS	ASN	P942	P942	N710	S605	R454	E281	D40
GLY	LEU	L948	L948	E725	N606	R457	N282	
ASP	ASP	Q949	Q949	P715	L611	K462	T299	P57
LEU	LEU	D950	D950	E725	N616	E465	T302	W64
ASN	ASN	V951	V951	T732	T618	R466	Q311	F65
GLY	GLY	N953	N953	K733	C617	D467	G311	I68
VAL	VAL	H954	H954	C743	T618	N477	T316	SER
LYS	LYS	N955	N955	C749	A623	K478	S316	GLY
GLY	GLY	K969	K969	Y756	D627	P479	N317	ASN
VAL	VAL	F970	F970	L763	Q628	C480	V327	GLY
LYS	LYS	G971	G971	A771	L629	M481	R328	THR
HIS	HIS	S974	S974	K786	S640	C482	N354	K77
TYR	TYR	S975	S975	F802	V642	V483	R355	R78
THR	THR	F981	F981	I805	G648	N487	K356	I95
		D985	D985	L828	C649	L492	R357	E96
		R995	R995	ALA	I651	F497	C361	K97
		V1008	V1008	ASP	S689	E516	S366	
		K1157	K1157	ALA	Y660	H519	V367	
		N1158	N1158	GLY		A520	A372	
		H1159	H1159				P373	
		T1160	T1160				F374	
		S1161	S1161				F375	
		P1162	P1162					
		ASP	ASP					

● Molecule 1: Spike glycoprotein



MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	LEU	VAL	SER	Q14	C15	V16	N17	L18	T19	T20	R21	T22	Q23	L24	P25	N30	T33	R34	Y37	D40	K41	V42	L54	W64	F65	H66	V67	I68	SER	GLY	THR	ASN	GLY	THR	K77	R78	N87	D88	G89	K97	R102
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- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



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

Chain G: 100%



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

Chain H: 50% 50%



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

Chain K: 100%



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

Chain L: 50% 50%



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

Chain M: 100%



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

Chain N: 



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

Chain P: 



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

Chain Q: 



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

Chain R: 



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

Chain S: 



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

Chain T: 



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



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



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



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



- Molecule 3: beta-D-mannopyranose-(1-4)-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, Not provided	
Number of particles used	371808	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (\AA)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	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	0.18	1/8837 (0.0%)	0.47	4/12019 (0.0%)
1	B	0.19	0/8837	0.49	4/12019 (0.0%)
1	C	0.19	0/8977	0.48	3/12207 (0.0%)
All	All	0.19	1/26651 (0.0%)	0.48	11/36245 (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	2
1	B	0	1
1	C	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	LEU	C-N	6.04	1.40	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	942	PRO	N-CA-CB	9.96	110.19	101.83
1	C	942	PRO	N-CA-CB	9.92	110.16	101.83
1	B	892	PRO	N-CA-CB	7.84	110.26	103.36
1	A	892	PRO	N-CA-CB	7.75	110.53	103.33
1	A	156	VAL	N-CA-C	-7.68	103.78	111.77

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	GLU	Peptide
1	A	133	PHE	Peptide
1	B	1117	THR	Peptide
1	C	330	PRO	Peptide
1	C	359	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8632	0	8437	122	0
1	B	8632	0	8436	114	0
1	C	8770	0	8564	142	0
2	D	28	0	25	2	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
3	I	39	0	34	0	0
3	J	39	0	34	0	0
3	O	39	0	34	1	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
4	A	140	0	128	4	0
4	B	126	0	115	0	0
4	C	154	0	141	1	0
All	All	27041	0	26341	366	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 7.

The worst 5 of 366 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:O	1:A:185:ASN:HB2	1.82	0.80
1:A:254:SER:N	4:A:1301:NAG:HO6	1.84	0.75
1:B:790:LYS:HZ3	1:C:704:SER:HB2	1.54	0.72
1:A:134:GLN:HB2	1:A:157:TYR:HB2	1.73	0.71
1:B:433:VAL:HG12	1:B:512:VAL:HG12	1.73	0.69

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	1088/1270 (86%)	1016 (93%)	72 (7%)	0	100	100
1	B	1088/1270 (86%)	997 (92%)	90 (8%)	1 (0%)	48	81
1	C	1107/1270 (87%)	1013 (92%)	94 (8%)	0	100	100
All	All	3283/3810 (86%)	3026 (92%)	256 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	942	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	964/1113 (87%)	964 (100%)	0	100	100
1	B	964/1113 (87%)	963 (100%)	1 (0%)	92	94
1	C	976/1113 (88%)	975 (100%)	1 (0%)	92	94
All	All	2904/3339 (87%)	2902 (100%)	2 (0%)	92	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	C	613	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	675	GLN
1	C	751	ASN
1	C	957	GLN
1	A	193	ASN
1	A	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	1.56	2 (14%)	17,19,21	1.09	1 (5%)
2	NAG	D	2	2	14,14,15	0.47	0	17,19,21	0.44	0
2	NAG	E	1	2,1	14,14,15	1.17	1 (7%)	17,19,21	1.78	1 (5%)
2	NAG	E	2	2	14,14,15	0.95	1 (7%)	17,19,21	1.18	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	F	2	2	14,14,15	0.26	0	17,19,21	0.40	0
2	NAG	G	1	2	14,14,15	0.33	0	17,19,21	0.90	1 (5%)
2	NAG	G	2	2	14,14,15	0.36	0	17,19,21	0.41	0
2	NAG	H	1	2,1	14,14,15	0.63	0	17,19,21	0.71	0
2	NAG	H	2	2	14,14,15	0.65	0	17,19,21	1.96	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.30	0	17,19,21	0.50	0
3	NAG	I	2	3	14,14,15	1.23	1 (7%)	17,19,21	1.56	1 (5%)
3	BMA	I	3	3	11,11,12	0.74	0	15,15,17	0.76	0
3	NAG	J	1	3,1	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	J	2	3	14,14,15	1.38	1 (7%)	17,19,21	1.40	1 (5%)
3	BMA	J	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.35	3 (20%)
2	NAG	K	1	2,1	14,14,15	0.62	1 (7%)	17,19,21	0.58	0
2	NAG	K	2	2	14,14,15	0.40	0	17,19,21	0.61	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	L	2	2	14,14,15	1.09	1 (7%)	17,19,21	1.14	1 (5%)
2	NAG	M	1	2,1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	M	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	N	1	2,1	14,14,15	0.32	0	17,19,21	0.77	1 (5%)
2	NAG	N	2	2	14,14,15	0.36	0	17,19,21	0.41	0
3	NAG	O	1	3	14,14,15	0.44	0	17,19,21	0.74	1 (5%)
3	NAG	O	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	BMA	O	3	3	11,11,12	1.28	2 (18%)	15,15,17	1.60	3 (20%)
2	NAG	P	1	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	P	2	2	14,14,15	0.30	0	17,19,21	0.35	0
2	NAG	Q	1	2,1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	Q	2	2	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	R	1	2,1	14,14,15	0.35	0	17,19,21	0.35	0
2	NAG	R	2	2	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	S	1	2,1	14,14,15	0.46	0	17,19,21	0.87	1 (5%)
2	NAG	S	2	2	14,14,15	1.34	1 (7%)	17,19,21	1.71	2 (11%)
2	NAG	T	1	2,1	14,14,15	0.28	0	17,19,21	0.57	0
2	NAG	T	2	2	14,14,15	0.29	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	U	1	3	14,14,15	0.67	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	U	2	3	14,14,15	0.38	0	17,19,21	0.36	0
3	BMA	U	3	3	11,11,12	0.63	0	15,15,17	0.85	0
3	NAG	V	1	3,1	14,14,15	0.27	0	17,19,21	0.76	1 (5%)
3	NAG	V	2	3	14,14,15	0.26	0	17,19,21	0.69	0
3	BMA	V	3	3	11,11,12	0.75	0	15,15,17	0.83	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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	5/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
2	NAG	P	1	2	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	4/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	1/6/23/26	0/1/1/1
3	BMA	U	3	3	-	2/2/19/22	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O5-C1	5.05	1.51	1.43
3	J	2	NAG	O5-C1	4.84	1.51	1.43
2	S	2	NAG	O5-C1	4.80	1.51	1.43
3	I	2	NAG	O5-C1	4.46	1.50	1.43
2	E	1	NAG	O5-C1	4.27	1.50	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	6.92	121.57	112.19
2	H	2	NAG	C2-N2-C7	6.89	132.71	122.90
3	I	2	NAG	C1-O5-C5	6.21	120.61	112.19
2	S	2	NAG	C1-O5-C5	6.17	120.55	112.19
3	J	2	NAG	C1-O5-C5	5.57	119.73	112.19

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

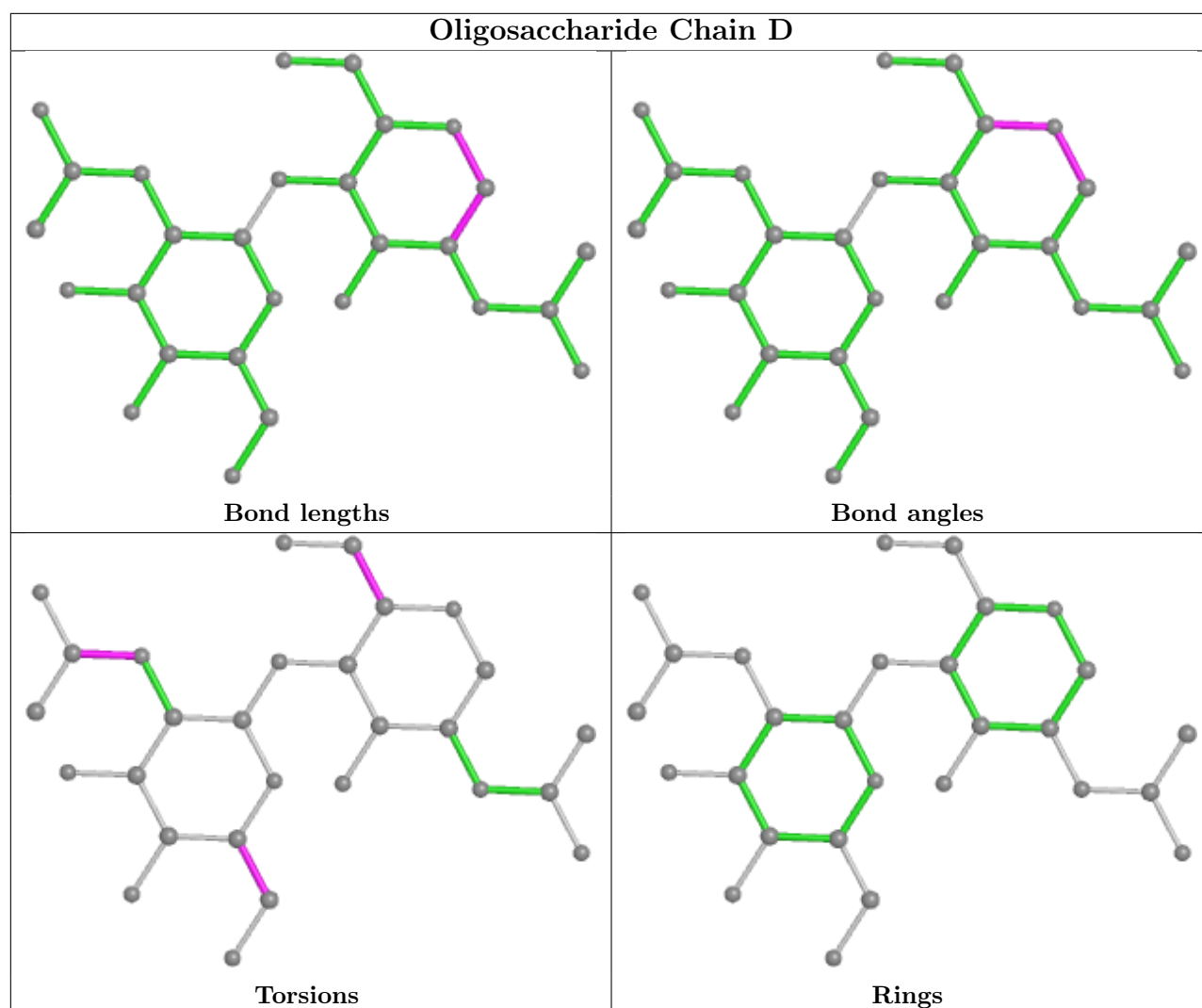
Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

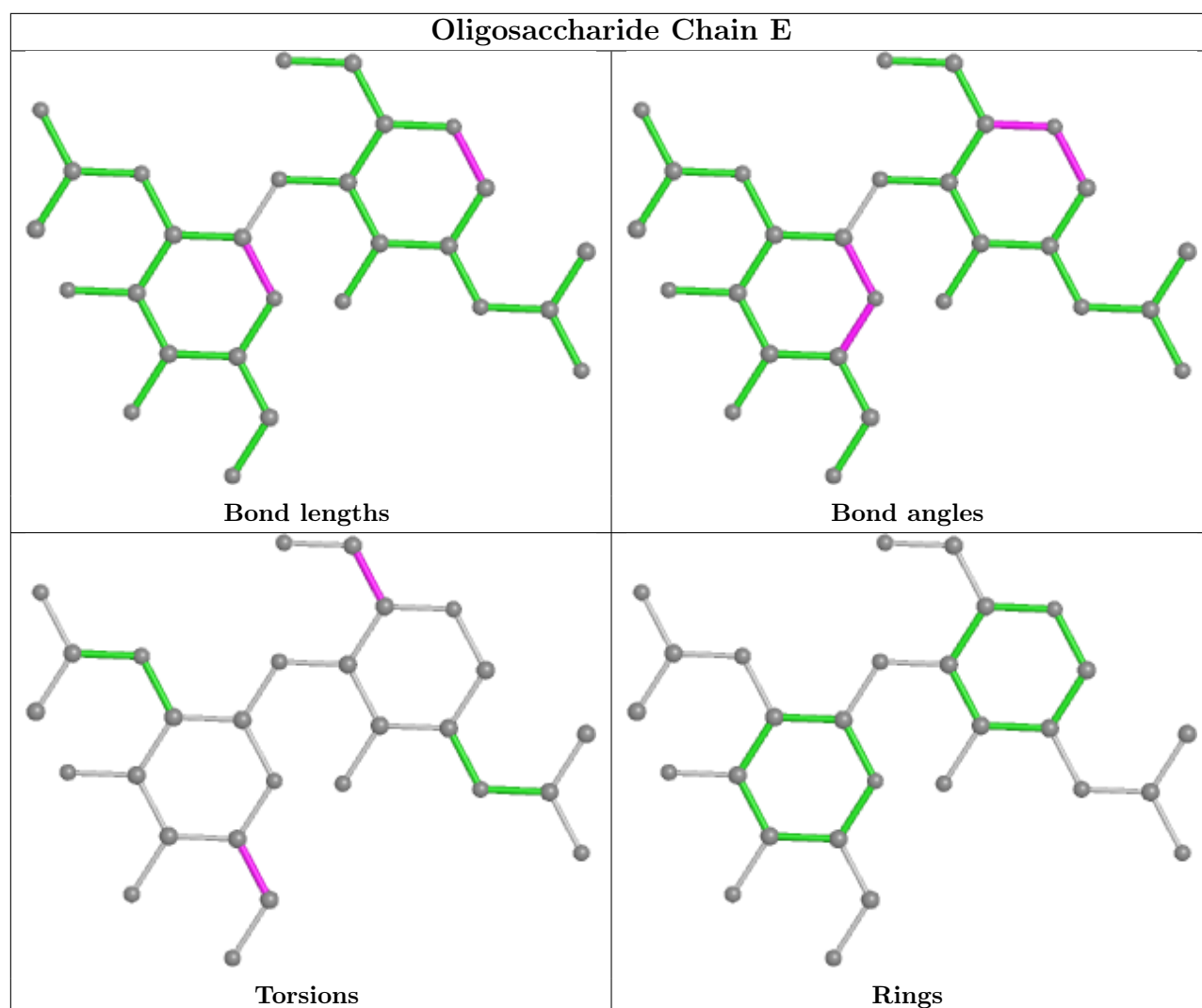
There are no ring outliers.

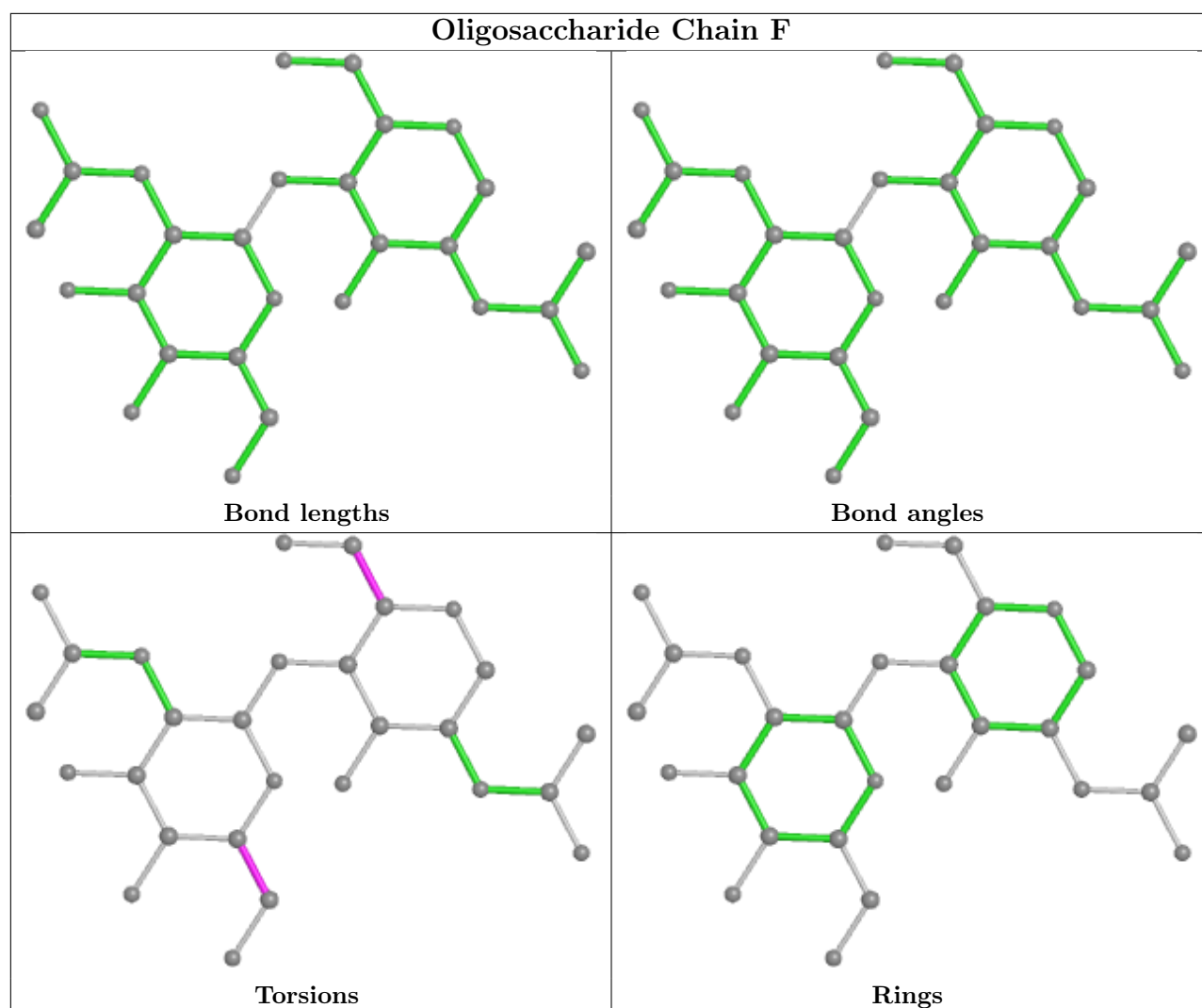
7 monomers are involved in 6 short contacts:

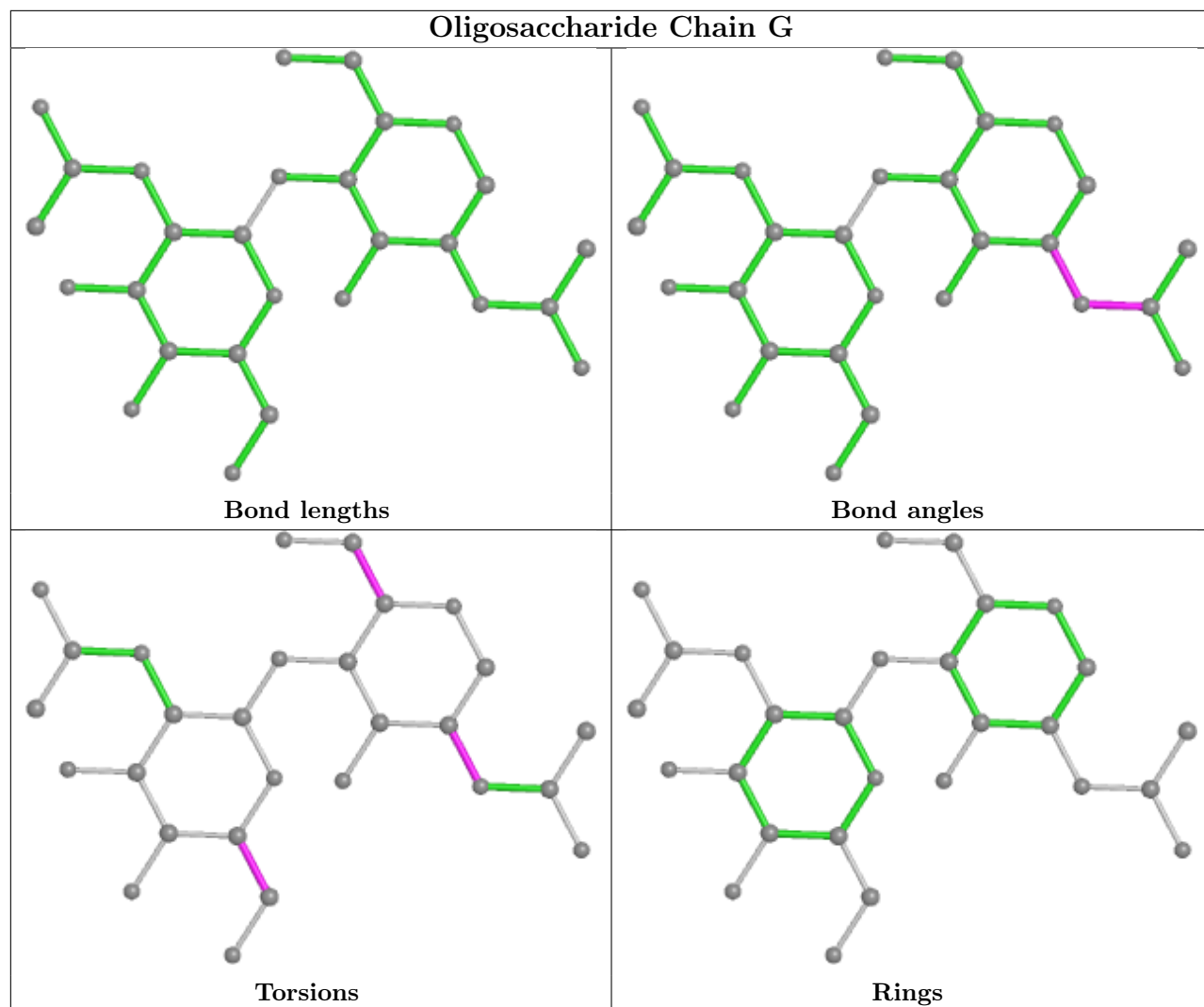
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	2	NAG	1	0
2	D	2	NAG	2	0
2	H	1	NAG	1	0
2	G	2	NAG	1	0
2	H	2	NAG	1	0
2	Q	1	NAG	1	0
2	D	1	NAG	2	0

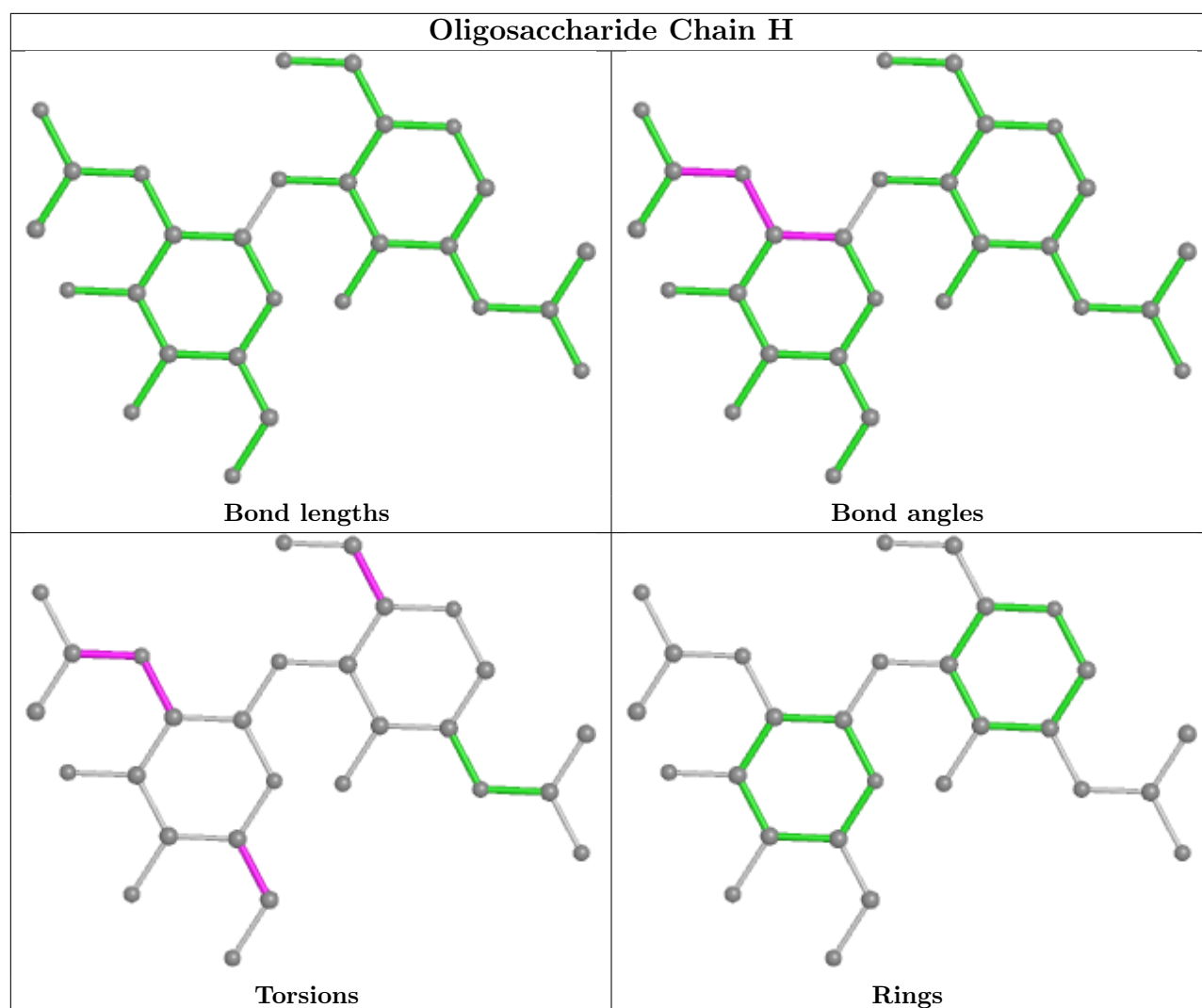
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

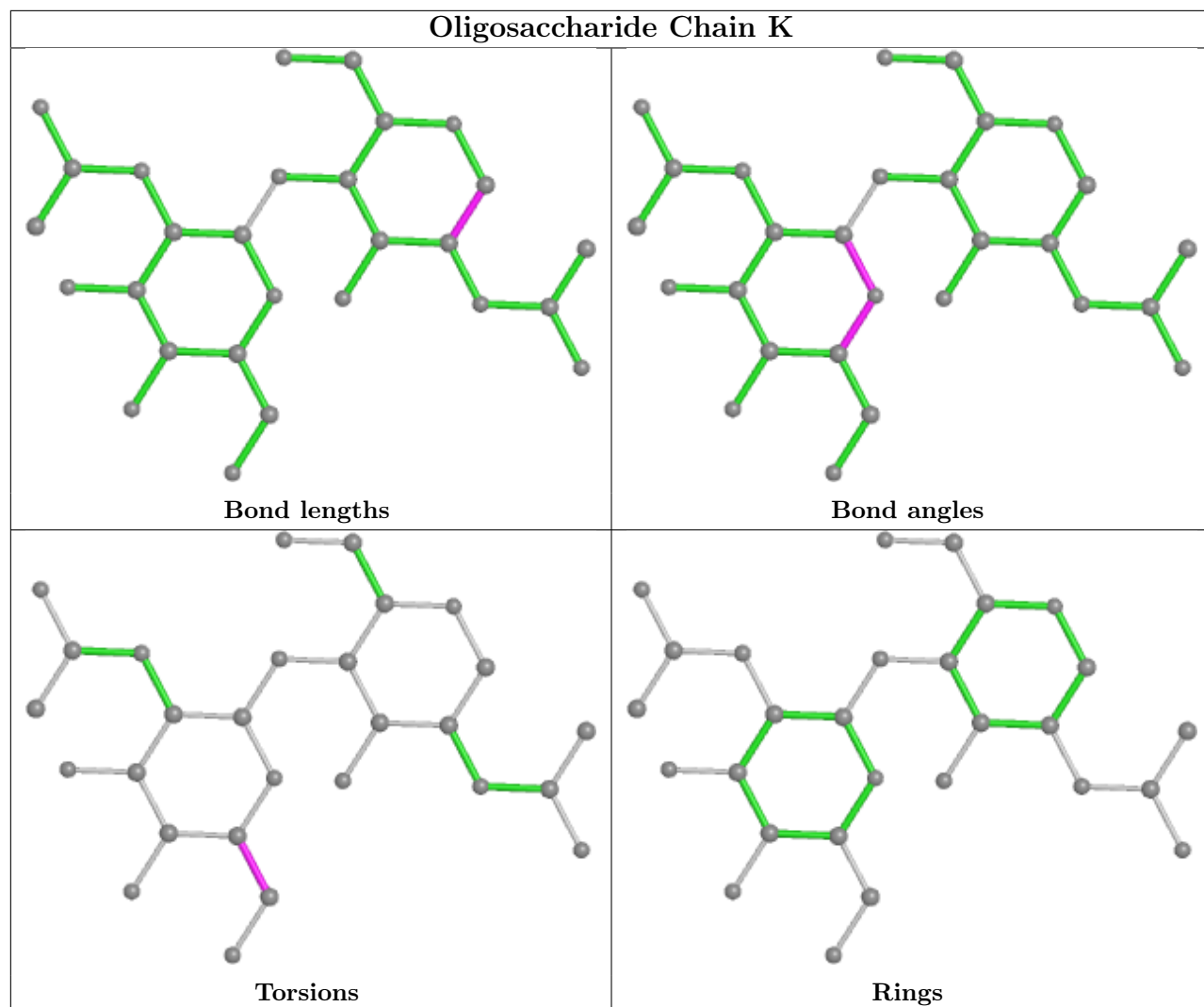


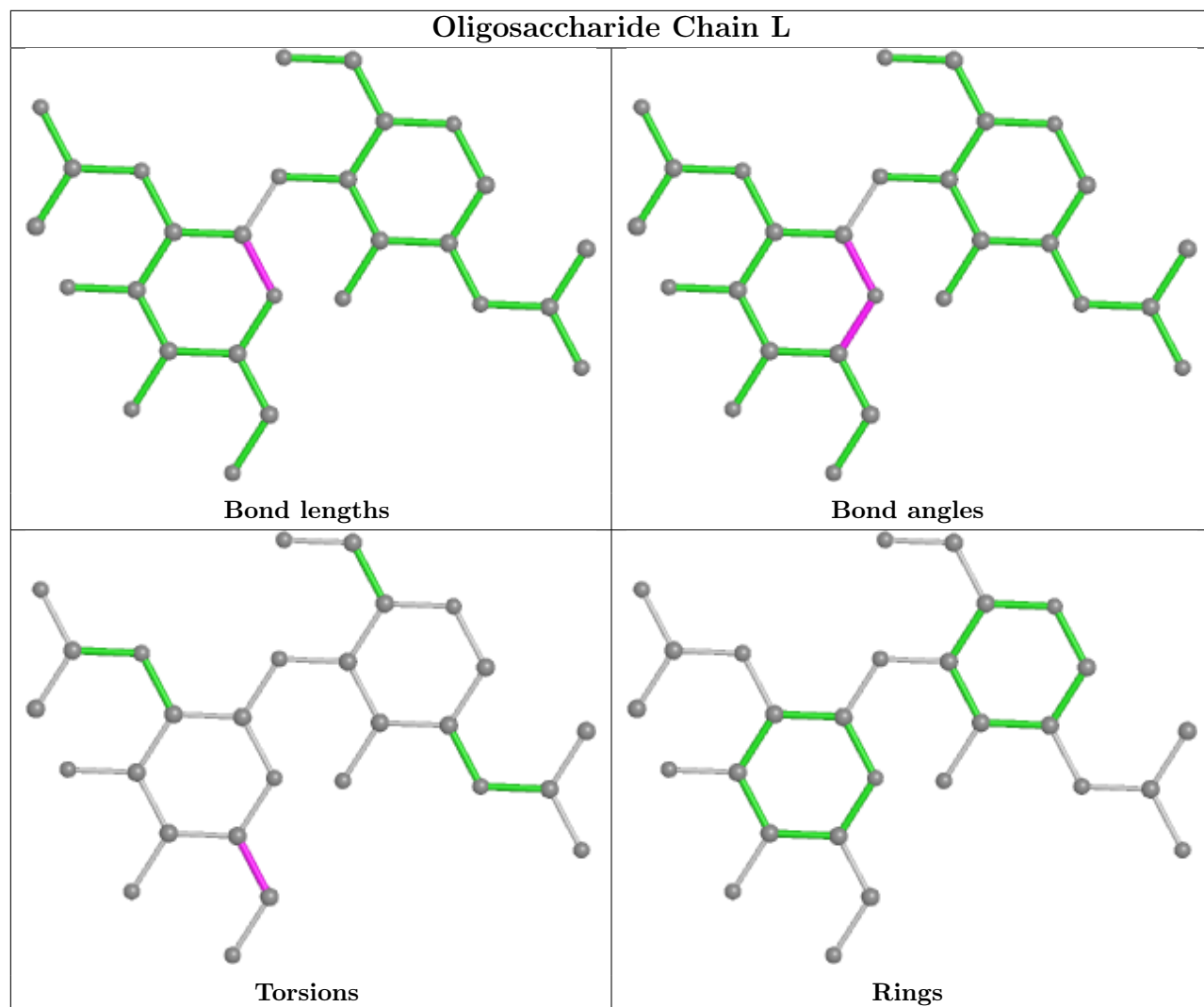


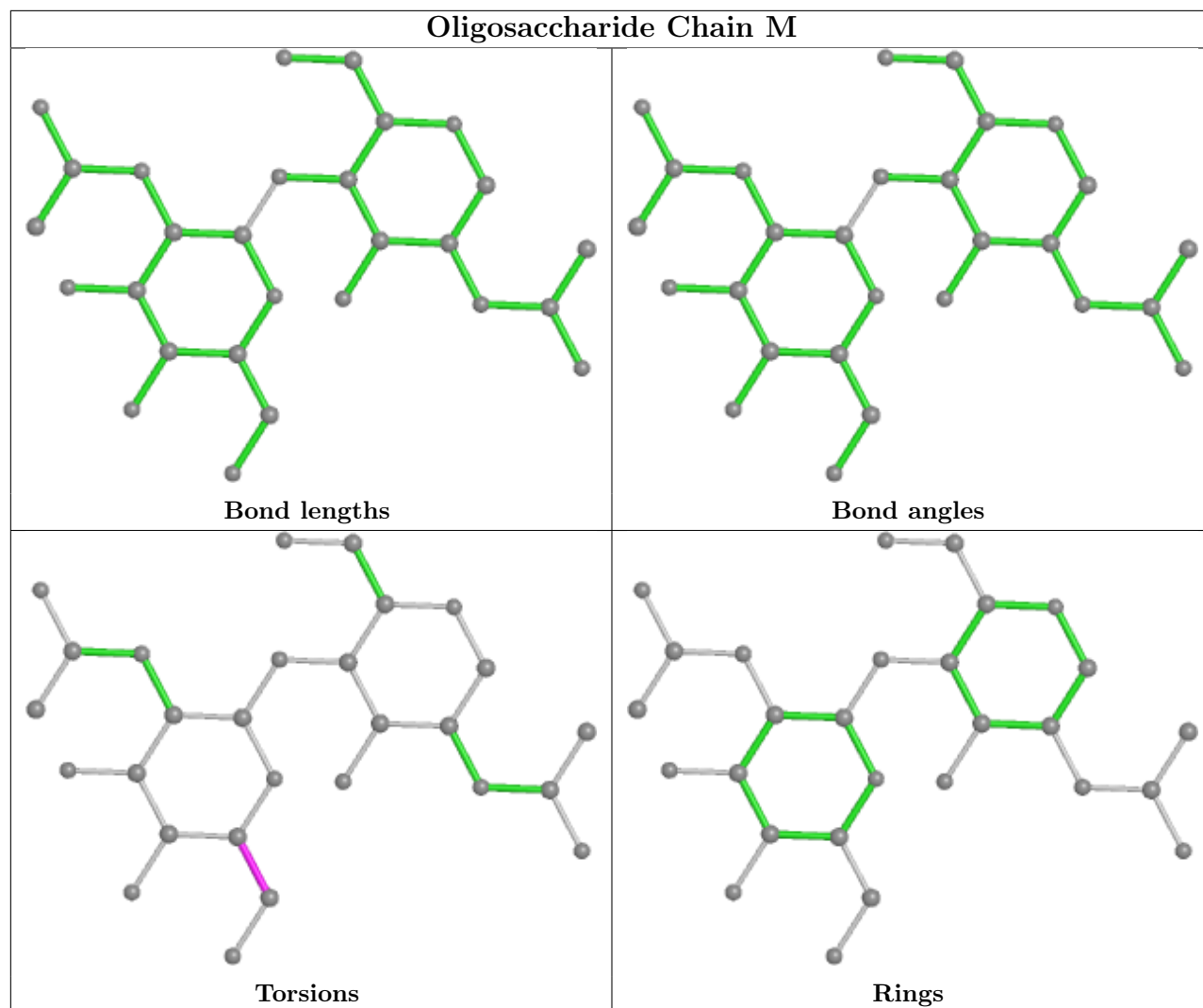


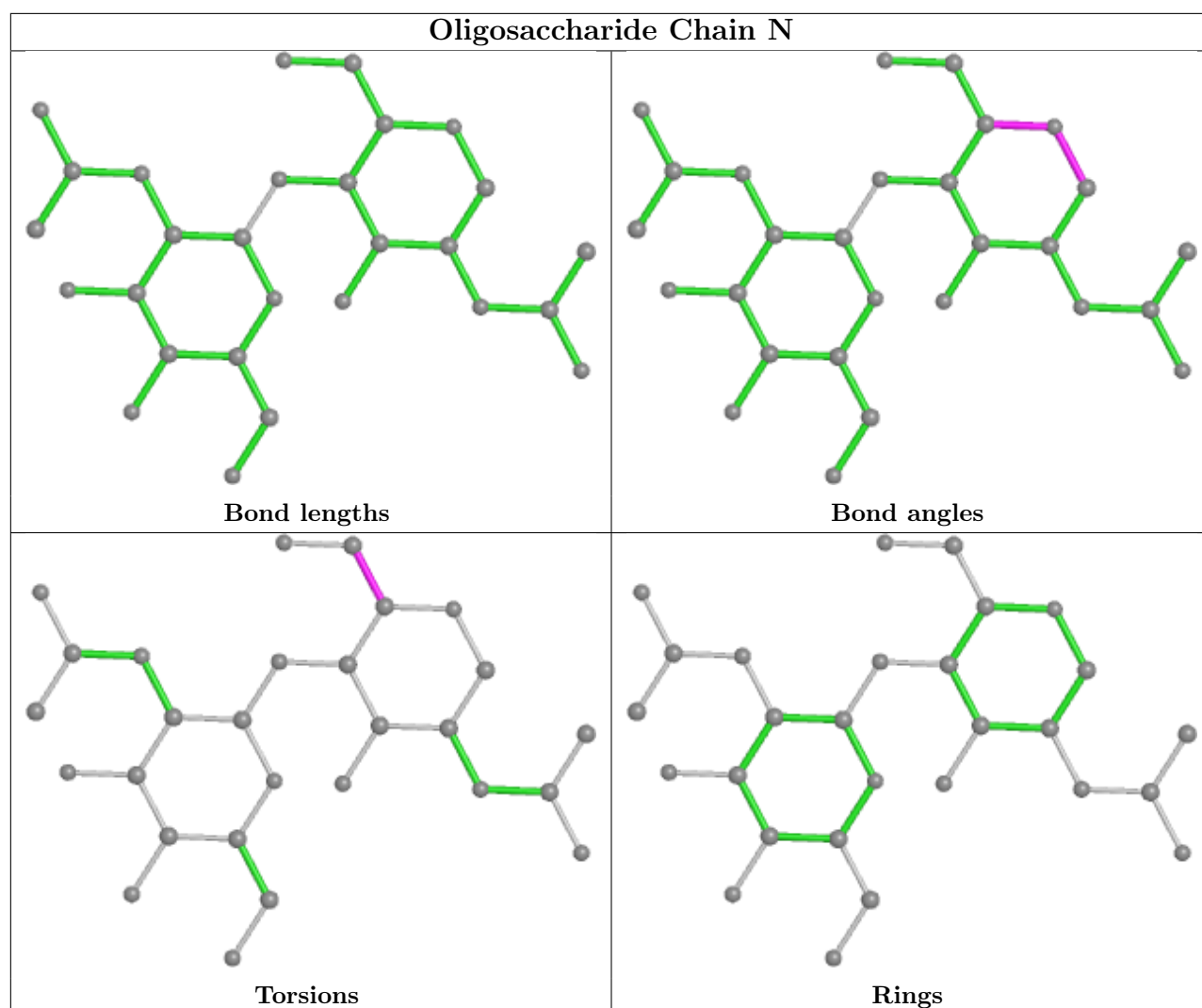


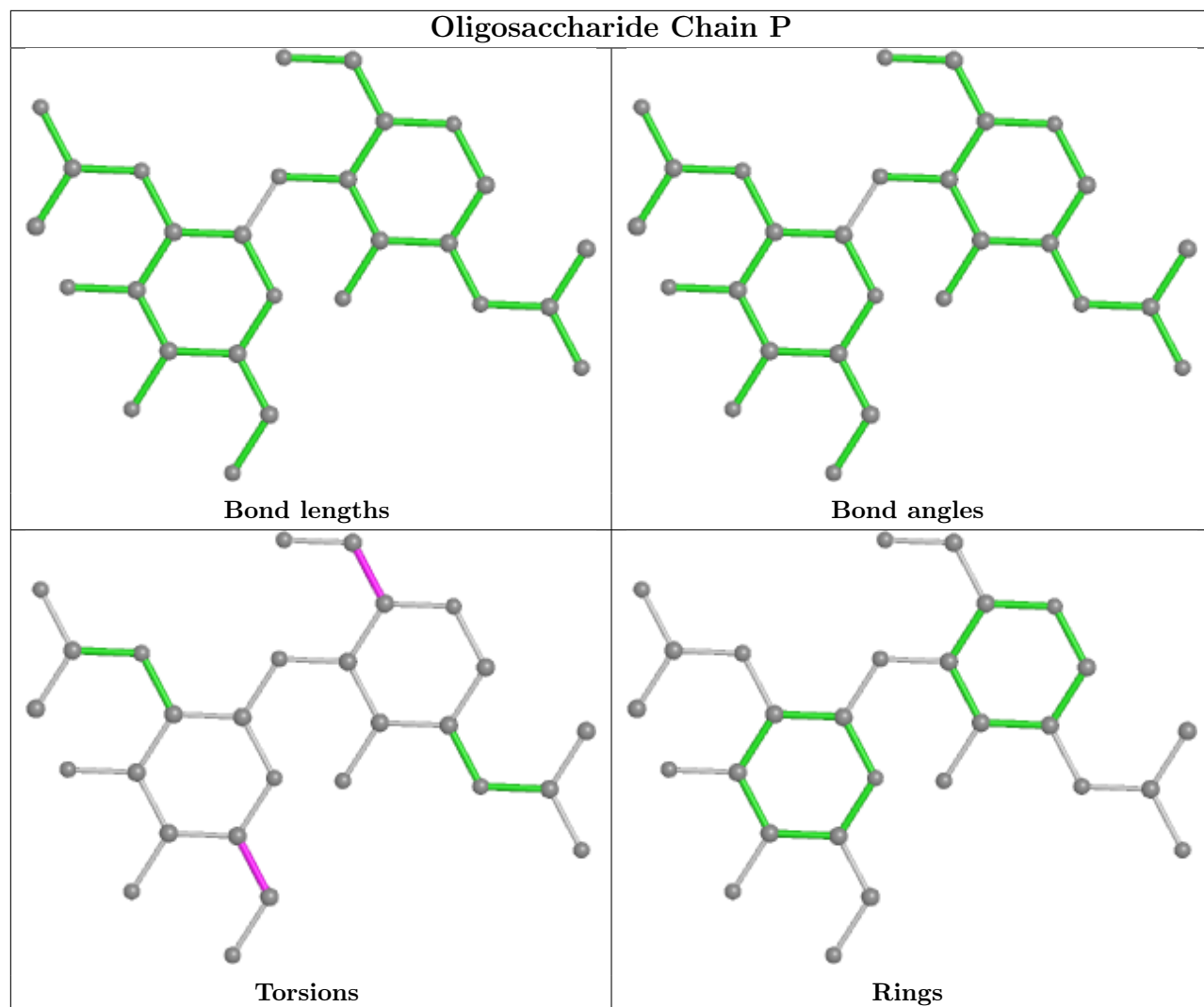


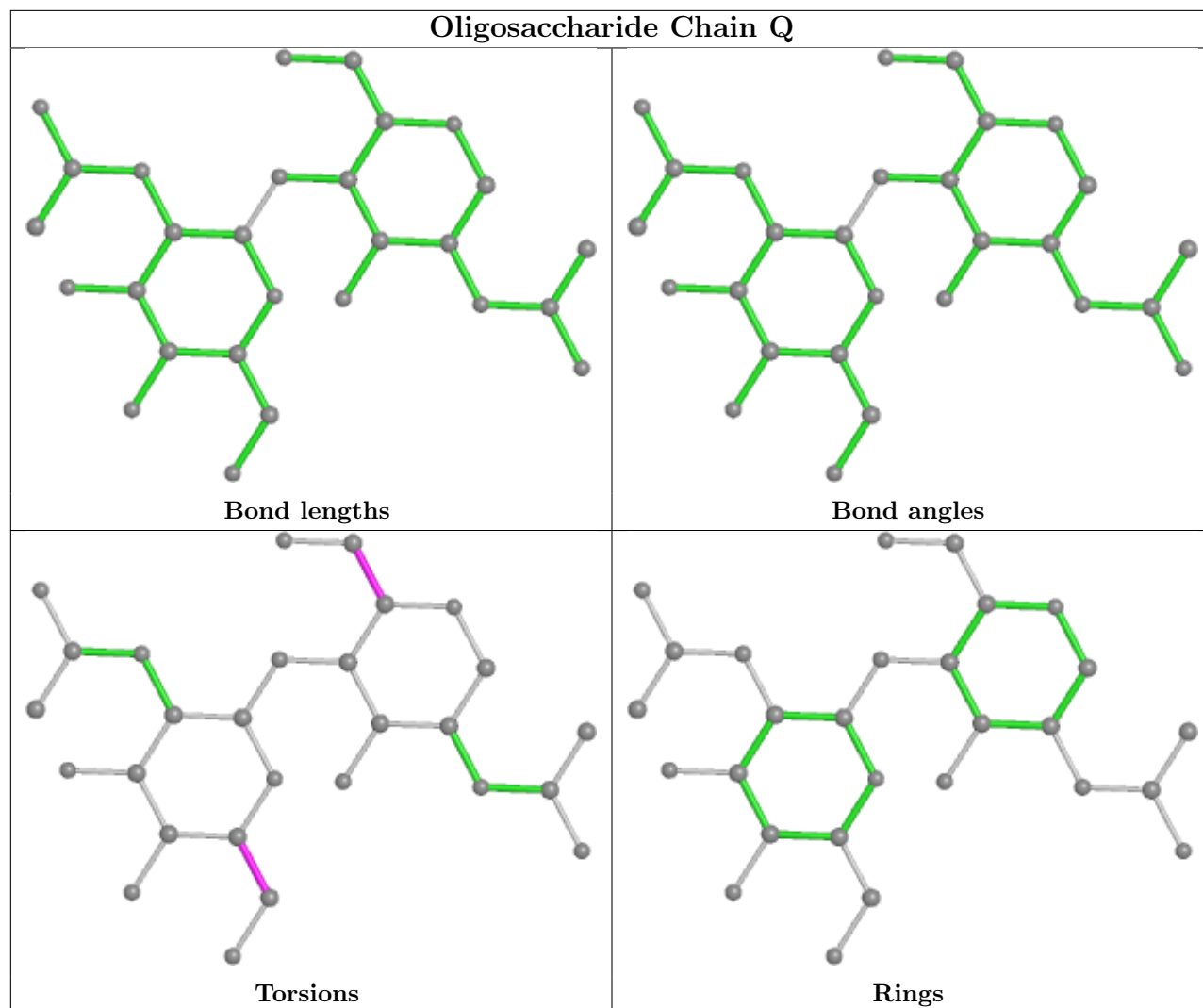


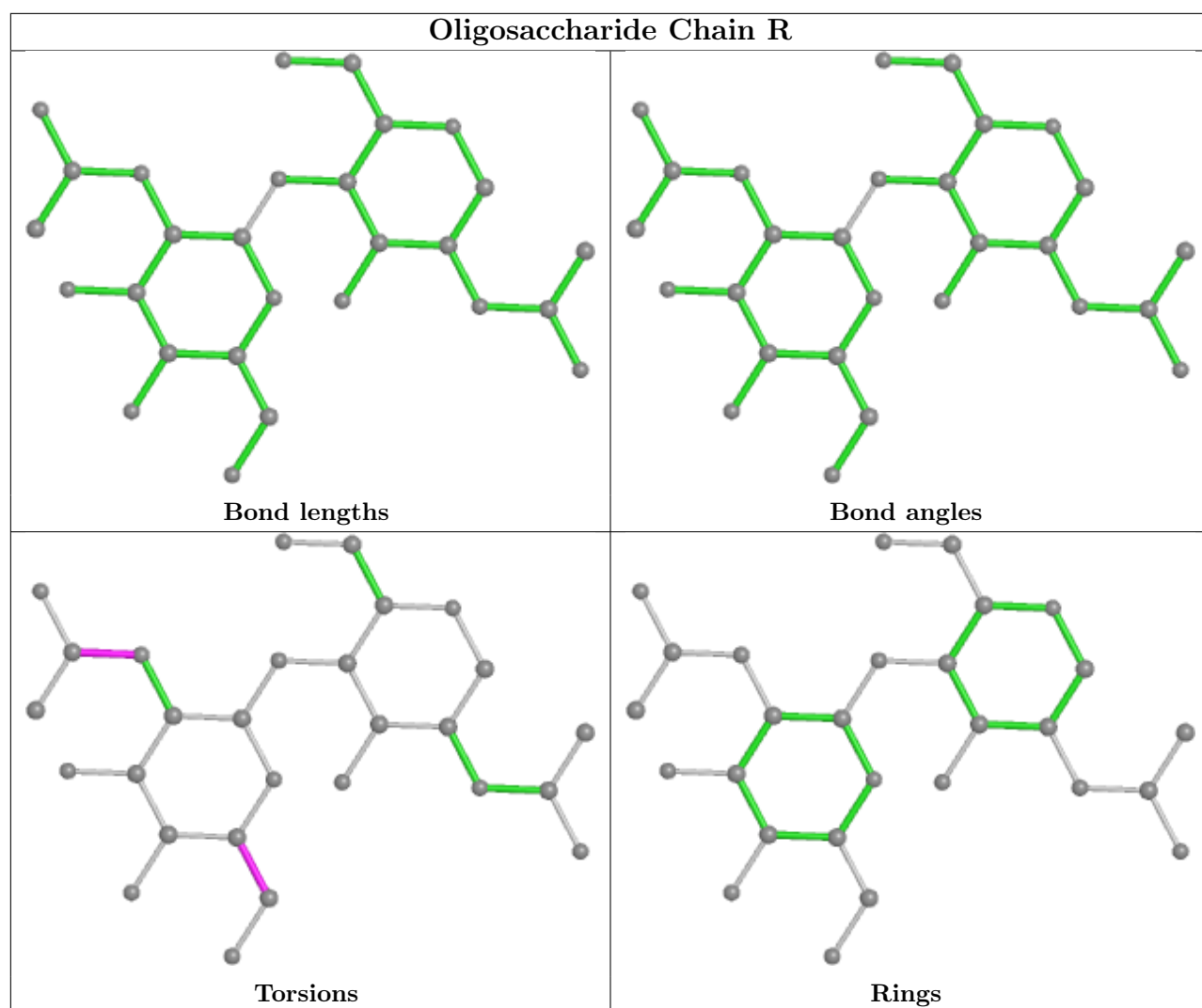


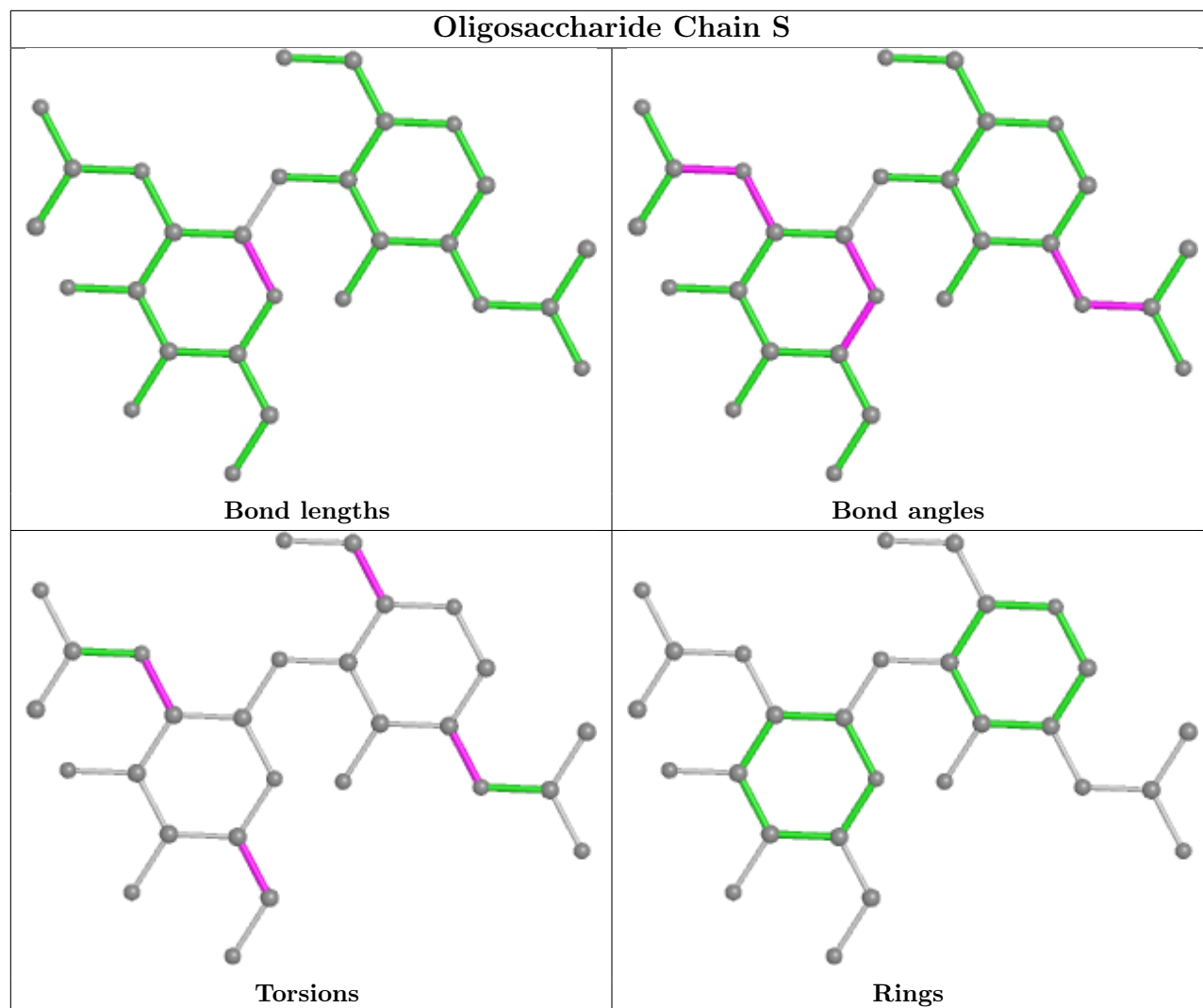


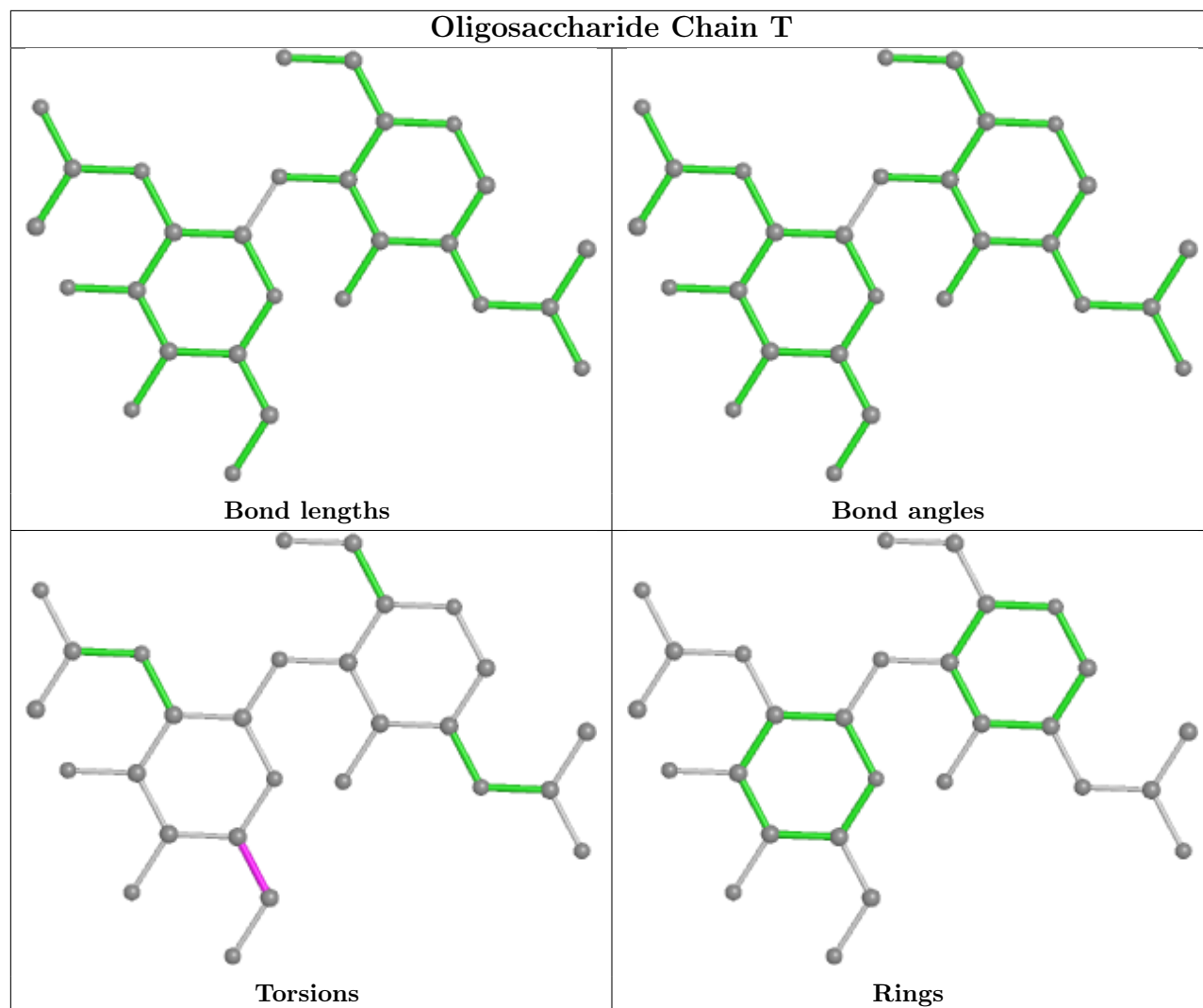


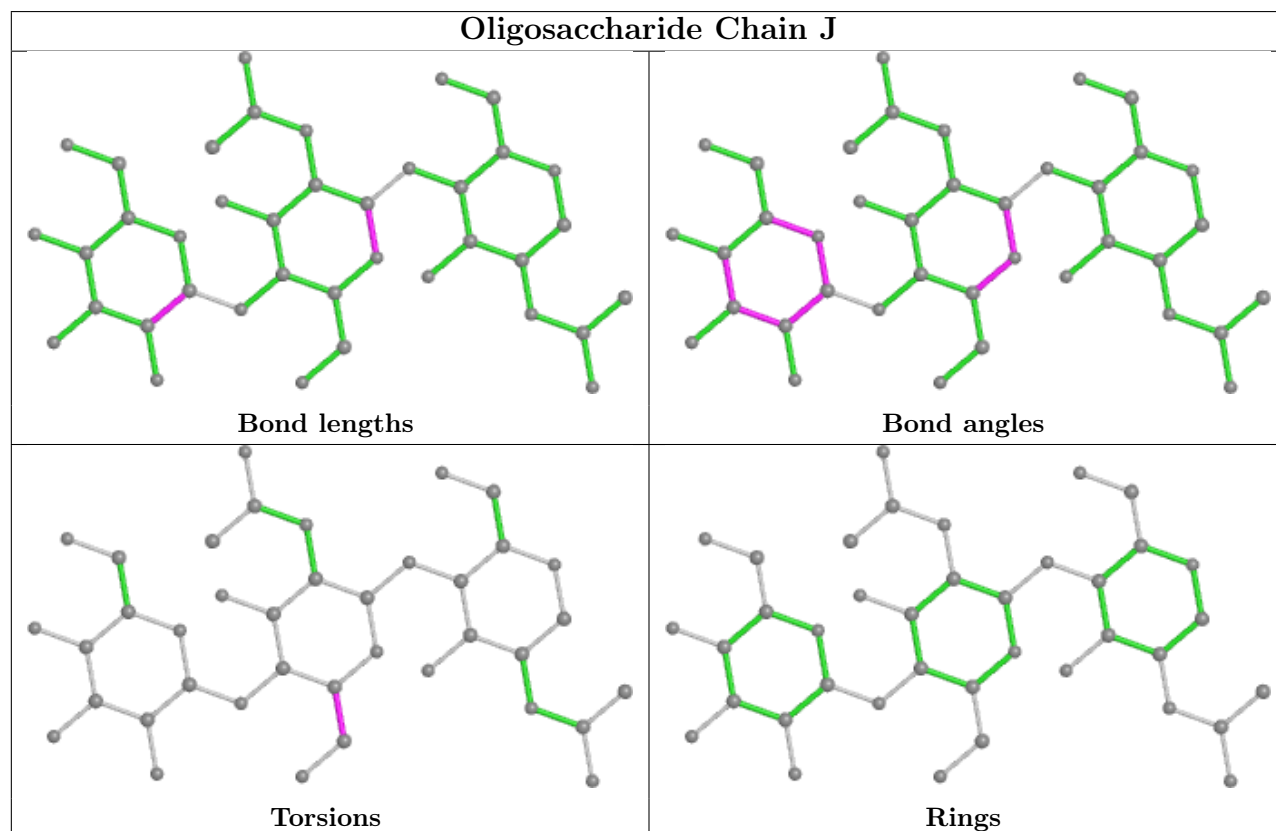
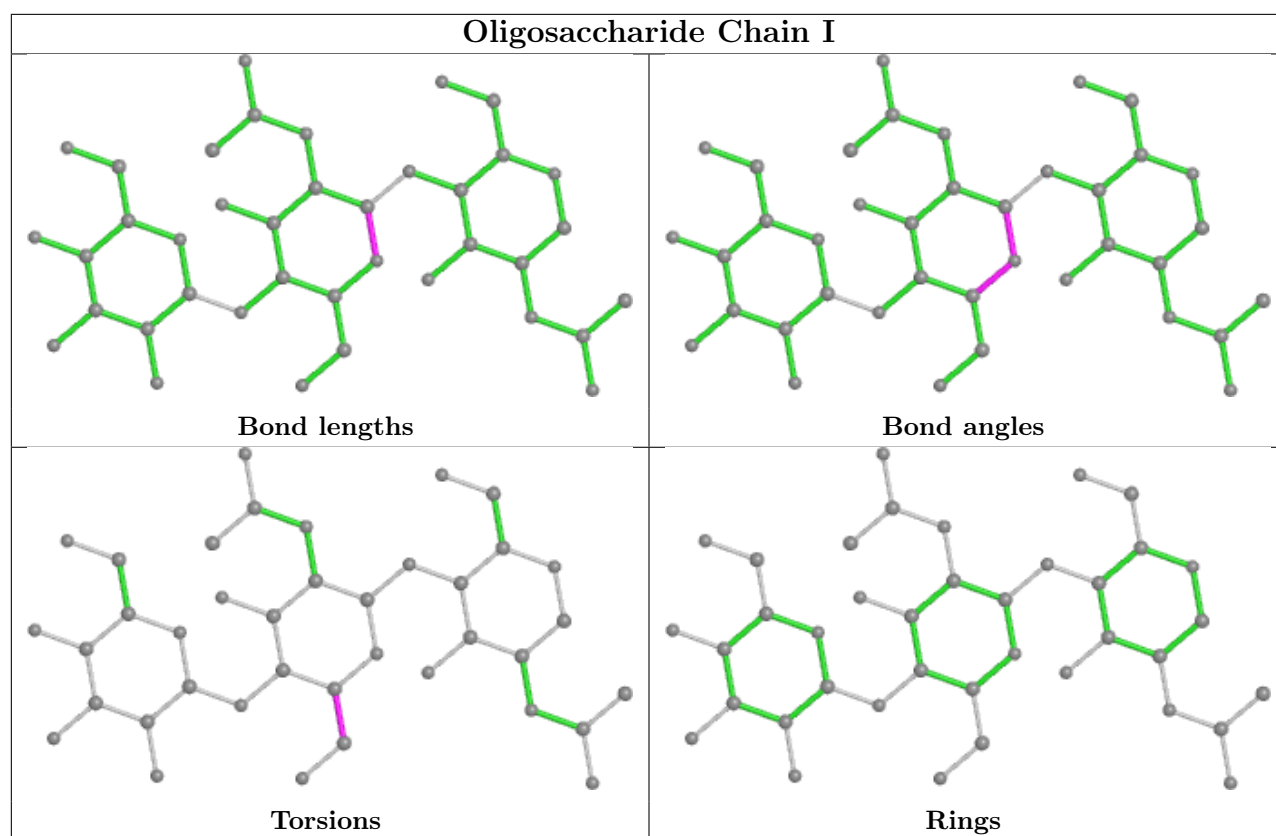


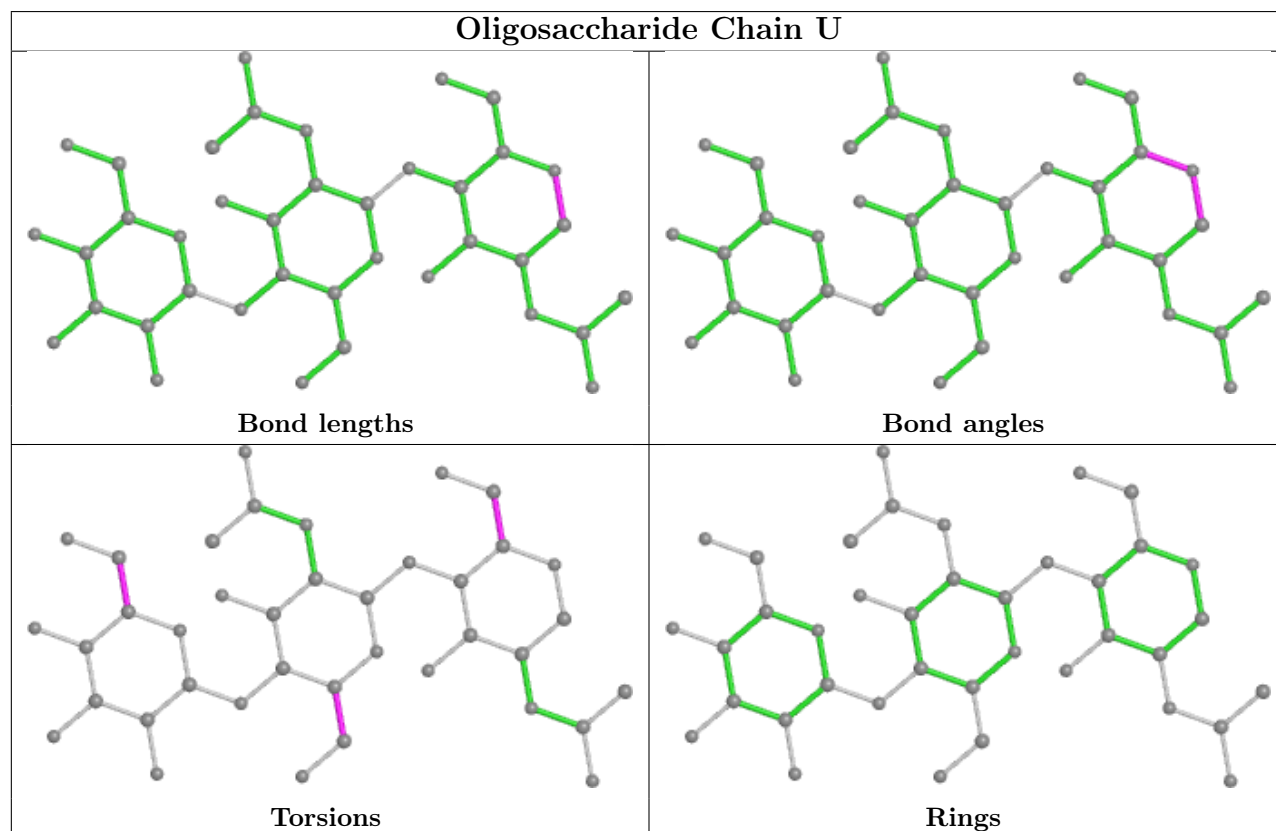
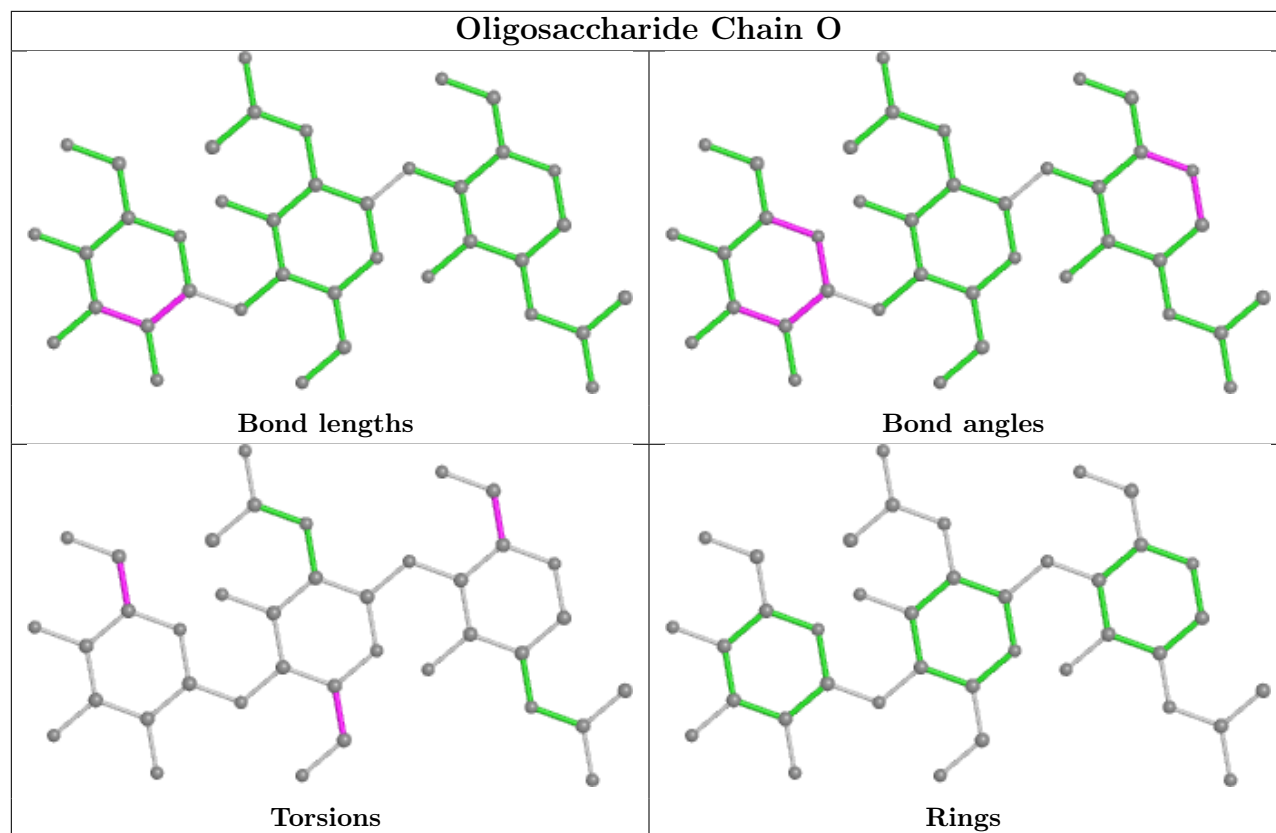


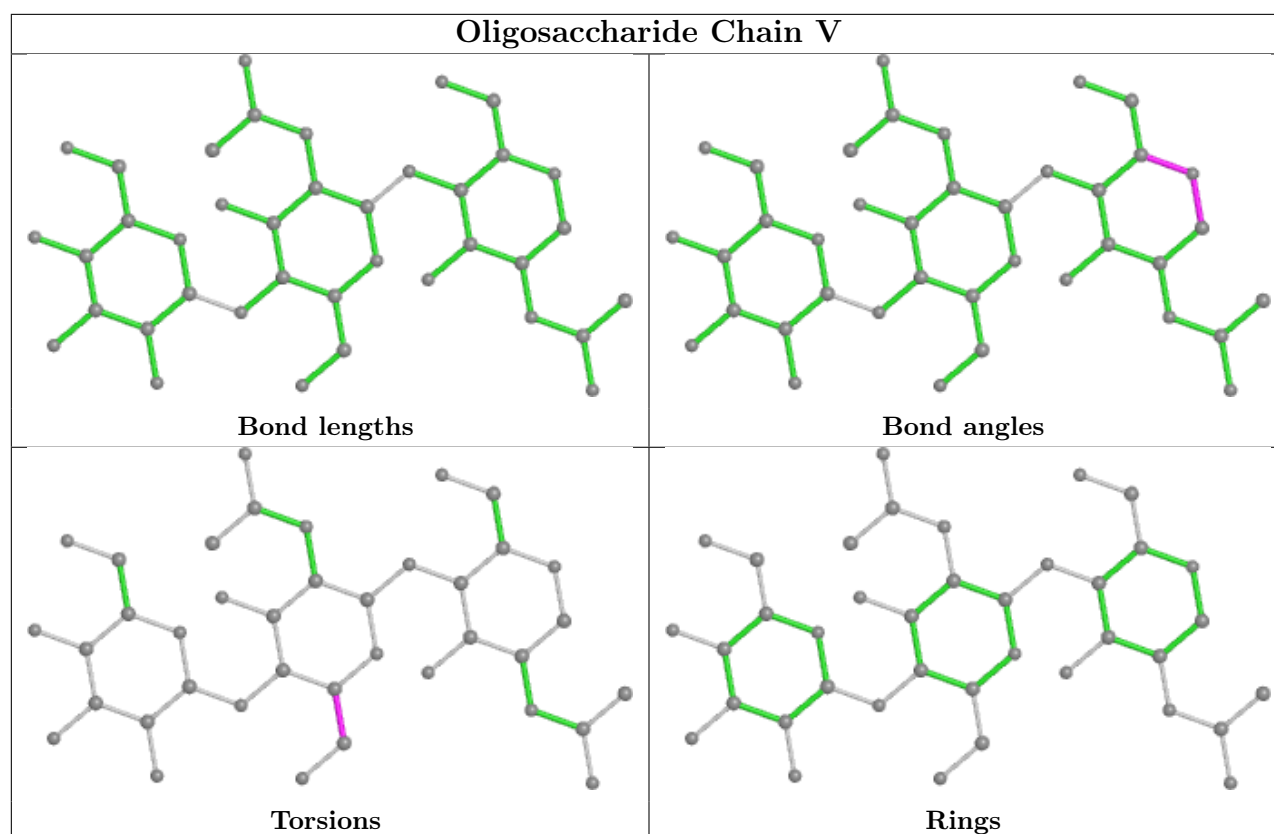












5.6 Ligand geometry [i](#)

30 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	$\# Z > 2$
4	NAG	B	1306	1	14,14,15	0.48	0	17,19,21	0.45	0
4	NAG	C	1308	1	14,14,15	0.53	0	17,19,21	0.53	0
4	NAG	A	1301	1	14,14,15	0.36	0	17,19,21	0.49	0
4	NAG	B	1309	1	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	B	1303	1	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	B	1302	-	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	C	1305	1	14,14,15	1.09	1 (7%)	17,19,21	1.17	1 (5%)
4	NAG	C	1311	1	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	A	1302	1	14,14,15	0.25	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	1304	1	14,14,15	0.40	0	17,19,21	0.30	0
4	NAG	A	1308	1	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	B	1301	1	14,14,15	0.34	0	17,19,21	0.47	0
4	NAG	C	1307	1	14,14,15	0.30	0	17,19,21	0.49	0
4	NAG	A	1307	1	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	C	1303	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	A	1305	1	14,14,15	0.34	0	17,19,21	0.51	0
4	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	0.94	2 (11%)
4	NAG	A	1310	-	14,14,15	0.53	0	17,19,21	0.46	0
4	NAG	C	1309	1	14,14,15	1.11	1 (7%)	17,19,21	1.46	1 (5%)
4	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	B	1307	1	14,14,15	0.54	0	17,19,21	0.44	0
4	NAG	A	1309	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	B	1308	1	14,14,15	0.25	0	17,19,21	0.38	0
4	NAG	C	1302	1	14,14,15	1.18	1 (7%)	17,19,21	1.47	1 (5%)
4	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	C	1301	1	14,14,15	0.33	0	17,19,21	0.60	1 (5%)
4	NAG	C	1306	1	14,14,15	0.64	0	17,19,21	0.82	1 (5%)
4	NAG	C	1304	-	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	C	1310	-	14,14,15	0.93	1 (7%)	17,19,21	1.04	1 (5%)

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
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1310	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	-	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1302	NAG	O5-C1	4.30	1.50	1.43
4	C	1309	NAG	O5-C1	4.00	1.50	1.43
4	C	1305	NAG	O5-C1	3.51	1.49	1.43
4	C	1310	NAG	O5-C1	2.78	1.48	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1302	NAG	C1-O5-C5	5.83	120.10	112.19
4	C	1309	NAG	C1-O5-C5	5.78	120.03	112.19
4	C	1305	NAG	C1-O5-C5	4.63	118.46	112.19
4	C	1310	NAG	C1-O5-C5	4.07	117.70	112.19
4	C	1306	NAG	C2-N2-C7	2.40	126.33	122.90

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1301	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1308	NAG	1	0
4	A	1301	NAG	2	0
4	A	1302	NAG	1	0
4	A	1310	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.

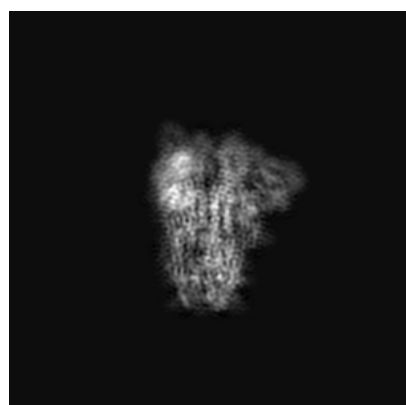
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32479. These allow visual inspection of the internal detail of the map and identification of artifacts.

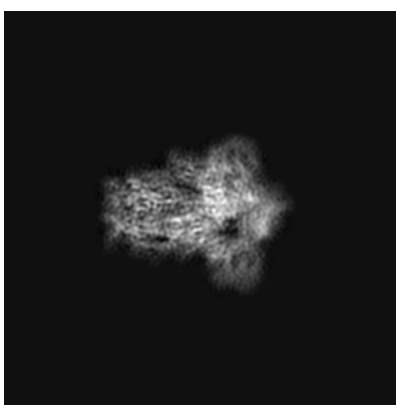
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

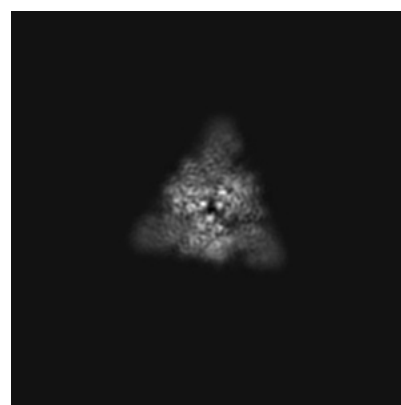
6.1.1 Primary map



X



Y



Z

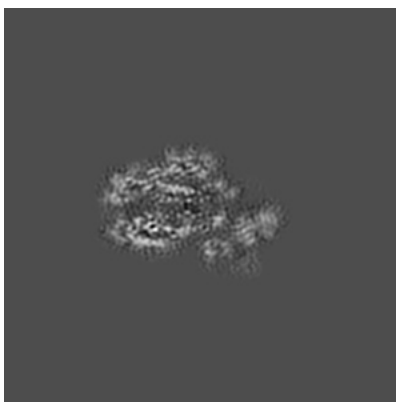
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

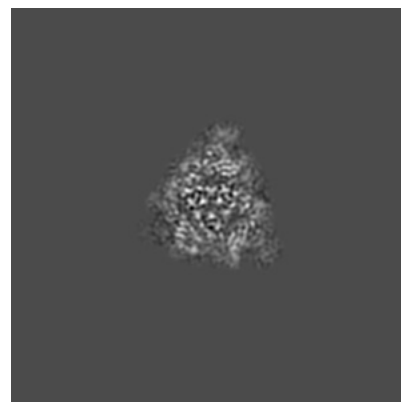
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

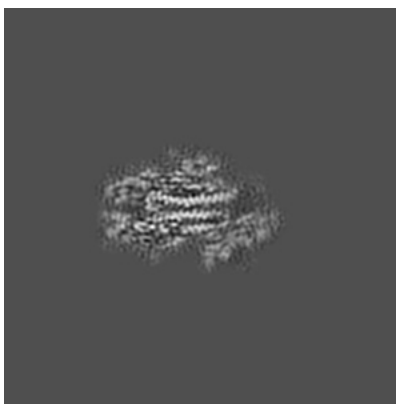
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

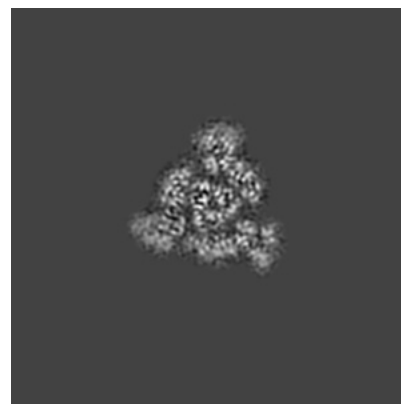
6.3.1 Primary map



X Index: 166



Y Index: 164

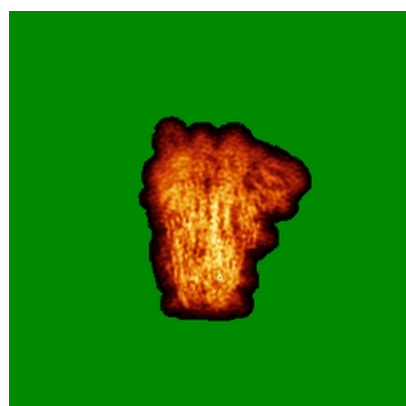


Z Index: 171

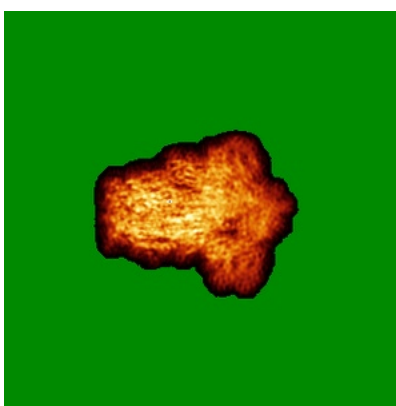
The images above show the largest variance slices of the map in three orthogonal directions.

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

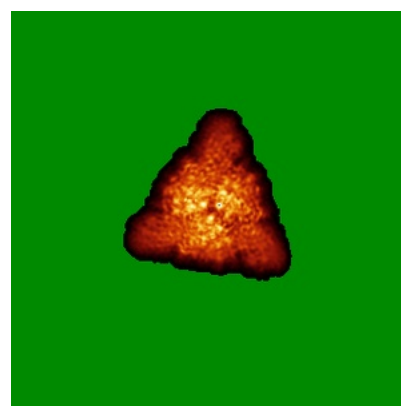
6.4.1 Primary map



X



Y

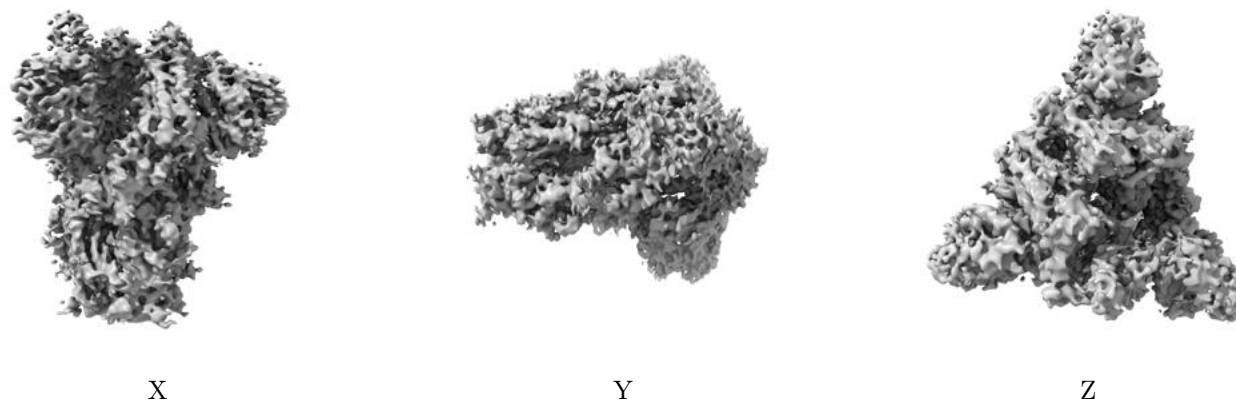


Z

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 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

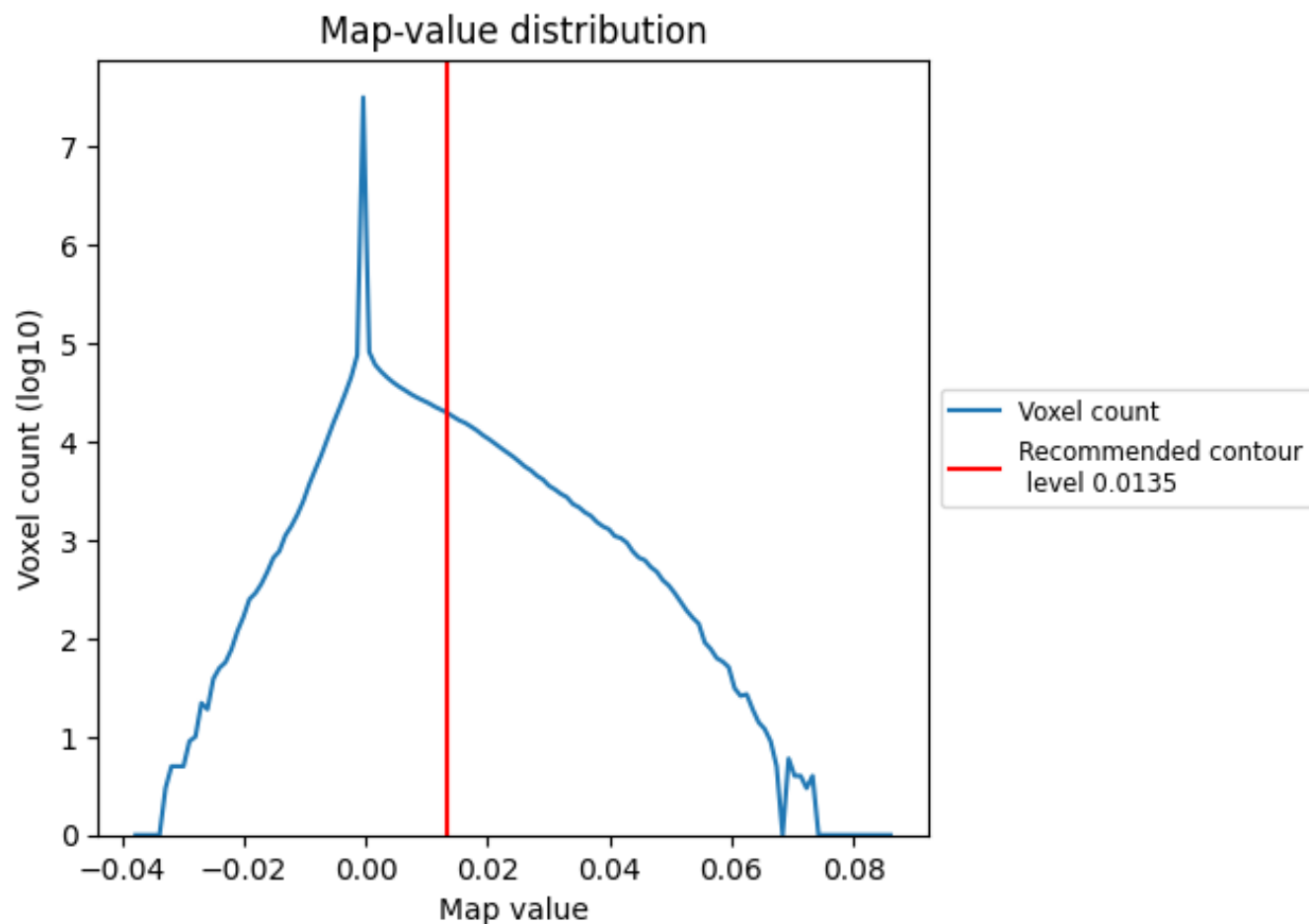
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

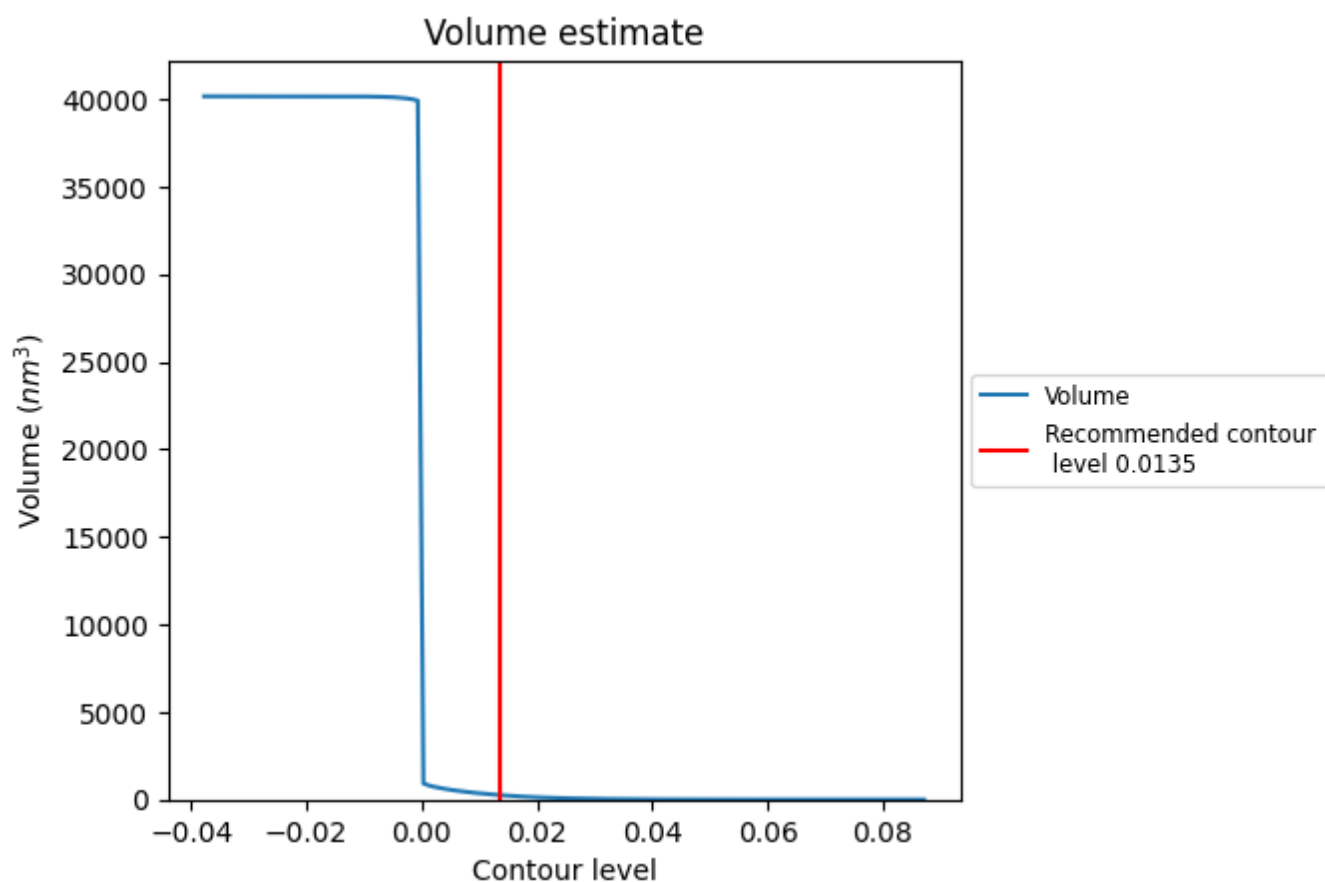
This section contains the results of statistical analysis of the map.

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.

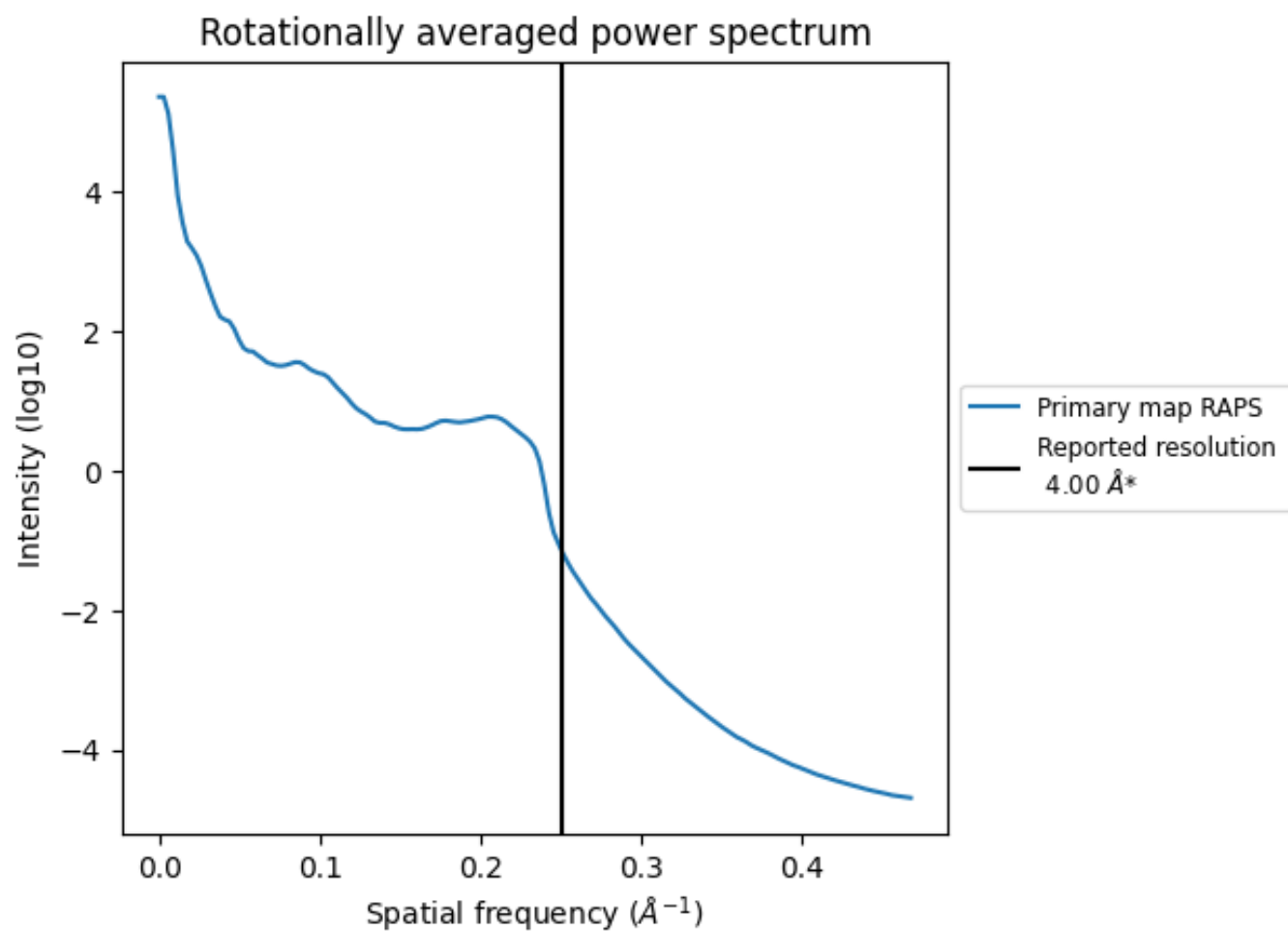
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 256 nm³; this corresponds to an approximate mass of 231 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

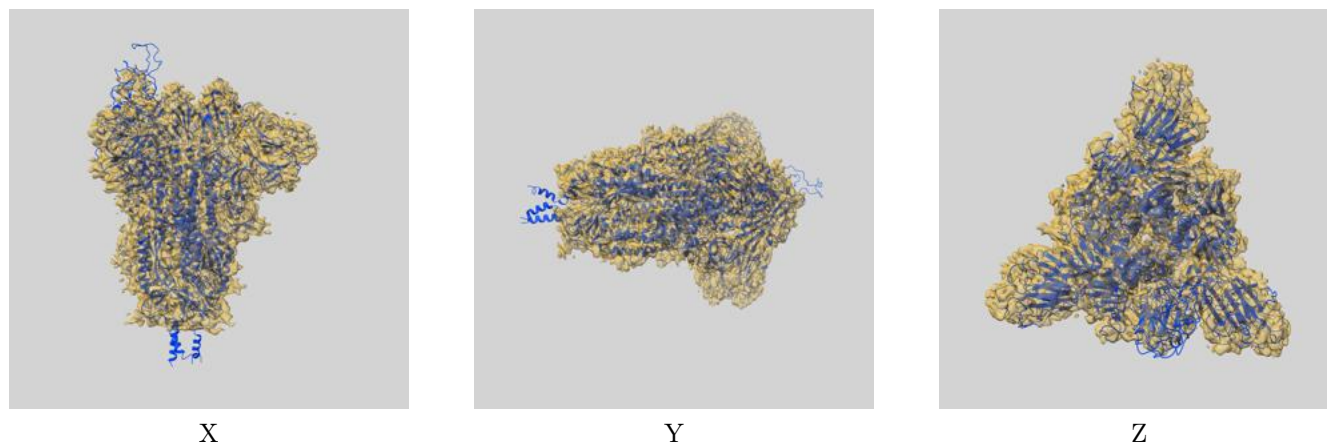
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

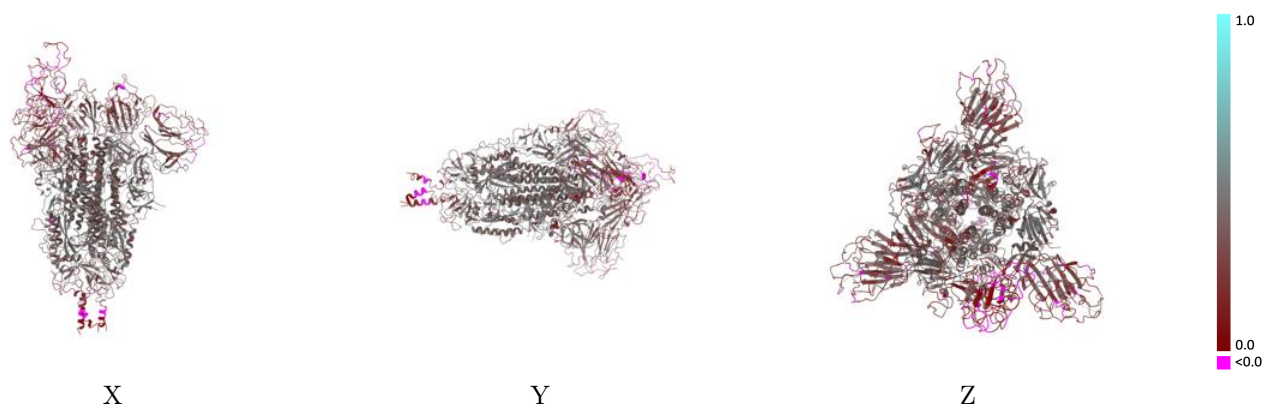
This section contains information regarding the fit between EMDB map EMD-32479 and PDB model 7WG7. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



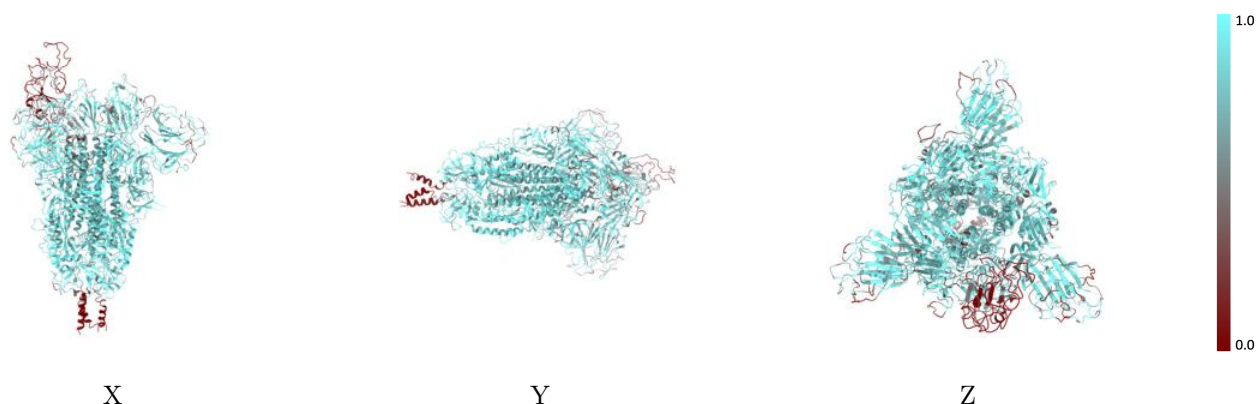
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



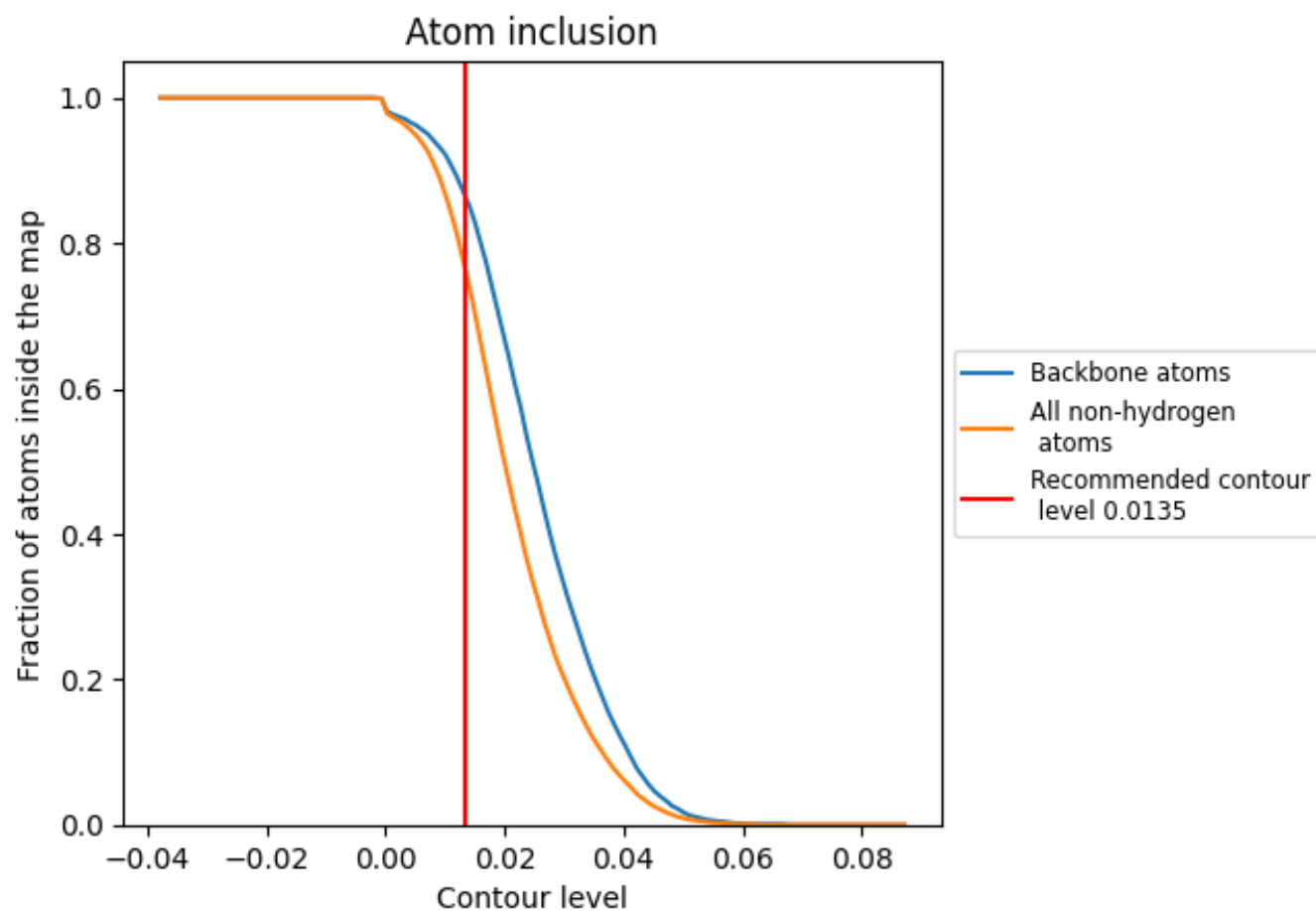
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0135).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.3380
A	 0.8110	 0.3580
B	 0.7870	 0.3440
C	 0.6950	 0.3120
D	 0.0710	 0.3190
E	 0.2140	 0.2010
F	 0.8210	 0.4670
G	 0.5000	 0.3100
H	 0.8570	 0.3330
I	 0.5900	 0.2400
J	 0.4360	 0.2370
K	 0.6070	 0.3750
L	 0.3930	 0.1630
M	 0.8570	 0.4690
N	 0.8930	 0.4560
O	 0.7180	 0.3920
P	 0.6070	 0.3930
Q	 0.3930	 0.3660
R	 0.5710	 0.3970
S	 0.3930	 0.3750
T	 0.8210	 0.4460
U	 0.6410	 0.3440
V	 0.5380	 0.2530

