



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 01:38 AM JST

PDB ID : 7CWU
EMDB ID : EMD-30488
Title : SARS-CoV-2 spike proteins trimer in complex with P17 and FC05 Fabs cocktail
Authors : Wang, X.; Wang, N.
Deposited on : 2020-08-31
Resolution : 3.50 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

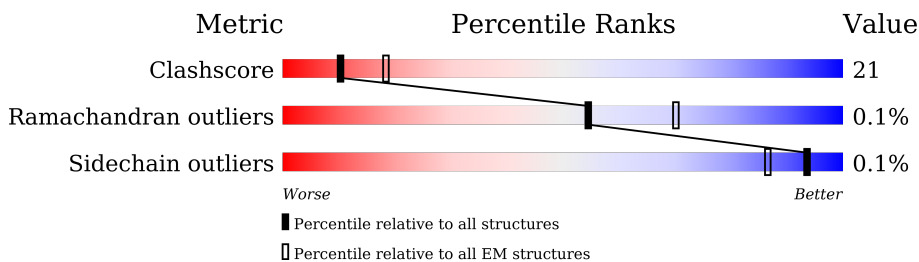
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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




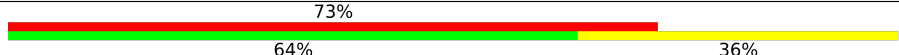






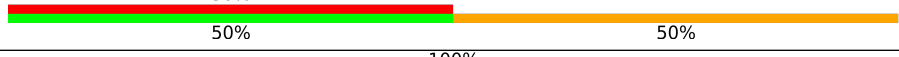
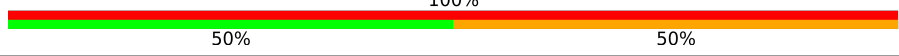

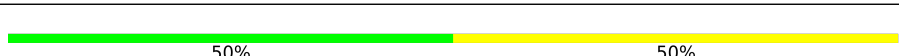
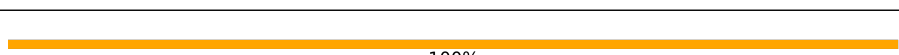
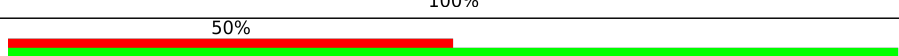
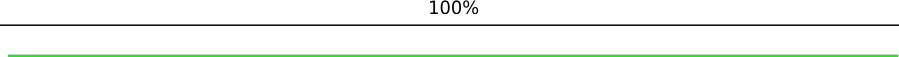
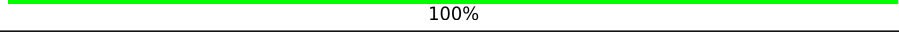

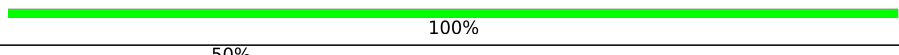
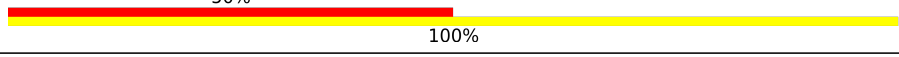


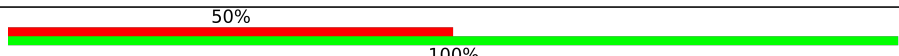
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	J	120	
1	N	120	
1	P	120	
2	F	109	
2	G	109	
2	I	109	
3	A	1273	
3	B	1273	

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Mol	Chain	Length	Quality of chain
3	C	1273	
4	H	120	
4	M	120	
4	O	120	
5	L	108	
5	R	108	
5	S	108	
6	D	2	
6	E	2	
6	K	2	
6	Q	2	
6	T	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	Y	2	
6	Z	2	
6	a	2	
6	b	2	
6	c	2	
6	d	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	D	1	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 36128 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 heavy chain of FC05 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	P	120	931	587	149	188	7	0	0
1	N	120	931	587	149	188	7	0	0
1	J	120	931	587	149	188	7	0	0

- Molecule 2 is a protein called light chain of FC05 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	109	789	492	132	163	2	0	0
2	G	109	789	492	132	163	2	0	0
2	F	109	789	492	132	163	2	0	0

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	1076	8392	5354	1405	1594	39	0	0
3	C	1070	8340	5321	1394	1586	39	0	0
3	A	1075	8387	5351	1404	1593	39	0	0

- Molecule 4 is a protein called heavy chain of P17 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	120	918	574	165	175	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
4	O	120	Total	C	N	O	S	0	0
			918	574	165	175	4		

- Molecule 5 is a protein called light chain of P17 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	108	Total	C	N	O	S	0	0
			817	511	137	167	2		
5	R	108	Total	C	N	O	S	0	0
			817	511	137	167	2		
5	S	108	Total	C	N	O	S	0	0
			817	511	137	167	2		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



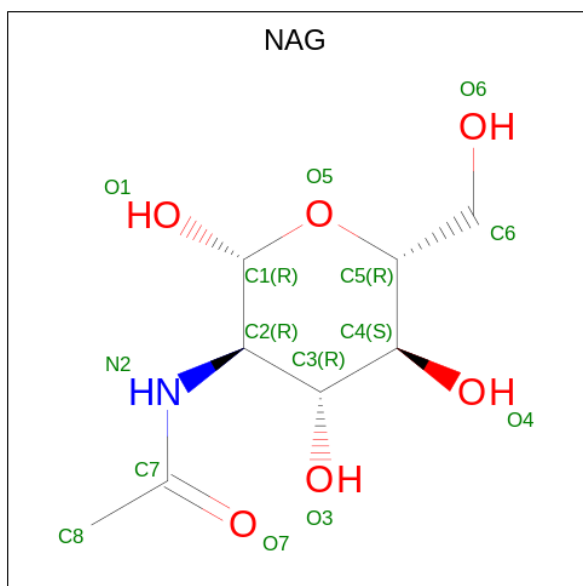
Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	2	Total	C	N	O	0	0
			28	16	2	10		
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	W	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	Y	2	Total 28	C 16	N 2	O 10	0	0
6	Z	2	Total 28	C 16	N 2	O 10	0	0
6	a	2	Total 28	C 16	N 2	O 10	0	0
6	b	2	Total 28	C 16	N 2	O 10	0	0
6	c	2	Total 28	C 16	N 2	O 10	0	0
6	d	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0
7	B	1	Total 70	C 40	N 5	O 25	0

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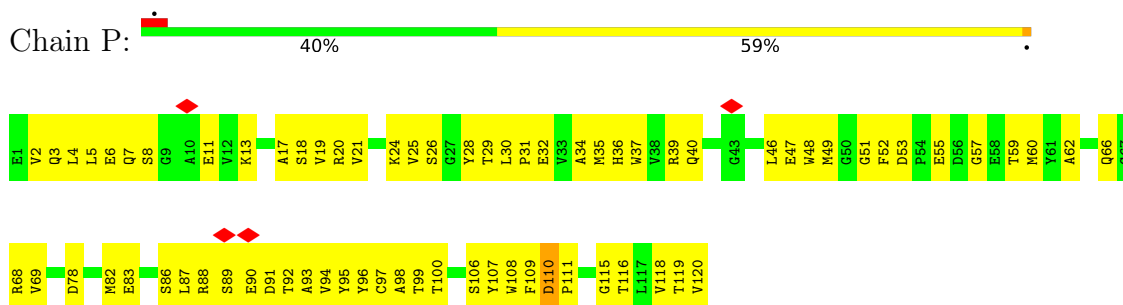
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	C	1	Total 84	48	6	30	0
7	C	1	Total 84	48	6	30	0
7	C	1	Total 84	48	6	30	0
7	C	1	Total 84	48	6	30	0
7	C	1	Total 84	48	6	30	0
7	C	1	Total 84	48	6	30	0
7	A	1	Total 70	40	5	25	0
7	A	1	Total 70	40	5	25	0
7	A	1	Total 70	40	5	25	0
7	A	1	Total 70	40	5	25	0
7	A	1	Total 70	40	5	25	0

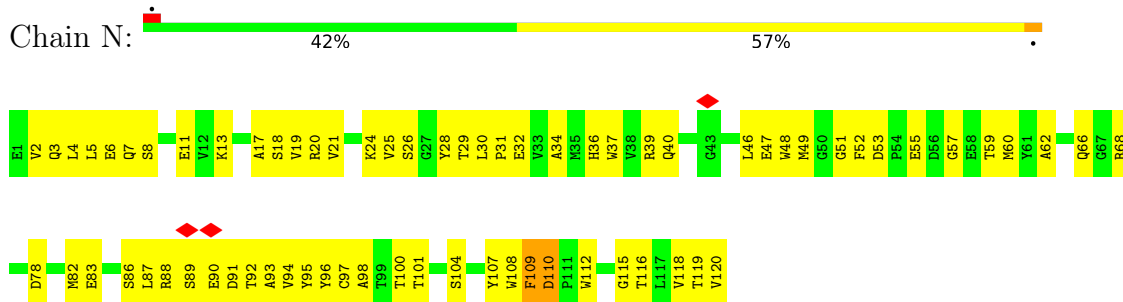
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

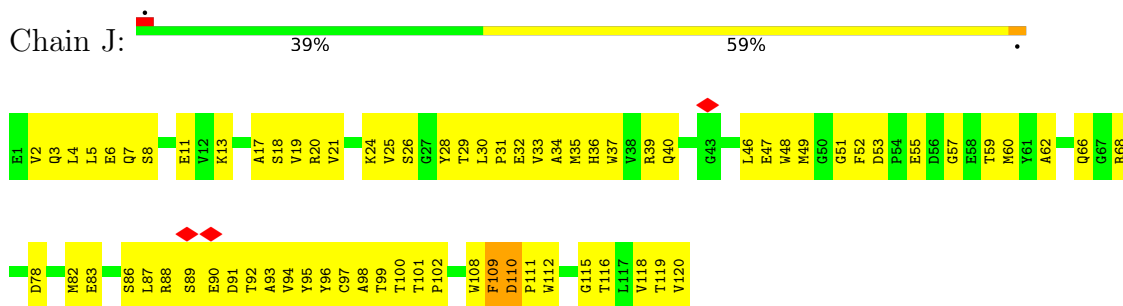
- Molecule 1: heavy chain of FC05 Fab



- Molecule 1: heavy chain of FC05 Fab

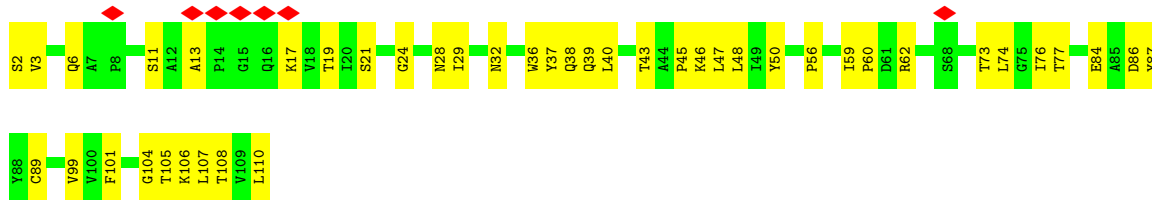


- Molecule 1: heavy chain of FC05 Fab

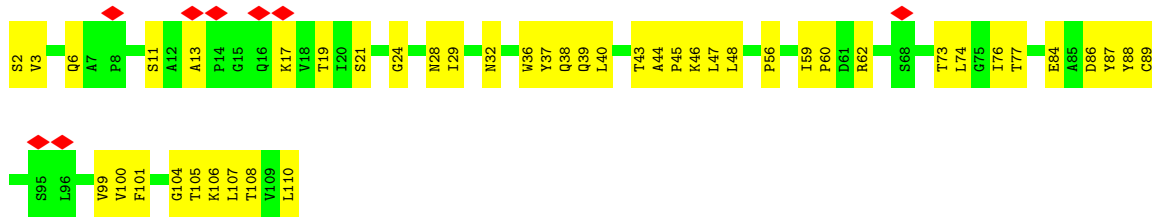


- Molecule 2: light chain of FC05 Fab

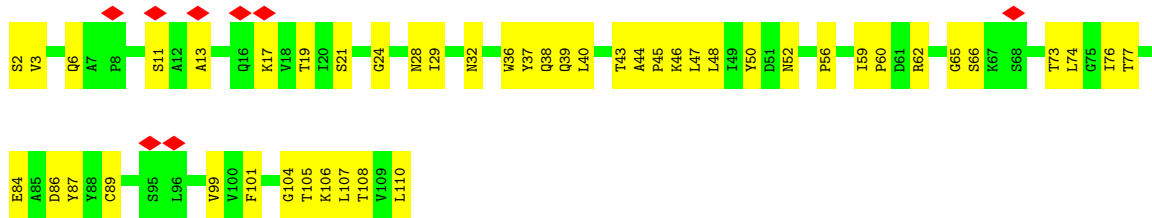




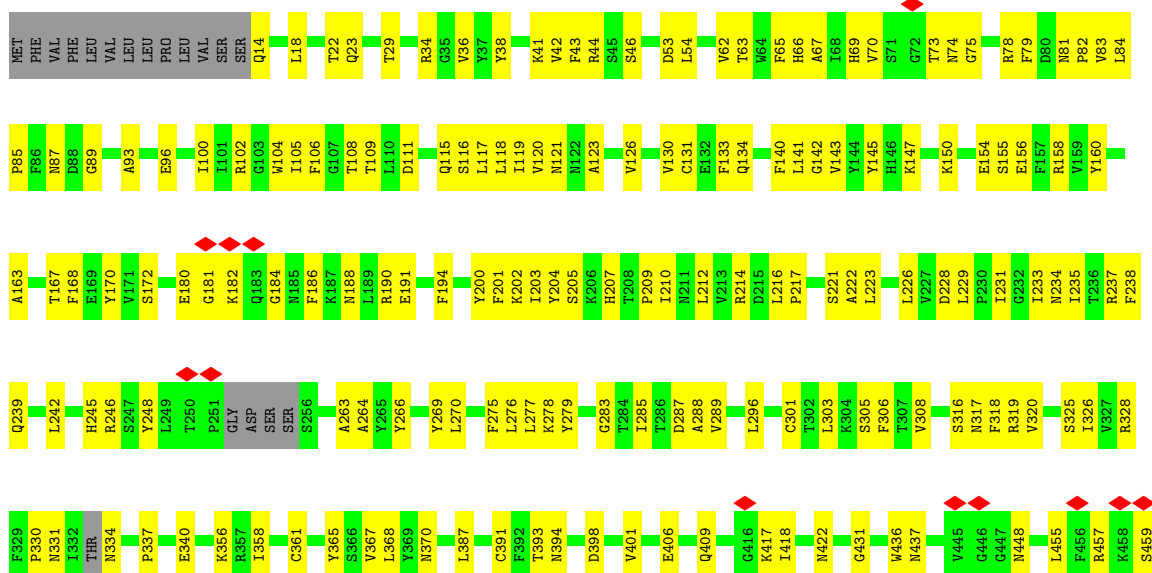
• Molecule 2: light chain of FC05 Fab

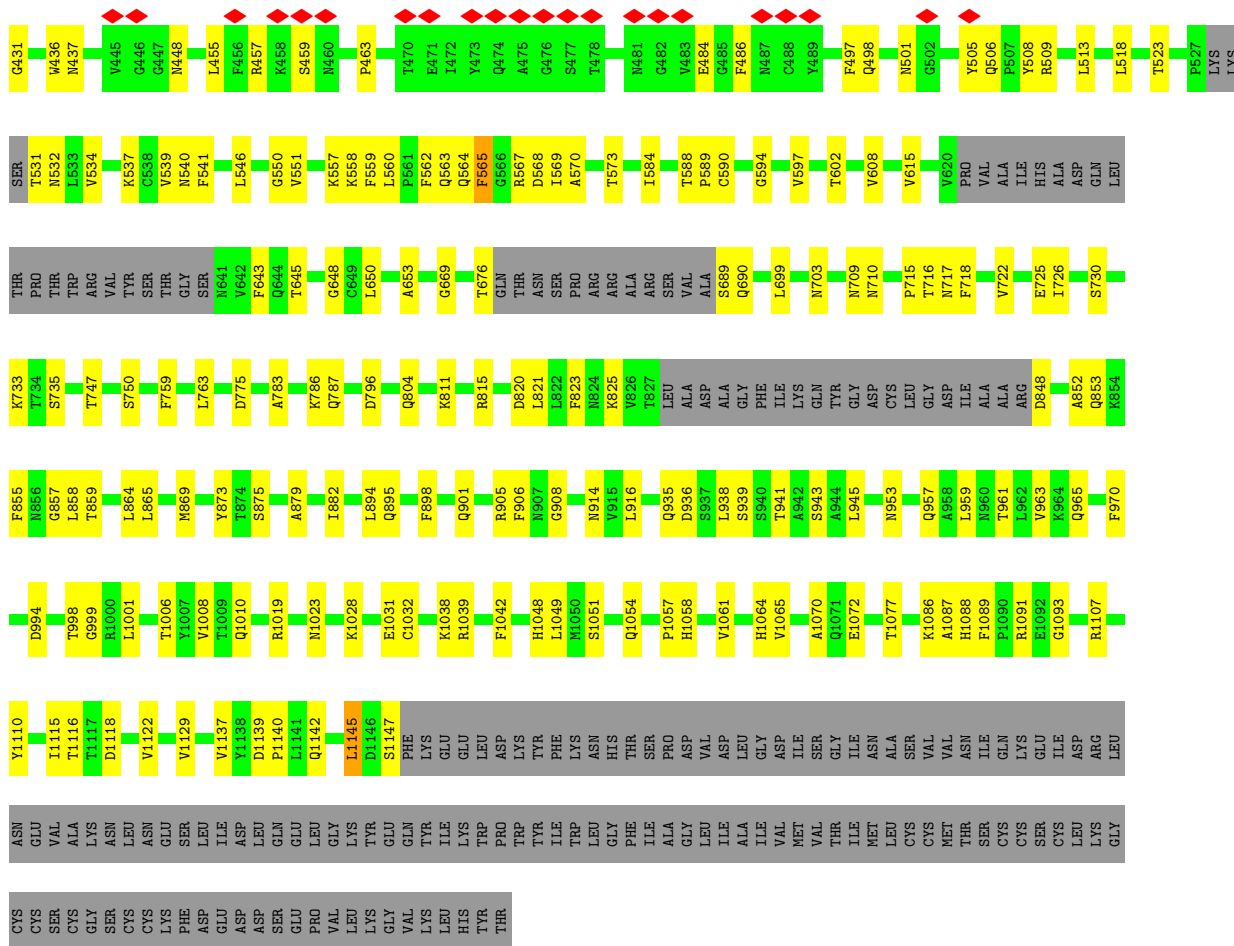


• Molecule 2: light chain of FC05 Fab

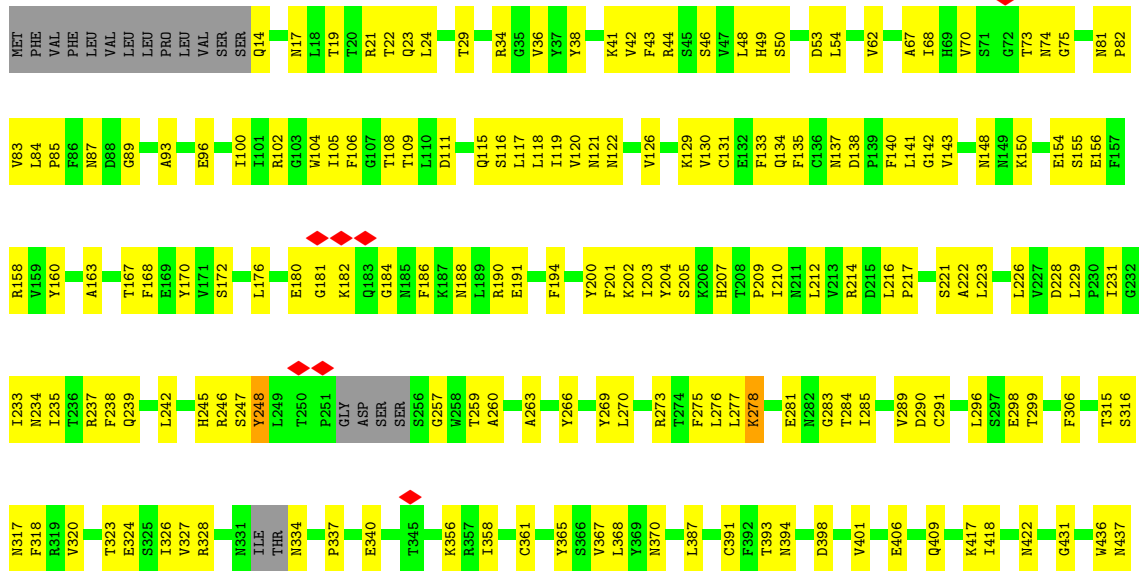


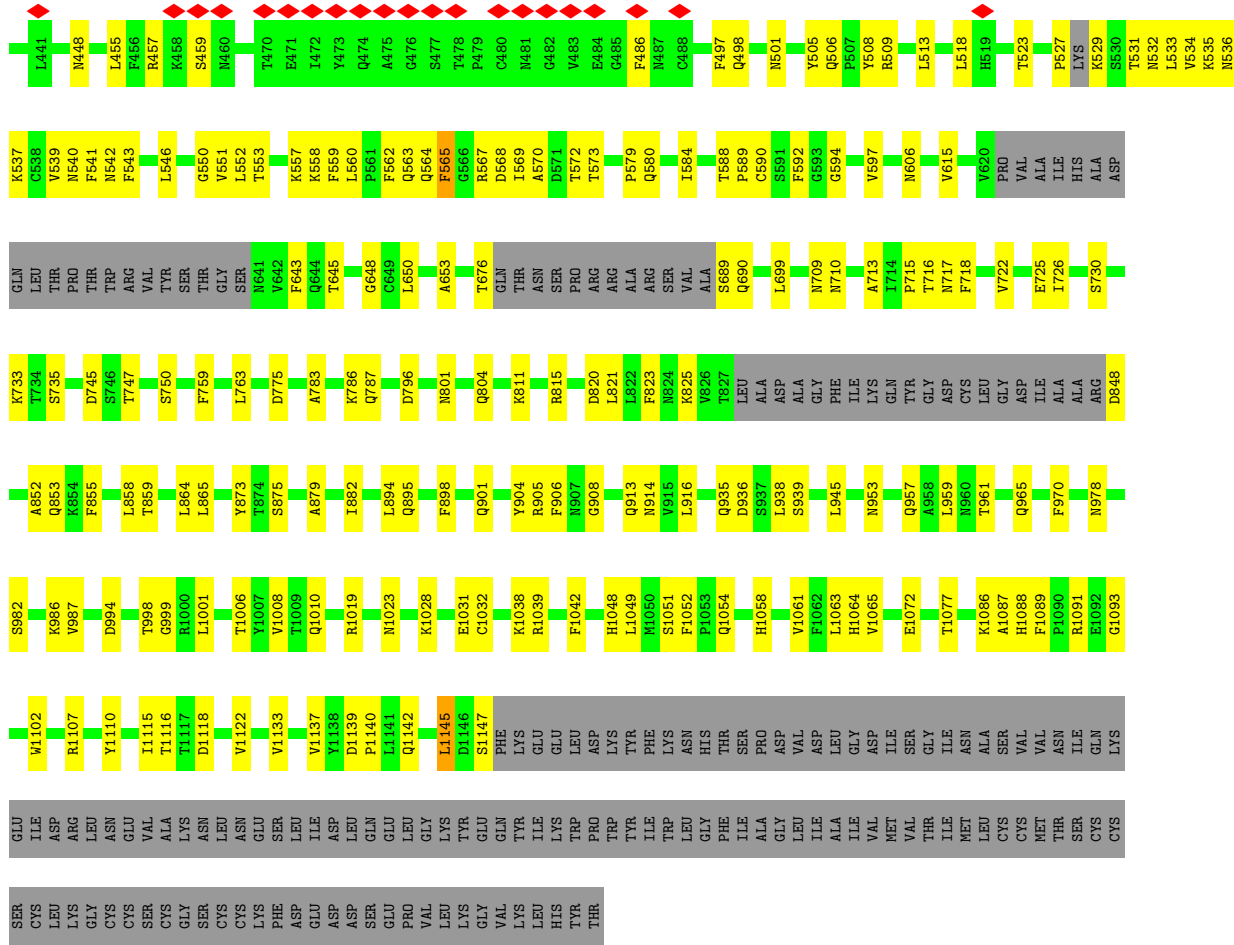
• Molecule 3: Spike glycoprotein



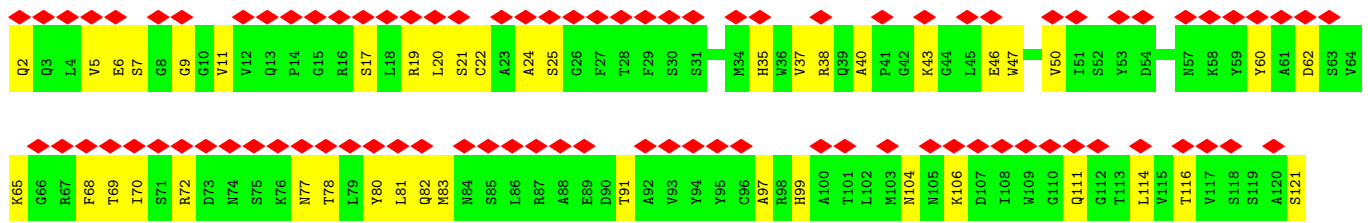
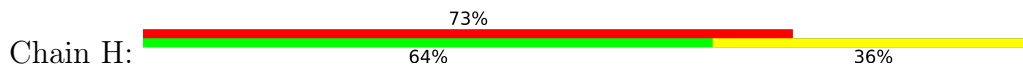


• Molecule 3: Spike glycoprotein

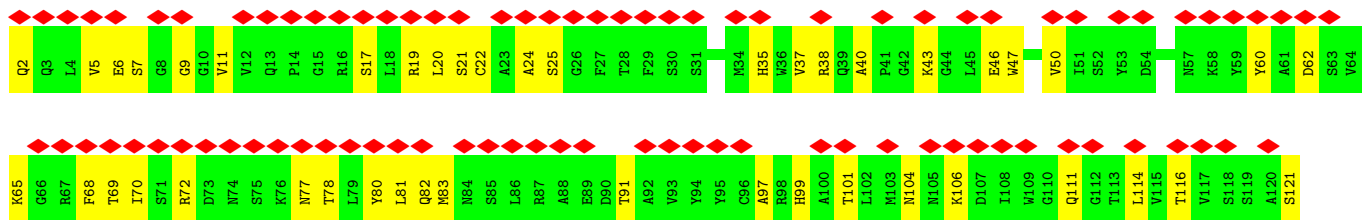
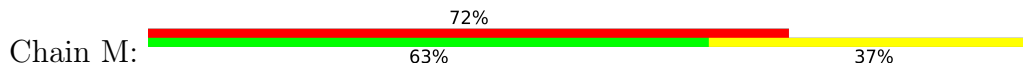




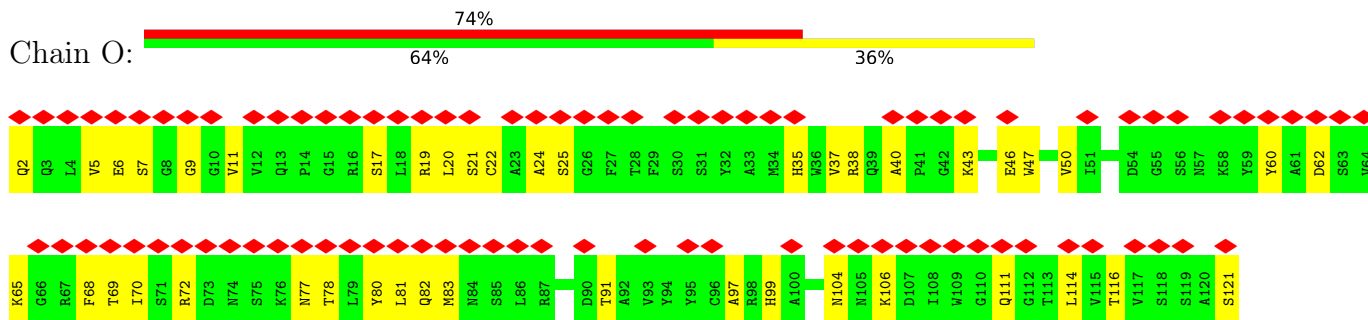
• Molecule 4: heavy chain of P17 Fab



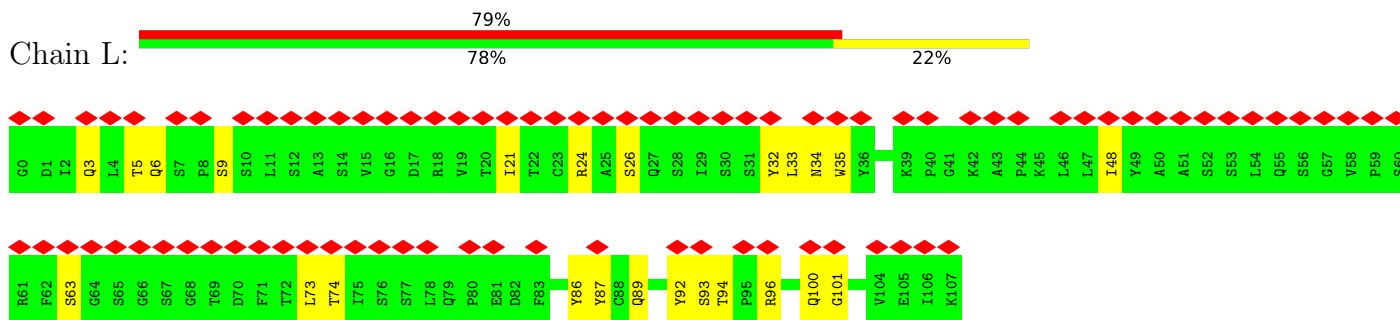
• Molecule 4: heavy chain of P17 Fab



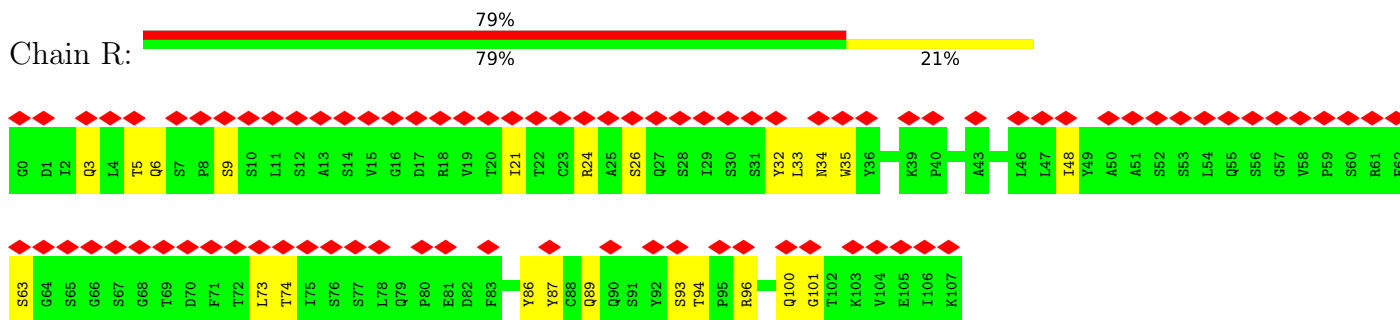
• Molecule 4: heavy chain of P17 Fab



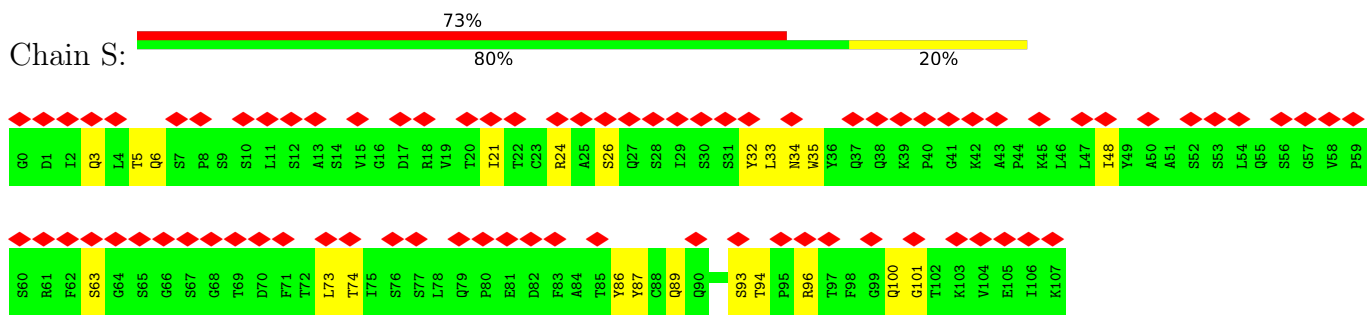
• Molecule 5: light chain of P17 Fab



• Molecule 5: light chain of P17 Fab



• Molecule 5: light chain of P17 Fab



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 50% 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 50% 100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain c:  100%

MAGE
MAGZ

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain d:  100%

MAGE
MAGZ

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99455	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0038	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	J	0.37	0/955	0.58	0/1299
1	N	0.37	0/955	0.59	1/1299 (0.1%)
1	P	0.36	0/955	0.57	0/1299
2	F	0.33	0/805	0.52	0/1097
2	G	0.32	0/805	0.52	0/1097
2	I	0.31	0/805	0.52	0/1097
3	A	0.45	0/8578	0.58	2/11671 (0.0%)
3	B	0.46	0/8583	0.58	1/11678 (0.0%)
3	C	0.44	0/8529	0.57	2/11606 (0.0%)
4	H	0.37	0/937	0.60	0/1269
4	M	0.37	0/937	0.60	0/1269
4	O	0.37	0/937	0.60	0/1269
5	L	0.38	0/834	0.59	0/1131
5	R	0.38	0/834	0.59	0/1131
5	S	0.38	0/834	0.59	0/1131
All	All	0.43	0/36283	0.58	6/49343 (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	J	0	1
1	N	0	1
1	P	0	2
3	A	0	5
3	B	0	3
3	C	0	4
4	H	0	1
4	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	O	0	1
All	All	0	19

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	110	ASP	CB-CA-C	5.51	121.42	110.40
3	C	848	ASP	CB-CG-OD2	5.26	123.03	118.30
3	A	848	ASP	CB-CG-OD2	5.17	122.95	118.30
3	B	387	LEU	CA-CB-CG	5.04	126.90	115.30
3	A	387	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	248	TYR	Peptide
1	J	8	SER	Peptide
1	N	8	SER	Peptide
1	P	110	ASP	Sidechain
1	P	8	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	931	0	878	77	0
1	N	931	0	878	78	0
1	P	931	0	878	122	0
2	F	789	0	768	48	0
2	G	789	0	768	41	0
2	I	789	0	768	51	0
3	A	8387	0	8173	366	0
3	B	8392	0	8175	390	0
3	C	8340	0	8121	412	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	918	0	885	25	0
4	M	918	0	885	27	0
4	O	918	0	885	26	0
5	L	817	0	800	18	0
5	R	817	0	800	17	0
5	S	817	0	800	15	0
6	D	28	0	25	7	0
6	E	28	0	25	1	0
6	K	28	0	25	1	0
6	Q	28	0	25	1	0
6	T	28	0	25	2	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
6	W	28	0	25	1	0
6	X	28	0	25	0	0
6	Y	28	0	25	5	0
6	Z	28	0	25	0	0
6	a	28	0	25	0	0
6	b	28	0	25	0	0
6	c	28	0	25	0	0
6	d	28	0	25	0	0
7	A	70	0	65	1	0
7	B	70	0	65	0	0
7	C	84	0	78	1	0
All	All	36128	0	35045	1515	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 1515 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:276:LEU:HD11	3:C:306:PHE:CE1	1.33	1.62
3:B:234:ASN:HD22	6:D:1:NAG:C1	1.10	1.62
3:C:234:ASN:HD22	6:E:1:NAG:C1	1.03	1.57
3:B:22:THR:CG2	3:B:78:ARG:HD2	1.28	1.57
3:B:63:THR:CG2	3:B:65:PHE:CZ	1.85	1.57

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	J	118/120 (98%)	108 (92%)	9 (8%)	1 (1%)	19	58
1	N	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	19	58
1	P	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
2	F	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
2	G	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
2	I	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
3	A	1061/1273 (83%)	980 (92%)	81 (8%)	0	100	100
3	B	1062/1273 (83%)	981 (92%)	81 (8%)	0	100	100
3	C	1056/1273 (83%)	983 (93%)	72 (7%)	1 (0%)	51	84
4	H	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
4	M	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
4	O	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
5	L	106/108 (98%)	97 (92%)	9 (8%)	0	100	100
5	R	106/108 (98%)	97 (92%)	9 (8%)	0	100	100
5	S	106/108 (98%)	97 (92%)	9 (8%)	0	100	100
All	All	4526/5190 (87%)	4184 (92%)	339 (8%)	3 (0%)	54	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	110	ASP
1	J	110	ASP
3	C	24	LEU

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	J	101/101 (100%)	100 (99%)	1 (1%)	76	88
1	N	101/101 (100%)	100 (99%)	1 (1%)	76	88
1	P	101/101 (100%)	101 (100%)	0	100	100
2	F	88/88 (100%)	88 (100%)	0	100	100
2	G	88/88 (100%)	88 (100%)	0	100	100
2	I	88/88 (100%)	88 (100%)	0	100	100
3	A	934/1112 (84%)	933 (100%)	1 (0%)	93	98
3	B	934/1112 (84%)	934 (100%)	0	100	100
3	C	928/1112 (84%)	928 (100%)	0	100	100
4	H	96/98 (98%)	96 (100%)	0	100	100
4	M	96/98 (98%)	96 (100%)	0	100	100
4	O	96/98 (98%)	96 (100%)	0	100	100
5	L	93/93 (100%)	93 (100%)	0	100	100
5	R	93/93 (100%)	93 (100%)	0	100	100
5	S	93/93 (100%)	93 (100%)	0	100	100
All	All	3930/4476 (88%)	3927 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	109	PHE
1	J	109	PHE
3	A	533	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	804	GLN

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Mol	Chain	Res	Type
4	O	84	ASN
3	A	239	GLN
4	O	39	GLN
4	M	39	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](#)

30 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$
6	NAG	D	1	3,6	14,14,15	1.20	1 (7%)	17,19,21	1.10	2 (11%)
6	NAG	D	2	6	14,14,15	0.35	0	17,19,21	0.44	0
6	NAG	E	1	3,6	14,14,15	1.65	1 (7%)	17,19,21	1.39	2 (11%)
6	NAG	E	2	6	14,14,15	0.21	0	17,19,21	0.52	0
6	NAG	K	1	3,6	14,14,15	1.66	1 (7%)	17,19,21	1.39	2 (11%)
6	NAG	K	2	6	14,14,15	0.22	0	17,19,21	0.50	0
6	NAG	Q	1	3,6	14,14,15	0.49	0	17,19,21	0.45	0
6	NAG	Q	2	6	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	T	1	3,6	14,14,15	0.30	0	17,19,21	1.00	1 (5%)
6	NAG	T	2	6	14,14,15	0.47	0	17,19,21	1.21	2 (11%)
6	NAG	U	1	3,6	14,14,15	0.46	0	17,19,21	0.39	0
6	NAG	U	2	6	14,14,15	0.29	0	17,19,21	0.43	0
6	NAG	V	1	3,6	14,14,15	0.52	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	V	2	6	14,14,15	0.34	0	17,19,21	0.39	0
6	NAG	W	1	3,6	14,14,15	0.47	0	17,19,21	0.45	0
6	NAG	W	2	6	14,14,15	0.27	0	17,19,21	0.36	0
6	NAG	X	1	3,6	14,14,15	0.43	0	17,19,21	0.45	0
6	NAG	X	2	6	14,14,15	0.29	0	17,19,21	0.37	0
6	NAG	Y	1	3,6	14,14,15	0.27	0	17,19,21	0.69	0
6	NAG	Y	2	6	14,14,15	0.26	0	17,19,21	0.70	0
6	NAG	Z	1	3,6	14,14,15	0.33	0	17,19,21	0.49	0
6	NAG	Z	2	6	14,14,15	0.32	0	17,19,21	0.40	0
6	NAG	a	1	3,6	14,14,15	0.49	0	17,19,21	0.44	0
6	NAG	a	2	6	14,14,15	0.17	0	17,19,21	0.45	0
6	NAG	b	1	3,6	14,14,15	0.50	0	17,19,21	0.39	0
6	NAG	b	2	6	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	c	1	3,6	14,14,15	0.50	0	17,19,21	0.51	0
6	NAG	c	2	6	14,14,15	0.26	0	17,19,21	0.38	0
6	NAG	d	1	3,6	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	d	2	6	14,14,15	0.33	0	17,19,21	0.39	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
6	NAG	D	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	E	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
6	NAG	K	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	NAG	Q	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	T	1	3,6	-	3/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	NAG	U	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
6	NAG	V	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	X	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Y	1	3,6	-	3/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	NAG	b	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	b	2	6	-	2/6/23/26	0/1/1/1
6	NAG	c	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	c	2	6	-	1/6/23/26	0/1/1/1
6	NAG	d	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1	NAG	O5-C1	-5.99	1.34	1.43
6	E	1	NAG	O5-C1	-5.96	1.34	1.43
6	D	1	NAG	O5-C1	-3.88	1.37	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	2	NAG	C1-O5-C5	3.71	117.21	112.19
6	K	1	NAG	C3-C4-C5	3.67	116.79	110.24
6	E	1	NAG	C3-C4-C5	3.65	116.76	110.24
6	D	1	NAG	C3-C4-C5	3.22	115.98	110.24
6	T	1	NAG	C4-C3-C2	-2.63	107.16	111.02

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	T	1	NAG	C8-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2

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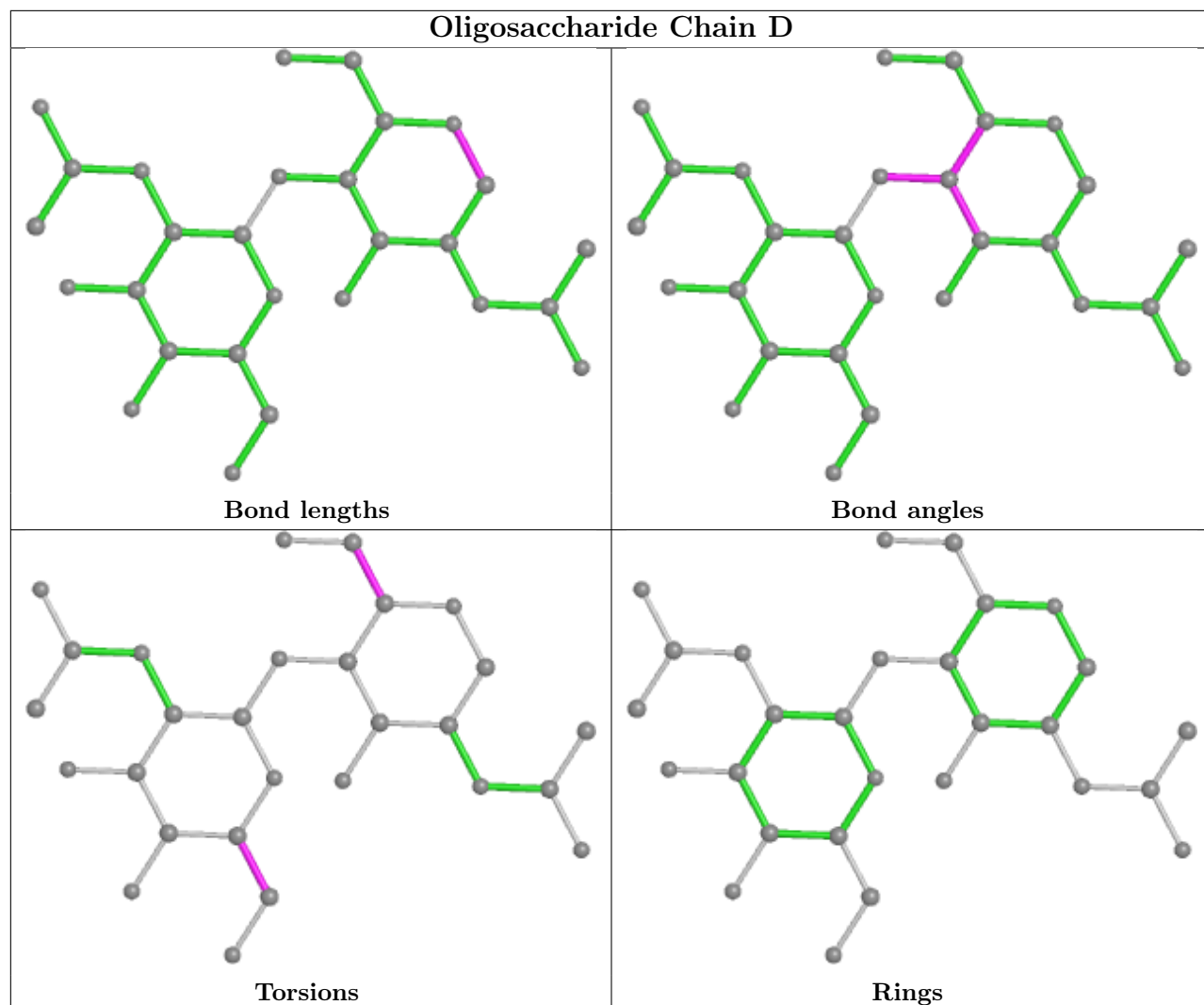
Mol	Chain	Res	Type	Atoms
6	Z	2	NAG	O5-C5-C6-O6

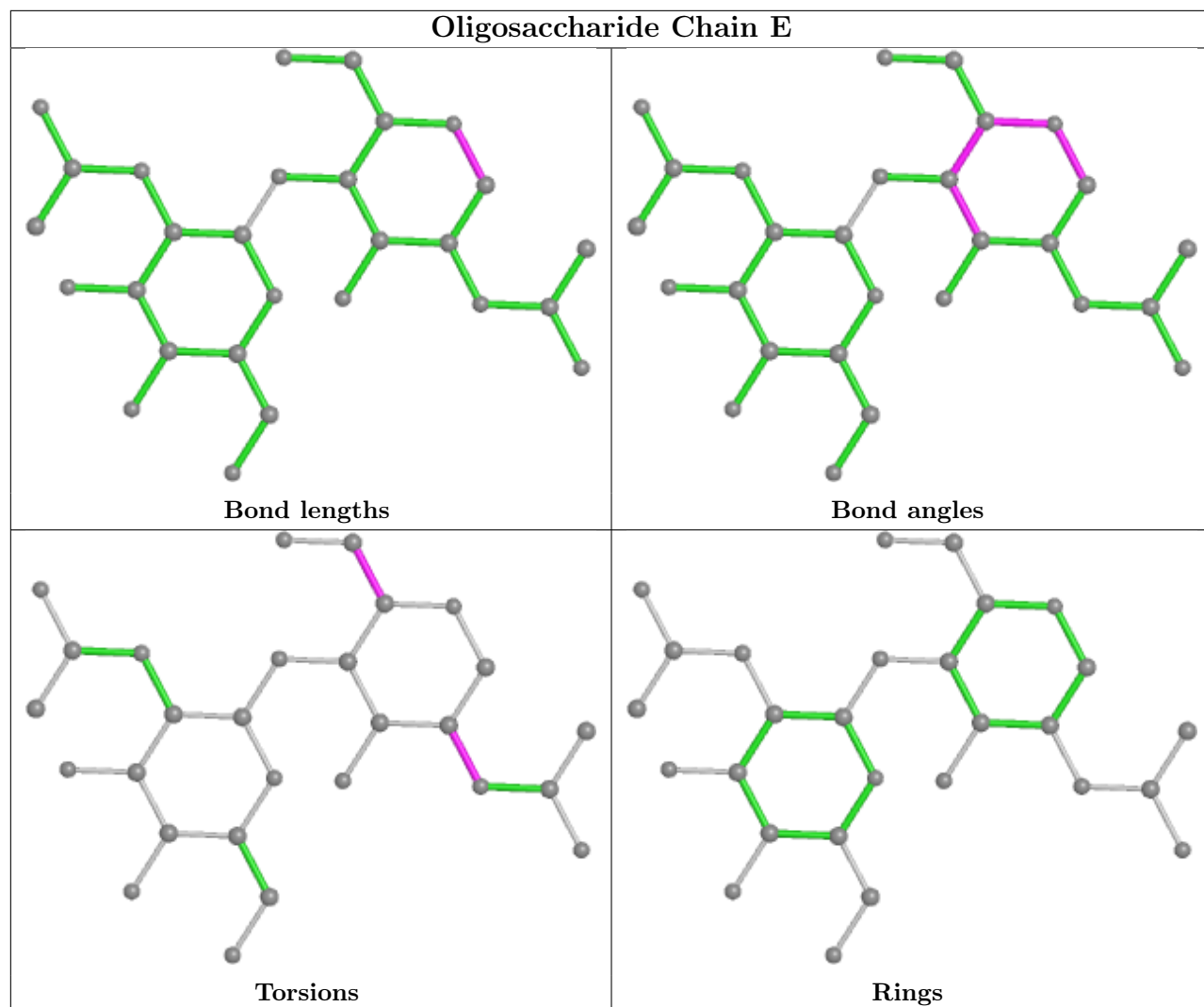
There are no ring outliers.

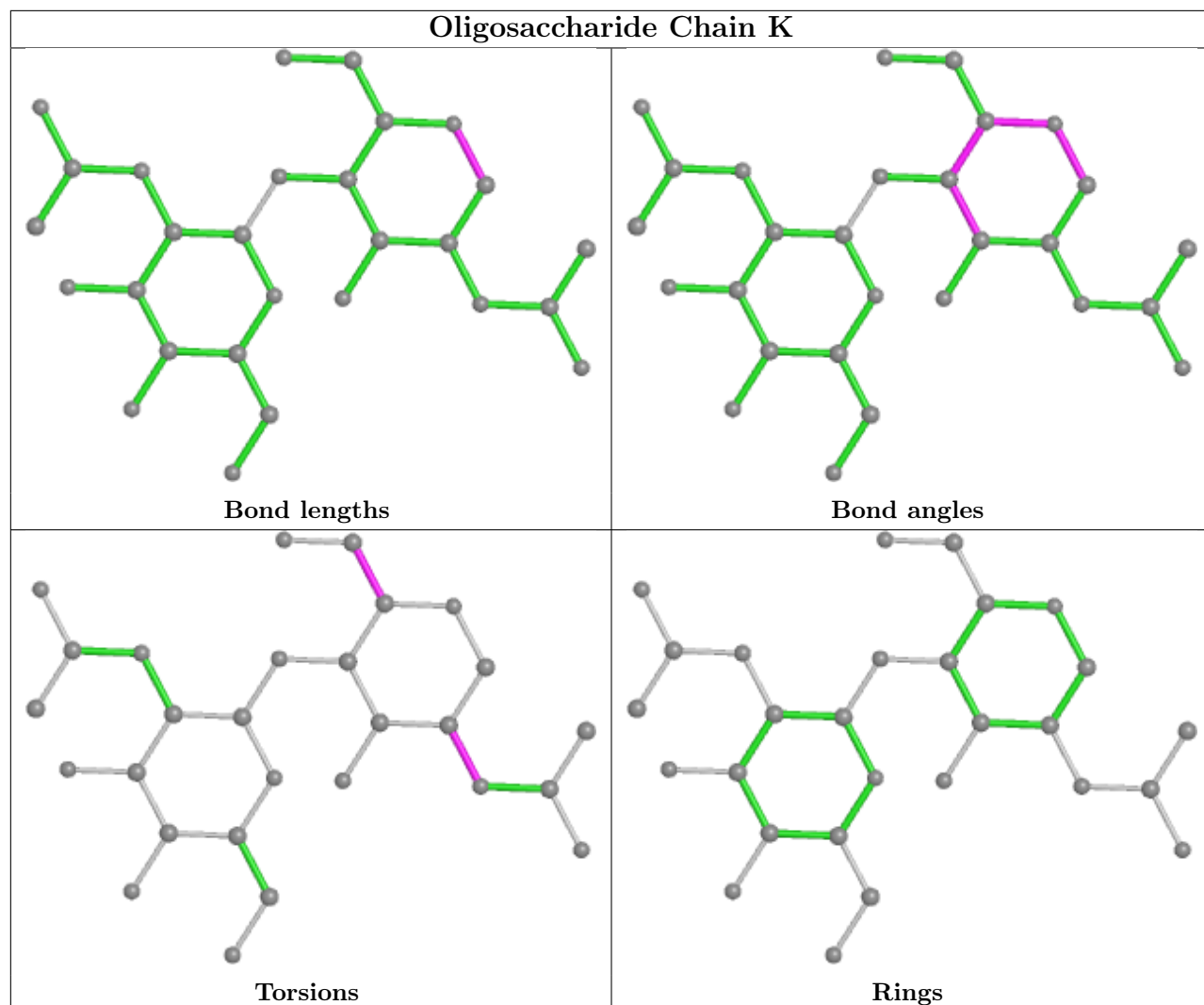
9 monomers are involved in 18 short contacts:

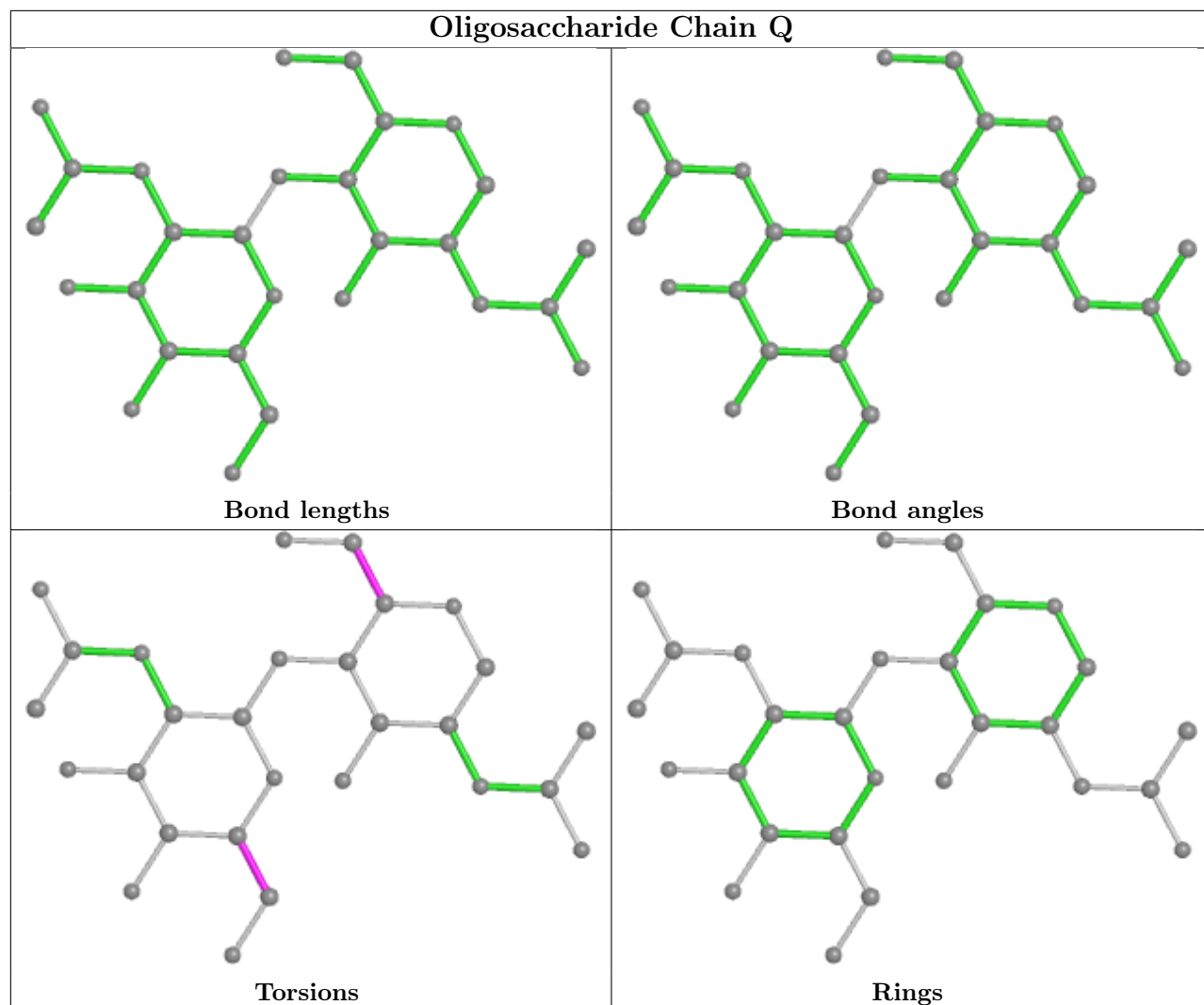
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Y	2	NAG	2	0
6	Y	1	NAG	3	0
6	T	2	NAG	2	0
6	Q	1	NAG	1	0
6	T	1	NAG	2	0
6	W	1	NAG	1	0
6	D	1	NAG	7	0
6	K	1	NAG	1	0
6	E	1	NAG	1	0

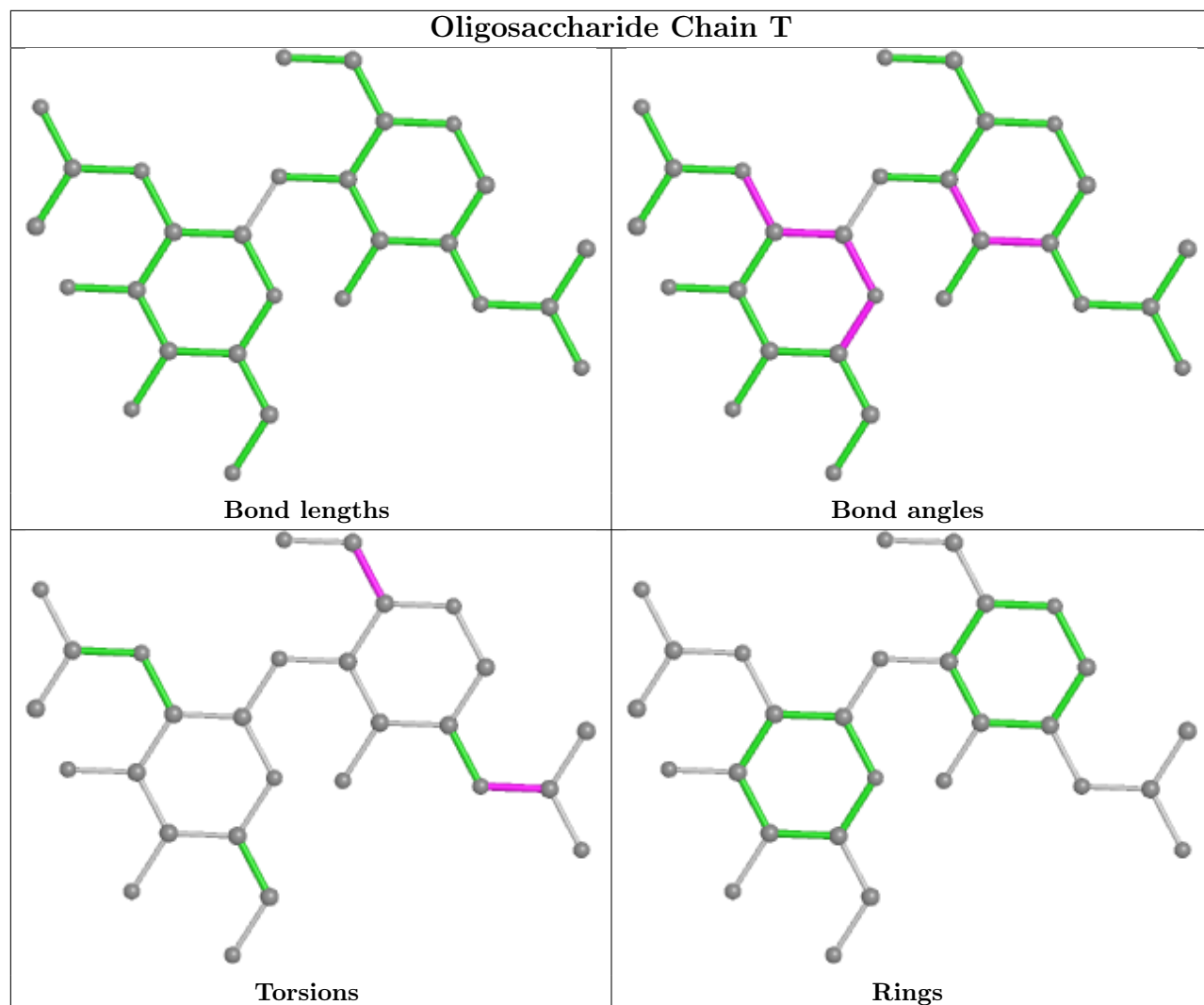
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

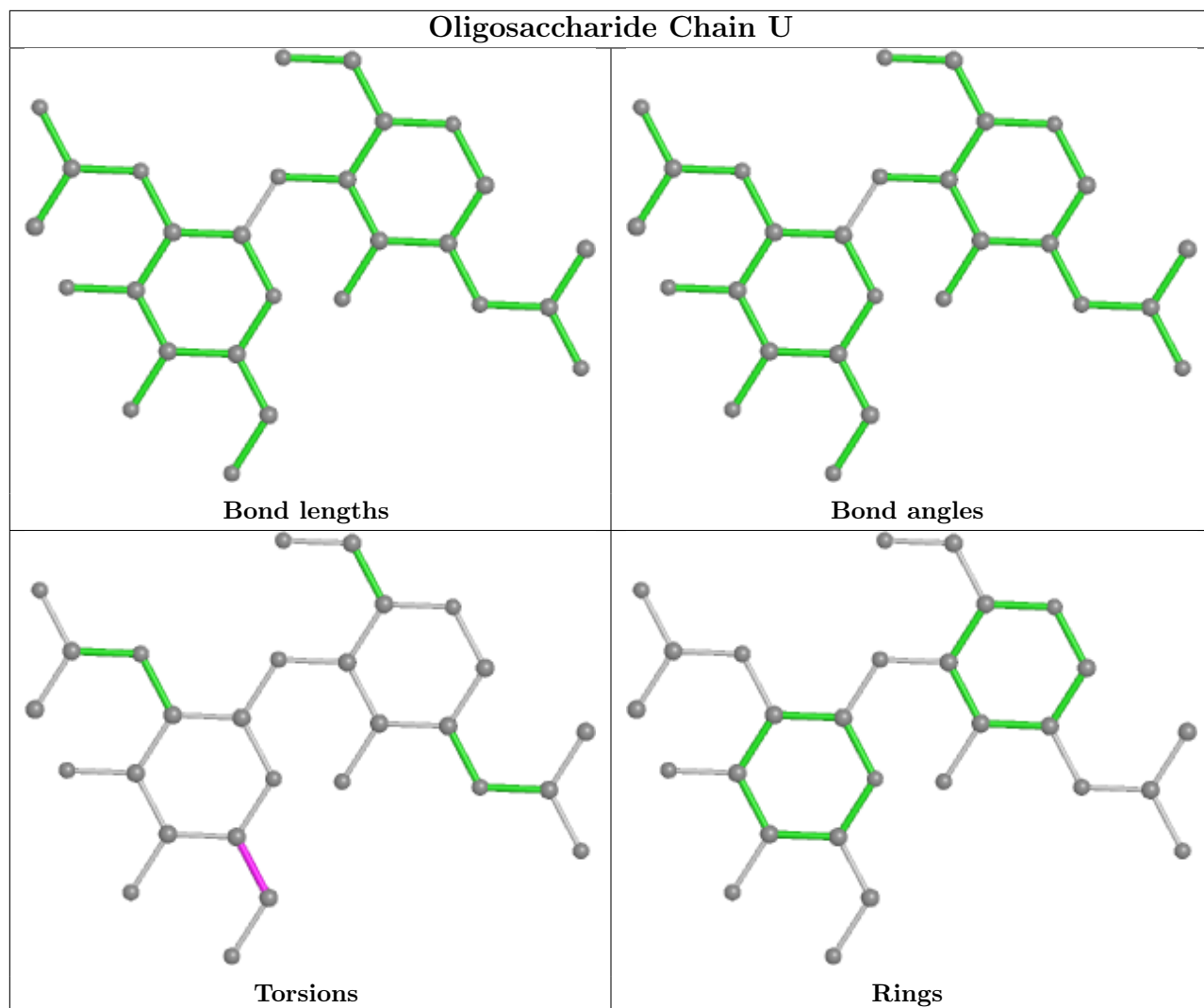


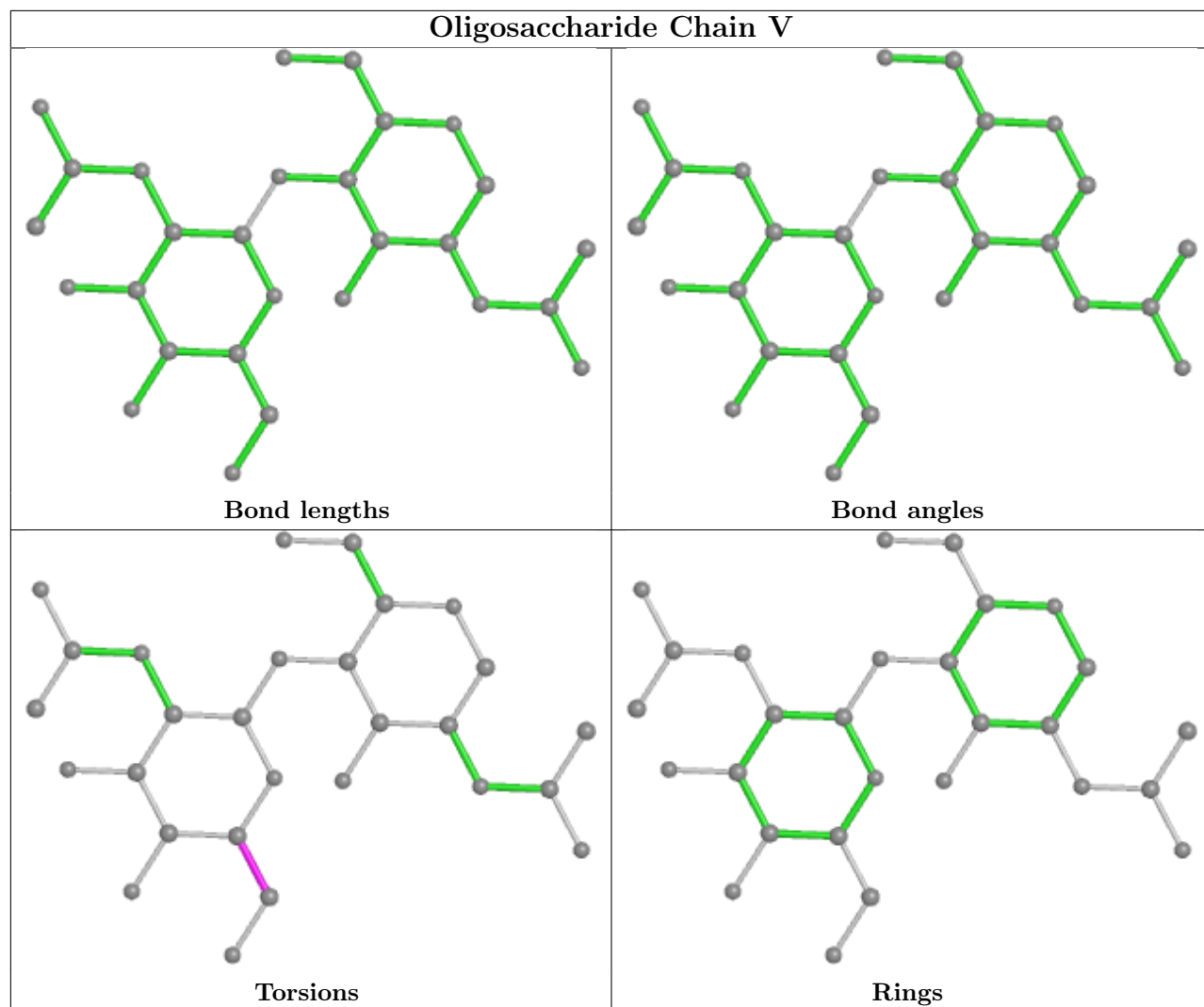


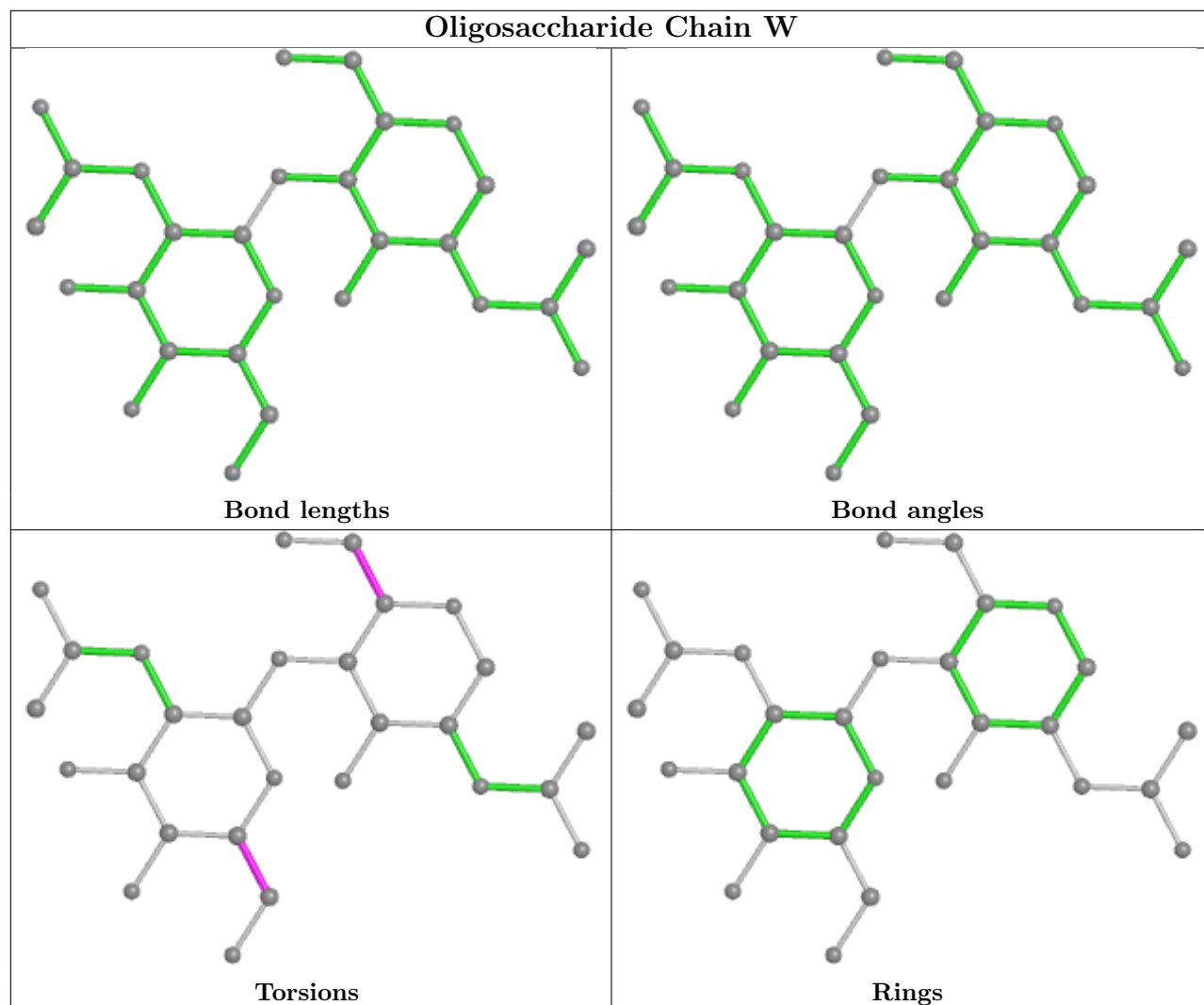


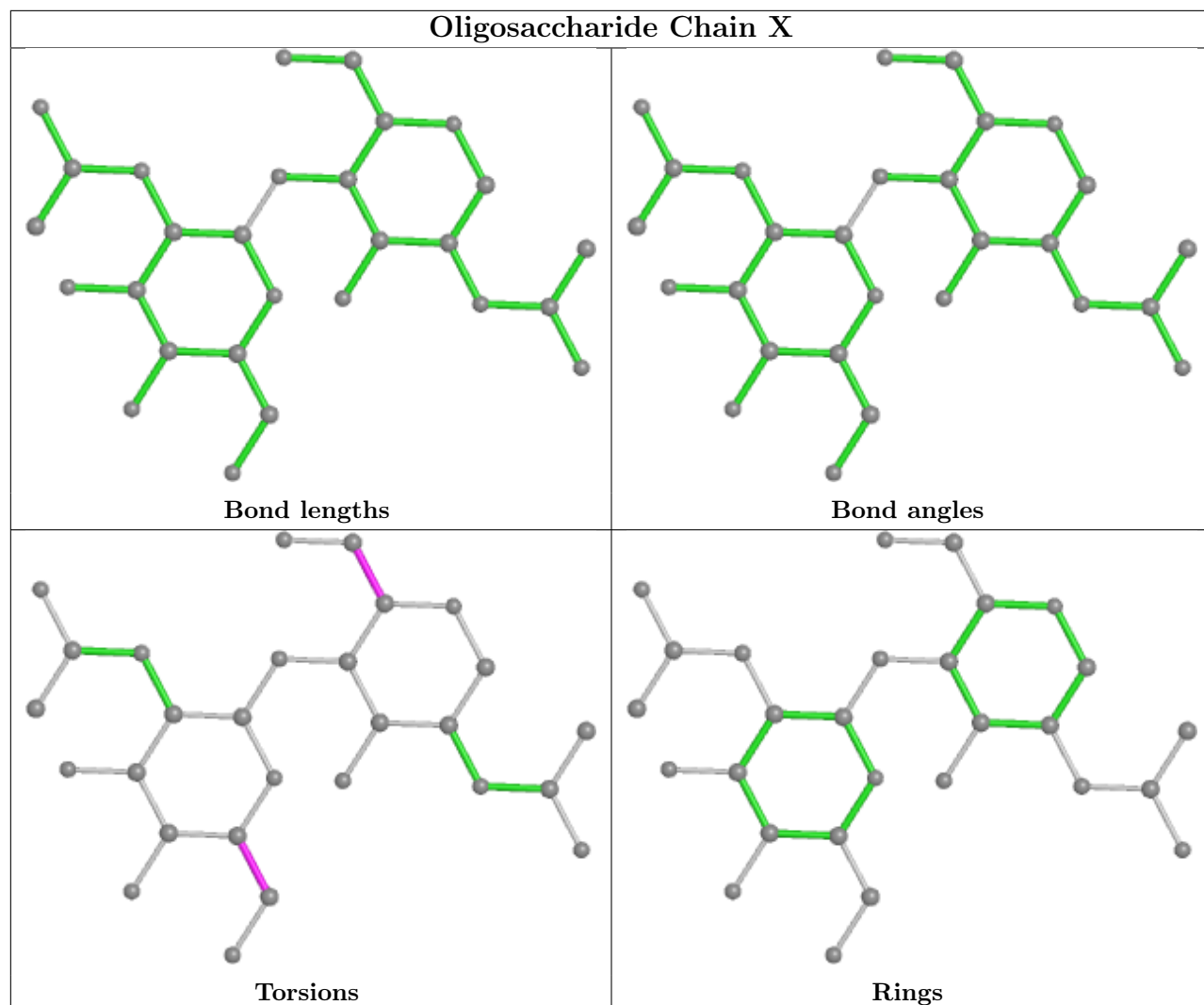


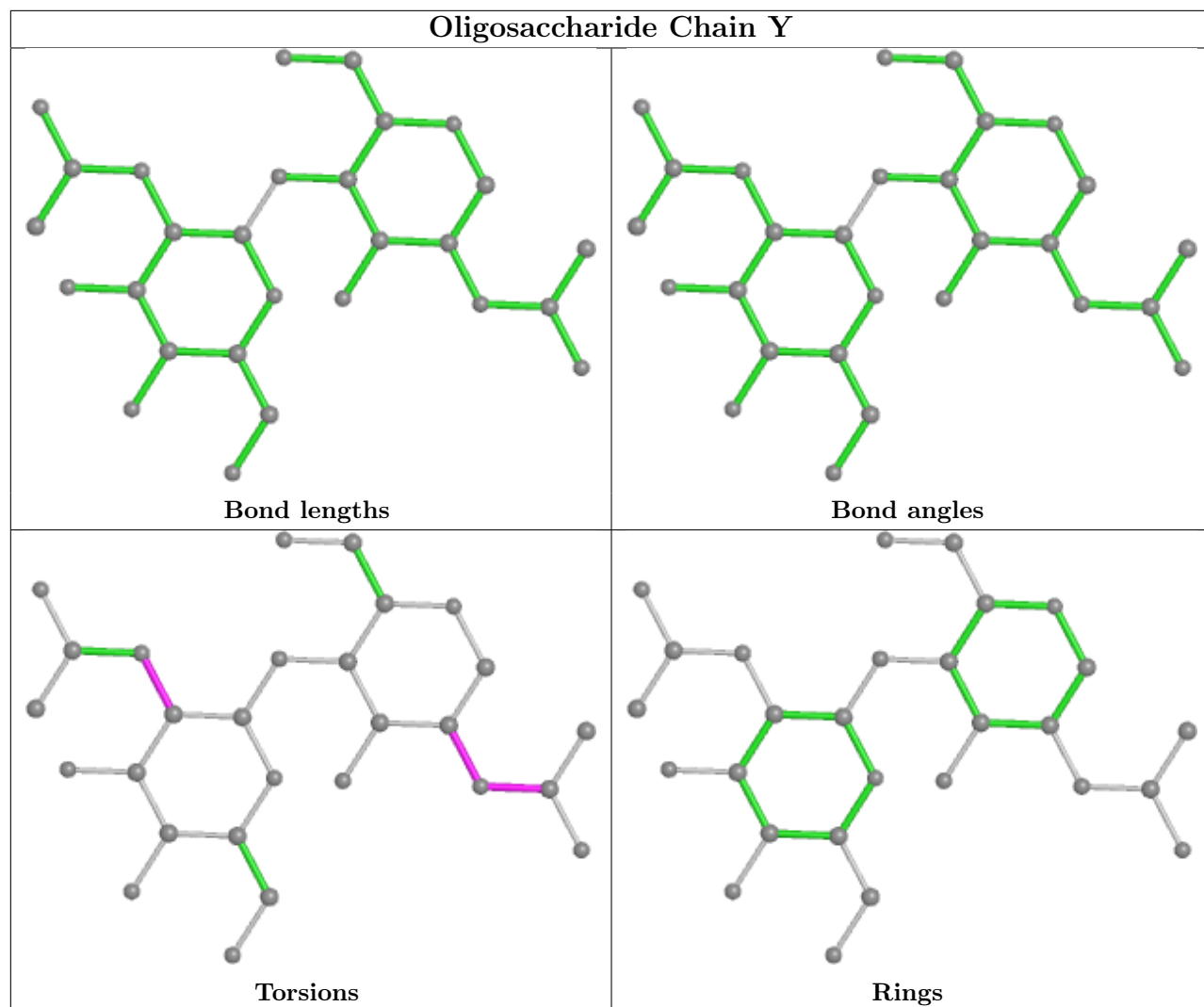


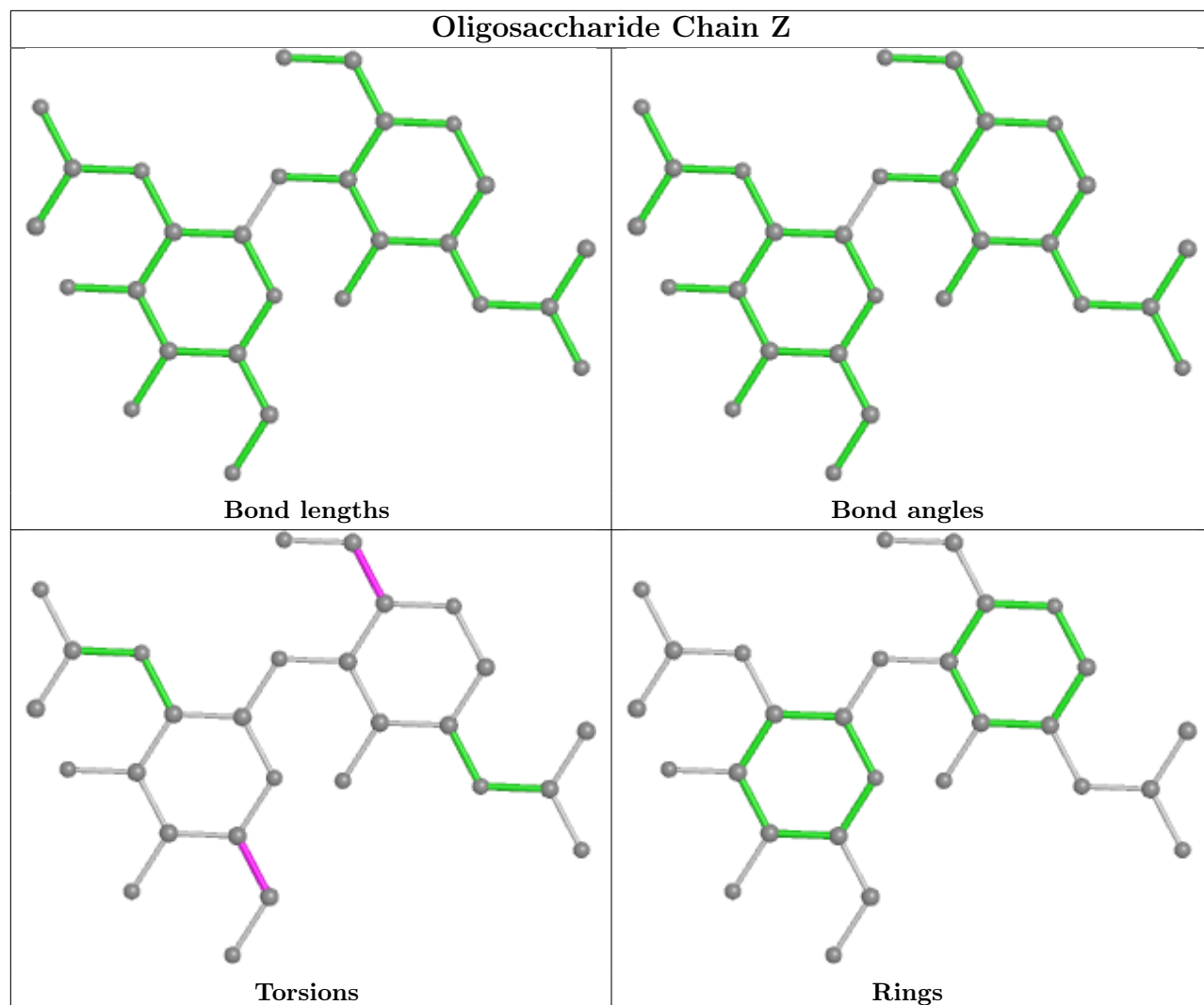


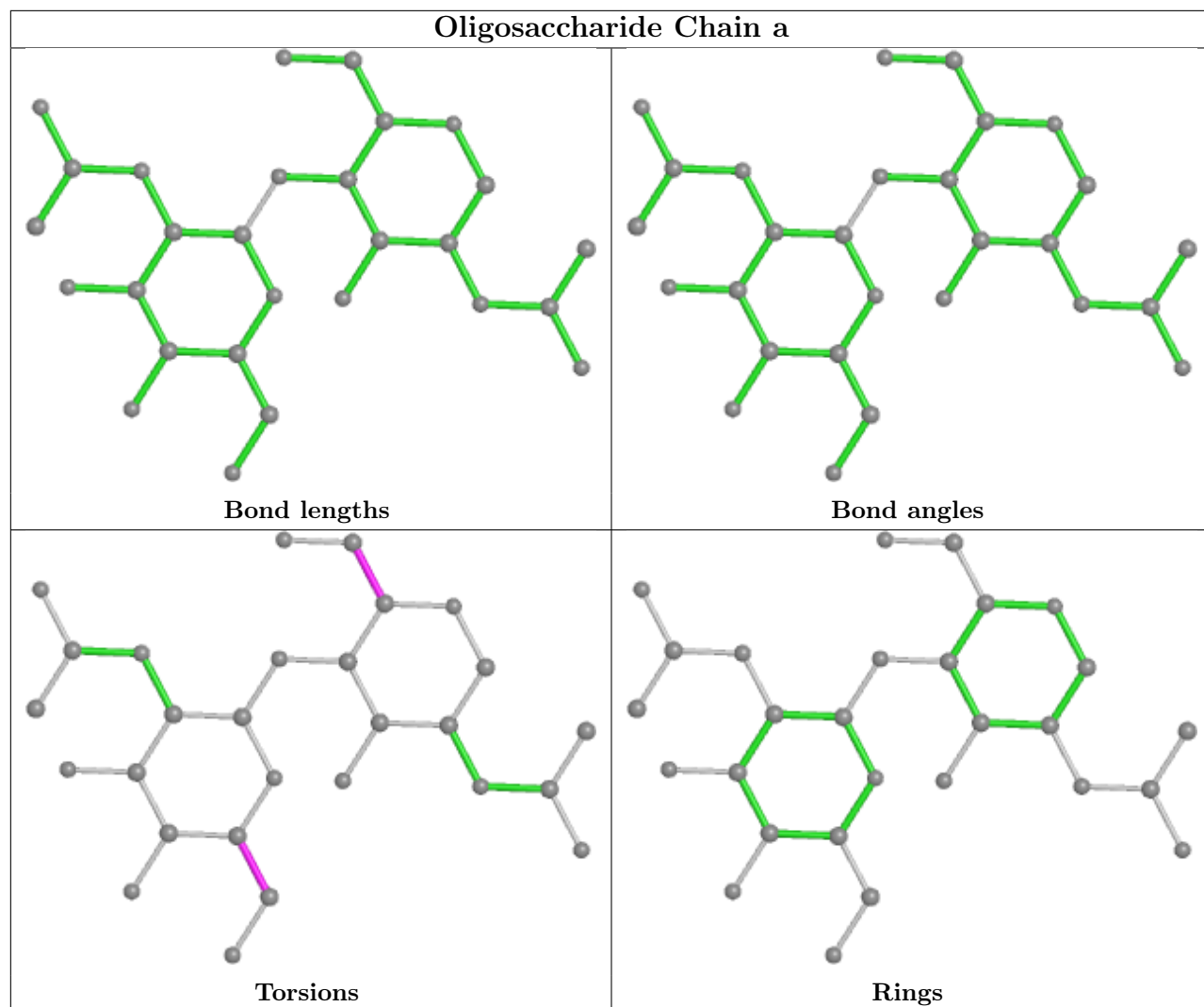


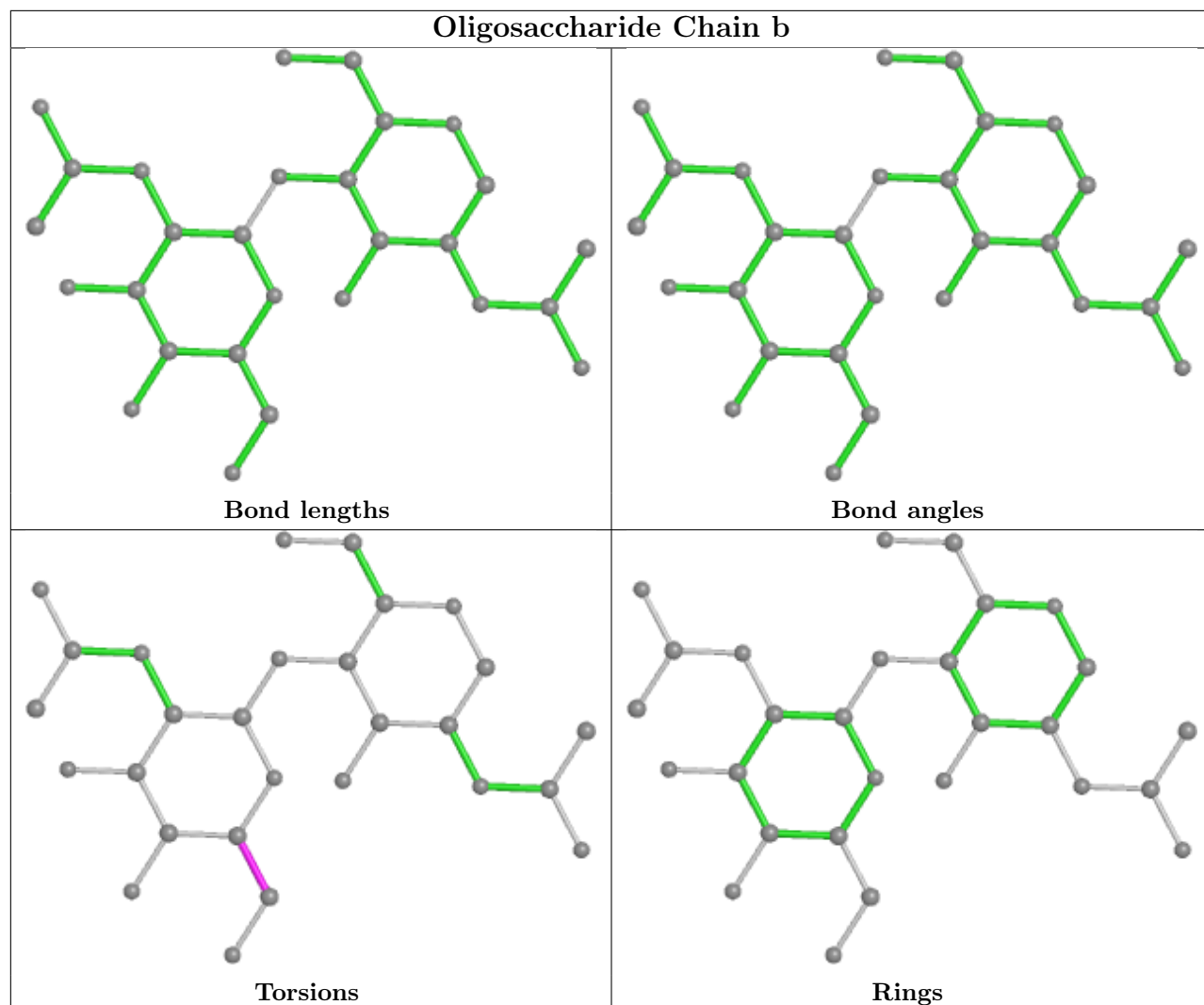


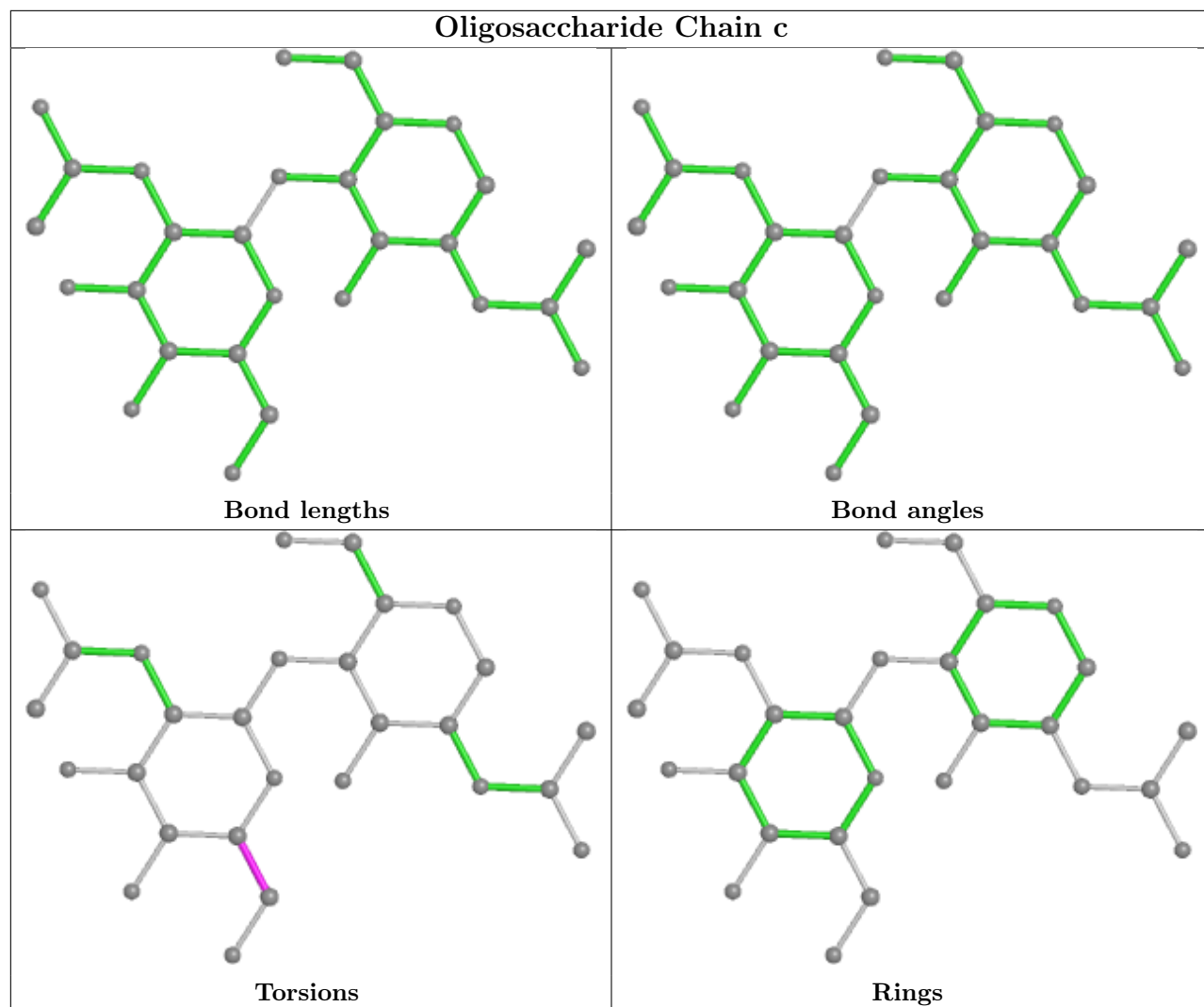


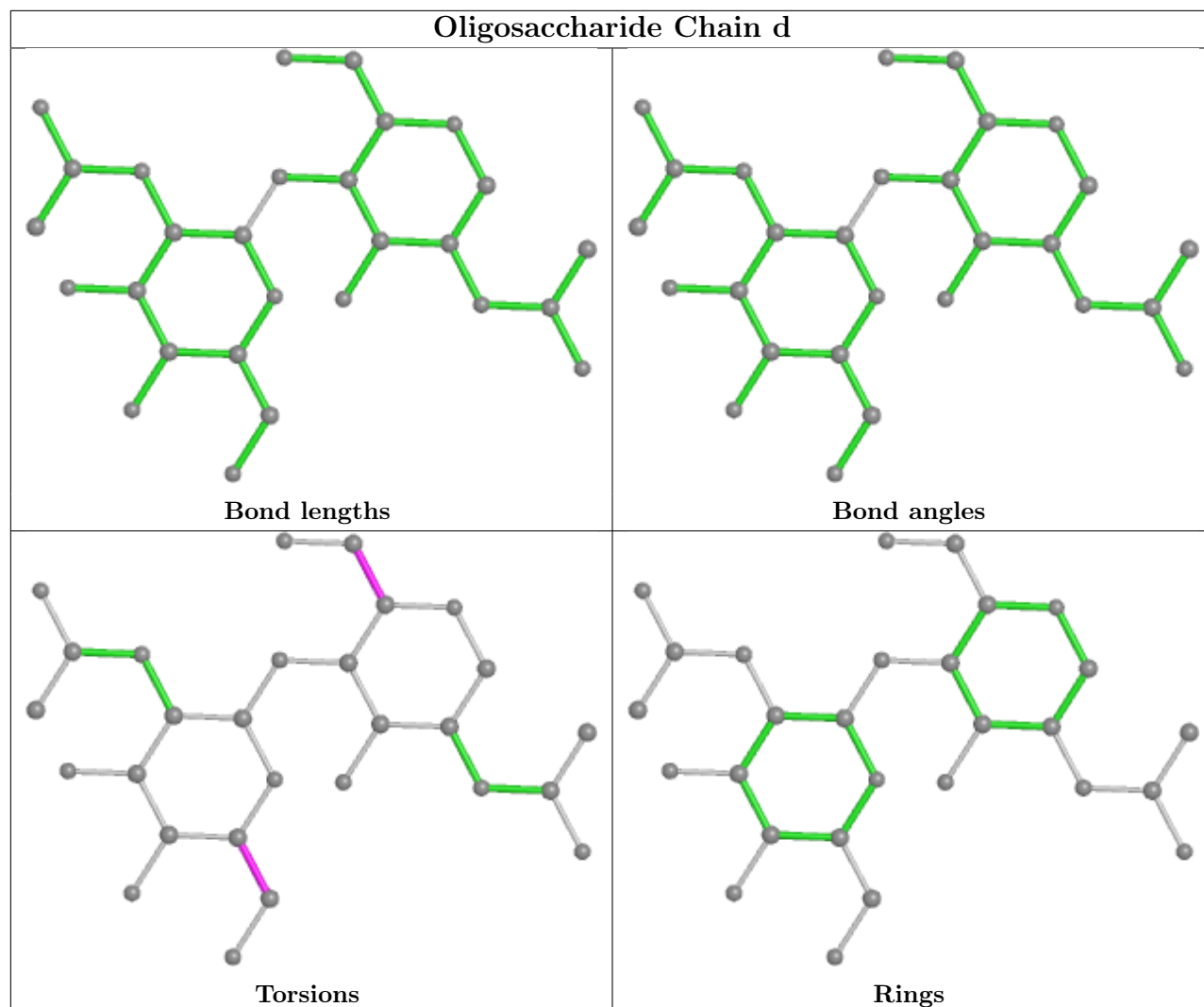












5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
7	NAG	A	1303	3	14,14,15	0.18	0	17,19,21	0.44	0
7	NAG	B	1303	3	14,14,15	0.31	0	17,19,21	0.37	0
7	NAG	C	1301	3	14,14,15	0.35	0	17,19,21	0.38	0
7	NAG	C	1302	3	14,14,15	0.22	0	17,19,21	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	1301	3	14,14,15	0.22	0	17,19,21	0.35	0
7	NAG	B	1302	3	14,14,15	0.67	0	17,19,21	0.44	0
7	NAG	A	1305	3	14,14,15	0.23	0	17,19,21	0.61	0
7	NAG	B	1304	3	14,14,15	0.48	0	17,19,21	0.51	0
7	NAG	C	1304	3	14,14,15	0.21	0	17,19,21	0.43	0
7	NAG	A	1304	3	14,14,15	0.58	0	17,19,21	0.37	0
7	NAG	A	1302	3	14,14,15	0.49	0	17,19,21	0.49	0
7	NAG	B	1305	3	14,14,15	0.25	0	17,19,21	0.51	0
7	NAG	B	1301	3	14,14,15	0.39	0	17,19,21	0.41	0
7	NAG	C	1306	3	14,14,15	0.22	0	17,19,21	0.59	0
7	NAG	C	1305	3	14,14,15	0.57	0	17,19,21	0.36	0
7	NAG	C	1303	3	14,14,15	0.46	0	17,19,21	0.48	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
7	NAG	A	1303	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1303	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1301	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1302	3	-	0/6/23/26	0/1/1/1
7	NAG	A	1301	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1302	3	-	2/6/23/26	0/1/1/1
7	NAG	A	1305	3	-	1/6/23/26	0/1/1/1
7	NAG	B	1304	3	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	3	-	0/6/23/26	0/1/1/1
7	NAG	A	1304	3	-	2/6/23/26	0/1/1/1
7	NAG	A	1302	3	-	1/6/23/26	0/1/1/1
7	NAG	B	1305	3	-	1/6/23/26	0/1/1/1
7	NAG	B	1301	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1306	3	-	1/6/23/26	0/1/1/1
7	NAG	C	1305	3	-	2/6/23/26	0/1/1/1
7	NAG	C	1303	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1302	NAG	O5-C5-C6-O6
7	C	1305	NAG	C4-C5-C6-O6
7	A	1304	NAG	C4-C5-C6-O6
7	C	1305	NAG	O5-C5-C6-O6
7	A	1304	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1304	NAG	1	0
7	C	1305	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.

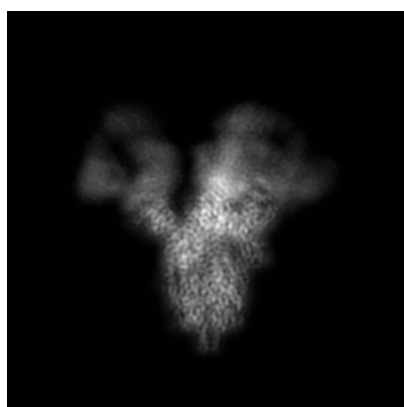
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30488. These allow visual inspection of the internal detail of the map and identification of artifacts.

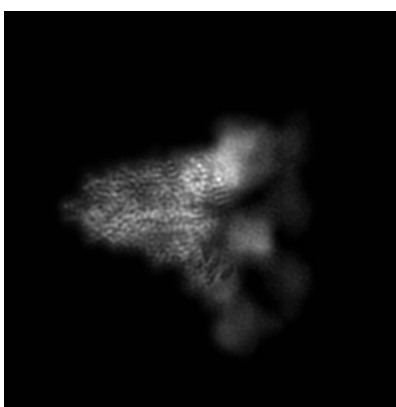
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

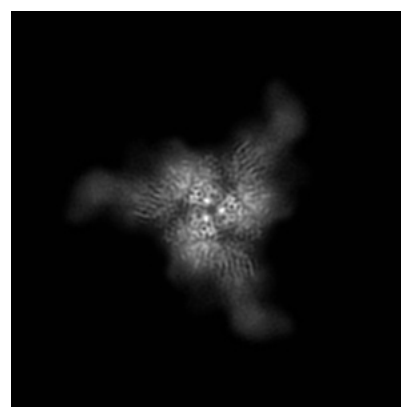
6.1.1 Primary map



X



Y

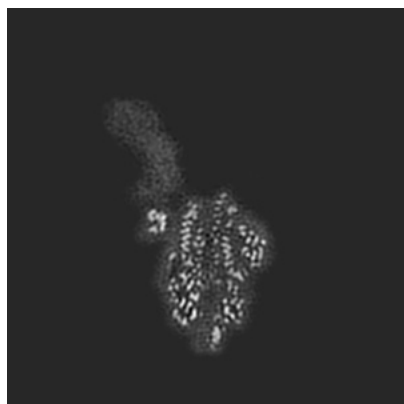


Z

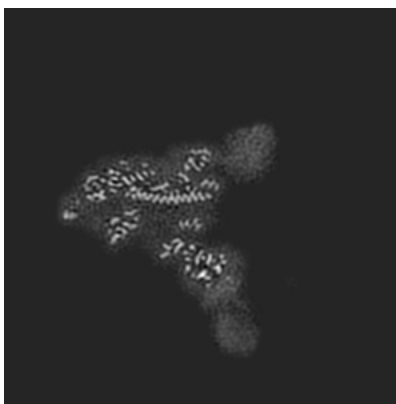
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

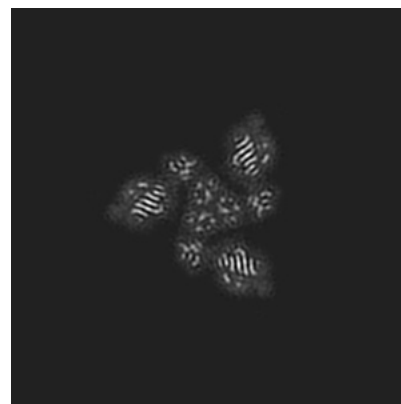
6.2.1 Primary map



X Index: 150



Y Index: 150

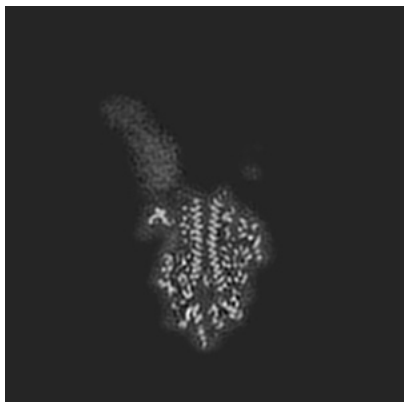


Z Index: 150

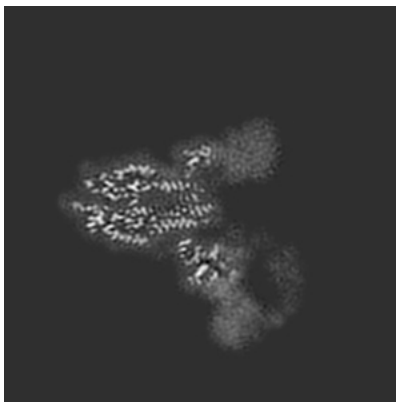
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

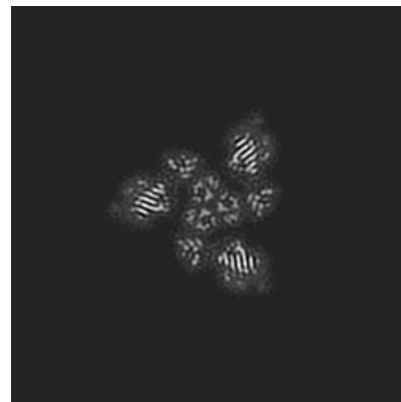
6.3.1 Primary map



X Index: 146



Y Index: 159



Z Index: 149

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

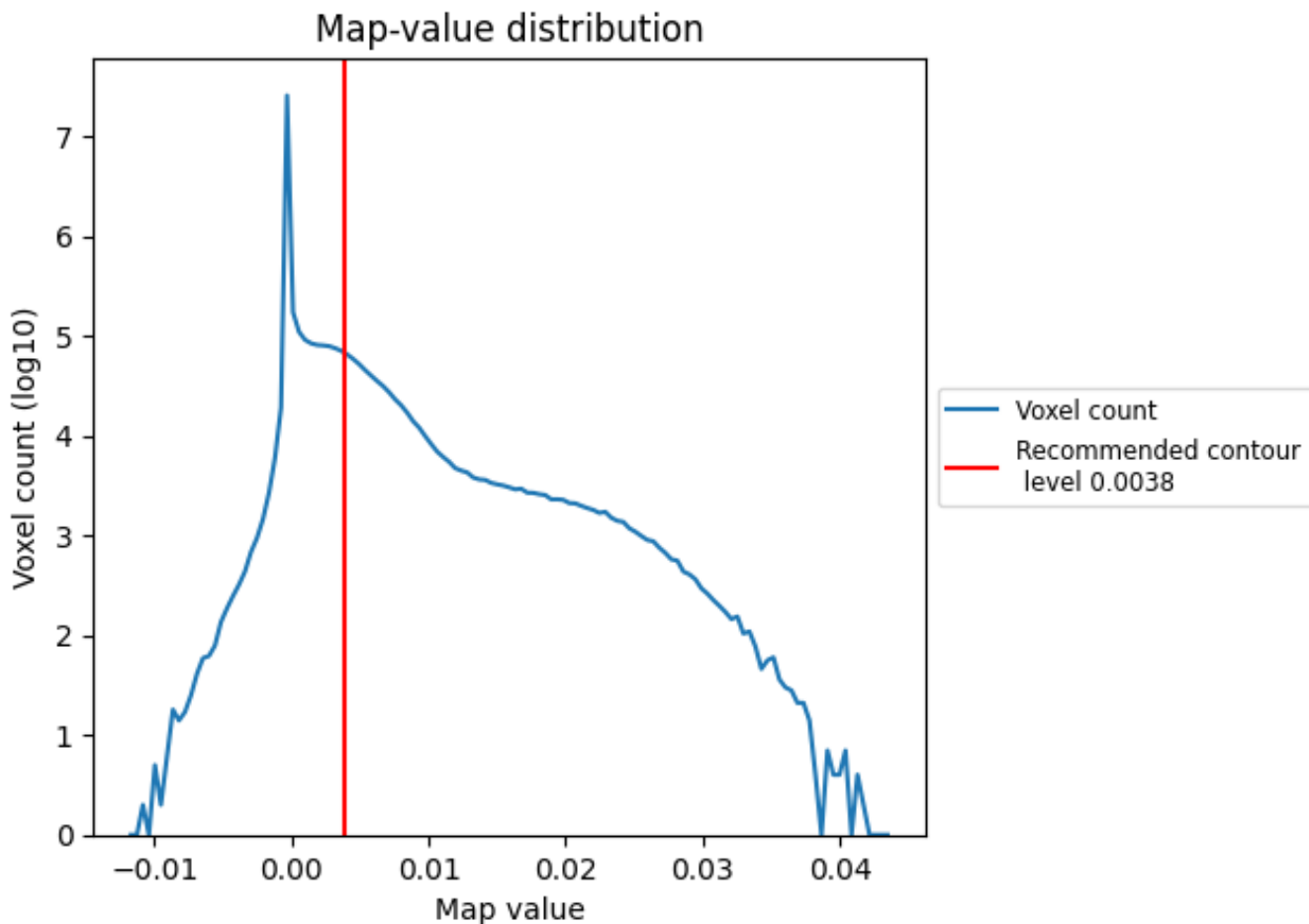
6.5 Mask visualisation

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

7 Map analysis [i](#)

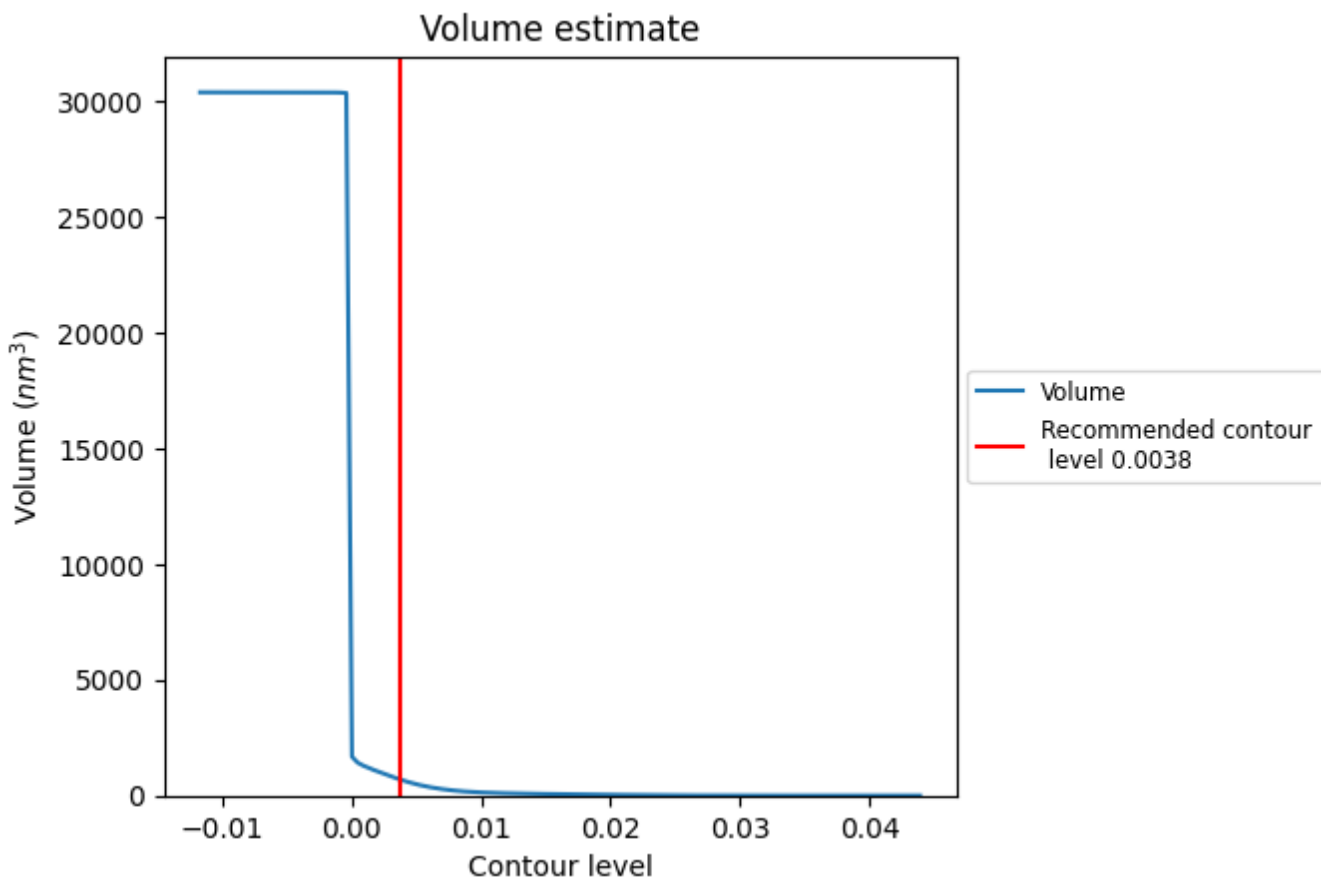
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

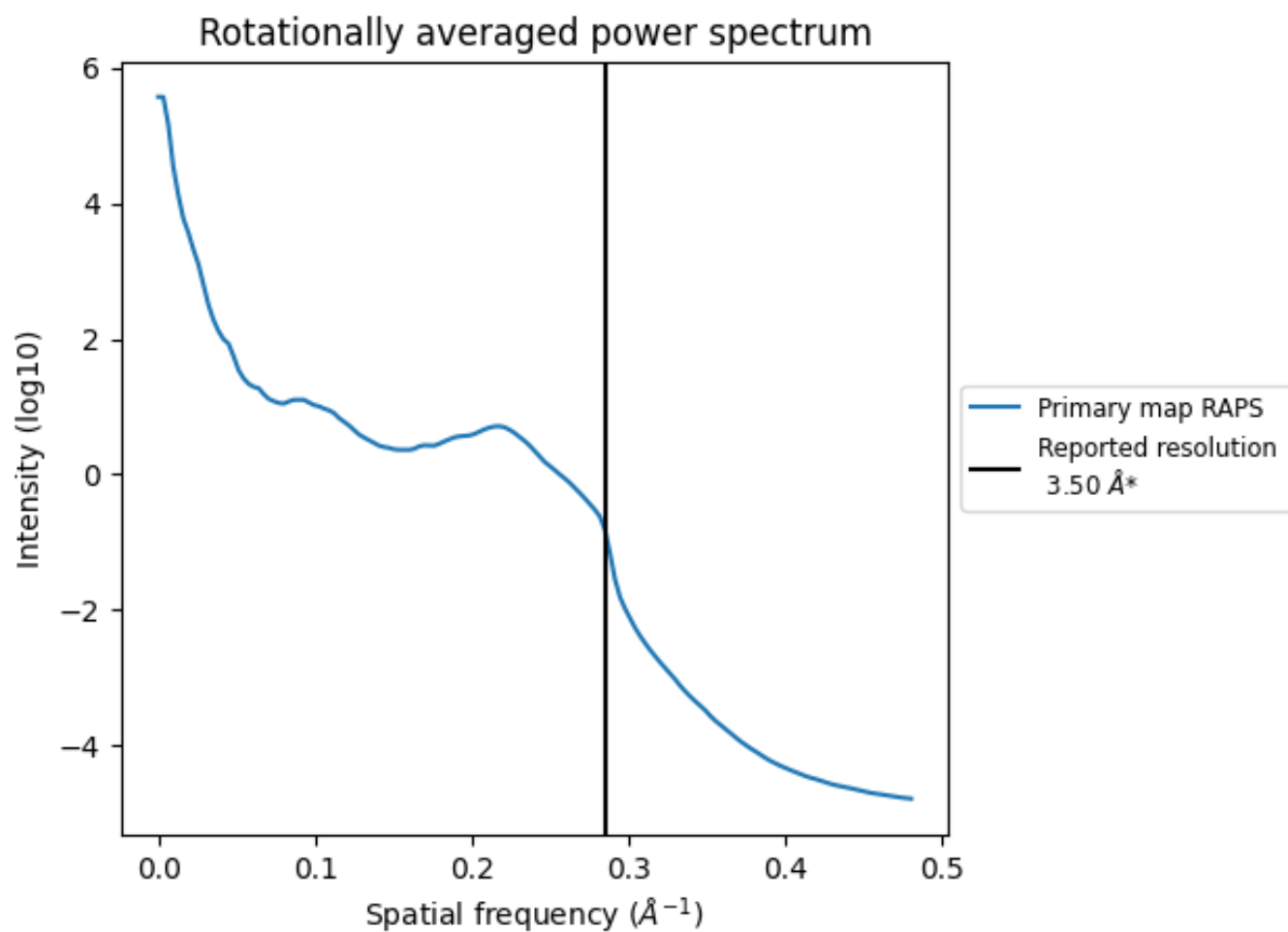
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 685 nm³; this corresponds to an approximate mass of 618 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 0.286 Å⁻¹

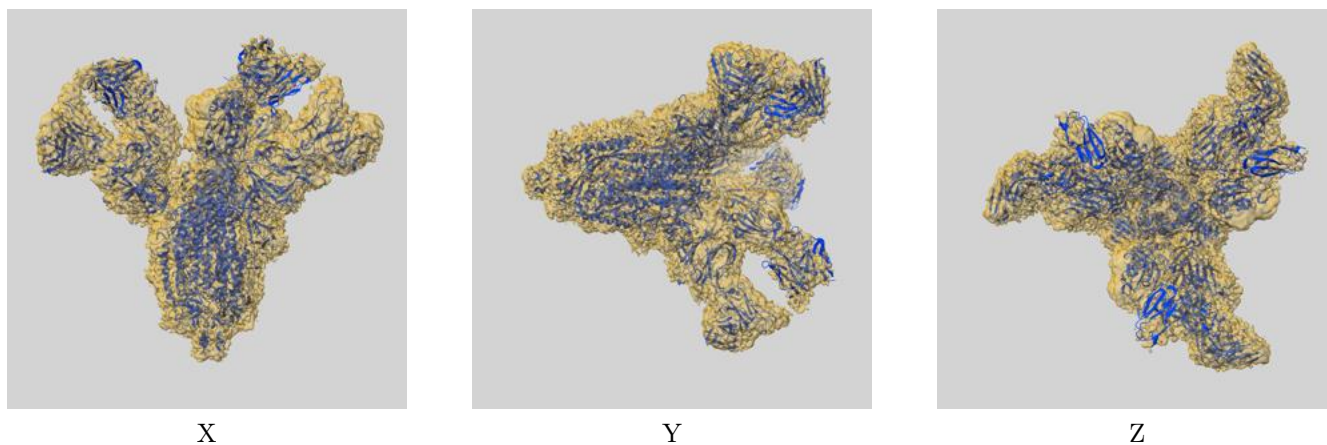
8 Fourier-Shell correlation

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-30488 and PDB model 7CWU. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



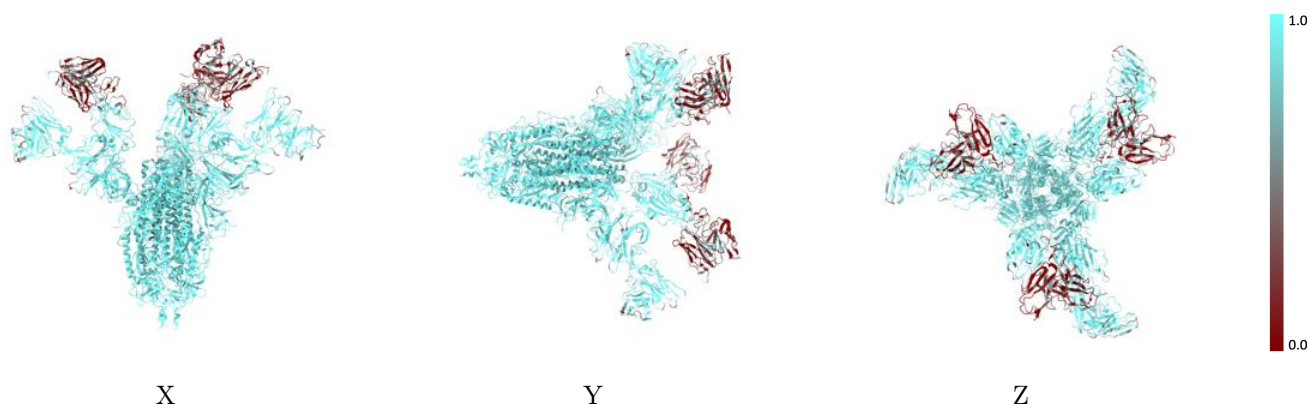
The images above show the 3D surface view of the map at the recommended contour level 0.0038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



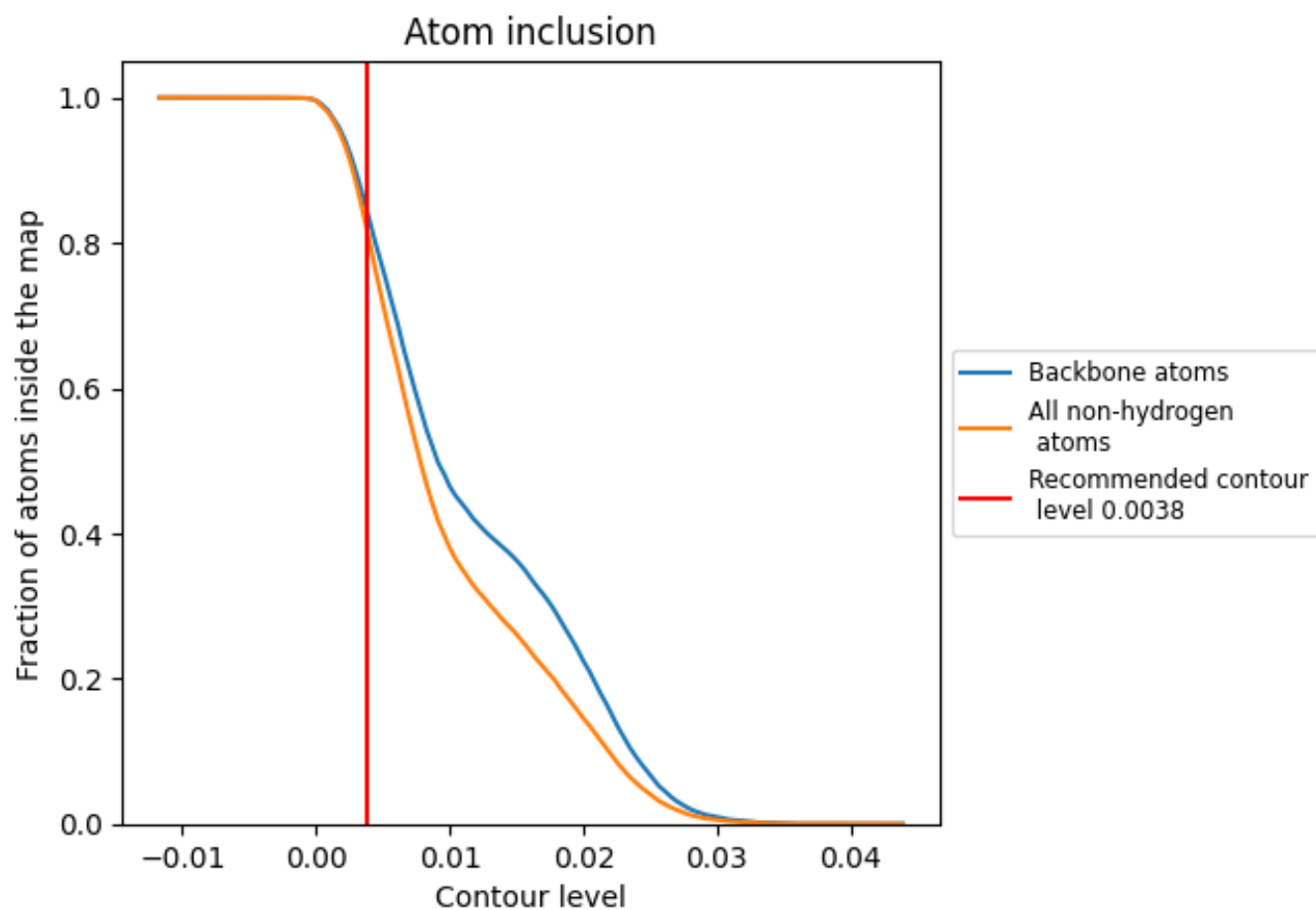
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0038).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.0038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8202	 0.2090
A	 0.9267	 0.2780
B	 0.9244	 0.2760
C	 0.9252	 0.2800
D	 0.3571	 0.0950
E	 0.1429	 -0.0030
F	 0.8522	 0.0320
G	 0.8509	 0.0340
H	 0.2662	 0.0260
I	 0.8586	 0.0310
J	 0.9179	 0.0700
K	 0.1071	 -0.0260
L	 0.2282	 0.0230
M	 0.2662	 0.0270
N	 0.9135	 0.0690
O	 0.2472	 0.0460
P	 0.9168	 0.0600
Q	 0.8571	 0.2950
R	 0.2344	 0.0190
S	 0.2668	 0.0240
T	 0.7143	 0.2010
U	 0.6071	 0.2830
V	 0.8571	 0.4150
W	 0.7857	 0.2720
X	 0.7143	 0.3390
Y	 0.5714	 0.2640
Z	 0.8571	 0.4090
a	 0.7857	 0.3010
b	 0.5714	 0.3010
c	 0.7500	 0.3580
d	 0.8571	 0.4230

