



wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 10:36 AM EST

PDB ID : 8CY7
EMDB ID : EMD-27069
Title : SARS-CoV-2 Spike protein in complex with a pan-sarbecovirus nanobody 2-34
Authors : Huang, W.; Taylor, D.
Deposited on : 2022-05-23
Resolution : 2.90 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:

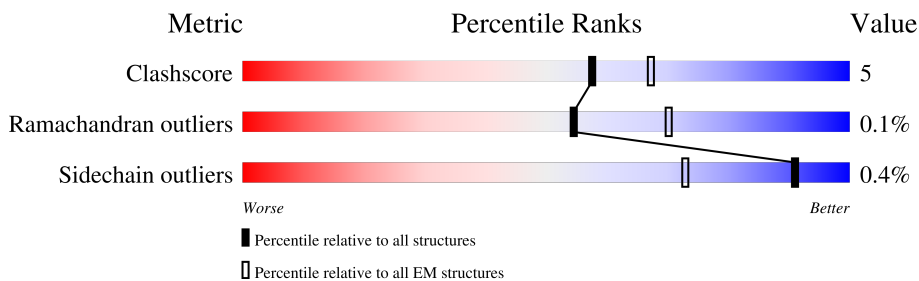
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.90 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.



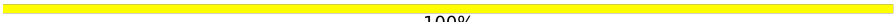
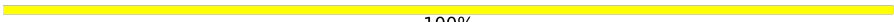
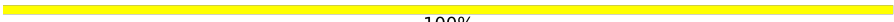
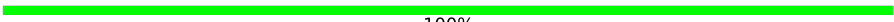
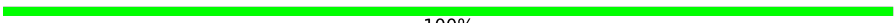

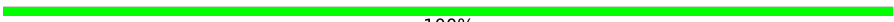
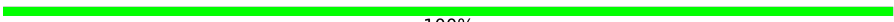


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	1273	73% 9% 18%
1	B	1273	73% 9% 18%
1	C	1273	72% 10% 18%
2	D	121	89% 11%
2	E	121	87% 13%
2	F	121	83% 16%
3	G	2	100%
3	H	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	J	2	 100%
3	K	2	 100%
3	L	2	 100%
3	M	2	 100%
3	N	2	 50% 50%
3	O	2	 100%
3	P	2	 100%
3	Q	2	 100%
3	R	2	 50% 50%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 55418 atoms, of which 27035 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
			Total	C	H	N	O	S		
1	A	1050	16148	5234	7953	1365	1559	37	0	0
1	B	1050	16161	5236	7962	1366	1560	37	0	0
1	C	1050	16160	5236	7961	1366	1560	37	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called pan-sarbecovirus nanobody 2-38.

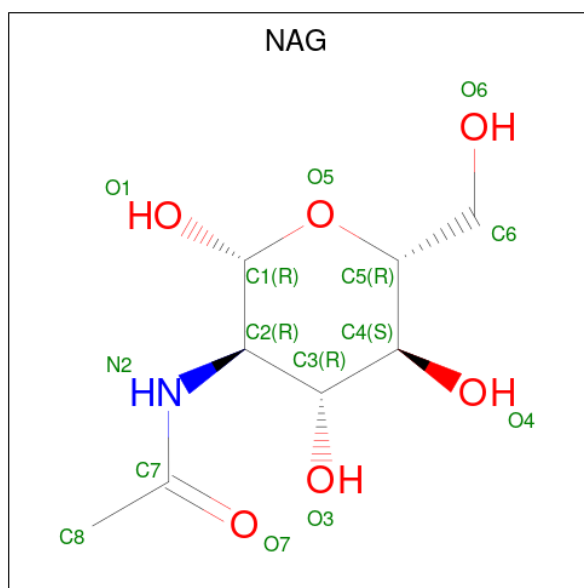
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	121	1809	575	891	161	178	4	0	0
2	E	121	1809	575	891	161	178	4	0	0
2	F	121	1809	575	891	161	178	4	0	0

- Molecule 3 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
3	G	2	Total	C	H	N	O	0	0
			51	16	23	2	10		
3	H	2	Total	C	N	O		0	0
			28	16	2	10			
3	I	2	Total	C	N	O		0	0
			28	16	2	10			
3	J	2	Total	C	N	O		0	0
			28	16	2	10			
3	K	2	Total	C	H	N	O	0	0
			52	16	24	2	10		
3	L	2	Total	C	H	N	O	0	0
			37	16	9	2	10		
3	M	2	Total	C	H	N	O	0	0
			38	16	10	2	10		
3	N	2	Total	C	N	O		0	0
			28	16	2	10			
3	O	2	Total	C	H	N	O	0	0
			49	16	21	2	10		
3	P	2	Total	C	H	N	O	0	0
			52	16	24	2	10		
3	Q	2	Total	C	N	O		0	0
			28	16	2	10			
3	R	2	Total	C	N	O		0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	A	1	Total	C	H	N	O	0
			380	136	142	17	85	
4	B	1	Total	C	H	N	O	0
			327	120	117	15	75	
4	B	1	Total	C	H	N	O	0
			327	120	117	15	75	
4	B	1	Total	C	H	N	O	0
			327	120	117	15	75	
4	B	1	Total	C	H	N	O	0
			327	120	117	15	75	
4	B	1	Total	C	H	N	O	0
			327	120	117	15	75	

Continued on next page...

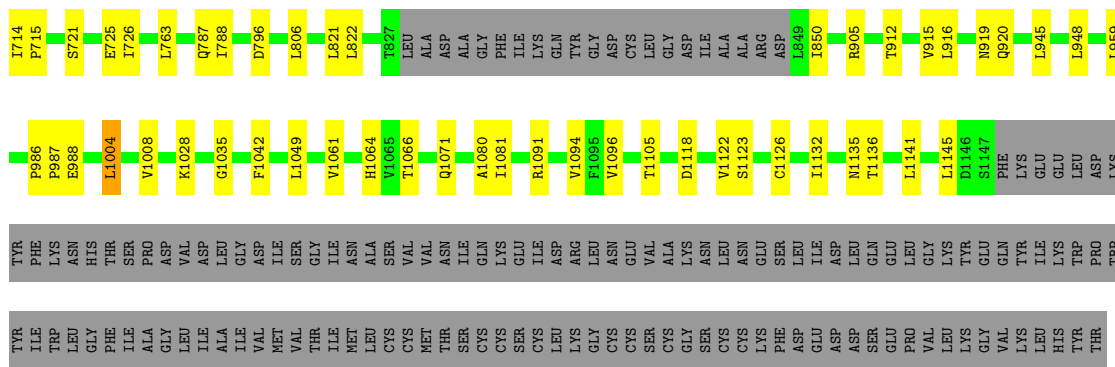
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	B	1	Total 327	C 120	H 117	N 15	O 75	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0
4	C	1	Total 368	C 144	H 116	N 18	O 90	0

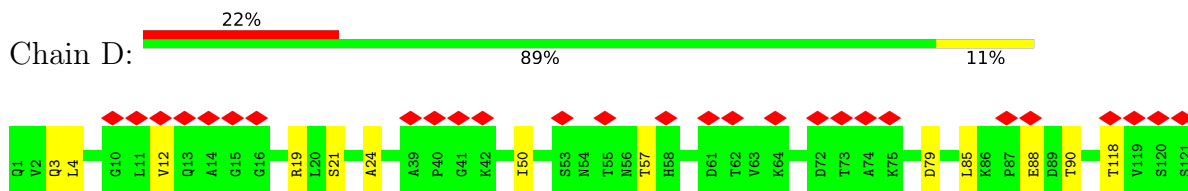
Continued on next page...

Continued from previous page...

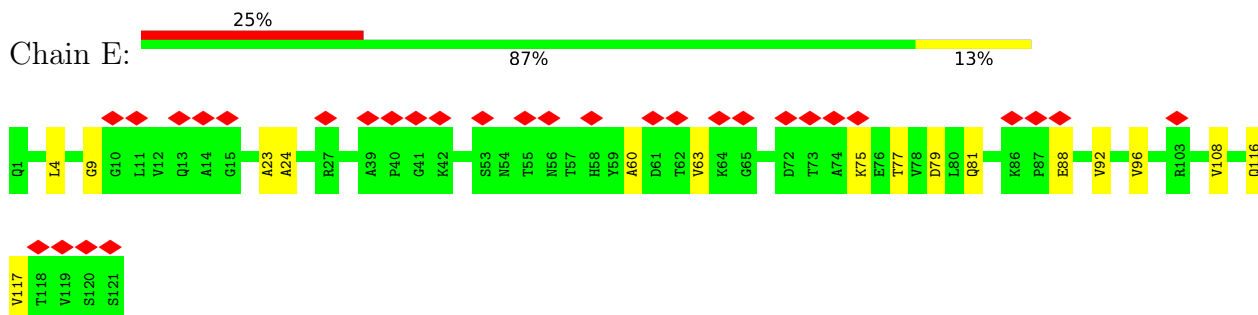
Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	H	N	O	0
			368	144	116	18	90	
4	C	1	Total	C	H	N	O	0
			368	144	116	18	90	
4	C	1	Total	C	H	N	O	0
			368	144	116	18	90	
4	C	1	Total	C	H	N	O	0
			368	144	116	18	90	
4	C	1	Total	C	H	N	O	0
			368	144	116	18	90	
4	C	1	Total	C	H	N	O	0
			368	144	116	18	90	



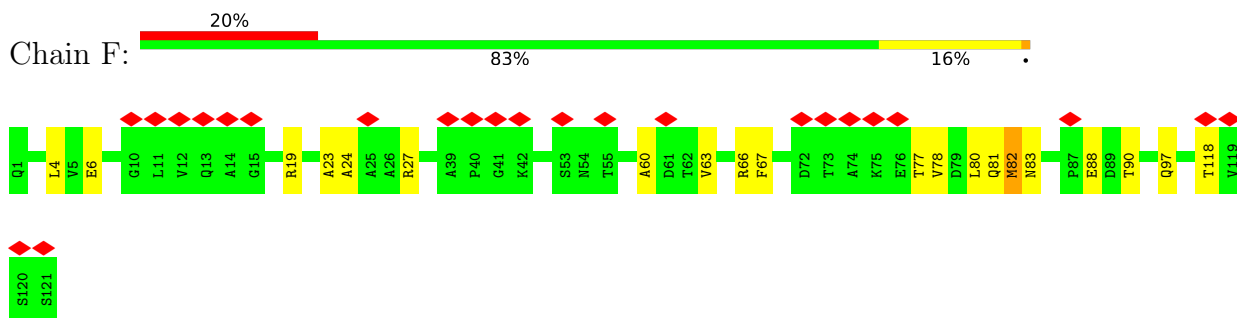
• Molecule 2: pan-sarbecovirus nanobody 2-38



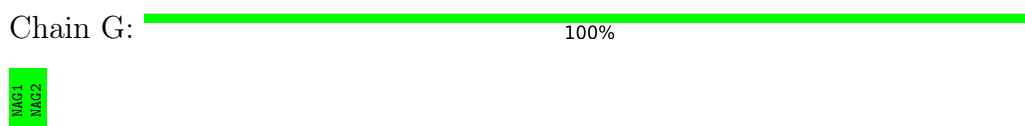
• Molecule 2: pan-sarbecovirus nanobody 2-38



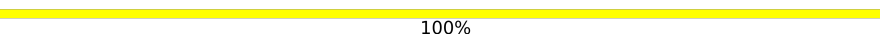
• Molecule 2: pan-sarbecovirus nanobody 2-38



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

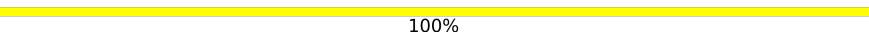


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

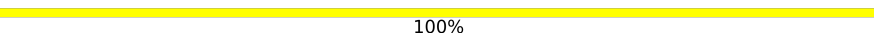
MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain N:  50% 50%

MAG1
MAG2

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

Chain O:  100%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21902	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 ($e^-/\text{\AA}^2$)	31.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.868	Depositor
Minimum map value	-0.298	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	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: 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	0.25	0/8388	0.50	11/11424 (0.1%)
1	B	0.26	0/8392	0.58	19/11429 (0.2%)
1	C	0.25	0/8392	0.57	24/11429 (0.2%)
2	D	0.25	0/937	0.48	0/1270
2	E	0.25	0/937	0.48	0/1270
2	F	0.24	0/937	0.48	0/1270
All	All	0.25	0/27983	0.54	54/38092 (0.1%)

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	VAL	CG1-CB-CG2	6.84	121.85	110.90
1	B	1094	VAL	CG1-CB-CG2	6.81	121.80	110.90
1	B	1068	VAL	CG1-CB-CG2	6.80	121.78	110.90
1	C	227	VAL	CG1-CB-CG2	6.79	121.76	110.90
1	C	1094	VAL	CG1-CB-CG2	6.78	121.75	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8195	7953	7964	77	0
1	B	8199	7962	7975	69	0
1	C	8199	7961	7972	81	0
2	D	918	891	892	8	0
2	E	918	891	892	11	0
2	F	918	891	892	13	0
3	G	28	23	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	4	0
3	J	28	0	25	1	0
3	K	28	24	25	1	0
3	L	28	9	25	0	0
3	M	28	10	25	0	0
3	N	28	0	25	1	0
3	O	28	21	25	0	0
3	P	28	24	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	4	0
4	A	238	142	221	6	0
4	B	210	117	195	4	0
4	C	252	116	234	9	0
All	All	28383	27035	27537	277	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 277 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:I:1:NAG:H83	3:I:1:NAG:H3	1.50	0.91
3:R:2:NAG:H3	3:R:2:NAG:H83	1.56	0.88
4:C:1312:NAG:H83	4:C:1312:NAG:H3	1.56	0.88
4:C:1315:NAG:H3	4:C:1315:NAG:H83	1.55	0.85
1:C:581:THR:HG23	1:C:583:GLU:OE1	1.83	0.79

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	1038/1273 (82%)	997 (96%)	41 (4%)	0	100	100
1	B	1038/1273 (82%)	995 (96%)	42 (4%)	1 (0%)	51	82
1	C	1038/1273 (82%)	993 (96%)	41 (4%)	4 (0%)	34	66
2	D	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
2	E	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
2	F	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
All	All	3471/4182 (83%)	3336 (96%)	130 (4%)	5 (0%)	54	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	621	PRO
1	B	332	ILE
1	C	332	ILE
1	C	592	PHE
1	C	624	ILE

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	914/1112 (82%)	911 (100%)	3 (0%)	92	98
1	B	915/1112 (82%)	913 (100%)	2 (0%)	93	98
1	C	915/1112 (82%)	911 (100%)	4 (0%)	91	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	95/95 (100%)	94 (99%)	1 (1%)	73	92
2	E	95/95 (100%)	95 (100%)	0	100	100
2	F	95/95 (100%)	94 (99%)	1 (1%)	73	92
All	All	3029/3621 (84%)	3018 (100%)	11 (0%)	91	97

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	343	ASN
1	C	603	ASN
2	F	82	MET
2	D	19	ARG
1	B	603	ASN

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

Mol	Chain	Res	Type
1	A	774	GLN
1	B	675	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](#)

24 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
3	NAG	G	1	3,1	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	G	2	3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	H	1	3,1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	I	1	3,1	14,14,15	0.38	0	17,19,21	0.64	0
3	NAG	I	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	J	1	3,1	14,14,15	0.22	0	17,19,21	0.36	0
3	NAG	J	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	K	1	3,1	14,14,15	0.24	0	17,19,21	0.47	0
3	NAG	K	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	L	1	3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	L	2	3	14,14,15	0.23	0	17,19,21	0.39	0
3	NAG	M	1	3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	M	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	N	1	3,1	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	N	2	3	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	O	1	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	O	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	P	1	3,1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	P	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	Q	1	3,1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	R	1	3,1	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	R	2	3	14,14,15	0.24	0	17,19,21	0.52	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
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	1	3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	NAG	M	1	3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	NAG	O	1	3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	R	2	3	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 12 short contacts:

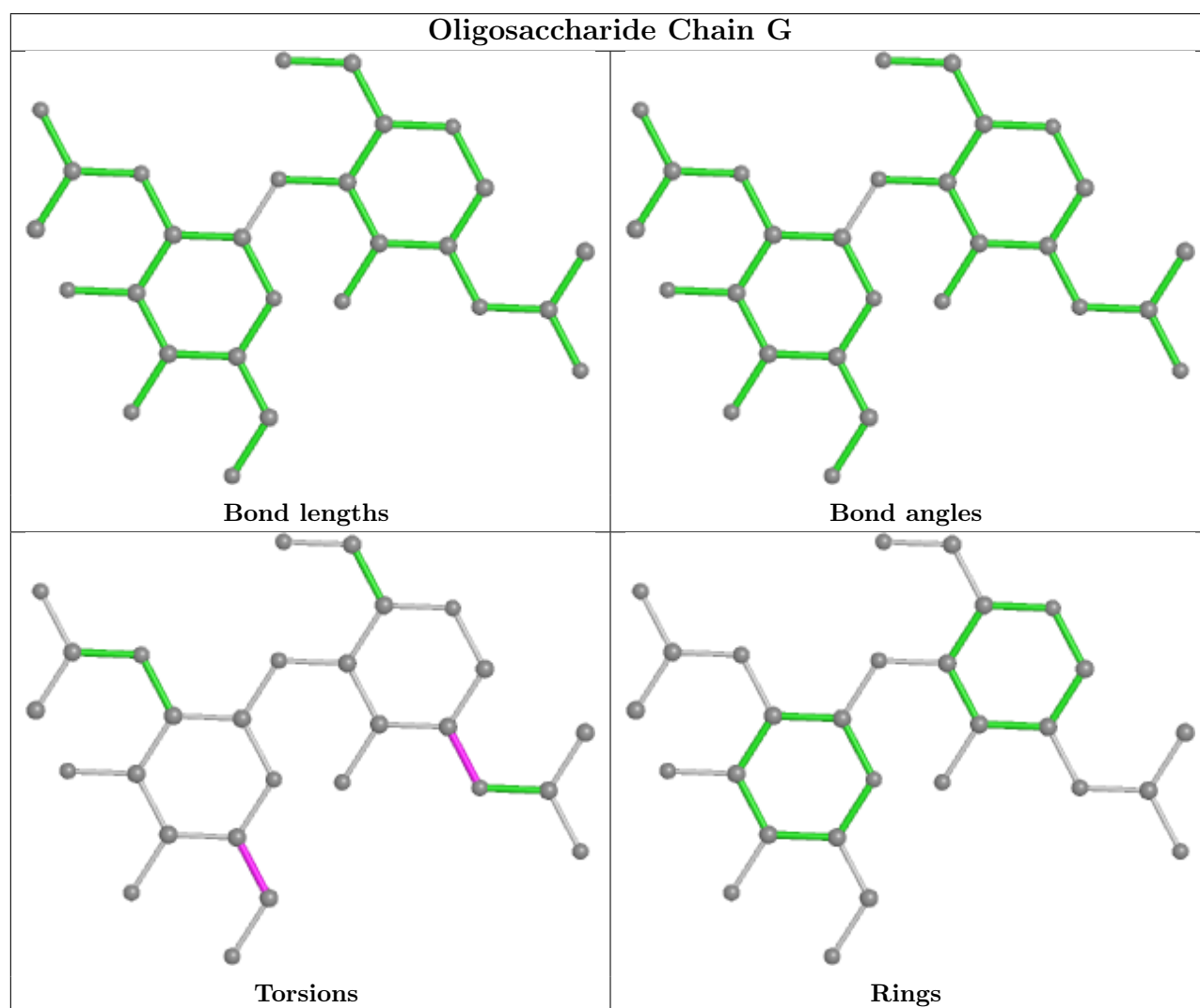
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	2	NAG	4	0
3	K	2	NAG	1	0
3	K	1	NAG	1	0
3	N	1	NAG	1	0
3	H	1	NAG	1	0
3	I	1	NAG	4	0
3	J	1	NAG	1	0

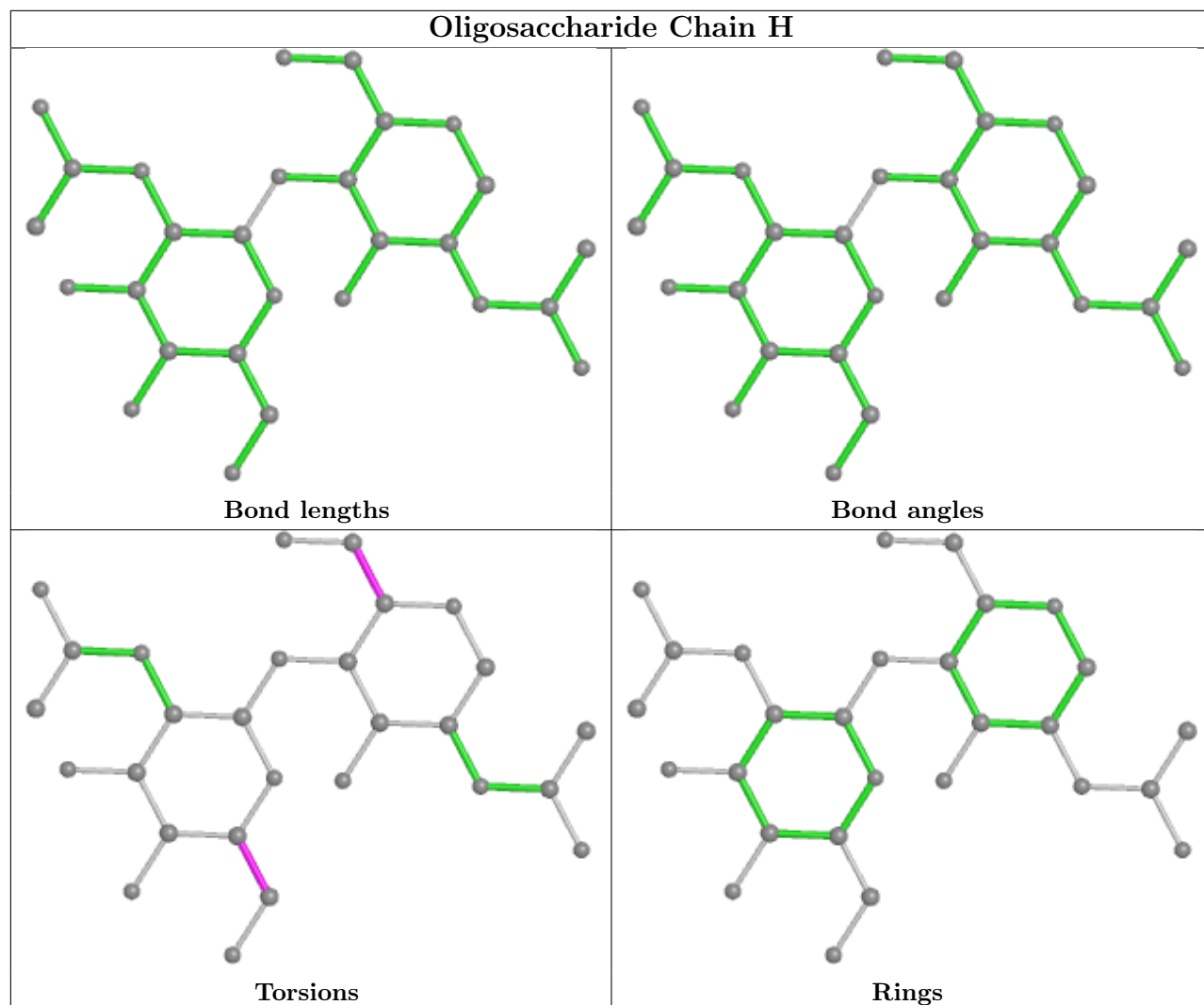
Continued on next page...

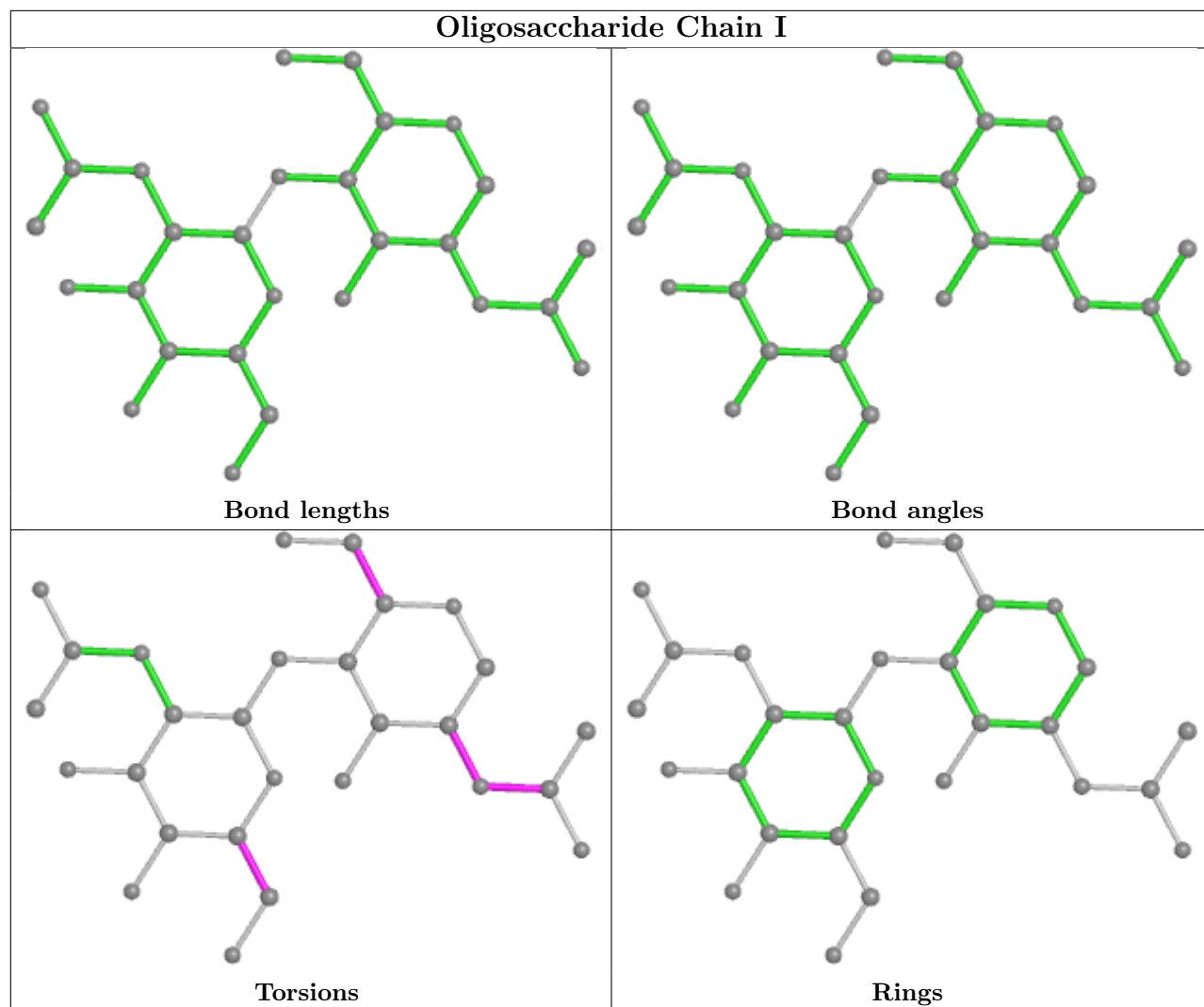
Continued from previous page...

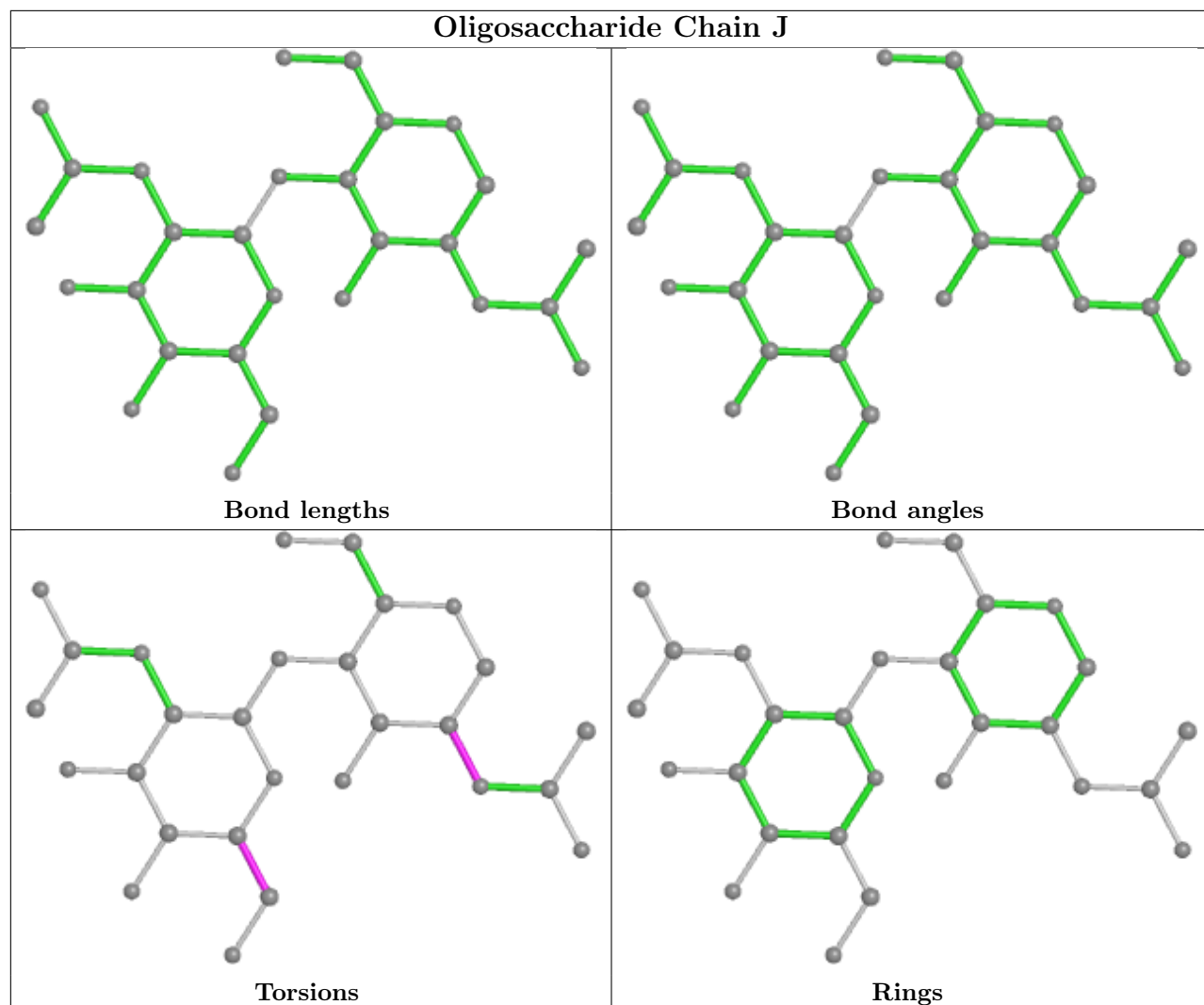
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2	NAG	1	0
3	J	2	NAG	1	0
3	I	2	NAG	1	0

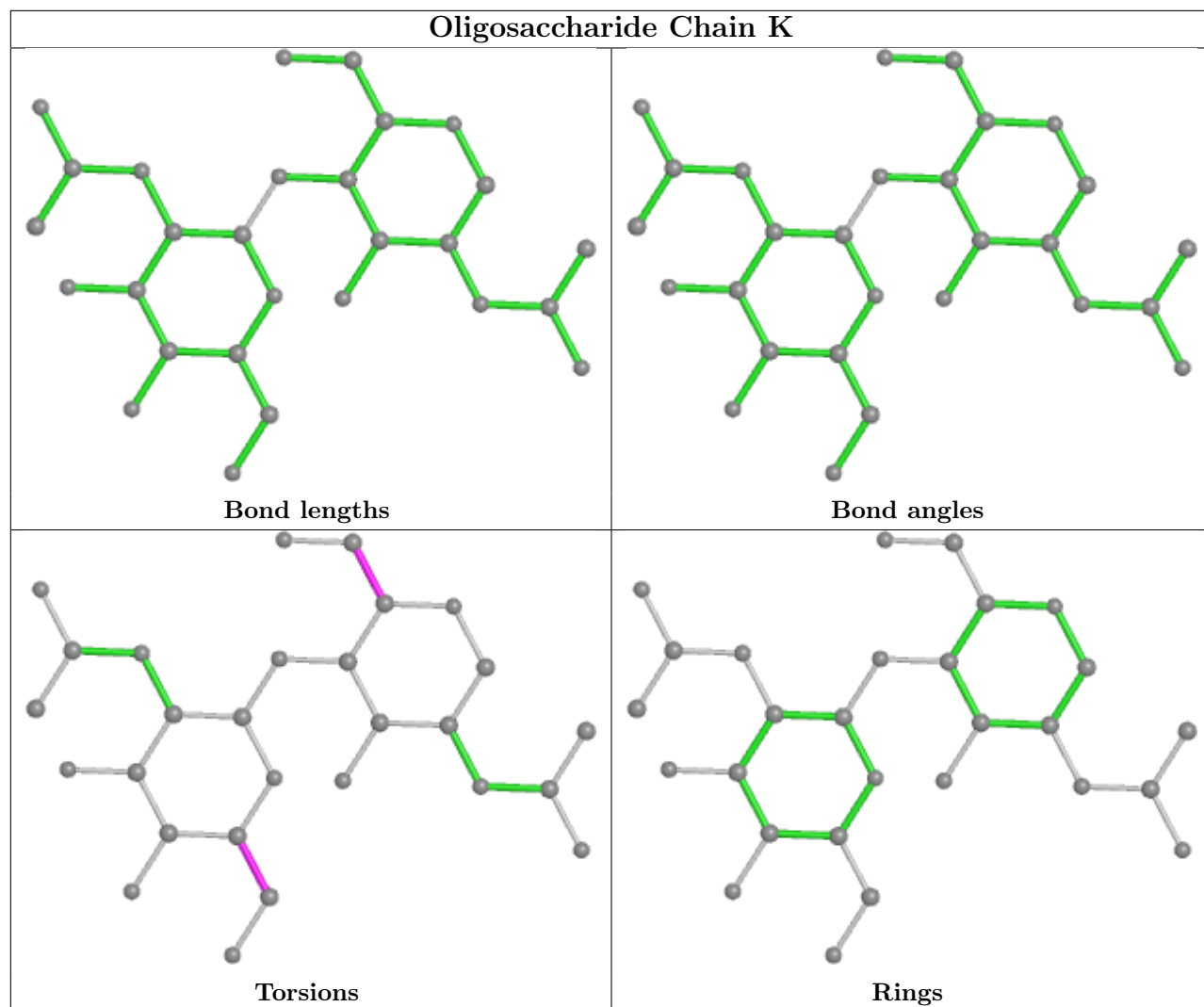
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

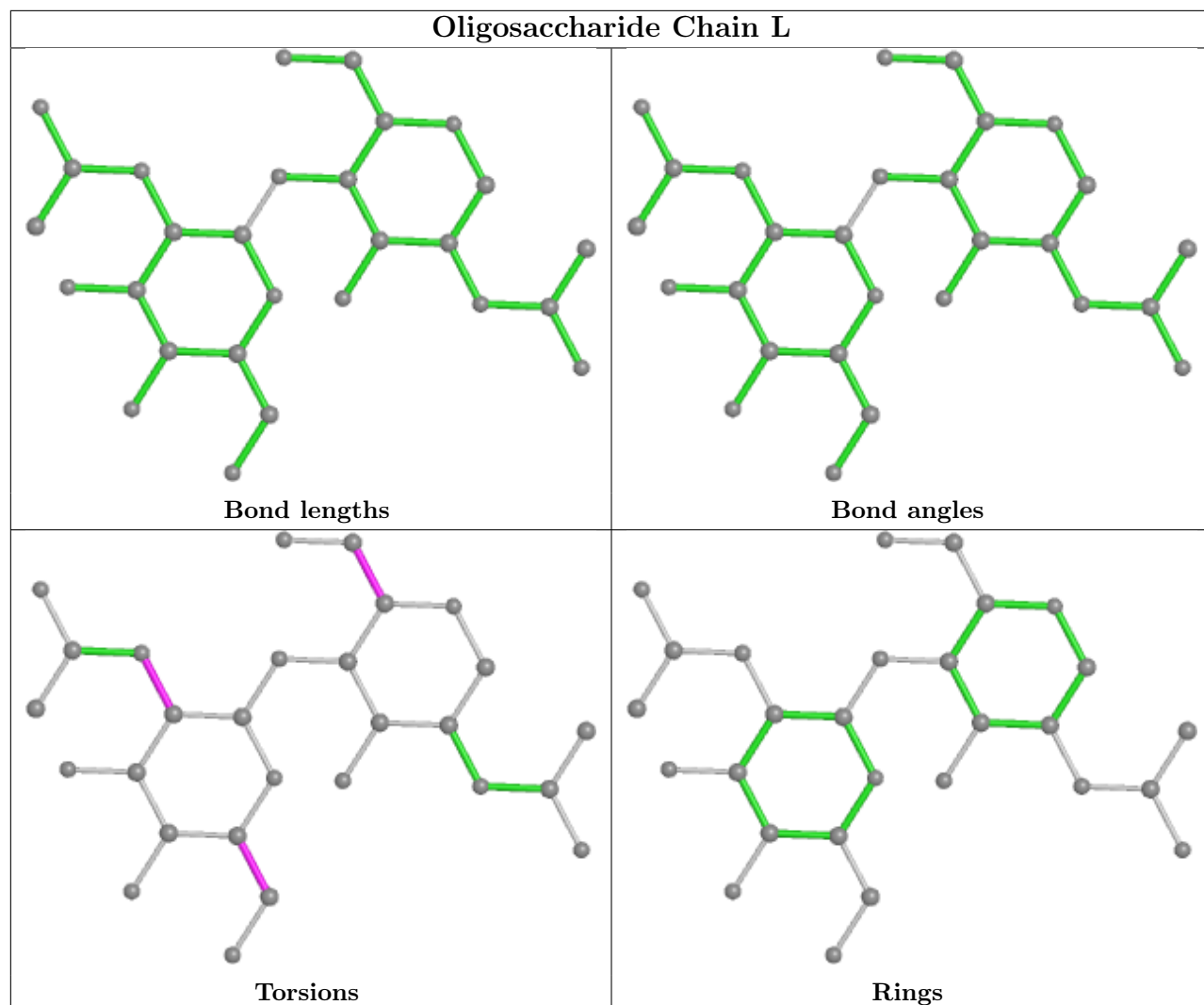


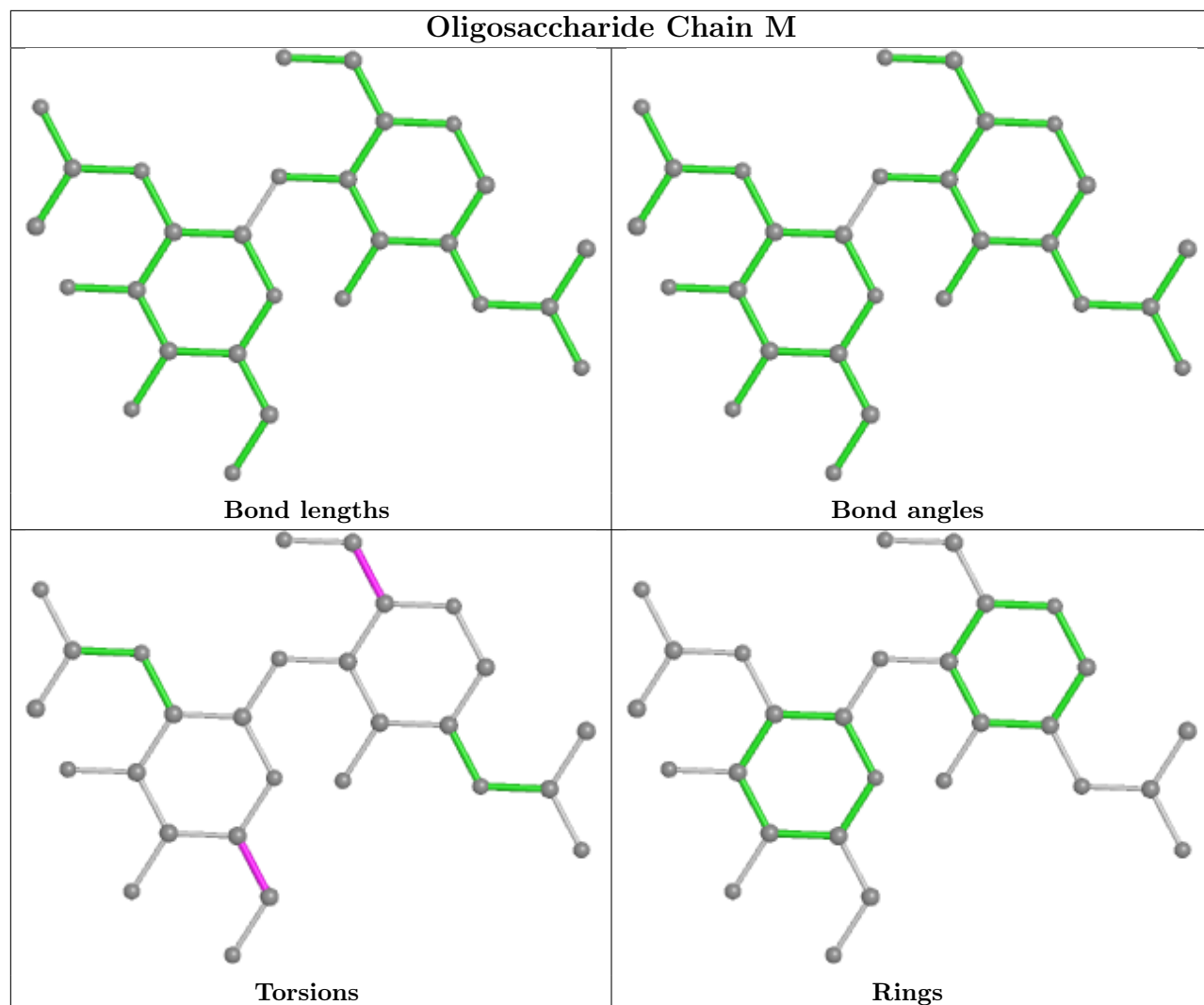


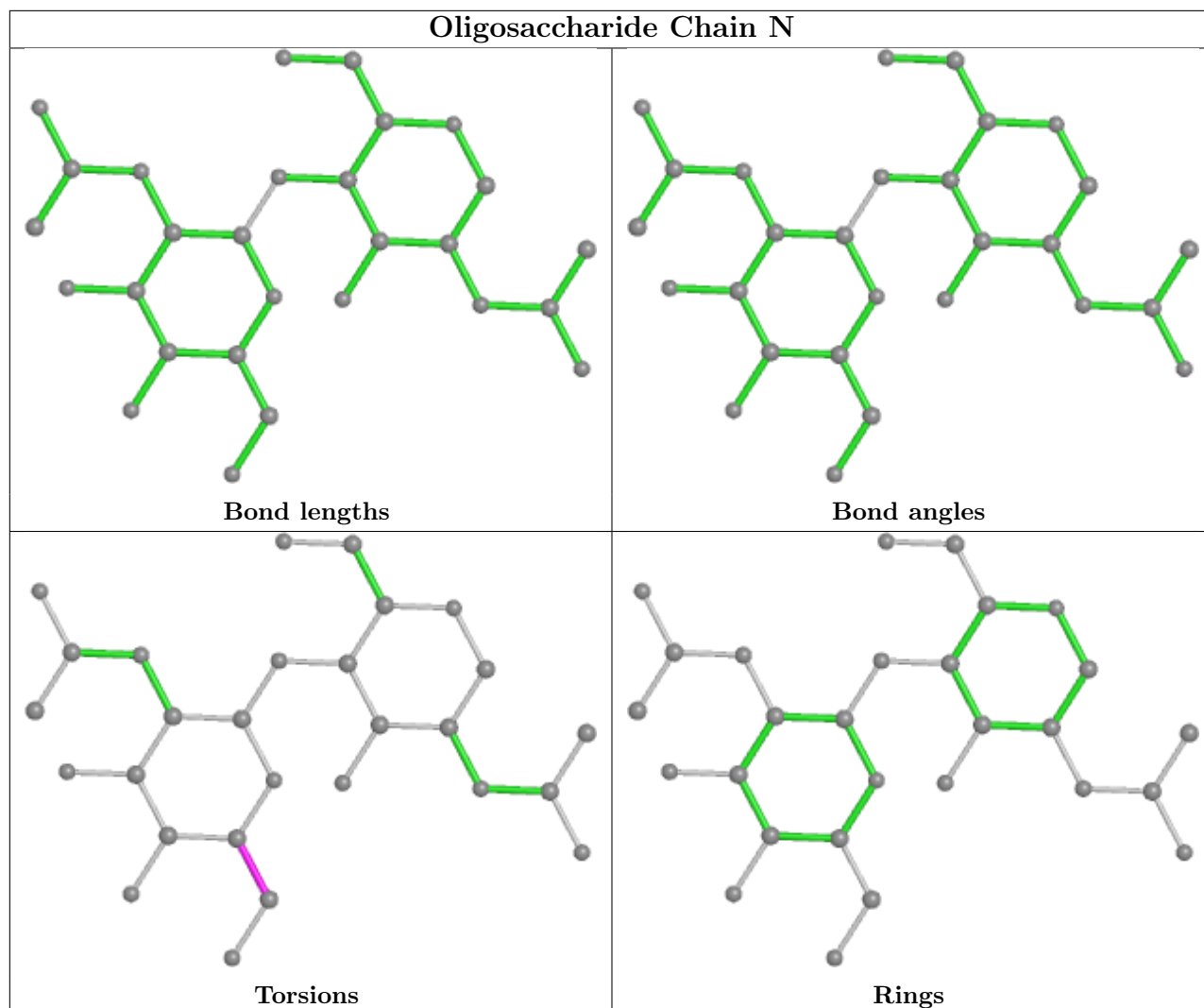


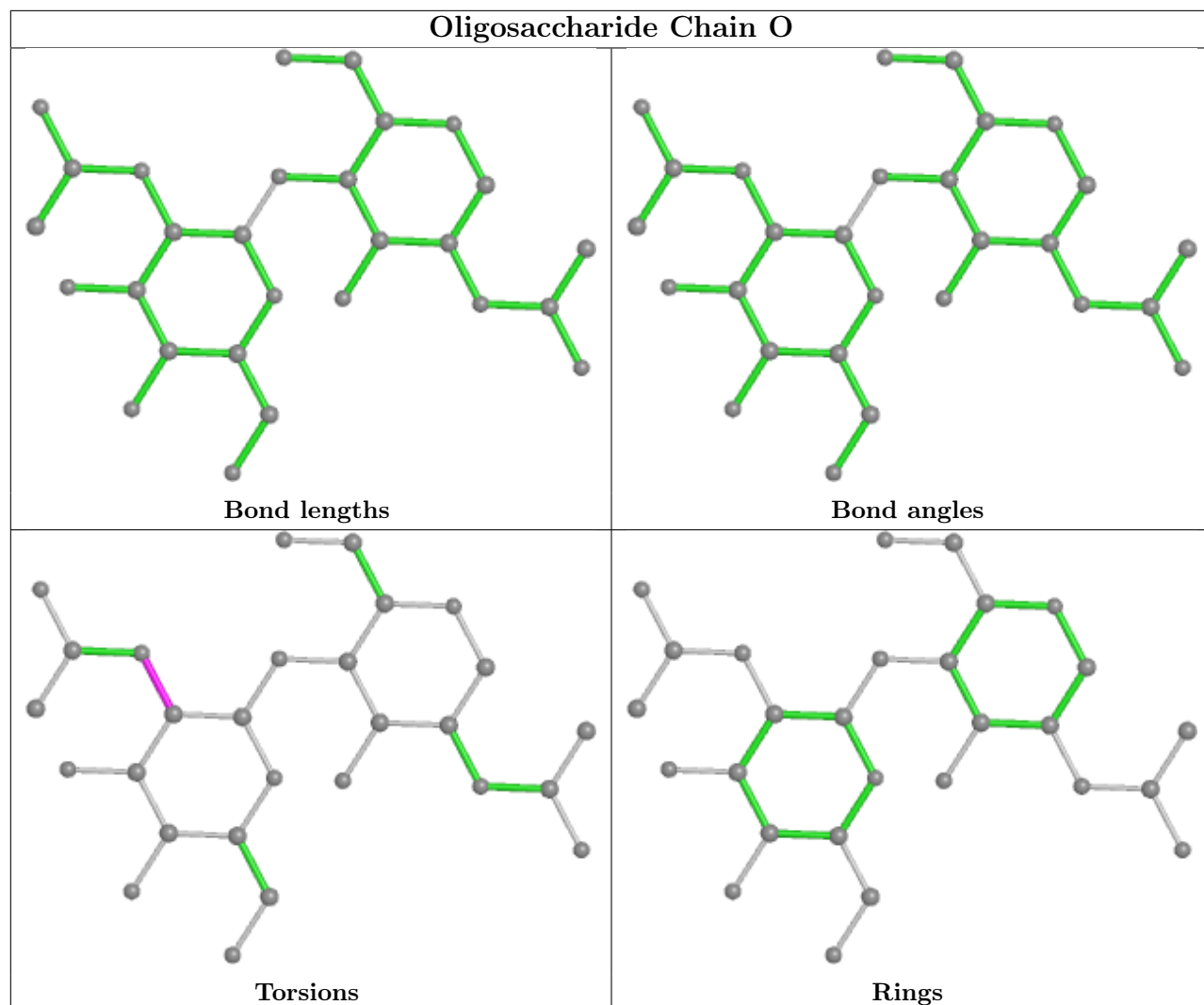


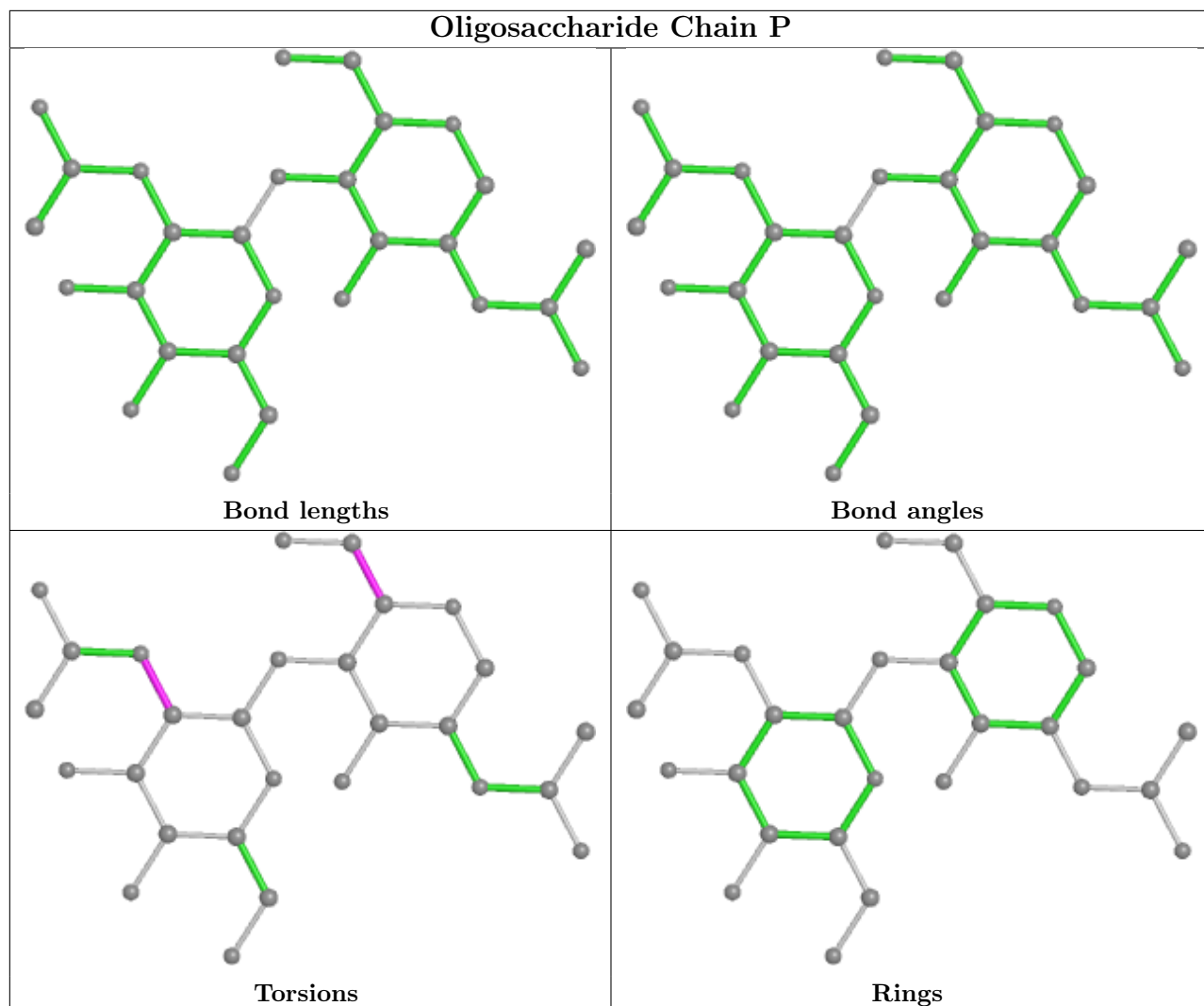


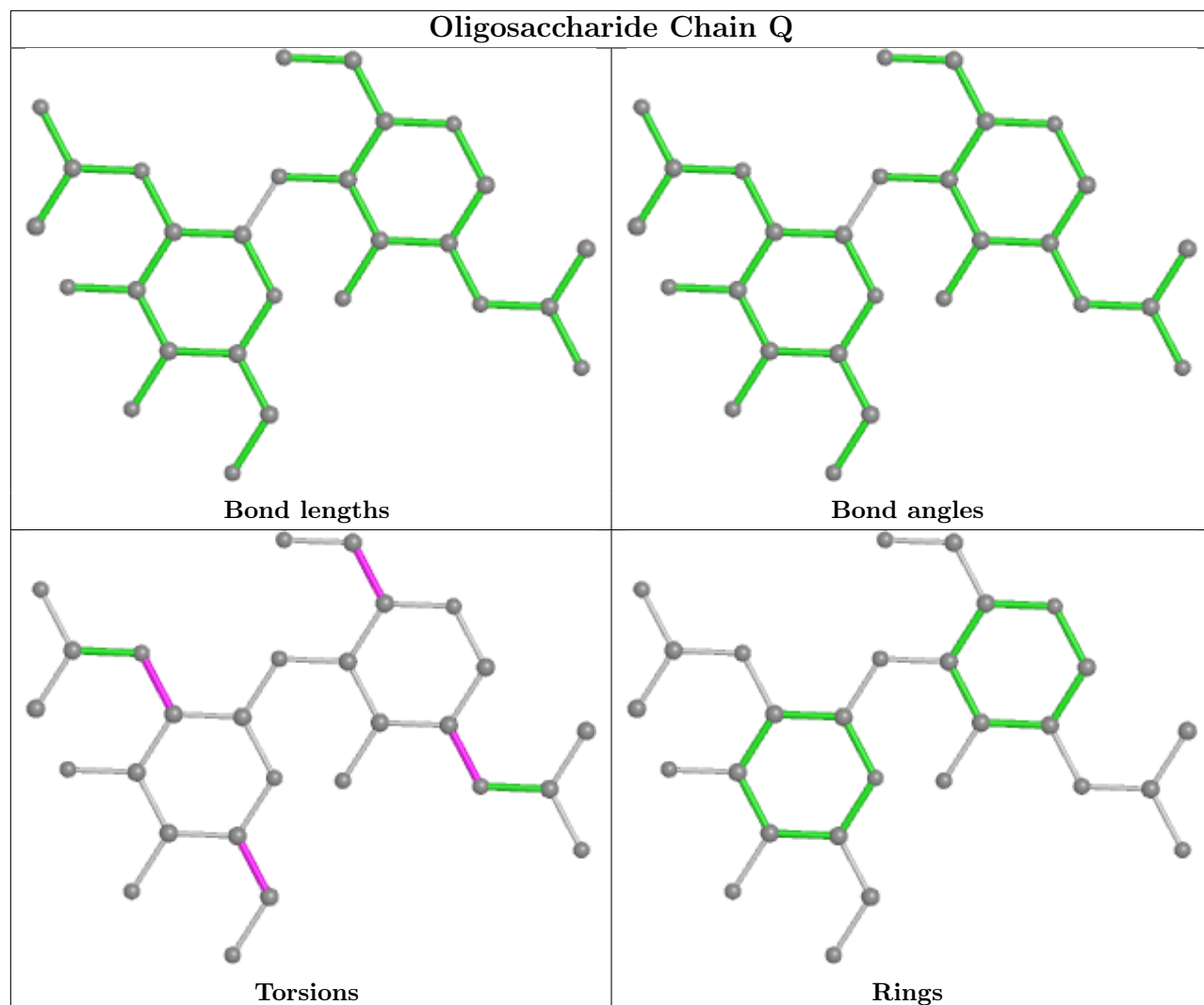


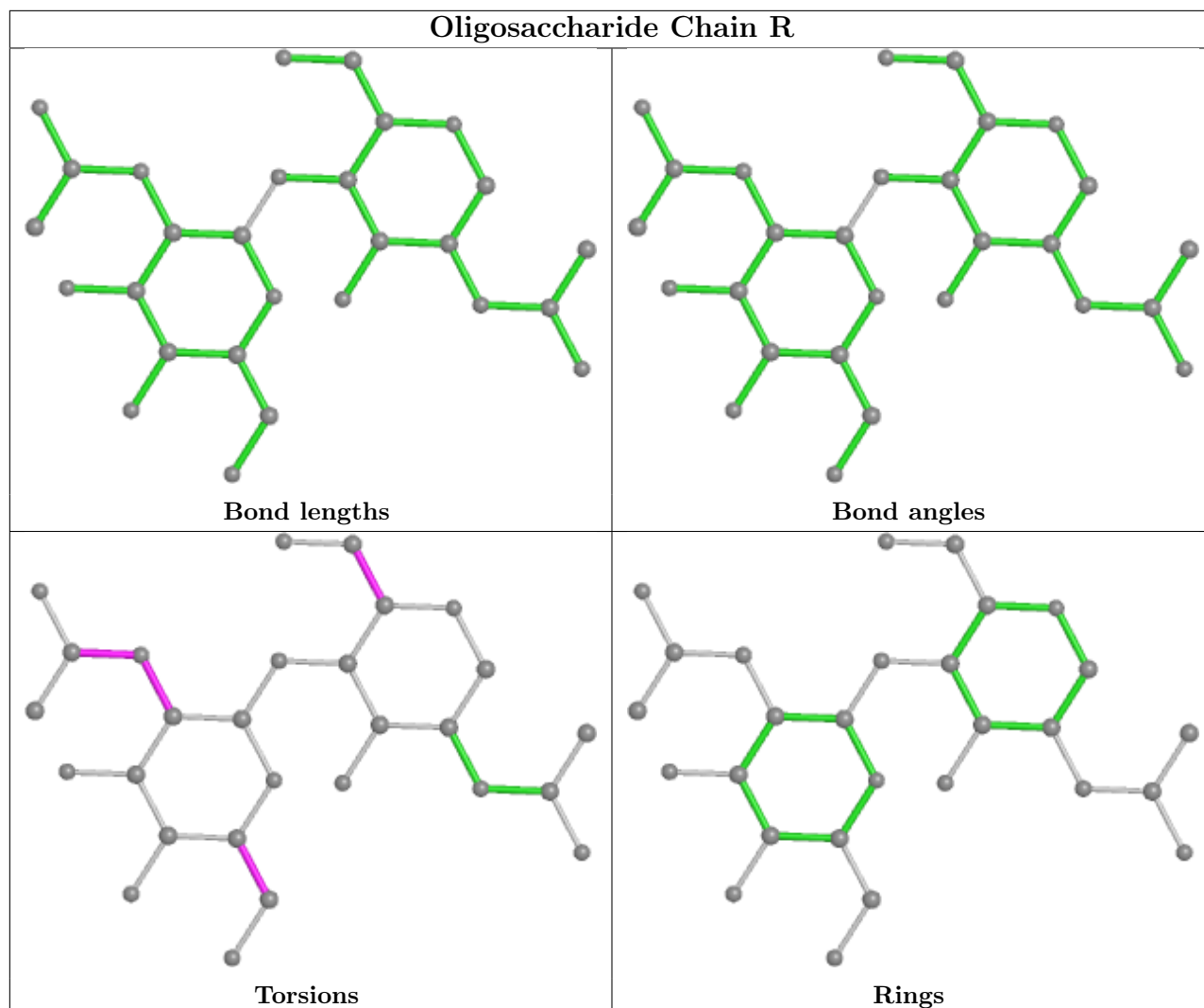












5.6 Ligand geometry [i](#)

50 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	A	1305	-	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	C	1318	-	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	A	1315	-	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	A	1316	1	14,14,15	0.24	0	17,19,21	0.37	0

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	0.30	0	17,19,21	0.41	0
4	NAG	C	1304	1	14,14,15	0.54	0	17,19,21	0.78	1 (5%)
4	NAG	C	1306	1	14,14,15	0.25	0	17,19,21	0.38	0
4	NAG	C	1312	1	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	C	1315	-	14,14,15	0.23	0	17,19,21	0.53	0
4	NAG	A	1314	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1314	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1302	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	A	1309	1	14,14,15	0.20	0	17,19,21	0.52	0
4	NAG	B	1309	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	C	1311	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	A	1311	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.38	0
4	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	A	1310	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	C	1301	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	B	1302	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	B	1307	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	A	1312	-	14,14,15	0.27	0	17,19,21	0.85	1 (5%)
4	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	1303	-	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	B	1312	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1301	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	B	1315	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	B	1311	-	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	C	1310	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	C	1317	-	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1310	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	C	1303	-	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	A	1307	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	1308	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	A	1313	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	A	1308	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	C	1305	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	1305	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	C	1313	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1309	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	B	1313	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1314	1	14,14,15	0.21	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1316	-	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	A	1304	1	14,14,15	0.26	0	17,19,21	0.38	0
4	NAG	A	1317	-	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	C	1307	1	14,14,15	0.24	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
4	NAG	A	1305	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1318	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1315	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1315	-	-	5/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1309	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1310	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	-	-	5/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1315	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1311	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1317	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1314	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1316	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1317	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1304	NAG	C1-O5-C5	2.90	116.12	112.19
4	A	1312	NAG	C2-N2-C7	2.67	126.71	122.90

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1313	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	A	1313	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1317	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1316	NAG	3	0
4	B	1306	NAG	1	0
4	C	1312	NAG	4	0
4	C	1315	NAG	4	0
4	B	1314	NAG	1	0
4	A	1312	NAG	3	0
4	B	1312	NAG	1	0
4	B	1308	NAG	1	0
4	C	1307	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.

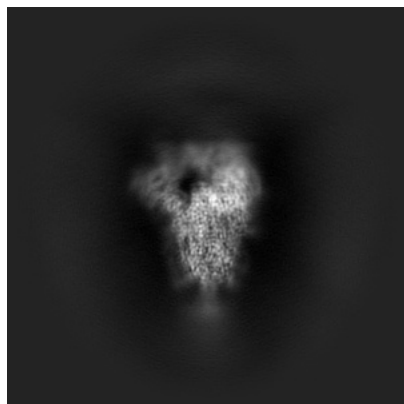
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27069. These allow visual inspection of the internal detail of the map and identification of artifacts.

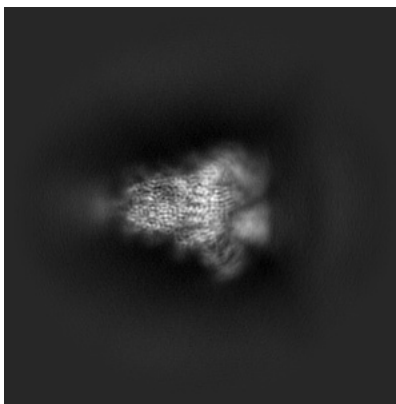
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

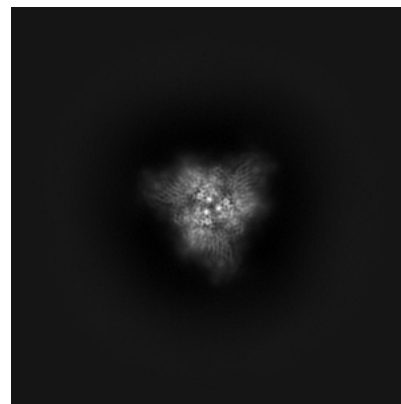
6.1.1 Primary map



X

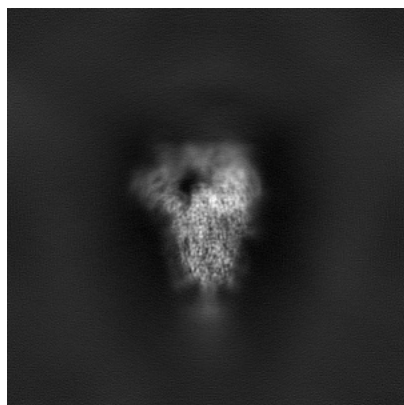


Y

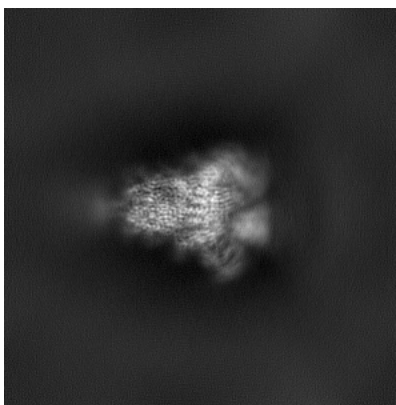


Z

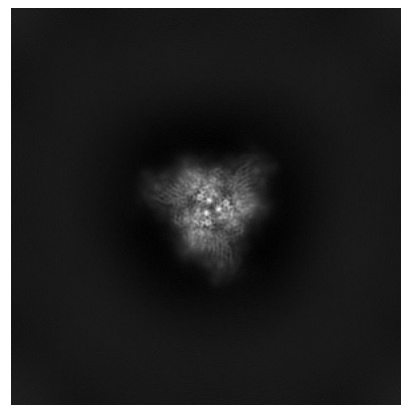
6.1.2 Raw map



X



Y

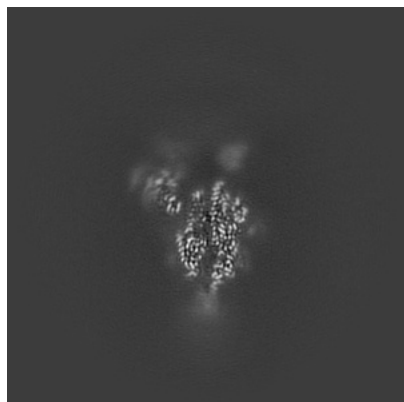


Z

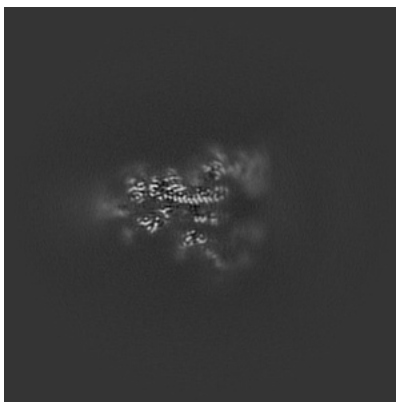
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

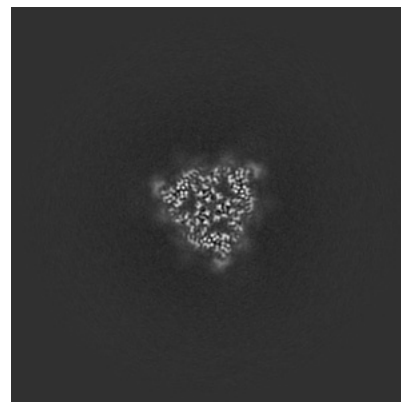
6.2.1 Primary map



X Index: 200

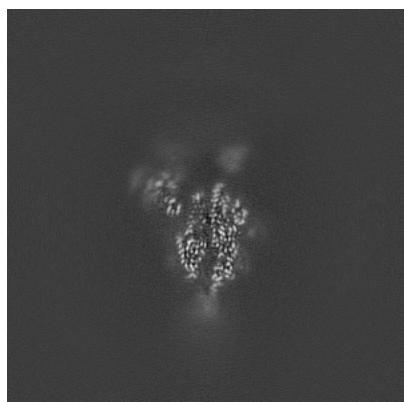


Y Index: 200

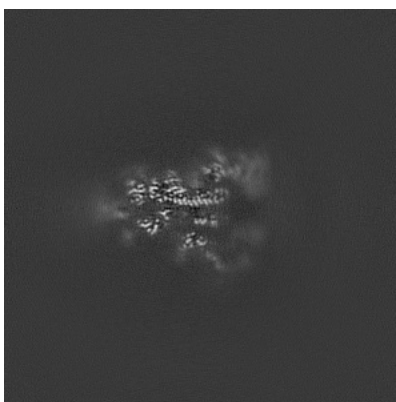


Z Index: 200

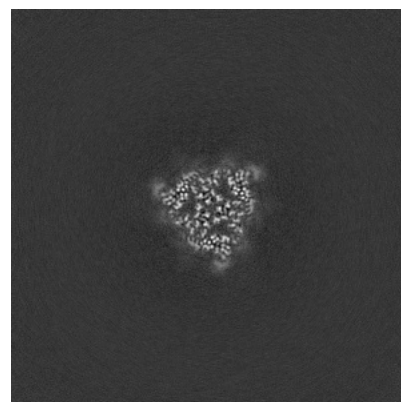
6.2.2 Raw map



X Index: 200



Y Index: 200

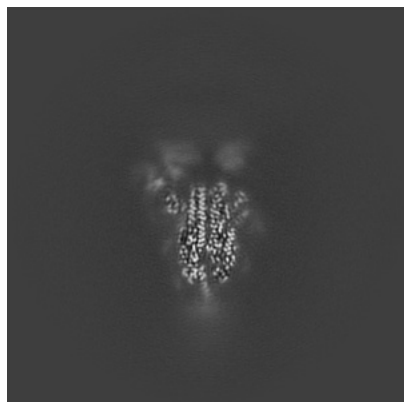


Z Index: 200

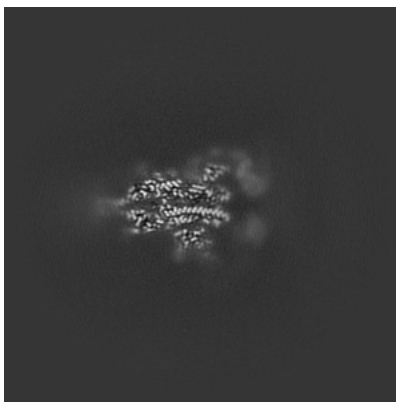
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

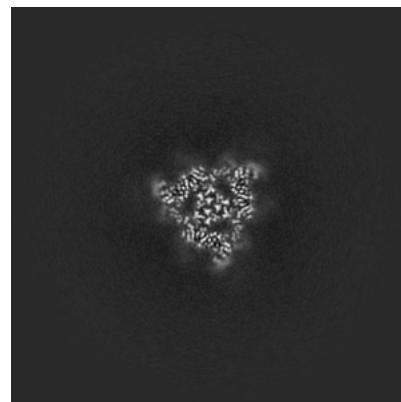
6.3.1 Primary map



X Index: 195

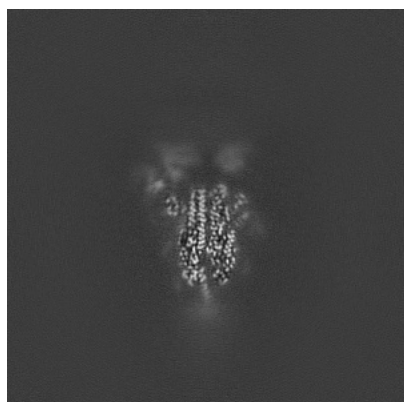


Y Index: 194

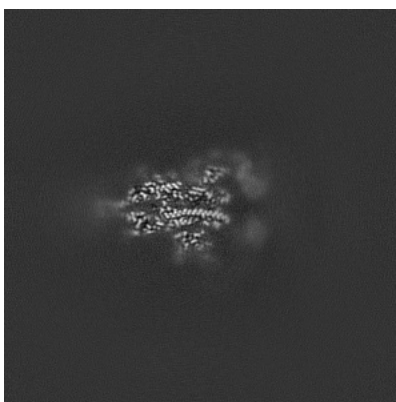


Z Index: 202

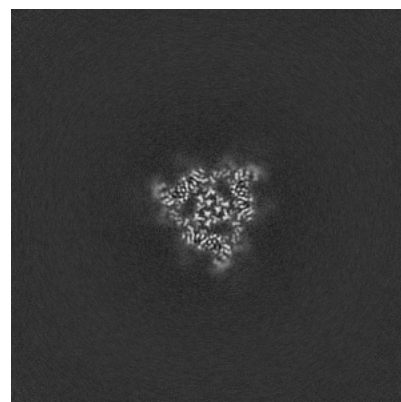
6.3.2 Raw map



X Index: 195



Y Index: 194

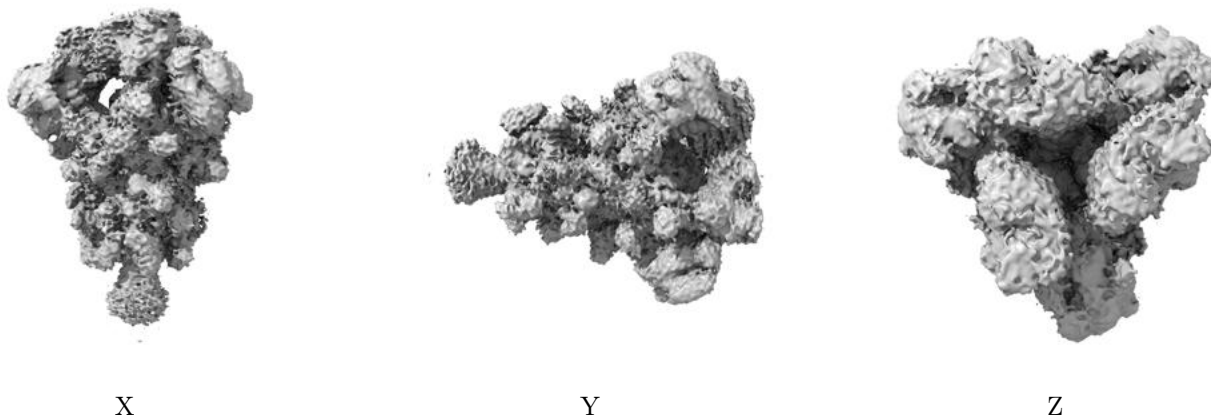


Z Index: 202

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

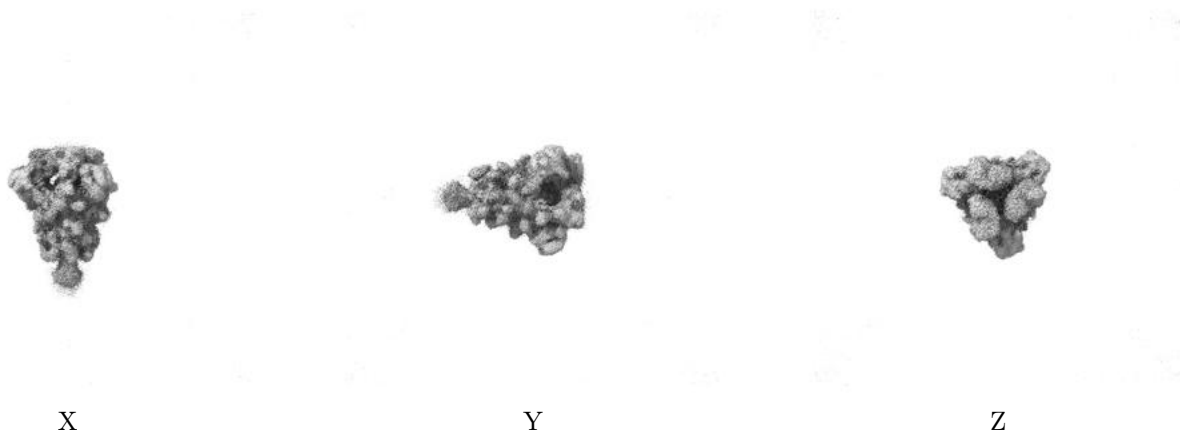
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

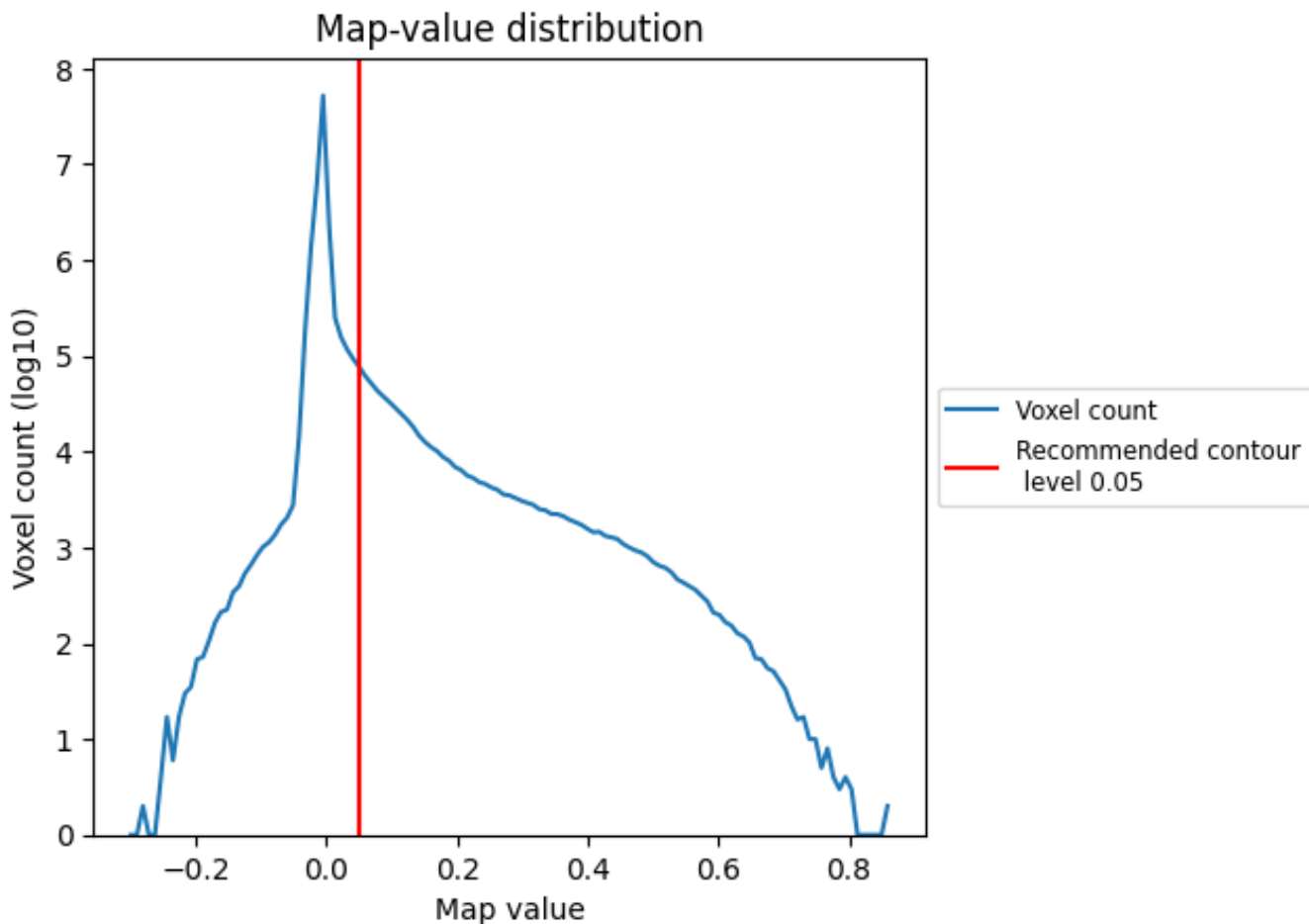
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

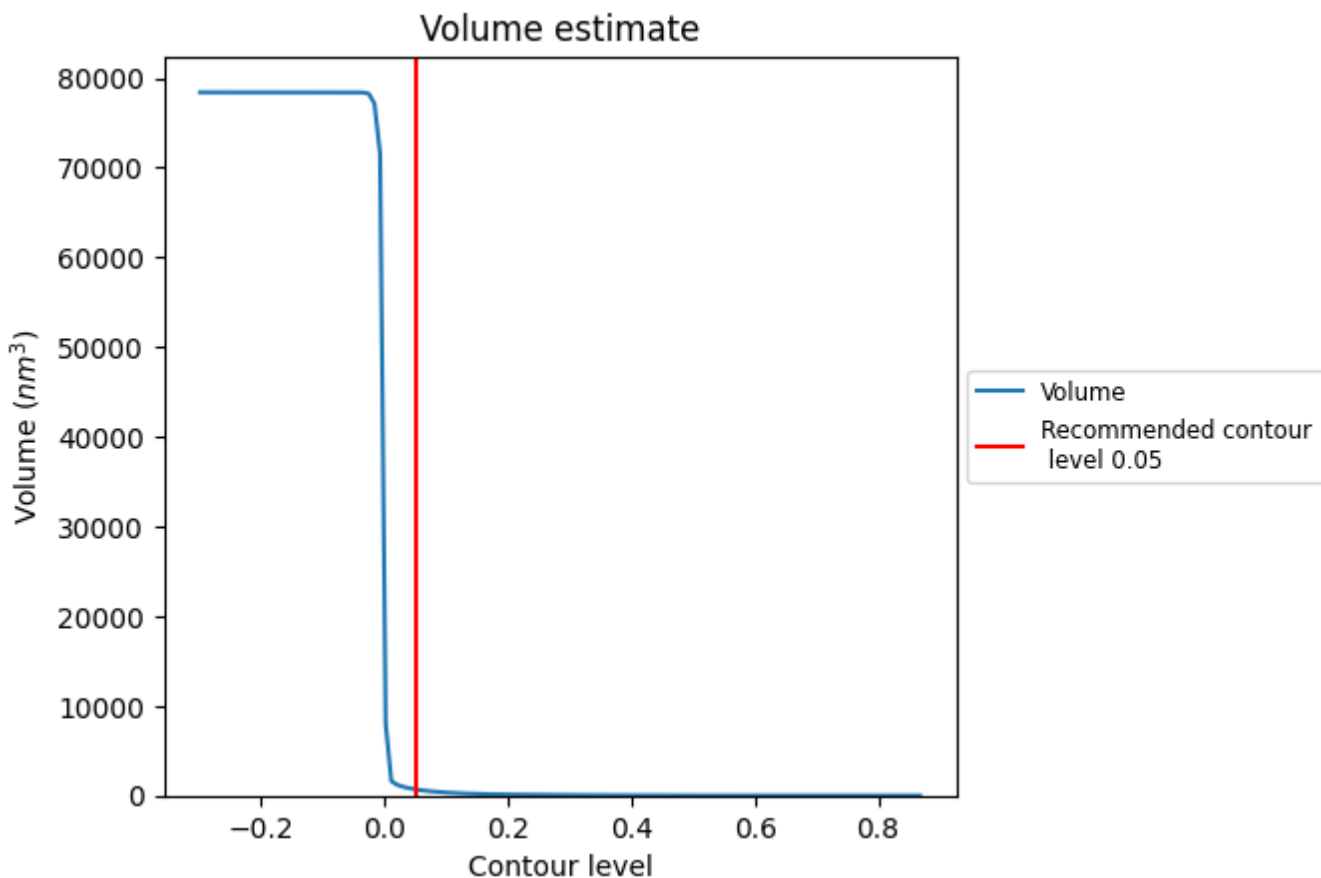
This section contains the results of statistical analysis of the map.

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.

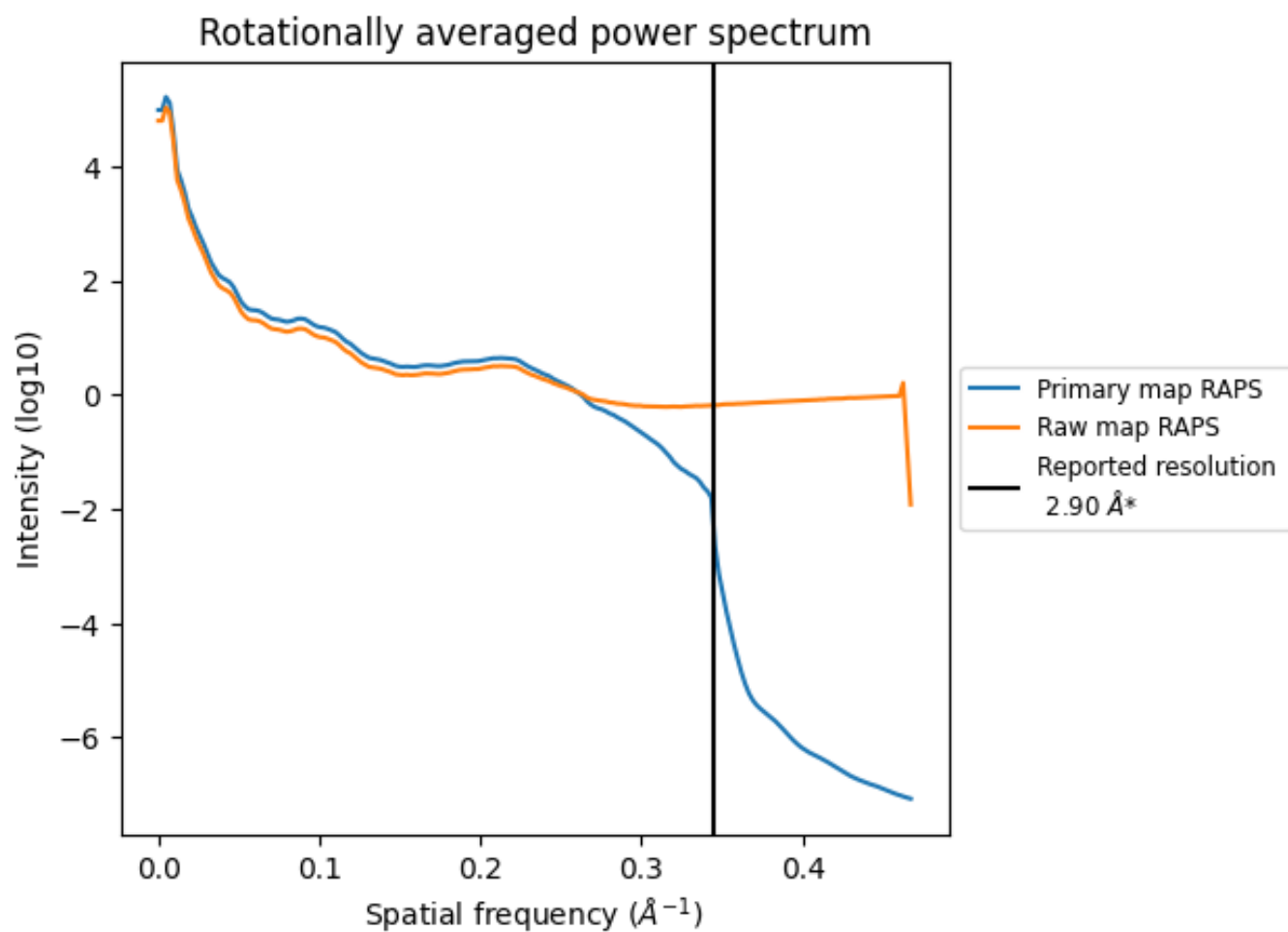
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 696 nm³; this corresponds to an approximate mass of 629 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](#)

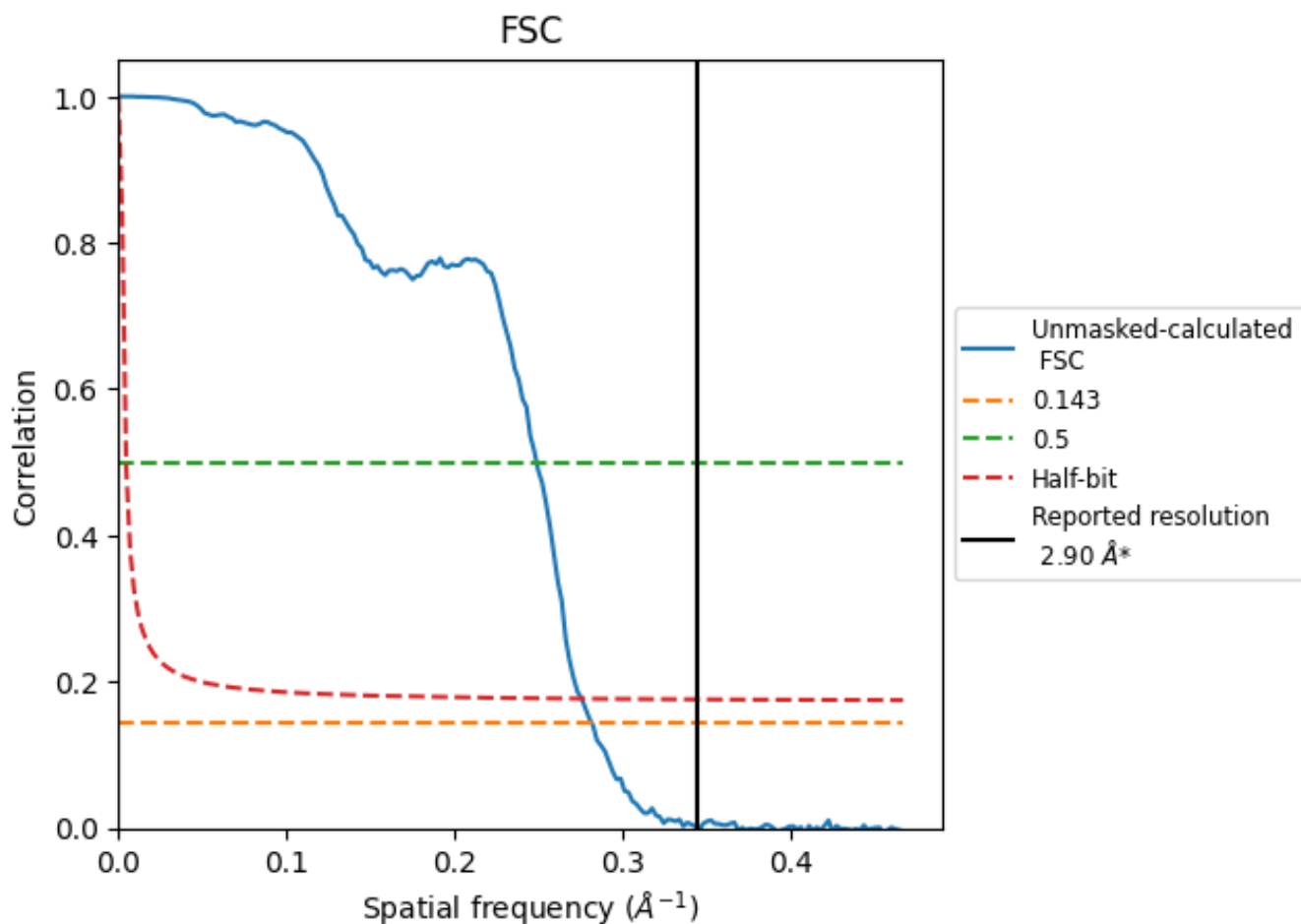


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

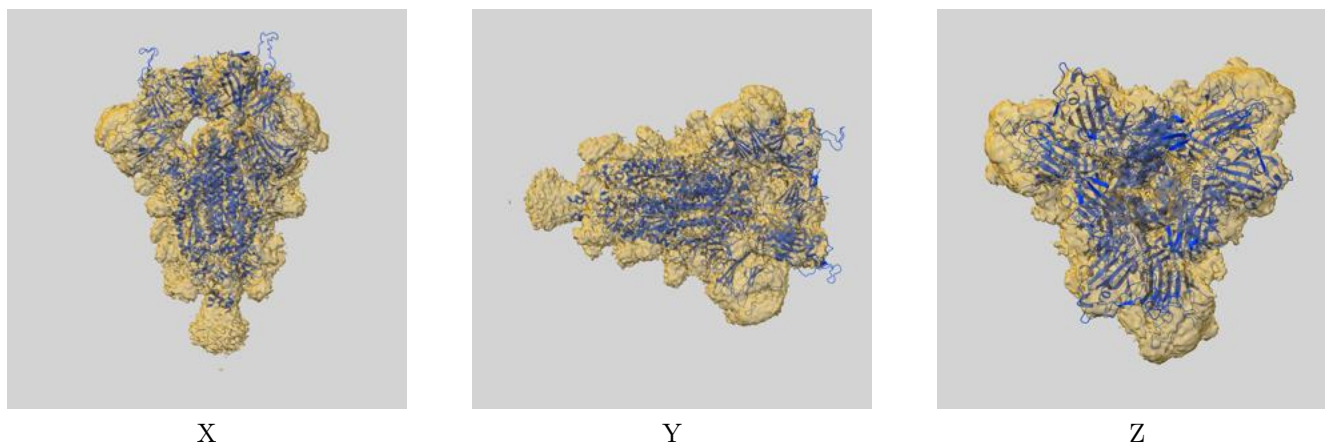
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.55	4.02	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.55 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

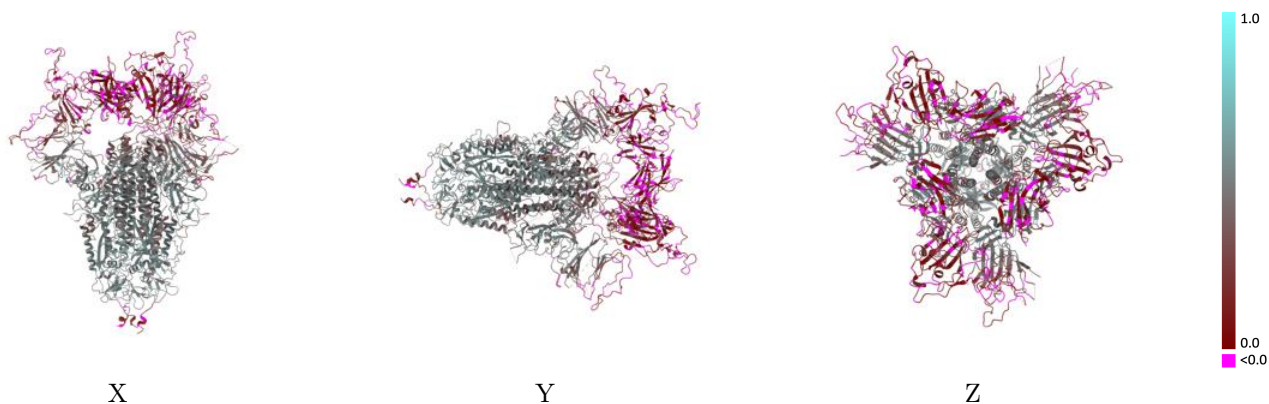
This section contains information regarding the fit between EMDB map EMD-27069 and PDB model 8CY7. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



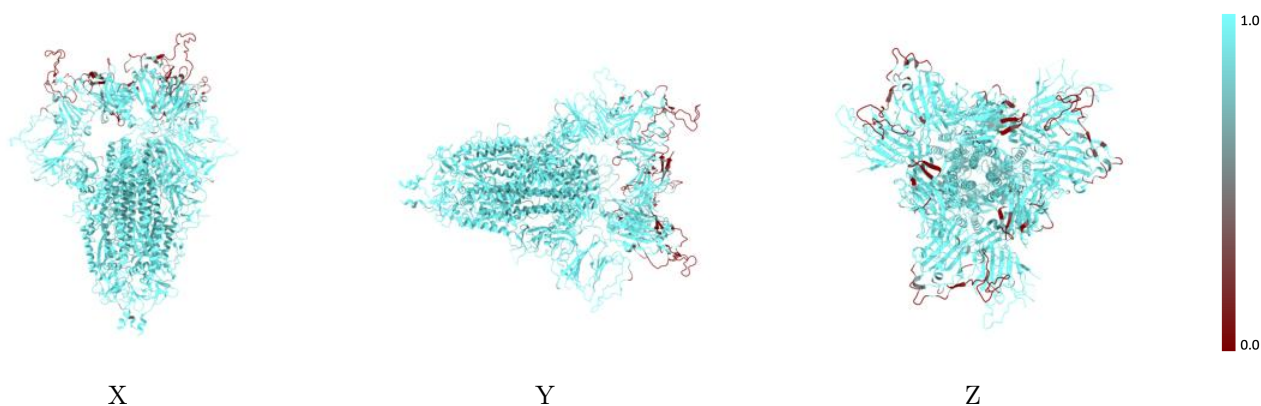
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



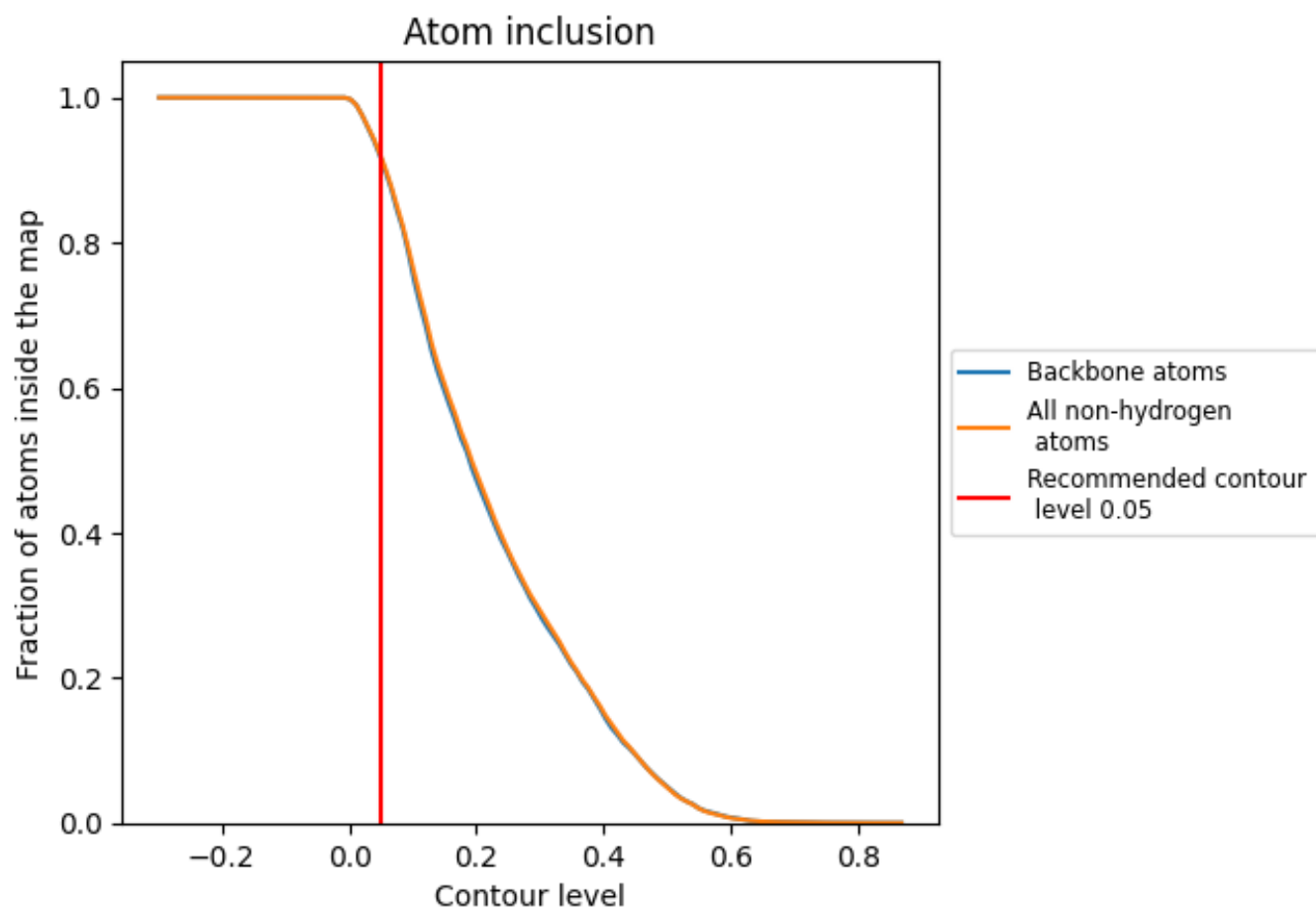
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9186	 0.3300
A	 0.9341	 0.3610
B	 0.9345	 0.3660
C	 0.9319	 0.3540
D	 0.7639	 0.0520
E	 0.7450	 0.0590
F	 0.7784	 0.0640
G	 0.9643	 0.3590
H	 1.0000	 0.2320
I	 0.7500	 0.1380
J	 0.9643	 0.3240
K	 1.0000	 0.3720
L	 0.9286	 0.2820
M	 1.0000	 0.1720
N	 1.0000	 0.3940
O	 0.7500	 0.1630
P	 1.0000	 0.4080
Q	 0.7857	 0.1080
R	 1.0000	 0.3950

