



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 7LCN / pdb_00007lcn
EMDB ID : EMD-23277
Title : Structure of SARS-CoV-2 S protein in complex with N-terminal domain anti-body DH1050.1
Authors : Manne, K.; Acharya, P.
Deposited on : 2021-01-11
Resolution : 3.35 Å(reported)
Based on initial model : 6VXX

This is a Full wwPDB EM Validation 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:

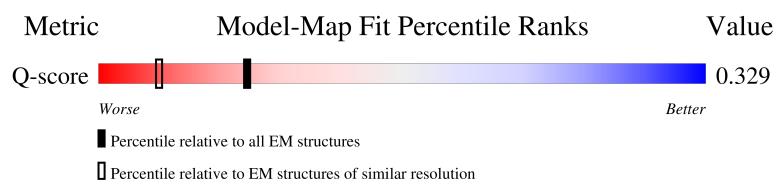
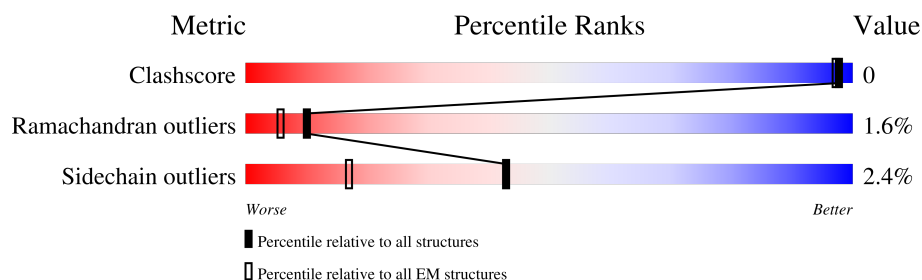
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.35 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14390 (2.85 - 3.85)

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	1121	
1	C	1121	
1	K	1121	
2	B	223	

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Mol	Chain	Length	Quality of chain
2	H	223	55% 93% 6%
2	M	223	63% 88% 9%
3	D	216	55% 94% 6%
3	L	216	46% 92% 7%
3	S	216	55% 92% 7%
4	E	2	50% 100%
4	F	2	50% 50%
4	G	2	100%
4	I	2	100%
4	J	2	100%
4	N	2	50% 100%
4	O	2	50% 50%
4	P	2	100%
4	Q	2	100%
4	R	2	100%
4	T	2	50% 100%
4	V	2	100%
4	W	2	100%
4	X	2	100%
4	Y	2	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 67117 atoms, of which 33049 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	C	993	Total	C	H	N	O	S	0	0
			15370	4979	7580	1294	1483	34		
1	A	993	Total	C	H	N	O	S	0	0
			15370	4979	7580	1294	1483	34		
1	K	993	Total	C	H	N	O	S	0	0
			15370	4979	7580	1294	1483	34		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called DH1050.1 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	223	Total	C	H	N	O	S	0	0
			3297	1053	1630	274	332	8		
2	B	223	Total	C	H	N	O	S	0	0
			3297	1053	1630	274	332	8		
2	M	223	Total	C	H	N	O	S	0	0
			3298	1053	1631	274	332	8		

- Molecule 3 is a protein called DH1050.1 light chain.

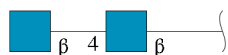
Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	216	Total	C	H	N	O	S	0	0
			3143	999	1538	266	334	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	216	Total	C	H	N	O	S	0	0
			3143	999	1538	266	334	6		
3	S	216	Total	C	H	N	O	S	0	0
			3143	999	1538	266	334	6		

- Molecule 4 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
4	N	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	O	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	P	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	Q	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	R	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	E	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	F	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	G	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	I	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	J	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	T	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	V	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	W	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	X	2	Total	C	H	N	O		0	0
			53	16	25	2	10			
4	Y	2	Total	C	H	N	O		0	0
			53	16	25	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

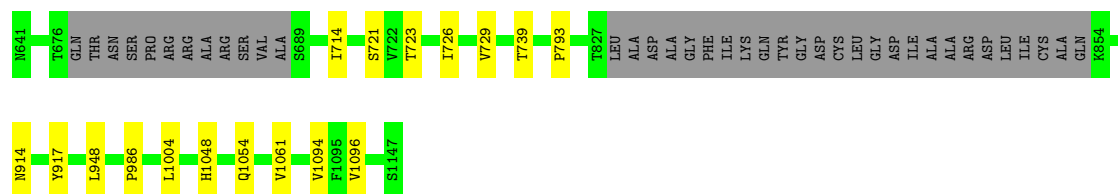


Mol	Chain	Residues	Atoms					AltConf
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

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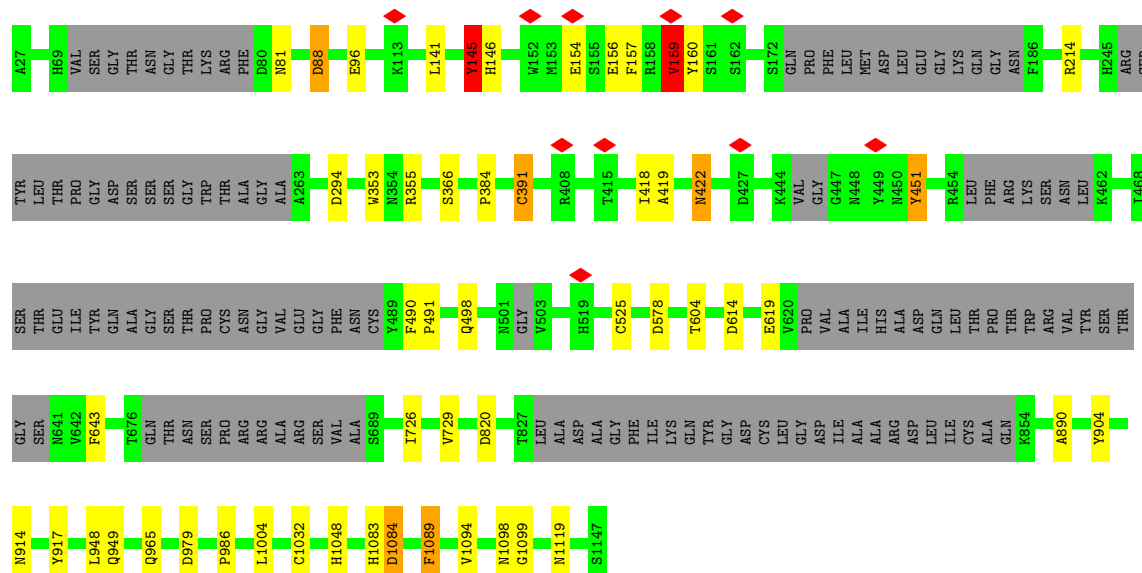
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Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	A	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0
5	K	1	Total 27	C 8	H 13	N 1	O 5	0



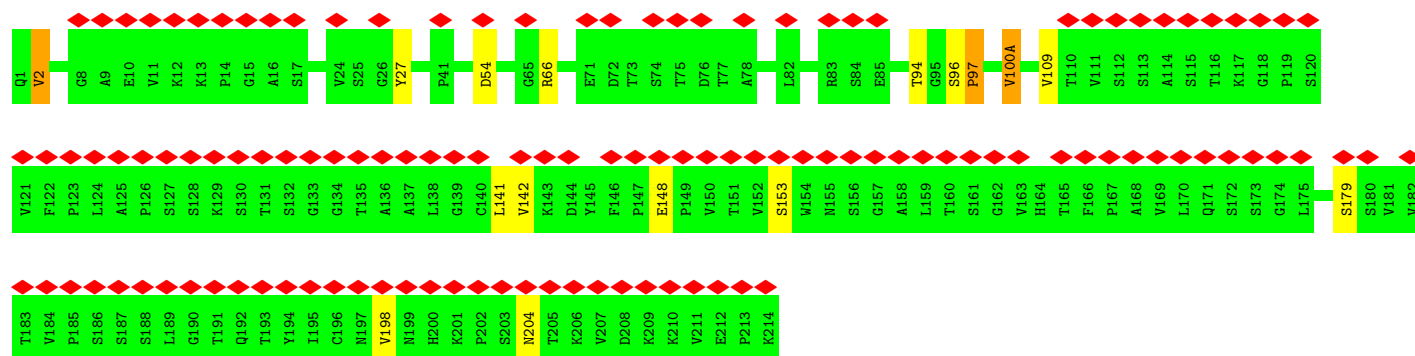
• Molecule 1: Spike glycoprotein

Chain K: 84% .. 11%



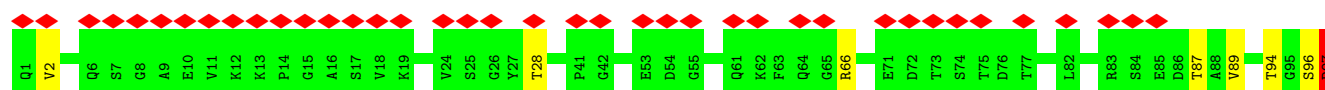
• Molecule 2: DH1050.1 heavy chain

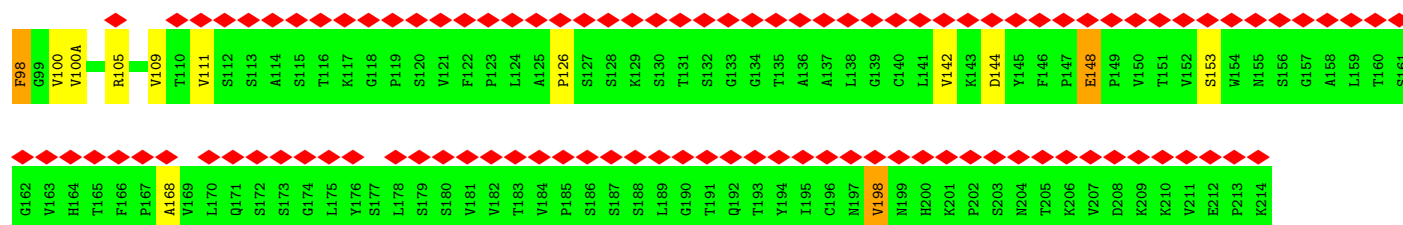
Chain H: 55% 93% 6% .



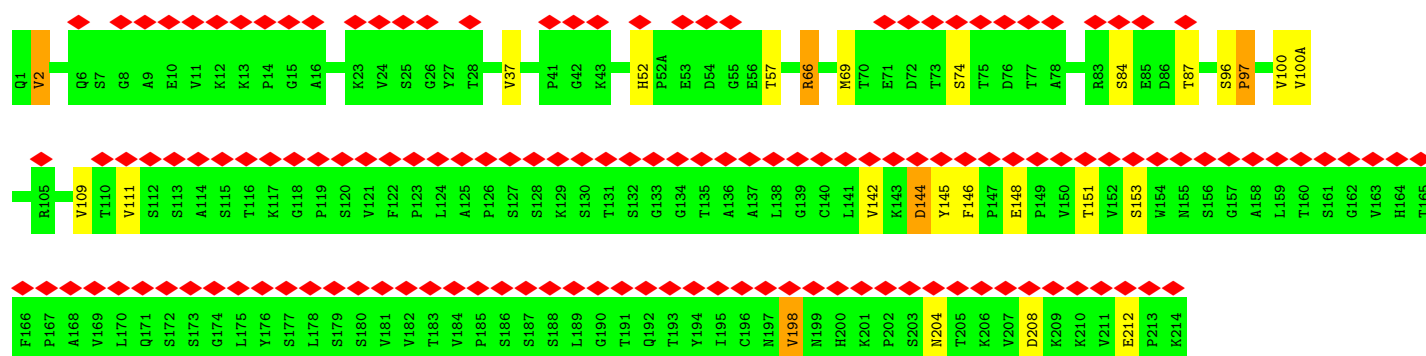
• Molecule 2: DH1050.1 heavy chain

Chain B: 64% 91% 8% .

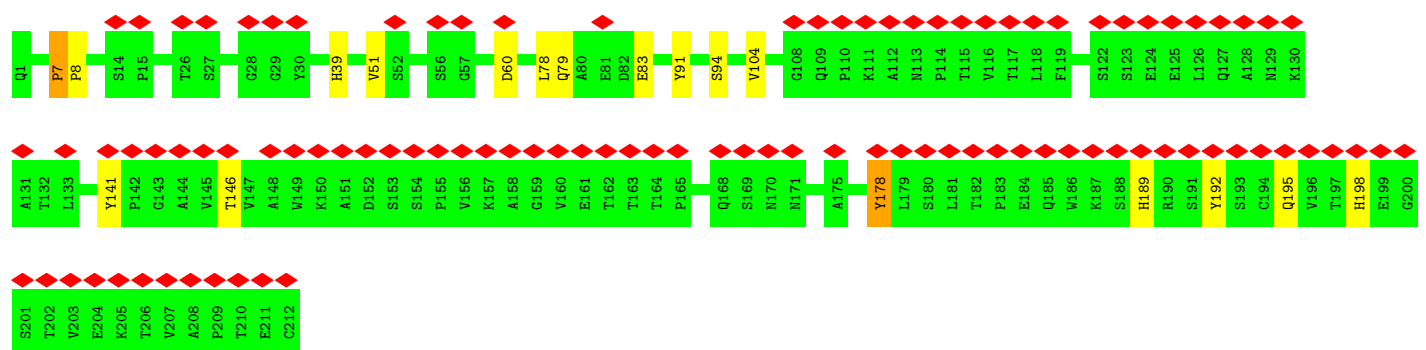
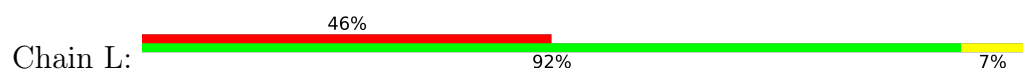




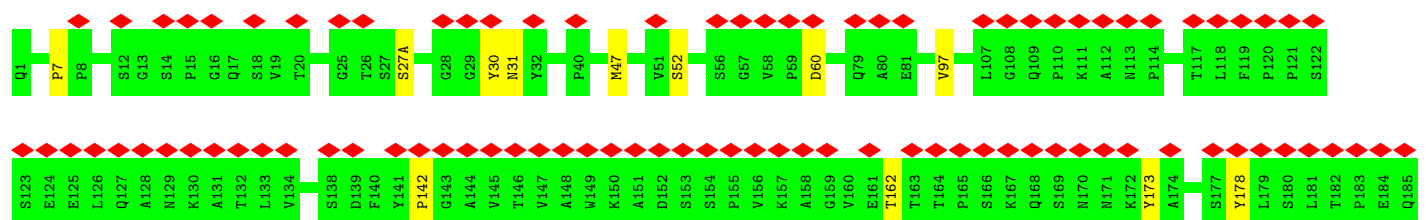
• Molecule 2: DH1050.1 heavy chain



• Molecule 3: DH1050.1 light chain

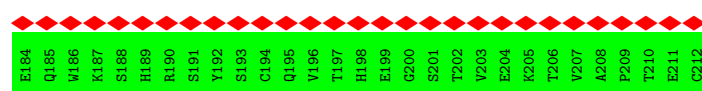
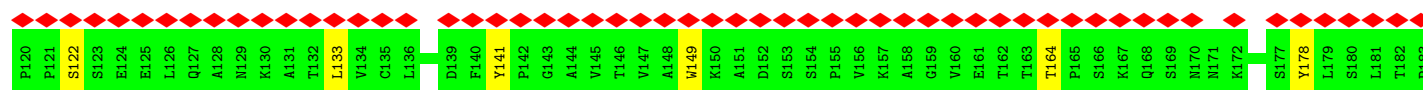
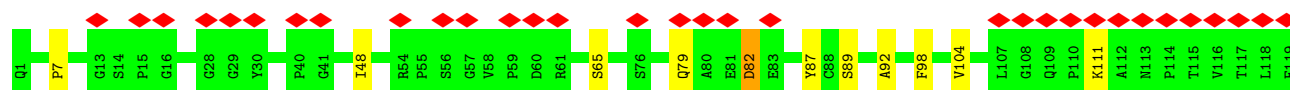
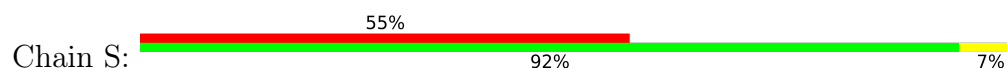


• Molecule 3: DH1050.1 light chain





- Molecule 3: DH1050.1 light chain



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



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



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



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



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

Chain R:  100%

NAG1
NAG2

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

Chain E:  100%

NAG1
NAG2

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

Chain F:  50% 50%

NAG1
NAG2

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

Chain G:  100%

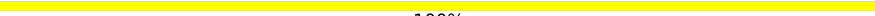
NAG1
NAG2

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

Chain I:  100%

NAG1
NAG2

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

Chain J:  100%

NAG1
NAG2

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



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



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



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



- Molecule 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	426025	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 ($e^-/\text{\AA}^2$)	65.09	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.705	Depositor
Minimum map value	-0.698	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.194	Depositor
Map size ($\text{\AA}$)	338.56, 338.56, 338.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

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	0.75	0/7966	1.29	14/10835 (0.1%)
1	C	0.75	0/7966	1.30	15/10835 (0.1%)
1	K	0.75	0/7966	1.30	18/10835 (0.2%)
2	B	0.86	0/1710	1.49	10/2331 (0.4%)
2	H	0.85	0/1710	1.45	4/2331 (0.2%)
2	M	0.87	0/1710	1.50	9/2331 (0.4%)
3	D	0.82	0/1646	1.43	3/2248 (0.1%)
3	L	0.84	1/1646 (0.1%)	1.44	4/2248 (0.2%)
3	S	0.83	1/1646 (0.1%)	1.42	2/2248 (0.1%)
All	All	0.78	2/33966 (0.0%)	1.35	79/46242 (0.2%)

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	4
1	C	0	4
1	K	0	4
2	H	0	1
2	M	0	1
3	D	0	1
3	L	0	2
3	S	0	2
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	7	PRO	CA-C	5.13	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	7	PRO	CA-C	5.00	1.56	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	VAL	CA-CB-CG1	13.36	133.12	110.40
3	S	7	PRO	N-CA-C	13.14	126.73	110.70
2	M	100(A)	VAL	CA-CB-CG1	13.12	132.71	110.40
2	B	100(A)	VAL	CA-CB-CG1	12.83	132.20	110.40
2	B	2	VAL	CA-CB-CG1	12.71	132.01	110.40
2	M	2	VAL	CA-CB-CG1	12.61	131.84	110.40
3	L	7	PRO	N-CA-C	12.41	125.84	110.70
2	H	100(A)	VAL	CA-CB-CG1	12.40	131.48	110.40
1	C	159	VAL	CA-CB-CG1	12.18	131.10	110.40
1	A	159	VAL	CA-CB-CG1	12.15	131.06	110.40
1	K	159	VAL	CA-CB-CG1	11.90	130.63	110.40
3	D	7	PRO	N-CA-C	11.60	124.85	110.70
2	B	98	PHE	CA-CB-CG	8.72	122.52	113.80
2	H	97	PRO	CA-N-CD	-7.88	100.97	112.00
1	A	391	CYS	N-CA-C	7.40	120.42	109.24
2	M	97	PRO	CA-N-CD	-7.14	102.00	112.00
1	C	319	ARG	CD-NE-CZ	6.63	133.68	124.40
1	C	331	ASN	CA-CB-CG	6.44	119.04	112.60
1	C	384	PRO	CA-C-N	6.44	128.81	120.44
1	C	384	PRO	C-N-CA	6.44	128.81	120.44
1	C	391	CYS	N-CA-C	6.43	118.95	109.24
1	K	1098	ASN	CA-CB-CG	6.12	118.72	112.60
3	L	198	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	K	391	CYS	N-CA-C	6.09	118.32	109.07
3	S	82	ASP	CA-CB-CG	6.07	118.67	112.60
2	M	212	GLU	N-CA-C	5.97	113.39	108.07
1	A	106	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	347	PHE	CA-CB-CG	5.84	119.64	113.80
3	D	198	HIS	CB-CG-CD2	-5.83	123.62	131.20
2	M	52	HIS	CA-CB-CG	5.82	119.62	113.80
1	A	986	PRO	N-CA-C	5.79	117.77	110.70
1	A	391	CYS	CA-CB-SG	5.78	127.68	114.40
1	C	578	ASP	CA-CB-CG	5.74	118.34	112.60
2	B	144	ASP	CA-CB-CG	5.74	118.34	112.60
2	B	66	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	K	88	ASP	CA-CB-CG	5.67	118.27	112.60
1	K	986	PRO	N-CA-C	5.65	117.59	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	THR	N-CA-C	5.46	117.13	110.41
1	K	979	ASP	CA-CB-CG	5.41	118.01	112.60
3	L	189	HIS	CB-CG-CD2	-5.41	124.17	131.20
2	B	97	PRO	CA-N-CD	-5.39	104.45	112.00
1	K	391	CYS	CA-CB-SG	5.38	126.78	114.40
1	A	1054	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	A	578	ASP	CB-CA-C	5.37	118.05	109.62
2	M	144	ASP	CA-CB-CG	5.35	117.95	112.60
1	C	1098	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	384	PRO	CA-C-N	5.30	127.34	120.44
1	A	384	PRO	C-N-CA	5.30	127.34	120.44
1	A	157	PHE	CA-CB-CG	5.28	119.08	113.80
1	K	384	PRO	CA-C-N	5.28	127.30	120.44
1	K	384	PRO	C-N-CA	5.28	127.30	120.44
1	K	1048	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	C	138	ASP	CA-C-N	5.24	126.39	119.84
1	C	138	ASP	C-N-CA	5.24	126.39	119.84
2	M	66	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	C	1085	GLY	CA-C-N	5.23	128.27	120.95
1	C	1085	GLY	C-N-CA	5.23	128.27	120.95
3	L	195	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	K	451	TYR	CA-C-N	5.22	128.28	120.87
1	K	451	TYR	C-N-CA	5.22	128.28	120.87
1	K	1089	PHE	CA-CB-CG	5.22	119.02	113.80
2	B	148	GLU	CB-CA-C	5.21	120.43	110.17
1	C	331	ASN	CB-CG-ND2	-5.17	108.64	116.40
3	D	7	PRO	CB-CA-C	5.15	117.20	110.92
2	B	126	PRO	CA-C-N	5.14	128.37	120.82
2	B	126	PRO	C-N-CA	5.14	128.37	120.82
2	H	66	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	C	986	PRO	N-CA-C	5.09	116.91	110.70
1	K	965	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	1048	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	K	643	PHE	CA-CB-CG	5.05	118.85	113.80
1	K	949	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	M	57	THR	CA-C-N	5.05	127.27	120.50
2	M	57	THR	C-N-CA	5.05	127.27	120.50
1	A	245	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	K	490	PHE	CA-C-N	5.02	126.12	119.84
1	K	490	PHE	C-N-CA	5.02	126.12	119.84
1	C	1064	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	A	329	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	TYR	Sidechain
1	A	279	TYR	Sidechain
1	A	355	ARG	Sidechain
1	A	451	TYR	Sidechain
1	C	145	TYR	Sidechain
1	C	279	TYR	Sidechain
1	C	355	ARG	Sidechain
1	C	451	TYR	Sidechain
3	D	178	TYR	Sidechain
2	H	27	TYR	Sidechain
1	K	145	TYR	Sidechain
1	K	355	ARG	Sidechain
1	K	451	TYR	Sidechain
1	K	904	TYR	Sidechain
3	L	141	TYR	Sidechain
3	L	91	TYR	Sidechain
2	M	66	ARG	Sidechain
3	S	178	TYR	Sidechain
3	S	87	TYR	Sidechain

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	7790	7580	7580	8	0
1	C	7790	7580	7580	9	0
1	K	7790	7580	7580	10	0
2	B	1667	1630	1630	0	0
2	H	1667	1630	1630	2	0
2	M	1667	1631	1630	0	0
3	D	1605	1538	1538	2	0
3	L	1605	1538	1538	2	0
3	S	1605	1538	1538	3	0
4	E	28	25	25	0	0
4	F	28	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	28	25	25	0	0
4	I	28	25	25	0	0
4	J	28	25	25	0	0
4	N	28	25	25	0	0
4	O	28	25	25	0	0
4	P	28	25	25	0	0
4	Q	28	25	25	0	0
4	R	28	25	25	0	0
4	T	28	25	25	0	0
4	V	28	25	25	0	0
4	W	28	25	25	0	0
4	X	28	25	25	0	0
4	Y	28	25	25	0	0
5	A	154	143	143	0	0
5	C	154	143	143	1	0
5	K	154	143	143	0	0
All	All	34068	33049	33048	30	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 0.

All (30) 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:726:ILE:HG22	1:A:948:LEU:HD13	1.68	0.73
1:C:123:ALA:HB3	5:C:1302:NAG:H83	1.88	0.55
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.89	0.54
1:K:418:ILE:HG23	1:K:422:ASN:HD21	1.76	0.50
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.92	0.50
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.93	0.50
1:K:391:CYS:HB2	1:K:525:CYS:HA	1.94	0.50
3:S:133:LEU:HD23	3:S:149:TRP:CZ3	2.47	0.49
1:C:726:ILE:CG2	1:C:948:LEU:HD13	2.44	0.48
3:S:111:LYS:HE2	3:S:141:TYR:CE1	2.49	0.48
3:S:89:SER:HB2	3:S:98:PHE:CD2	2.50	0.47
1:C:245:HIS:HA	2:H:100(A):VAL:HB	1.97	0.46
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.51	0.46
1:A:726:ILE:HG23	1:A:1061:VAL:HG22	1.97	0.45
1:K:1083:HIS:CG	1:K:1084:ASP:H	2.35	0.45
1:C:1089:PHE:CE2	1:K:914:ASN:HA	2.52	0.44
1:A:914:ASN:HA	1:K:1089:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:142:PRO:HD3	3:D:173:TYR:CD1	2.53	0.43
1:C:666:ILE:HD12	1:C:670:ILE:HG22	2.01	0.43
1:C:1089:PHE:CE2	1:K:917:TYR:CD2	3.07	0.43
1:K:726:ILE:HG22	1:K:948:LEU:HD13	2.01	0.42
1:C:143:VAL:HG22	1:C:144:TYR:H	1.85	0.42
2:H:179:SER:HB3	3:L:178:TYR:CE1	2.55	0.42
1:A:917:TYR:CD2	1:K:1089:PHE:CE2	3.09	0.41
1:A:714:ILE:HD12	1:A:1096:VAL:HG11	2.02	0.41
1:K:418:ILE:H	1:K:418:ILE:HD12	1.85	0.41
1:K:353:TRP:CD1	1:K:353:TRP:H	2.38	0.41
3:D:30:TYR:CG	3:D:31:ASN:N	2.90	0.40
1:A:391:CYS:CB	1:A:525:CYS:HA	2.50	0.40
3:L:7:PRO:HA	3:L:8:PRO:HD3	1.93	0.40

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	A	971/1121 (87%)	870 (90%)	91 (9%)	10 (1%)	12	38
1	C	971/1121 (87%)	885 (91%)	78 (8%)	8 (1%)	16	44
1	K	971/1121 (87%)	877 (90%)	80 (8%)	14 (1%)	9	30
2	B	221/223 (99%)	183 (83%)	29 (13%)	9 (4%)	2	14
2	H	221/223 (99%)	191 (86%)	23 (10%)	7 (3%)	3	17
2	M	221/223 (99%)	190 (86%)	20 (9%)	11 (5%)	1	10
3	D	214/216 (99%)	180 (84%)	31 (14%)	3 (1%)	9	30
3	L	214/216 (99%)	186 (87%)	24 (11%)	4 (2%)	6	25
3	S	214/216 (99%)	194 (91%)	19 (9%)	1 (0%)	24	52
All	All	4218/4680 (90%)	3756 (89%)	395 (9%)	67 (2%)	10	28

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	97	PRO
2	H	148	GLU
2	B	97	PRO
2	B	148	GLU
2	M	96	SER
2	M	97	PRO
2	M	148	GLU
2	H	96	SER
2	H	153	SER
2	B	100	VAL
1	K	145	TYR
1	K	146	HIS
1	K	156	GLU
1	K	890	ALA
2	M	153	SER
2	M	198	VAL
1	C	123	ALA
1	C	150	LYS
3	L	83	GLU
2	B	87	THR
2	B	168	ALA
2	B	198	VAL
1	K	614	ASP
2	M	84	SER
2	M	144	ASP
1	C	157	PHE
1	C	603	ASN
1	C	604	THR
1	C	614	ASP
2	H	54	ASP
1	A	146	HIS
1	A	158	ARG
1	A	603	ASN
2	B	105	ARG
2	B	153	SER
1	K	157	PHE
1	K	419	ALA
1	K	1084	ASP
2	M	87	THR
1	C	139	PRO
2	H	204	ASN
3	L	60	ASP

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Mol	Chain	Res	Type
3	L	94	SER
1	A	141	LEU
1	A	145	TYR
1	A	156	GLU
1	A	165	ASN
1	A	604	THR
3	D	27(A)	SER
3	D	60	ASP
1	K	141	LEU
1	K	604	THR
3	S	92	ALA
3	D	52	SER
2	M	204	ASN
1	K	491	PRO
2	M	146	PHE
1	C	159	VAL
1	K	729	VAL
2	M	100	VAL
2	B	96	SER
1	K	1099	GLY
2	H	198	VAL
3	L	51	VAL
1	A	793	PRO
1	A	729	VAL
1	K	159	VAL

5.3.2 Protein sidechains ⓘ

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	872/972 (90%)	858 (98%)	14 (2%)	55	67
1	C	872/972 (90%)	857 (98%)	15 (2%)	53	67
1	K	872/972 (90%)	853 (98%)	19 (2%)	45	63
2	B	189/189 (100%)	181 (96%)	8 (4%)	26	52
2	H	189/189 (100%)	184 (97%)	5 (3%)	40	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	189/189 (100%)	178 (94%)	11 (6%)	18	45
3	D	182/182 (100%)	178 (98%)	4 (2%)	45	63
3	L	182/182 (100%)	175 (96%)	7 (4%)	29	55
3	S	182/182 (100%)	175 (96%)	7 (4%)	29	55
All	All	3729/4029 (93%)	3639 (98%)	90 (2%)	43	62

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	84	LEU
1	C	143	VAL
1	C	145	TYR
1	C	159	VAL
1	C	160	TYR
1	C	202	LYS
1	C	366	SER
1	C	382	VAL
1	C	505	TYR
1	C	578	ASP
1	C	603	ASN
1	C	619	GLU
1	C	738	CYS
1	C	739	THR
1	C	1004	LEU
2	H	2	VAL
2	H	94	THR
2	H	109	VAL
2	H	141	LEU
2	H	142	VAL
3	L	39	HIS
3	L	78	LEU
3	L	79	GLN
3	L	104	VAL
3	L	146	THR
3	L	178	TYR
3	L	192	TYR
1	A	81	ASN
1	A	116	SER
1	A	156	GLU
1	A	159	VAL
1	A	160	TYR

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Mol	Chain	Res	Type
1	A	366	SER
1	A	578	ASP
1	A	603	ASN
1	A	619	GLU
1	A	721	SER
1	A	723	THR
1	A	739	THR
1	A	1004	LEU
1	A	1094	VAL
2	B	89	VAL
2	B	94	THR
2	B	97	PRO
2	B	98	PHE
2	B	109	VAL
2	B	111	VAL
2	B	142	VAL
2	B	198	VAL
3	D	47	MET
3	D	97	VAL
3	D	162	THR
3	D	196	VAL
1	K	81	ASN
1	K	88	ASP
1	K	96	GLU
1	K	145	TYR
1	K	154	GLU
1	K	159	VAL
1	K	160	TYR
1	K	214	ARG
1	K	294	ASP
1	K	366	SER
1	K	422	ASN
1	K	498	GLN
1	K	578	ASP
1	K	619	GLU
1	K	820	ASP
1	K	1004	LEU
1	K	1032	CYS
1	K	1094	VAL
1	K	1119	ASN
2	M	2	VAL
2	M	37	VAL

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Mol	Chain	Res	Type
2	M	69	MET
2	M	74	SER
2	M	109	VAL
2	M	111	VAL
2	M	142	VAL
2	M	145	TYR
2	M	151	THR
2	M	198	VAL
2	M	208	ASP
3	S	48	ILE
3	S	65	SER
3	S	79	GLN
3	S	82	ASP
3	S	104	VAL
3	S	122	SER
3	S	164	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	134	GLN
1	C	149	ASN
1	C	188	ASN
1	C	196	ASN
1	C	388	ASN
1	C	540	ASN
1	C	607	GLN
1	C	914	ASN
1	C	919	ASN
1	C	935	GLN
1	C	957	GLN
1	C	992	GLN
1	C	1002	GLN
2	H	64	GLN
3	L	69	ASN
3	L	170	ASN
1	A	52	GLN
1	A	115	GLN
1	A	134	GLN
1	A	146	HIS
1	A	164	ASN
1	A	196	ASN

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Mol	Chain	Res	Type
1	A	211	ASN
1	A	314	GLN
1	A	422	ASN
1	A	448	ASN
1	A	450	ASN
1	A	519	HIS
1	A	536	ASN
1	A	540	ASN
1	A	606	ASN
1	A	613	GLN
1	A	641	ASN
1	A	658	ASN
1	A	907	ASN
1	A	913	GLN
1	A	957	GLN
1	A	1002	GLN
2	B	204	ASN
3	D	127	GLN
3	D	171	ASN
1	K	52	GLN
1	K	148	ASN
1	K	388	ASN
1	K	450	ASN
1	K	613	GLN
1	K	655	HIS
1	K	690	GLN
1	K	755	GLN
1	K	907	ASN
1	K	913	GLN
1	K	935	GLN
1	K	1048	HIS
3	S	129	ASN
3	S	171	ASN
3	S	189	HIS

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 ⓘ

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
4	NAG	E	1	4,1	14,14,15	1.30	2 (14%)	17,19,21	0.98	0
4	NAG	E	2	4	14,14,15	1.15	1 (7%)	17,19,21	0.87	0
4	NAG	F	1	4,1	14,14,15	0.94	0	17,19,21	0.80	0
4	NAG	F	2	4	14,14,15	1.14	1 (7%)	17,19,21	0.72	0
4	NAG	G	1	4,1	14,14,15	1.09	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	G	2	4	14,14,15	1.13	1 (7%)	17,19,21	0.66	0
4	NAG	I	1	4,1	14,14,15	1.21	1 (7%)	17,19,21	1.03	0
4	NAG	I	2	4	14,14,15	1.09	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	J	1	4,1	14,14,15	1.32	3 (21%)	17,19,21	0.75	0
4	NAG	J	2	4	14,14,15	1.13	1 (7%)	17,19,21	1.07	1 (5%)
4	NAG	N	1	4,1	14,14,15	1.42	3 (21%)	17,19,21	1.12	1 (5%)
4	NAG	N	2	4	14,14,15	1.33	2 (14%)	17,19,21	0.84	0
4	NAG	O	1	4,1	14,14,15	0.97	0	17,19,21	0.76	0
4	NAG	O	2	4	14,14,15	1.16	1 (7%)	17,19,21	0.71	0
4	NAG	P	1	4,1	14,14,15	1.11	1 (7%)	17,19,21	0.83	1 (5%)
4	NAG	P	2	4	14,14,15	1.28	3 (21%)	17,19,21	0.98	1 (5%)
4	NAG	Q	1	4,1	14,14,15	1.23	1 (7%)	17,19,21	1.11	1 (5%)
4	NAG	Q	2	4	14,14,15	1.24	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	R	1	4,1	14,14,15	1.30	2 (14%)	17,19,21	0.58	0
4	NAG	R	2	4	14,14,15	1.13	1 (7%)	17,19,21	1.23	1 (5%)
4	NAG	T	1	4,1	14,14,15	1.25	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	T	2	4	14,14,15	1.27	2 (14%)	17,19,21	0.76	0
4	NAG	V	1	4,1	14,14,15	1.03	0	17,19,21	0.87	1 (5%)
4	NAG	V	2	4	14,14,15	1.23	1 (7%)	17,19,21	1.19	1 (5%)
4	NAG	W	1	4,1	14,14,15	1.13	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	W	2	4	14,14,15	1.17	1 (7%)	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	X	1	4,1	14,14,15	1.25	1 (7%)	17,19,21	0.96	0
4	NAG	X	2	4	14,14,15	1.13	1 (7%)	17,19,21	0.76	0
4	NAG	Y	1	4,1	14,14,15	1.18	1 (7%)	17,19,21	0.70	0
4	NAG	Y	2	4	14,14,15	1.10	1 (7%)	17,19,21	1.17	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	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	2	NAG	O5-C5	3.05	1.49	1.43
4	N	2	NAG	O5-C5	2.96	1.49	1.43
4	X	2	NAG	O5-C5	2.90	1.49	1.43
4	P	2	NAG	O5-C5	2.82	1.48	1.43
4	N	1	NAG	O5-C5	2.79	1.48	1.43
4	J	2	NAG	O5-C5	2.78	1.48	1.43
4	I	2	NAG	O5-C5	2.77	1.48	1.43
4	T	2	NAG	O5-C5	2.77	1.48	1.43
4	Q	2	NAG	O5-C5	2.76	1.48	1.43
4	X	1	NAG	O5-C5	2.73	1.48	1.43
4	Q	1	NAG	O5-C5	2.69	1.48	1.43
4	E	1	NAG	O5-C5	2.64	1.48	1.43
4	R	2	NAG	O5-C5	2.64	1.48	1.43
4	I	1	NAG	O5-C5	2.59	1.48	1.43
4	F	2	NAG	O5-C5	2.52	1.48	1.43
4	E	2	NAG	O5-C5	2.51	1.48	1.43
4	J	1	NAG	C1-C2	2.50	1.55	1.52
4	O	2	NAG	O5-C5	2.47	1.48	1.43
4	T	1	NAG	C1-C2	2.47	1.55	1.52
4	R	1	NAG	O5-C5	2.46	1.48	1.43
4	Y	2	NAG	O5-C5	2.41	1.48	1.43
4	W	2	NAG	O5-C5	2.38	1.48	1.43
4	Y	1	NAG	O5-C5	2.36	1.48	1.43
4	W	1	NAG	O5-C5	2.36	1.48	1.43
4	G	2	NAG	O5-C5	2.35	1.48	1.43
4	J	1	NAG	O5-C5	2.30	1.47	1.43
4	N	1	NAG	O4-C4	2.27	1.48	1.43
4	P	2	NAG	C1-C2	2.24	1.55	1.52
4	E	1	NAG	O4-C4	2.21	1.48	1.43
4	N	1	NAG	C1-C2	2.21	1.55	1.52
4	G	1	NAG	O5-C5	2.18	1.47	1.43
4	N	2	NAG	C1-C2	2.18	1.55	1.52
4	R	1	NAG	C1-C2	2.15	1.55	1.52
4	P	1	NAG	O5-C5	2.12	1.47	1.43
4	J	1	NAG	O5-C1	2.10	1.47	1.43
4	P	2	NAG	O5-C1	2.07	1.47	1.43
4	Q	2	NAG	O5-C1	2.02	1.47	1.43
4	T	2	NAG	O5-C1	2.01	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	2	NAG	C1-O5-C5	4.20	117.81	112.19
4	Y	2	NAG	C1-O5-C5	3.76	117.23	112.19
4	N	1	NAG	C1-O5-C5	3.69	117.14	112.19
4	Q	1	NAG	C1-O5-C5	3.38	116.71	112.19
4	V	2	NAG	C1-O5-C5	3.35	116.68	112.19
4	J	2	NAG	C1-O5-C5	3.24	116.53	112.19
4	P	2	NAG	C1-O5-C5	3.24	116.53	112.19
4	G	1	NAG	C1-O5-C5	2.96	116.15	112.19
4	I	2	NAG	C1-O5-C5	2.87	116.03	112.19
4	W	1	NAG	C1-O5-C5	2.67	115.76	112.19
4	T	1	NAG	C1-O5-C5	2.58	115.64	112.19
4	Q	2	NAG	C1-O5-C5	2.34	115.33	112.19
4	P	1	NAG	C1-O5-C5	2.32	115.30	112.19
4	V	1	NAG	C1-O5-C5	2.29	115.25	112.19

There are no chirality outliers.

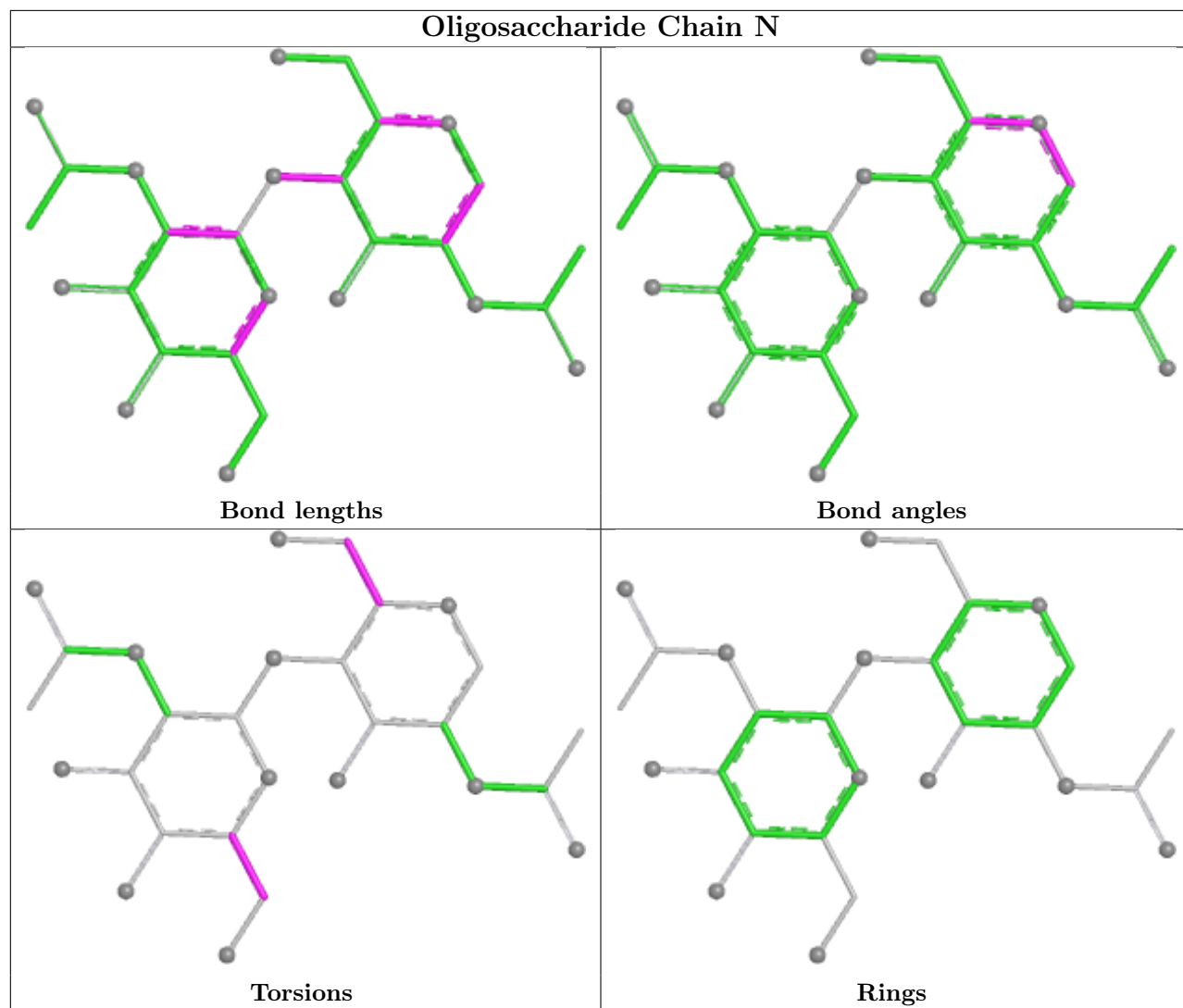
All (10) torsion outliers are listed below:

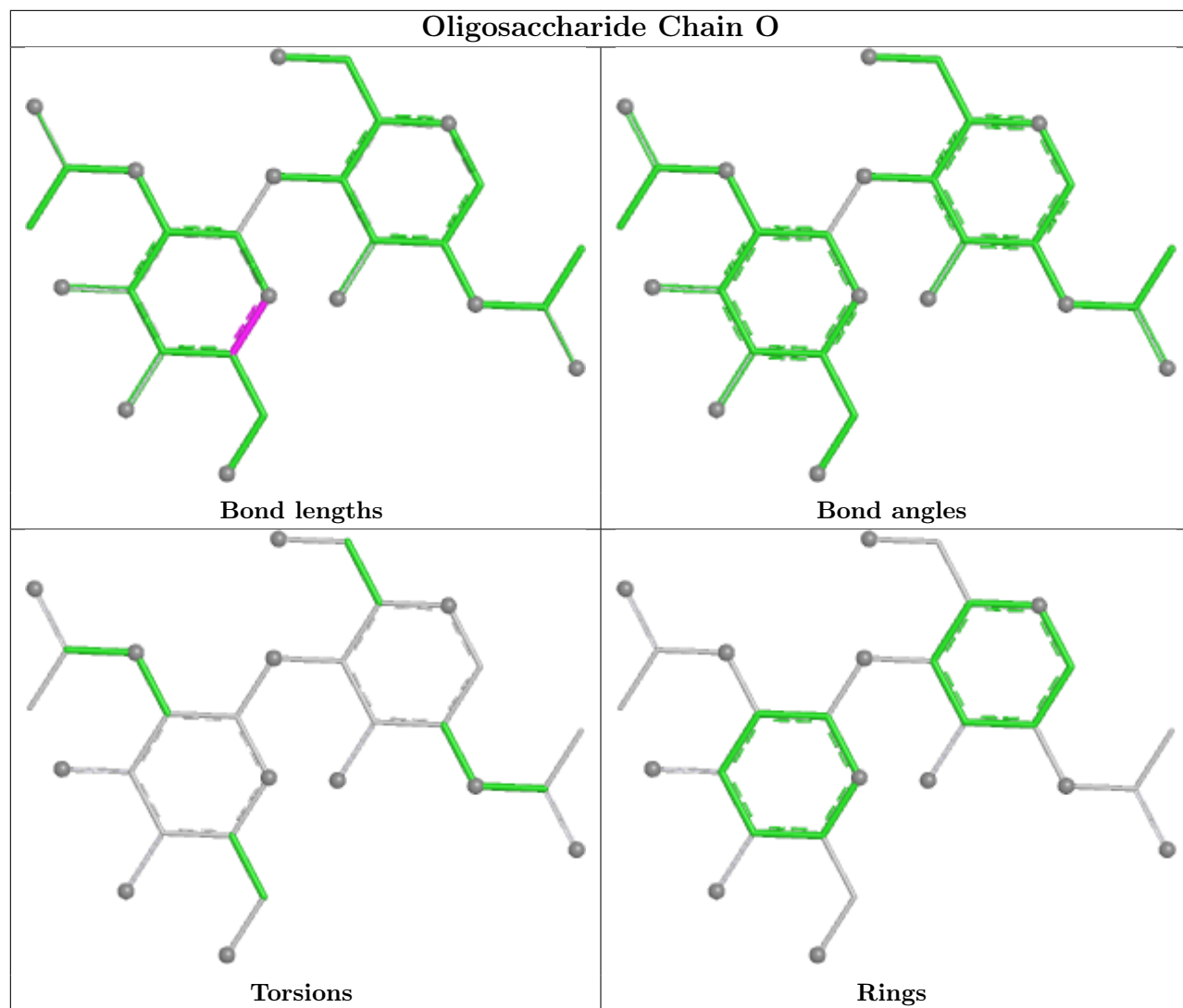
Mol	Chain	Res	Type	Atoms
4	W	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C1-C2-N2-C7

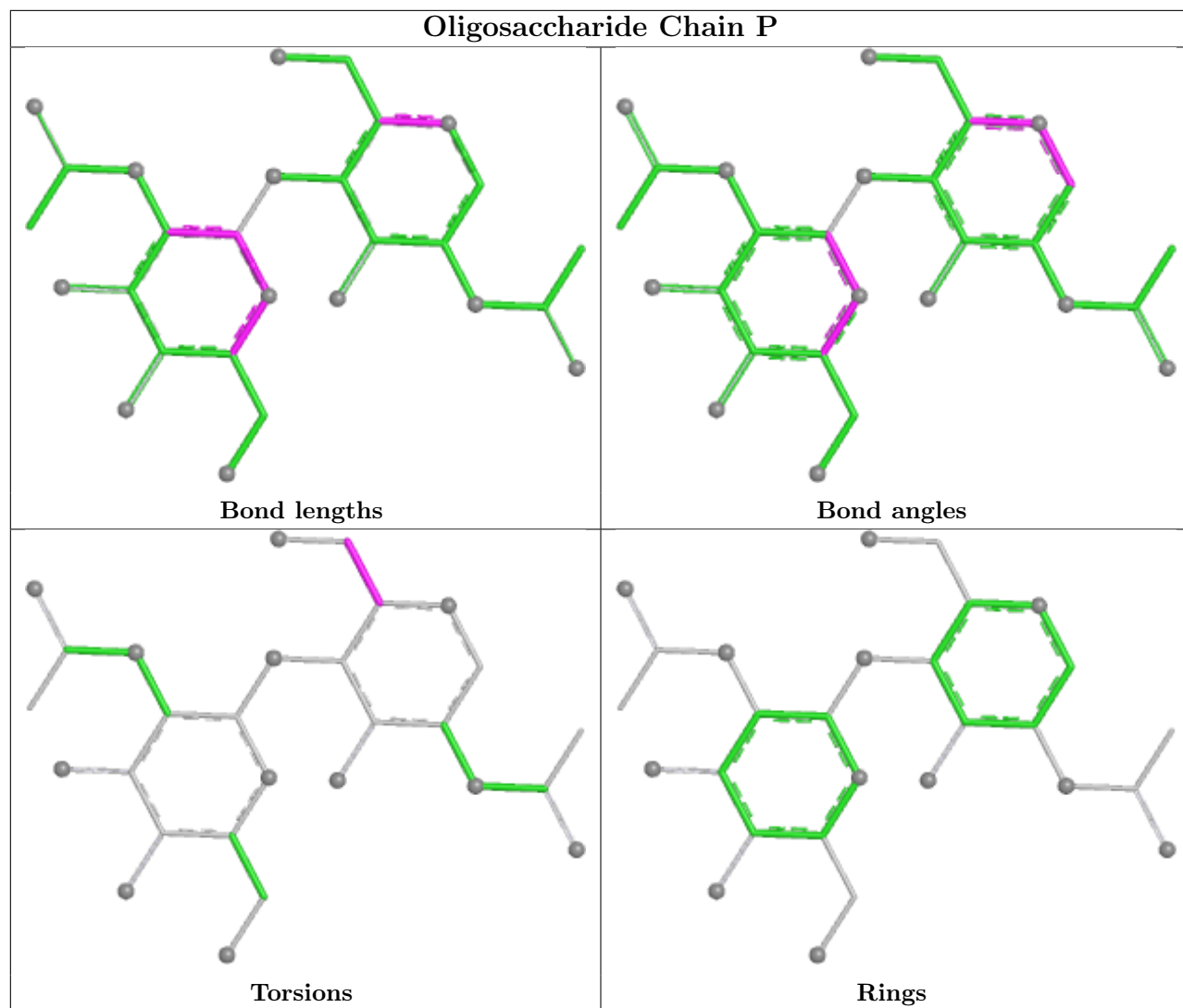
There are no ring outliers.

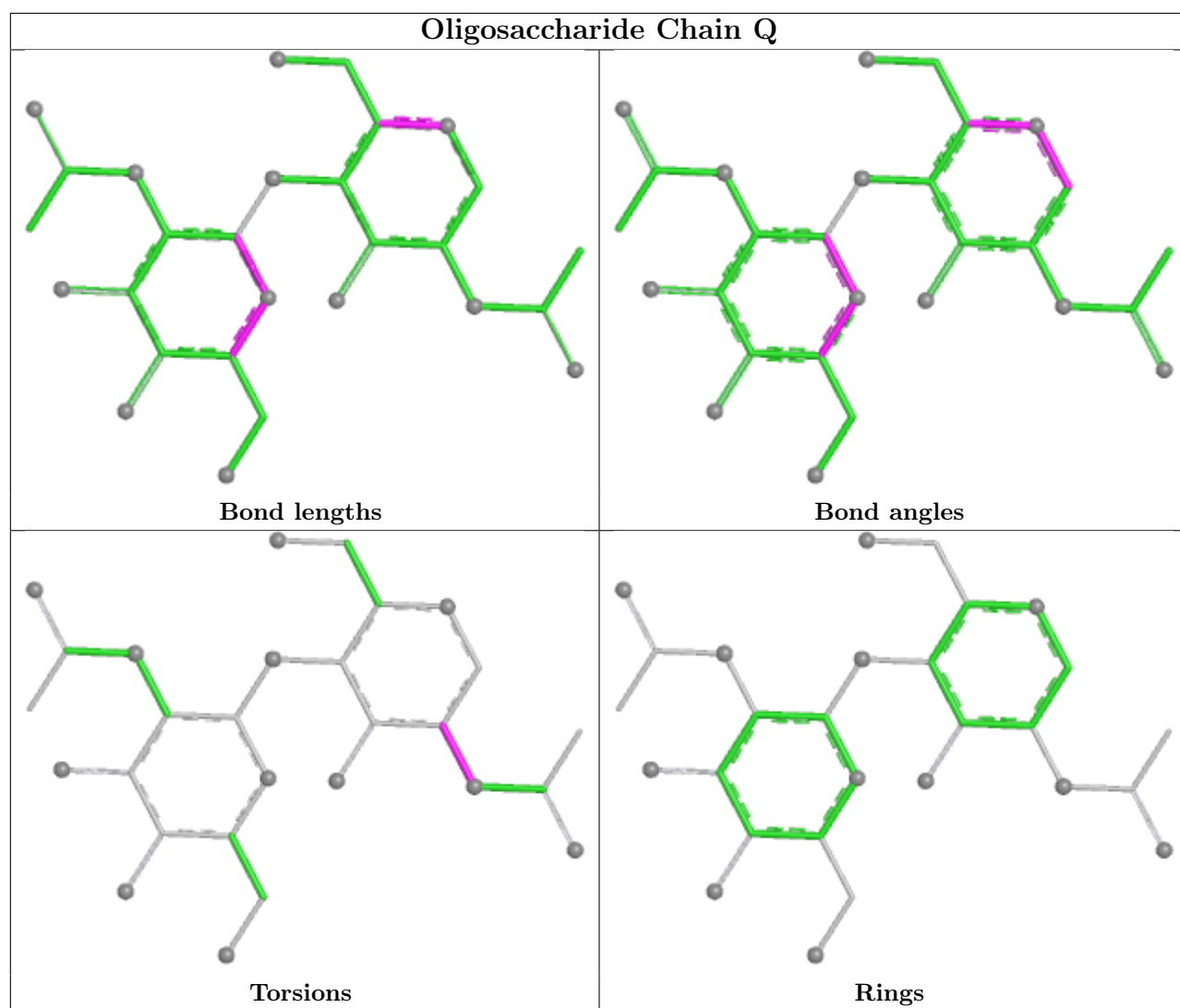
No monomer is involved in short contacts.

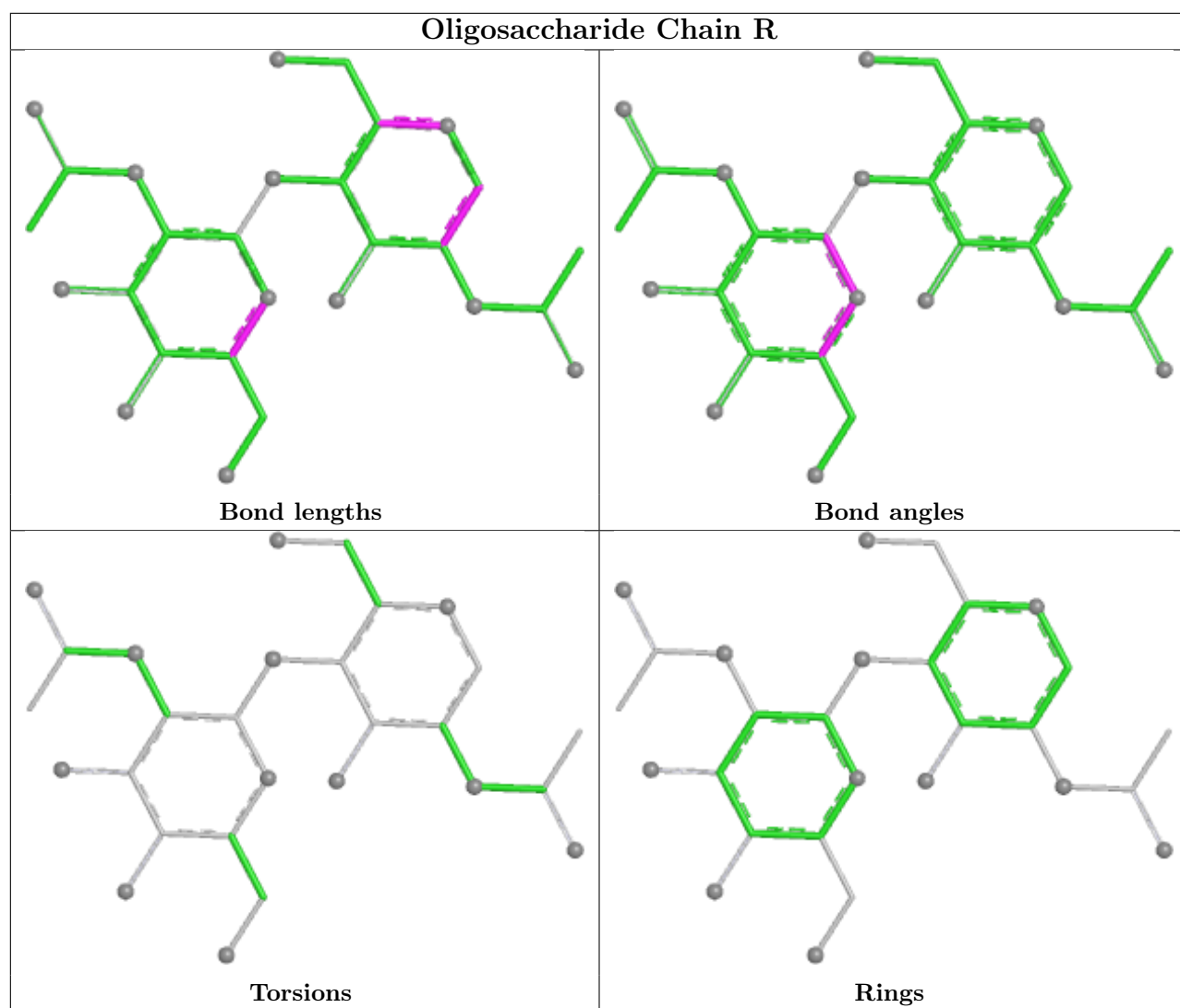
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

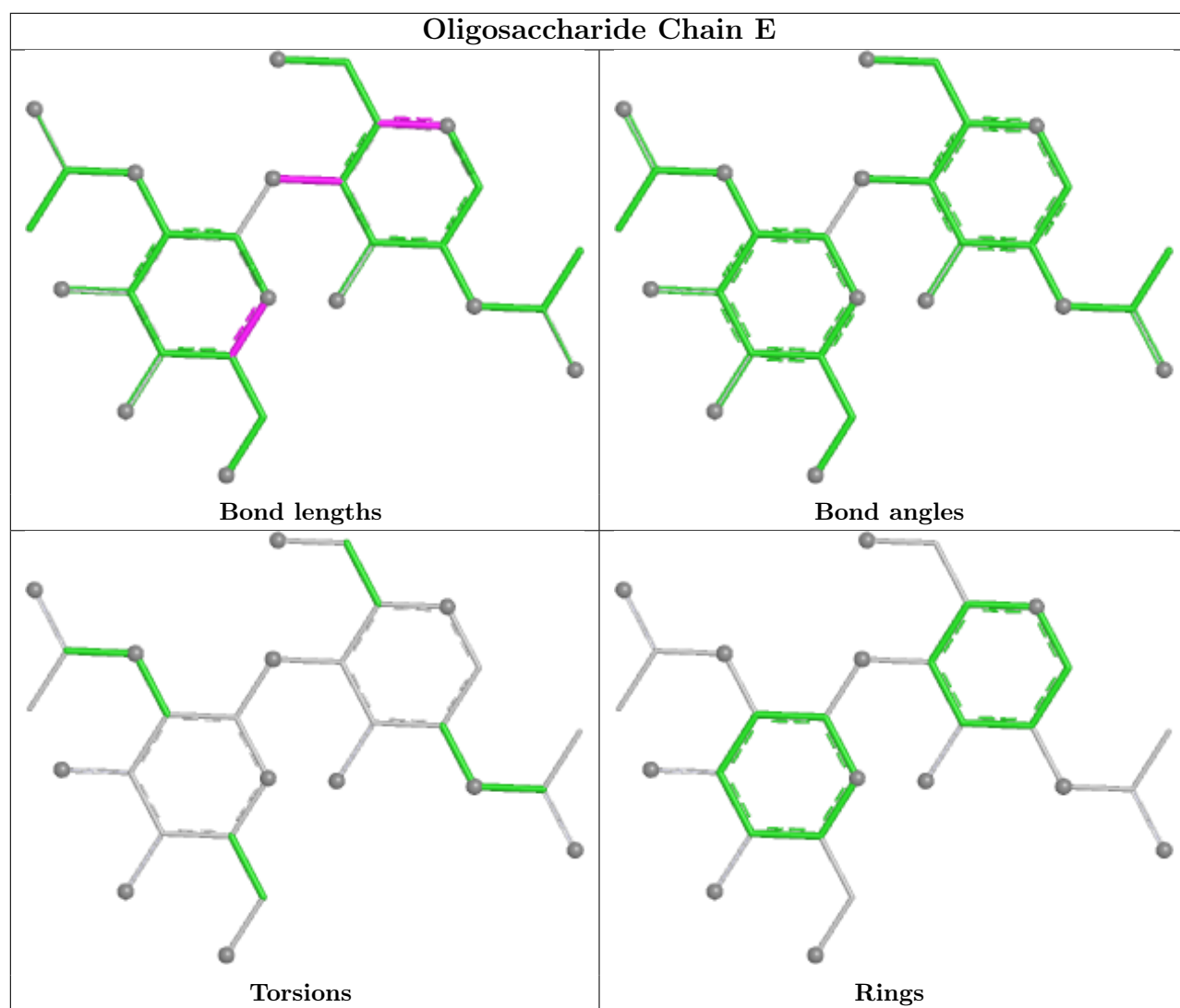


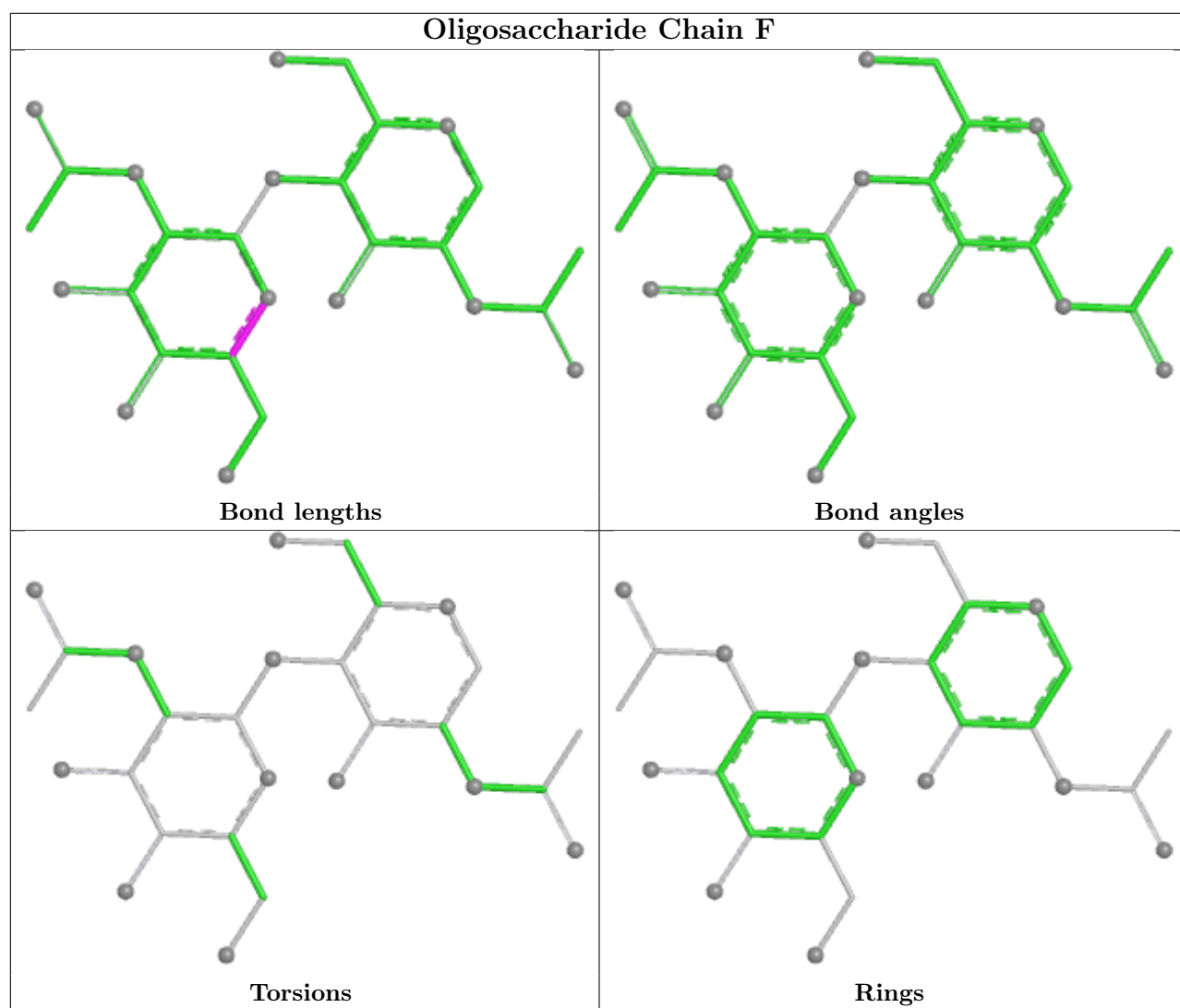


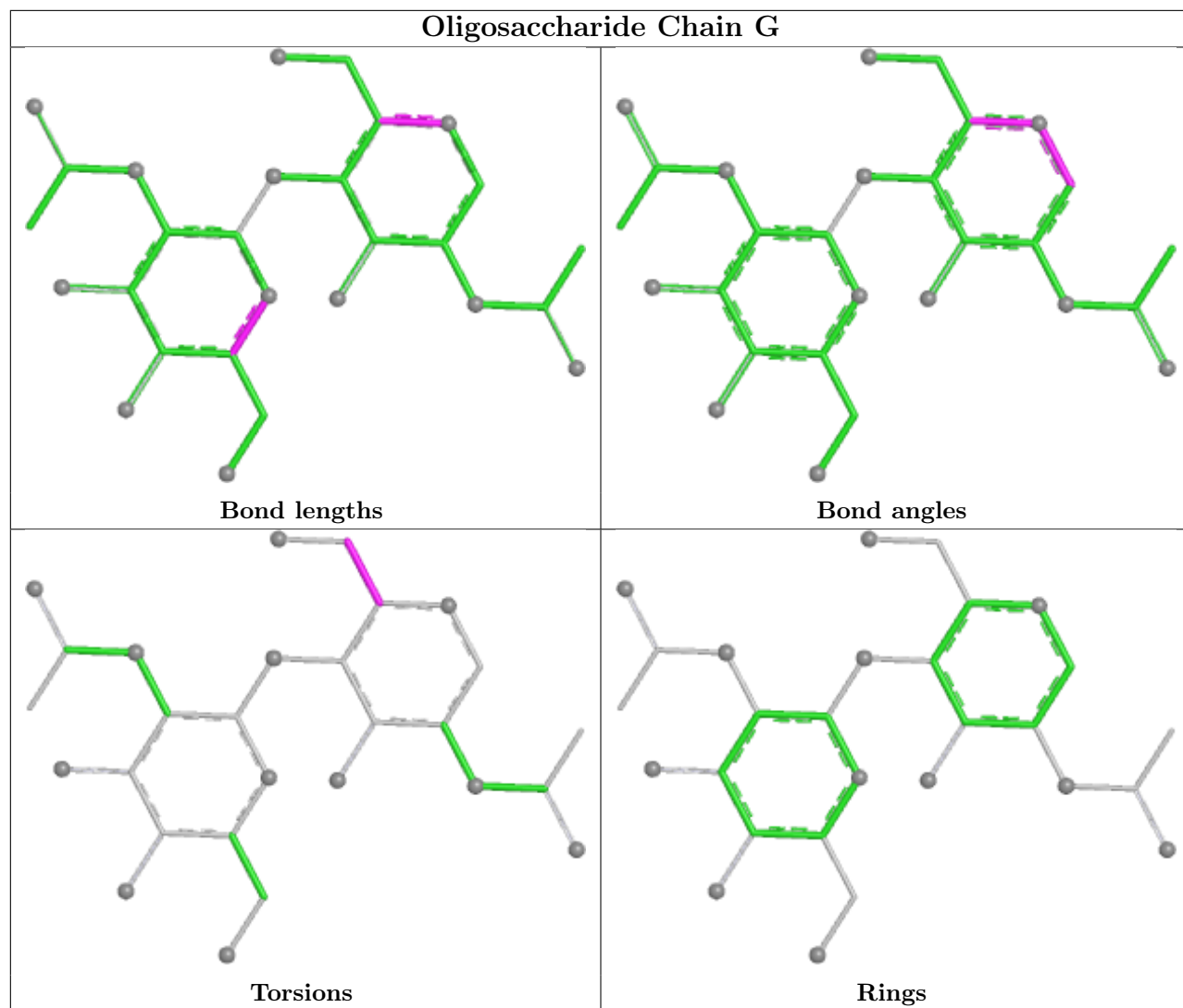


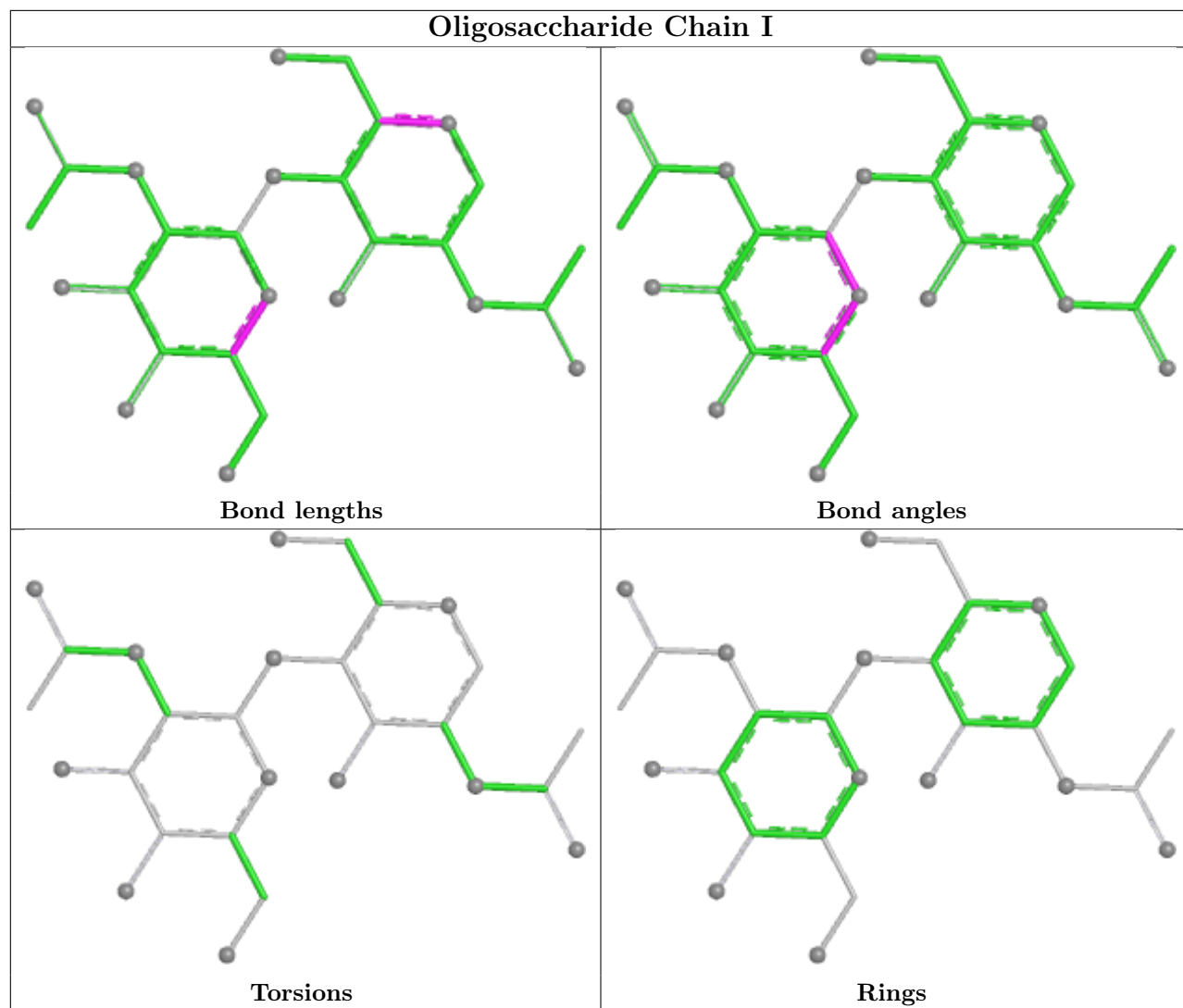


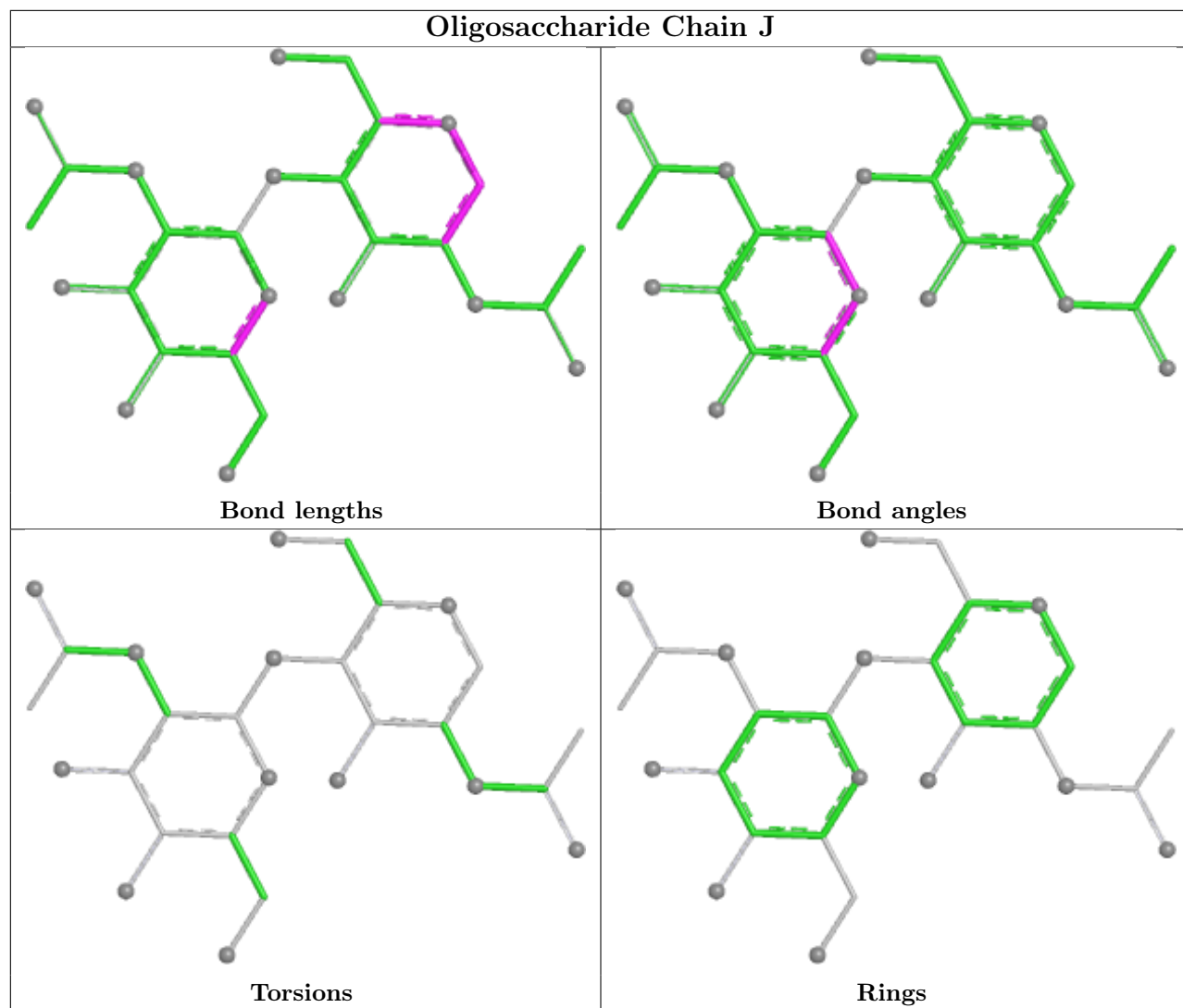


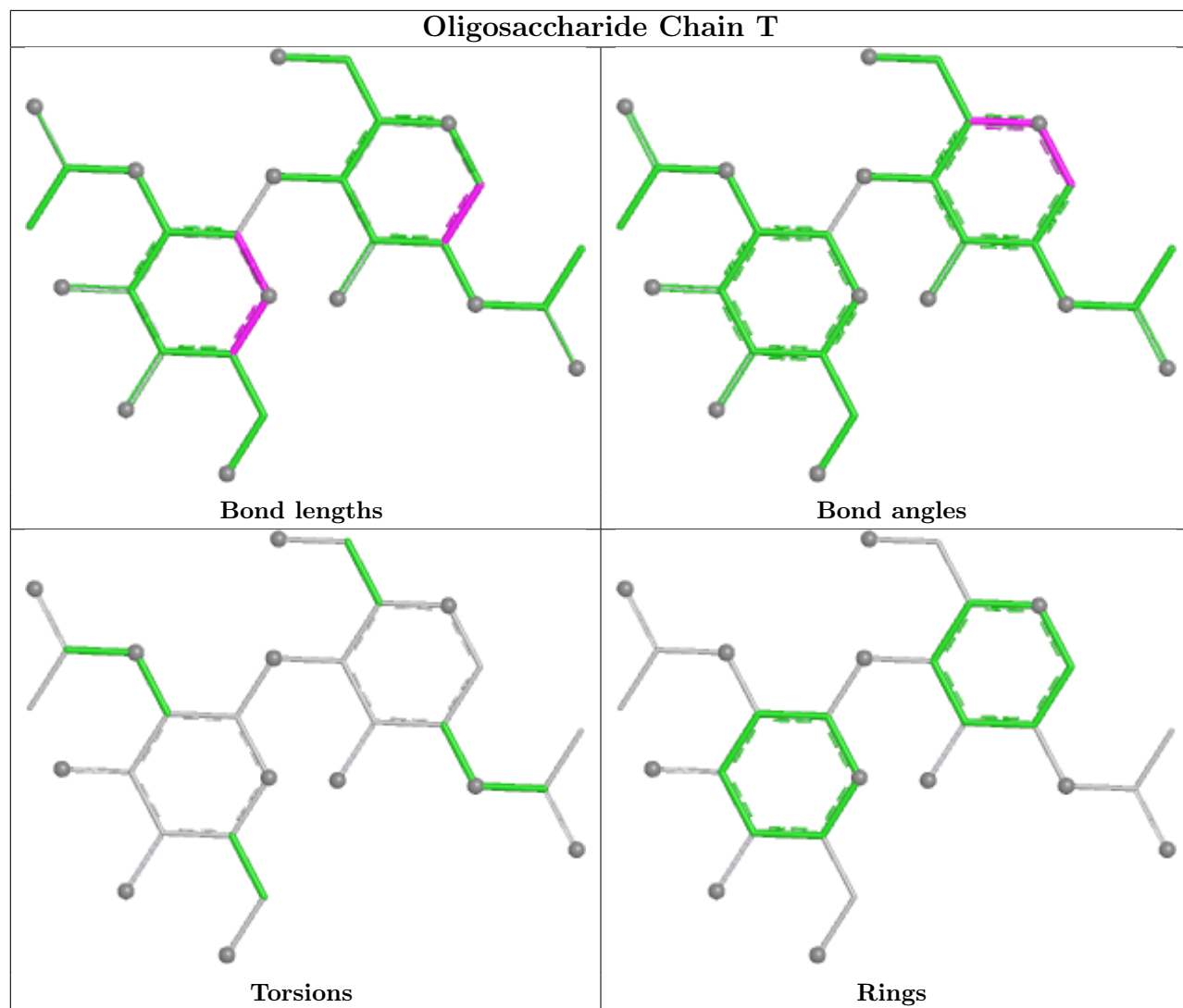


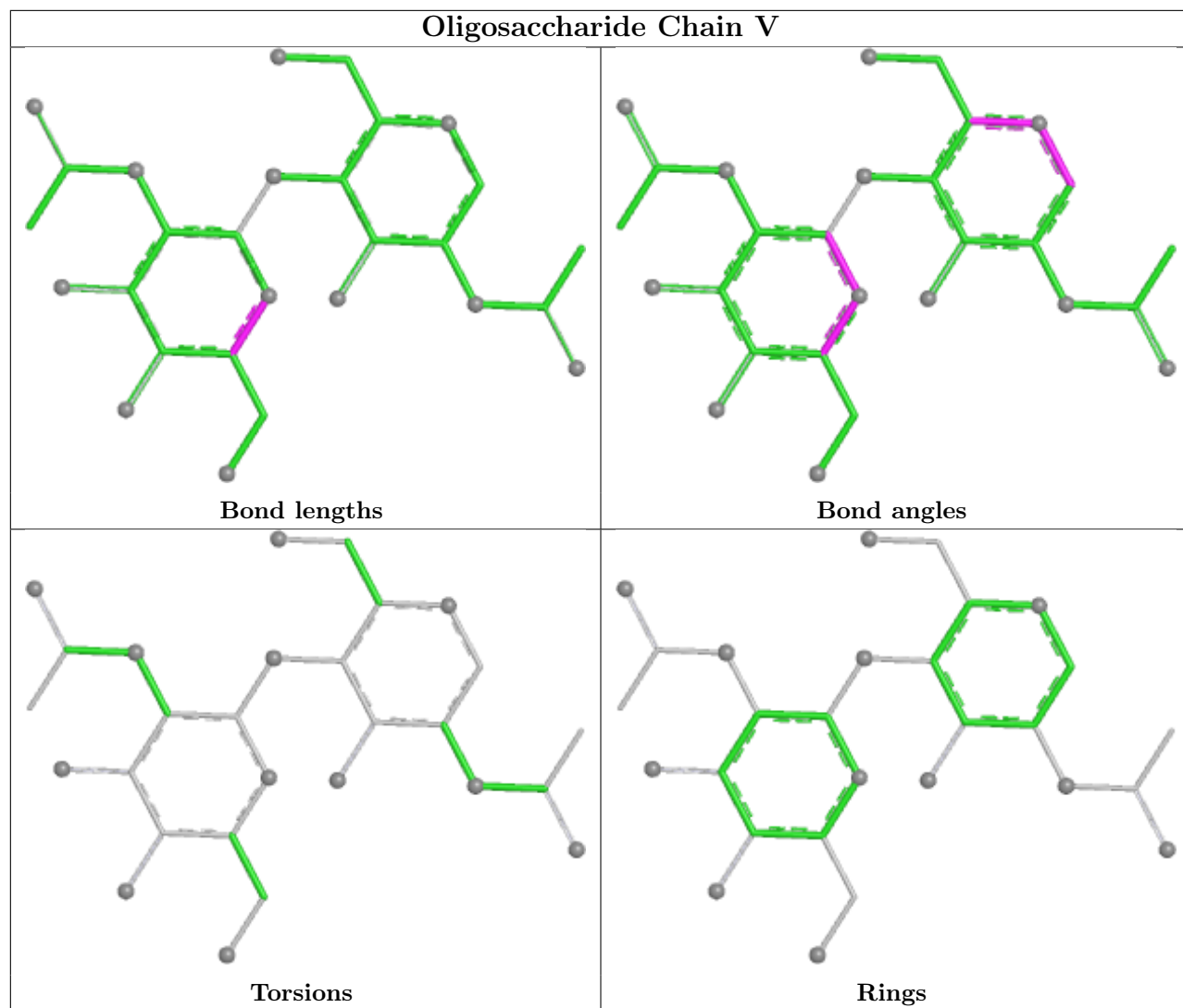


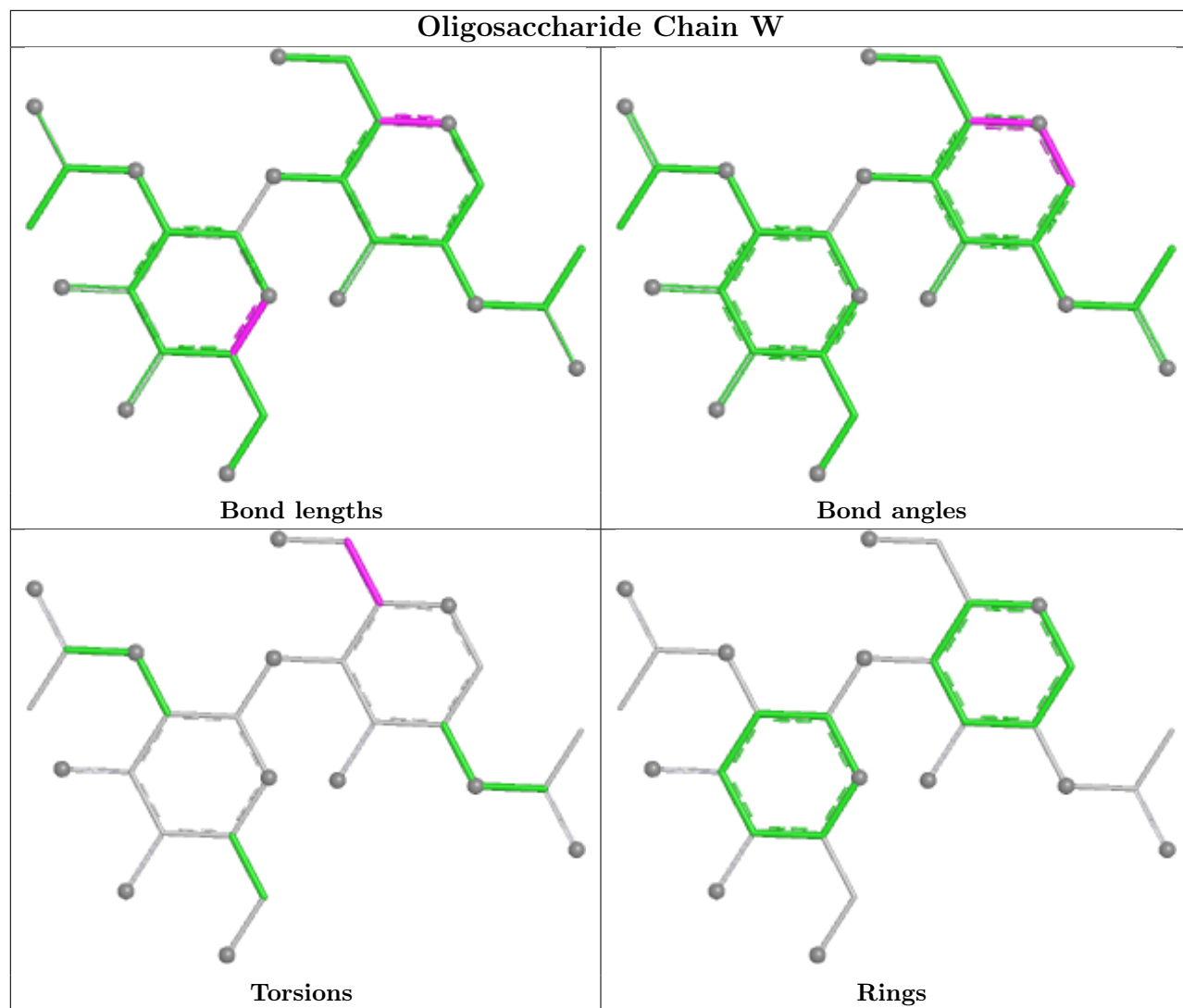


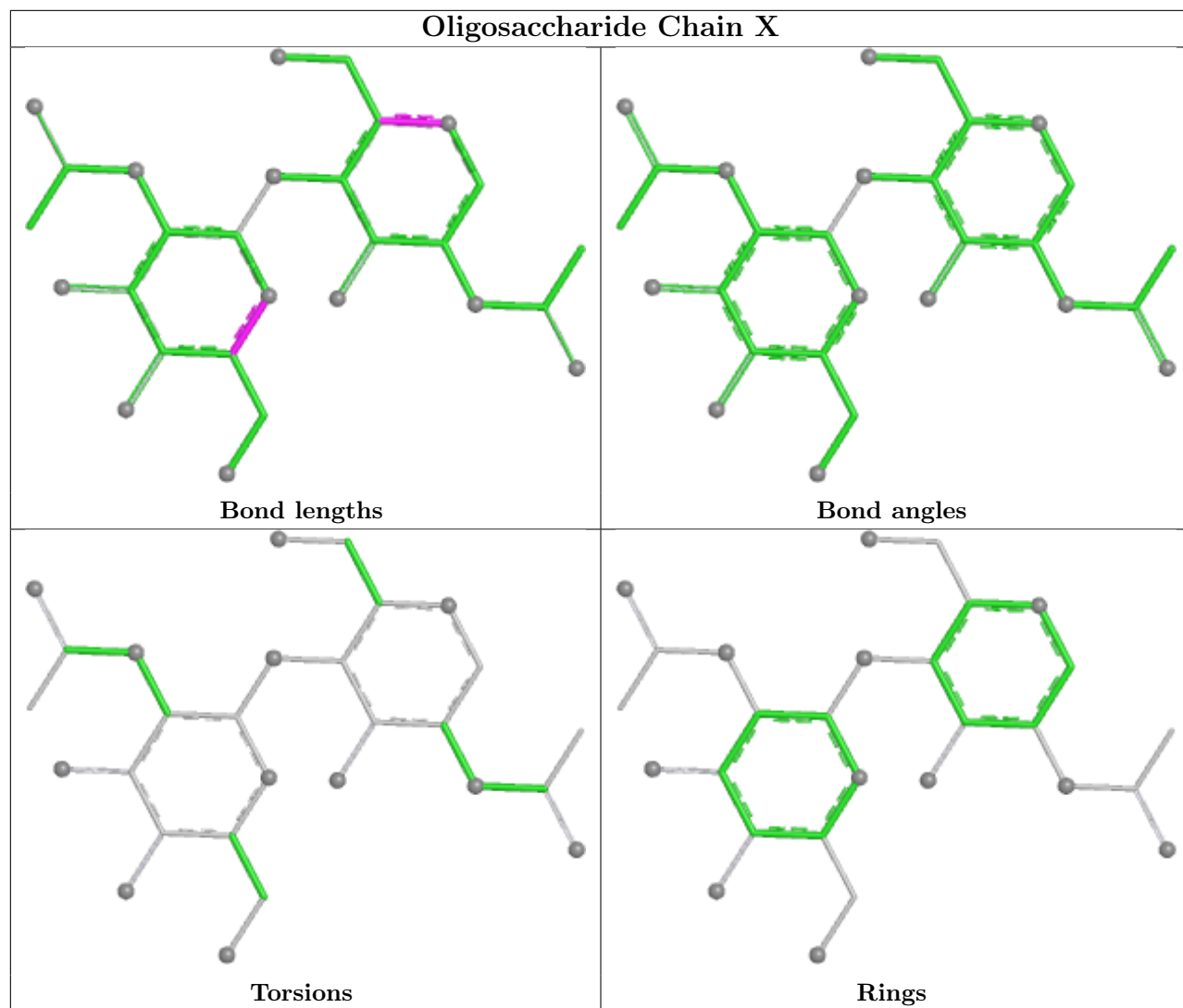


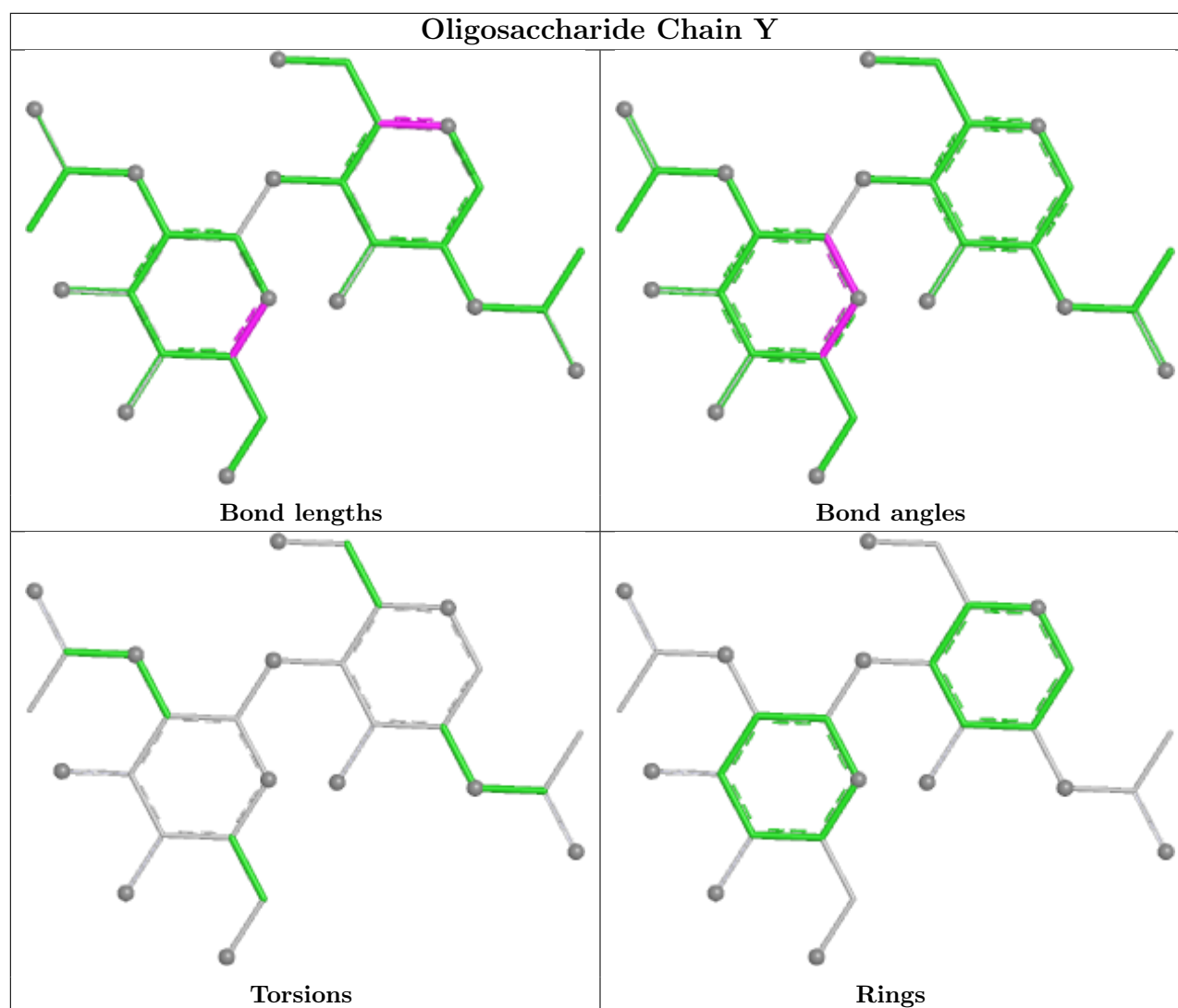












5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
5	NAG	K	1307	1	14,14,15	1.29	2 (14%)	17,19,21	0.85	1 (5%)
5	NAG	K	1303	1	14,14,15	1.28	3 (21%)	17,19,21	0.80	0
5	NAG	K	1309	1	14,14,15	1.18	2 (14%)	17,19,21	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1302	1	14,14,15	1.19	2 (14%)	17,19,21	0.82	0
5	NAG	K	1305	1	14,14,15	1.20	1 (7%)	17,19,21	0.76	0
5	NAG	A	1308	1	14,14,15	1.38	3 (21%)	17,19,21	1.03	1 (5%)
5	NAG	C	1304	1	14,14,15	1.27	2 (14%)	17,19,21	0.70	0
5	NAG	C	1307	1	14,14,15	1.07	2 (14%)	17,19,21	0.97	1 (5%)
5	NAG	K	1302	1	14,14,15	1.22	2 (14%)	17,19,21	0.74	0
5	NAG	C	1310	1	14,14,15	1.14	2 (14%)	17,19,21	1.39	1 (5%)
5	NAG	C	1305	1	14,14,15	1.21	1 (7%)	17,19,21	0.79	0
5	NAG	A	1302	1	14,14,15	1.38	2 (14%)	17,19,21	1.26	3 (17%)
5	NAG	K	1301	1	14,14,15	1.27	2 (14%)	17,19,21	0.72	0
5	NAG	K	1310	1	14,14,15	1.16	1 (7%)	17,19,21	1.12	1 (5%)
5	NAG	C	1306	1	14,14,15	1.25	1 (7%)	17,19,21	0.73	0
5	NAG	K	1304	1	14,14,15	1.30	2 (14%)	17,19,21	0.75	0
5	NAG	A	1311	1	14,14,15	1.21	2 (14%)	17,19,21	0.95	1 (5%)
5	NAG	C	1309	1	14,14,15	1.02	1 (7%)	17,19,21	0.77	0
5	NAG	C	1301	1	14,14,15	1.19	2 (14%)	17,19,21	0.60	0
5	NAG	K	1311	1	14,14,15	1.18	2 (14%)	17,19,21	0.77	1 (5%)
5	NAG	C	1308	1	14,14,15	1.22	2 (14%)	17,19,21	0.86	1 (5%)
5	NAG	A	1301	1	14,14,15	1.09	2 (14%)	17,19,21	0.72	0
5	NAG	C	1303	1	14,14,15	1.30	3 (21%)	17,19,21	0.72	0
5	NAG	A	1303	1	14,14,15	1.15	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	A	1309	1	14,14,15	1.10	2 (14%)	17,19,21	0.86	1 (5%)
5	NAG	K	1306	1	14,14,15	1.26	2 (14%)	17,19,21	0.69	0
5	NAG	A	1304	1	14,14,15	1.30	2 (14%)	17,19,21	0.91	0
5	NAG	A	1305	1	14,14,15	1.30	3 (21%)	17,19,21	0.93	1 (5%)
5	NAG	K	1308	1	14,14,15	1.24	2 (14%)	17,19,21	0.87	1 (5%)
5	NAG	A	1307	1	14,14,15	1.09	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	A	1310	1	14,14,15	1.13	2 (14%)	17,19,21	0.63	0
5	NAG	A	1306	1	14,14,15	1.20	1 (7%)	17,19,21	0.89	0
5	NAG	C	1311	1	14,14,15	1.29	3 (21%)	17,19,21	1.37	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
5	NAG	K	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	K	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	K	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	K	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	K	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	K	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	K	1310	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	K	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	K	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	K	1306	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	K	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	1/6/23/26	0/1/1/1

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1302	NAG	O5-C5	3.13	1.49	1.43
5	K	1303	NAG	O5-C5	2.91	1.49	1.43
5	C	1301	NAG	O5-C5	2.88	1.49	1.43
5	K	1308	NAG	O5-C5	2.83	1.48	1.43
5	A	1308	NAG	C1-C2	2.83	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1311	NAG	C1-C2	2.79	1.56	1.52
5	A	1306	NAG	O5-C5	2.77	1.48	1.43
5	C	1302	NAG	O5-C5	2.76	1.48	1.43
5	A	1305	NAG	O5-C5	2.74	1.48	1.43
5	K	1307	NAG	O5-C5	2.72	1.48	1.43
5	C	1303	NAG	O5-C5	2.72	1.48	1.43
5	C	1305	NAG	O5-C5	2.69	1.48	1.43
5	A	1304	NAG	C1-C2	2.69	1.56	1.52
5	C	1306	NAG	O5-C5	2.68	1.48	1.43
5	K	1304	NAG	O5-C5	2.66	1.48	1.43
5	K	1310	NAG	O5-C5	2.65	1.48	1.43
5	K	1305	NAG	O5-C5	2.62	1.48	1.43
5	C	1308	NAG	O5-C5	2.61	1.48	1.43
5	A	1308	NAG	O5-C5	2.59	1.48	1.43
5	C	1304	NAG	O5-C5	2.59	1.48	1.43
5	K	1306	NAG	O5-C5	2.57	1.48	1.43
5	K	1304	NAG	C1-C2	2.53	1.55	1.52
5	K	1309	NAG	O5-C5	2.52	1.48	1.43
5	A	1311	NAG	O5-C5	2.51	1.48	1.43
5	K	1311	NAG	O5-C5	2.50	1.48	1.43
5	K	1311	NAG	C1-C2	2.48	1.55	1.52
5	A	1304	NAG	O5-C5	2.48	1.48	1.43
5	A	1309	NAG	O5-C5	2.47	1.48	1.43
5	K	1302	NAG	C1-C2	2.47	1.55	1.52
5	A	1303	NAG	O5-C5	2.46	1.48	1.43
5	K	1301	NAG	C1-C2	2.46	1.55	1.52
5	K	1307	NAG	C1-C2	2.45	1.55	1.52
5	A	1307	NAG	O5-C5	2.40	1.48	1.43
5	A	1308	NAG	O5-C1	2.37	1.47	1.43
5	C	1311	NAG	O5-C5	2.33	1.48	1.43
5	A	1305	NAG	C1-C2	2.33	1.55	1.52
5	K	1301	NAG	O5-C5	2.29	1.47	1.43
5	C	1304	NAG	C1-C2	2.27	1.55	1.52
5	K	1306	NAG	C1-C2	2.24	1.55	1.52
5	C	1303	NAG	C1-C2	2.24	1.55	1.52
5	K	1302	NAG	O5-C5	2.24	1.47	1.43
5	C	1310	NAG	O5-C5	2.22	1.47	1.43
5	C	1311	NAG	O5-C1	2.21	1.47	1.43
5	C	1309	NAG	O5-C5	2.20	1.47	1.43
5	A	1301	NAG	O5-C5	2.18	1.47	1.43
5	A	1310	NAG	O5-C5	2.17	1.47	1.43
5	C	1308	NAG	C1-C2	2.13	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1303	NAG	O5-C1	2.12	1.47	1.43
5	A	1302	NAG	C1-C2	2.11	1.55	1.52
5	K	1303	NAG	C1-C2	2.11	1.55	1.52
5	K	1309	NAG	C1-C2	2.07	1.55	1.52
5	A	1311	NAG	C1-C2	2.07	1.55	1.52
5	C	1303	NAG	O5-C1	2.07	1.47	1.43
5	C	1302	NAG	C1-C2	2.06	1.55	1.52
5	C	1310	NAG	C1-C2	2.05	1.55	1.52
5	A	1301	NAG	C1-C2	2.04	1.55	1.52
5	A	1309	NAG	C1-C2	2.04	1.55	1.52
5	C	1307	NAG	C1-C2	2.03	1.55	1.52
5	C	1307	NAG	O5-C5	2.02	1.47	1.43
5	A	1305	NAG	O5-C1	2.01	1.47	1.43
5	A	1310	NAG	C1-C2	2.01	1.55	1.52
5	K	1308	NAG	C1-C2	2.00	1.55	1.52
5	C	1301	NAG	C1-C2	2.00	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1310	NAG	C1-O5-C5	5.22	119.18	112.19
5	C	1311	NAG	C1-O5-C5	4.42	118.11	112.19
5	A	1307	NAG	C1-O5-C5	3.67	117.11	112.19
5	A	1308	NAG	C1-O5-C5	3.60	117.02	112.19
5	K	1309	NAG	C1-O5-C5	3.60	117.02	112.19
5	K	1310	NAG	C1-O5-C5	3.42	116.77	112.19
5	C	1307	NAG	C1-O5-C5	3.02	116.24	112.19
5	A	1309	NAG	C1-O5-C5	2.90	116.07	112.19
5	A	1305	NAG	C1-O5-C5	2.88	116.05	112.19
5	A	1303	NAG	C1-O5-C5	2.88	116.04	112.19
5	C	1308	NAG	C1-O5-C5	2.65	115.73	112.19
5	K	1308	NAG	C1-O5-C5	2.46	115.49	112.19
5	K	1307	NAG	C1-O5-C5	2.37	115.37	112.19
5	A	1302	NAG	C1-O5-C5	2.23	115.17	112.19
5	K	1311	NAG	C1-O5-C5	2.17	115.10	112.19
5	A	1311	NAG	C1-O5-C5	2.14	115.05	112.19
5	A	1302	NAG	C1-C2-N2	2.11	113.77	110.43
5	A	1302	NAG	C2-N2-C7	2.05	125.65	122.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1302	NAG	C1-C2-N2-C7
5	C	1310	NAG	O5-C5-C6-O6
5	K	1310	NAG	O5-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	C	1302	NAG	C1-C2-N2-C7
5	K	1301	NAG	O5-C5-C6-O6
5	K	1306	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	C	1302	NAG	C3-C2-N2-C7
5	K	1302	NAG	C3-C2-N2-C7
5	C	1311	NAG	C1-C2-N2-C7
5	A	1303	NAG	C1-C2-N2-C7
5	A	1308	NAG	C1-C2-N2-C7
5	K	1302	NAG	C1-C2-N2-C7
5	K	1303	NAG	C1-C2-N2-C7
5	K	1304	NAG	C1-C2-N2-C7
5	K	1309	NAG	C1-C2-N2-C7
5	K	1309	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1302	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.

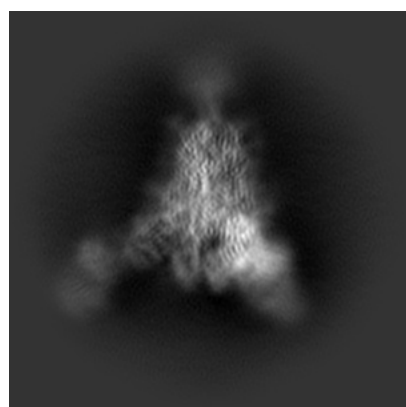
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23277. These allow visual inspection of the internal detail of the map and identification of artifacts.

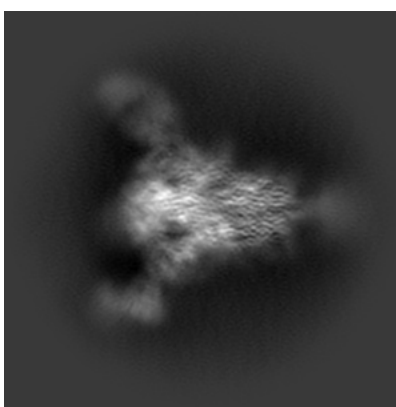
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

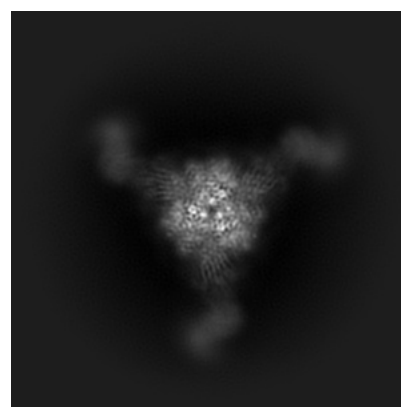
6.1.1 Primary map



X



Y

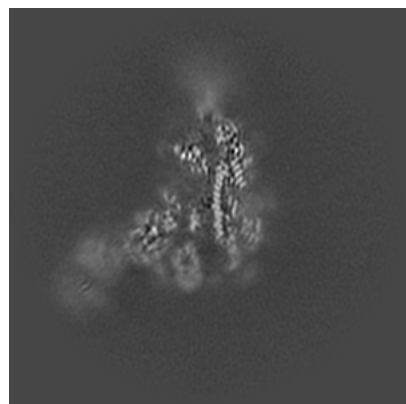


Z

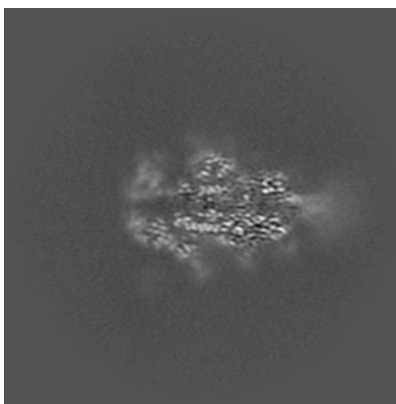
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

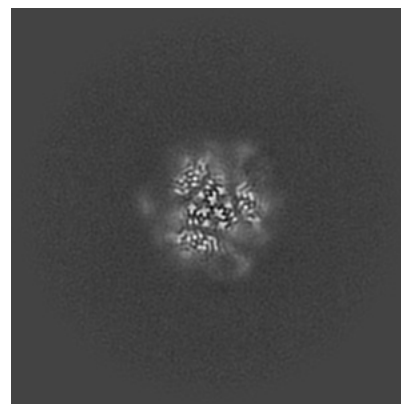
6.2.1 Primary map



X Index: 160



Y Index: 160

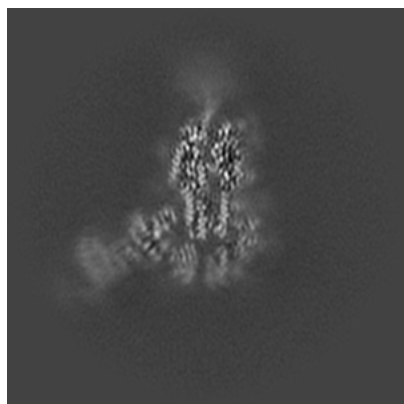


Z Index: 160

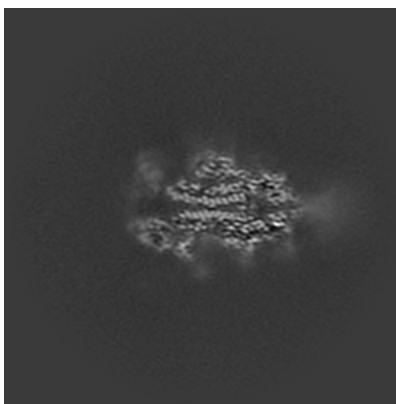
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

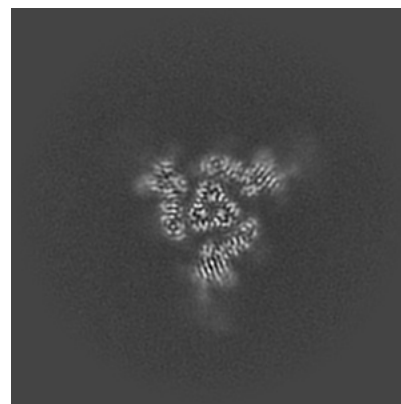
6.3.1 Primary map



X Index: 168



Y Index: 157

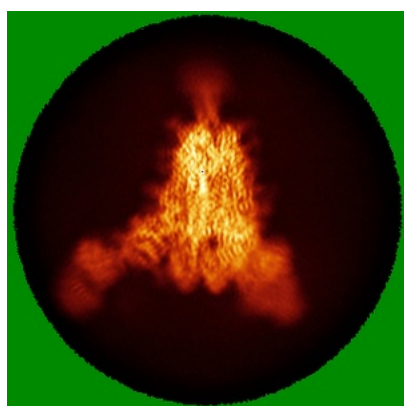


Z Index: 143

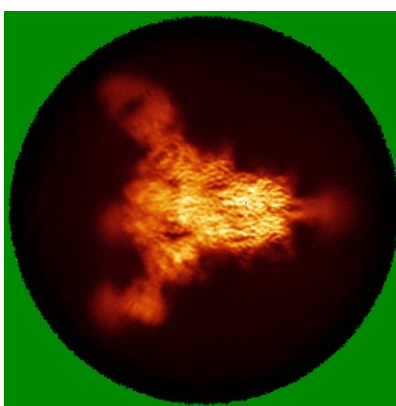
The images above show the largest variance slices of the map in three orthogonal directions.

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

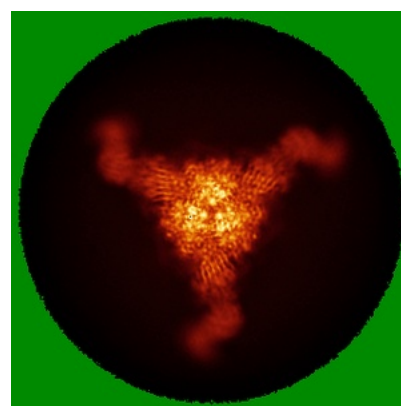
6.4.1 Primary map



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

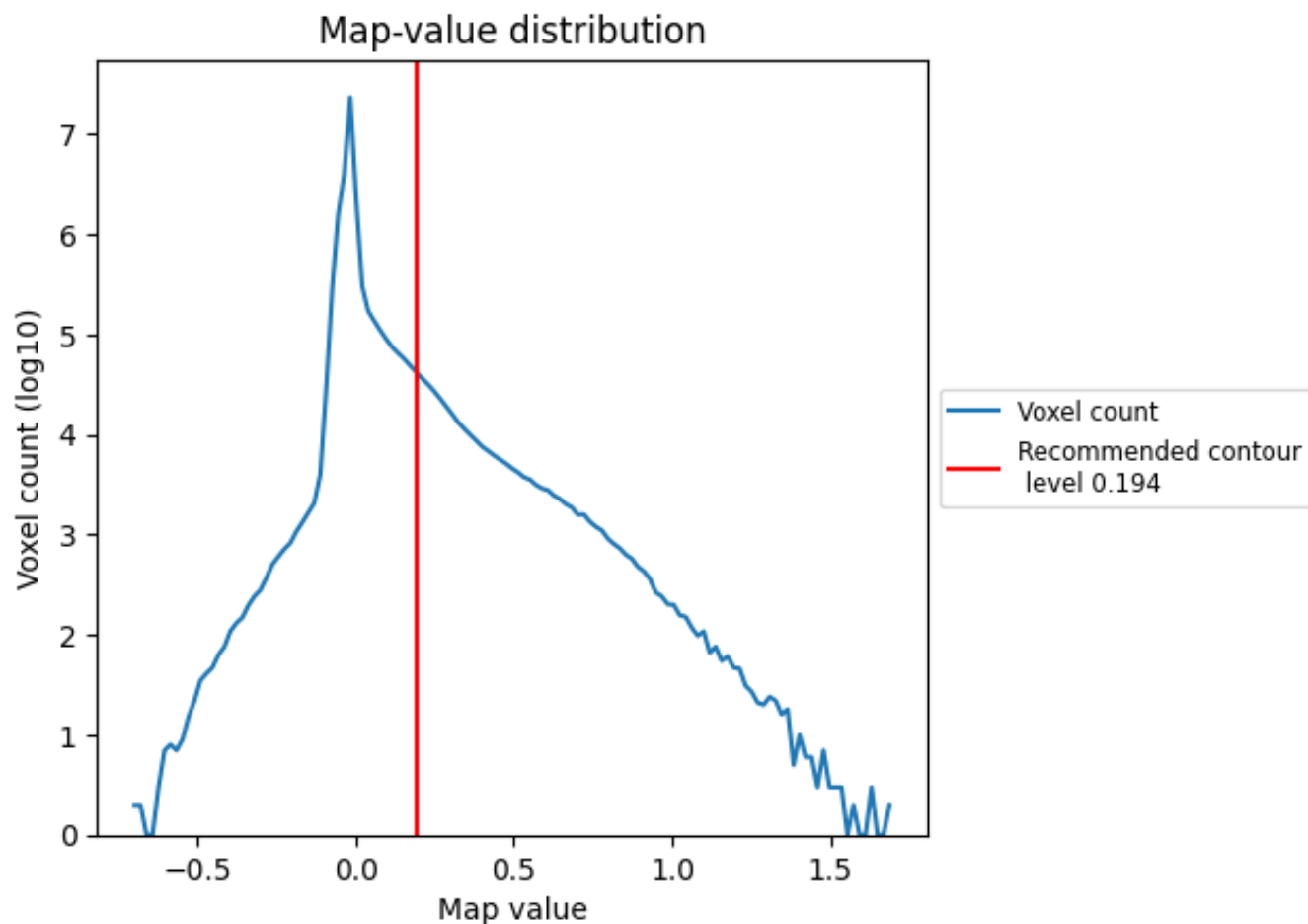
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

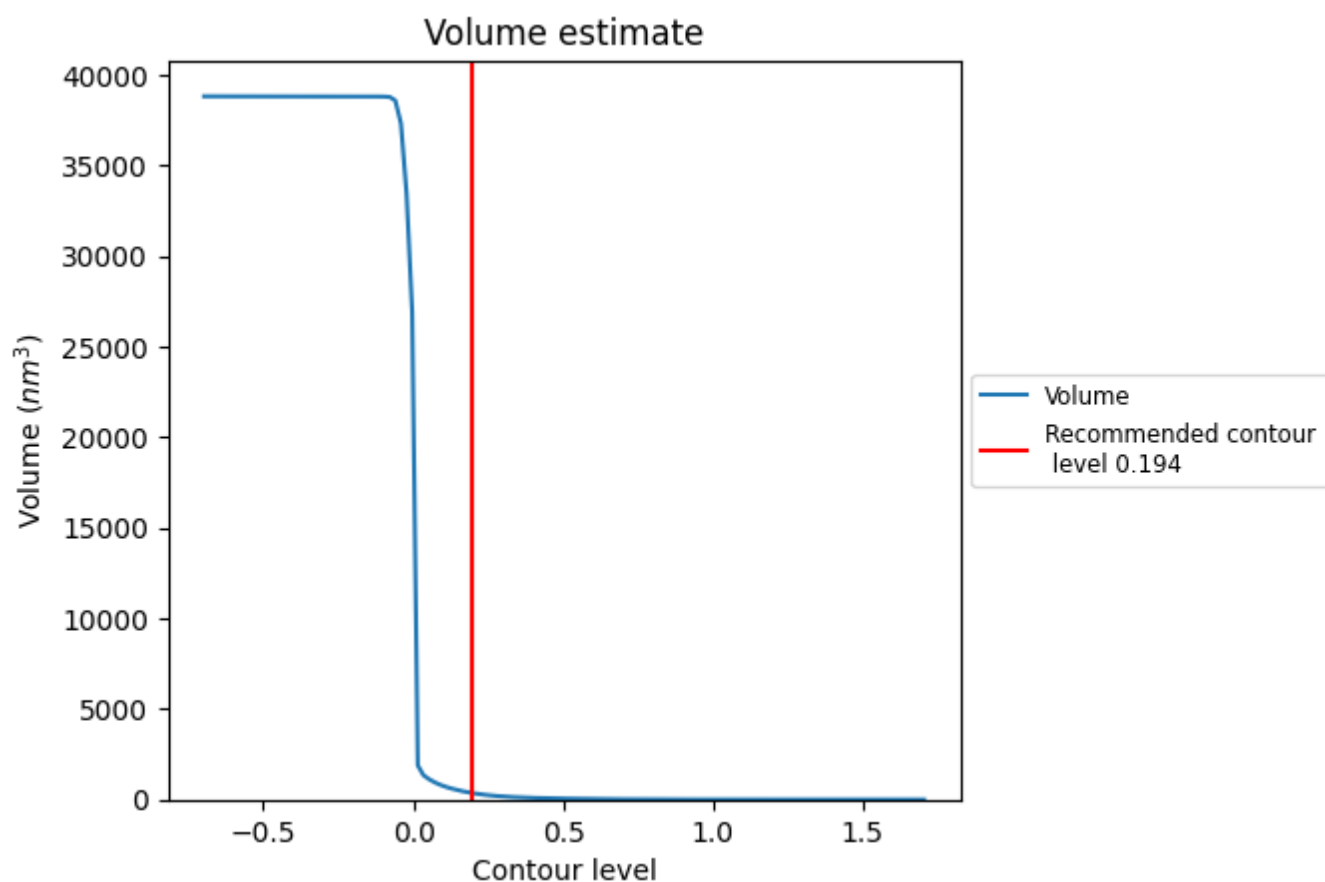
This section contains the results of statistical analysis of the map.

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.

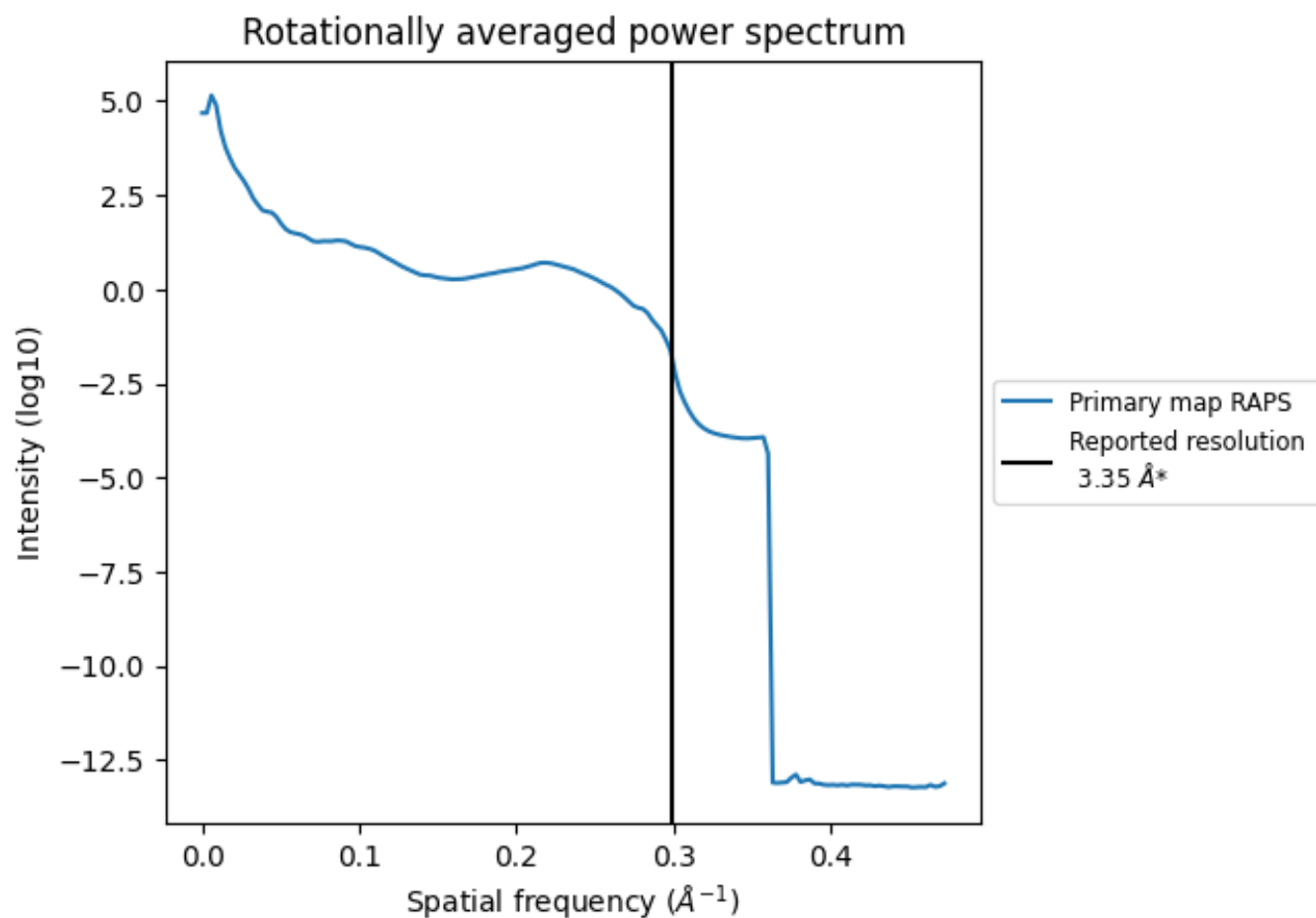
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 369 nm^3 ; this corresponds to an approximate mass of 334 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 0.299 $\text{\AA}^{-1}$

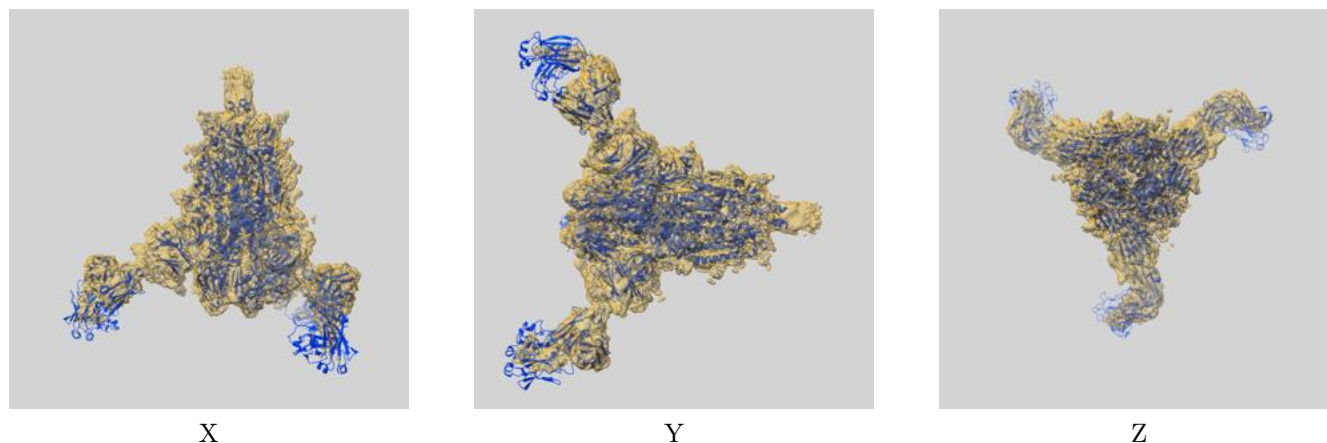
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

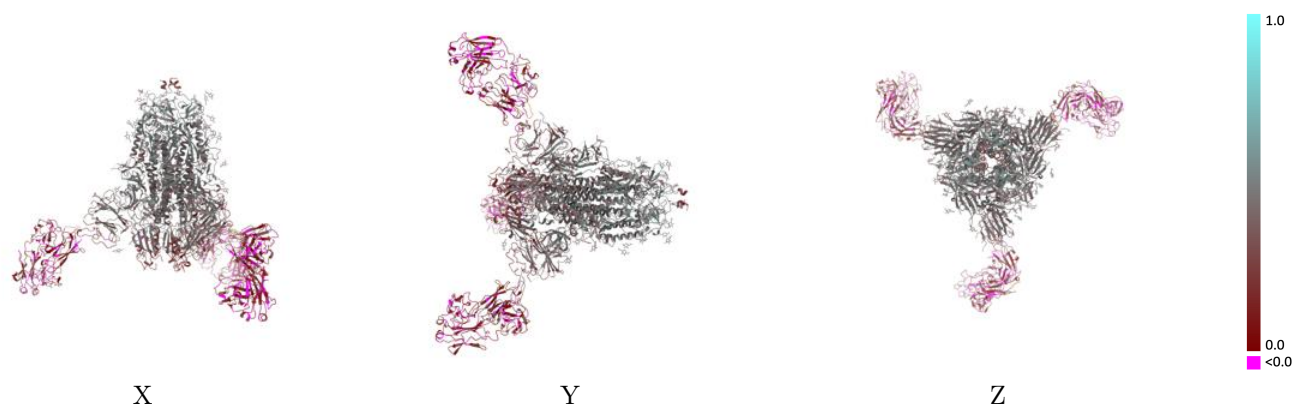
This section contains information regarding the fit between EMDB map EMD-23277 and PDB model 7LCN. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



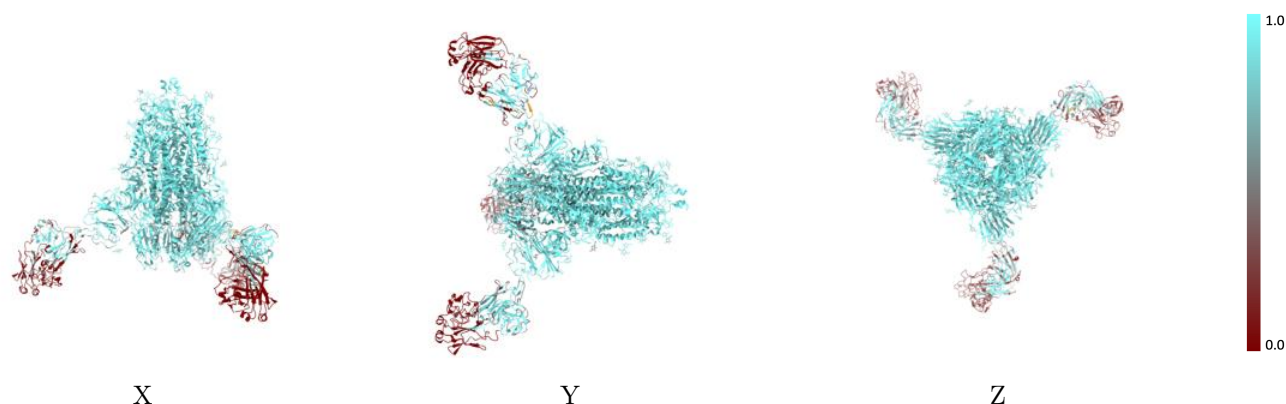
The images above show the 3D surface view of the map at the recommended contour level 0.194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



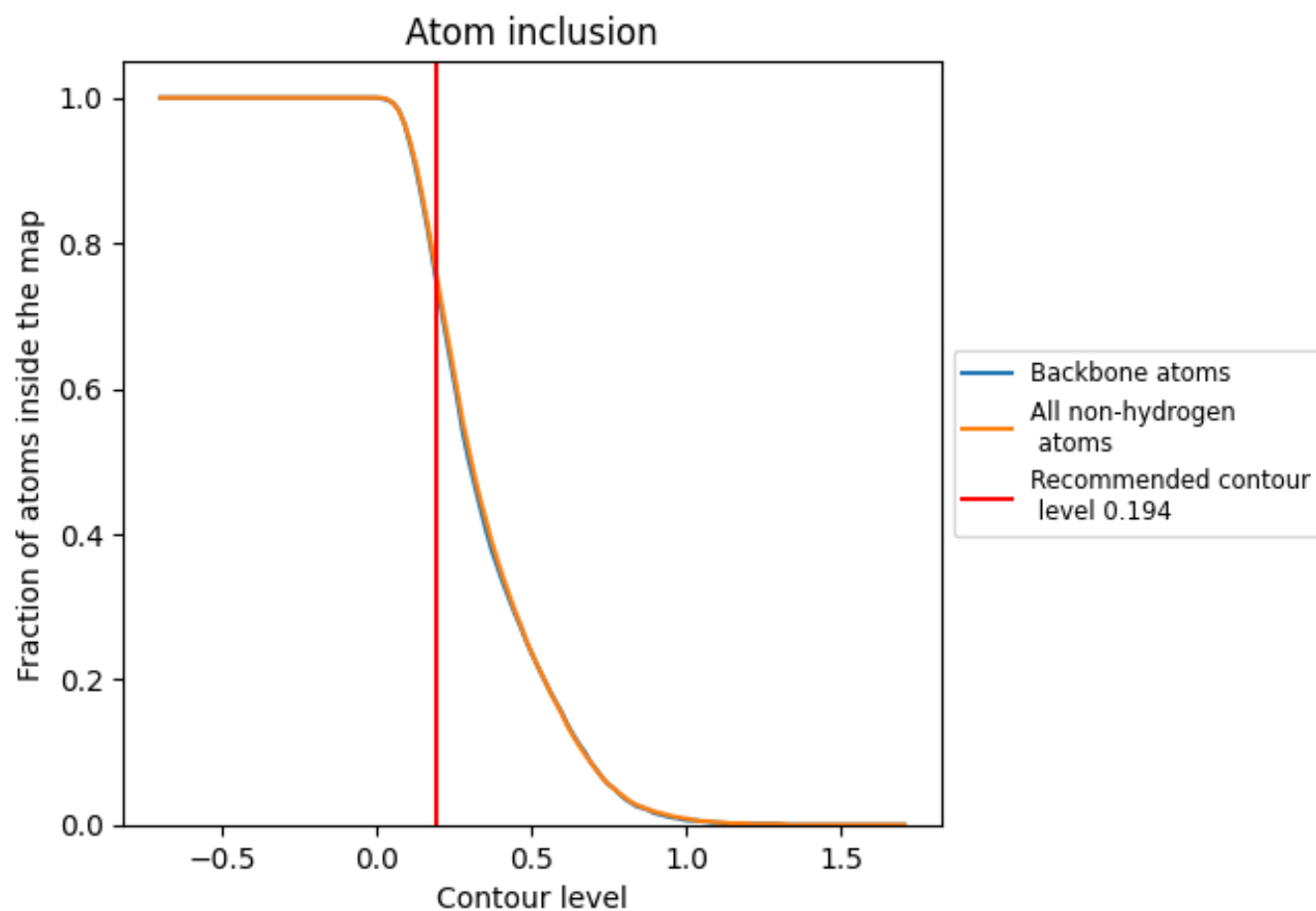
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.194).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 75% 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 (0.194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7540	 0.3290
A	 0.9110	 0.4130
B	 0.3260	 0.1260
C	 0.9080	 0.4120
D	 0.3980	 0.1160
E	 0.2140	 0.3970
F	 0.9290	 0.4900
G	 0.8930	 0.4350
H	 0.4070	 0.1360
I	 0.9290	 0.4200
J	 0.8570	 0.4240
K	 0.9070	 0.4110
L	 0.4700	 0.1310
M	 0.3380	 0.1160
N	 0.2500	 0.2920
O	 0.9290	 0.4950
P	 0.8930	 0.4150
Q	 1.0000	 0.4780
R	 0.8570	 0.4670
S	 0.4000	 0.1070
T	 0.2140	 0.3290
V	 0.9640	 0.4700
W	 0.8930	 0.4500
X	 0.8930	 0.4160
Y	 0.8210	 0.4570

