



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:10 AM UTC

PDB ID : 6ZOX / pdb_00006zox
EMDB ID : EMD-11329
Title : Structure of Disulphide-stabilized SARS-CoV-2 Spike Protein Trimer (x2 disulphide-bond mutant, G413C, V987C, single Arg S1/S2 cleavage site)
Authors : Xiong, X.; Qu, K.; Scheres, S.H.W.; Briggs, J.A.G.
Deposited on : 2020-07-08
Resolution : 3.00 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:

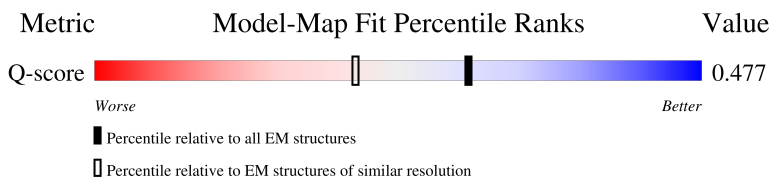
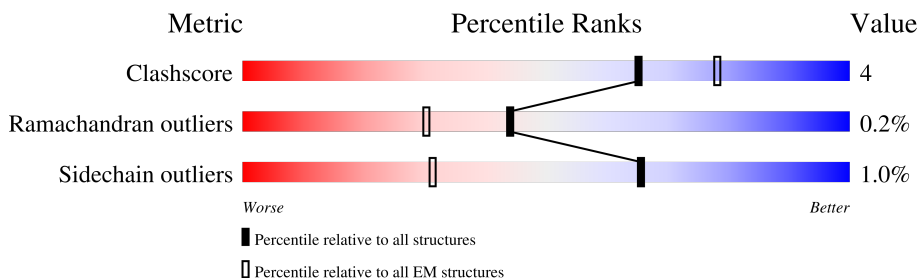
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	1247	
1	B	1247	
1	C	1247	
2	D	2	

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24696 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0
			7938	5066	1319	1514	39		
1	B	1017	Total	C	N	O	S	0	0
			7938	5066	1319	1514	39		
1	C	1017	Total	C	N	O	S	0	0
			7938	5066	1319	1514	39		

There are 177 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	413	CYS	GLY	engineered mutation	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	987	CYS	VAL	engineered mutation	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	413	CYS	GLY	engineered mutation	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	987	CYS	VAL	engineered mutation	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	413	CYS	GLY	engineered mutation	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	987	CYS	VAL	engineered mutation	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2

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



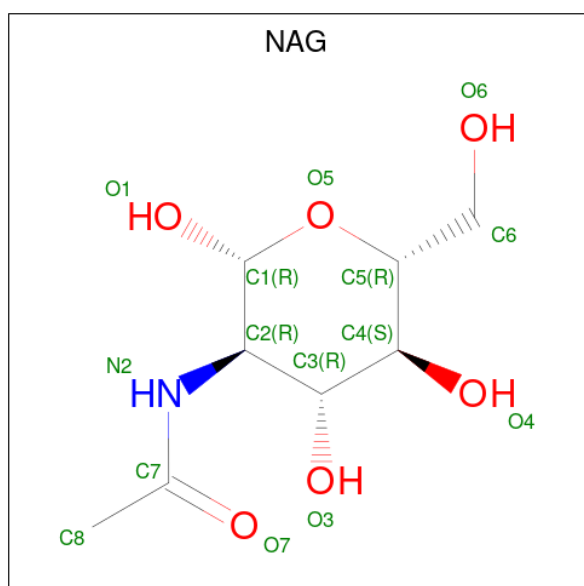
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

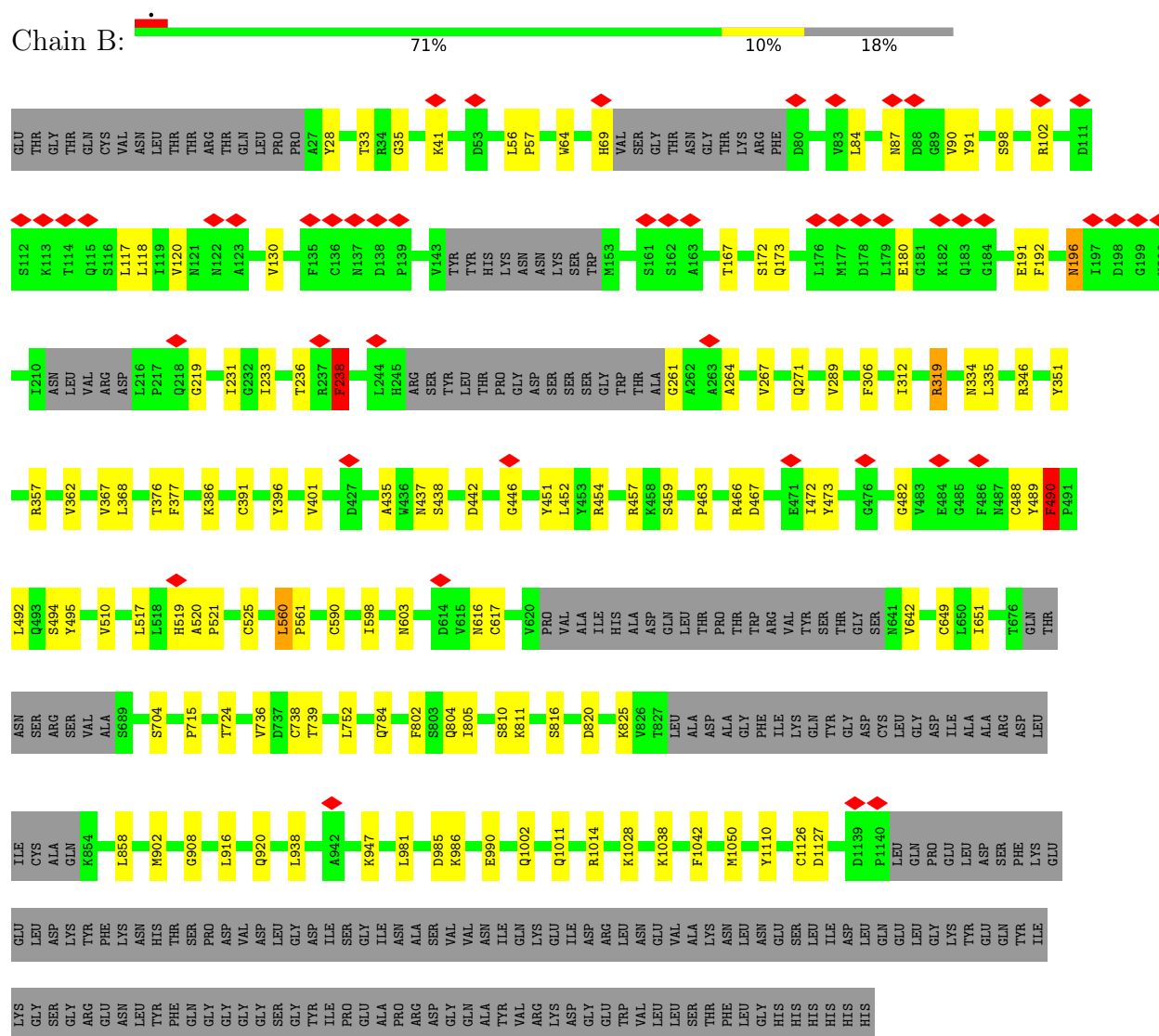
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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C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

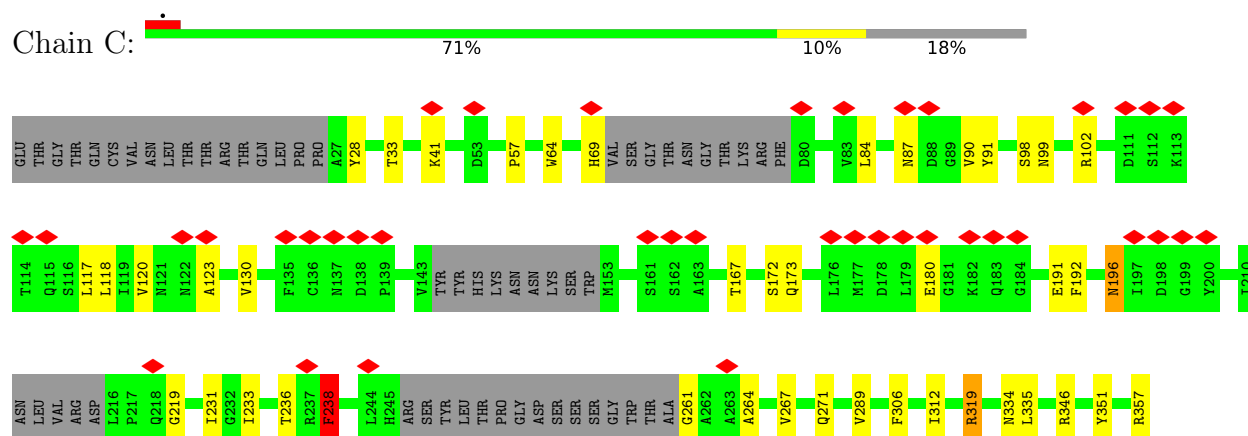
- Molecule 1: Spike glycoprotein

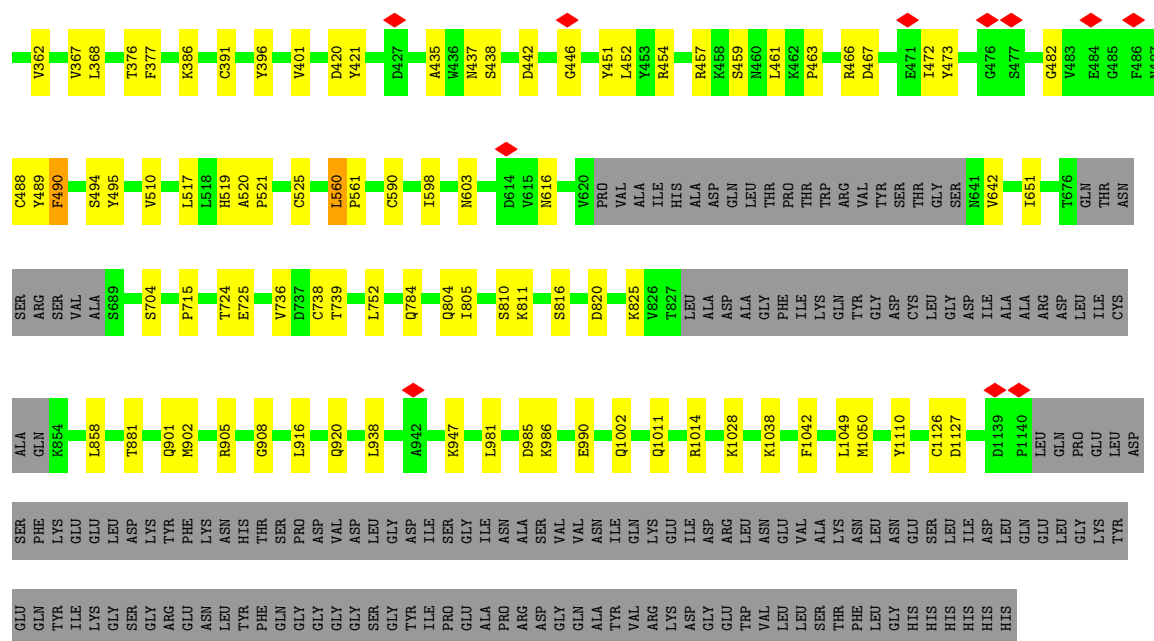
Chain B:



- Molecule 1: Spike glycoprotein

Chain C:





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



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



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



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





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



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



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



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



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



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





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



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



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



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



- Molecule 2: 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, C3	Depositor
Number of particles used	162468	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.131	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0257	Depositor
Map size (Å)	271.616, 271.616, 271.616	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	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	0.48	0/8115	0.99	23/11034 (0.2%)
1	B	0.48	0/8115	0.99	23/11034 (0.2%)
1	C	0.48	0/8115	0.99	23/11034 (0.2%)
All	All	0.48	0/24345	0.99	69/33102 (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	3
1	B	0	3
1	C	0	3
All	All	0	9

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	525	CYS	CA-CB-SG	8.92	134.92	114.40
1	C	525	CYS	CA-CB-SG	8.92	134.92	114.40
1	A	525	CYS	CA-CB-SG	8.90	134.87	114.40
1	A	102	ARG	CA-CB-CG	7.90	129.89	114.10
1	C	102	ARG	CA-CB-CG	7.90	129.89	114.10
1	A	616	ASN	N-CA-C	-7.89	97.77	110.32
1	B	102	ARG	CA-CB-CG	7.88	129.87	114.10
1	C	616	ASN	N-CA-C	-7.87	97.81	110.32
1	B	616	ASN	N-CA-C	-7.85	97.84	110.32
1	C	377	PHE	N-CA-CB	-7.24	99.45	112.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	PHE	N-CA-CB	-7.23	99.47	112.27
1	A	377	PHE	N-CA-CB	-7.22	99.49	112.27
1	C	238	PHE	N-CA-CB	-6.94	100.07	111.66
1	A	238	PHE	N-CA-CB	-6.93	100.09	111.66
1	A	560	LEU	CB-CA-C	6.90	119.46	109.11
1	B	238	PHE	N-CA-CB	-6.89	100.15	111.66
1	B	560	LEU	CB-CA-C	6.88	119.43	109.11
1	C	560	LEU	CB-CA-C	6.87	119.41	109.11
1	C	335	LEU	CA-C-N	6.56	129.80	120.49
1	C	335	LEU	C-N-CA	6.56	129.80	120.49
1	A	335	LEU	CA-C-N	6.52	129.75	120.49
1	A	335	LEU	C-N-CA	6.52	129.75	120.49
1	B	335	LEU	CA-C-N	6.51	129.74	120.49
1	B	335	LEU	C-N-CA	6.51	129.74	120.49
1	B	391	CYS	CA-CB-SG	6.09	128.41	114.40
1	C	391	CYS	CA-CB-SG	6.08	128.39	114.40
1	A	391	CYS	CA-CB-SG	6.07	128.37	114.40
1	A	490	PHE	CB-CA-C	6.02	117.36	108.87
1	C	490	PHE	CB-CA-C	6.00	117.33	108.87
1	B	490	PHE	CB-CA-C	5.99	117.31	108.87
1	B	377	PHE	N-CA-C	5.83	118.28	107.60
1	A	377	PHE	N-CA-C	5.83	118.27	107.60
1	C	377	PHE	N-CA-C	5.82	118.25	107.60
1	B	446	GLY	CA-C-N	5.80	132.78	121.41
1	B	446	GLY	C-N-CA	5.80	132.78	121.41
1	A	446	GLY	CA-C-N	5.79	132.76	121.41
1	A	446	GLY	C-N-CA	5.79	132.76	121.41
1	C	446	GLY	CA-C-N	5.78	132.73	121.41
1	C	446	GLY	C-N-CA	5.78	132.73	121.41
1	C	319	ARG	CA-CB-CG	5.70	125.50	114.10
1	A	1127	ASP	CA-C-N	5.69	128.18	122.66
1	A	1127	ASP	C-N-CA	5.69	128.18	122.66
1	B	319	ARG	CA-CB-CG	5.69	125.48	114.10
1	C	1127	ASP	CA-C-N	5.69	128.18	122.66
1	C	1127	ASP	C-N-CA	5.69	128.18	122.66
1	B	1127	ASP	CA-C-N	5.68	128.17	122.66
1	B	1127	ASP	C-N-CA	5.68	128.17	122.66
1	A	319	ARG	CA-CB-CG	5.67	125.43	114.10
1	A	490	PHE	N-CA-C	-5.63	102.97	110.07
1	B	490	PHE	N-CA-C	-5.62	102.99	110.07
1	A	238	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	238	PHE	CA-CB-CG	5.60	119.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	490	PHE	N-CA-C	-5.60	103.01	110.07
1	C	238	PHE	CA-CB-CG	5.55	119.36	113.80
1	A	102	ARG	CB-CA-C	-5.51	99.34	109.15
1	B	102	ARG	CB-CA-C	-5.50	99.35	109.15
1	C	102	ARG	CB-CA-C	-5.49	99.38	109.15
1	B	495	TYR	N-CA-C	-5.39	101.39	109.95
1	A	495	TYR	N-CA-C	-5.37	101.41	109.95
1	C	495	TYR	N-CA-C	-5.37	101.42	109.95
1	B	463	PRO	CA-C-N	5.22	131.24	123.05
1	B	463	PRO	C-N-CA	5.22	131.24	123.05
1	C	463	PRO	CA-C-N	5.22	131.24	123.05
1	C	463	PRO	C-N-CA	5.22	131.24	123.05
1	A	463	PRO	CA-C-N	5.19	131.20	123.05
1	A	463	PRO	C-N-CA	5.19	131.20	123.05
1	B	704	SER	N-CA-C	-5.10	101.44	109.50
1	C	704	SER	N-CA-C	-5.10	101.44	109.50
1	A	704	SER	N-CA-C	-5.08	101.47	109.50

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	PHE	Sidechain
1	A	517	LEU	Peptide
1	A	947	LYS	Mainchain
1	B	490	PHE	Sidechain
1	B	517	LEU	Peptide
1	B	947	LYS	Mainchain
1	C	490	PHE	Sidechain
1	C	517	LEU	Peptide
1	C	947	LYS	Mainchain

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	7938	0	7725	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7938	0	7725	67	0
1	C	7938	0	7725	70	0
2	D	28	0	25	2	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	2	0
2	J	28	0	25	0	0
2	K	28	0	25	1	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	2	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
3	A	154	0	143	3	0
3	B	154	0	143	3	0
3	C	154	0	143	3	0
All	All	24696	0	23979	195	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 4.

All (195) 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:C:442:ASP:OD1	1:C:451:TYR:OH	2.02	0.78
1:A:442:ASP:OD1	1:A:451:TYR:OH	2.02	0.76
1:B:346:ARG:NH2	1:B:451:TYR:OH	2.18	0.76
1:A:346:ARG:NH2	1:A:451:TYR:OH	2.19	0.76
1:C:346:ARG:NH2	1:C:451:TYR:OH	2.19	0.76
1:A:319:ARG:NH2	1:A:590:CYS:O	2.20	0.75
1:B:319:ARG:NH2	1:B:590:CYS:O	2.20	0.75
1:C:319:ARG:NH2	1:C:590:CYS:O	2.20	0.75
1:B:442:ASP:OD1	1:B:451:TYR:OH	2.02	0.75
1:B:752:LEU:HD21	1:B:990:GLU:OE1	1.90	0.71
1:C:752:LEU:HD21	1:C:990:GLU:OE1	1.90	0.71
1:A:752:LEU:HD21	1:A:990:GLU:OE1	1.90	0.70
1:B:98:SER:OG	1:B:180:GLU:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:825:LYS:NZ	1:C:938:LEU:O	2.19	0.69
1:A:98:SER:OG	1:A:180:GLU:O	2.10	0.69
1:A:33:THR:OG1	1:A:219:GLY:O	2.10	0.68
1:A:825:LYS:NZ	1:A:938:LEU:O	2.19	0.68
1:C:98:SER:OG	1:C:180:GLU:O	2.10	0.67
1:C:33:THR:OG1	1:C:219:GLY:O	2.10	0.67
1:B:825:LYS:NZ	1:B:938:LEU:O	2.19	0.67
1:B:33:THR:OG1	1:B:219:GLY:O	2.10	0.66
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.29	0.66
1:A:457:ARG:NE	1:A:467:ASP:OD1	2.29	0.65
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.28	0.65
1:C:457:ARG:NE	1:C:467:ASP:OD1	2.29	0.65
1:B:457:ARG:NE	1:B:467:ASP:OD1	2.29	0.65
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.29	0.65
1:A:466:ARG:NH1	1:B:231:ILE:O	2.31	0.64
1:C:172:SER:OG	1:C:173:GLN:OE1	2.17	0.63
1:A:172:SER:OG	1:A:173:GLN:OE1	2.17	0.63
1:B:172:SER:OG	1:B:173:GLN:OE1	2.17	0.63
1:B:466:ARG:NH1	1:C:231:ILE:O	2.32	0.62
1:A:357:ARG:NH2	1:A:396:TYR:OH	2.33	0.62
1:A:231:ILE:O	1:C:466:ARG:NH1	2.32	0.62
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.83	0.61
1:A:457:ARG:NH2	2:I:1:NAG:O7	2.33	0.61
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.33	0.61
1:C:357:ARG:NH2	1:C:396:TYR:OH	2.33	0.61
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.83	0.61
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.33	0.61
1:A:367:VAL:HG23	1:A:368:LEU:HD12	1.83	0.61
1:B:357:ARG:NH2	1:B:396:TYR:OH	2.33	0.61
1:C:457:ARG:NH2	2:D:1:NAG:O7	2.33	0.61
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.34	0.60
1:B:457:ARG:NH2	2:N:1:NAG:O7	2.35	0.59
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.33	0.59
1:A:804:GLN:NE2	2:F:1:NAG:O6	2.36	0.59
1:A:902:MET:SD	1:A:1050:MET:HE3	2.43	0.59
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.34	0.59
1:B:902:MET:SD	1:B:1050:MET:HE3	2.43	0.59
1:A:196:ASN:O	1:A:196:ASN:ND2	2.36	0.59
1:B:804:GLN:NE2	2:K:1:NAG:O6	2.36	0.59
1:C:804:GLN:NE2	2:P:1:NAG:O6	2.36	0.59
1:B:472:ILE:HD11	1:B:482:GLY:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASN:O	1:C:196:ASN:ND2	2.36	0.58
1:C:472:ILE:HD11	1:C:482:GLY:H	1.69	0.58
1:C:902:MET:SD	1:C:1050:MET:HE3	2.43	0.58
1:B:196:ASN:O	1:B:196:ASN:ND2	2.36	0.58
1:A:472:ILE:HD11	1:A:482:GLY:H	1.69	0.57
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.40	0.57
1:B:90:VAL:HG21	1:B:238:PHE:CE1	2.40	0.57
1:C:90:VAL:HG21	1:C:238:PHE:CE1	2.40	0.57
1:A:715:PRO:O	1:A:1110:TYR:N	2.38	0.57
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.87	0.56
1:B:715:PRO:O	1:B:1110:TYR:N	2.38	0.56
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.87	0.56
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.87	0.56
1:C:715:PRO:O	1:C:1110:TYR:N	2.38	0.55
1:B:312:ILE:HD12	1:B:598:ILE:HD11	1.89	0.55
1:C:312:ILE:HD12	1:C:598:ILE:HD11	1.89	0.54
1:A:312:ILE:HD12	1:A:598:ILE:HD11	1.89	0.54
1:C:334:ASN:O	1:C:362:VAL:HG12	2.07	0.54
1:C:236:THR:HG21	2:N:1:NAG:H5	1.90	0.54
1:B:236:THR:HG21	2:I:1:NAG:H5	1.90	0.54
1:A:334:ASN:O	1:A:362:VAL:HG12	2.07	0.53
1:B:334:ASN:O	1:B:362:VAL:HG12	2.07	0.53
1:A:805:ILE:O	1:A:816:SER:OG	2.26	0.53
1:A:236:THR:HG21	2:D:1:NAG:H5	1.90	0.53
1:A:981:LEU:O	1:C:386:LYS:NZ	2.43	0.52
1:A:386:LYS:NZ	1:B:981:LEU:O	2.43	0.51
1:A:472:ILE:HD12	1:A:488:CYS:SG	2.51	0.51
1:A:28:TYR:O	3:A:1301:NAG:H82	2.11	0.51
1:C:472:ILE:HD12	1:C:488:CYS:SG	2.51	0.51
1:B:472:ILE:HD12	1:B:488:CYS:SG	2.51	0.50
1:C:28:TYR:O	3:C:1301:NAG:H82	2.11	0.50
1:C:130:VAL:HG21	1:C:231:ILE:HG23	1.93	0.50
1:B:386:LYS:NZ	1:C:981:LEU:O	2.43	0.50
1:A:167:THR:HG21	1:C:466:ARG:HH22	1.77	0.50
1:B:130:VAL:HG21	1:B:231:ILE:HG23	1.93	0.50
1:B:28:TYR:O	3:B:1301:NAG:H82	2.11	0.50
1:C:916:LEU:O	1:C:920:GLN:N	2.45	0.50
1:A:130:VAL:HG21	1:A:231:ILE:HG23	1.93	0.50
3:B:1309:NAG:H3	3:B:1309:NAG:H83	1.95	0.49
1:A:84:LEU:HD13	1:A:267:VAL:HG21	1.95	0.49
1:A:738:CYS:SG	1:A:739:THR:N	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:ILE:O	1:C:816:SER:OG	2.26	0.49
1:A:916:LEU:O	1:A:920:GLN:N	2.45	0.49
1:B:916:LEU:O	1:B:920:GLN:N	2.45	0.49
3:A:1309:NAG:H3	3:A:1309:NAG:H83	1.95	0.49
1:B:738:CYS:SG	1:B:739:THR:N	2.86	0.49
3:C:1309:NAG:H83	3:C:1309:NAG:H3	1.95	0.49
1:B:435:ALA:CB	1:B:510:VAL:HG12	2.43	0.48
1:C:84:LEU:HD13	1:C:267:VAL:HG21	1.95	0.48
1:C:738:CYS:SG	1:C:739:THR:N	2.86	0.48
1:A:435:ALA:CB	1:A:510:VAL:HG12	2.43	0.48
1:C:435:ALA:CB	1:C:510:VAL:HG12	2.43	0.48
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.34	0.48
1:C:642:VAL:HG13	1:C:651:ILE:HG22	1.95	0.48
1:B:519:HIS:O	1:C:41:LYS:HB2	2.14	0.48
1:B:84:LEU:HD13	1:B:267:VAL:HG21	1.95	0.47
1:A:167:THR:HG21	1:C:466:ARG:NH2	2.30	0.47
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.79	0.47
1:A:642:VAL:HG13	1:A:651:ILE:HG22	1.96	0.47
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.79	0.47
1:C:452:LEU:HD13	1:C:494:SER:HB2	1.96	0.47
1:C:91:TYR:OH	1:C:191:GLU:OE2	2.33	0.47
1:C:985:ASP:OD1	1:C:986:LYS:N	2.45	0.47
1:B:642:VAL:HG13	1:B:651:ILE:HG22	1.96	0.47
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.79	0.47
1:A:519:HIS:O	1:B:41:LYS:HB2	2.15	0.47
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.33	0.47
1:A:473:TYR:N	1:A:489:TYR:O	2.43	0.47
1:A:452:LEU:HD13	1:A:494:SER:HB2	1.97	0.46
1:A:985:ASP:OD1	1:A:986:LYS:N	2.45	0.46
1:B:91:TYR:OH	1:B:191:GLU:OE2	2.33	0.46
1:B:452:LEU:HD13	1:B:494:SER:HB2	1.97	0.46
3:A:1321:NAG:H81	1:C:351:TYR:OH	2.15	0.46
1:B:466:ARG:HH22	1:C:167:THR:HG21	1.81	0.45
1:A:41:LYS:HB2	1:C:519:HIS:O	2.16	0.45
1:A:466:ARG:HH22	1:B:167:THR:HG21	1.82	0.45
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.48	0.44
1:B:805:ILE:O	1:B:816:SER:OG	2.26	0.44
1:B:985:ASP:OD1	1:B:986:LYS:N	2.45	0.44
1:C:401:VAL:HG21	1:C:451:TYR:CE1	2.53	0.44
1:C:473:TYR:N	1:C:489:TYR:O	2.43	0.44
1:C:736:VAL:HG22	1:C:858:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:HG23	1:A:306:PHE:CZ	2.53	0.44
1:A:401:VAL:HG21	1:A:451:TYR:CE1	2.53	0.44
1:B:736:VAL:HG22	1:B:858:LEU:CD2	2.48	0.44
1:B:401:VAL:HG21	1:B:451:TYR:CE1	2.53	0.43
1:C:289:VAL:HG23	1:C:306:PHE:CZ	2.53	0.43
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.44	0.43
1:C:457:ARG:NH1	1:C:459:SER:O	2.49	0.43
1:B:289:VAL:HG23	1:B:306:PHE:CZ	2.53	0.43
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.53	0.42
1:C:1011:GLN:OE1	1:C:1014:ARG:NH1	2.53	0.42
1:A:118:LEU:CD2	1:A:120:VAL:HG23	2.50	0.42
1:C:118:LEU:CD2	1:C:120:VAL:HG23	2.50	0.42
1:A:117:LEU:HB2	1:A:233:ILE:HD11	2.02	0.42
1:B:117:LEU:HB2	1:B:233:ILE:HD11	2.02	0.42
1:B:736:VAL:HG13	1:B:858:LEU:HD23	2.01	0.42
1:A:881:THR:O	1:A:901:GLN:NE2	2.51	0.42
1:B:118:LEU:CD2	1:B:120:VAL:HG23	2.50	0.42
1:C:117:LEU:HB2	1:C:233:ILE:HD11	2.02	0.42
1:C:420:ASP:O	1:C:461:LEU:N	2.53	0.42
1:C:736:VAL:HG13	1:C:858:LEU:HD23	2.01	0.42
1:C:881:THR:O	1:C:901:GLN:NE2	2.51	0.42
1:B:437:ASN:OD1	1:B:438:SER:N	2.53	0.42
1:B:473:TYR:N	1:B:489:TYR:O	2.43	0.41
1:A:466:ARG:NH2	1:B:167:THR:HG21	2.35	0.41
1:B:466:ARG:NH2	1:C:167:THR:HG21	2.35	0.41
1:A:560:LEU:HD23	1:A:561:PRO:HD2	2.02	0.41
1:B:35:GLY:HA3	1:B:56:LEU:HB3	2.03	0.41
1:C:99:ASN:HD22	1:C:123:ALA:HB2	1.84	0.41
1:A:437:ASN:OD1	1:A:438:SER:N	2.53	0.41
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.53	0.41
1:A:99:ASN:HD22	1:A:123:ALA:HB2	1.84	0.41
1:A:736:VAL:HG13	1:A:858:LEU:HD23	2.01	0.41
1:C:57:PRO:HG3	1:C:271:GLN:NE2	2.36	0.41
1:C:172:SER:OG	1:C:173:GLN:N	2.54	0.41
1:A:454:ARG:NH1	1:A:467:ASP:O	2.54	0.41
1:B:617:CYS:HB3	1:B:649:CYS:HB3	2.03	0.41
1:C:437:ASN:OD1	1:C:438:SER:N	2.53	0.41
1:C:454:ARG:NH1	1:C:467:ASP:O	2.54	0.41
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.44	0.41
1:A:420:ASP:O	1:A:461:LEU:N	2.53	0.41
1:A:35:GLY:HA3	1:A:56:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PRO:HG3	1:A:271:GLN:NE2	2.36	0.40
1:B:560:LEU:HD23	1:B:561:PRO:HD2	2.02	0.40
1:B:802:PHE:CD2	1:B:805:ILE:HD11	2.57	0.40
1:C:725:GLU:CD	1:C:1028:LYS:HZ2	2.29	0.40
1:A:39:PRO:HG3	1:A:51:THR:HG21	2.03	0.40
1:A:351:TYR:OH	3:B:1321:NAG:H81	2.21	0.40
1:B:69:HIS:N	1:B:261:GLY:O	2.54	0.40
1:B:454:ARG:NH1	1:B:467:ASP:O	2.54	0.40
1:C:69:HIS:N	1:C:261:GLY:O	2.54	0.40
1:C:560:LEU:HD23	1:C:561:PRO:HD2	2.02	0.40
1:A:935:GLN:O	1:A:939:SER:N	2.48	0.40
1:A:1028:LYS:O	1:A:1032:CYS:N	2.46	0.40
1:B:351:TYR:OH	3:C:1321:NAG:H81	2.22	0.40
1:C:420:ASP:OD1	1:C:421:TYR:N	2.55	0.40
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.57	0.40
1:B:57:PRO:HG3	1:B:271:GLN:NE2	2.36	0.40
1:B:457:ARG:NH1	1:B:459:SER:O	2.49	0.40
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.57	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	1001/1247 (80%)	963 (96%)	36 (4%)	2 (0%)	43	76
1	B	1001/1247 (80%)	963 (96%)	36 (4%)	2 (0%)	43	76
1	C	1001/1247 (80%)	963 (96%)	36 (4%)	2 (0%)	43	76
All	All	3003/3741 (80%)	2889 (96%)	108 (4%)	6 (0%)	44	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	B	87	ASN
1	C	87	ASN
1	A	1126	CYS
1	B	1126	CYS
1	C	1126	CYS

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	887/1082 (82%)	878 (99%)	9 (1%)	68	84
1	B	887/1082 (82%)	878 (99%)	9 (1%)	68	84
1	C	887/1082 (82%)	878 (99%)	9 (1%)	68	84
All	All	2661/3246 (82%)	2634 (99%)	27 (1%)	65	84

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	PHE
1	A	196	ASN
1	A	238	PHE
1	A	376	THR
1	A	603	ASN
1	A	724	THR
1	A	784	GLN
1	A	810	SER
1	A	1002	GLN
1	B	192	PHE
1	B	196	ASN
1	B	238	PHE
1	B	376	THR
1	B	603	ASN
1	B	724	THR
1	B	784	GLN
1	B	810	SER

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Mol	Chain	Res	Type
1	B	1002	GLN
1	C	192	PHE
1	C	196	ASN
1	C	238	PHE
1	C	376	THR
1	C	603	ASN
1	C	724	THR
1	C	784	GLN
1	C	810	SER
1	C	1002	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	536	ASN
1	A	564	GLN
1	A	764	ASN
1	A	804	GLN
1	A	1058	HIS
1	A	1088	HIS
1	A	1108	ASN
1	B	196	ASN
1	B	536	ASN
1	B	564	GLN
1	B	764	ASN
1	B	787	GLN
1	B	804	GLN
1	B	1088	HIS
1	B	1108	ASN
1	C	196	ASN
1	C	536	ASN
1	C	564	GLN
1	C	764	ASN
1	C	787	GLN
1	C	804	GLN
1	C	1108	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

30 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.26	0	17,19,21	0.67	0
2	NAG	D	2	2	14,14,15	0.48	0	17,19,21	0.61	0
2	NAG	E	1	2,1	14,14,15	0.17	0	17,19,21	0.60	0
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.62	0
2	NAG	F	1	2,1	14,14,15	0.21	0	17,19,21	0.62	0
2	NAG	F	2	2	14,14,15	0.16	0	17,19,21	0.63	0
2	NAG	G	1	2,1	14,14,15	0.16	0	17,19,21	0.58	0
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.60	0
2	NAG	H	1	2,1	14,14,15	0.23	0	17,19,21	0.58	0
2	NAG	H	2	2	14,14,15	0.16	0	17,19,21	0.64	0
2	NAG	I	1	2,1	14,14,15	0.26	0	17,19,21	0.67	0
2	NAG	I	2	2	14,14,15	0.50	0	17,19,21	0.62	0
2	NAG	J	1	2,1	14,14,15	0.19	0	17,19,21	0.59	0
2	NAG	J	2	2	14,14,15	0.26	0	17,19,21	0.63	0
2	NAG	K	1	2,1	14,14,15	0.21	0	17,19,21	0.62	0
2	NAG	K	2	2	14,14,15	0.15	0	17,19,21	0.61	0
2	NAG	L	1	2,1	14,14,15	0.17	0	17,19,21	0.58	0
2	NAG	L	2	2	14,14,15	0.25	0	17,19,21	0.59	0
2	NAG	M	1	2,1	14,14,15	0.22	0	17,19,21	0.58	0
2	NAG	M	2	2	14,14,15	0.17	0	17,19,21	0.64	0
2	NAG	N	1	2,1	14,14,15	0.26	0	17,19,21	0.68	0
2	NAG	N	2	2	14,14,15	0.49	0	17,19,21	0.61	0
2	NAG	O	1	2,1	14,14,15	0.17	0	17,19,21	0.61	0
2	NAG	O	2	2	14,14,15	0.26	0	17,19,21	0.62	0
2	NAG	P	1	2,1	14,14,15	0.21	0	17,19,21	0.62	0
2	NAG	P	2	2	14,14,15	0.15	0	17,19,21	0.62	0
2	NAG	Q	1	2,1	14,14,15	0.16	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Q	2	2	14,14,15	0.27	0	17,19,21	0.60	0
2	NAG	R	1	2,1	14,14,15	0.22	0	17,19,21	0.58	0
2	NAG	R	2	2	14,14,15	0.17	0	17,19,21	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	3/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	R	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6

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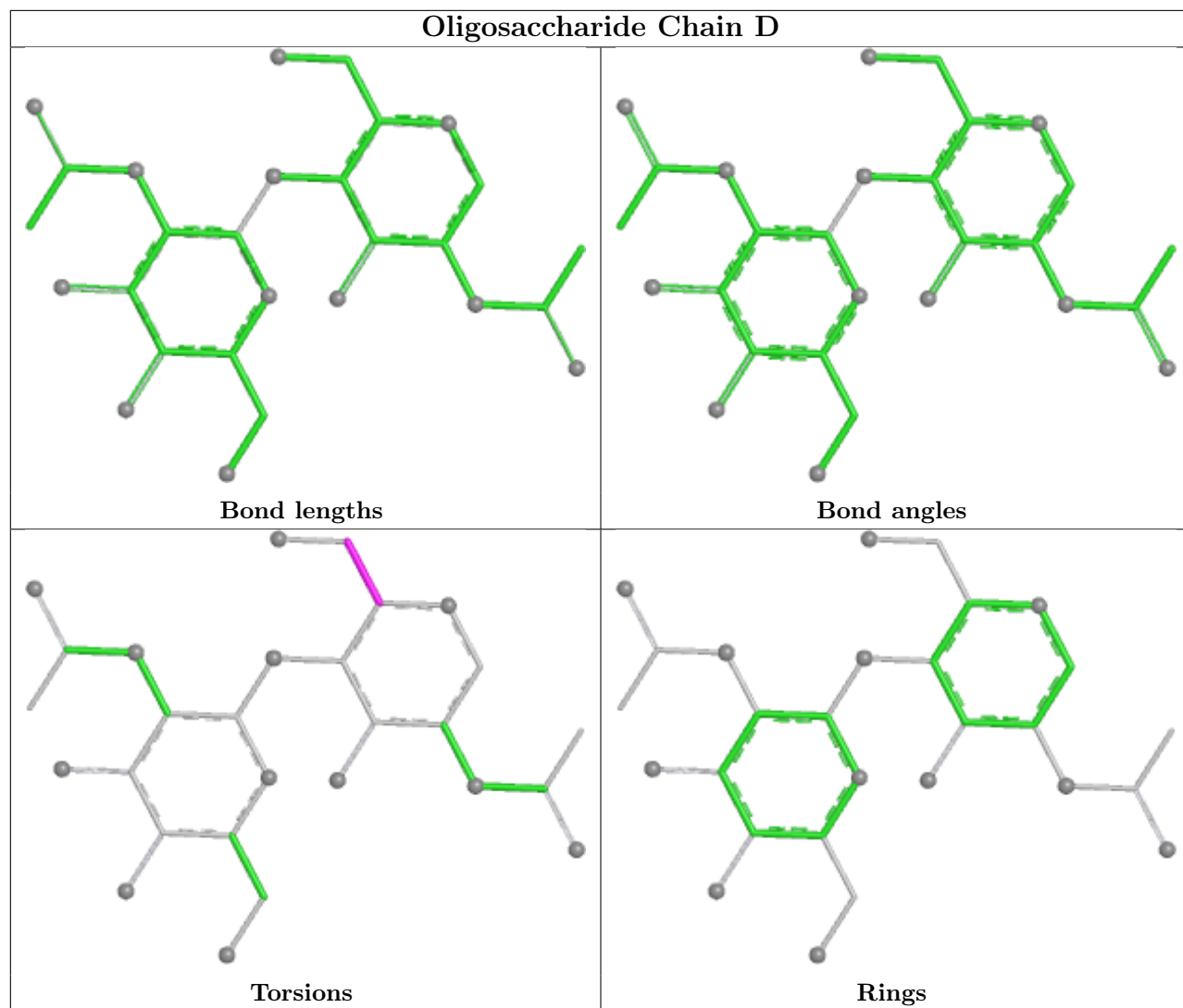
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	K	2	NAG	C1-C2-N2-C7
2	M	2	NAG	C1-C2-N2-C7
2	P	2	NAG	C1-C2-N2-C7
2	R	2	NAG	C1-C2-N2-C7

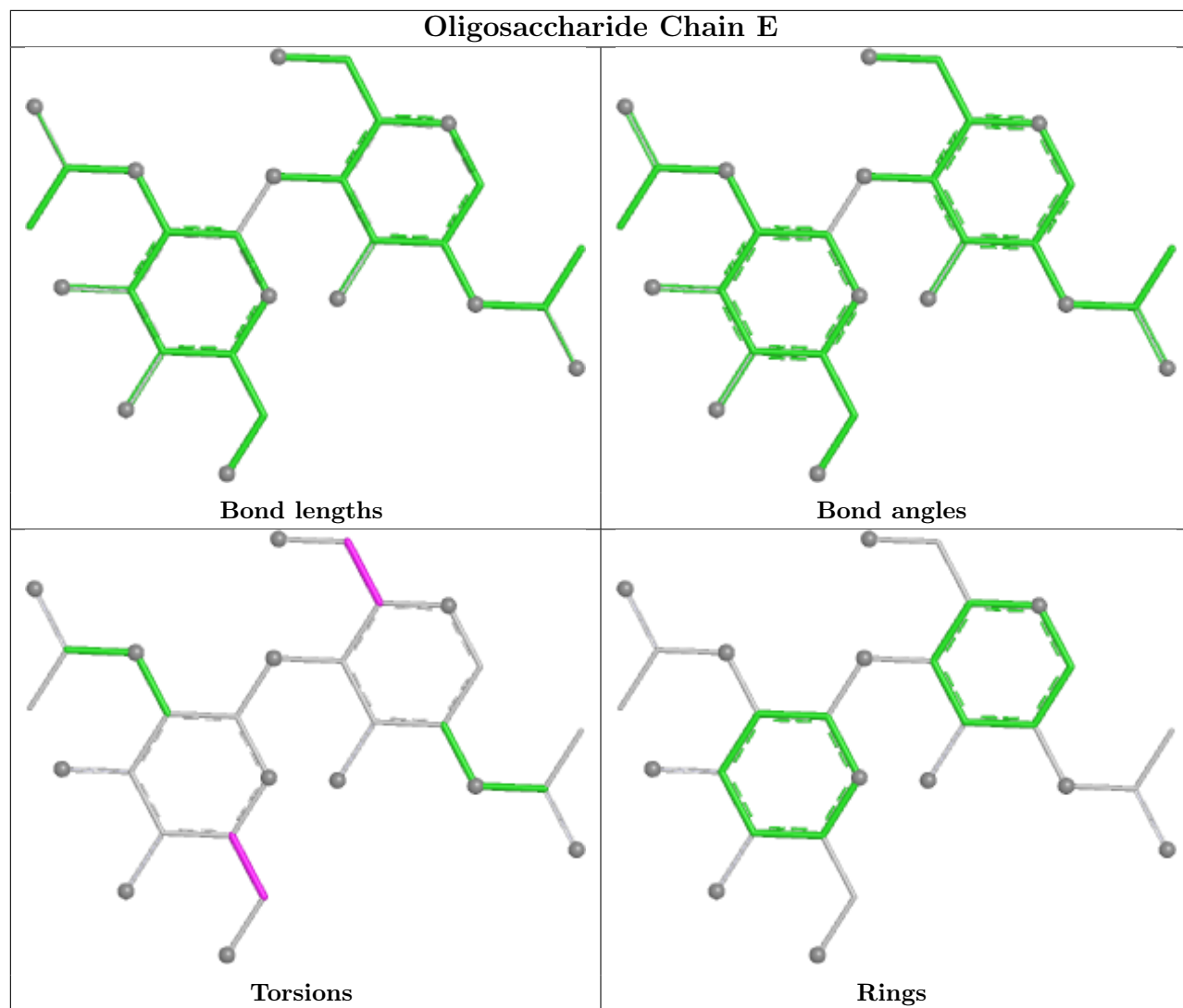
There are no ring outliers.

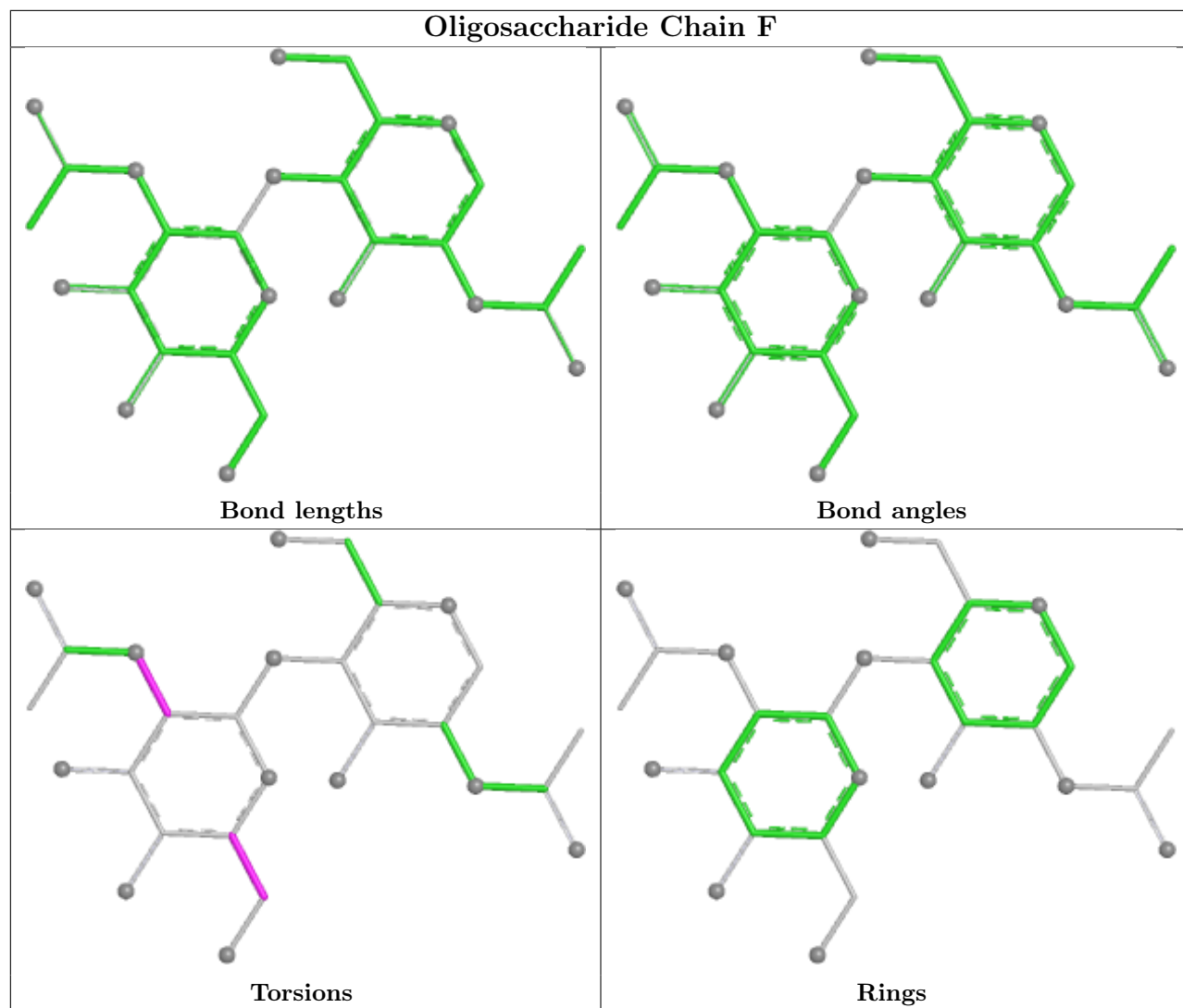
6 monomers are involved in 9 short contacts:

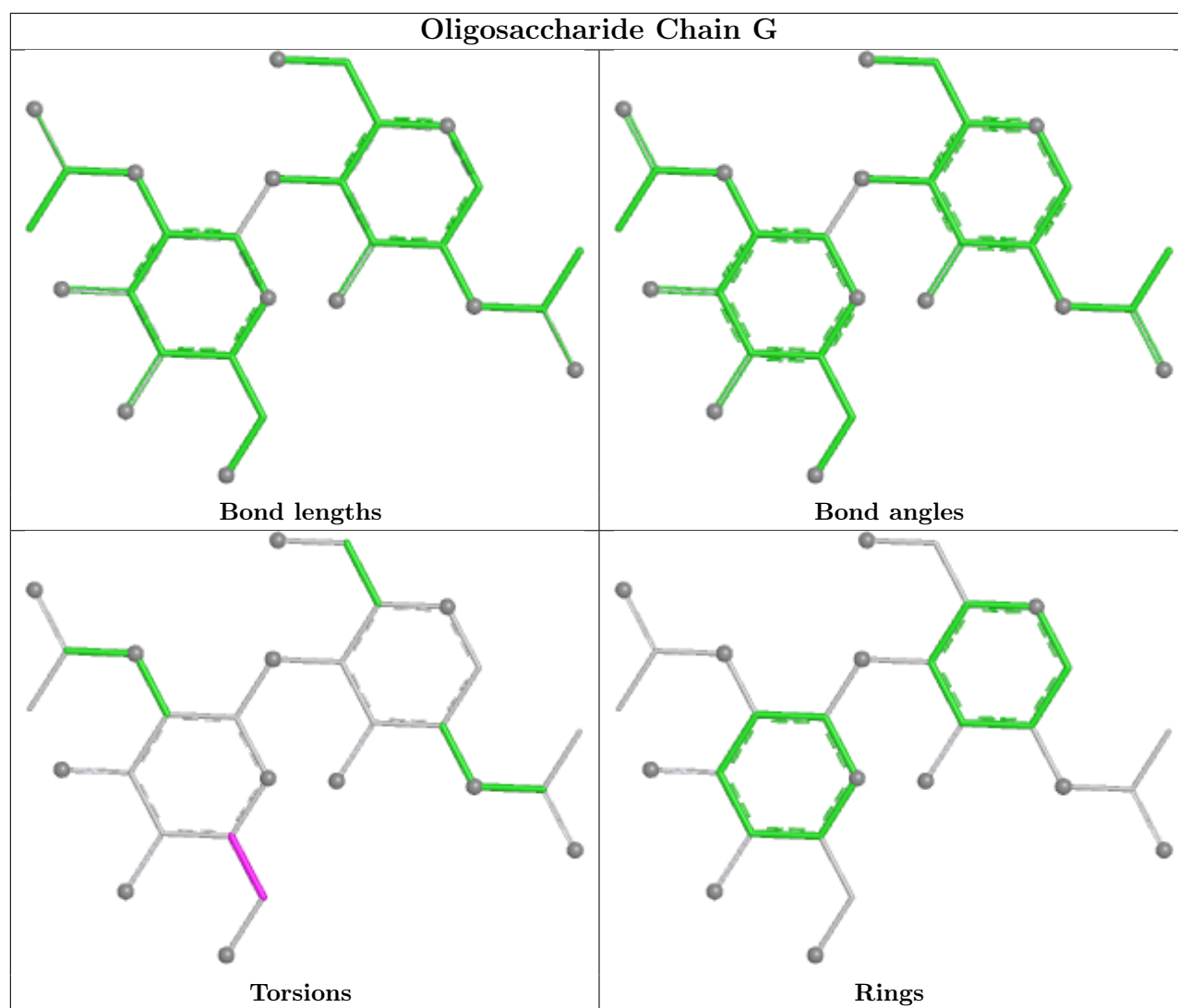
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	NAG	1	0
2	K	1	NAG	1	0
2	N	1	NAG	2	0
2	D	1	NAG	2	0
2	F	1	NAG	1	0
2	I	1	NAG	2	0

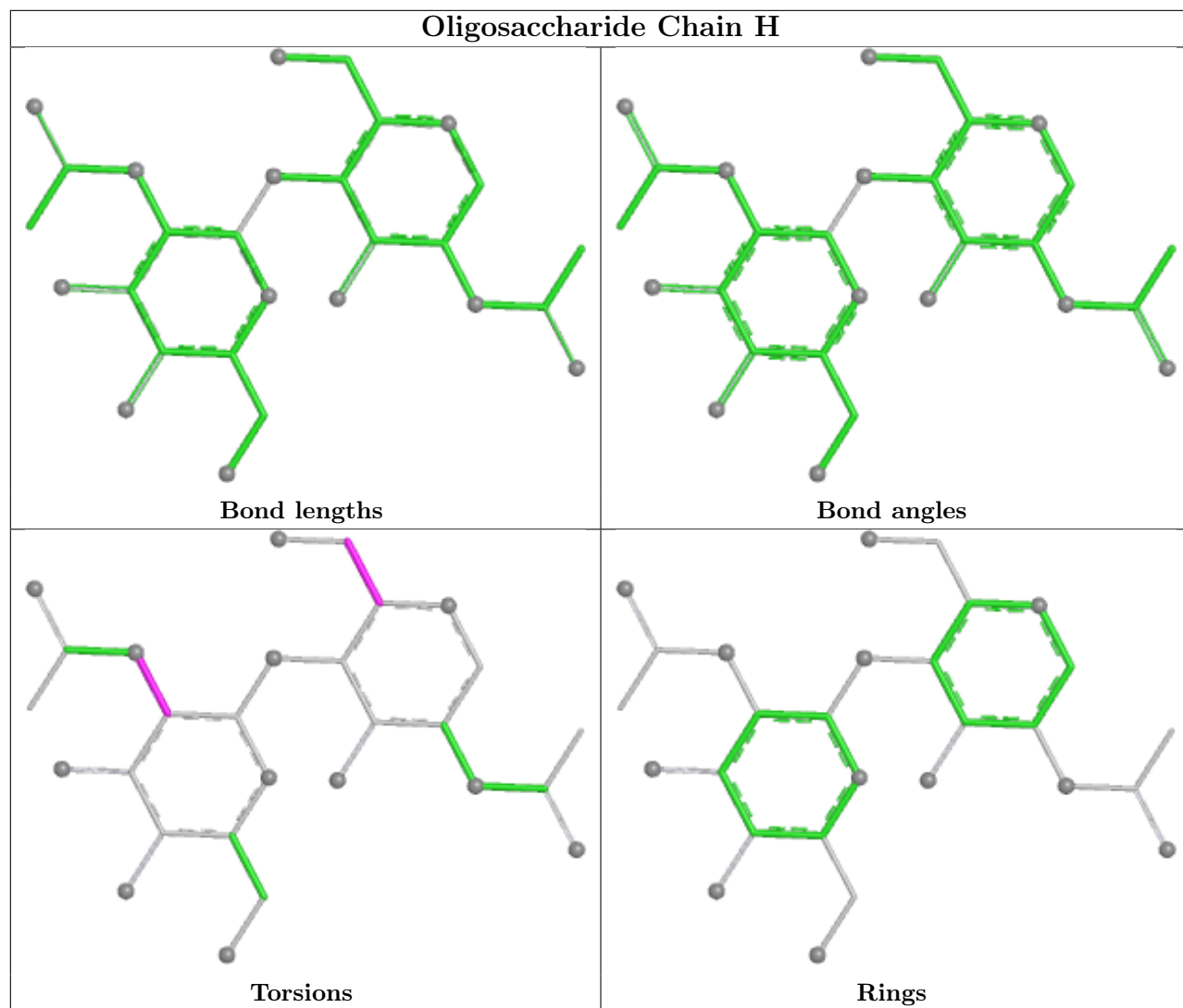
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

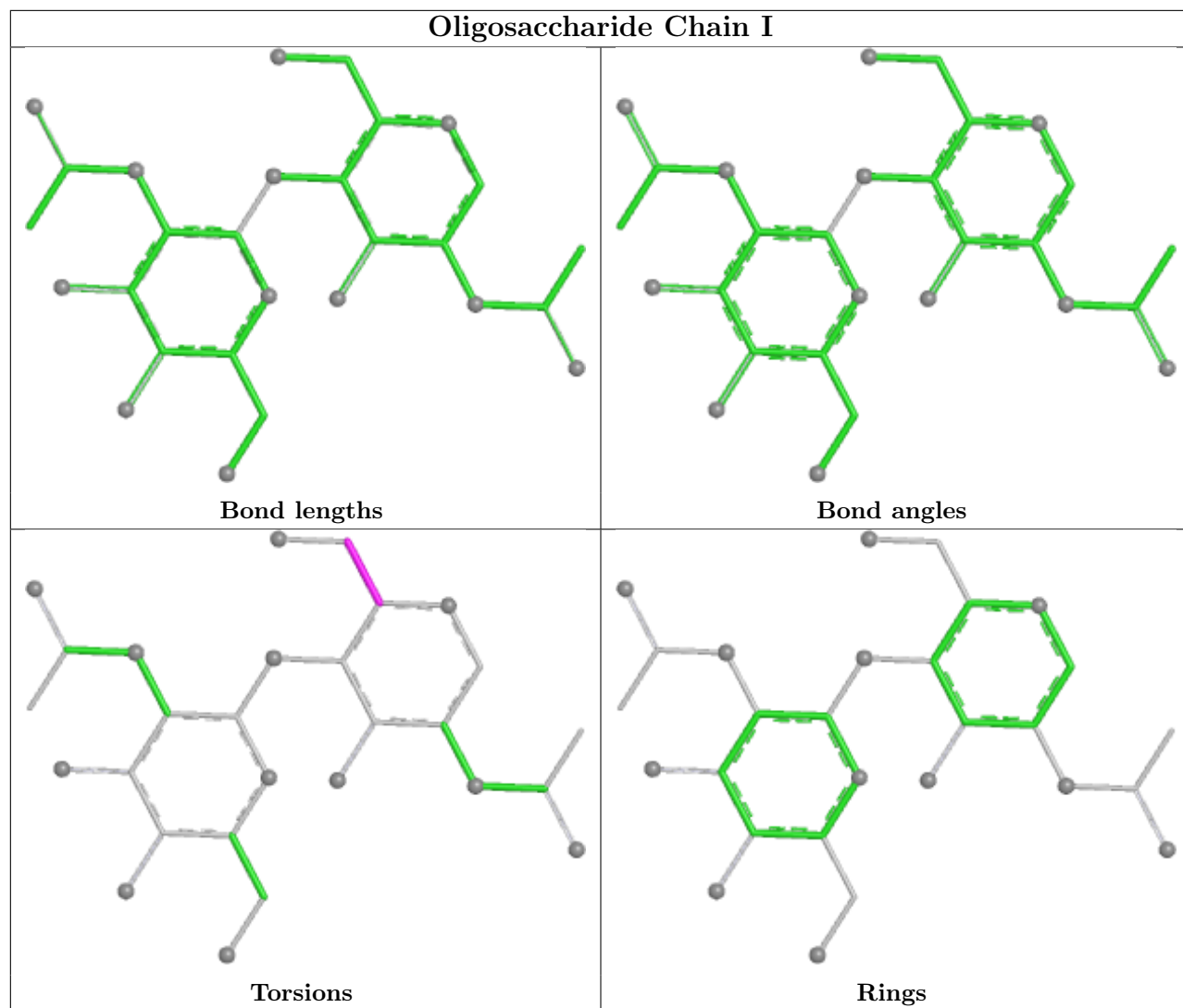


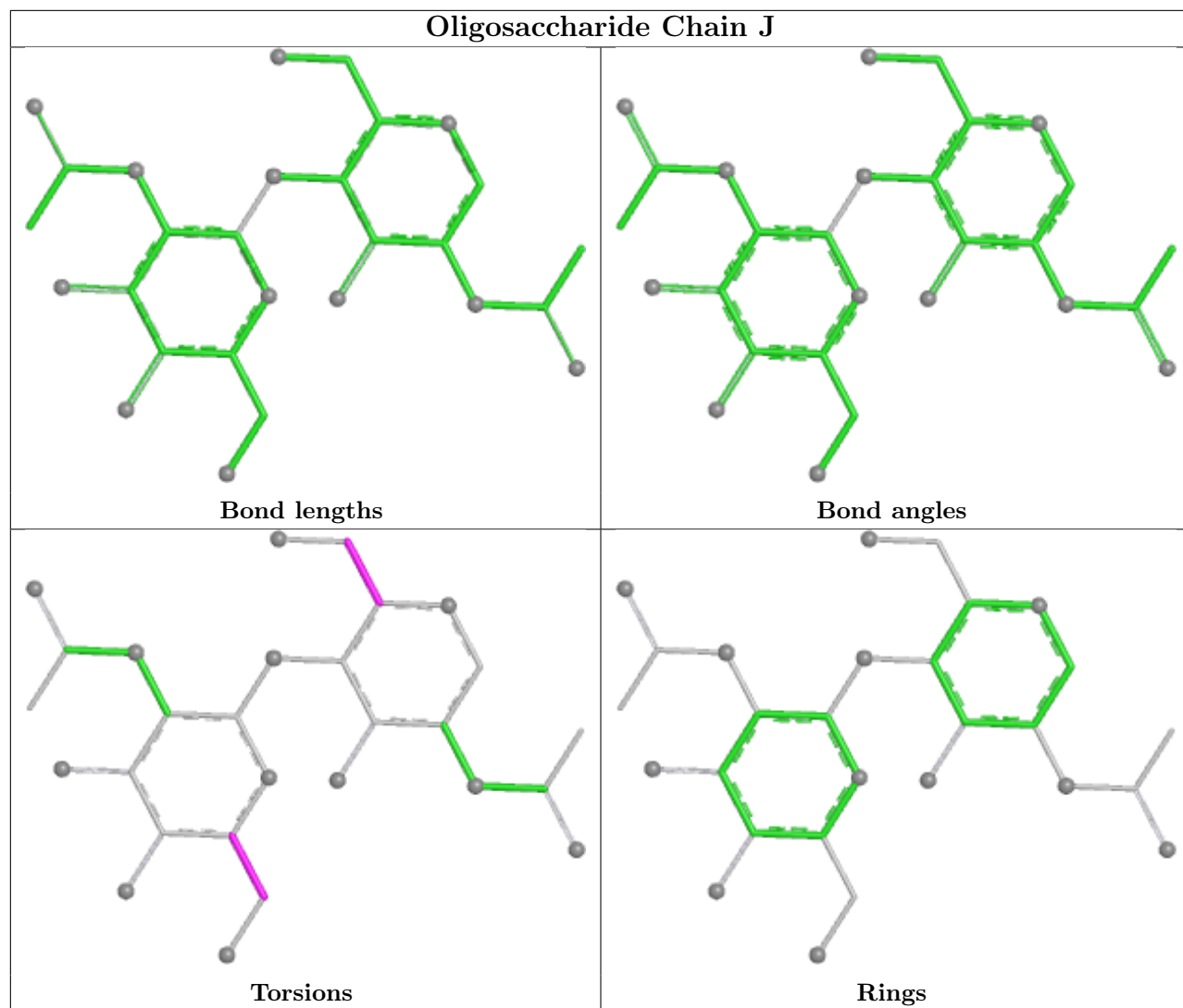


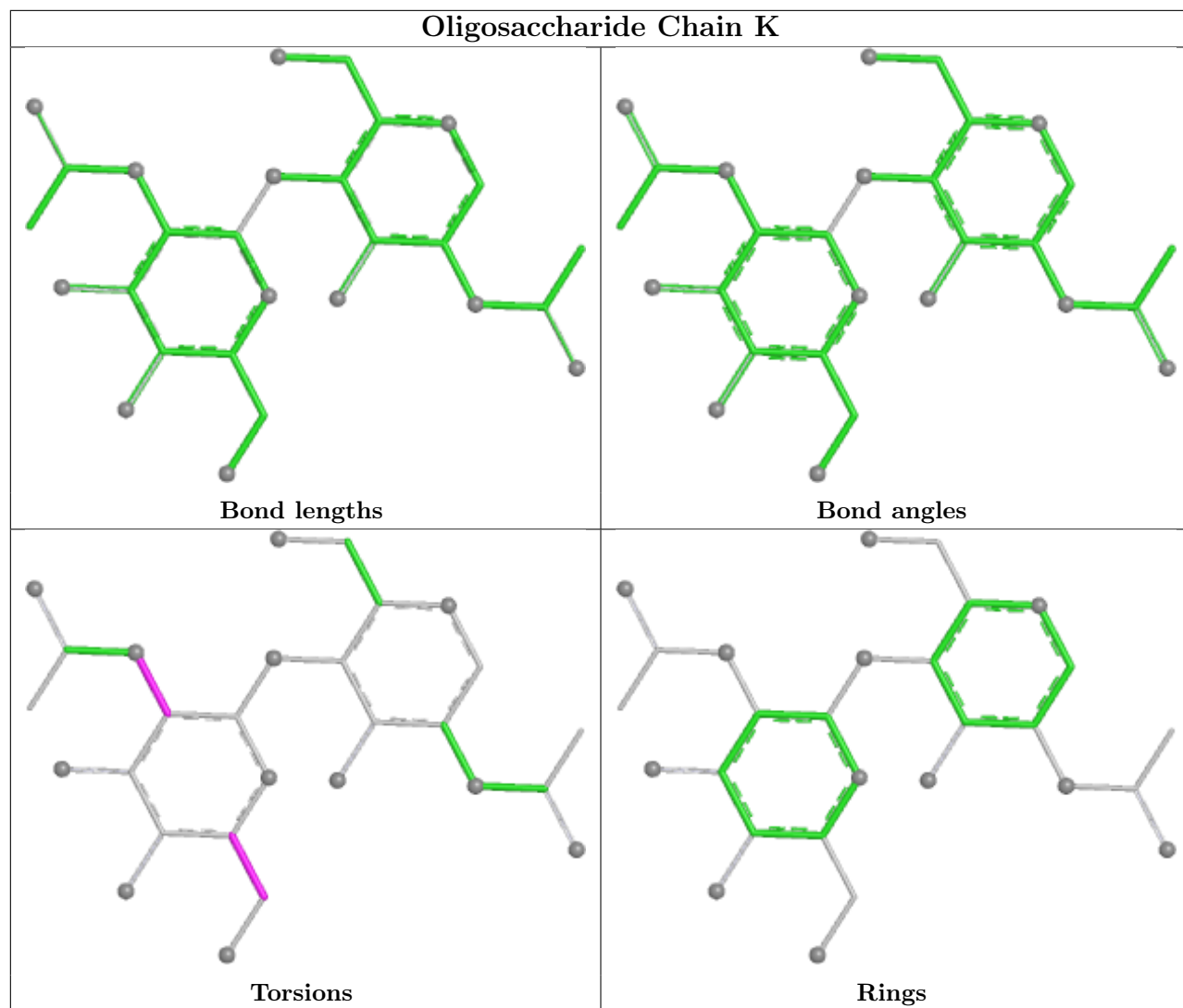


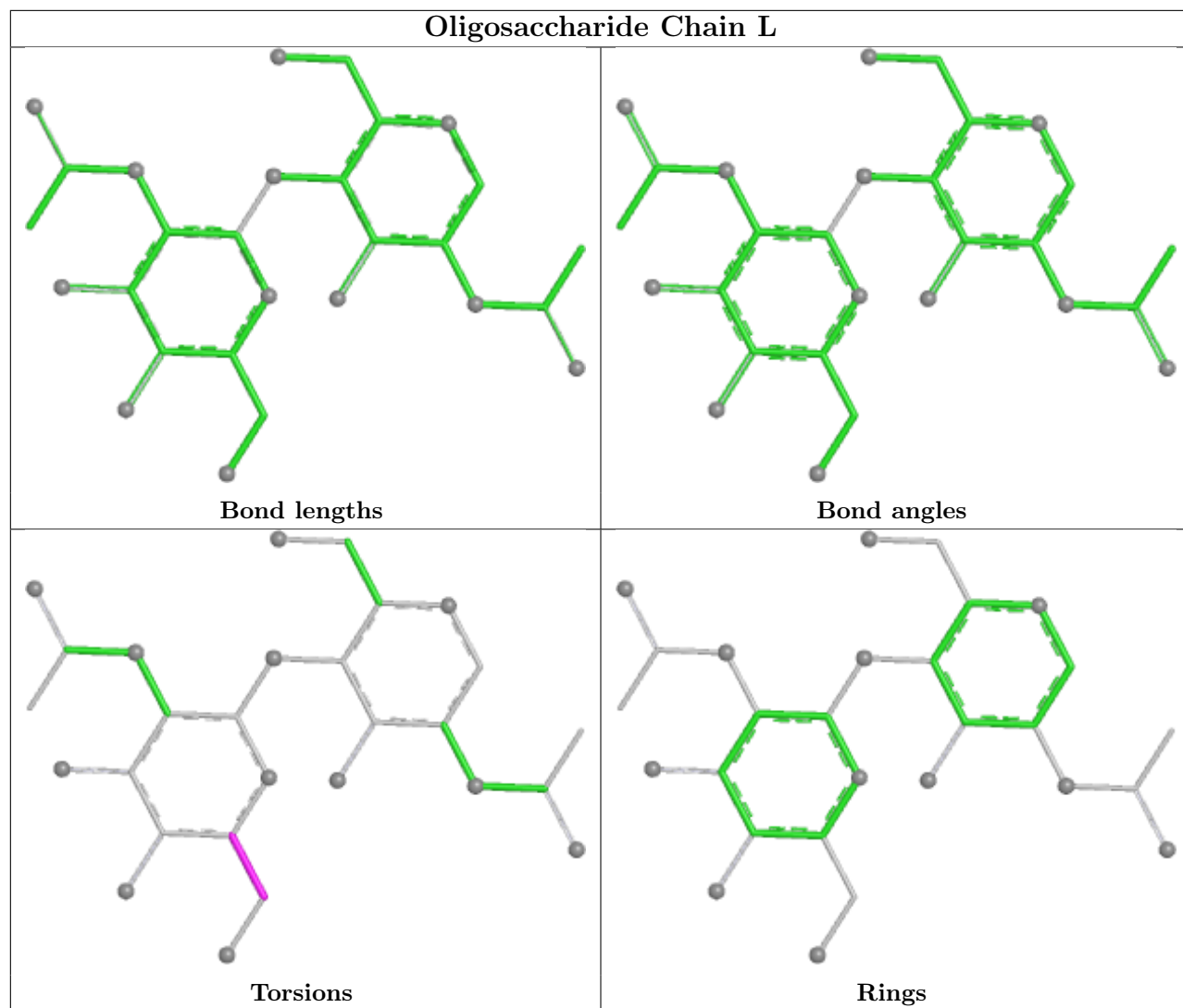


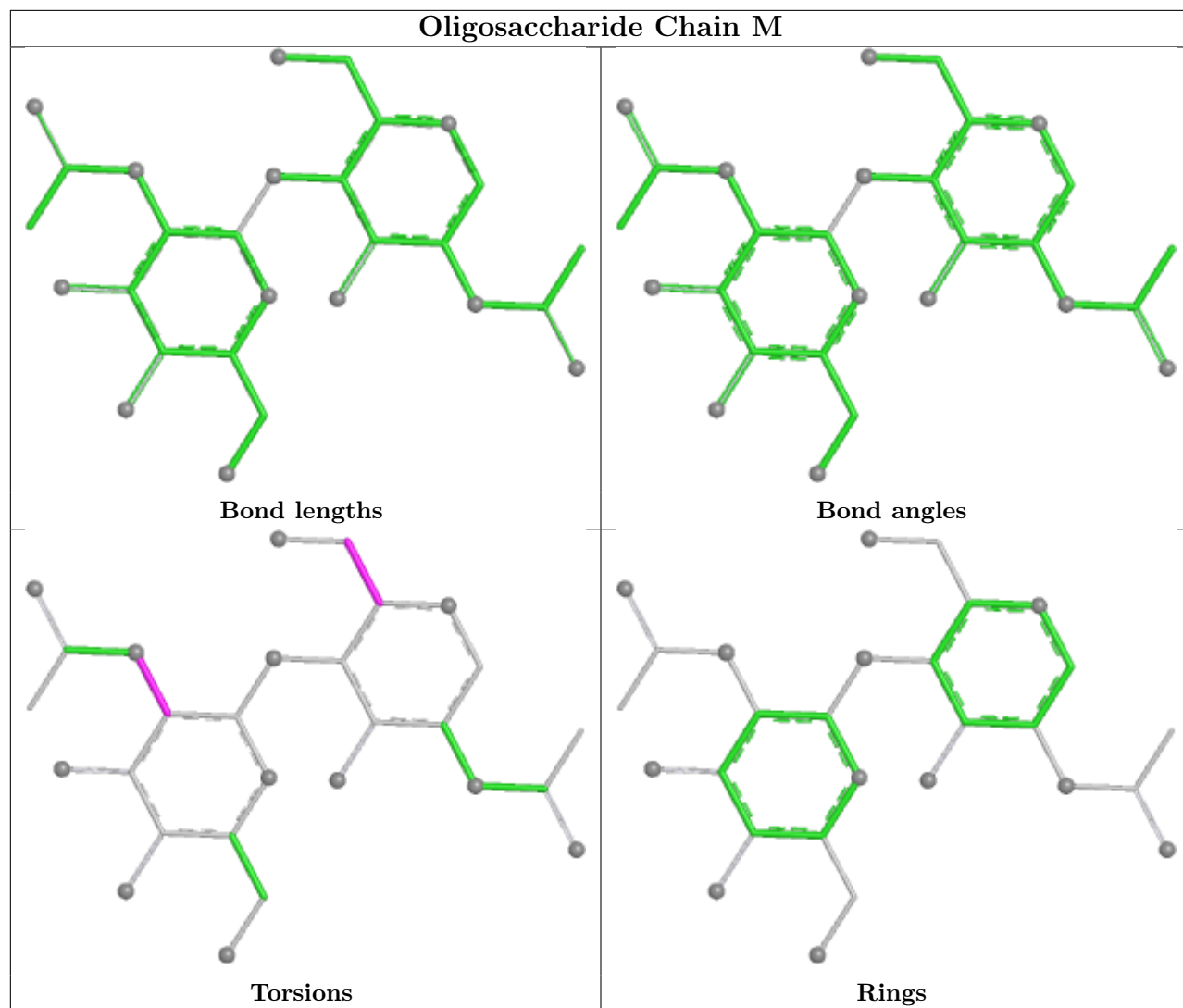


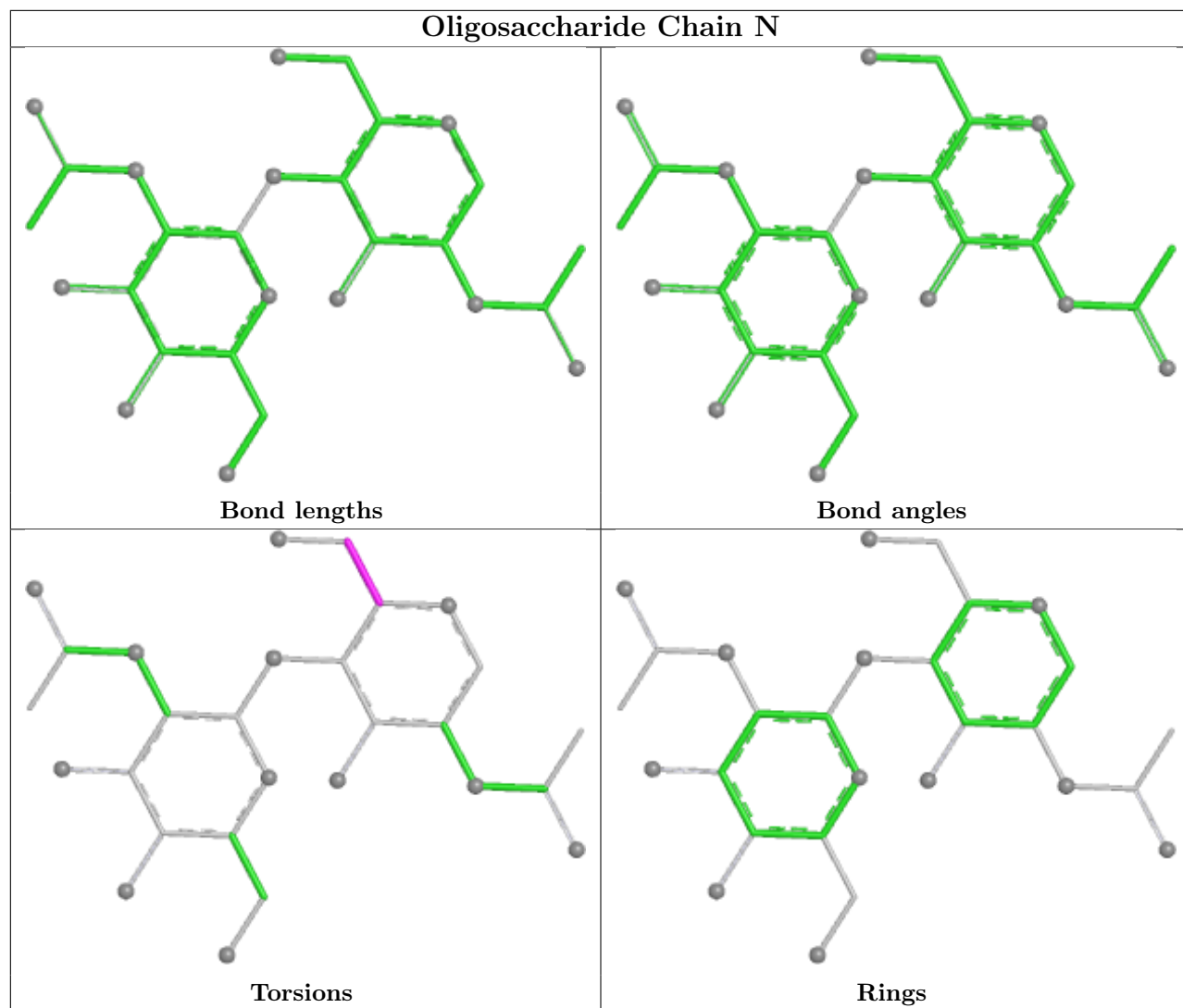


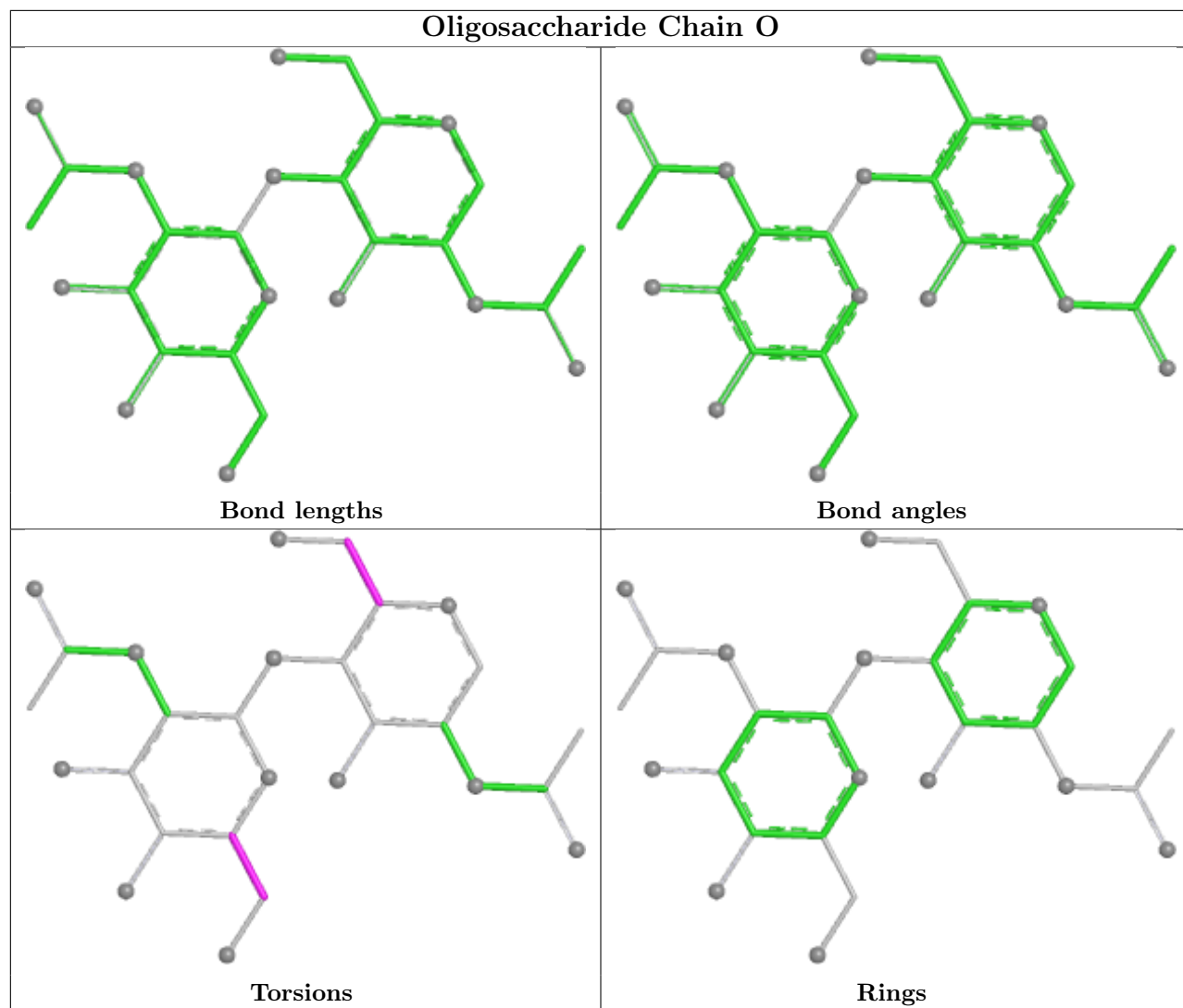


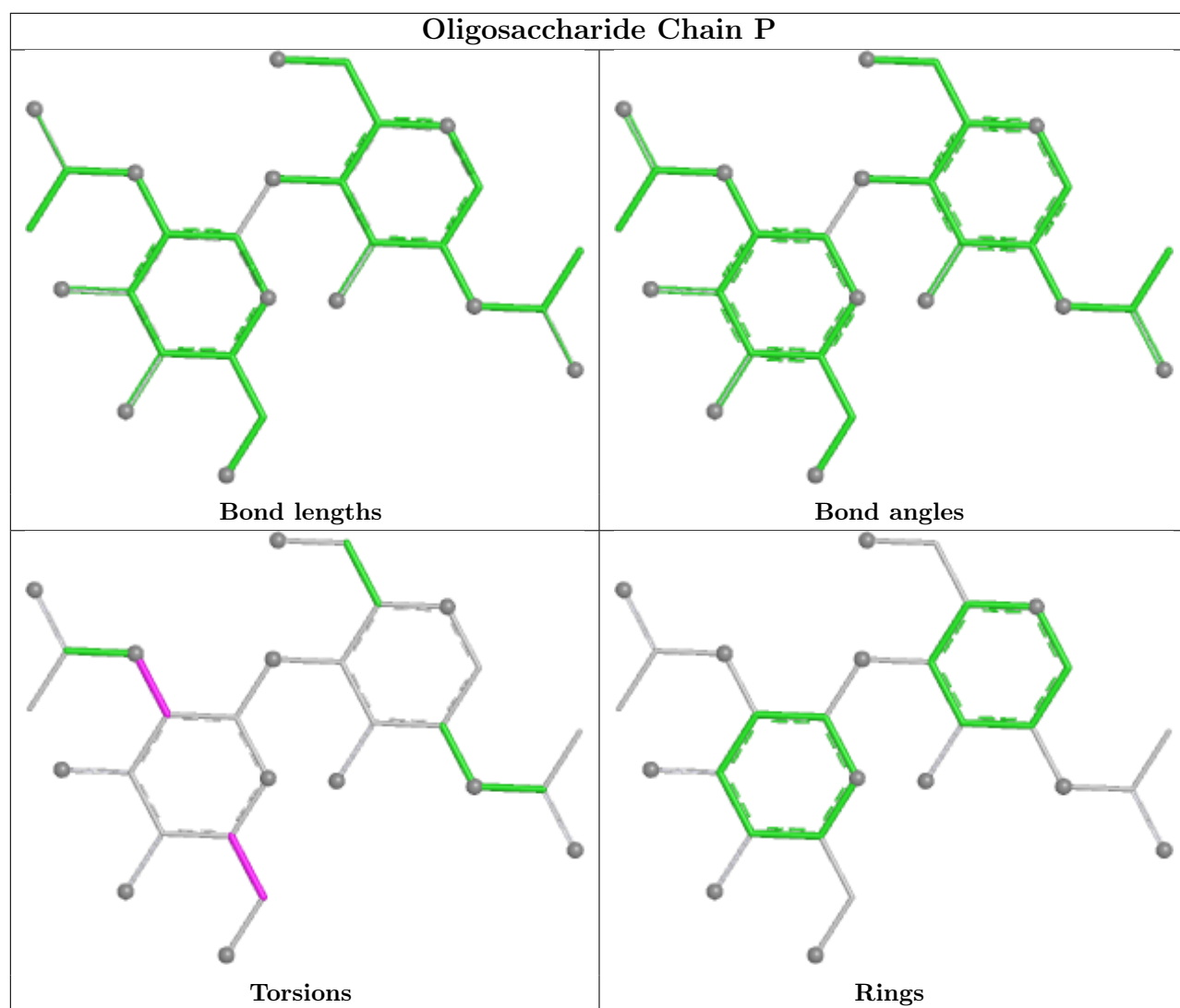


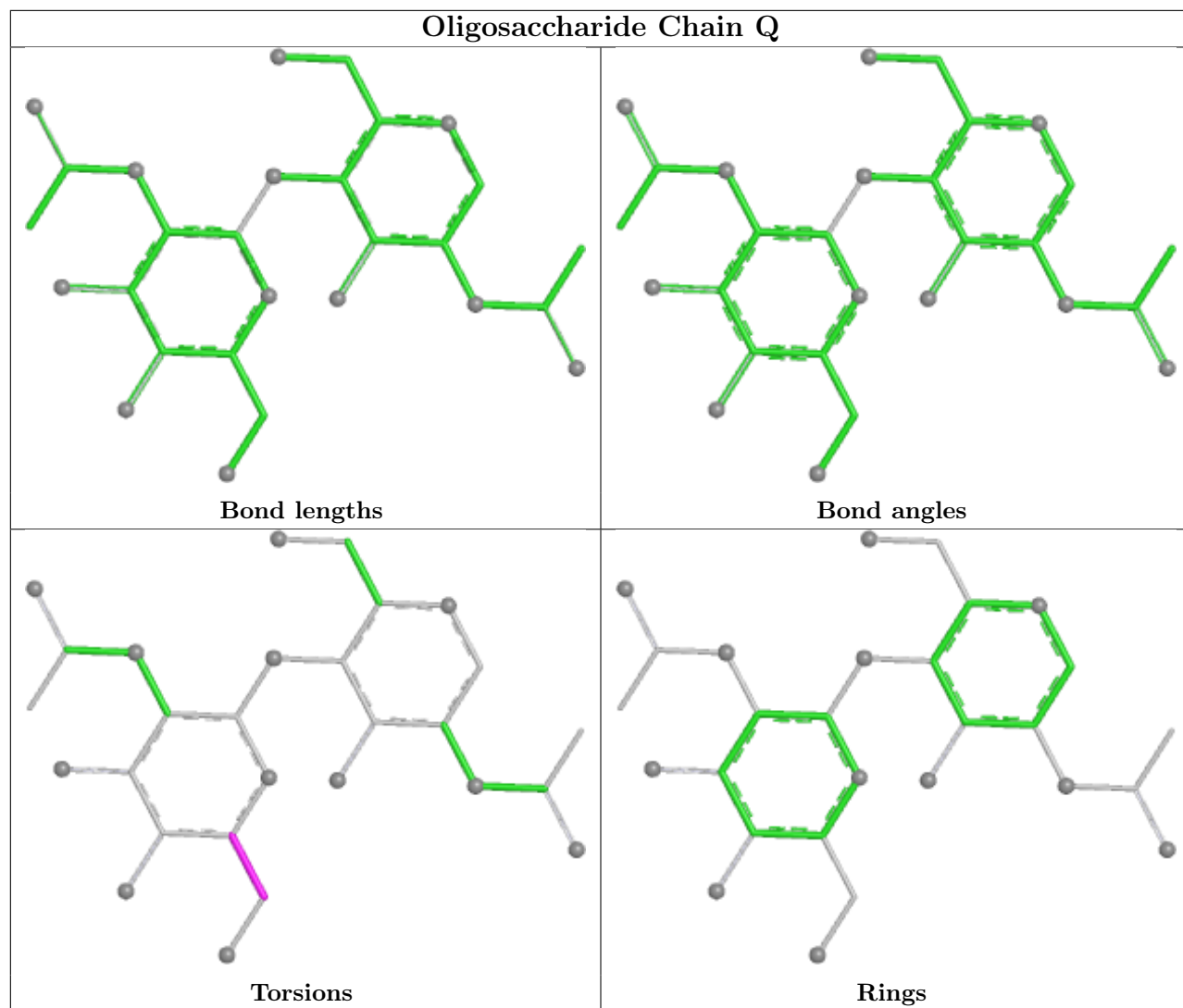


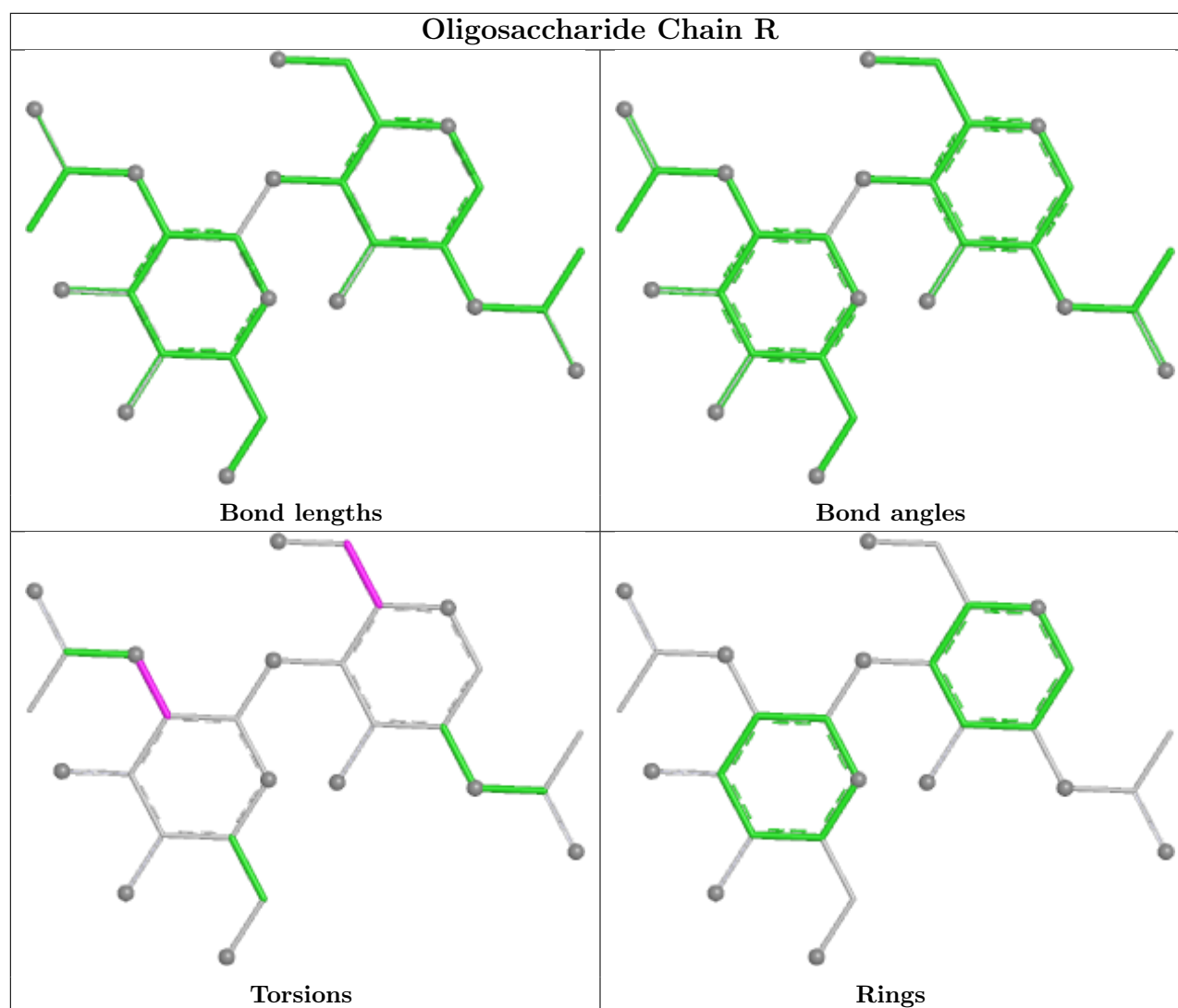












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	NAG	C	1308	1	14,14,15	0.37	0	17,19,21	0.52	0
3	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.57	0
3	NAG	B	1308	1	14,14,15	0.37	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1302	1	14,14,15	0.34	0	17,19,21	1.00	1 (5%)
3	NAG	A	1308	1	14,14,15	0.37	0	17,19,21	0.52	0
3	NAG	A	1321	1	14,14,15	0.32	0	17,19,21	0.73	0
3	NAG	C	1307	1	14,14,15	0.19	0	17,19,21	0.66	0
3	NAG	C	1305	1	14,14,15	0.48	0	17,19,21	0.59	0
3	NAG	B	1305	1	14,14,15	0.48	0	17,19,21	0.60	0
3	NAG	B	1301	1	14,14,15	0.75	0	17,19,21	0.59	0
3	NAG	B	1316	1	14,14,15	0.15	0	17,19,21	0.66	0
3	NAG	C	1301	1	14,14,15	0.74	0	17,19,21	0.59	0
3	NAG	C	1311	1	14,14,15	0.30	0	17,19,21	0.54	0
3	NAG	A	1307	1	14,14,15	0.19	0	17,19,21	0.65	0
3	NAG	B	1311	1	14,14,15	0.29	0	17,19,21	0.54	0
3	NAG	A	1316	1	14,14,15	0.15	0	17,19,21	0.66	0
3	NAG	B	1321	1	14,14,15	0.33	0	17,19,21	0.73	0
3	NAG	C	1321	1	14,14,15	0.32	0	17,19,21	0.73	0
3	NAG	A	1305	1	14,14,15	0.48	0	17,19,21	0.59	0
3	NAG	C	1309	1	14,14,15	0.33	0	17,19,21	1.65	2 (11%)
3	NAG	B	1306	1	14,14,15	0.58	1 (7%)	17,19,21	0.52	0
3	NAG	A	1302	1	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
3	NAG	B	1302	1	14,14,15	0.33	0	17,19,21	0.99	1 (5%)
3	NAG	B	1309	1	14,14,15	0.32	0	17,19,21	1.64	2 (11%)
3	NAG	A	1310	1	14,14,15	0.28	0	17,19,21	0.57	0
3	NAG	A	1301	1	14,14,15	0.73	0	17,19,21	0.59	0
3	NAG	B	1307	1	14,14,15	0.20	0	17,19,21	0.65	0
3	NAG	C	1316	1	14,14,15	0.14	0	17,19,21	0.66	0
3	NAG	C	1306	1	14,14,15	0.58	1 (7%)	17,19,21	0.52	0
3	NAG	A	1311	1	14,14,15	0.29	0	17,19,21	0.54	0
3	NAG	A	1309	1	14,14,15	0.32	0	17,19,21	1.65	2 (11%)
3	NAG	C	1310	1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	A	1306	1	14,14,15	0.58	1 (7%)	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	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1321	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1316	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1321	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1321	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	6/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	6/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1316	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	6/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1306	NAG	O5-C1	2.05	1.47	1.43
3	C	1306	NAG	O5-C1	2.05	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1306	NAG	O5-C1	2.04	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1309	NAG	C2-N2-C7	5.24	129.92	122.90
3	C	1309	NAG	C2-N2-C7	5.23	129.91	122.90
3	B	1309	NAG	C2-N2-C7	5.22	129.89	122.90
3	C	1302	NAG	C2-N2-C7	3.28	127.29	122.90
3	B	1302	NAG	C2-N2-C7	3.26	127.27	122.90
3	A	1302	NAG	C2-N2-C7	3.24	127.24	122.90
3	A	1309	NAG	C1-C2-N2	2.80	114.84	110.43
3	C	1309	NAG	C1-C2-N2	2.77	114.80	110.43
3	B	1309	NAG	C1-C2-N2	2.77	114.80	110.43

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1306	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1302	NAG	O5-C5-C6-O6
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	A	1309	NAG	C8-C7-N2-C2
3	A	1309	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	B	1309	NAG	C8-C7-N2-C2
3	B	1309	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	C	1309	NAG	C8-C7-N2-C2
3	C	1309	NAG	O7-C7-N2-C2
3	A	1316	NAG	O5-C5-C6-O6
3	B	1316	NAG	O5-C5-C6-O6
3	C	1316	NAG	O5-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	B	1316	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	A	1316	NAG	C4-C5-C6-O6
3	C	1316	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	A	1321	NAG	O5-C5-C6-O6
3	B	1321	NAG	O5-C5-C6-O6
3	C	1321	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1309	NAG	O5-C5-C6-O6
3	A	1305	NAG	C1-C2-N2-C7
3	A	1321	NAG	C1-C2-N2-C7
3	B	1305	NAG	C1-C2-N2-C7
3	B	1321	NAG	C1-C2-N2-C7
3	C	1305	NAG	C1-C2-N2-C7
3	C	1321	NAG	C1-C2-N2-C7
3	B	1311	NAG	O5-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	A	1305	NAG	C3-C2-N2-C7
3	A	1309	NAG	C3-C2-N2-C7
3	B	1305	NAG	C3-C2-N2-C7
3	B	1309	NAG	C3-C2-N2-C7
3	C	1305	NAG	C3-C2-N2-C7
3	C	1309	NAG	C3-C2-N2-C7
3	C	1302	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	A	1309	NAG	C1-C2-N2-C7
3	B	1309	NAG	C1-C2-N2-C7
3	C	1309	NAG	C1-C2-N2-C7
3	A	1321	NAG	C3-C2-N2-C7
3	B	1321	NAG	C3-C2-N2-C7
3	C	1321	NAG	C3-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1321	NAG	1	0
3	B	1301	NAG	1	0
3	C	1301	NAG	1	0
3	B	1321	NAG	1	0
3	C	1321	NAG	1	0
3	C	1309	NAG	1	0
3	B	1309	NAG	1	0
3	A	1301	NAG	1	0
3	A	1309	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.

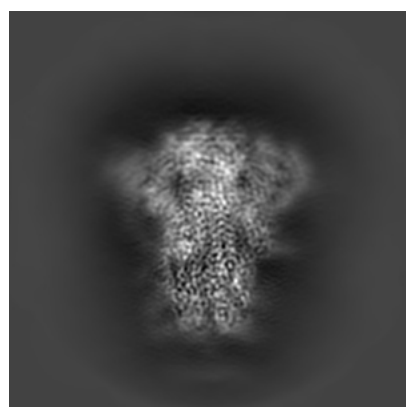
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11329. These allow visual inspection of the internal detail of the map and identification of artifacts.

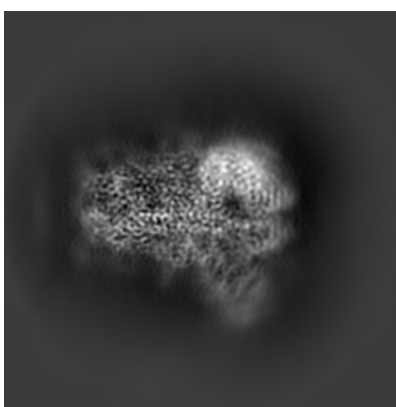
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

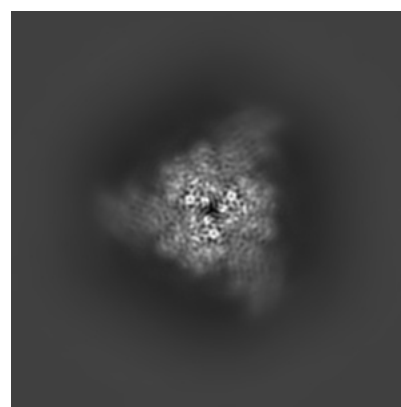
6.1.1 Primary map



X



Y

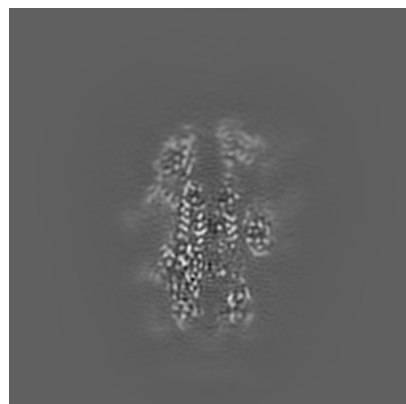


Z

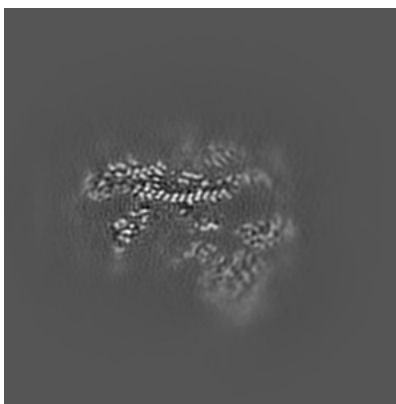
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

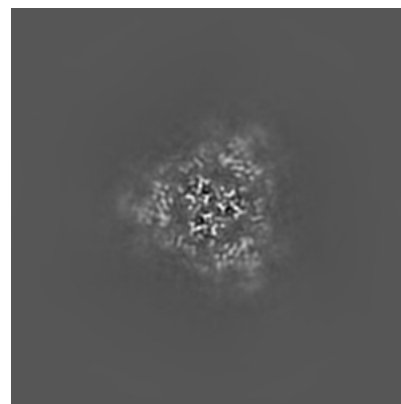
6.2.1 Primary map



X Index: 128



Y Index: 128

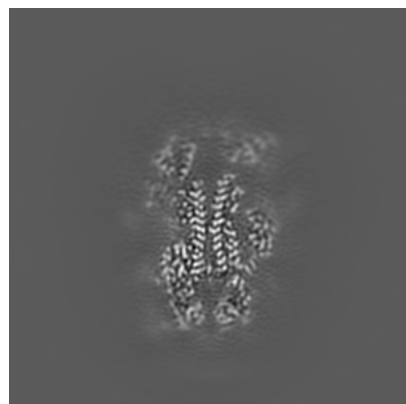


Z Index: 128

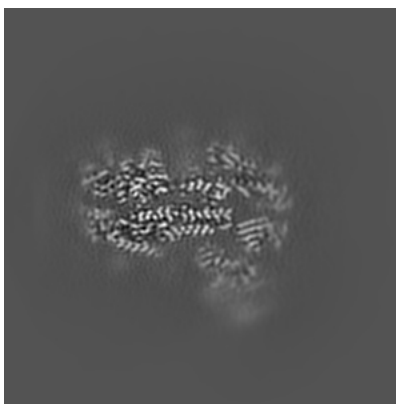
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

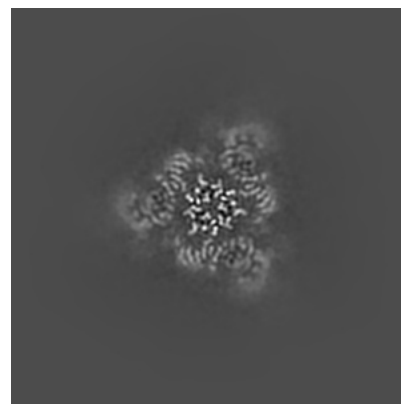
6.3.1 Primary map



X Index: 125



Y Index: 135

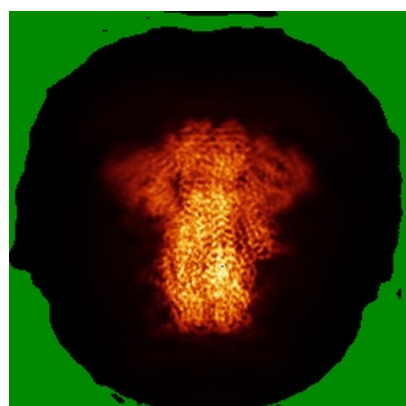


Z Index: 133

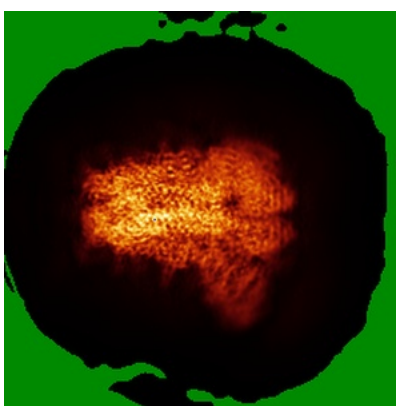
The images above show the largest variance slices of the map in three orthogonal directions.

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

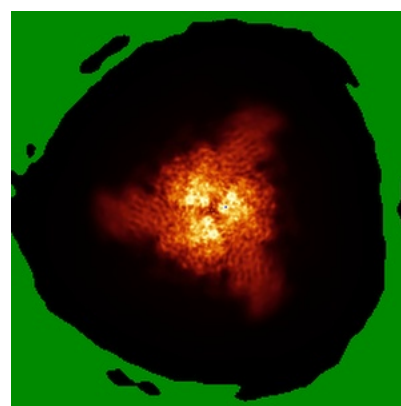
6.4.1 Primary map



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 0.0257. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

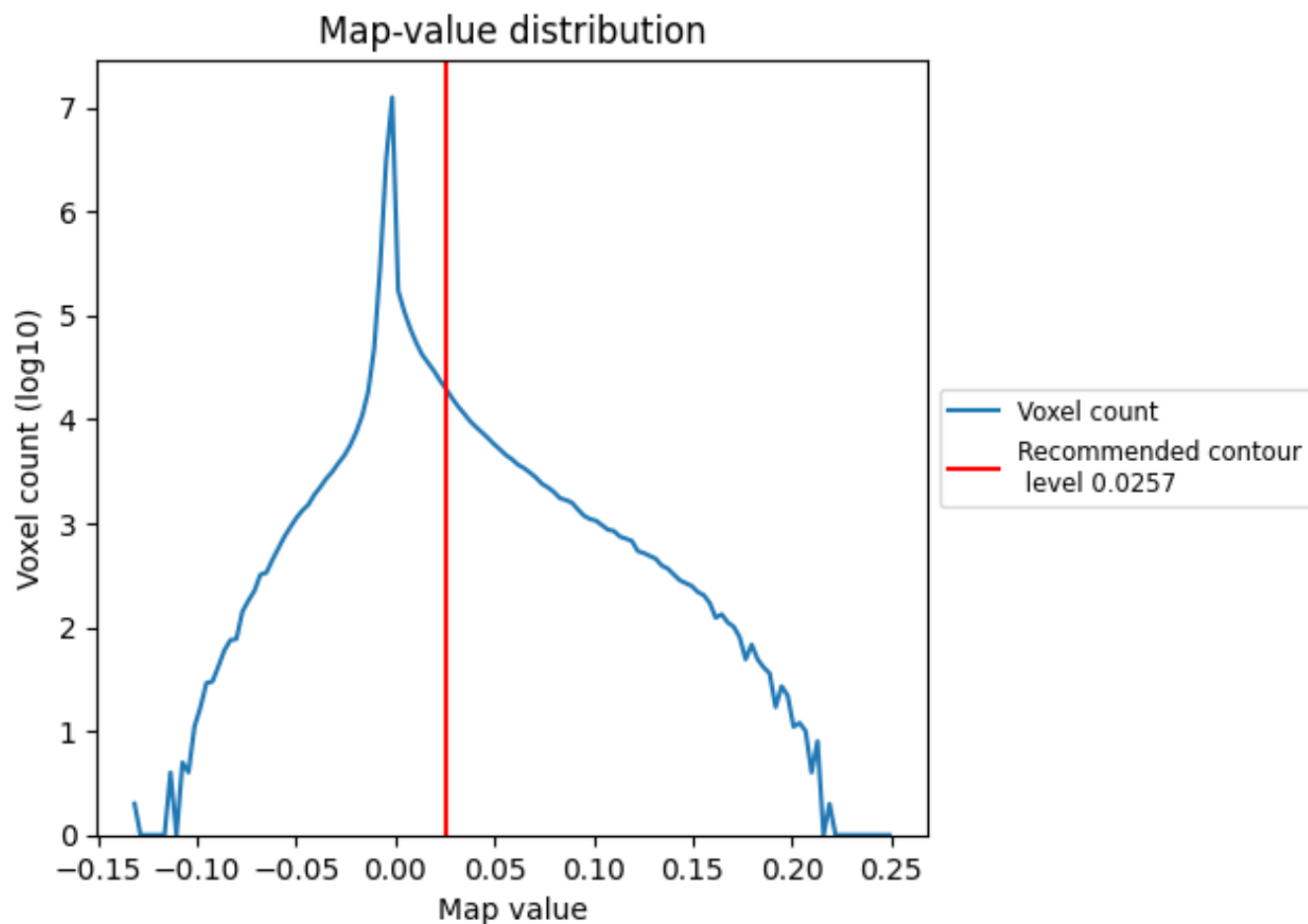
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

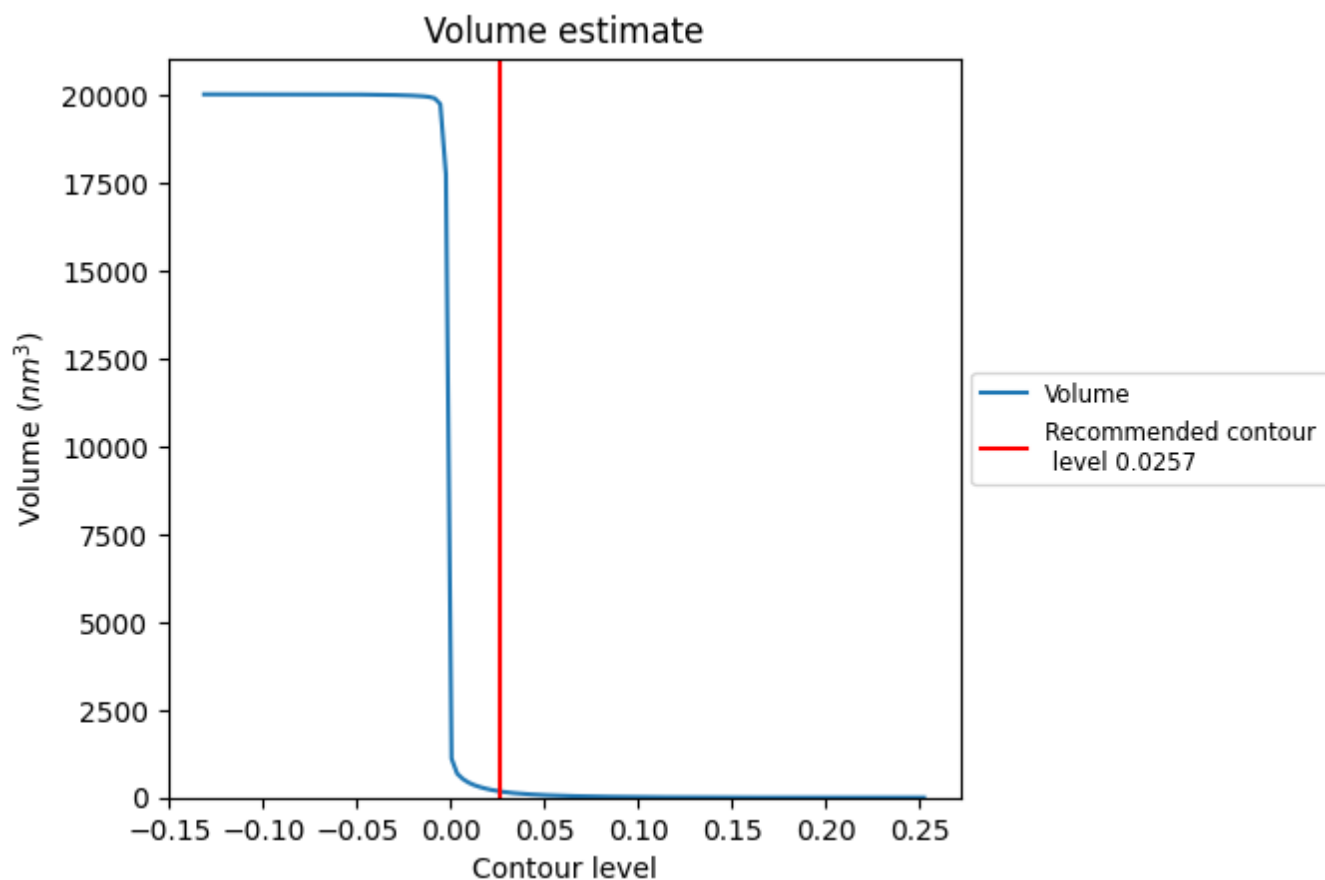
This section contains the results of statistical analysis of the map.

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.

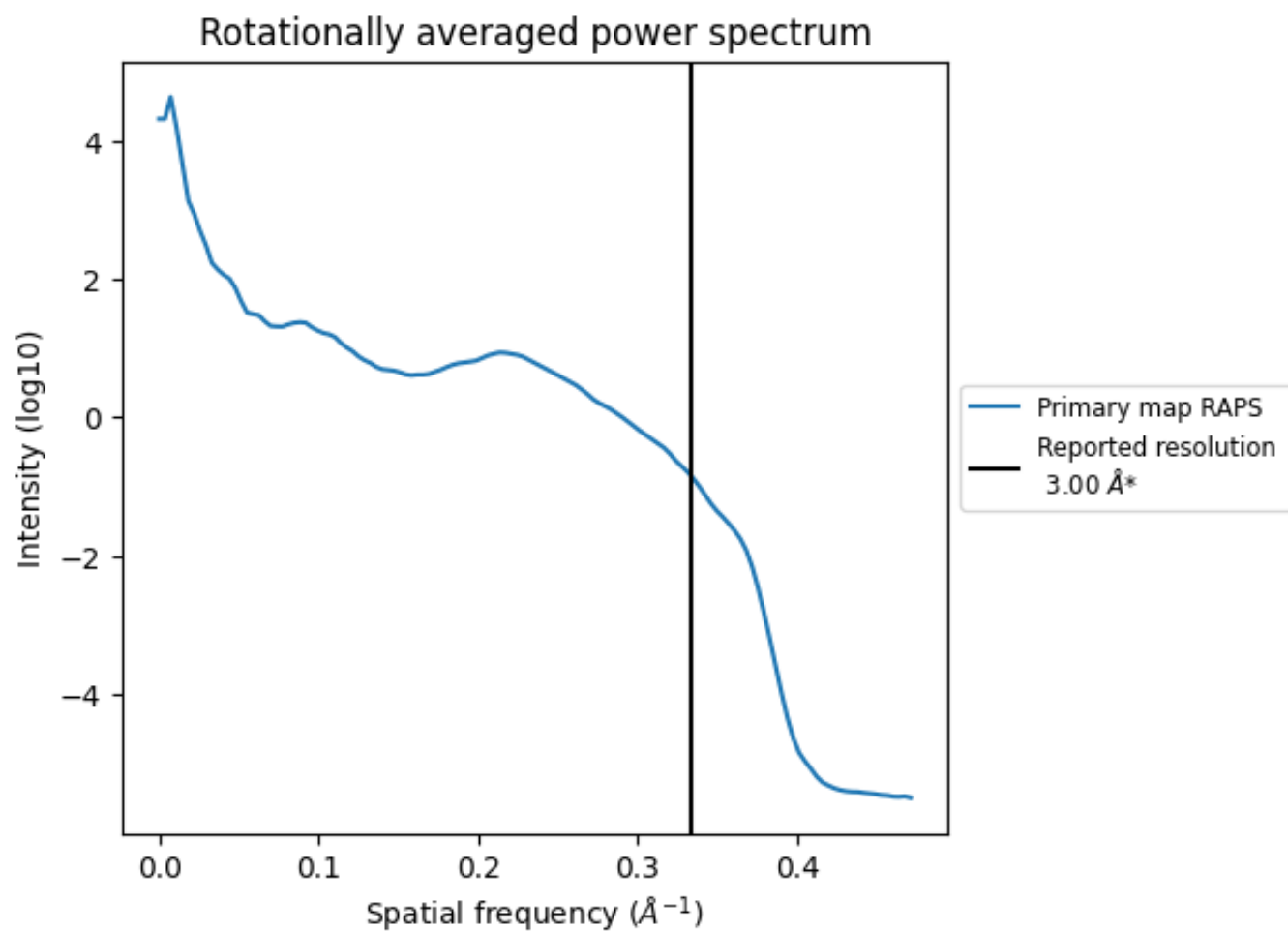
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm^3 ; this corresponds to an approximate mass of 163 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 0.333 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

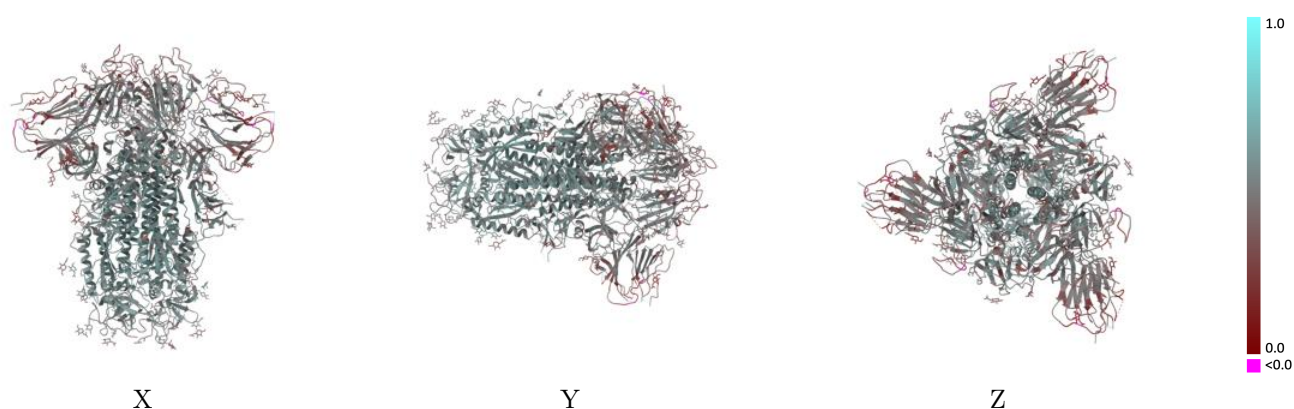
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11329 and PDB model 6ZOX. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

This section was not generated.

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

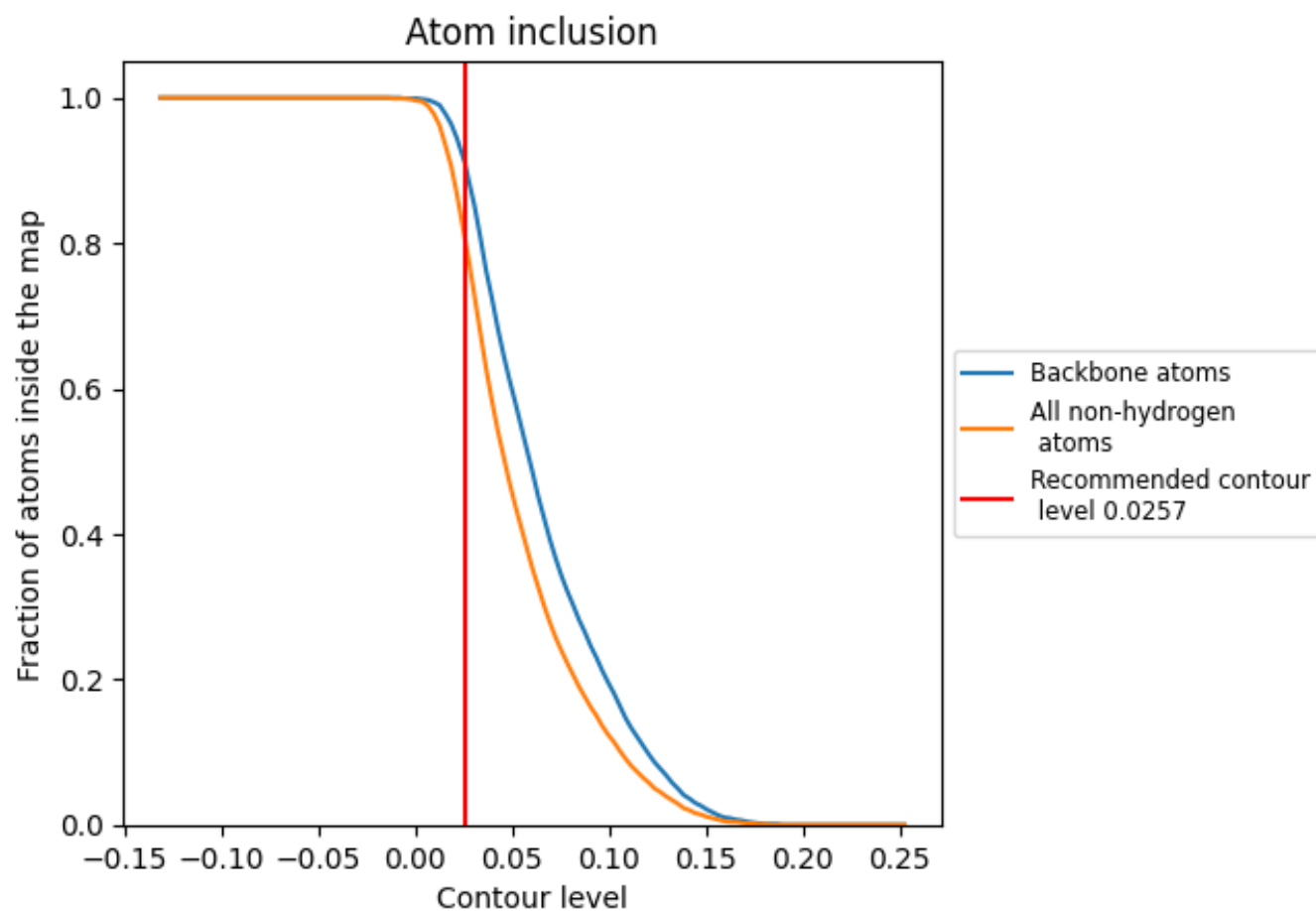


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 80% 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 (0.0257) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8040	 0.4770
A	 0.8090	 0.4790
B	 0.8080	 0.4780
C	 0.8090	 0.4780
D	 0.0360	 0.3760
E	 0.7860	 0.5190
F	 0.7860	 0.4300
G	 0.5000	 0.4380
H	 0.5000	 0.4340
I	 0.0710	 0.3850
J	 0.7500	 0.5100
K	 0.7860	 0.4300
L	 0.5000	 0.4430
M	 0.4640	 0.4350
N	 0.0710	 0.3770
O	 0.7860	 0.5130
P	 0.7860	 0.4310
Q	 0.5000	 0.4450
R	 0.5360	 0.4090

