



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 04:50 PM EDT

PDB ID : 6B7N
EMDB ID : EMD-7063
Title : Cryo-electron microscopy structure of porcine delta coronavirus spike protein in the pre-fusion state
Authors : Shang, J.; Zheng, Y.; Yang, Y.; Liu, C.; Geng, Q.; Tai, W.; Du, L.; Zhou, Y.; Zhang, W.; Li, F.
Deposited on : 2017-10-04
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

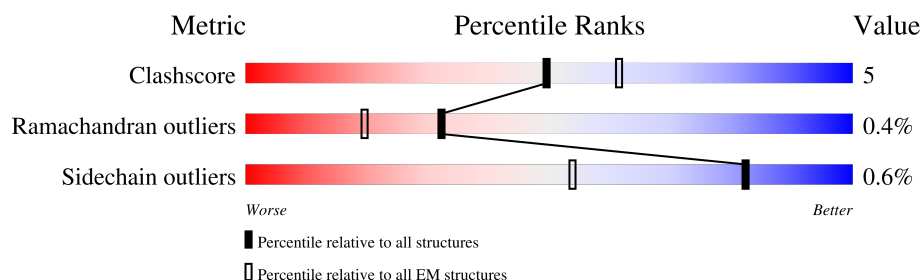
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



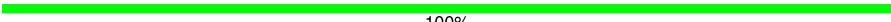


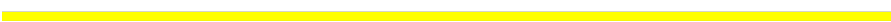






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1107	<div> <div>7%</div> <div>73%</div> <div>14%</div> <div>13%</div> </div>
1	B	1107	<div> <div>7%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
1	C	1107	<div> <div>6%</div> <div>73%</div> <div>14%</div> <div>13%</div> </div>
2	D	2	<div> <div>100%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>
2	H	2	<div> <div>50%</div> <div>100%</div> </div>
2	I	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	2	 100%
2	K	2	 50% 50%
2	M	2	 50% 100%
2	N	2	 100%
2	O	2	 50% 50%
2	P	2	 50% 50%
2	R	2	 50% 100%
3	G	3	 67% 33%
3	L	3	 33% 67%
3	Q	3	 33% 67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22215 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 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	966	Total	C	N	O	S	0	0
			7139	4521	1184	1394	40		
1	B	966	Total	C	N	O	S	0	0
			7139	4521	1184	1394	40		
1	C	966	Total	C	N	O	S	0	0
			7139	4521	1184	1394	40		

There are 333 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ILE	VAL	conflict	UNP A0A075E3D7
A	553	ILE	THR	conflict	UNP A0A075E3D7
A	583	THR	ALA	conflict	UNP A0A075E3D7
A	642	LYS	GLN	conflict	UNP A0A075E3D7
A	1018	ASP	-	expression tag	UNP A0A075E3D7
A	1019	VAL	-	expression tag	UNP A0A075E3D7
A	1020	ASN	-	expression tag	UNP A0A075E3D7
A	1021	GLN	-	expression tag	UNP A0A075E3D7
A	1022	THR	-	expression tag	UNP A0A075E3D7
A	1023	VAL	-	expression tag	UNP A0A075E3D7
A	1024	SER	-	expression tag	UNP A0A075E3D7
A	1025	ASP	-	expression tag	UNP A0A075E3D7
A	1026	ILE	-	expression tag	UNP A0A075E3D7
A	1027	ILE	-	expression tag	UNP A0A075E3D7
A	1028	ASP	-	expression tag	UNP A0A075E3D7
A	1029	ASN	-	expression tag	UNP A0A075E3D7
A	1030	LEU	-	expression tag	UNP A0A075E3D7
A	1031	PRO	-	expression tag	UNP A0A075E3D7
A	1032	THR	-	expression tag	UNP A0A075E3D7
A	1033	ALA	-	expression tag	UNP A0A075E3D7
A	1034	THR	-	expression tag	UNP A0A075E3D7
A	1035	PRO	-	expression tag	UNP A0A075E3D7
A	1036	PRO	-	expression tag	UNP A0A075E3D7
A	1037	GLN	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1038	TRP	-	expression tag	UNP A0A075E3D7
A	1039	ASP	-	expression tag	UNP A0A075E3D7
A	1040	VAL	-	expression tag	UNP A0A075E3D7
A	1041	GLY	-	expression tag	UNP A0A075E3D7
A	1042	ILE	-	expression tag	UNP A0A075E3D7
A	1043	TYR	-	expression tag	UNP A0A075E3D7
A	1044	ASN	-	expression tag	UNP A0A075E3D7
A	1045	ASN	-	expression tag	UNP A0A075E3D7
A	1046	THR	-	expression tag	UNP A0A075E3D7
A	1047	ILE	-	expression tag	UNP A0A075E3D7
A	1048	LEU	-	expression tag	UNP A0A075E3D7
A	1049	ASN	-	expression tag	UNP A0A075E3D7
A	1050	LEU	-	expression tag	UNP A0A075E3D7
A	1051	THR	-	expression tag	UNP A0A075E3D7
A	1052	VAL	-	expression tag	UNP A0A075E3D7
A	1053	GLU	-	expression tag	UNP A0A075E3D7
A	1054	ILE	-	expression tag	UNP A0A075E3D7
A	1055	ASN	-	expression tag	UNP A0A075E3D7
A	1056	ASP	-	expression tag	UNP A0A075E3D7
A	1057	LEU	-	expression tag	UNP A0A075E3D7
A	1058	GLN	-	expression tag	UNP A0A075E3D7
A	1059	GLU	-	expression tag	UNP A0A075E3D7
A	1060	ARG	-	expression tag	UNP A0A075E3D7
A	1061	SER	-	expression tag	UNP A0A075E3D7
A	1062	LYS	-	expression tag	UNP A0A075E3D7
A	1063	ASN	-	expression tag	UNP A0A075E3D7
A	1064	LEU	-	expression tag	UNP A0A075E3D7
A	1065	SER	-	expression tag	UNP A0A075E3D7
A	1066	GLN	-	expression tag	UNP A0A075E3D7
A	1067	ILE	-	expression tag	UNP A0A075E3D7
A	1068	ALA	-	expression tag	UNP A0A075E3D7
A	1069	ASP	-	expression tag	UNP A0A075E3D7
A	1070	ARG	-	expression tag	UNP A0A075E3D7
A	1071	LEU	-	expression tag	UNP A0A075E3D7
A	1072	GLN	-	expression tag	UNP A0A075E3D7
A	1073	ASN	-	expression tag	UNP A0A075E3D7
A	1074	TYR	-	expression tag	UNP A0A075E3D7
A	1075	ILE	-	expression tag	UNP A0A075E3D7
A	1076	ASP	-	expression tag	UNP A0A075E3D7
A	1077	ASN	-	expression tag	UNP A0A075E3D7
A	1078	VAL	-	expression tag	UNP A0A075E3D7
A	1079	ASP	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1080	ILE	-	expression tag	UNP A0A075E3D7
A	1081	LYS	-	expression tag	UNP A0A075E3D7
A	1082	GLN	-	expression tag	UNP A0A075E3D7
A	1083	ILE	-	expression tag	UNP A0A075E3D7
A	1084	GLU	-	expression tag	UNP A0A075E3D7
A	1085	ASP	-	expression tag	UNP A0A075E3D7
A	1086	LYS	-	expression tag	UNP A0A075E3D7
A	1087	ILE	-	expression tag	UNP A0A075E3D7
A	1088	GLU	-	expression tag	UNP A0A075E3D7
A	1089	GLU	-	expression tag	UNP A0A075E3D7
A	1090	ILE	-	expression tag	UNP A0A075E3D7
A	1091	LEU	-	expression tag	UNP A0A075E3D7
A	1092	SER	-	expression tag	UNP A0A075E3D7
A	1093	LYS	-	expression tag	UNP A0A075E3D7
A	1094	ILE	-	expression tag	UNP A0A075E3D7
A	1095	TYR	-	expression tag	UNP A0A075E3D7
A	1096	HIS	-	expression tag	UNP A0A075E3D7
A	1097	ILE	-	expression tag	UNP A0A075E3D7
A	1098	GLU	-	expression tag	UNP A0A075E3D7
A	1099	ASN	-	expression tag	UNP A0A075E3D7
A	1100	GLU	-	expression tag	UNP A0A075E3D7
A	1101	ILE	-	expression tag	UNP A0A075E3D7
A	1102	ALA	-	expression tag	UNP A0A075E3D7
A	1103	ARG	-	expression tag	UNP A0A075E3D7
A	1104	ILE	-	expression tag	UNP A0A075E3D7
A	1105	LYS	-	expression tag	UNP A0A075E3D7
A	1106	LYS	-	expression tag	UNP A0A075E3D7
A	1107	LEU	-	expression tag	UNP A0A075E3D7
A	1108	ILE	-	expression tag	UNP A0A075E3D7
A	1109	GLY	-	expression tag	UNP A0A075E3D7
A	1110	GLU	-	expression tag	UNP A0A075E3D7
A	1111	ILE	-	expression tag	UNP A0A075E3D7
A	1112	GLY	-	expression tag	UNP A0A075E3D7
A	1113	GLY	-	expression tag	UNP A0A075E3D7
A	1114	GLY	-	expression tag	UNP A0A075E3D7
A	1115	GLY	-	expression tag	UNP A0A075E3D7
A	1116	SER	-	expression tag	UNP A0A075E3D7
A	1117	HIS	-	expression tag	UNP A0A075E3D7
A	1118	HIS	-	expression tag	UNP A0A075E3D7
A	1119	HIS	-	expression tag	UNP A0A075E3D7
A	1120	HIS	-	expression tag	UNP A0A075E3D7
A	1121	HIS	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1122	HIS	-	expression tag	UNP A0A075E3D7
A	1123	HIS	-	expression tag	UNP A0A075E3D7
A	1124	HIS	-	expression tag	UNP A0A075E3D7
B	111	ILE	VAL	conflict	UNP A0A075E3D7
B	553	ILE	THR	conflict	UNP A0A075E3D7
B	583	THR	ALA	conflict	UNP A0A075E3D7
B	642	LYS	GLN	conflict	UNP A0A075E3D7
B	1018	ASP	-	expression tag	UNP A0A075E3D7
B	1019	VAL	-	expression tag	UNP A0A075E3D7
B	1020	ASN	-	expression tag	UNP A0A075E3D7
B	1021	GLN	-	expression tag	UNP A0A075E3D7
B	1022	THR	-	expression tag	UNP A0A075E3D7
B	1023	VAL	-	expression tag	UNP A0A075E3D7
B	1024	SER	-	expression tag	UNP A0A075E3D7
B	1025	ASP	-	expression tag	UNP A0A075E3D7
B	1026	ILE	-	expression tag	UNP A0A075E3D7
B	1027	ILE	-	expression tag	UNP A0A075E3D7
B	1028	ASP	-	expression tag	UNP A0A075E3D7
B	1029	ASN	-	expression tag	UNP A0A075E3D7
B	1030	LEU	-	expression tag	UNP A0A075E3D7
B	1031	PRO	-	expression tag	UNP A0A075E3D7
B	1032	THR	-	expression tag	UNP A0A075E3D7
B	1033	ALA	-	expression tag	UNP A0A075E3D7
B	1034	THR	-	expression tag	UNP A0A075E3D7
B	1035	PRO	-	expression tag	UNP A0A075E3D7
B	1036	PRO	-	expression tag	UNP A0A075E3D7
B	1037	GLN	-	expression tag	UNP A0A075E3D7
B	1038	TRP	-	expression tag	UNP A0A075E3D7
B	1039	ASP	-	expression tag	UNP A0A075E3D7
B	1040	VAL	-	expression tag	UNP A0A075E3D7
B	1041	GLY	-	expression tag	UNP A0A075E3D7
B	1042	ILE	-	expression tag	UNP A0A075E3D7
B	1043	TYR	-	expression tag	UNP A0A075E3D7
B	1044	ASN	-	expression tag	UNP A0A075E3D7
B	1045	ASN	-	expression tag	UNP A0A075E3D7
B	1046	THR	-	expression tag	UNP A0A075E3D7
B	1047	ILE	-	expression tag	UNP A0A075E3D7
B	1048	LEU	-	expression tag	UNP A0A075E3D7
B	1049	ASN	-	expression tag	UNP A0A075E3D7
B	1050	LEU	-	expression tag	UNP A0A075E3D7
B	1051	THR	-	expression tag	UNP A0A075E3D7
B	1052	VAL	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1053	GLU	-	expression tag	UNP A0A075E3D7
B	1054	ILE	-	expression tag	UNP A0A075E3D7
B	1055	ASN	-	expression tag	UNP A0A075E3D7
B	1056	ASP	-	expression tag	UNP A0A075E3D7
B	1057	LEU	-	expression tag	UNP A0A075E3D7
B	1058	GLN	-	expression tag	UNP A0A075E3D7
B	1059	GLU	-	expression tag	UNP A0A075E3D7
B	1060	ARG	-	expression tag	UNP A0A075E3D7
B	1061	SER	-	expression tag	UNP A0A075E3D7
B	1062	LYS	-	expression tag	UNP A0A075E3D7
B	1063	ASN	-	expression tag	UNP A0A075E3D7
B	1064	LEU	-	expression tag	UNP A0A075E3D7
B	1065	SER	-	expression tag	UNP A0A075E3D7
B	1066	GLN	-	expression tag	UNP A0A075E3D7
B	1067	ILE	-	expression tag	UNP A0A075E3D7
B	1068	ALA	-	expression tag	UNP A0A075E3D7
B	1069	ASP	-	expression tag	UNP A0A075E3D7
B	1070	ARG	-	expression tag	UNP A0A075E3D7
B	1071	LEU	-	expression tag	UNP A0A075E3D7
B	1072	GLN	-	expression tag	UNP A0A075E3D7
B	1073	ASN	-	expression tag	UNP A0A075E3D7
B	1074	TYR	-	expression tag	UNP A0A075E3D7
B	1075	ILE	-	expression tag	UNP A0A075E3D7
B	1076	ASP	-	expression tag	UNP A0A075E3D7
B	1077	ASN	-	expression tag	UNP A0A075E3D7
B	1078	VAL	-	expression tag	UNP A0A075E3D7
B	1079	ASP	-	expression tag	UNP A0A075E3D7
B	1080	ILE	-	expression tag	UNP A0A075E3D7
B	1081	LYS	-	expression tag	UNP A0A075E3D7
B	1082	GLN	-	expression tag	UNP A0A075E3D7
B	1083	ILE	-	expression tag	UNP A0A075E3D7
B	1084	GLU	-	expression tag	UNP A0A075E3D7
B	1085	ASP	-	expression tag	UNP A0A075E3D7
B	1086	LYS	-	expression tag	UNP A0A075E3D7
B	1087	ILE	-	expression tag	UNP A0A075E3D7
B	1088	GLU	-	expression tag	UNP A0A075E3D7
B	1089	GLU	-	expression tag	UNP A0A075E3D7
B	1090	ILE	-	expression tag	UNP A0A075E3D7
B	1091	LEU	-	expression tag	UNP A0A075E3D7
B	1092	SER	-	expression tag	UNP A0A075E3D7
B	1093	LYS	-	expression tag	UNP A0A075E3D7
B	1094	ILE	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1095	TYR	-	expression tag	UNP A0A075E3D7
B	1096	HIS	-	expression tag	UNP A0A075E3D7
B	1097	ILE	-	expression tag	UNP A0A075E3D7
B	1098	GLU	-	expression tag	UNP A0A075E3D7
B	1099	ASN	-	expression tag	UNP A0A075E3D7
B	1100	GLU	-	expression tag	UNP A0A075E3D7
B	1101	ILE	-	expression tag	UNP A0A075E3D7
B	1102	ALA	-	expression tag	UNP A0A075E3D7
B	1103	ARG	-	expression tag	UNP A0A075E3D7
B	1104	ILE	-	expression tag	UNP A0A075E3D7
B	1105	LYS	-	expression tag	UNP A0A075E3D7
B	1106	LYS	-	expression tag	UNP A0A075E3D7
B	1107	LEU	-	expression tag	UNP A0A075E3D7
B	1108	ILE	-	expression tag	UNP A0A075E3D7
B	1109	GLY	-	expression tag	UNP A0A075E3D7
B	1110	GLU	-	expression tag	UNP A0A075E3D7
B	1111	ILE	-	expression tag	UNP A0A075E3D7
B	1112	GLY	-	expression tag	UNP A0A075E3D7
B	1113	GLY	-	expression tag	UNP A0A075E3D7
B	1114	GLY	-	expression tag	UNP A0A075E3D7
B	1115	GLY	-	expression tag	UNP A0A075E3D7
B	1116	SER	-	expression tag	UNP A0A075E3D7
B	1117	HIS	-	expression tag	UNP A0A075E3D7
B	1118	HIS	-	expression tag	UNP A0A075E3D7
B	1119	HIS	-	expression tag	UNP A0A075E3D7
B	1120	HIS	-	expression tag	UNP A0A075E3D7
B	1121	HIS	-	expression tag	UNP A0A075E3D7
B	1122	HIS	-	expression tag	UNP A0A075E3D7
B	1123	HIS	-	expression tag	UNP A0A075E3D7
B	1124	HIS	-	expression tag	UNP A0A075E3D7
C	111	ILE	VAL	conflict	UNP A0A075E3D7
C	553	ILE	THR	conflict	UNP A0A075E3D7
C	583	THR	ALA	conflict	UNP A0A075E3D7
C	642	LYS	GLN	conflict	UNP A0A075E3D7
C	1018	ASP	-	expression tag	UNP A0A075E3D7
C	1019	VAL	-	expression tag	UNP A0A075E3D7
C	1020	ASN	-	expression tag	UNP A0A075E3D7
C	1021	GLN	-	expression tag	UNP A0A075E3D7
C	1022	THR	-	expression tag	UNP A0A075E3D7
C	1023	VAL	-	expression tag	UNP A0A075E3D7
C	1024	SER	-	expression tag	UNP A0A075E3D7
C	1025	ASP	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1026	ILE	-	expression tag	UNP A0A075E3D7
C	1027	ILE	-	expression tag	UNP A0A075E3D7
C	1028	ASP	-	expression tag	UNP A0A075E3D7
C	1029	ASN	-	expression tag	UNP A0A075E3D7
C	1030	LEU	-	expression tag	UNP A0A075E3D7
C	1031	PRO	-	expression tag	UNP A0A075E3D7
C	1032	THR	-	expression tag	UNP A0A075E3D7
C	1033	ALA	-	expression tag	UNP A0A075E3D7
C	1034	THR	-	expression tag	UNP A0A075E3D7
C	1035	PRO	-	expression tag	UNP A0A075E3D7
C	1036	PRO	-	expression tag	UNP A0A075E3D7
C	1037	GLN	-	expression tag	UNP A0A075E3D7
C	1038	TRP	-	expression tag	UNP A0A075E3D7
C	1039	ASP	-	expression tag	UNP A0A075E3D7
C	1040	VAL	-	expression tag	UNP A0A075E3D7
C	1041	GLY	-	expression tag	UNP A0A075E3D7
C	1042	ILE	-	expression tag	UNP A0A075E3D7
C	1043	TYR	-	expression tag	UNP A0A075E3D7
C	1044	ASN	-	expression tag	UNP A0A075E3D7
C	1045	ASN	-	expression tag	UNP A0A075E3D7
C	1046	THR	-	expression tag	UNP A0A075E3D7
C	1047	ILE	-	expression tag	UNP A0A075E3D7
C	1048	LEU	-	expression tag	UNP A0A075E3D7
C	1049	ASN	-	expression tag	UNP A0A075E3D7
C	1050	LEU	-	expression tag	UNP A0A075E3D7
C	1051	THR	-	expression tag	UNP A0A075E3D7
C	1052	VAL	-	expression tag	UNP A0A075E3D7
C	1053	GLU	-	expression tag	UNP A0A075E3D7
C	1054	ILE	-	expression tag	UNP A0A075E3D7
C	1055	ASN	-	expression tag	UNP A0A075E3D7
C	1056	ASP	-	expression tag	UNP A0A075E3D7
C	1057	LEU	-	expression tag	UNP A0A075E3D7
C	1058	GLN	-	expression tag	UNP A0A075E3D7
C	1059	GLU	-	expression tag	UNP A0A075E3D7
C	1060	ARG	-	expression tag	UNP A0A075E3D7
C	1061	SER	-	expression tag	UNP A0A075E3D7
C	1062	LYS	-	expression tag	UNP A0A075E3D7
C	1063	ASN	-	expression tag	UNP A0A075E3D7
C	1064	LEU	-	expression tag	UNP A0A075E3D7
C	1065	SER	-	expression tag	UNP A0A075E3D7
C	1066	GLN	-	expression tag	UNP A0A075E3D7
C	1067	ILE	-	expression tag	UNP A0A075E3D7

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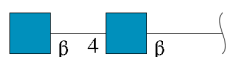
Chain	Residue	Modelled	Actual	Comment	Reference
C	1068	ALA	-	expression tag	UNP A0A075E3D7
C	1069	ASP	-	expression tag	UNP A0A075E3D7
C	1070	ARG	-	expression tag	UNP A0A075E3D7
C	1071	LEU	-	expression tag	UNP A0A075E3D7
C	1072	GLN	-	expression tag	UNP A0A075E3D7
C	1073	ASN	-	expression tag	UNP A0A075E3D7
C	1074	TYR	-	expression tag	UNP A0A075E3D7
C	1075	ILE	-	expression tag	UNP A0A075E3D7
C	1076	ASP	-	expression tag	UNP A0A075E3D7
C	1077	ASN	-	expression tag	UNP A0A075E3D7
C	1078	VAL	-	expression tag	UNP A0A075E3D7
C	1079	ASP	-	expression tag	UNP A0A075E3D7
C	1080	ILE	-	expression tag	UNP A0A075E3D7
C	1081	LYS	-	expression tag	UNP A0A075E3D7
C	1082	GLN	-	expression tag	UNP A0A075E3D7
C	1083	ILE	-	expression tag	UNP A0A075E3D7
C	1084	GLU	-	expression tag	UNP A0A075E3D7
C	1085	ASP	-	expression tag	UNP A0A075E3D7
C	1086	LYS	-	expression tag	UNP A0A075E3D7
C	1087	ILE	-	expression tag	UNP A0A075E3D7
C	1088	GLU	-	expression tag	UNP A0A075E3D7
C	1089	GLU	-	expression tag	UNP A0A075E3D7
C	1090	ILE	-	expression tag	UNP A0A075E3D7
C	1091	LEU	-	expression tag	UNP A0A075E3D7
C	1092	SER	-	expression tag	UNP A0A075E3D7
C	1093	LYS	-	expression tag	UNP A0A075E3D7
C	1094	ILE	-	expression tag	UNP A0A075E3D7
C	1095	TYR	-	expression tag	UNP A0A075E3D7
C	1096	HIS	-	expression tag	UNP A0A075E3D7
C	1097	ILE	-	expression tag	UNP A0A075E3D7
C	1098	GLU	-	expression tag	UNP A0A075E3D7
C	1099	ASN	-	expression tag	UNP A0A075E3D7
C	1100	GLU	-	expression tag	UNP A0A075E3D7
C	1101	ILE	-	expression tag	UNP A0A075E3D7
C	1102	ALA	-	expression tag	UNP A0A075E3D7
C	1103	ARG	-	expression tag	UNP A0A075E3D7
C	1104	ILE	-	expression tag	UNP A0A075E3D7
C	1105	LYS	-	expression tag	UNP A0A075E3D7
C	1106	LYS	-	expression tag	UNP A0A075E3D7
C	1107	LEU	-	expression tag	UNP A0A075E3D7
C	1108	ILE	-	expression tag	UNP A0A075E3D7
C	1109	GLY	-	expression tag	UNP A0A075E3D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1110	GLU	-	expression tag	UNP A0A075E3D7
C	1111	ILE	-	expression tag	UNP A0A075E3D7
C	1112	GLY	-	expression tag	UNP A0A075E3D7
C	1113	GLY	-	expression tag	UNP A0A075E3D7
C	1114	GLY	-	expression tag	UNP A0A075E3D7
C	1115	GLY	-	expression tag	UNP A0A075E3D7
C	1116	SER	-	expression tag	UNP A0A075E3D7
C	1117	HIS	-	expression tag	UNP A0A075E3D7
C	1118	HIS	-	expression tag	UNP A0A075E3D7
C	1119	HIS	-	expression tag	UNP A0A075E3D7
C	1120	HIS	-	expression tag	UNP A0A075E3D7
C	1121	HIS	-	expression tag	UNP A0A075E3D7
C	1122	HIS	-	expression tag	UNP A0A075E3D7
C	1123	HIS	-	expression tag	UNP A0A075E3D7
C	1124	HIS	-	expression tag	UNP A0A075E3D7

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



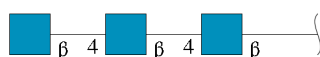
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16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

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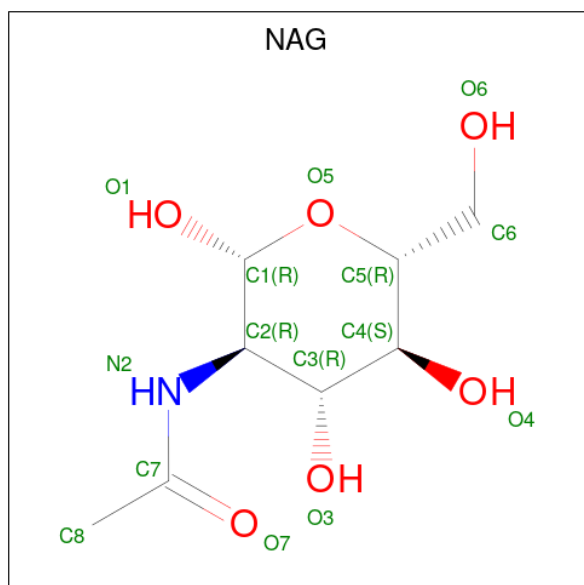
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	3	Total	C	N	O	0	0
			42	24	3	15		
3	L	3	Total	C	N	O	0	0
			42	24	3	15		
3	Q	3	Total	C	N	O	0	0
			42	24	3	15		

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

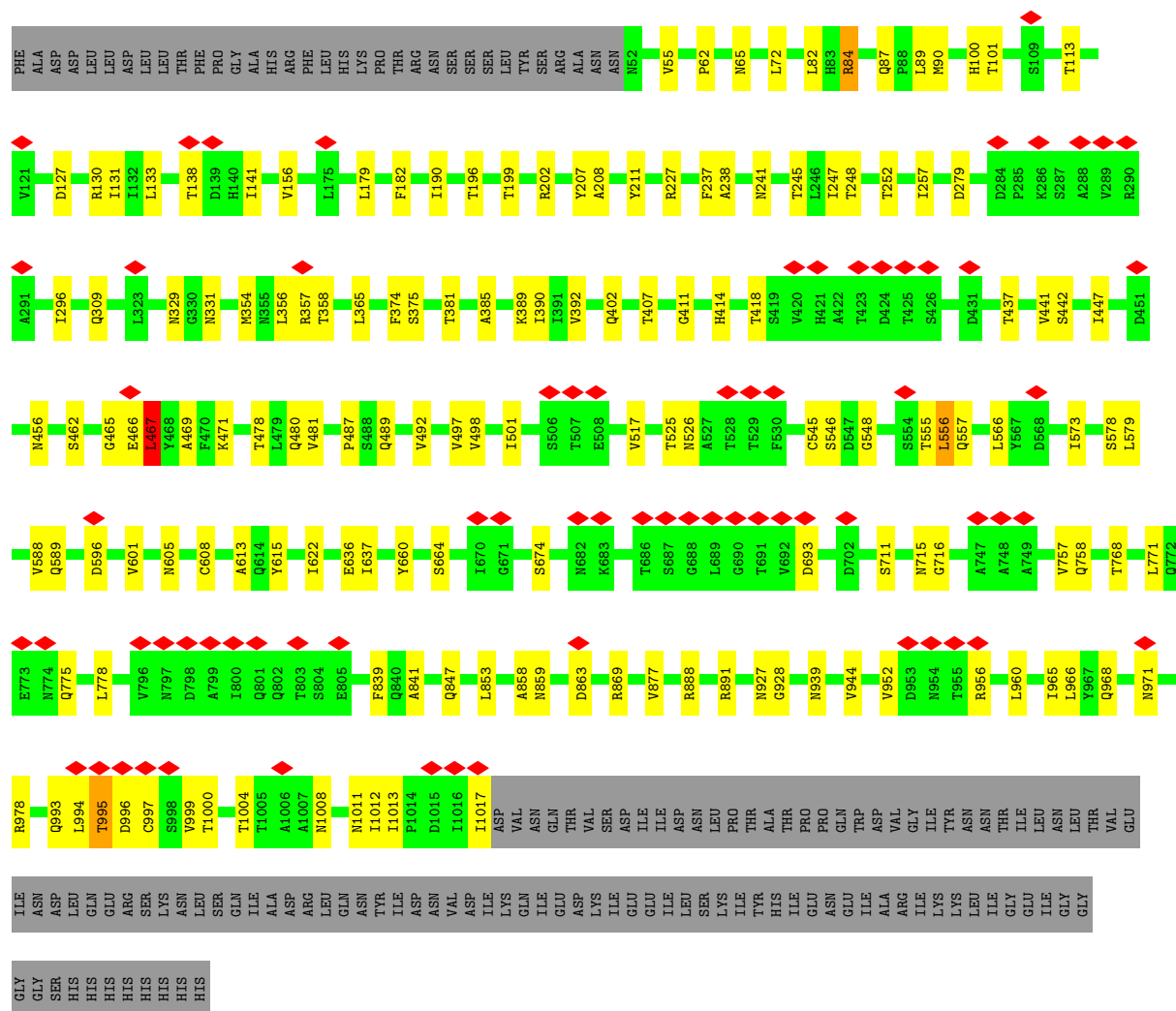


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4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

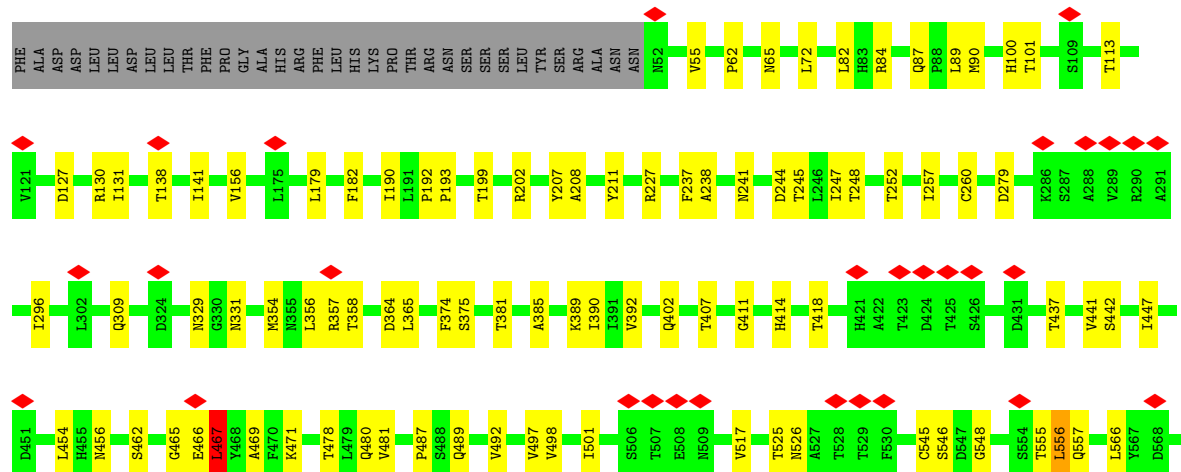
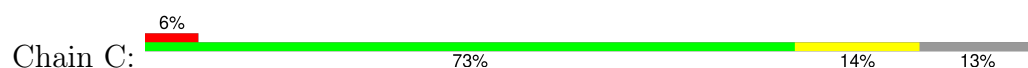
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	



• Molecule 1: Spike protein





WORLD WIDE
PDB
PROTEIN DATA BANK

Chain I:  100%

NAG1
NAG2

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

Chain J:  100%

NAG1
NAG2

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

Chain K:  50% 50%

NAG1
NAG2

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

Chain M:  50% 100%

NAG1
NAG2

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

Chain N:  100%

NAG1
NAG2

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

Chain O:  50% 50%

NAG1
NAG2

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

Chain P:  50% 50%



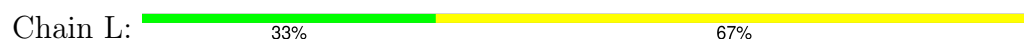
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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	87002	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.136	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0468	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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	0.43	1/7270 (0.0%)	0.65	1/9959 (0.0%)
1	B	0.43	1/7270 (0.0%)	0.65	1/9959 (0.0%)
1	C	0.43	1/7270 (0.0%)	0.65	1/9959 (0.0%)
All	All	0.43	3/21810 (0.0%)	0.65	3/29877 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
All	All	0	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	517	VAL	C-N	-5.46	1.21	1.34
1	A	517	VAL	C-N	-5.44	1.21	1.34
1	B	517	VAL	C-N	-5.41	1.21	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	LEU	CA-CB-CG	9.88	138.02	115.30
1	A	467	LEU	CA-CB-CG	9.87	138.00	115.30
1	C	467	LEU	CA-CB-CG	9.86	137.98	115.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	THR	Peptide
1	A	358	THR	Peptide
1	A	418	THR	Peptide
1	A	466	GLU	Peptide
1	A	555	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7139	0	6840	86	0
1	B	7139	0	6840	83	0
1	C	7139	0	6840	83	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	R	28	0	25	0	0
3	G	42	0	37	1	0
3	L	42	0	37	0	0
3	Q	42	0	37	0	0
4	A	112	0	104	1	0
4	B	112	0	104	1	0
4	C	112	0	104	1	0
All	All	22215	0	21243	238	0

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

The worst 5 of 238 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:859:ASN:O	1:A:863:ASP:HB2	1.87	0.74
1:B:859:ASN:O	1:B:863:ASP:HB2	1.87	0.74
1:C:859:ASN:O	1:C:863:ASP:HB2	1.87	0.74
1:B:456:ASN:ND2	1:C:252:THR:O	2.25	0.70
1:A:72:LEU:H	1:A:87:GLN:HE22	1.40	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	964/1107 (87%)	843 (87%)	117 (12%)	4 (0%)	30	61
1	B	964/1107 (87%)	844 (88%)	116 (12%)	4 (0%)	30	61
1	C	964/1107 (87%)	844 (88%)	116 (12%)	4 (0%)	30	61
All	All	2892/3321 (87%)	2531 (88%)	349 (12%)	12 (0%)	32	61

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	LEU
1	A	557	GLN
1	A	996	ASP
1	B	467	LEU
1	B	557	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	771/975 (79%)	766 (99%)	5 (1%)	84	90
1	B	771/975 (79%)	766 (99%)	5 (1%)	84	90
1	C	771/975 (79%)	766 (99%)	5 (1%)	84	90
All	All	2313/2925 (79%)	2298 (99%)	15 (1%)	82	90

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	331	ASN
1	C	365	LEU
1	B	365	LEU
1	C	994	LEU
1	C	84	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	402	GLN
1	C	939	ASN
1	B	939	ASN
1	C	1011	ASN
1	C	402	GLN

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 ⓘ

33 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	1,2	14,14,15	0.71	1 (7%)	17,19,21	2.77	4 (23%)
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.67	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.27	0	17,19,21	0.56	0
2	NAG	E	2	2	14,14,15	0.23	0	17,19,21	0.64	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.34	0	17,19,21	0.73	1 (5%)
2	NAG	F	2	2	14,14,15	0.21	0	17,19,21	0.60	0
3	NAG	G	1	1,3	14,14,15	0.50	0	17,19,21	1.04	1 (5%)
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.57	0
3	NAG	G	3	3	14,14,15	0.45	0	17,19,21	0.69	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.46	0	17,19,21	0.66	0
2	NAG	H	2	2	14,14,15	0.23	0	17,19,21	0.51	0
2	NAG	I	1	1,2	14,14,15	0.65	0	17,19,21	2.82	4 (23%)
2	NAG	I	2	2	14,14,15	0.23	0	17,19,21	0.66	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.28	0	17,19,21	0.54	0
2	NAG	J	2	2	14,14,15	0.31	0	17,19,21	0.60	0
2	NAG	K	1	1,2	14,14,15	0.43	0	17,19,21	0.75	1 (5%)
2	NAG	K	2	2	14,14,15	0.19	0	17,19,21	0.59	0
3	NAG	L	1	1,3	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
3	NAG	L	2	3	14,14,15	0.23	0	17,19,21	0.58	0
3	NAG	L	3	3	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.46	0	17,19,21	0.65	0
2	NAG	M	2	2	14,14,15	0.21	0	17,19,21	0.55	0
2	NAG	N	1	1,2	14,14,15	0.76	1 (7%)	17,19,21	2.78	5 (29%)
2	NAG	N	2	2	14,14,15	0.26	0	17,19,21	0.65	1 (5%)
2	NAG	O	1	1,2	14,14,15	0.32	0	17,19,21	0.55	0
2	NAG	O	2	2	14,14,15	0.21	0	17,19,21	0.62	1 (5%)
2	NAG	P	1	1,2	14,14,15	0.36	0	17,19,21	0.72	0
2	NAG	P	2	2	14,14,15	0.21	0	17,19,21	0.60	0
3	NAG	Q	1	1,3	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.58	0
3	NAG	Q	3	3	14,14,15	0.43	0	17,19,21	0.68	1 (5%)
2	NAG	R	1	1,2	14,14,15	0.48	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	R	2	2	14,14,15	0.23	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	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	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	3	3	-	4/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	3	3	-	4/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	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	1,2	-	4/6/23/26	0/1/1/1
2	NAG	P	2	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	3	3	-	4/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	NAG	O5-C1	-2.28	1.39	1.43
2	D	1	NAG	O5-C1	-2.12	1.40	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	8.42	134.18	122.90
2	N	1	NAG	C2-N2-C7	8.41	134.17	122.90
2	I	1	NAG	C2-N2-C7	8.39	134.14	122.90
2	I	1	NAG	C1-C2-N2	5.02	118.35	110.43
2	N	1	NAG	C1-C2-N2	4.87	118.11	110.43

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

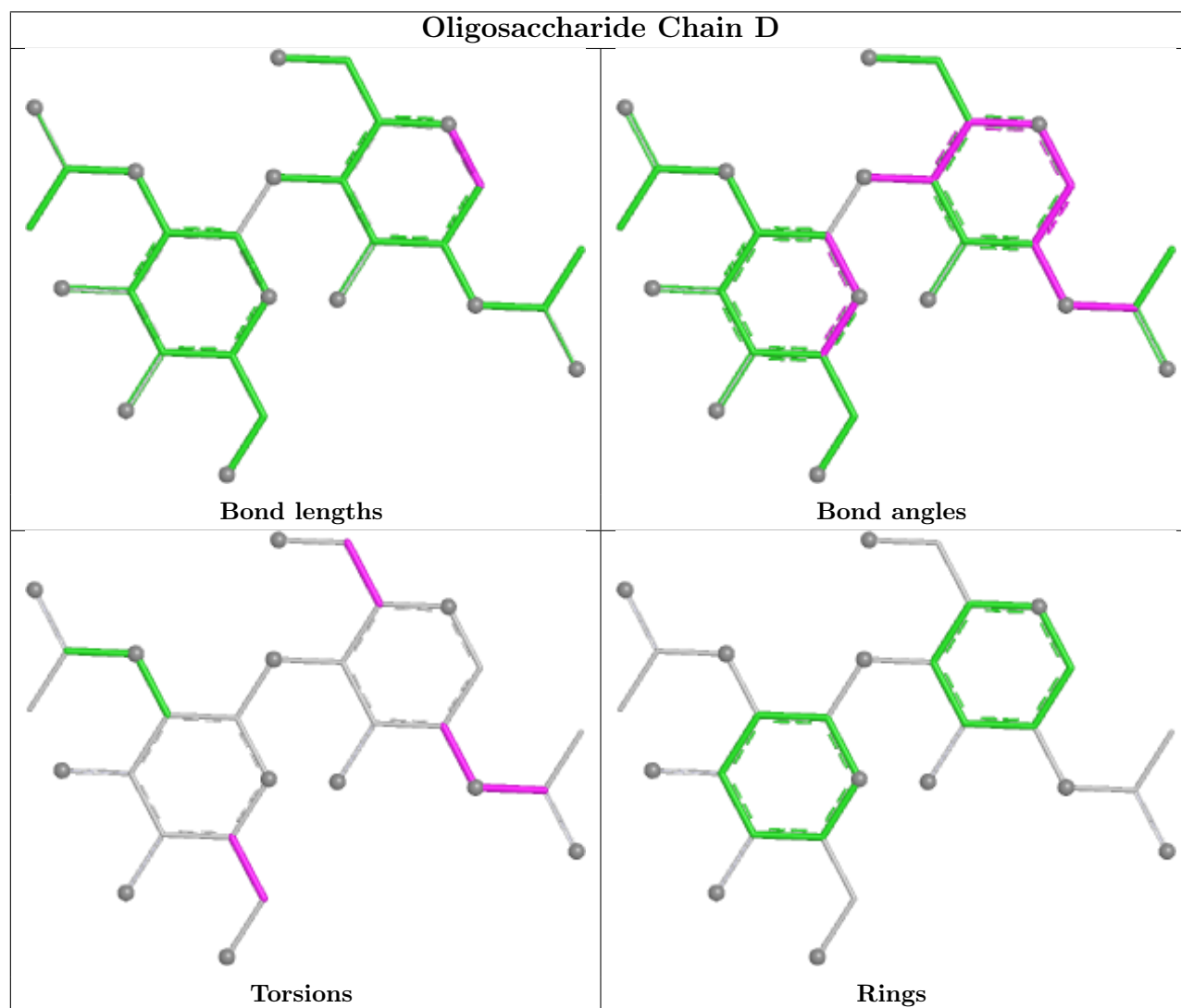
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6

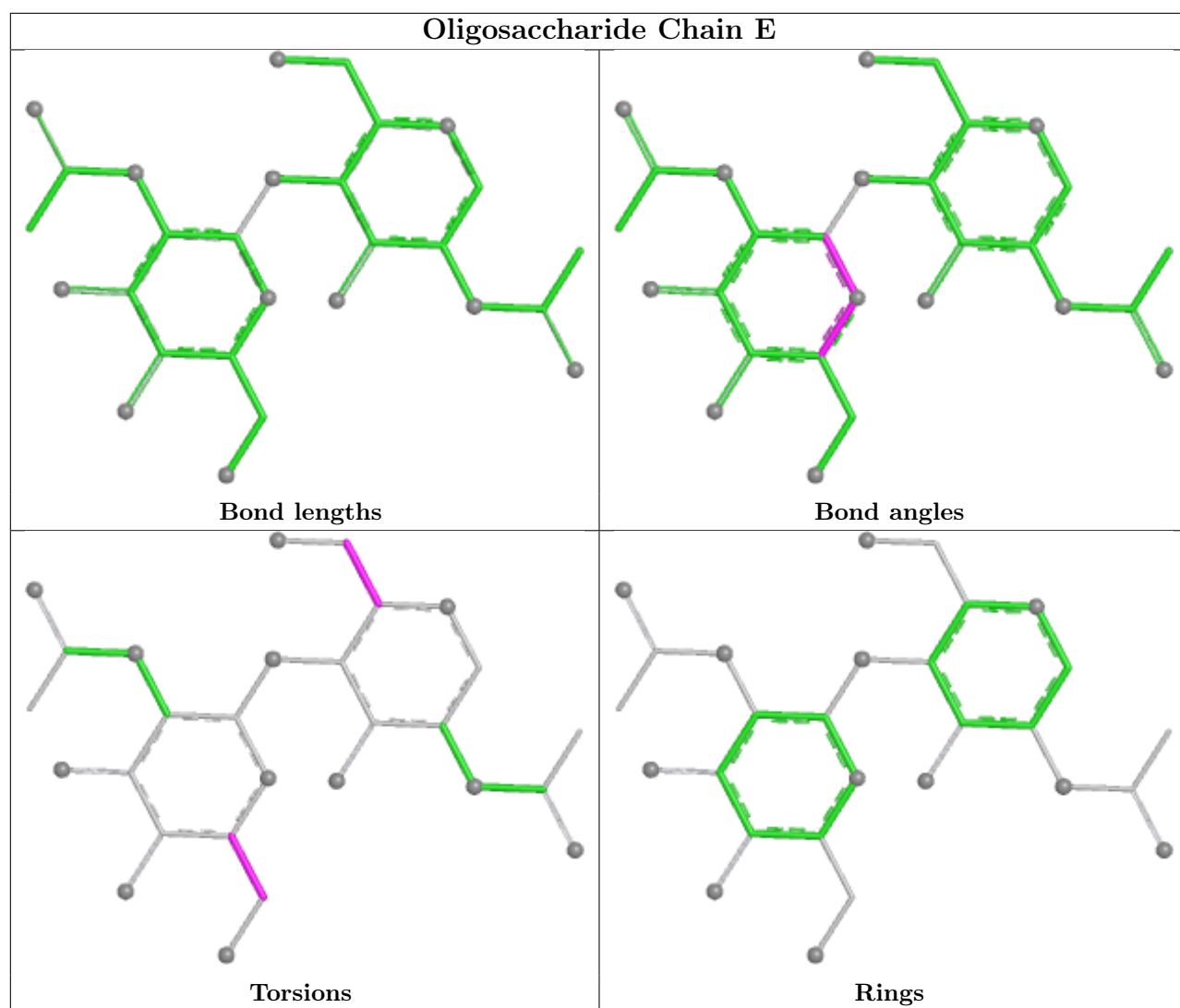
There are no ring outliers.

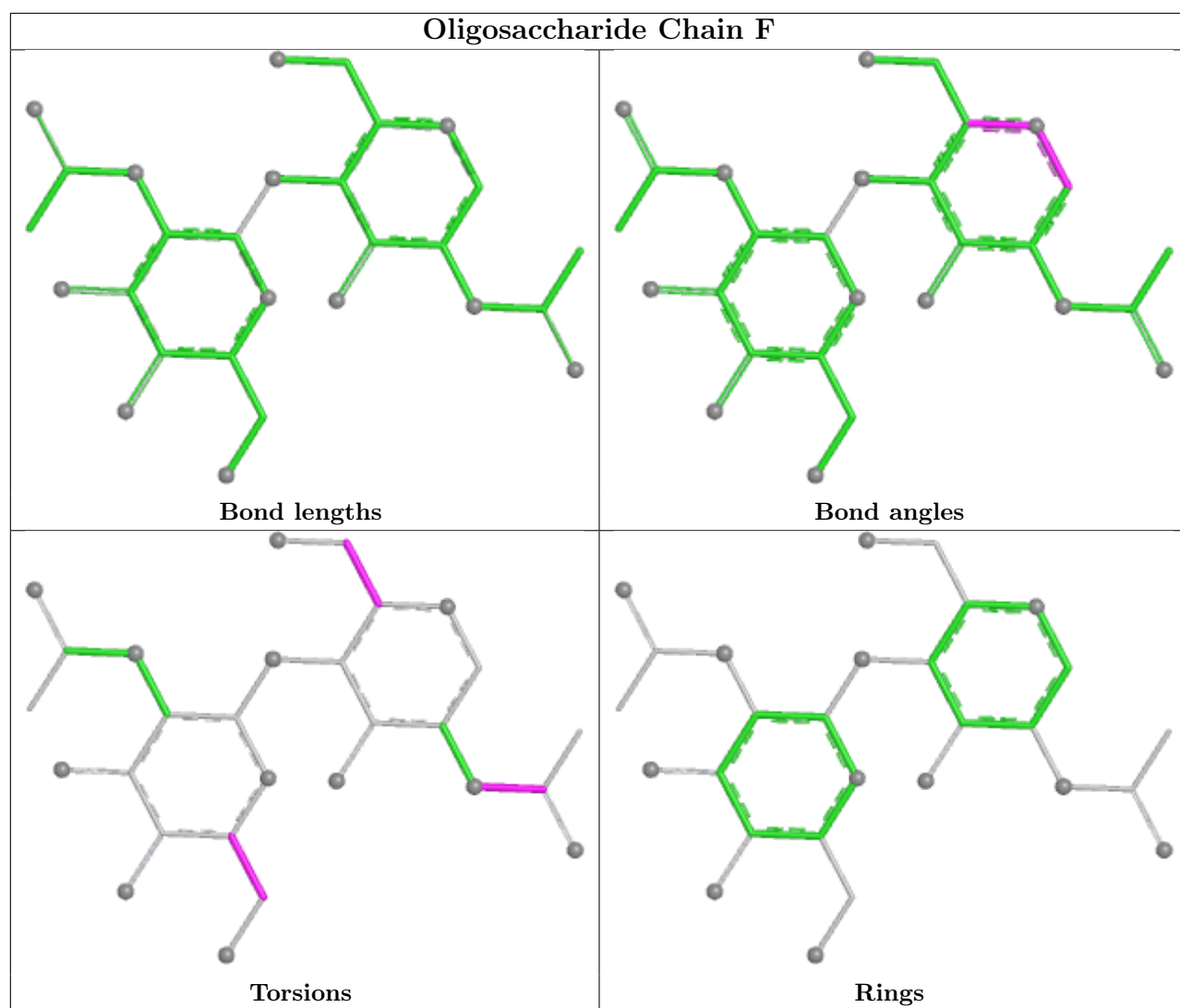
4 monomers are involved in 3 short contacts:

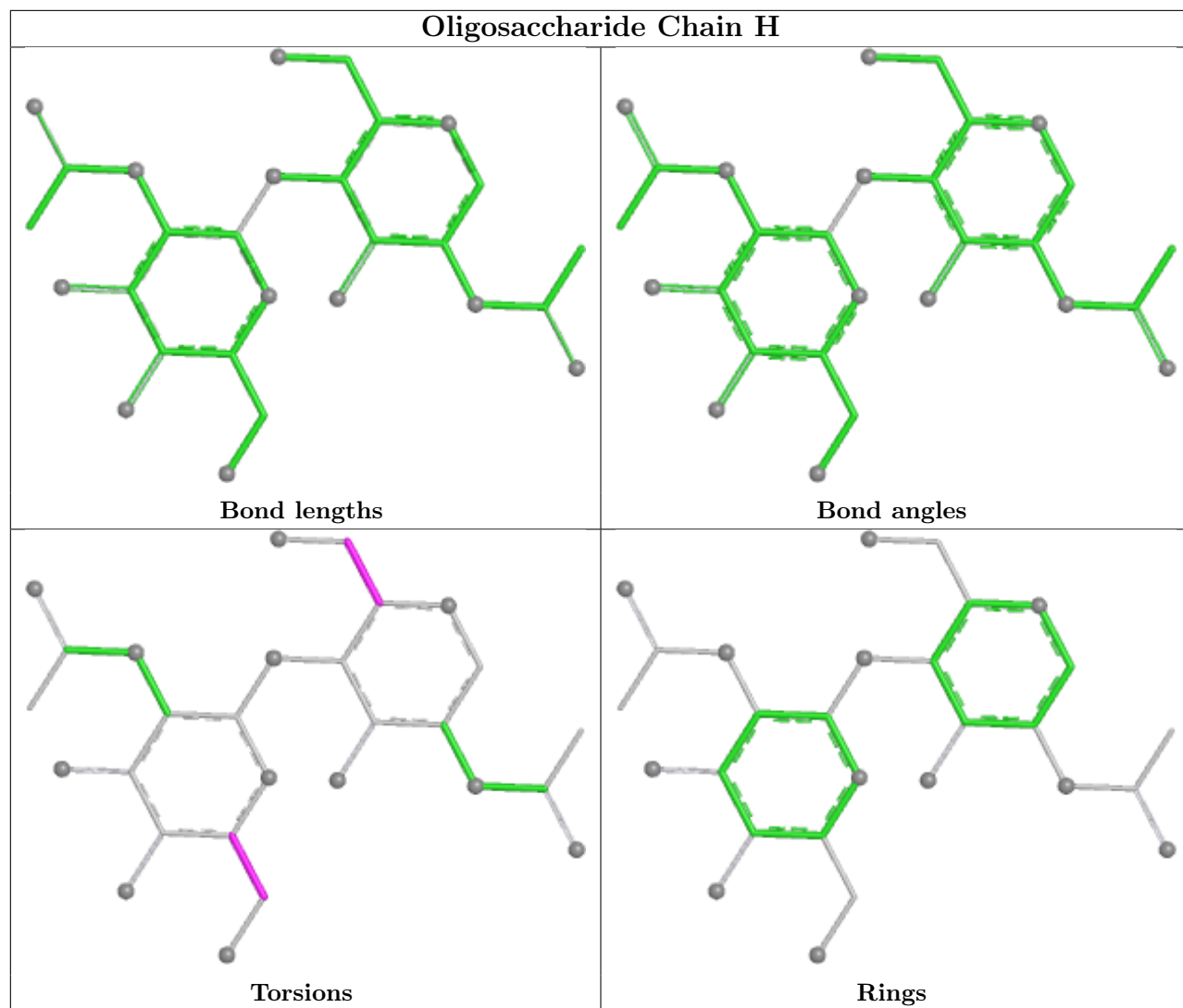
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0
2	P	1	NAG	1	0
3	G	2	NAG	1	0
2	F	1	NAG	1	0

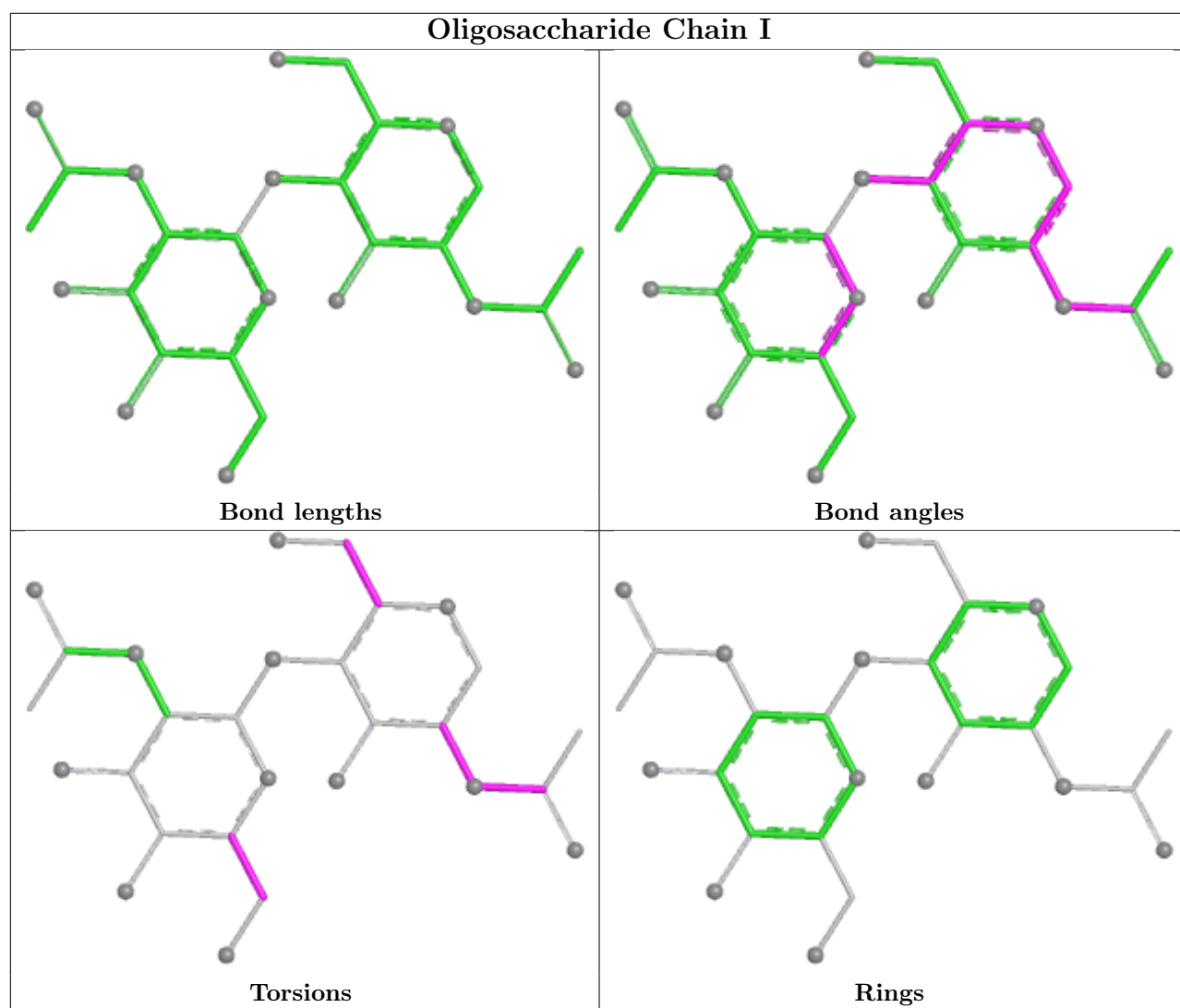
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

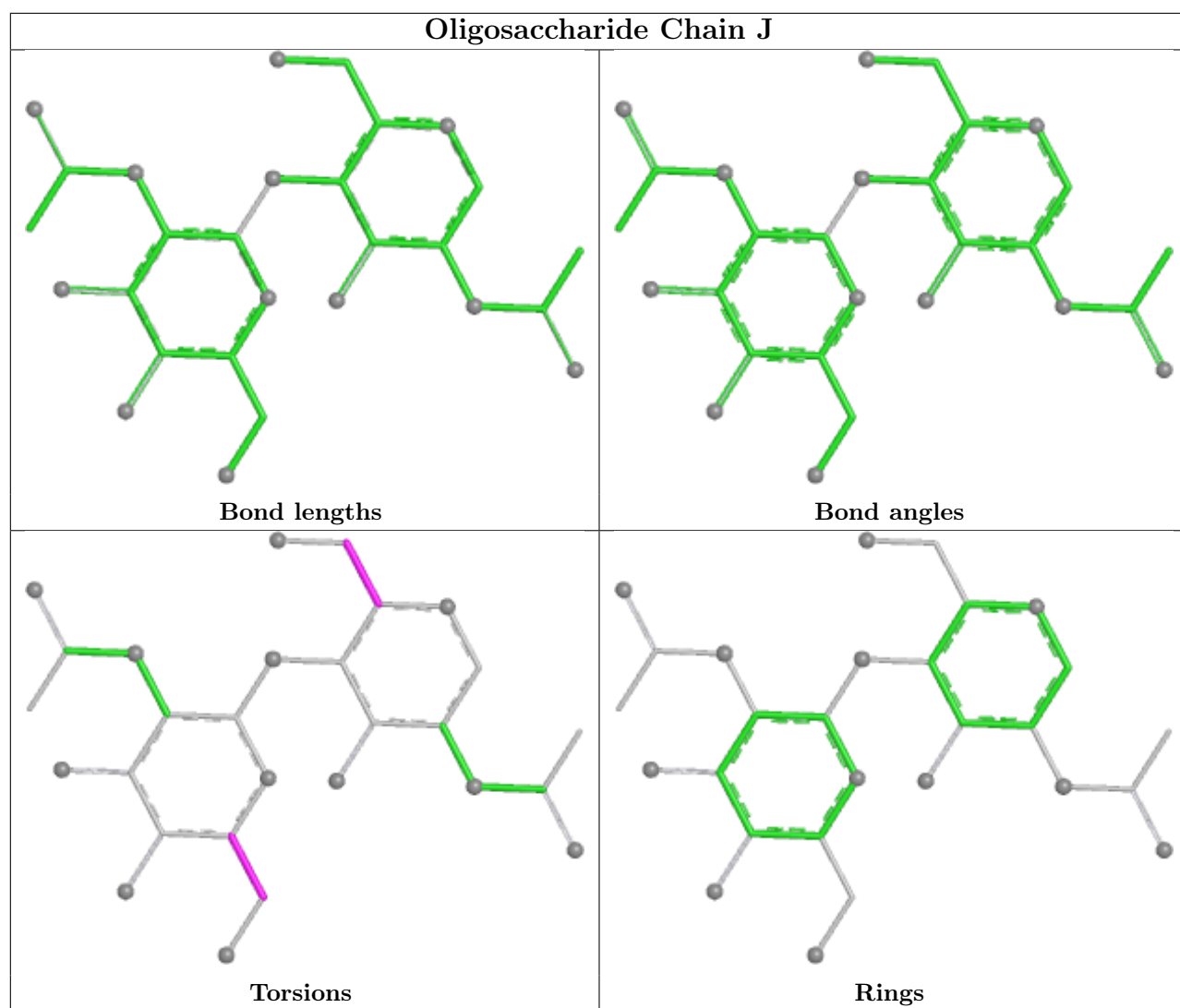


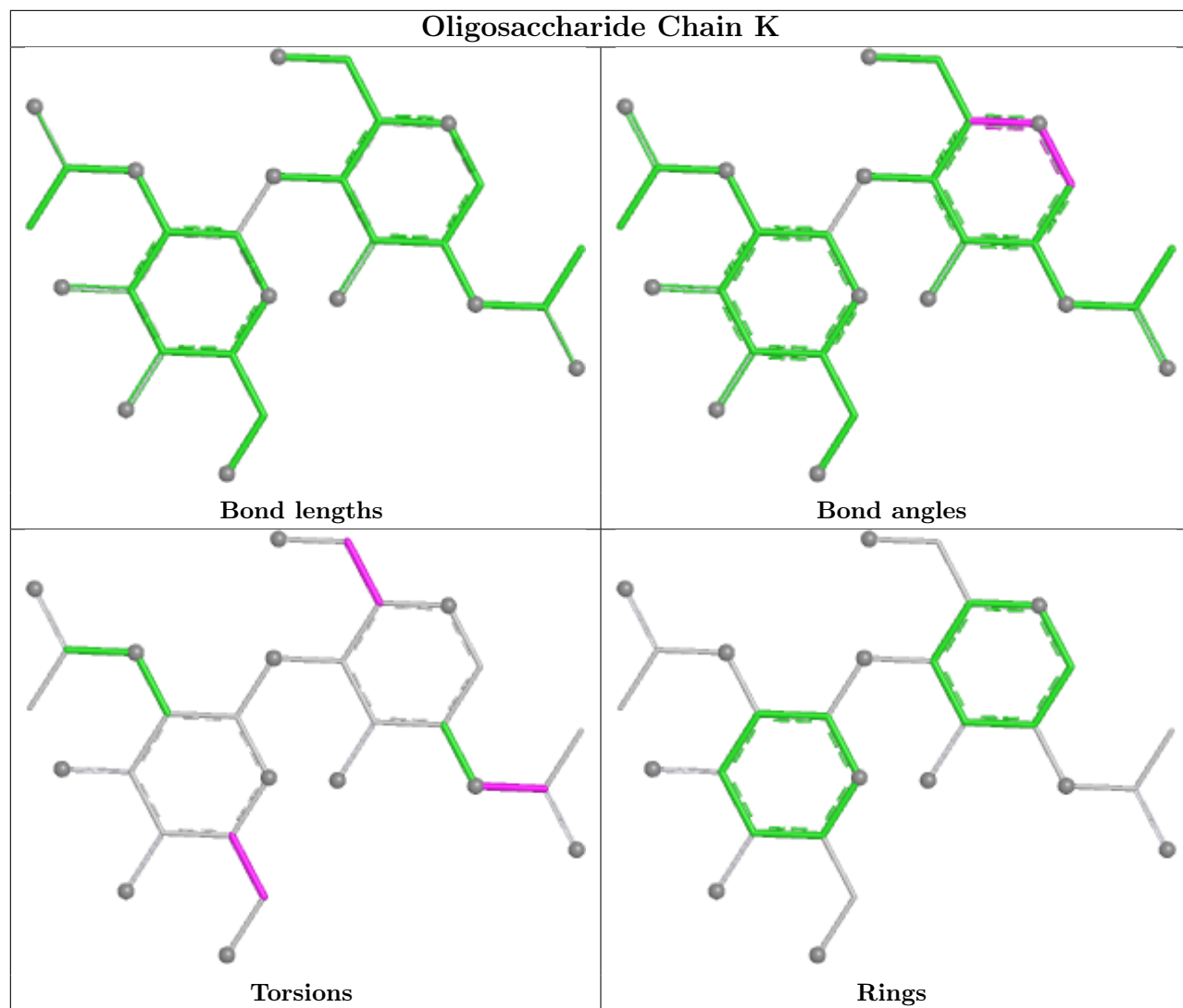


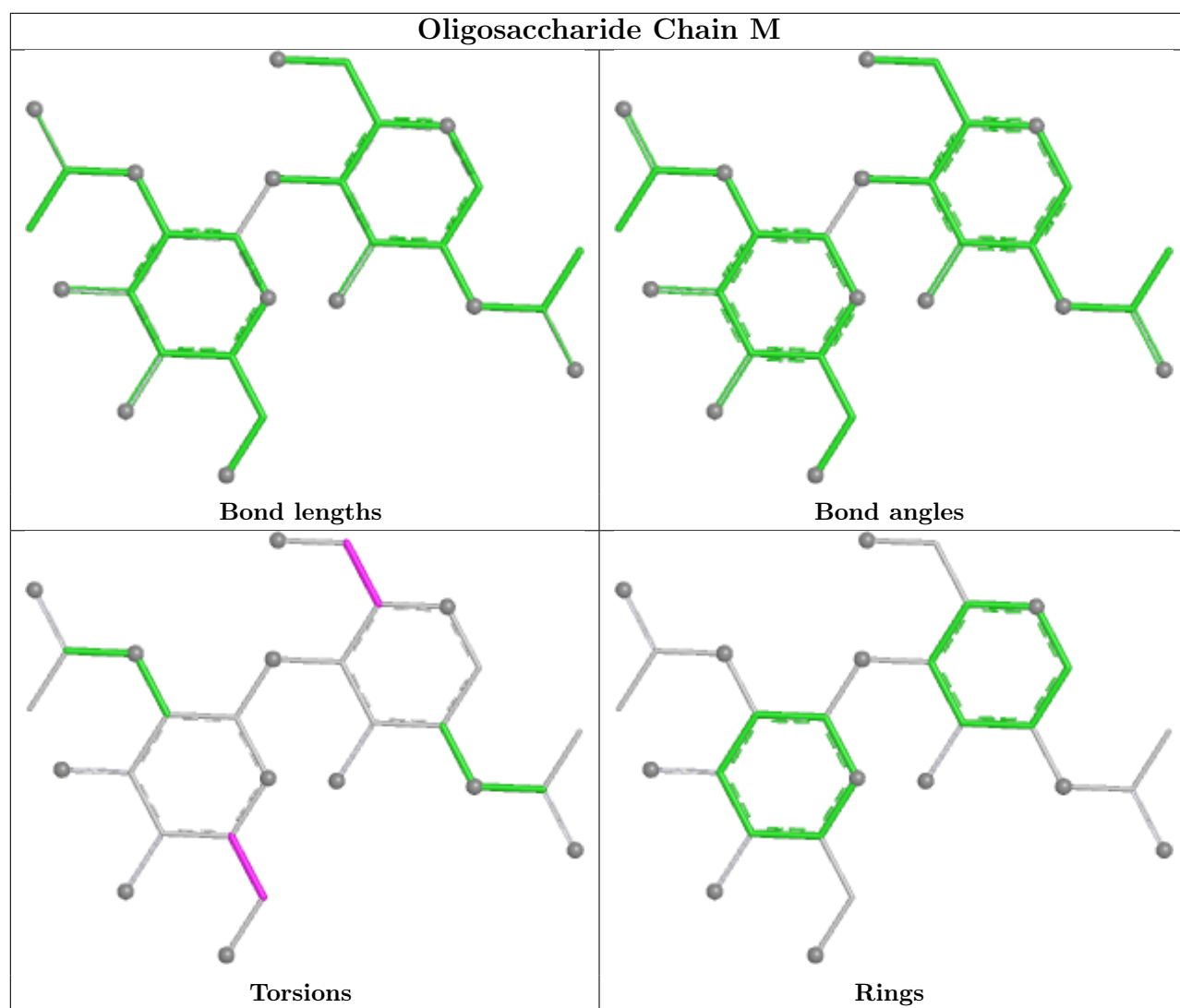


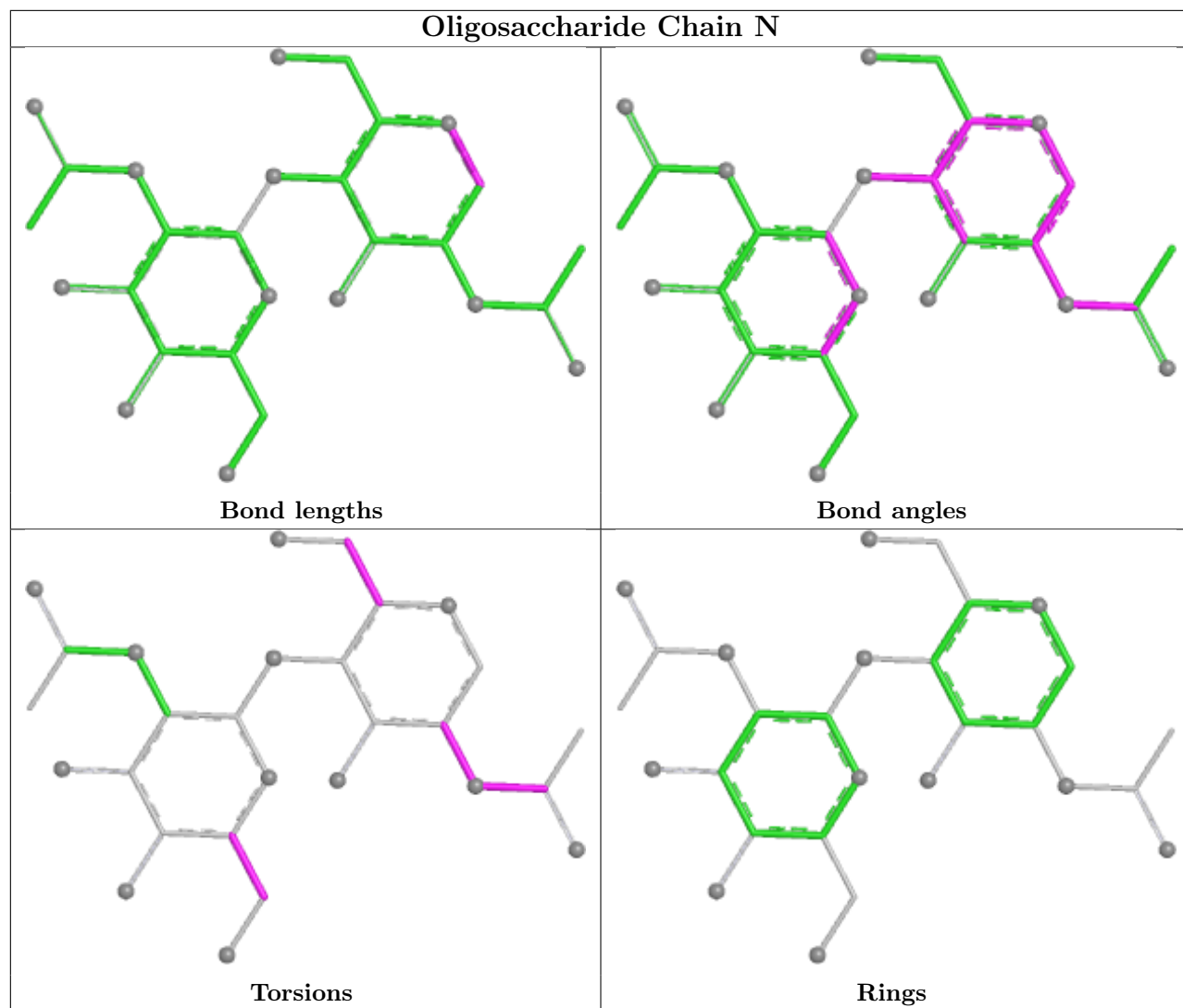


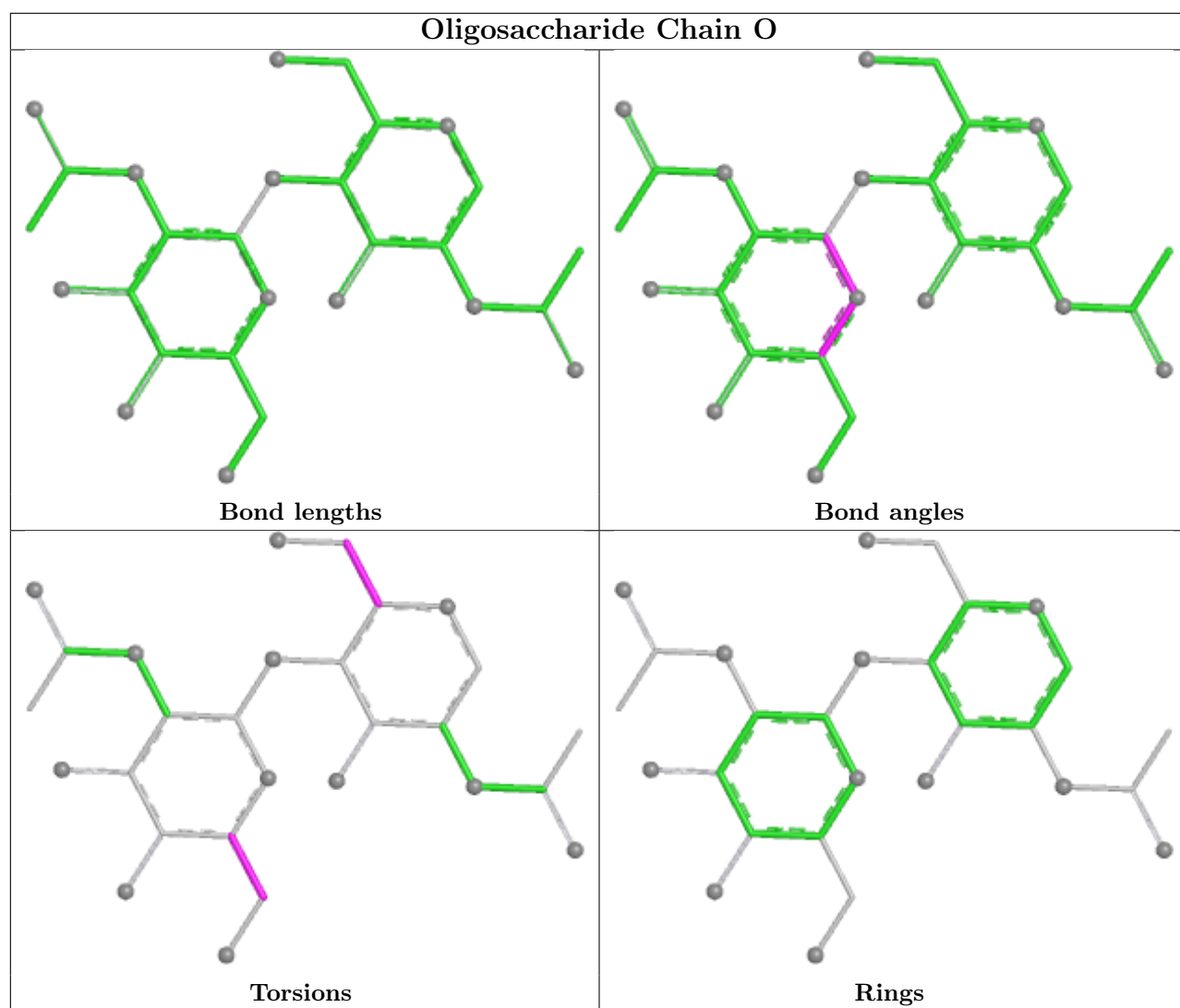


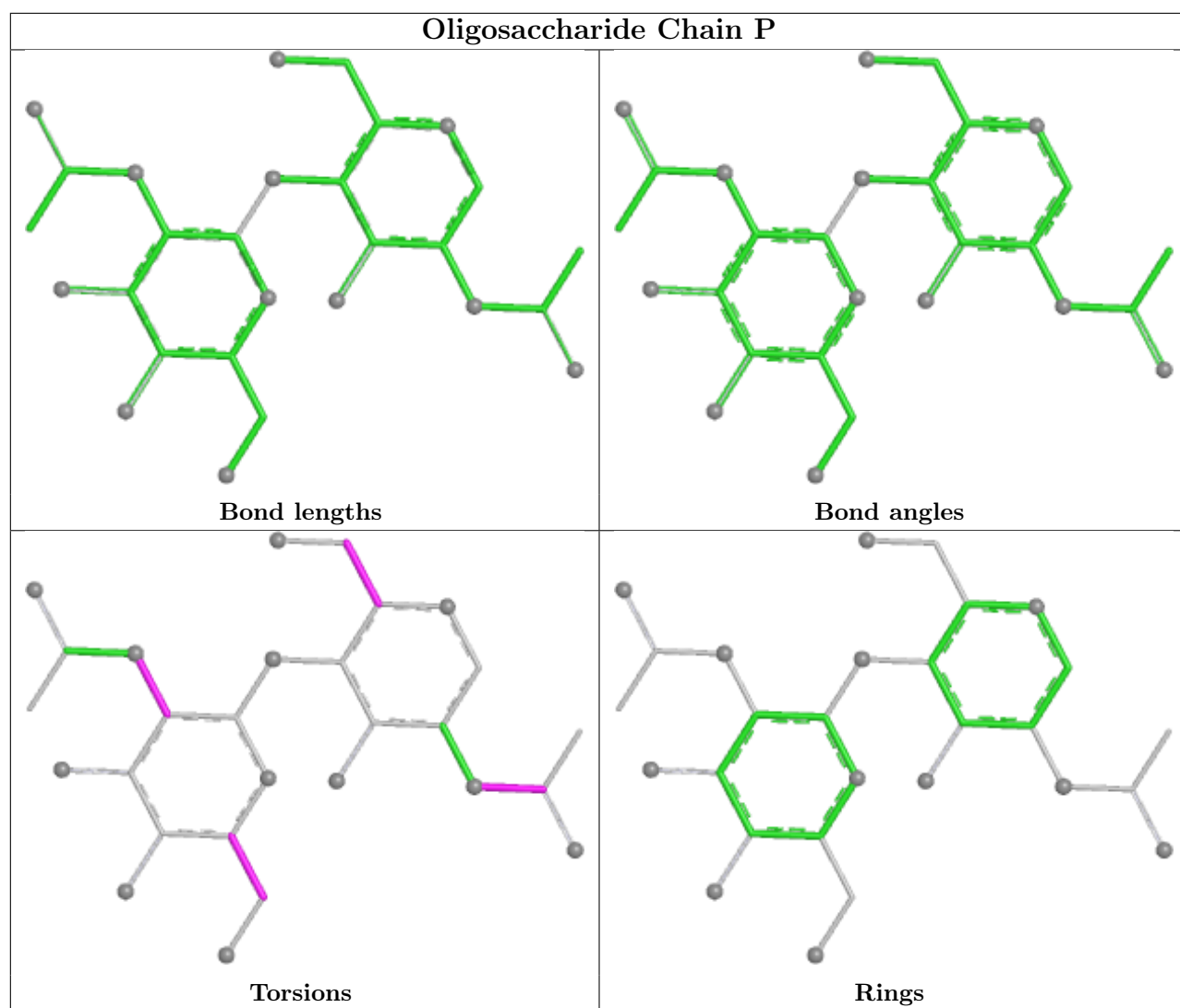


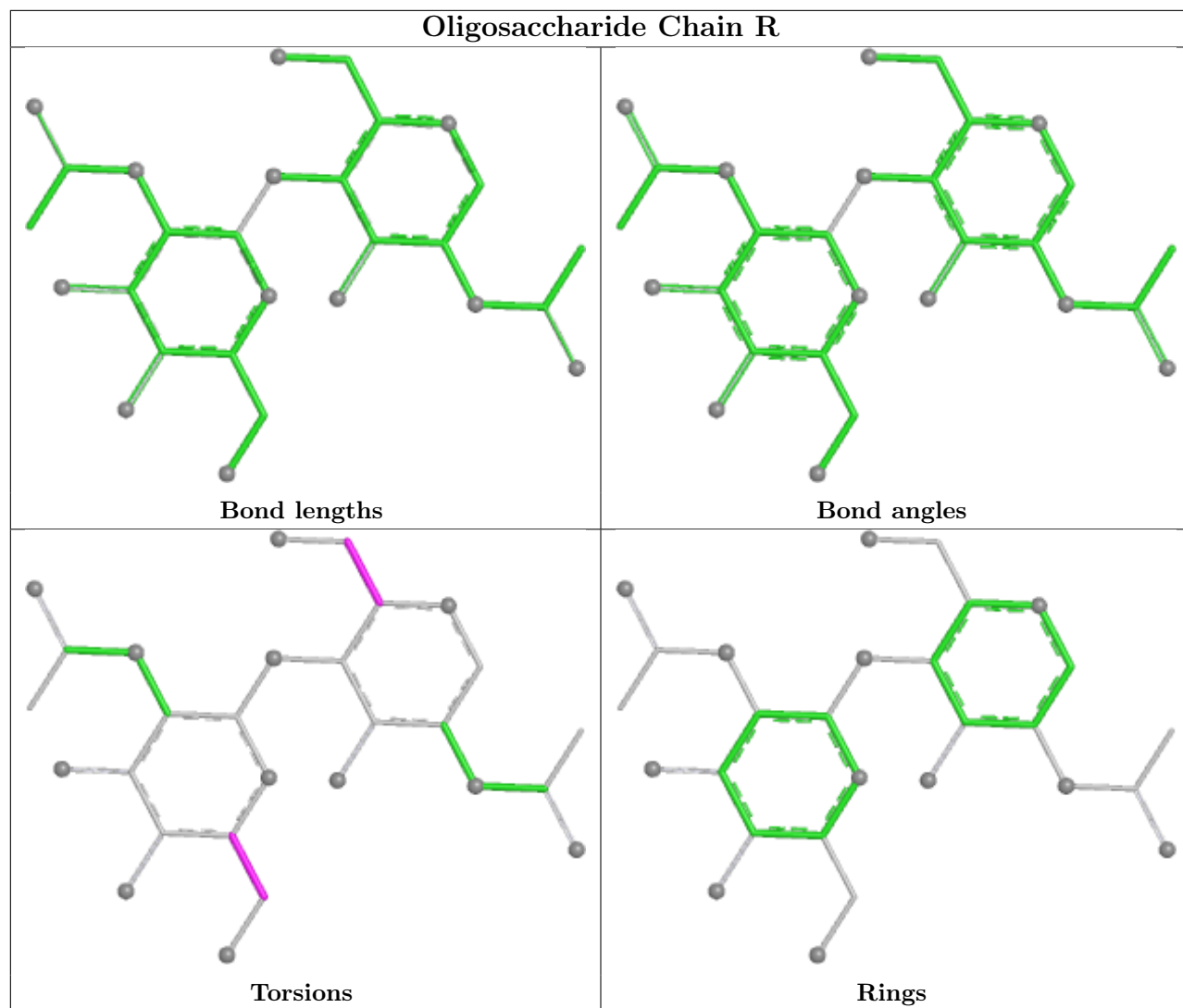


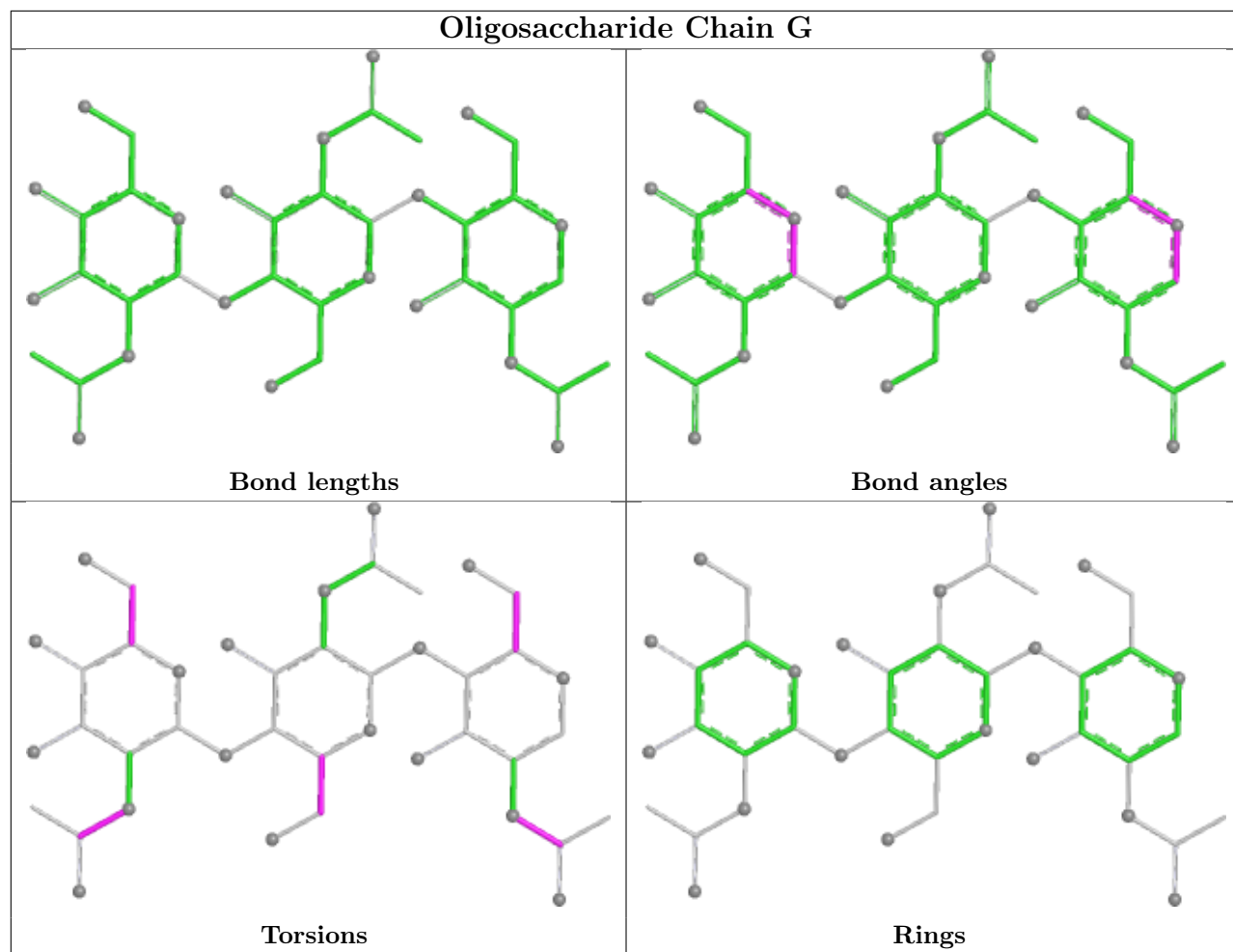


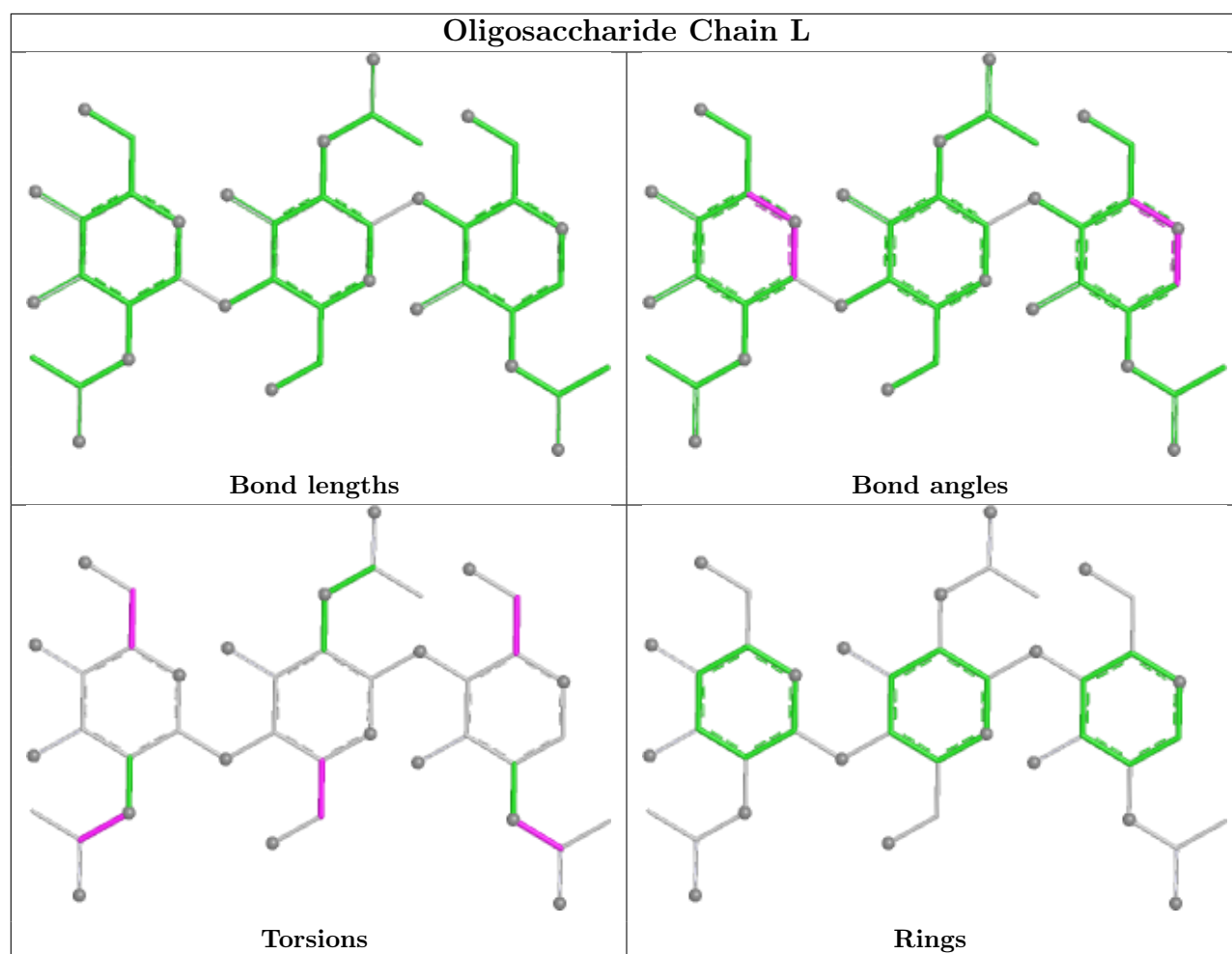


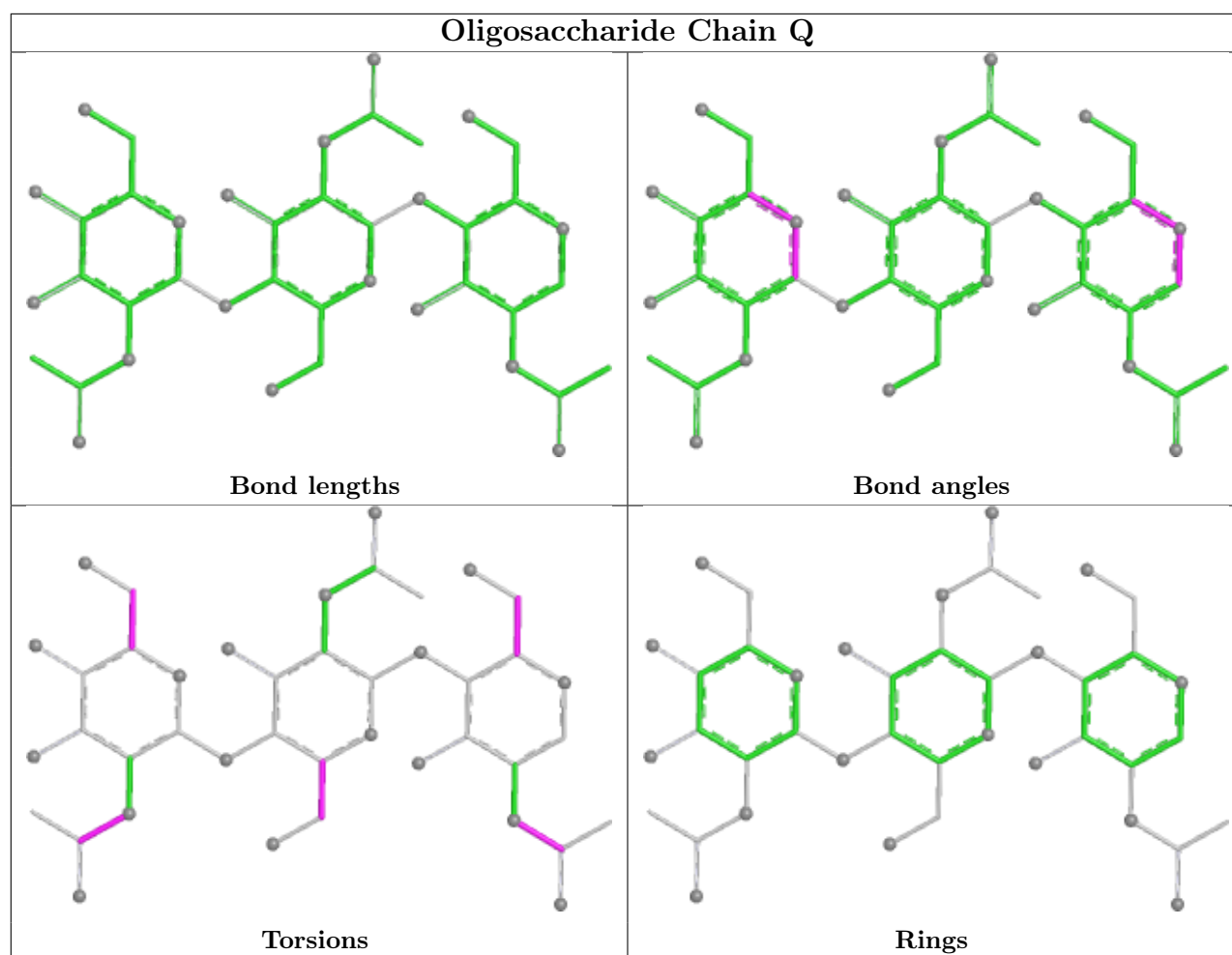












5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1209	1	14,14,15	0.39	0	17,19,21	0.61	0
4	NAG	B	1208	1	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	A	1207	1	14,14,15	0.87	1 (7%)	17,19,21	2.36	3 (17%)
4	NAG	C	1205	1	14,14,15	0.21	0	17,19,21	0.59	0
4	NAG	B	1207	1	14,14,15	0.84	1 (7%)	17,19,21	2.36	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1217	1	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
4	NAG	A	1208	1	14,14,15	0.21	0	17,19,21	0.51	0
4	NAG	C	1208	1	14,14,15	0.21	0	17,19,21	0.52	0
4	NAG	C	1206	1	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
4	NAG	A	1209	1	14,14,15	0.32	0	17,19,21	0.65	0
4	NAG	A	1210	1	14,14,15	0.41	0	17,19,21	0.40	0
4	NAG	B	1210	1	14,14,15	0.44	0	17,19,21	0.40	0
4	NAG	C	1207	1	14,14,15	0.84	1 (7%)	17,19,21	2.36	3 (17%)
4	NAG	A	1217	1	14,14,15	0.50	0	17,19,21	0.94	1 (5%)
4	NAG	C	1211	1	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	B	1206	1	14,14,15	0.55	0	17,19,21	0.66	0
4	NAG	B	1209	1	14,14,15	0.26	0	17,19,21	0.63	0
4	NAG	B	1211	1	14,14,15	0.27	0	17,19,21	0.58	0
4	NAG	A	1205	1	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	C	1217	1	14,14,15	0.53	0	17,19,21	0.94	1 (5%)
4	NAG	A	1211	1	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	C	1210	1	14,14,15	0.38	0	17,19,21	0.39	0
4	NAG	A	1206	1	14,14,15	0.60	0	17,19,21	0.69	1 (5%)
4	NAG	B	1205	1	14,14,15	0.30	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1209	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1208	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1207	1	-	6/6/23/26	0/1/1/1
4	NAG	C	1205	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1207	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1217	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1208	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1208	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1206	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1209	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1210	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1210	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1207	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1217	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1211	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1206	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1209	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1211	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1205	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1217	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1211	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1210	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1206	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1205	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1207	NAG	C1-C2	2.69	1.56	1.52
4	C	1207	NAG	C1-C2	2.55	1.55	1.52
4	B	1207	NAG	C1-C2	2.49	1.55	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1207	NAG	C2-N2-C7	8.34	134.08	122.90
4	C	1207	NAG	C2-N2-C7	8.29	134.00	122.90
4	A	1207	NAG	C2-N2-C7	8.28	133.99	122.90
4	C	1207	NAG	C1-C2-N2	4.06	116.83	110.43
4	A	1207	NAG	C1-C2-N2	4.05	116.82	110.43

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1211	NAG	O5-C5-C6-O6
4	B	1211	NAG	O5-C5-C6-O6
4	A	1211	NAG	O5-C5-C6-O6
4	B	1205	NAG	O5-C5-C6-O6
4	C	1205	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1217	NAG	1	0
4	A	1217	NAG	1	0
4	C	1217	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.

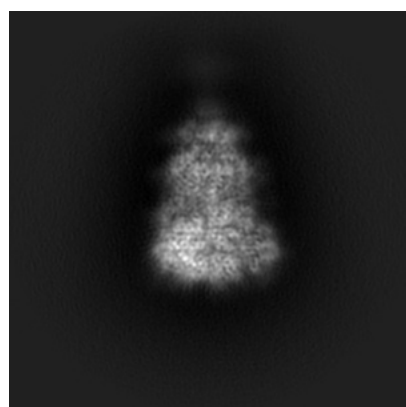
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7063. These allow visual inspection of the internal detail of the map and identification of artifacts.

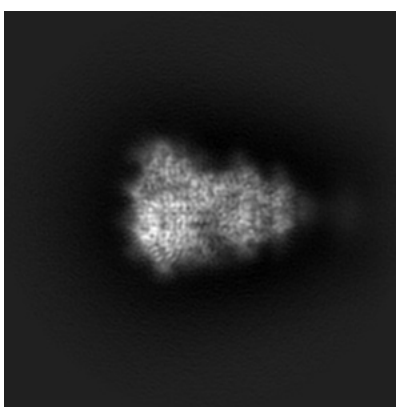
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

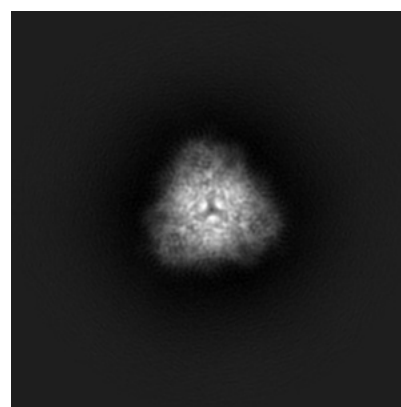
6.1.1 Primary map



X



Y

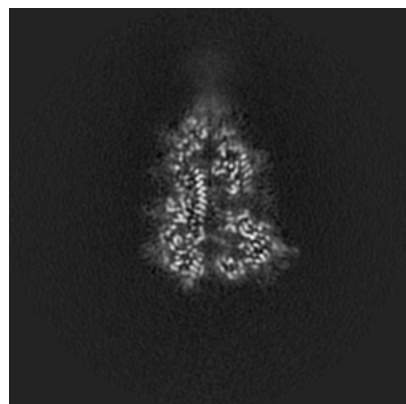


Z

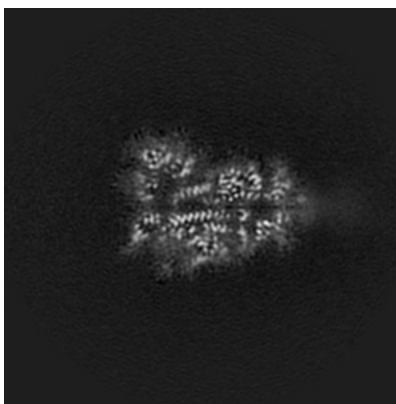
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

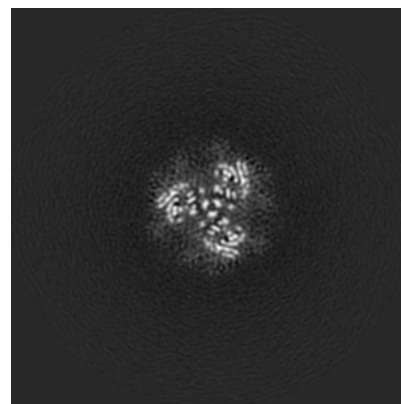
6.2.1 Primary map



X Index: 128



Y Index: 128

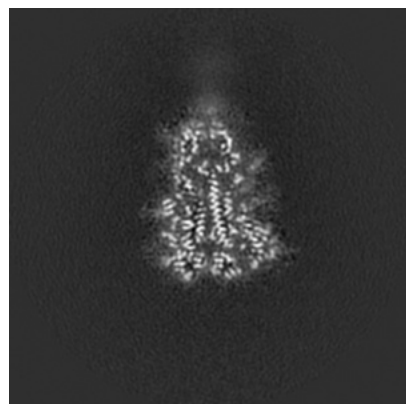


Z Index: 128

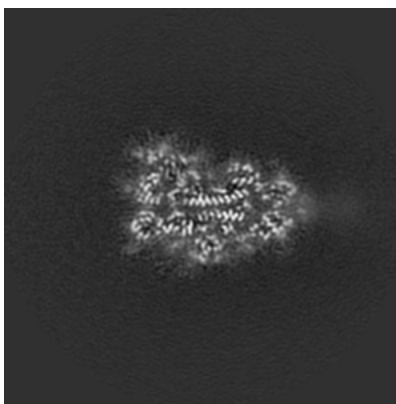
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

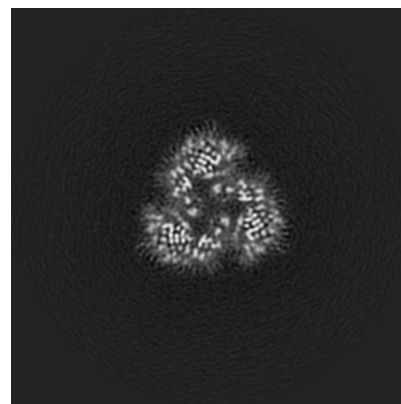
6.3.1 Primary map



X Index: 132



Y Index: 132

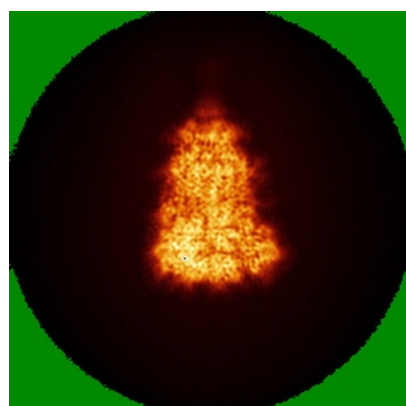


Z Index: 104

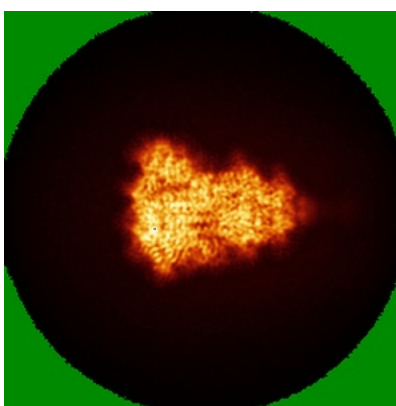
The images above show the largest variance slices of the map in three orthogonal directions.

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

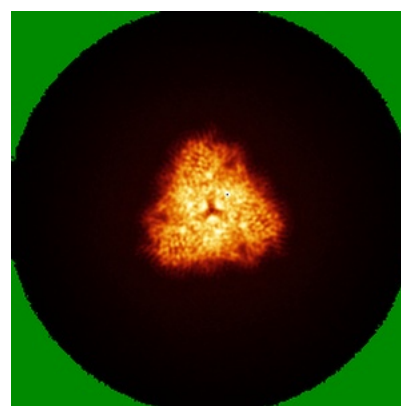
6.4.1 Primary map



X



Y

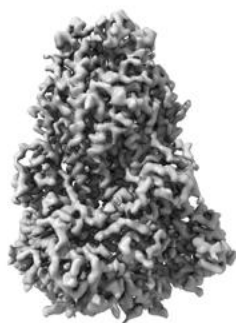


Z

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](#)

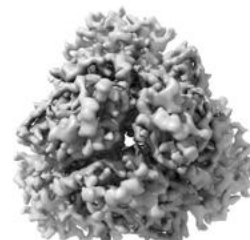
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0468. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

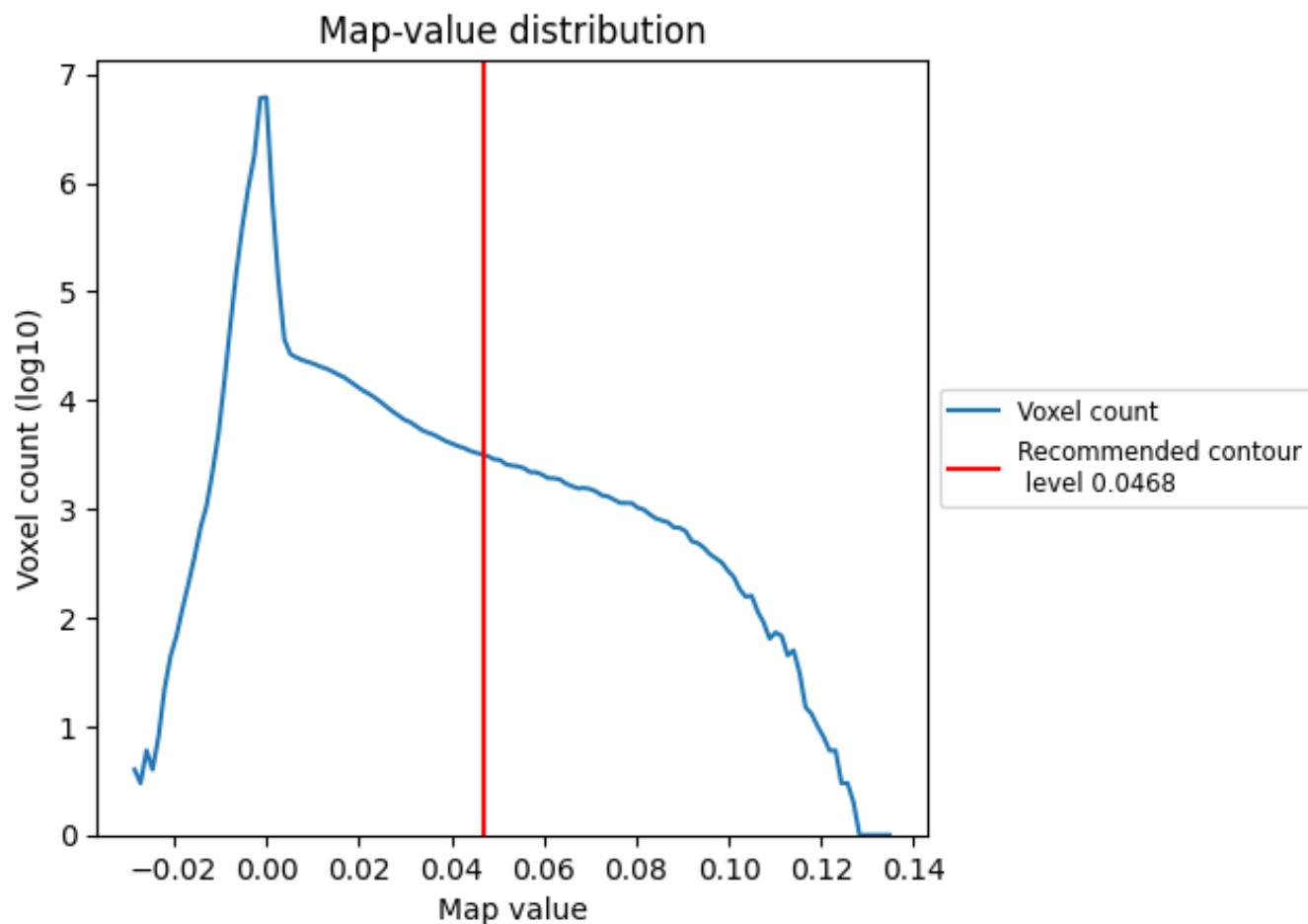
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

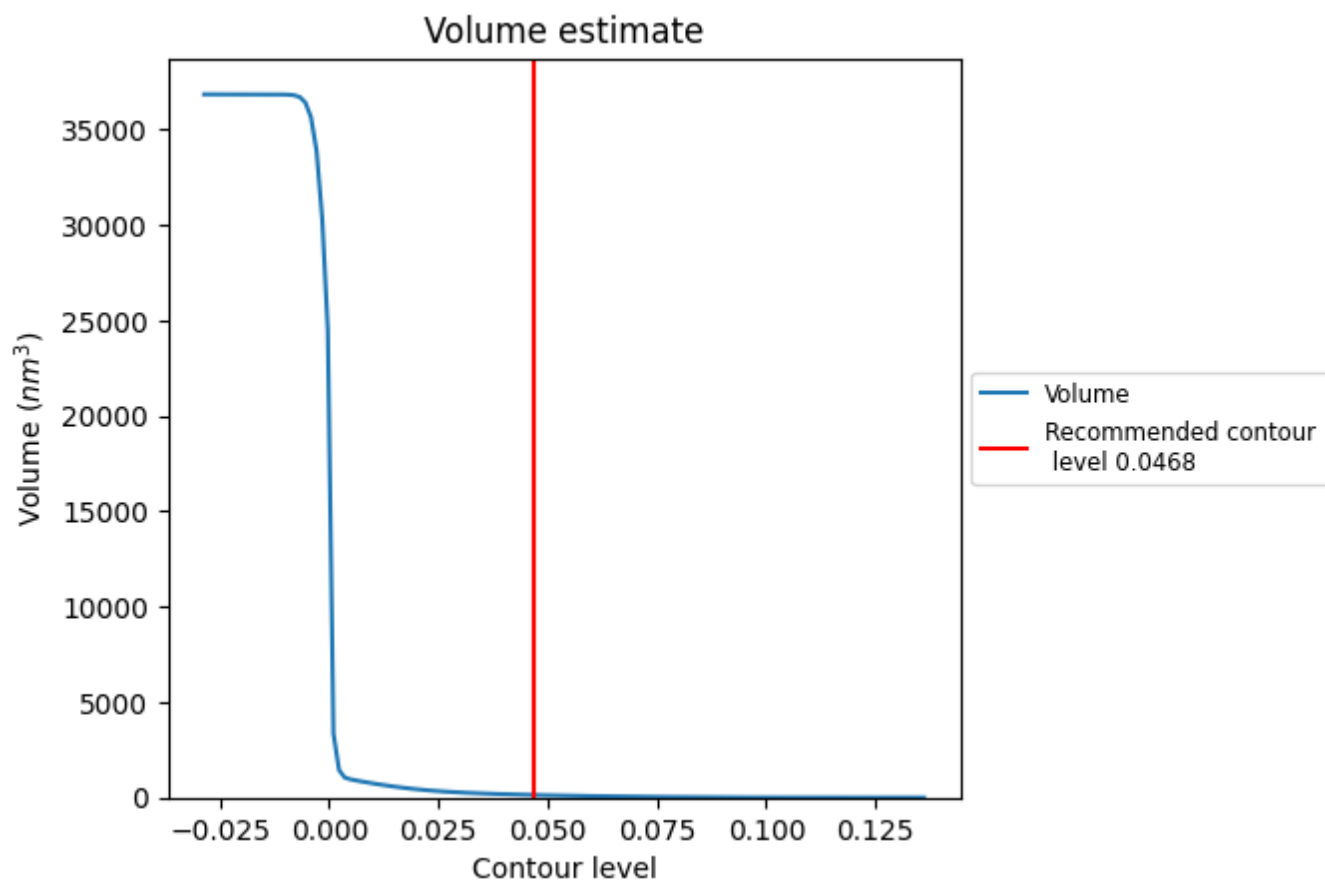
This section contains the results of statistical analysis of the map.

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.

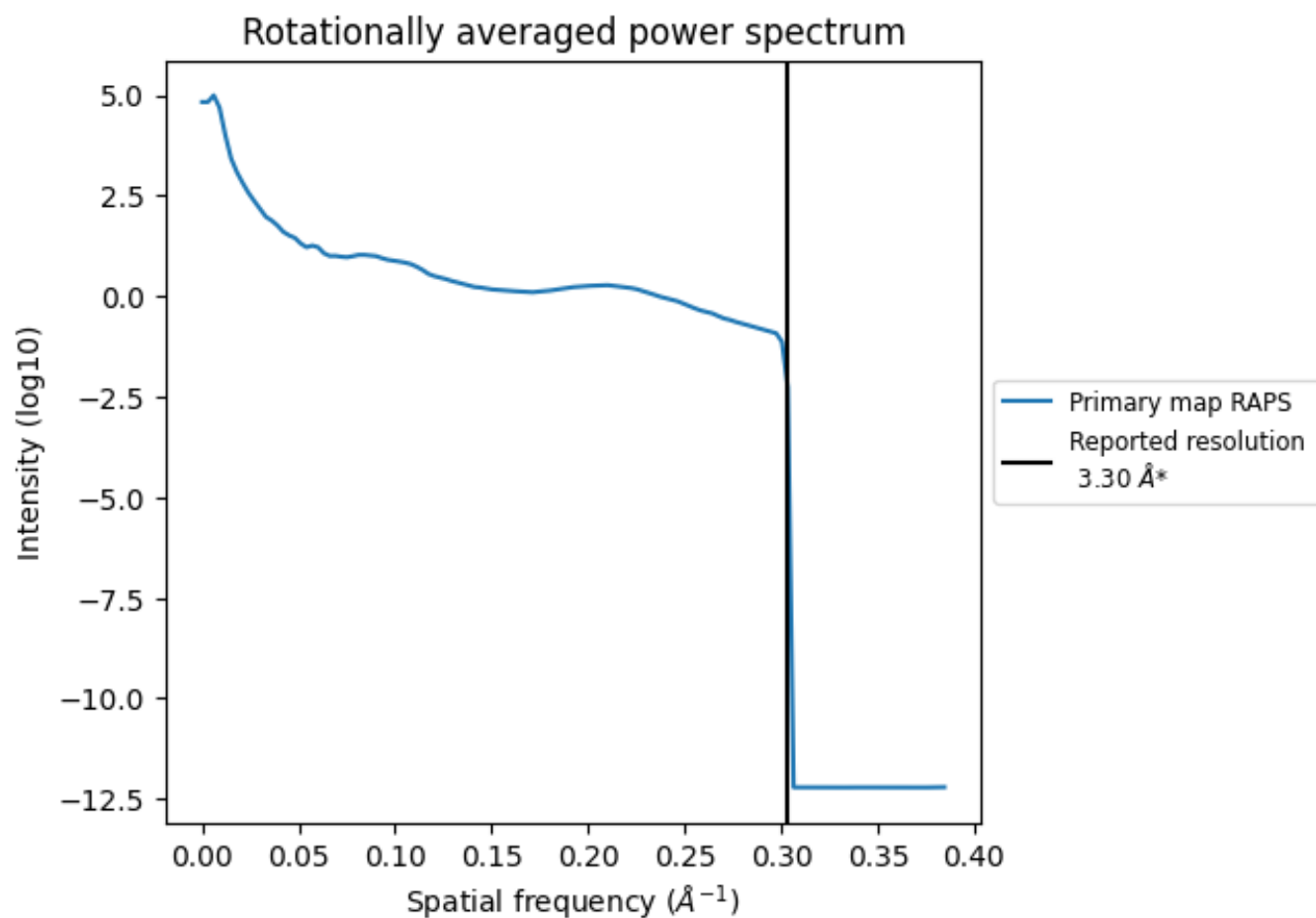
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 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 0.303 Å⁻¹

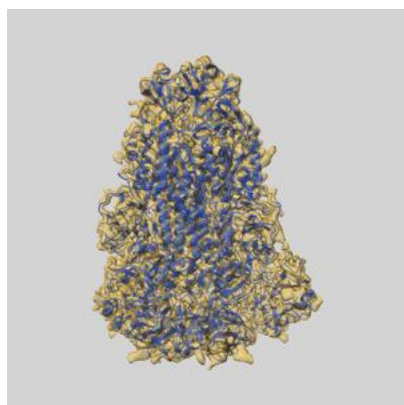
8 Fourier-Shell correlation ⓘ

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

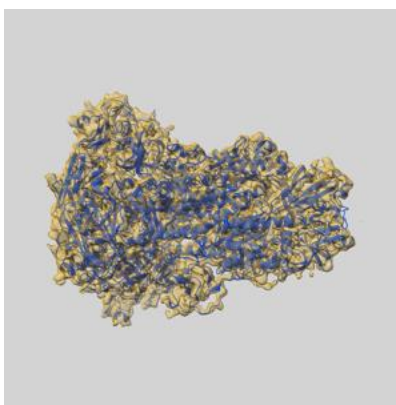
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7063 and PDB model 6B7N. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

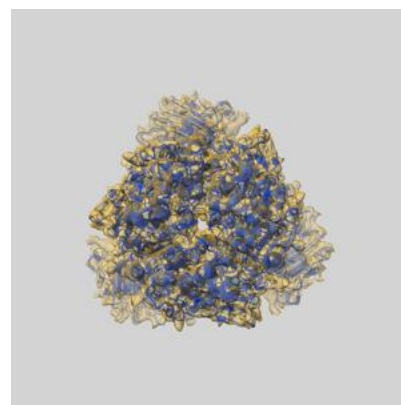
9.1 Map-model overlay [i](#)



X



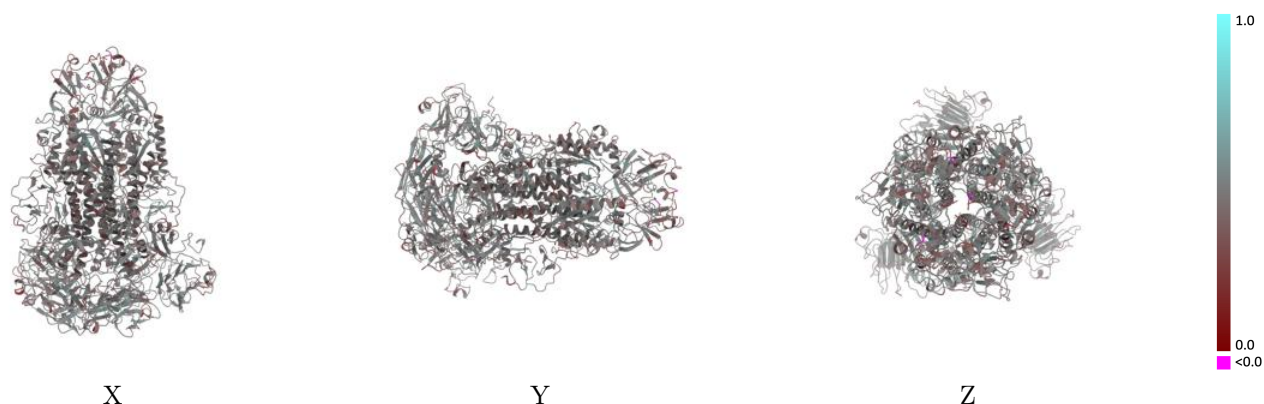
Y



Z

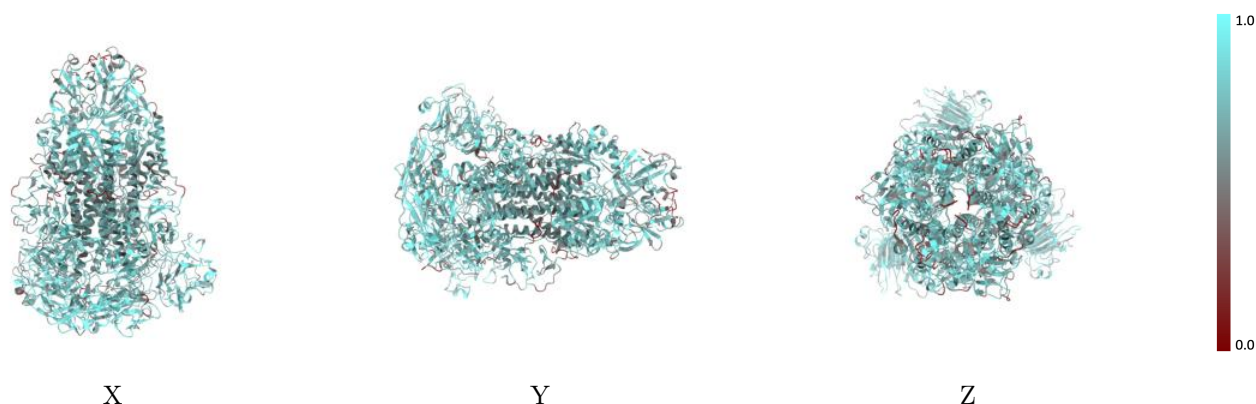
The images above show the 3D surface view of the map at the recommended contour level 0.0468 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



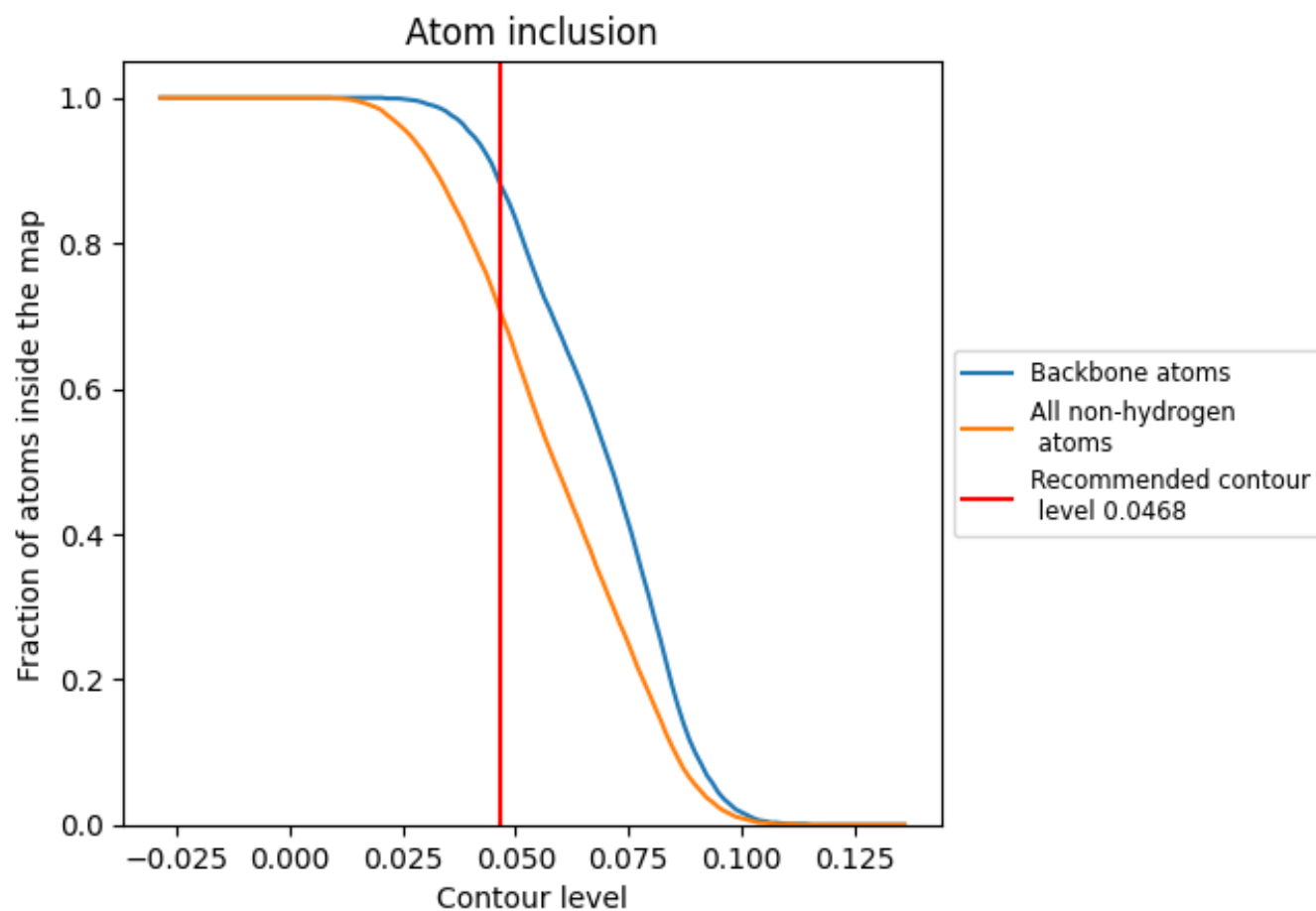
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0468).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (0.0468) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7040	 0.4470
A	 0.7050	 0.4460
B	 0.7070	 0.4480
C	 0.7060	 0.4470
D	 0.6790	 0.4500
E	 0.6430	 0.4430
F	 0.5710	 0.4770
G	 0.6670	 0.4550
H	 0.3930	 0.4130
I	 0.7140	 0.4740
J	 0.6430	 0.4720
K	 0.6070	 0.4780
L	 0.6670	 0.4600
M	 0.3930	 0.4260
N	 0.7140	 0.4680
O	 0.6430	 0.4640
P	 0.6070	 0.4730
Q	 0.6910	 0.4620
R	 0.3930	 0.4200

