



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 02:48 PM EDT

PDB ID : 9OG4 / pdb_00009og4
EMDB ID : EMD-70451
Title : SARS-COV-2-6P-MUT7 S PROTEIN-DY-III-281 complex closed conformation
Authors : Chandravanshi, M.; Niu, L.; Tolbert, W.D.; Pazgier, M.
Deposited on : 2025-04-30
Resolution : 3.56 Å(reported)
Based on initial model : 7RU1

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:

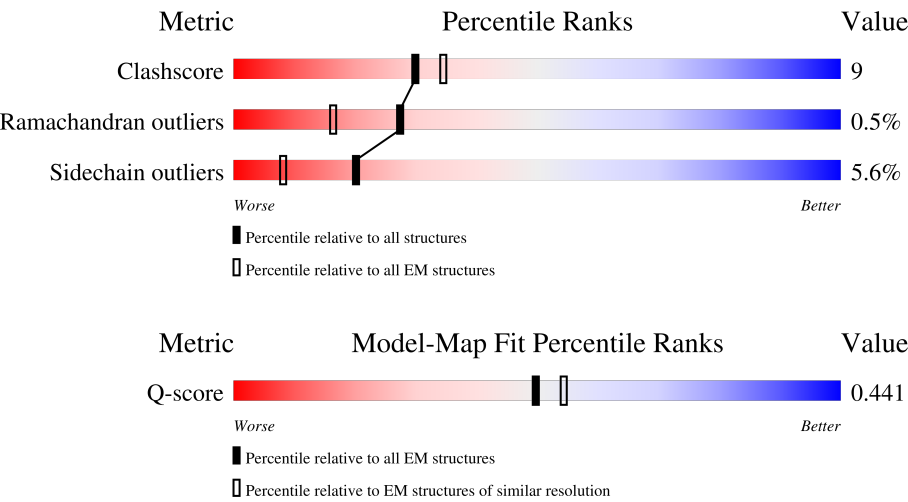
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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.




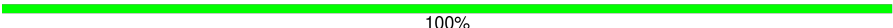

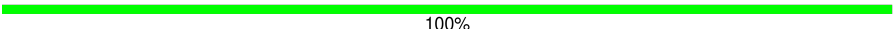
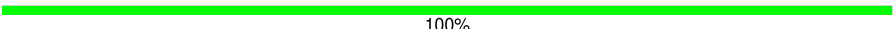
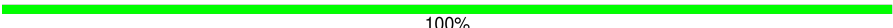



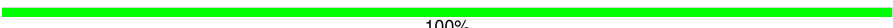


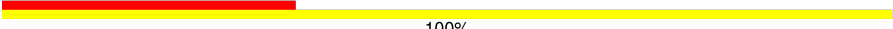



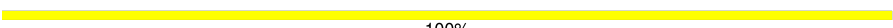
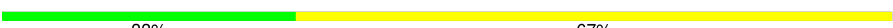
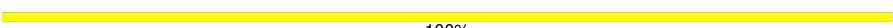
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12750 (3.06 - 4.06)

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	1280	<div><div></div><div>61%19%•18%</div></div>
1	B	1280	<div><div></div><div>65%18%•16%</div></div>
1	C	1280	<div><div></div><div>60%18%•20%</div></div>
2	D	2	<div><div></div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
2	E	2	 50% 50%
2	G	2	 100%
2	H	2	 50% 50%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 50% 50%
2	N	2	 50% 50%
2	O	2	 50% 50%
2	P	2	 100%
2	Q	2	 50% 50%
2	T	2	 50% 50%
3	F	3	 33% 100%
3	I	3	 33% 67%
3	R	3	 67% 33%
3	S	3	 33% 67%
3	U	3	 100%
3	V	3	 33% 67%
3	W	3	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25594 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	1053	Total	C	N	O	S	0	0
			8217	5240	1368	1569	40		
1	C	1025	Total	C	N	O	S	0	0
			7998	5105	1325	1529	39		
1	B	1079	Total	C	N	O	S	0	0
			8434	5379	1407	1606	42		

There are 249 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	705	CYS	VAL	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	883	CYS	THR	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	ALA	-	expression tag	UNP P0DTC2
A	1252	TRP	-	expression tag	UNP P0DTC2
A	1253	SER	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	PRO	-	expression tag	UNP P0DTC2
A	1256	GLN	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	LYS	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	GLY	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	ALA	-	expression tag	UNP P0DTC2
A	1273	TRP	-	expression tag	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	PRO	-	expression tag	UNP P0DTC2
A	1277	GLN	-	expression tag	UNP P0DTC2
A	1278	PHE	-	expression tag	UNP P0DTC2
A	1279	GLU	-	expression tag	UNP P0DTC2
A	1280	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	705	CYS	VAL	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	883	CYS	THR	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	ALA	-	expression tag	UNP P0DTC2
C	1252	TRP	-	expression tag	UNP P0DTC2
C	1253	SER	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	PRO	-	expression tag	UNP P0DTC2
C	1256	GLN	-	expression tag	UNP P0DTC2
C	1257	PHE	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	LYS	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	GLY	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	SER	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1265	GLY	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	ALA	-	expression tag	UNP P0DTC2
C	1273	TRP	-	expression tag	UNP P0DTC2
C	1274	SER	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	PRO	-	expression tag	UNP P0DTC2
C	1277	GLN	-	expression tag	UNP P0DTC2
C	1278	PHE	-	expression tag	UNP P0DTC2
C	1279	GLU	-	expression tag	UNP P0DTC2
C	1280	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	705	CYS	VAL	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	883	CYS	THR	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	ALA	-	expression tag	UNP P0DTC2
B	1252	TRP	-	expression tag	UNP P0DTC2
B	1253	SER	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	PRO	-	expression tag	UNP P0DTC2
B	1256	GLN	-	expression tag	UNP P0DTC2
B	1257	PHE	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	LYS	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	GLY	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	SER	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	ALA	-	expression tag	UNP P0DTC2
B	1273	TRP	-	expression tag	UNP P0DTC2
B	1274	SER	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	PRO	-	expression tag	UNP P0DTC2
B	1277	GLN	-	expression tag	UNP P0DTC2
B	1278	PHE	-	expression tag	UNP P0DTC2
B	1279	GLU	-	expression tag	UNP P0DTC2
B	1280	LYS	-	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.



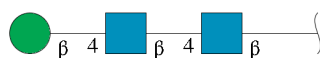
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	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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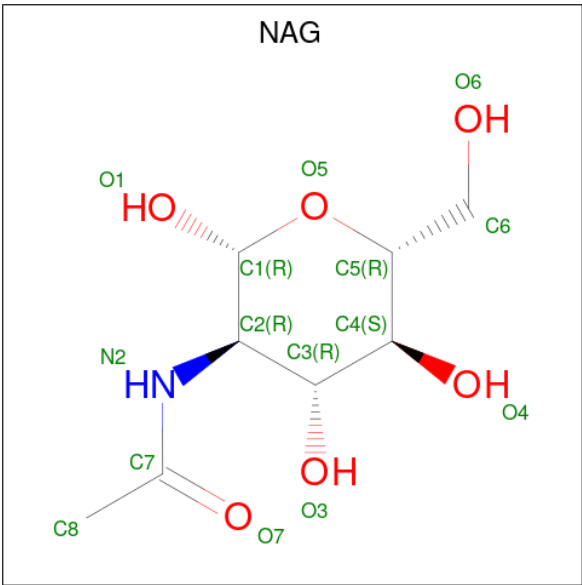
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(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	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	R	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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	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	
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	B	1	Total	C	N	O	0
			14	8	1	5	

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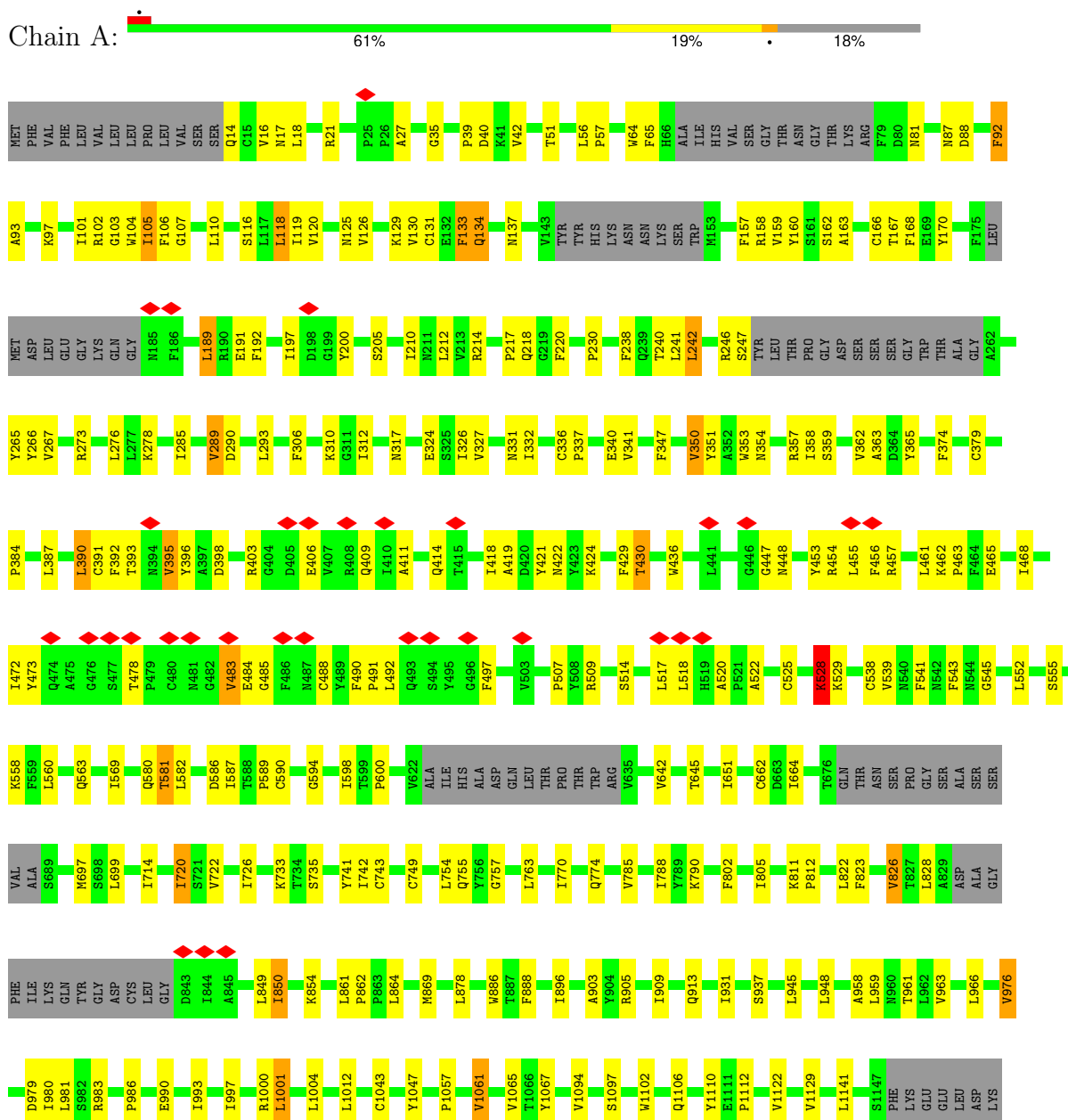
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein







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

Chain D:  100%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%



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

Chain M:



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

Chain N:



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

Chain O:



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

Chain P:



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

Chain Q:



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

Chain T:



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

Chain F:  33% 100%



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

Chain I:  33% 67%



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

Chain R:  67% 67% 33%



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

Chain S:  33% 33% 67%



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

Chain U:  100%



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

Chain V:  33% 67%



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

Chain W:

100%

MAG1
MAG2
EMJ3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.798	Depositor
Minimum map value	-0.399	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.079	Depositor
Map size (Å)	331.13602, 331.13602, 331.13602	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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, BMA

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	0.16	0/8404	0.34	0/11441
1	B	0.14	0/8629	0.32	0/11744
1	C	0.14	0/8182	0.31	0/11138
All	All	0.14	0/25215	0.32	0/34323

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8217	0	8011	171	0
1	B	8434	0	8212	151	0
1	C	7998	0	7773	149	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	28	0	25	1	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	T	28	0	25	0	0
3	F	39	0	34	0	0
3	I	39	0	34	0	0
3	R	39	0	34	0	0
3	S	39	0	34	0	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
3	W	39	0	34	0	0
4	A	56	0	52	0	0
4	B	126	0	117	2	0
4	C	126	0	117	3	0
All	All	25594	0	24845	447	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 9.

All (447) 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:B:318:PHE:HB3	1:B:593:GLY:HA3	1.58	0.86
1:C:406:GLU:HG2	1:C:418:ILE:HG13	1.60	0.84
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.61	0.82
1:C:201:PHE:HB3	1:C:229:LEU:HB3	1.66	0.78
1:C:105:ILE:HB	1:C:239:GLN:HB2	1.67	0.76
1:B:115:GLN:HB2	1:B:233:ILE:HG12	1.68	0.76
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.68	0.76
1:A:409:GLN:HA	1:A:414:GLN:HG2	1.68	0.75
1:B:42:VAL:HG11	1:B:44:ARG:HE	1.53	0.74
1:A:483:VAL:HG12	1:A:485:GLY:H	1.53	0.74
1:B:847:ARG:HB2	1:B:854:LYS:HD2	1.68	0.73
1:C:560:LEU:HD22	1:C:562:PHE:HD1	1.54	0.72
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.72	0.72
1:A:457:ARG:HH12	1:A:461:LEU:HB3	1.53	0.71
1:A:105:ILE:HG23	1:A:118:LEU:HA	1.71	0.71
1:A:276:LEU:HB3	1:A:289:VAL:HG13	1.73	0.70
1:B:189:LEU:HB2	1:B:210:ILE:HD13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:HB2	1:A:563:GLN:HG3	1.73	0.70
1:C:393:THR:HG22	1:C:522:ALA:HA	1.74	0.69
1:C:213:VAL:HG13	1:C:214:ARG:HG2	1.77	0.66
1:B:320:VAL:HA	1:B:631:PRO:HG2	1.78	0.65
1:A:896:ILE:HG13	1:B:712:ILE:HG13	1.77	0.65
1:A:757:GLY:HA3	1:B:965:GLN:HE22	1.60	0.65
1:C:276:LEU:HD11	1:C:301:CYS:HA	1.78	0.65
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.79	0.65
1:A:478:THR:HG21	1:A:488:CYS:HB3	1.79	0.64
1:C:1103:PHE:HZ	2:M:1:NAG:H62	1.62	0.64
1:B:16:VAL:HG23	4:B:1301:NAG:H82	1.80	0.64
1:C:86:PHE:HB2	1:C:238:PHE:HD2	1.63	0.64
1:B:886:TRP:CD1	1:B:886:TRP:H	2.16	0.63
1:C:560:LEU:HB3	1:C:563:GLN:HG3	1.81	0.62
1:A:391:CYS:H	1:A:518:LEU:HD21	1.63	0.62
1:B:327:VAL:HG12	1:B:542:ASN:HB3	1.81	0.62
1:A:518:LEU:HD22	1:A:545:GLY:HA3	1.79	0.62
1:A:699:LEU:HD21	1:C:869:MET:HG2	1.82	0.62
1:A:14:GLN:HA	1:A:158:ARG:HH21	1.65	0.61
1:B:19:THR:HG23	1:B:20:THR:HG23	1.81	0.61
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.83	0.61
1:B:18:LEU:HD11	1:B:244:LEU:HD11	1.83	0.61
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.82	0.61
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.83	0.61
1:A:133:PHE:HB3	1:A:163:ALA:H	1.65	0.61
1:B:214:ARG:HH21	1:B:215:ASP:HB2	1.64	0.61
1:A:35:GLY:HA3	1:A:56:LEU:HD23	1.83	0.60
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.83	0.60
1:C:378:LYS:HB3	1:C:380:TYR:HE1	1.66	0.60
1:B:193:VAL:HG13	1:B:204:TYR:HB2	1.82	0.60
1:C:1129:VAL:HG13	1:B:917:TYR:HB3	1.84	0.60
1:A:220:PHE:HE2	1:A:285:ILE:HG22	1.66	0.60
1:A:210:ILE:HD12	1:A:217:PRO:HG3	1.84	0.59
1:C:659:SER:HB3	1:C:698:SER:HB3	1.85	0.59
1:C:404:GLY:HA3	1:C:505:TYR:HA	1.85	0.59
1:C:742:ILE:HD13	1:C:1000:ARG:HB3	1.83	0.59
1:B:409:GLN:HE22	1:B:416:GLY:HA3	1.68	0.59
1:A:411:ALA:HB3	1:A:414:GLN:HB2	1.85	0.59
1:A:429:PHE:HE1	1:A:514:SER:HB2	1.68	0.58
1:B:200:TYR:HB3	1:B:230:PRO:HA	1.85	0.58
1:C:234:ASN:HB3	4:C:1307:NAG:O5	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ILE:HD11	1:B:239:GLN:HB3	1.85	0.58
1:A:354:ASN:O	1:A:398:ASP:HA	2.03	0.58
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.86	0.58
1:C:353:TRP:HB3	1:C:400:PHE:HB3	1.84	0.58
1:B:100:ILE:HG23	1:B:243:ALA:H	1.69	0.58
1:B:529:LYS:HE3	1:B:530:SER:H	1.68	0.58
1:B:945:LEU:HD23	1:B:948:LEU:HD12	1.84	0.57
1:B:523:THR:HG23	1:B:524:VAL:HG12	1.86	0.57
1:B:81:ASN:HD21	1:B:242:LEU:HD13	1.68	0.57
1:A:390:LEU:HB3	1:A:518:LEU:HD11	1.87	0.57
1:A:869:MET:HG2	1:B:699:LEU:HD11	1.87	0.57
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.86	0.57
1:C:34:ARG:HD2	1:C:216:LEU:HD13	1.87	0.57
1:B:213:VAL:HG22	1:B:214:ARG:H	1.70	0.57
1:B:847:ARG:H	1:B:847:ARG:HE	1.52	0.57
1:A:770:ILE:O	1:A:774:GLN:HG2	2.05	0.57
1:C:318:PHE:H	1:C:593:GLY:HA3	1.70	0.57
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.86	0.57
1:B:403:ARG:HH11	1:B:495:TYR:HE2	1.53	0.57
1:B:452:LEU:HA	1:B:494:SER:HA	1.88	0.56
1:B:555:SER:HB3	1:B:584:ILE:HG22	1.86	0.56
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.87	0.56
1:A:324:GLU:H	1:A:539:VAL:HG12	1.71	0.56
1:C:656:VAL:HA	4:C:1309:NAG:H82	1.88	0.56
1:B:69:HIS:HA	1:B:77:LYS:HA	1.88	0.55
1:B:58:PHE:HD2	1:B:290:ASP:HB2	1.71	0.55
1:B:452:LEU:HD12	1:B:492:LEU:HB3	1.88	0.55
1:A:197:ILE:O	1:A:200:TYR:HB2	2.07	0.55
1:C:353:TRP:CD1	1:C:353:TRP:H	2.23	0.55
1:B:351:TYR:HB2	1:B:492:LEU:HD11	1.89	0.55
1:A:120:VAL:HG12	1:A:126:VAL:HG13	1.89	0.55
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.88	0.55
1:A:461:LEU:HD12	1:A:465:GLU:HB3	1.88	0.55
1:B:760:CYS:HA	1:B:763:LEU:HG	1.88	0.55
1:C:342:PHE:HE2	1:C:434:ILE:HG21	1.71	0.55
1:B:442:ASP:HB3	1:B:451:TYR:HE2	1.71	0.55
1:B:328:ARG:NH1	1:B:533:LEU:HB3	2.22	0.55
1:B:724:THR:HG23	1:B:934:ILE:HD11	1.88	0.55
1:C:592:PHE:HE2	1:B:857:GLY:H	1.53	0.54
1:B:185:ASN:HB3	1:B:187:LYS:HE2	1.89	0.54
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ILE:HG21	1:A:543:PHE:HE1	1.72	0.54
1:C:424:LYS:HB3	1:C:463:PRO:HA	1.90	0.54
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.88	0.54
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.71	0.54
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.73	0.54
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.90	0.54
1:C:233:ILE:HB	1:C:235:ILE:HD11	1.88	0.54
1:B:431:GLY:HA2	1:B:515:PHE:CD2	2.42	0.54
1:C:106:PHE:HZ	1:C:194:PHE:HD2	1.56	0.54
1:B:337:PRO:HD2	1:B:358:ILE:HG23	1.90	0.54
1:C:64:TRP:HZ3	1:C:214:ARG:HH22	1.55	0.54
1:C:560:LEU:HD11	1:B:223:LEU:HD23	1.90	0.54
1:B:124:THR:HG22	1:B:176:LEU:HD23	1.89	0.53
1:C:117:LEU:HD23	1:C:130:VAL:HG22	1.90	0.53
1:A:472:ILE:HG13	1:A:484:GLU:HG3	1.90	0.53
1:A:580:GLN:HG3	1:A:581:THR:H	1.73	0.53
1:A:823:PHE:HD1	1:A:1057:PRO:HG3	1.73	0.53
1:A:101:ILE:HA	1:A:242:LEU:HB3	1.90	0.53
1:A:785:VAL:HG11	1:A:888:PHE:HE2	1.73	0.53
1:A:1129:VAL:HG13	1:C:917:TYR:HB3	1.91	0.53
1:C:378:LYS:HB3	1:C:380:TYR:CE1	2.44	0.52
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.92	0.52
1:B:560:LEU:HB2	1:B:563:GLN:HG3	1.91	0.52
1:B:777:ASN:HD21	1:B:1019:ARG:HA	1.73	0.52
1:C:132:GLU:HB2	1:C:164:ASN:HB2	1.90	0.52
1:C:480:CYS:HB2	1:C:483:VAL:HG12	1.91	0.52
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.92	0.52
1:A:993:ILE:O	1:A:997:ILE:HG12	2.10	0.52
1:B:742:ILE:HG21	1:B:753:LEU:HD13	1.92	0.52
1:A:1110:TYR:CZ	1:A:1112:PRO:HG3	2.44	0.52
1:A:945:LEU:HD13	1:A:948:LEU:HD12	1.91	0.51
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.90	0.51
1:C:622:VAL:HG13	1:C:638:THR:H	1.75	0.51
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.92	0.51
1:C:1024:LEU:HD11	1:C:1028:LYS:HE2	1.93	0.51
1:B:97:LYS:NZ	1:B:188:ASN:H	2.09	0.51
1:A:976:VAL:HG13	1:A:979:ASP:HB2	1.92	0.51
1:A:983:ARG:HG2	1:B:390:LEU:HD11	1.92	0.51
1:C:105:ILE:HG13	1:C:241:LEU:HD11	1.93	0.51
1:C:332:ILE:HD13	1:C:360:ASN:HB3	1.92	0.51
1:C:206:LYS:HB3	1:C:223:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD11	1:C:233:ILE:HD13	1.92	0.51
1:C:553:THR:HG23	1:C:586:ASP:HB2	1.93	0.51
1:C:959:LEU:O	1:C:963:VAL:HG23	2.10	0.51
1:B:86:PHE:HE1	1:B:90:VAL:HG22	1.76	0.51
1:A:436:TRP:CZ3	1:A:509:ARG:HB2	2.46	0.50
1:B:821:LEU:HD22	1:B:935:GLN:HG3	1.92	0.50
1:B:130:VAL:HG12	1:B:168:PHE:HD2	1.76	0.50
1:B:770:ILE:O	1:B:774:GLN:HG2	2.11	0.50
1:A:430:THR:HG21	1:A:517:LEU:HD13	1.93	0.50
1:A:986:PRO:O	1:A:990:GLU:HG2	2.11	0.50
1:B:206:LYS:HE2	1:B:221:SER:HB3	1.93	0.50
1:B:642:VAL:HG23	1:B:651:ILE:HD11	1.93	0.50
1:C:64:TRP:HE1	1:C:264:ALA:HA	1.76	0.50
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.94	0.50
1:A:40:ASP:HB3	1:A:42:VAL:HG22	1.93	0.50
1:C:328:ARG:NH1	1:C:580:GLN:HG3	2.26	0.50
1:A:742:ILE:HG12	1:A:1000:ARG:HB3	1.94	0.50
1:B:452:LEU:HD23	1:B:452:LEU:H	1.77	0.50
1:C:329:PHE:CE2	1:C:528:LYS:HB3	2.47	0.50
1:C:329:PHE:HE2	1:C:528:LYS:HB3	1.76	0.50
1:A:642:VAL:HG22	1:A:651:ILE:HG12	1.94	0.49
1:A:790:LYS:H	1:A:790:LYS:HZ2	1.59	0.49
1:A:811:LYS:HD2	1:A:812:PRO:HD2	1.93	0.49
1:C:118:LEU:HD13	1:C:135:PHE:HE1	1.77	0.49
1:B:302:THR:HG21	1:B:315:THR:HG22	1.94	0.49
1:A:826:VAL:HG23	1:A:945:LEU:HD12	1.93	0.49
1:C:452:LEU:HD12	1:C:492:LEU:HD22	1.95	0.49
1:C:707:TYR:HE1	1:B:897:PRO:HA	1.77	0.49
1:B:171:VAL:HG12	1:B:171:VAL:O	2.12	0.49
1:A:81:ASN:OD1	1:A:242:LEU:HD21	2.11	0.49
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.95	0.49
1:C:168:PHE:CD2	1:C:231:ILE:HD11	2.48	0.49
1:B:319:ARG:HH12	1:B:589:PRO:HB2	1.77	0.49
1:A:379:CYS:SG	1:A:384:PRO:HG3	2.53	0.49
1:B:100:ILE:HA	1:B:243:ALA:HB3	1.95	0.49
1:C:110:LEU:HB3	1:C:135:PHE:HD2	1.77	0.49
1:B:328:ARG:HH21	1:B:580:GLN:HG3	1.77	0.49
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.52	0.49
1:A:129:LYS:HZ2	1:A:166:CYS:HB3	1.77	0.49
1:A:106:PHE:HA	1:A:238:PHE:HA	1.94	0.48
1:A:424:LYS:HB3	1:A:463:PRO:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLN:HB3	1:A:419:ALA:HB2	1.94	0.48
1:C:433:VAL:HG22	1:C:512:VAL:HG22	1.95	0.48
1:A:569:ILE:HD12	1:A:569:ILE:H	1.78	0.48
1:A:979:ASP:O	1:A:983:ARG:HB2	2.13	0.48
1:B:777:ASN:O	1:B:781:VAL:HG23	2.13	0.48
1:A:310:LYS:HG2	1:A:664:ILE:HD11	1.93	0.48
1:A:157:PHE:CG	1:A:157:PHE:O	2.66	0.48
1:A:351:TYR:HB2	1:A:454:ARG:HH12	1.79	0.48
1:A:353:TRP:CD1	1:A:353:TRP:H	2.31	0.48
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.49	0.48
1:B:33:THR:HA	1:B:58:PHE:HE1	1.78	0.48
1:B:441:LEU:HB3	1:B:509:ARG:HH21	1.78	0.48
1:A:357:ARG:HH11	1:A:396:TYR:HE1	1.61	0.48
1:C:160:TYR:H	1:C:160:TYR:HD1	1.61	0.48
1:C:336:CYS:HB3	1:C:361:CYS:HB2	1.67	0.48
1:B:452:LEU:HG	1:B:492:LEU:HD12	1.95	0.48
1:B:847:ARG:H	1:B:847:ARG:NE	2.11	0.48
1:A:528:LYS:HA	1:A:528:LYS:HD3	1.66	0.48
1:C:878:LEU:O	1:C:882:ILE:HD12	2.14	0.48
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.95	0.48
1:A:104:TRP:O	1:A:119:ILE:HB	2.13	0.48
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.65	0.48
1:C:418:ILE:HD13	1:C:422:ASN:HD21	1.79	0.47
1:C:118:LEU:HD11	1:C:159:VAL:HG11	1.95	0.47
1:A:131:CYS:HB2	1:A:133:PHE:CD2	2.49	0.47
1:B:103:GLY:HA3	1:B:119:ILE:O	2.13	0.47
1:A:869:MET:HG2	1:B:699:LEU:HD21	1.97	0.47
1:A:959:LEU:O	1:A:963:VAL:HG23	2.15	0.47
1:C:141:LEU:HD21	1:C:157:PHE:HE1	1.79	0.47
1:B:276:LEU:HB3	1:B:289:VAL:HG22	1.96	0.47
1:A:448:ASN:H	1:A:497:PHE:HB3	1.79	0.47
1:C:984:LEU:HB3	1:C:989:ALA:HB2	1.96	0.47
1:B:357:ARG:HD2	1:B:394:ASN:HD22	1.78	0.47
1:A:742:ILE:HD13	1:A:1001:LEU:HD12	1.96	0.47
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.50	0.47
1:A:886:TRP:H	1:A:886:TRP:CD1	2.32	0.47
1:C:1029:MET:HE2	1:C:1029:MET:HB2	1.80	0.47
1:B:886:TRP:HB3	1:B:1035:GLY:HA2	1.97	0.47
1:A:212:LEU:HG	1:A:214:ARG:HB3	1.96	0.47
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.97	0.47
1:A:189:LEU:HD21	1:A:210:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LEU:HB3	1:C:285:ILE:HD12	1.96	0.46
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.74	0.46
1:A:27:ALA:HB3	1:A:64:TRP:HE1	1.81	0.46
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.56	0.46
1:A:714:ILE:HD11	1:A:1094:VAL:HG21	1.96	0.46
1:A:864:LEU:HD21	1:B:697:MET:HE3	1.97	0.46
1:C:560:LEU:HD23	1:C:561:PRO:HD2	1.96	0.46
1:A:65:PHE:HB2	1:A:265:TYR:CE1	2.51	0.46
1:A:805:ILE:HB	1:A:878:LEU:HD21	1.98	0.46
1:A:983:ARG:O	1:B:382:VAL:HA	2.16	0.46
1:A:1094:VAL:HG12	1:C:904:TYR:OH	2.15	0.46
1:B:921:LYS:HD2	1:B:921:LYS:HA	1.68	0.46
1:B:490:PHE:HD1	1:B:491:PRO:HD2	1.80	0.46
1:B:852:ALA:HA	1:B:855:PHE:CE2	2.50	0.46
1:C:192:PHE:HB3	1:C:194:PHE:CE1	2.50	0.46
1:A:312:ILE:HD12	1:A:598:ILE:HG12	1.97	0.46
1:C:417:LYS:O	1:C:421:TYR:HB2	2.16	0.46
1:C:418:ILE:HG23	1:C:422:ASN:HD21	1.79	0.46
1:A:390:LEU:HB2	1:A:392:PHE:CE1	2.51	0.46
1:B:454:ARG:HD3	1:B:457:ARG:HG2	1.98	0.46
1:B:733:LYS:HE3	1:B:771:ALA:HB1	1.97	0.46
1:A:131:CYS:HA	1:A:166:CYS:HA	1.98	0.46
1:A:332:ILE:HG22	1:A:362:VAL:HG23	1.98	0.46
1:A:357:ARG:HD3	1:A:396:TYR:CE1	2.51	0.46
1:C:126:VAL:HG21	1:C:174:PRO:HD2	1.97	0.46
1:C:483:VAL:HG22	1:C:484:GLU:H	1.81	0.46
1:C:697:MET:SD	1:B:869:MET:HE1	2.55	0.46
1:B:327:VAL:HB	1:B:329:PHE:CE1	2.51	0.46
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.97	0.45
1:C:277:LEU:HB3	1:C:285:ILE:HG23	1.97	0.45
1:A:16:VAL:HG13	1:A:18:LEU:H	1.81	0.45
1:A:357:ARG:HE	1:A:359:SER:HB3	1.81	0.45
1:A:365:TYR:CD2	1:A:387:LEU:HG	2.51	0.45
1:C:922:LEU:HD11	1:C:926:GLN:HE21	1.80	0.45
1:A:589:PRO:HG3	1:C:855:PHE:HA	1.97	0.45
1:B:567:ARG:HG3	1:B:571:ASP:HA	1.98	0.45
1:B:165:ASN:HB2	4:B:1304:NAG:H2	1.99	0.45
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.97	0.45
1:C:92:PHE:HB3	1:C:192:PHE:HB2	1.99	0.45
1:C:94:SER:HB2	1:C:190:ARG:O	2.17	0.45
1:C:449:TYR:CE1	1:C:496:GLY:HA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:SER:HB2	1:C:586:ASP:OD1	2.17	0.45
1:C:623:ALA:O	1:C:625:HIS:N	2.49	0.45
1:B:352:ALA:HB1	1:B:466:ARG:HH21	1.81	0.45
1:C:578:ASP:HB3	1:C:581:THR:O	2.17	0.45
1:B:97:LYS:NZ	1:B:187:LYS:H	2.14	0.45
1:A:87:ASN:HB3	1:A:88:ASP:H	1.55	0.45
1:C:355:ARG:HE	1:C:396:TYR:HD2	1.65	0.45
1:A:103:GLY:HA3	1:A:241:LEU:HD23	1.99	0.45
1:A:16:VAL:HG22	1:A:17:ASN:H	1.82	0.44
1:A:168:PHE:CZ	1:A:170:TYR:HB2	2.52	0.44
1:A:754:LEU:HD23	1:A:754:LEU:HA	1.85	0.44
1:C:312:ILE:HG13	1:C:664:ILE:HG22	1.98	0.44
1:B:898:PHE:CZ	1:B:1050:MET:HE1	2.51	0.44
1:A:849:LEU:C	1:A:850:ILE:HG12	2.41	0.44
1:C:854:LYS:HD2	1:C:855:PHE:H	1.82	0.44
1:A:363:ALA:HB1	1:A:365:TYR:HE1	1.82	0.44
1:A:905:ARG:O	1:A:909:ILE:HG23	2.16	0.44
1:C:302:THR:HG21	1:C:315:THR:HG22	1.99	0.44
1:B:38:TYR:HE1	1:B:285:ILE:HG13	1.82	0.44
1:B:154:GLU:HB2	1:B:157:PHE:HE1	1.81	0.44
1:C:118:LEU:HD13	1:C:135:PHE:CE1	2.53	0.44
1:C:475:ALA:H	1:C:488:CYS:HA	1.82	0.44
1:C:84:LEU:HD13	1:C:84:LEU:HA	1.81	0.44
1:B:714:ILE:HD12	1:B:1096:VAL:HG21	1.98	0.44
1:A:350:VAL:HG11	1:A:403:ARG:HH12	1.83	0.44
1:A:365:TYR:HD2	1:A:387:LEU:HG	1.83	0.44
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.89	0.44
1:C:562:PHE:CE2	1:B:225:PRO:HG2	2.52	0.44
1:B:69:HIS:HD2	1:B:77:LYS:HD2	1.81	0.44
1:B:929:SER:O	1:B:933:LYS:HG2	2.18	0.44
1:A:453:TYR:CE1	1:A:455:LEU:HB2	2.52	0.44
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.99	0.44
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.85	0.44
1:B:790:LYS:HE3	1:B:790:LYS:HB3	1.80	0.44
1:A:191:GLU:O	1:A:205:SER:HA	2.17	0.44
1:A:374:PHE:HA	1:A:436:TRP:HB3	2.00	0.44
1:C:418:ILE:HD13	1:C:422:ASN:ND2	2.32	0.44
1:C:641:ASN:HB3	1:C:653:ALA:H	1.82	0.44
1:C:624:ILE:H	1:C:624:ILE:HG12	1.38	0.43
1:C:931:ILE:O	1:C:934:ILE:HG22	2.18	0.43
1:B:402:ILE:HD11	1:B:407:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:HD3	1:B:495:TYR:HE2	1.81	0.43
1:C:121:ASN:HA	1:C:126:VAL:HG13	2.00	0.43
1:C:452:LEU:HB3	1:C:492:LEU:HD22	1.99	0.43
1:C:1041:ASP:HB3	1:B:1030:SER:OG	2.18	0.43
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.89	0.43
1:C:205:SER:HB3	1:C:226:LEU:HD11	2.00	0.43
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.99	0.43
1:B:86:PHE:CE1	1:B:90:VAL:HG22	2.52	0.43
1:A:97:LYS:HA	1:A:97:LYS:HD3	1.76	0.43
1:A:129:LYS:HG3	1:A:168:PHE:O	2.18	0.43
1:B:117:LEU:HD13	1:B:231:ILE:HD11	2.01	0.43
1:A:347:PHE:CE2	1:A:509:ARG:HB3	2.53	0.43
1:C:320:VAL:HG12	1:C:591:SER:HB2	2.00	0.43
1:B:120:VAL:HB	1:B:127:VAL:HB	2.00	0.43
1:B:552:LEU:HG	1:B:585:LEU:HB3	1.99	0.43
1:A:447:GLY:HA2	1:A:497:PHE:HB3	2.00	0.43
1:C:61:ASN:HB3	4:C:1304:NAG:O5	2.18	0.43
1:A:134:GLN:H	1:A:162:SER:HB2	1.84	0.43
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.85	0.43
1:C:562:PHE:HE2	1:B:41:LYS:HG3	1.84	0.43
1:B:196:ASN:HB3	1:B:201:PHE:CD1	2.53	0.43
1:B:402:ILE:HD12	1:B:406:GLU:HG3	2.00	0.43
1:A:246:ARG:HB3	1:A:247:SER:H	1.64	0.43
1:A:357:ARG:HD3	1:A:396:TYR:HE1	1.83	0.43
1:A:422:ASN:HD21	1:A:454:ARG:H	1.65	0.43
1:B:991:VAL:O	1:B:995:ARG:HG3	2.19	0.43
1:A:107:GLY:HA2	1:A:116:SER:HA	2.01	0.43
1:A:406:GLU:HG2	1:A:418:ILE:HG13	2.01	0.43
1:A:456:PHE:HD2	1:A:491:PRO:HA	1.84	0.43
1:B:31:SER:HB3	1:B:56:LEU:HD21	2.01	0.43
1:A:102:ARG:H	1:A:242:LEU:HA	1.82	0.42
1:C:770:ILE:O	1:C:774:GLN:HG2	2.19	0.42
1:C:777:ASN:HD21	1:C:1019:ARG:HA	1.84	0.42
1:C:1086:LYS:HE2	1:C:1122:VAL:HG11	2.01	0.42
1:B:805:ILE:HB	1:B:878:LEU:HD11	2.00	0.42
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.54	0.42
1:C:473:TYR:H	1:C:491:PRO:HD3	1.85	0.42
1:C:621:PRO:HA	1:C:638:THR:HG23	2.01	0.42
1:C:741:TYR:CD2	1:C:1004:LEU:HD13	2.54	0.42
1:B:39:PRO:HG2	1:B:51:THR:HG21	2.00	0.42
1:A:456:PHE:HB3	1:A:473:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:CZ	1:A:507:PRO:HG3	2.55	0.42
1:A:39:PRO:HB3	1:A:51:THR:HG21	2.01	0.42
1:A:106:PHE:CD1	1:A:106:PHE:N	2.86	0.42
1:A:552:LEU:HB3	1:A:587:ILE:HG12	2.01	0.42
1:C:39:PRO:HG3	1:C:51:THR:HG21	2.00	0.42
1:C:614:ASP:O	1:C:615:VAL:HG22	2.19	0.42
1:B:357:ARG:HD2	1:B:394:ASN:ND2	2.34	0.42
1:B:117:LEU:HD11	1:B:119:ILE:HD11	2.01	0.42
1:A:212:LEU:HG	1:A:214:ARG:H	1.84	0.42
1:A:558:LYS:HD2	1:A:558:LYS:HA	1.82	0.42
1:A:790:LYS:HE3	1:A:790:LYS:HB3	1.96	0.42
1:C:263:ALA:HB1	1:C:265:TYR:CE2	2.53	0.42
1:C:326:ILE:HD13	1:C:326:ILE:HA	1.83	0.42
1:C:326:ILE:HG12	1:C:539:VAL:HG11	2.01	0.42
1:C:1046:GLY:HA2	1:B:890:ALA:HB1	2.01	0.42
1:B:69:HIS:HB2	1:B:77:LYS:HG3	2.02	0.42
1:B:141:LEU:HD12	1:B:142:GLY:H	1.83	0.42
1:B:770:ILE:HD11	1:B:1012:LEU:HA	2.02	0.42
1:A:290:ASP:HB3	1:A:293:LEU:HB2	2.01	0.42
1:A:326:ILE:HD13	1:A:326:ILE:HA	1.88	0.42
1:A:391:CYS:HB3	1:A:522:ALA:HB1	2.01	0.42
1:C:83:VAL:HG23	1:C:84:LEU:H	1.85	0.42
1:C:759:PHE:O	1:C:763:LEU:HG	2.19	0.42
1:B:981:LEU:HD23	1:B:981:LEU:HA	1.91	0.42
1:A:337:PRO:HB2	1:A:340:GLU:HB3	2.02	0.42
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.85	0.42
1:A:1097:SER:HB3	1:A:1102:TRP:CD2	2.55	0.42
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.60	0.42
1:C:100:ILE:HG21	1:C:242:LEU:HD23	2.02	0.42
1:B:1031:GLU:HG2	1:B:1037:SER:HB2	2.01	0.42
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.84	0.41
1:A:218:GLN:N	1:A:218:GLN:OE1	2.53	0.41
1:A:462:LYS:H	1:A:462:LYS:HG3	1.66	0.41
1:B:201:PHE:HB2	1:B:231:ILE:HG12	2.01	0.41
1:B:233:ILE:HD12	1:B:233:ILE:HA	1.82	0.41
1:B:886:TRP:CD1	1:B:886:TRP:N	2.85	0.41
1:A:93:ALA:HB3	1:A:266:TYR:HB2	2.02	0.41
1:C:537:LYS:HE2	1:C:537:LYS:HB2	1.91	0.41
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.91	0.41
1:A:276:LEU:HB3	1:A:289:VAL:CG1	2.46	0.41
1:C:431:GLY:HA2	1:C:515:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CE1	1:A:205:SER:HB3	2.55	0.41
1:A:490:PHE:HD1	1:A:492:LEU:H	1.68	0.41
1:A:555:SER:HA	1:A:586:ASP:HB2	2.02	0.41
1:C:898:PHE:CZ	1:C:1050:MET:HE1	2.55	0.41
1:C:1110:TYR:CZ	1:C:1112:PRO:HG3	2.56	0.41
1:B:578:ASP:HB3	1:B:581:THR:O	2.20	0.41
1:B:822:LEU:HD22	1:B:945:LEU:HD21	2.03	0.41
1:A:106:PHE:N	1:A:106:PHE:HD1	2.19	0.41
1:C:945:LEU:HD12	1:C:945:LEU:H	1.85	0.41
1:B:216:LEU:H	1:B:216:LEU:HD12	1.84	0.41
1:C:770:ILE:HD11	1:C:1012:LEU:HA	2.01	0.41
1:C:934:ILE:HD12	1:C:934:ILE:HA	1.81	0.41
1:B:421:TYR:HA	1:B:461:LEU:HD23	2.03	0.41
1:B:954:GLN:O	1:B:957:GLN:HB2	2.19	0.41
1:C:303:LEU:HD12	1:C:308:VAL:HG12	2.01	0.41
1:A:980:ILE:HD12	1:A:980:ILE:H	1.85	0.41
1:C:195:LYS:HE3	1:C:202:LYS:HE2	2.01	0.41
1:B:66:HIS:ND1	1:B:68:ILE:HB	2.35	0.41
1:B:903:ALA:HB1	1:B:913:GLN:HB3	2.01	0.41
1:A:21:ARG:HD2	1:A:21:ARG:HA	1.87	0.41
1:A:92:PHE:HD1	1:A:92:PHE:HA	1.78	0.41
1:A:131:CYS:HB2	1:A:133:PHE:HD2	1.86	0.41
1:A:697:MET:HE3	1:A:697:MET:HB2	1.95	0.41
1:A:735:SER:HB3	1:A:861:LEU:HD11	2.01	0.41
1:A:862:PRO:HG3	1:B:647:ALA:HB2	2.03	0.41
1:C:103:GLY:HA3	1:C:120:VAL:HA	2.03	0.41
1:C:121:ASN:HB3	1:C:126:VAL:HG13	2.02	0.41
1:C:295:PRO:O	1:C:299:THR:HG23	2.21	0.41
1:C:350:VAL:HA	1:C:400:PHE:HB2	2.02	0.41
1:C:1002:GLN:HB3	1:B:759:PHE:HZ	1.85	0.41
1:B:35:GLY:HA3	1:B:56:LEU:HD22	2.02	0.41
1:B:42:VAL:HG12	1:B:44:ARG:H	1.86	0.41
1:C:625:HIS:HB3	1:C:636:TYR:HD1	1.85	0.41
1:C:738:CYS:HB3	1:C:760:CYS:HB3	1.84	0.41
1:A:101:ILE:HD11	1:A:104:TRP:HE1	1.86	0.40
1:A:230:PRO:HG2	1:B:357:ARG:HH12	1.86	0.40
1:A:854:LYS:HB3	1:B:592:PHE:CZ	2.56	0.40
1:C:312:ILE:HG12	1:C:598:ILE:HG12	2.02	0.40
1:C:364:ASP:O	1:C:367:VAL:HG22	2.21	0.40
1:C:828:LEU:HD13	1:C:952:VAL:HG12	2.03	0.40
1:B:54:LEU:HA	1:B:272:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:866:THR:OG1	1:B:869:MET:HG3	2.21	0.40
1:C:26:PRO:HB2	1:C:27:ALA:H	1.61	0.40
1:C:194:PHE:N	1:C:194:PHE:CD1	2.89	0.40
1:B:298:GLU:HG2	1:B:315:THR:HB	2.03	0.40
1:A:92:PHE:HE2	1:A:104:TRP:NE1	2.20	0.40
1:A:741:TYR:CE1	1:A:966:LEU:HD13	2.57	0.40
1:B:387:LEU:HA	1:B:387:LEU:HD23	1.83	0.40
1:B:900:MET:HE3	1:B:900:MET:HB2	1.80	0.40
1:B:1043:CYS:HB2	1:B:1048:HIS:ND1	2.37	0.40
1:B:1105:THR:HG22	1:B:1112:PRO:HA	2.03	0.40
1:A:326:ILE:HB	1:A:541:PHE:HA	2.02	0.40
1:A:958:ALA:O	1:A:961:THR:HG22	2.21	0.40
1:C:1084:ASP:C	1:C:1086:LYS:H	2.28	0.40
1:B:1103:PHE:HZ	2:N:1:NAG:C7	2.34	0.40
1:A:278:LYS:HB2	1:A:306:PHE:CE2	2.57	0.40
1:A:453:TYR:HE1	1:A:455:LEU:HB2	1.86	0.40
1:A:733:LYS:HB3	1:A:733:LYS:HE2	1.91	0.40
1:C:93:ALA:HB2	1:C:266:TYR:HB2	2.03	0.40
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.98	0.40
1:B:1110:TYR:CZ	1:B:1112:PRO:HG3	2.56	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	1037/1280 (81%)	939 (90%)	94 (9%)	4 (0%)	30	62
1	B	1063/1280 (83%)	963 (91%)	96 (9%)	4 (0%)	30	62
1	C	1007/1280 (79%)	900 (89%)	101 (10%)	6 (1%)	22	56
All	All	3107/3840 (81%)	2802 (90%)	291 (9%)	14 (0%)	27	59

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	615	VAL
1	A	483	VAL
1	C	126	VAL
1	C	624	ILE
1	B	503	VAL
1	A	528	LYS
1	C	159	VAL
1	B	483	VAL
1	C	217	PRO
1	B	235	ILE
1	B	122	ASN
1	A	720	ILE
1	A	850	ILE
1	C	503	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	924/1108 (83%)	878 (95%)	46 (5%)	20	49
1	B	946/1108 (85%)	896 (95%)	50 (5%)	19	48
1	C	899/1108 (81%)	840 (93%)	59 (7%)	14	42
All	All	2769/3324 (83%)	2614 (94%)	155 (6%)	20	46

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	PHE
1	A	105	ILE
1	A	110	LEU
1	A	118	LEU
1	A	125	ASN
1	A	130	VAL
1	A	133	PHE

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Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	167	THR
1	A	189	LEU
1	A	240	THR
1	A	242	LEU
1	A	267	VAL
1	A	289	VAL
1	A	327	VAL
1	A	331	ASN
1	A	341	VAL
1	A	350	VAL
1	A	390	LEU
1	A	395	VAL
1	A	421	TYR
1	A	430	THR
1	A	468	ILE
1	A	525	CYS
1	A	528	LYS
1	A	529	LYS
1	A	581	THR
1	A	582	LEU
1	A	645	THR
1	A	720	ILE
1	A	755	GLN
1	A	763	LEU
1	A	788	ILE
1	A	826	VAL
1	A	828	LEU
1	A	931	ILE
1	A	937	SER
1	A	976	VAL
1	A	1001	LEU
1	A	1004	LEU
1	A	1043	CYS
1	A	1061	VAL
1	A	1106	GLN
1	A	1122	VAL
1	A	1141	LEU
1	C	47	VAL
1	C	61	ASN
1	C	81	ASN

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Mol	Chain	Res	Type
1	C	83	VAL
1	C	84	LEU
1	C	90	VAL
1	C	121	ASN
1	C	124	THR
1	C	141	LEU
1	C	216	LEU
1	C	227	VAL
1	C	233	ILE
1	C	236	THR
1	C	282	ASN
1	C	307	THR
1	C	312	ILE
1	C	345	THR
1	C	351	TYR
1	C	385	THR
1	C	391	CYS
1	C	392	PHE
1	C	415	THR
1	C	418	ILE
1	C	421	TYR
1	C	422	ASN
1	C	456	PHE
1	C	468	ILE
1	C	534	VAL
1	C	547	THR
1	C	576	VAL
1	C	577	ARG
1	C	615	VAL
1	C	622	VAL
1	C	624	ILE
1	C	642	VAL
1	C	650	LEU
1	C	651	ILE
1	C	734	THR
1	C	810	SER
1	C	828	LEU
1	C	864	LEU
1	C	878	LEU
1	C	902	MET
1	C	907	ASN
1	C	934	ILE

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Mol	Chain	Res	Type
1	C	937	SER
1	C	948	LEU
1	C	957	GLN
1	C	976	VAL
1	C	991	VAL
1	C	1000	ARG
1	C	1029	MET
1	C	1030	SER
1	C	1040	VAL
1	C	1075	PHE
1	C	1076	THR
1	C	1097	SER
1	C	1104	VAL
1	C	1128	VAL
1	B	33	THR
1	B	54	LEU
1	B	62	VAL
1	B	69	HIS
1	B	140	PHE
1	B	143	VAL
1	B	166	CYS
1	B	176	LEU
1	B	179	LEU
1	B	193	VAL
1	B	200	TYR
1	B	216	LEU
1	B	223	LEU
1	B	227	VAL
1	B	240	THR
1	B	267	VAL
1	B	291	CYS
1	B	350	VAL
1	B	395	VAL
1	B	401	VAL
1	B	455	LEU
1	B	461	LEU
1	B	498	GLN
1	B	524	VAL
1	B	533	LEU
1	B	547	THR
1	B	567	ARG
1	B	569	ILE

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Mol	Chain	Res	Type
1	B	599	THR
1	B	615	VAL
1	B	631	PRO
1	B	632	THR
1	B	635	VAL
1	B	697	MET
1	B	723	THR
1	B	753	LEU
1	B	770	ILE
1	B	788	ILE
1	B	847	ARG
1	B	878	LEU
1	B	886	TRP
1	B	900	MET
1	B	913	GLN
1	B	915	VAL
1	B	974	SER
1	B	990	GLU
1	B	1037	SER
1	B	1098	ASN
1	B	1104	VAL
1	B	1122	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	487	ASN
1	A	506	GLN
1	A	607	GLN
1	A	613	GLN
1	A	644	GLN
1	A	1011	GLN
1	C	125	ASN
1	C	239	GLN
1	C	334	ASN
1	C	422	ASN
1	C	437	ASN
1	C	506	GLN
1	C	607	GLN
1	C	625	HIS
1	C	804	GLN

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Mol	Chain	Res	Type
1	C	872	GLN
1	C	960	ASN
1	C	969	ASN
1	B	69	HIS
1	B	87	ASN
1	B	137	ASN
1	B	544	ASN
1	B	580	GLN
1	B	755	GLN
1	B	777	ASN
1	B	856	ASN
1	B	955	ASN
1	B	957	GLN
1	B	1011	GLN
1	B	1058	HIS
1	B	1125	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

47 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	0.73	0	17,19,21	1.07	2 (11%)
2	NAG	D	2	2	14,14,15	0.69	0	17,19,21	1.22	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	2,1	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
2	NAG	E	2	2	14,14,15	0.73	0	17,19,21	0.85	0
3	NAG	F	1	1,3	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
3	NAG	F	2	3	14,14,15	0.74	0	17,19,21	0.94	1 (5%)
3	BMA	F	3	3	11,11,12	0.84	0	15,15,17	2.06	4 (26%)
2	NAG	G	1	2,1	14,14,15	0.74	0	17,19,21	0.86	0
2	NAG	G	2	2	14,14,15	0.71	0	17,19,21	0.84	0
2	NAG	H	1	2,1	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
2	NAG	H	2	2	14,14,15	0.73	0	17,19,21	0.86	0
3	NAG	I	1	1,3	14,14,15	0.76	0	17,19,21	1.14	1 (5%)
3	NAG	I	2	3	14,14,15	0.73	0	17,19,21	0.86	0
3	BMA	I	3	3	11,11,12	0.85	0	15,15,17	2.13	3 (20%)
2	NAG	J	1	2,1	14,14,15	0.74	0	17,19,21	0.92	0
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.86	0
2	NAG	K	1	2,1	14,14,15	0.72	0	17,19,21	0.88	0
2	NAG	K	2	2	14,14,15	0.71	0	17,19,21	0.83	0
2	NAG	L	1	2,1	14,14,15	0.71	0	17,19,21	0.91	0
2	NAG	L	2	2	14,14,15	0.74	0	17,19,21	0.82	0
2	NAG	M	1	2,1	14,14,15	0.71	0	17,19,21	0.81	1 (5%)
2	NAG	M	2	2	14,14,15	0.74	0	17,19,21	0.84	0
2	NAG	N	1	2,1	14,14,15	0.78	0	17,19,21	2.06	3 (17%)
2	NAG	N	2	2	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
2	NAG	O	1	2,1	14,14,15	0.73	0	17,19,21	1.12	1 (5%)
2	NAG	O	2	2	14,14,15	0.75	0	17,19,21	0.90	0
2	NAG	P	1	2,1	14,14,15	0.76	0	17,19,21	0.83	0
2	NAG	P	2	2	14,14,15	0.71	0	17,19,21	0.87	0
2	NAG	Q	1	2,1	14,14,15	0.72	0	17,19,21	0.90	0
2	NAG	Q	2	2	14,14,15	0.73	0	17,19,21	0.89	1 (5%)
3	NAG	R	1	1,3	14,14,15	0.74	0	17,19,21	0.82	0
3	NAG	R	2	3	14,14,15	0.70	0	17,19,21	0.89	0
3	BMA	R	3	3	11,11,12	0.85	0	15,15,17	2.19	4 (26%)
3	NAG	S	1	1,3	14,14,15	0.73	0	17,19,21	0.81	0
3	NAG	S	2	3	14,14,15	0.70	0	17,19,21	0.90	1 (5%)
3	BMA	S	3	3	11,11,12	0.84	0	15,15,17	2.14	4 (26%)
2	NAG	T	1	2,1	14,14,15	0.72	0	17,19,21	1.10	1 (5%)
2	NAG	T	2	2	14,14,15	0.73	0	17,19,21	0.95	0
3	NAG	U	1	1,3	14,14,15	0.74	0	17,19,21	1.35	2 (11%)
3	NAG	U	2	3	14,14,15	0.72	0	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	U	3	3	11,11,12	0.87	0	15,15,17	2.15	3 (20%)
3	NAG	V	1	1,3	14,14,15	0.74	0	17,19,21	0.84	0
3	NAG	V	2	3	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
3	BMA	V	3	3	11,11,12	0.83	0	15,15,17	2.05	3 (20%)
3	NAG	W	1	1,3	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
3	NAG	W	2	3	14,14,15	0.70	0	17,19,21	0.96	1 (5%)
3	BMA	W	3	3	11,11,12	0.86	0	15,15,17	2.10	3 (20%)

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	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	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	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	0/2/19/22	0/1/1/1
2	NAG	T	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	1/2/19/22	0/1/1/1
3	NAG	W	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	3	BMA	C1-O5-C5	6.61	121.05	112.19
3	I	3	BMA	C1-O5-C5	6.60	121.03	112.19
3	U	3	BMA	C1-O5-C5	6.46	120.84	112.19
3	S	3	BMA	C1-O5-C5	6.41	120.77	112.19
3	V	3	BMA	C1-O5-C5	6.32	120.65	112.19
3	W	3	BMA	C1-O5-C5	6.21	120.51	112.19
3	F	3	BMA	C1-O5-C5	5.95	120.16	112.19
2	N	1	NAG	C2-N2-C7	5.10	129.74	122.90
2	N	1	NAG	C4-C3-C2	4.75	117.98	111.02
3	U	1	NAG	O5-C1-C2	-3.50	105.88	111.29
2	D	2	NAG	C2-N2-C7	3.40	127.45	122.90
2	N	1	NAG	C1-O5-C5	-3.05	108.10	112.19
2	D	1	NAG	O5-C1-C2	-2.97	106.69	111.29
3	I	1	NAG	C1-O5-C5	2.97	116.17	112.19
3	W	2	NAG	O5-C1-C2	-2.87	106.85	111.29
2	T	1	NAG	O5-C1-C2	-2.83	106.91	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O5-C1-C2	-2.68	107.15	111.29
2	O	1	NAG	O5-C1-C2	-2.68	107.15	111.29
3	F	3	BMA	C3-C4-C5	2.67	115.06	110.23
3	F	1	NAG	O5-C1-C2	-2.63	107.22	111.29
3	S	3	BMA	C3-C4-C5	2.62	114.98	110.23
3	U	3	BMA	C3-C4-C5	2.62	114.98	110.23
3	W	3	BMA	C3-C4-C5	2.61	114.97	110.23
3	R	3	BMA	C3-C4-C5	2.60	114.94	110.23
3	W	1	NAG	O5-C1-C2	-2.59	107.29	111.29
2	N	2	NAG	C1-O5-C5	2.55	115.61	112.19
3	R	3	BMA	C2-C3-C4	2.44	115.15	110.86
3	S	2	NAG	O5-C1-C2	-2.43	107.53	111.29
3	U	3	BMA	C2-C3-C4	2.42	115.12	110.86
3	F	2	NAG	O5-C1-C2	-2.42	107.55	111.29
3	F	3	BMA	C2-C3-C4	2.41	115.09	110.86
3	U	2	NAG	C1-O5-C5	2.37	115.36	112.19
3	V	2	NAG	O5-C1-C2	-2.36	107.64	111.29
3	W	3	BMA	C2-C3-C4	2.36	115.00	110.86
3	I	3	BMA	C3-C4-C5	2.30	114.41	110.23
3	S	3	BMA	C2-C3-C4	2.29	114.89	110.86
3	V	3	BMA	C2-C3-C4	2.22	114.77	110.86
3	I	3	BMA	C2-C3-C4	2.21	114.75	110.86
2	D	1	NAG	O4-C4-C3	-2.17	105.25	110.38
3	U	1	NAG	C3-C4-C5	2.14	114.11	110.23
2	H	1	NAG	O5-C1-C2	-2.07	108.09	111.29
3	R	3	BMA	O4-C4-C3	-2.06	105.51	110.38
3	F	3	BMA	O4-C4-C3	-2.05	105.55	110.38
3	S	3	BMA	O4-C4-C3	-2.04	105.57	110.38
3	V	3	BMA	C3-C4-C5	2.03	113.91	110.23
2	M	1	NAG	O5-C1-C2	-2.01	108.19	111.29
2	Q	2	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	3	BMA	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	N	1	NAG	C8-C7-N2-C2

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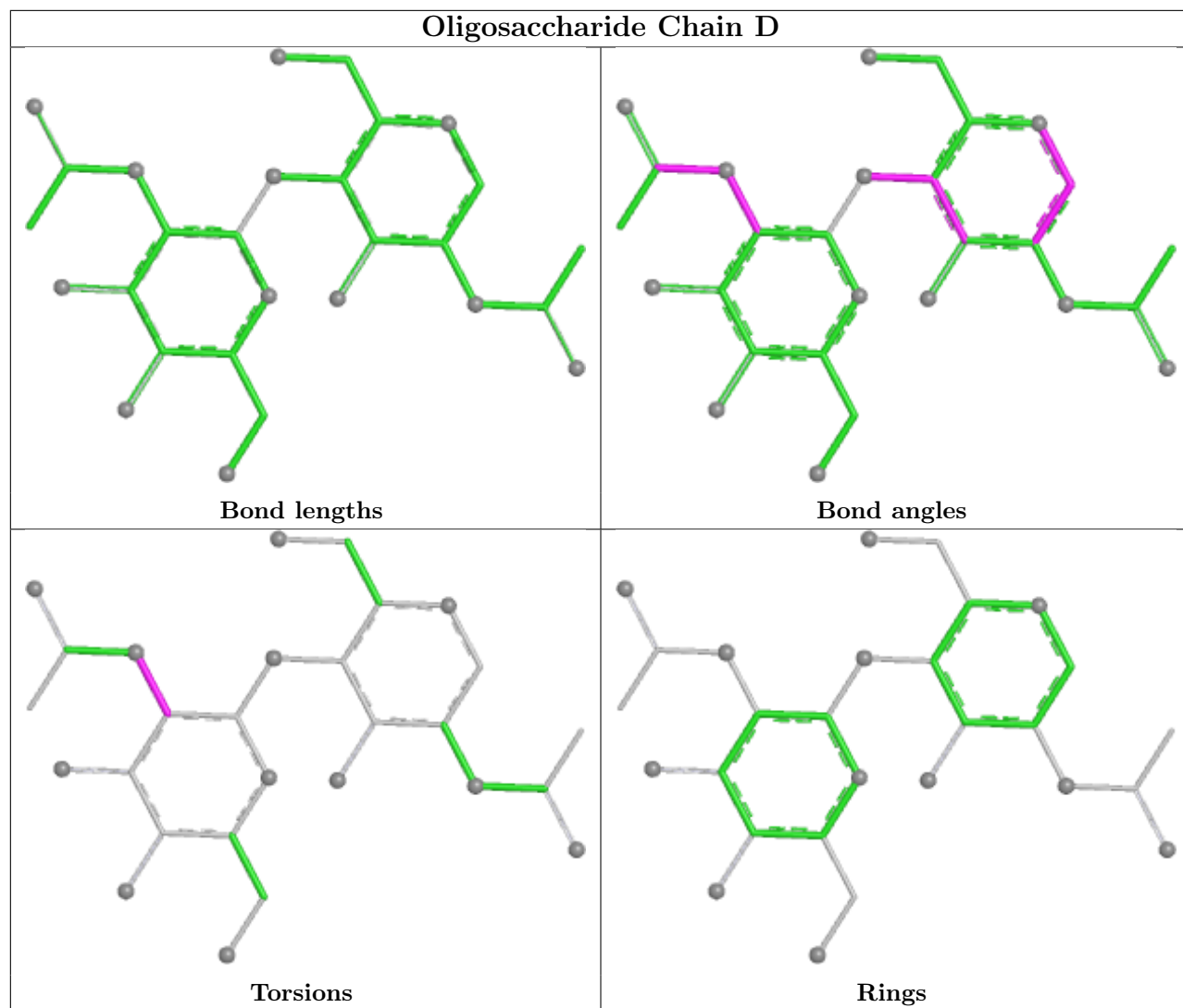
Mol	Chain	Res	Type	Atoms
2	N	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	V	3	BMA	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7
3	I	3	BMA	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6

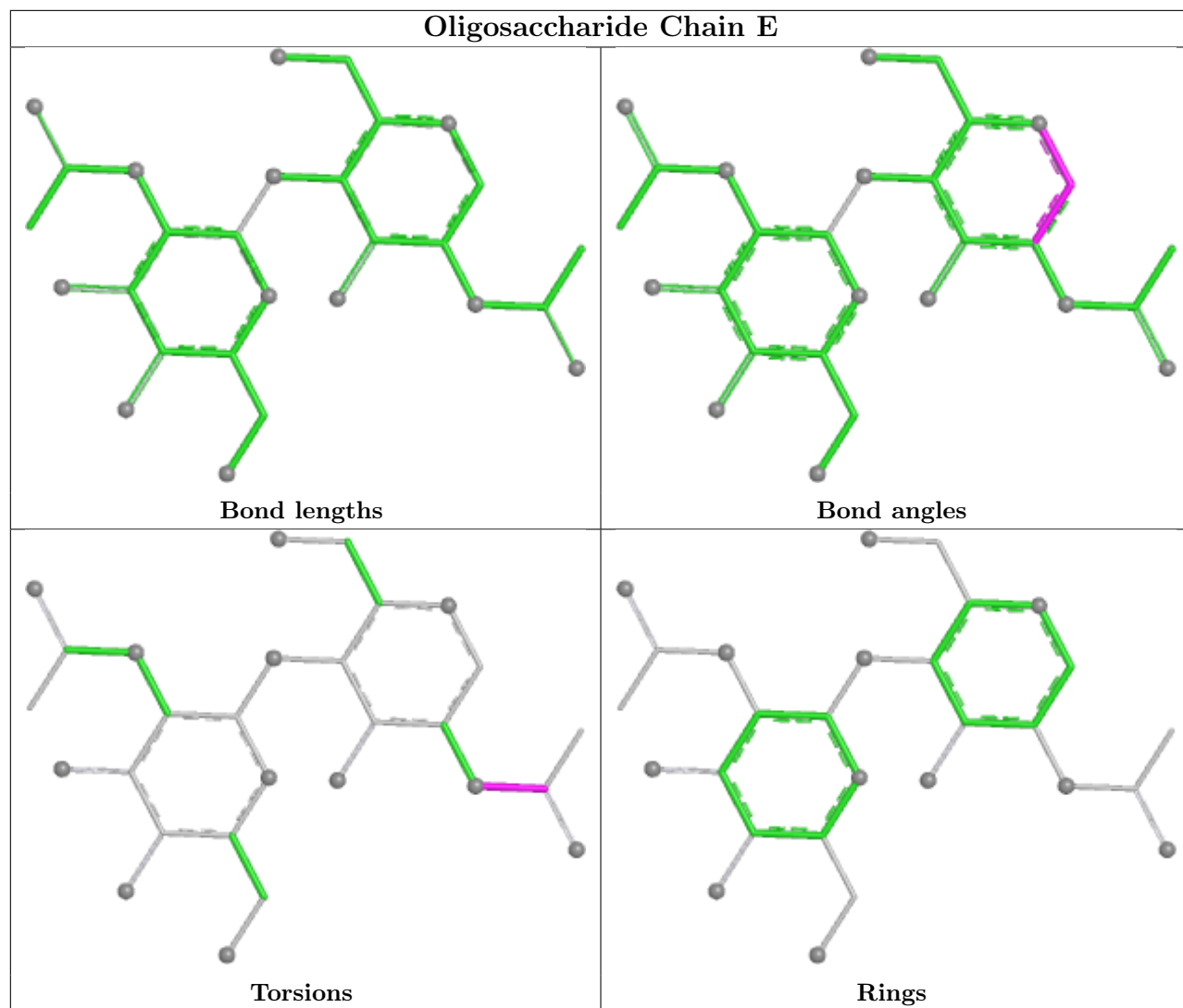
There are no ring outliers.

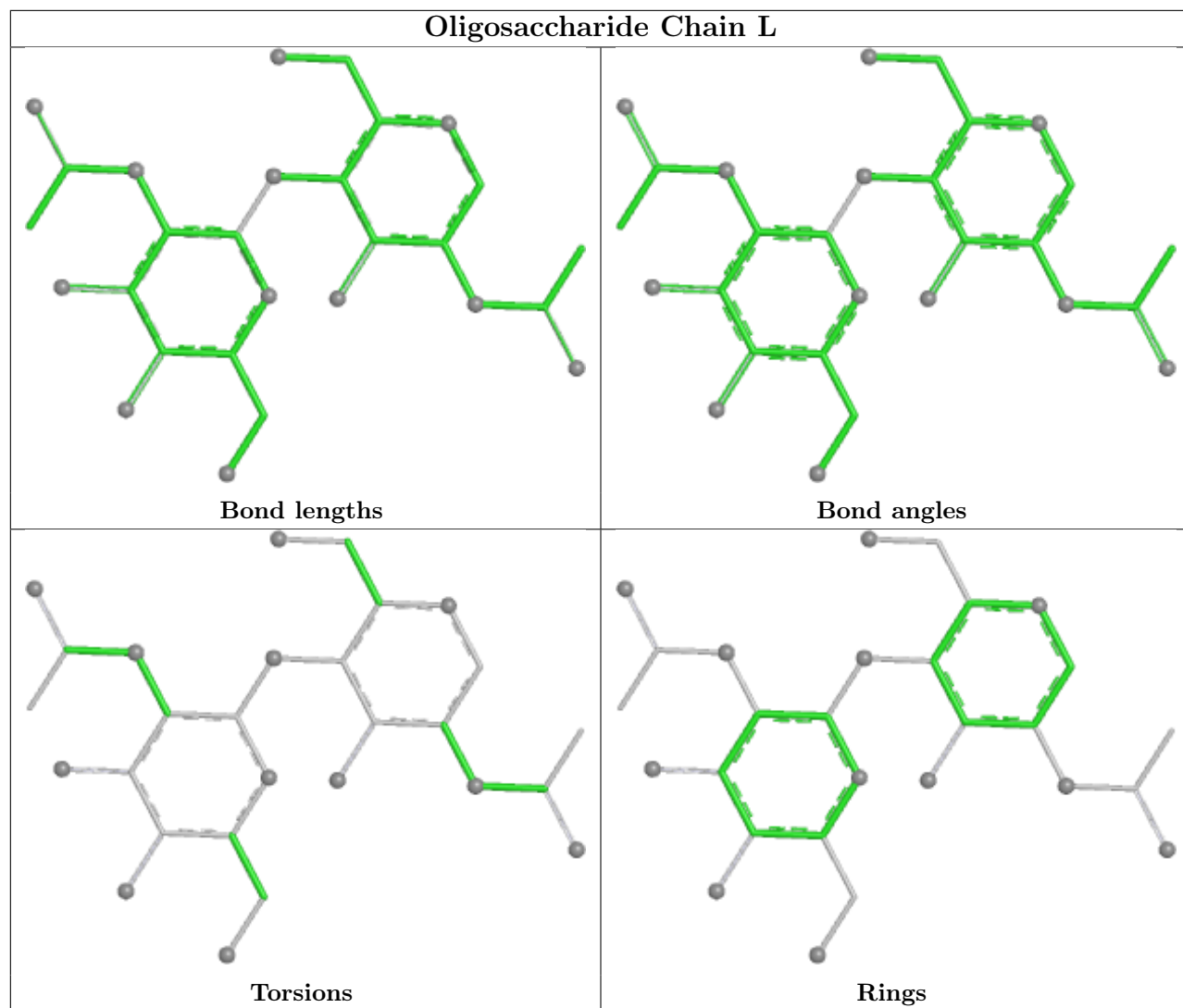
2 monomers are involved in 2 short contacts:

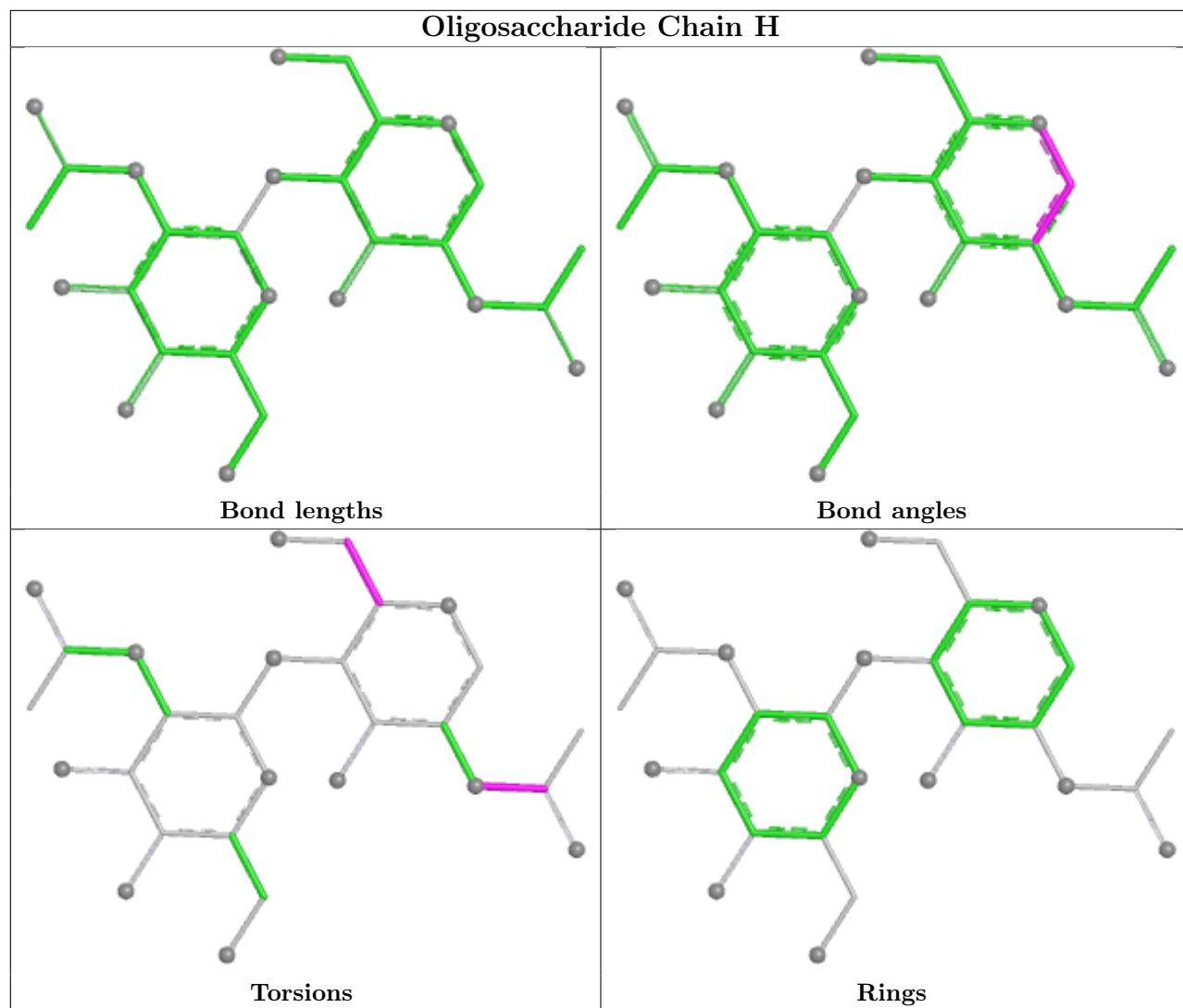
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	1	NAG	1	0
2	M	1	NAG	1	0

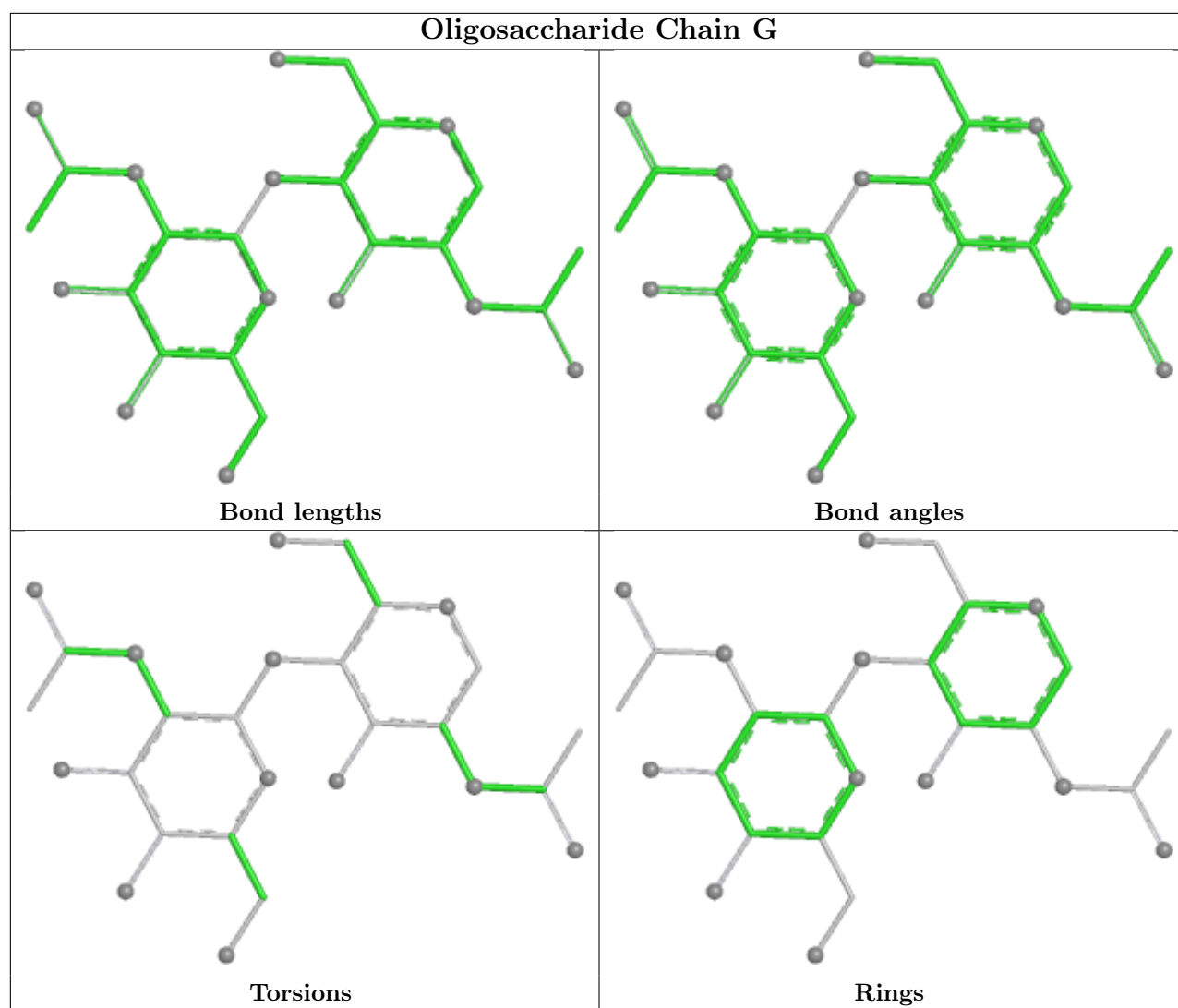
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

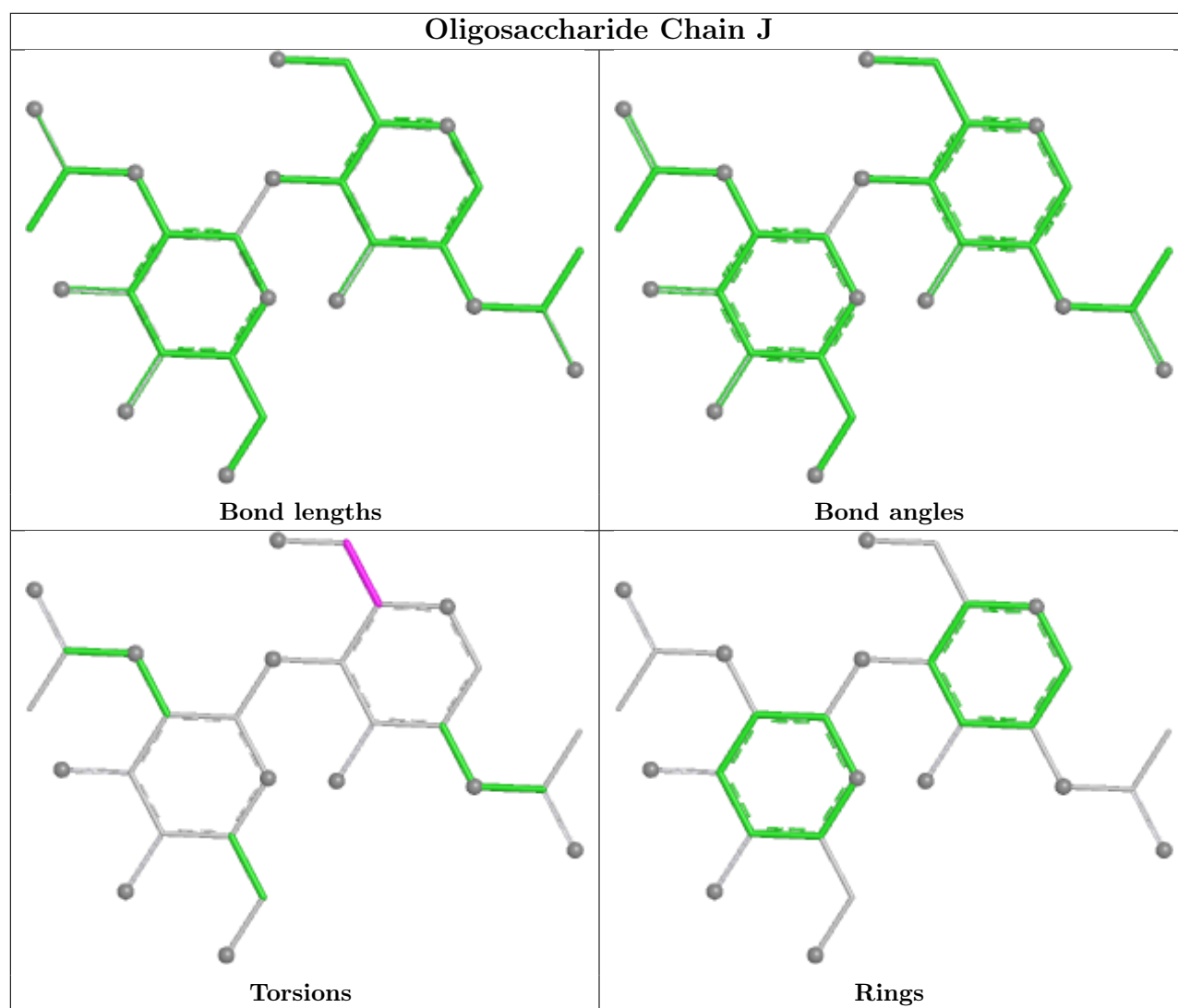


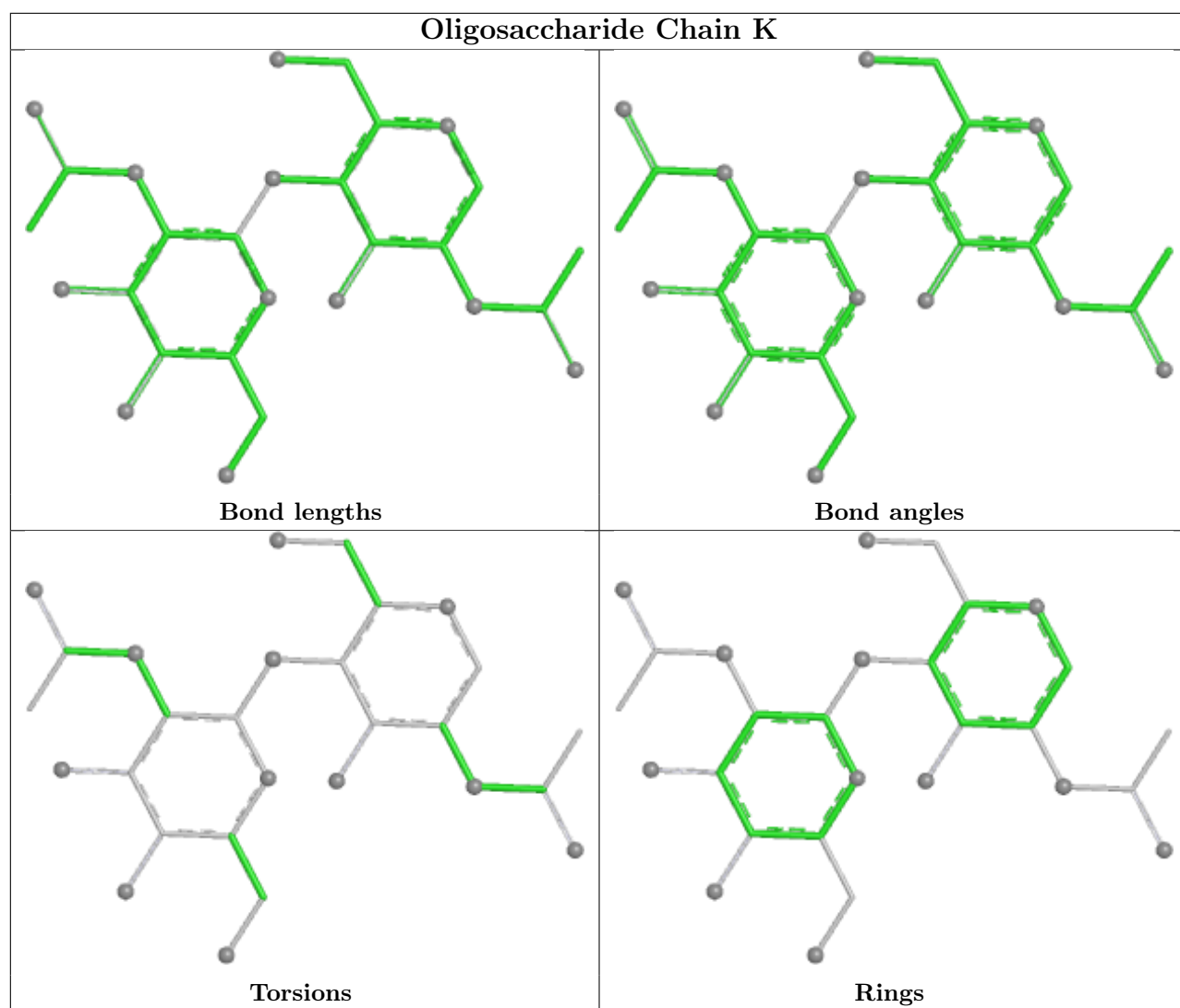


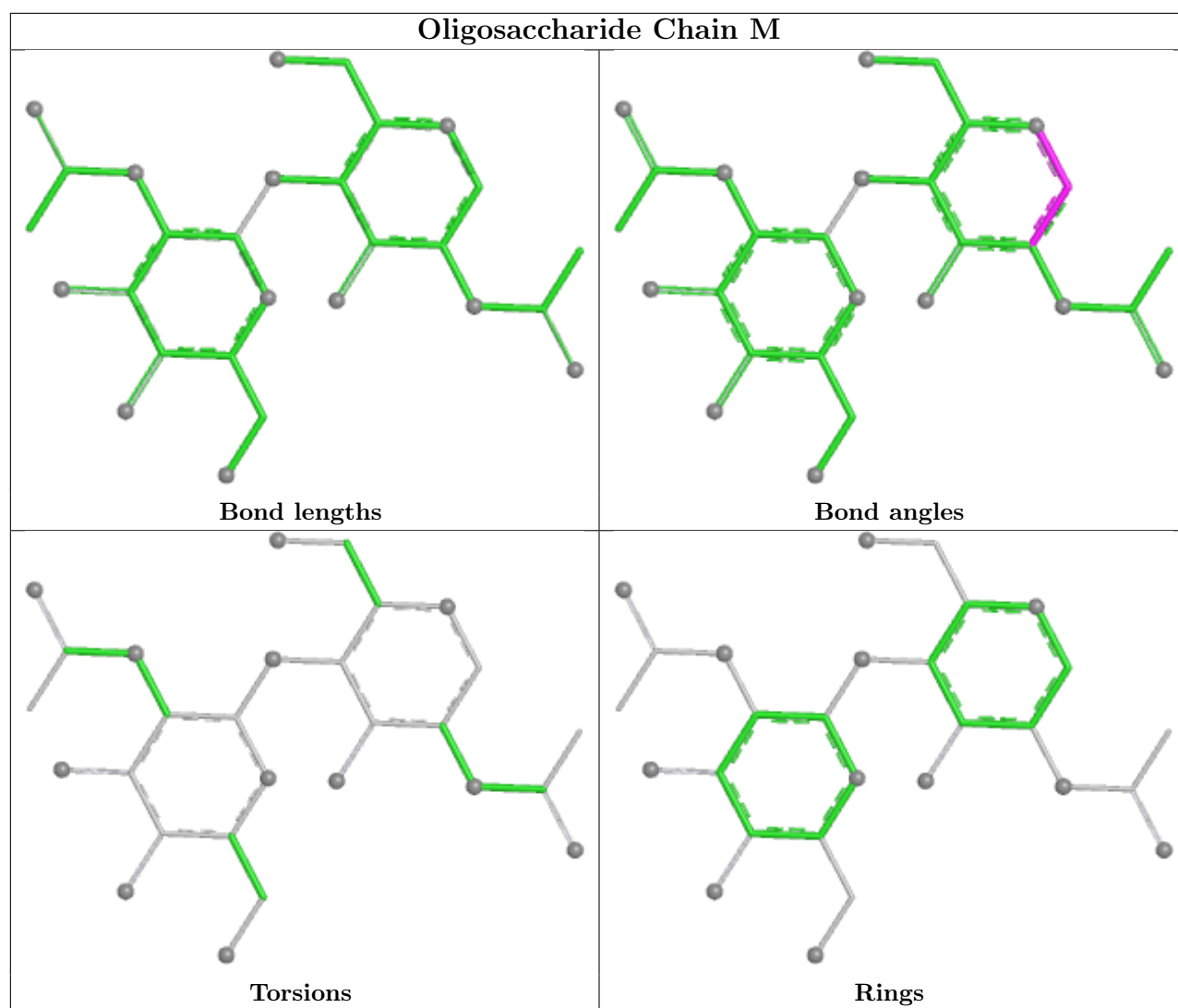


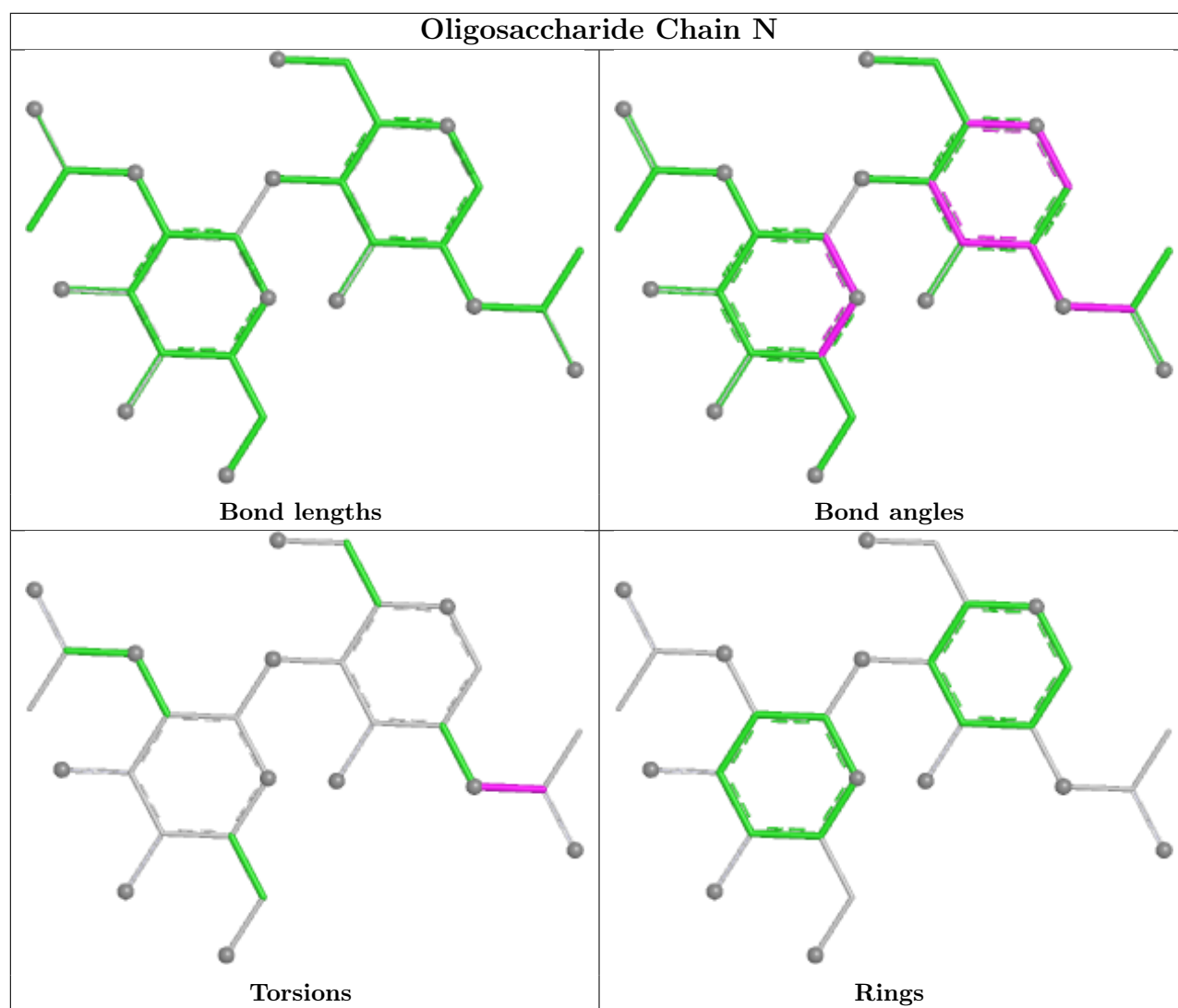


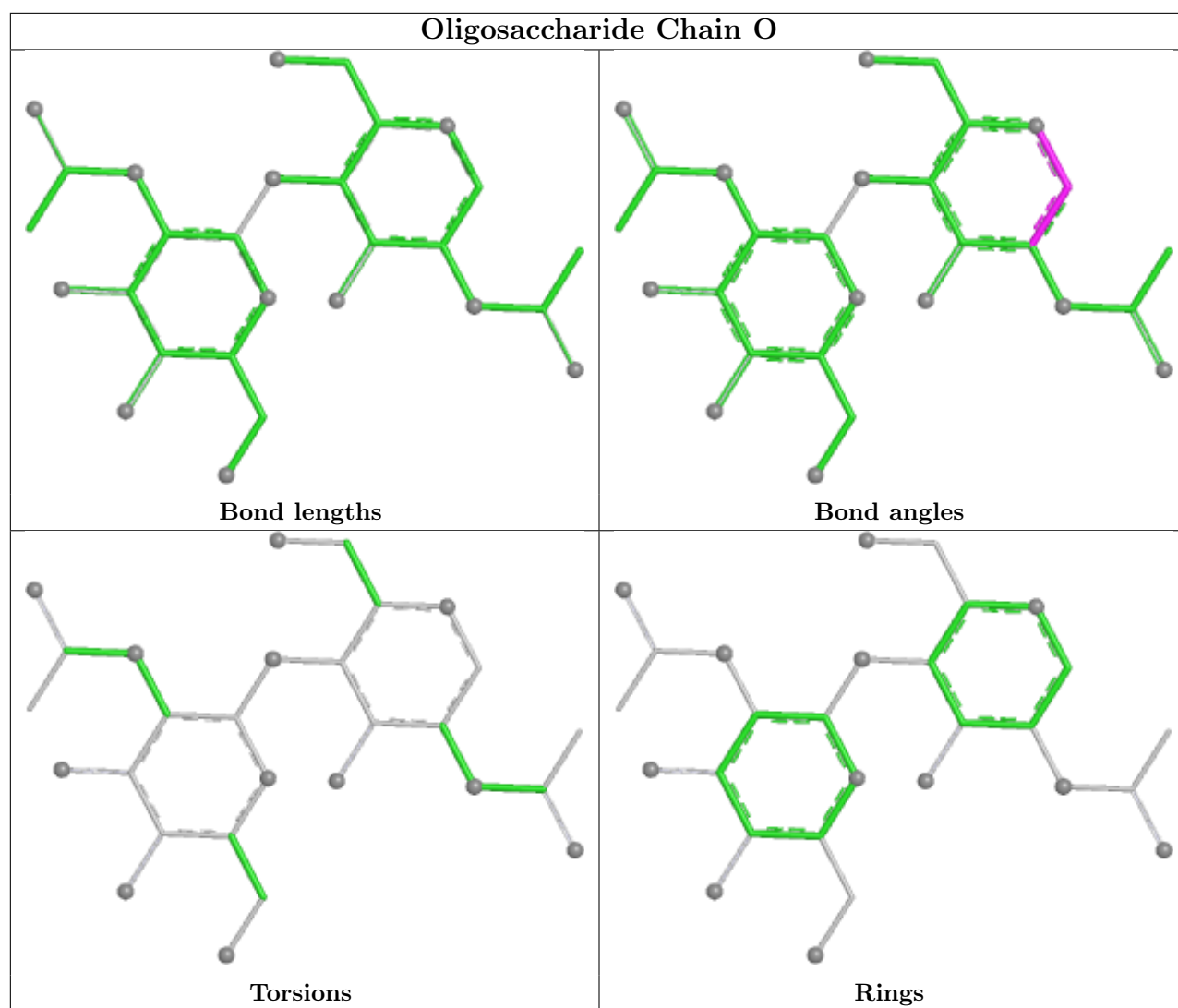


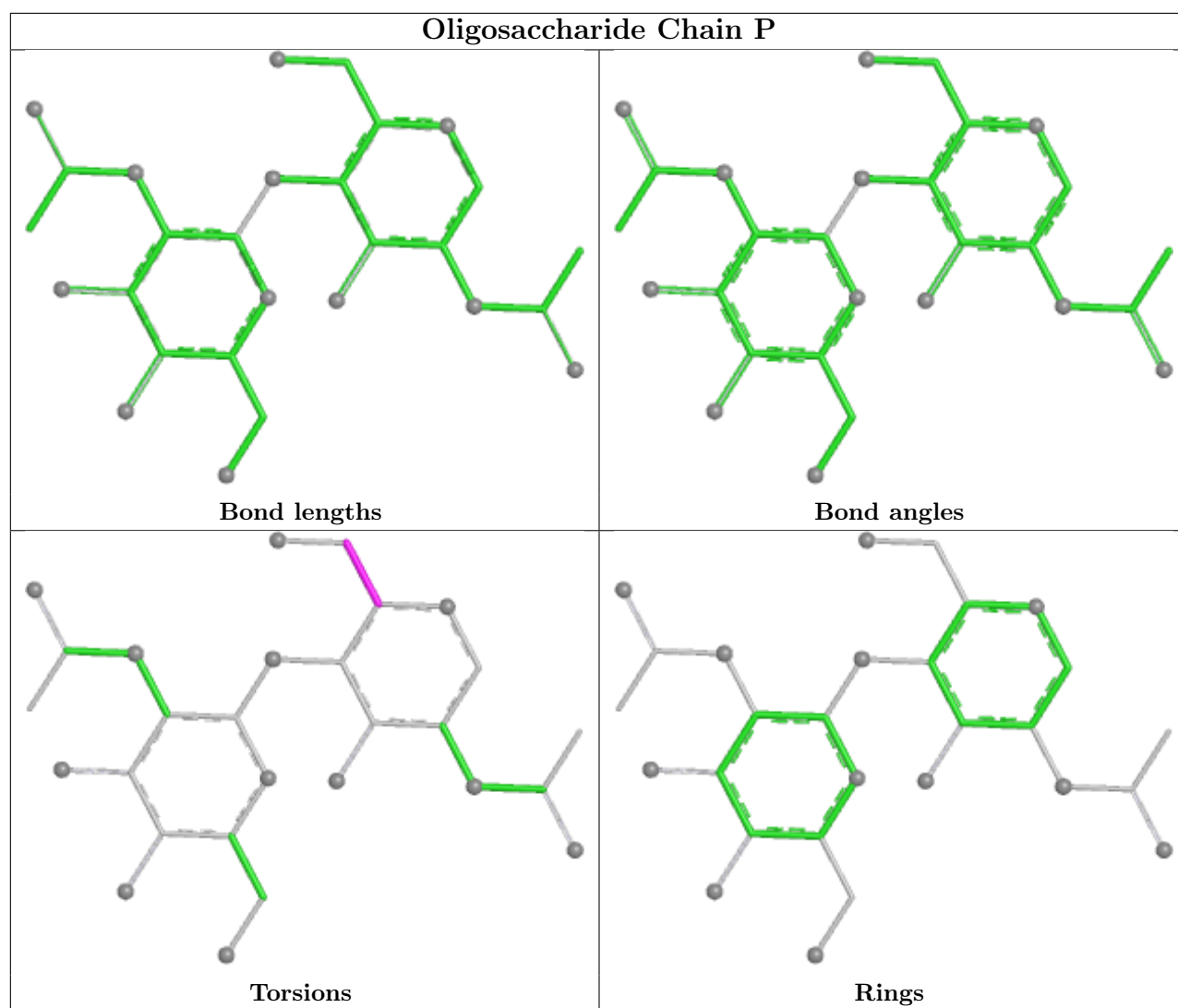


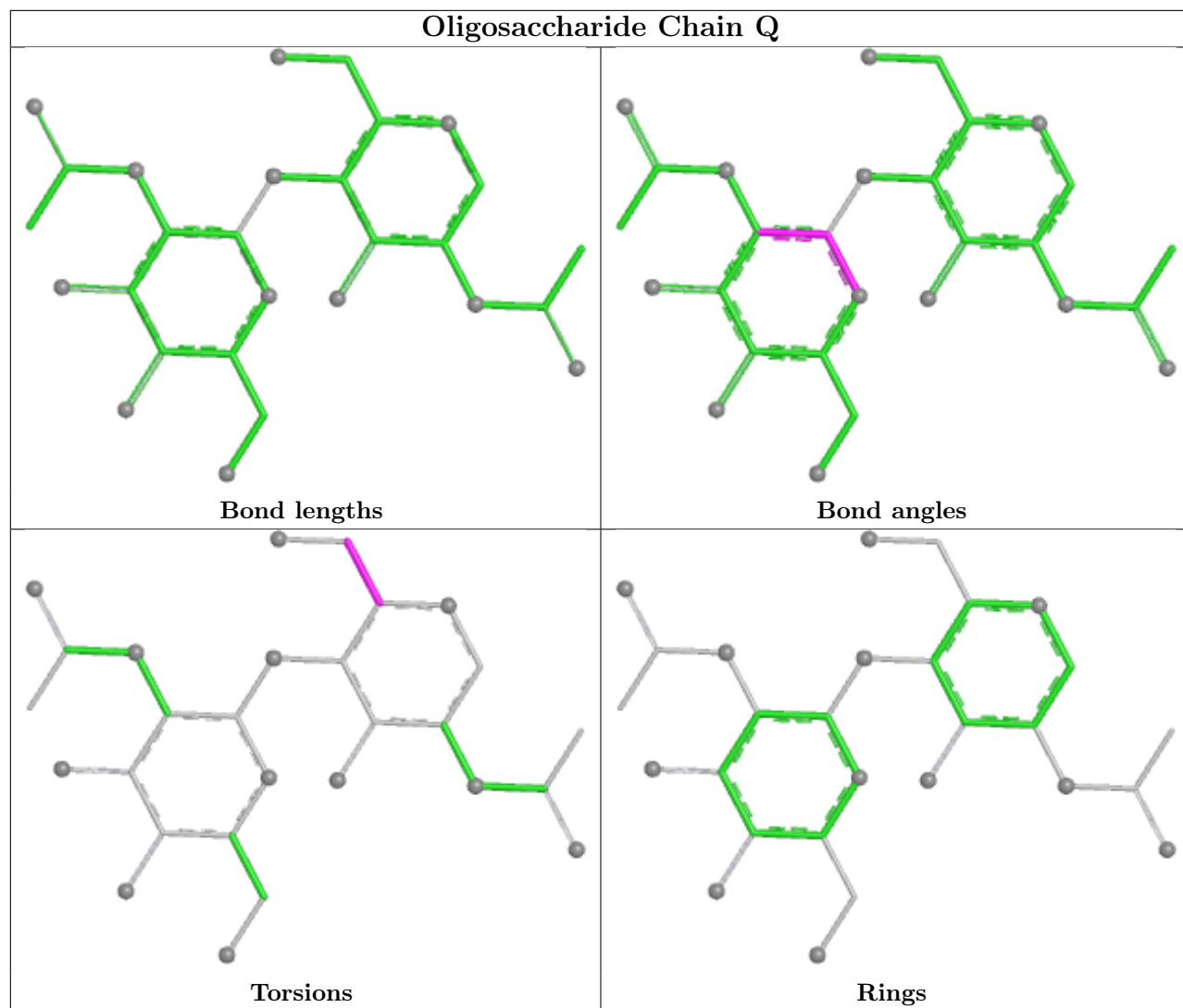


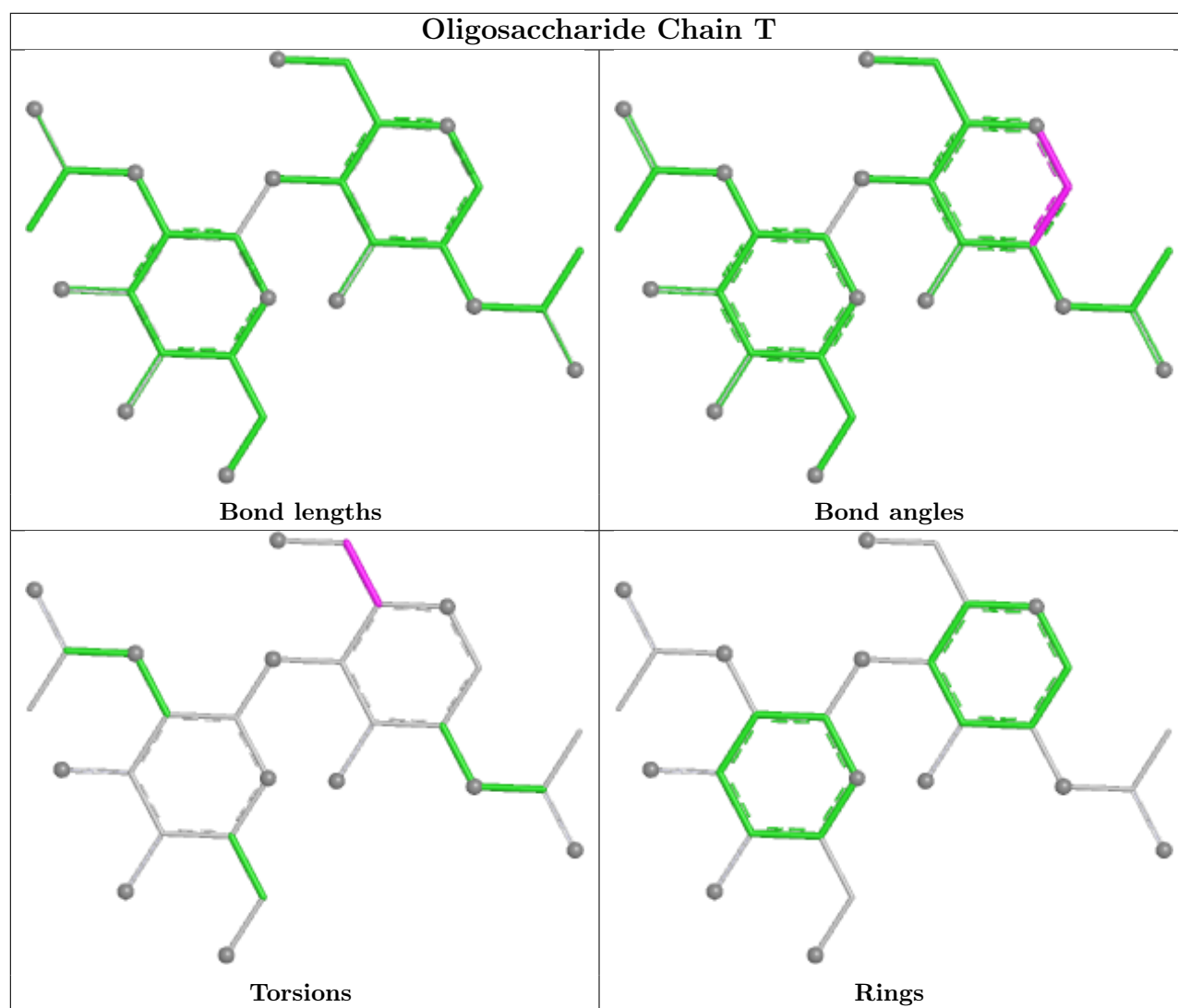


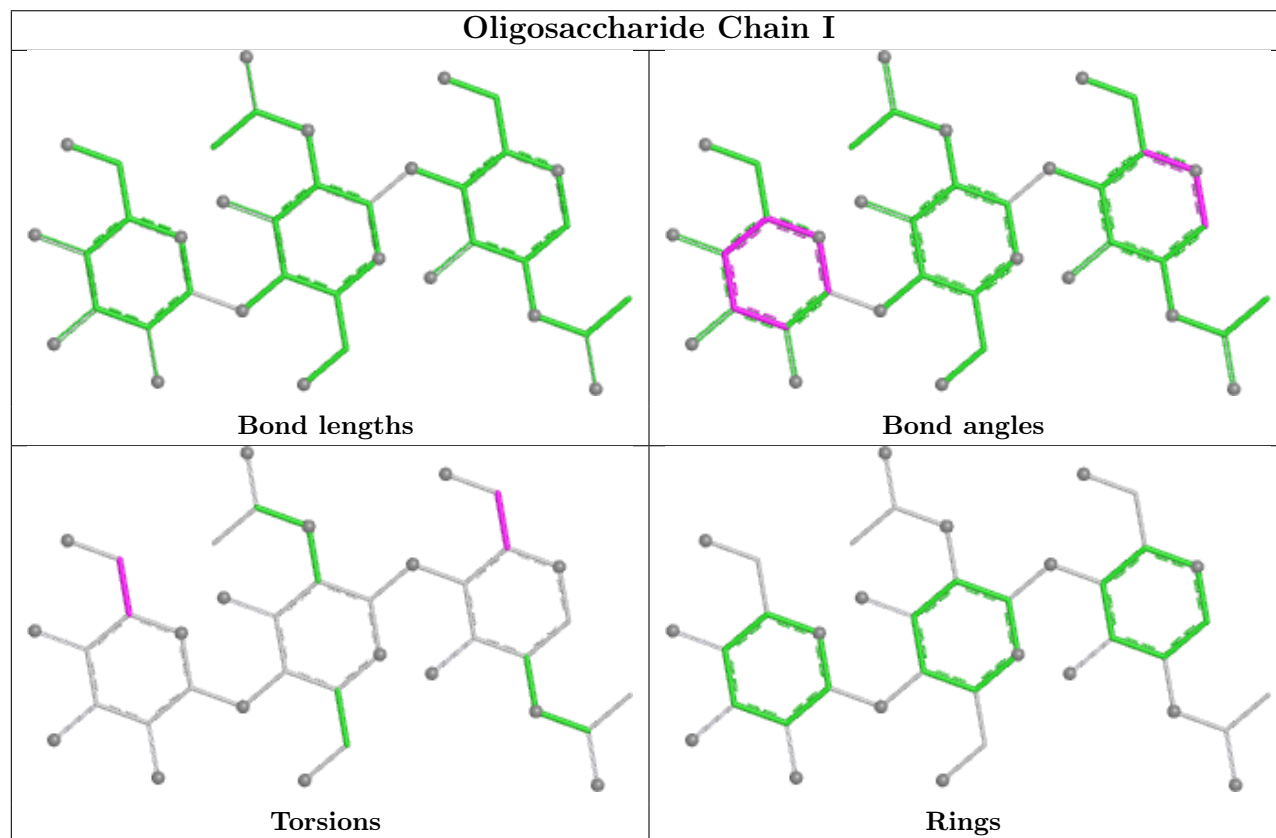
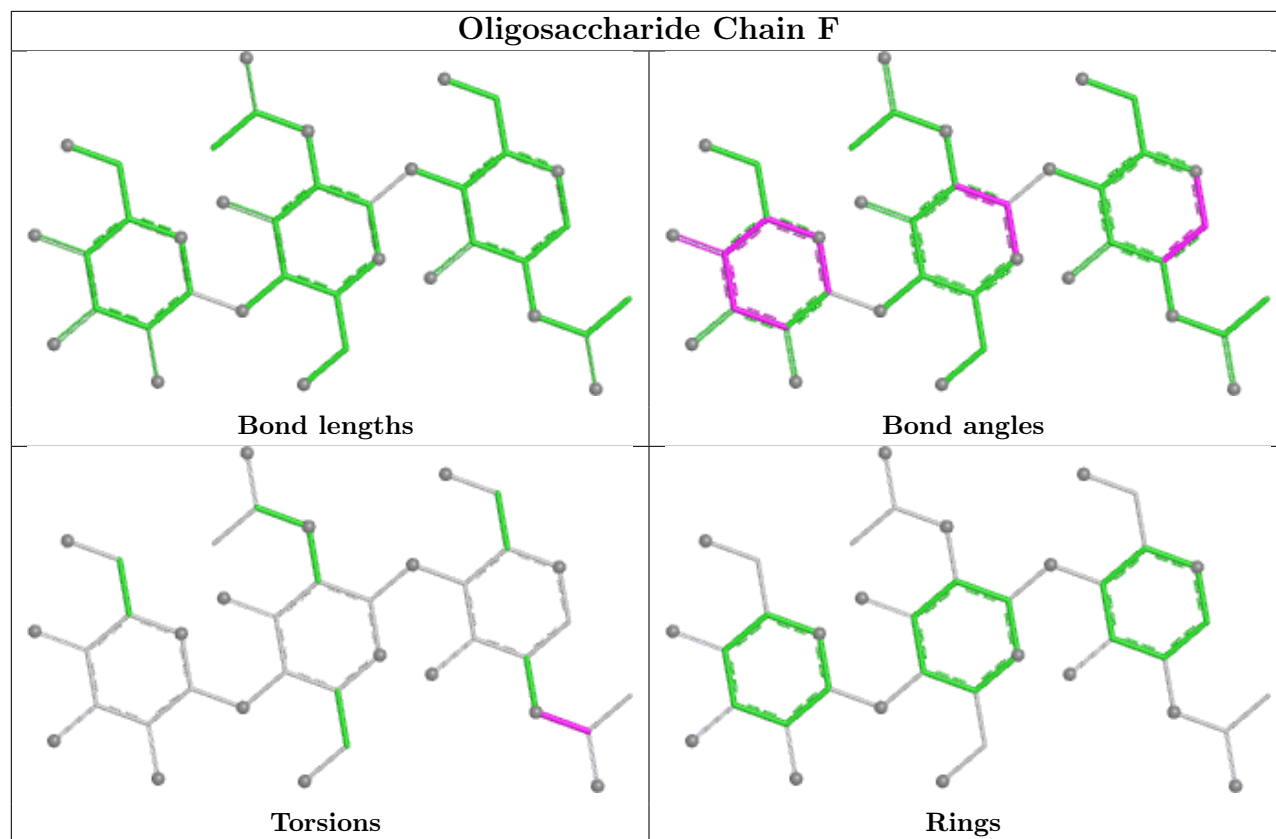


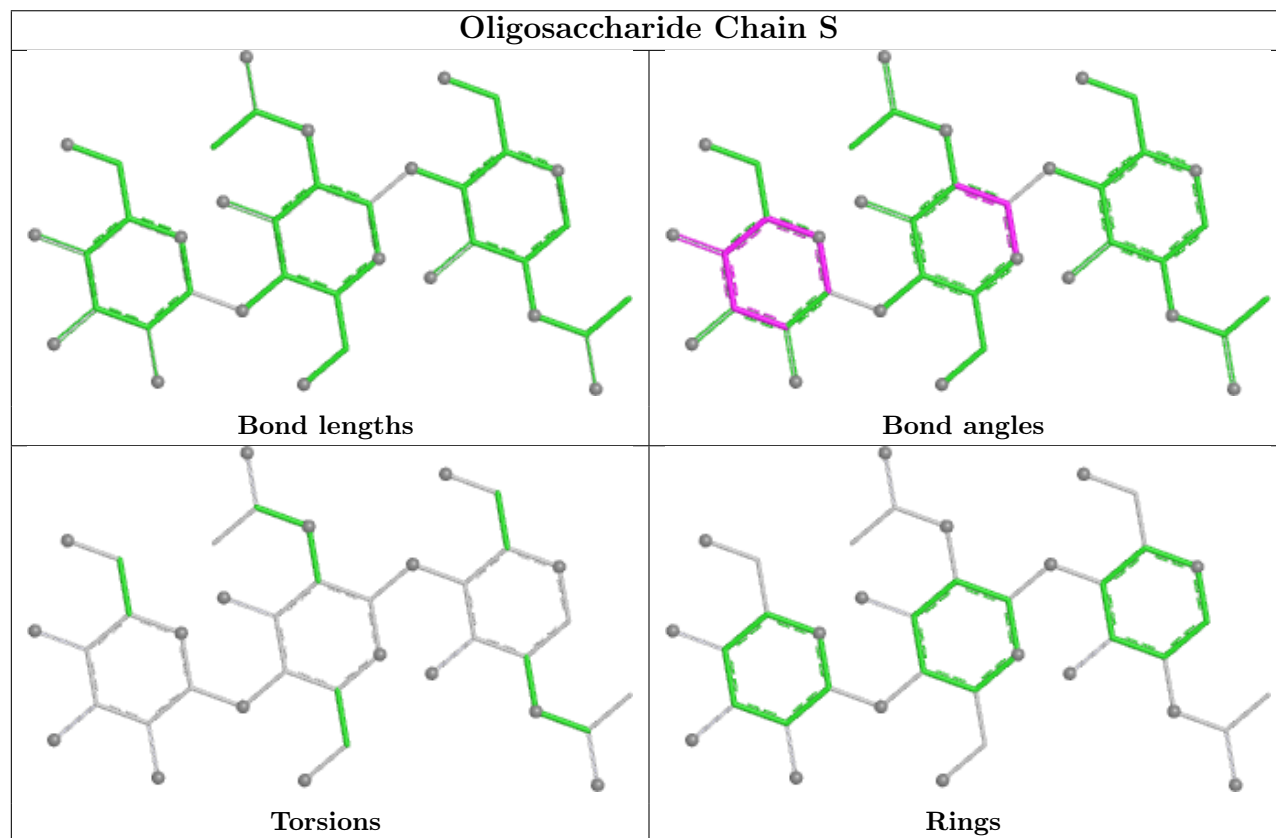
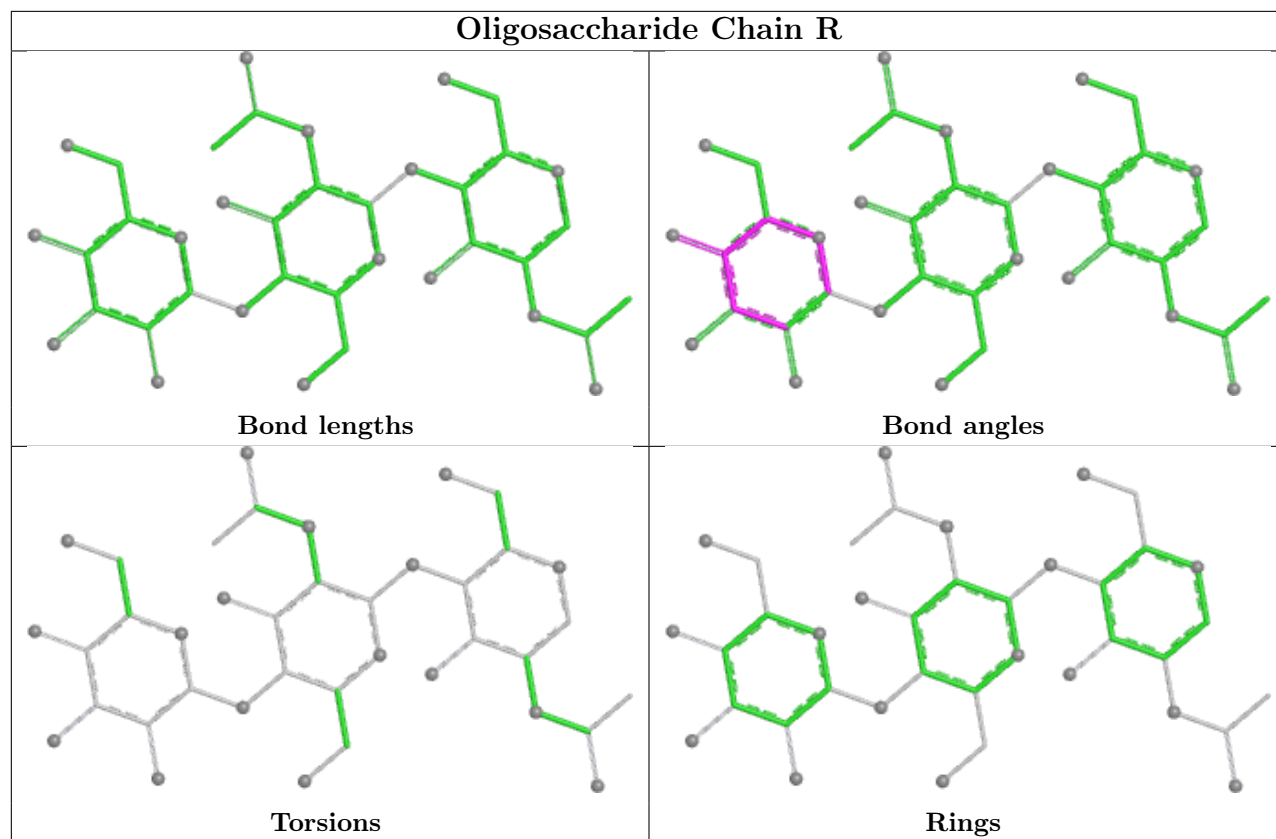


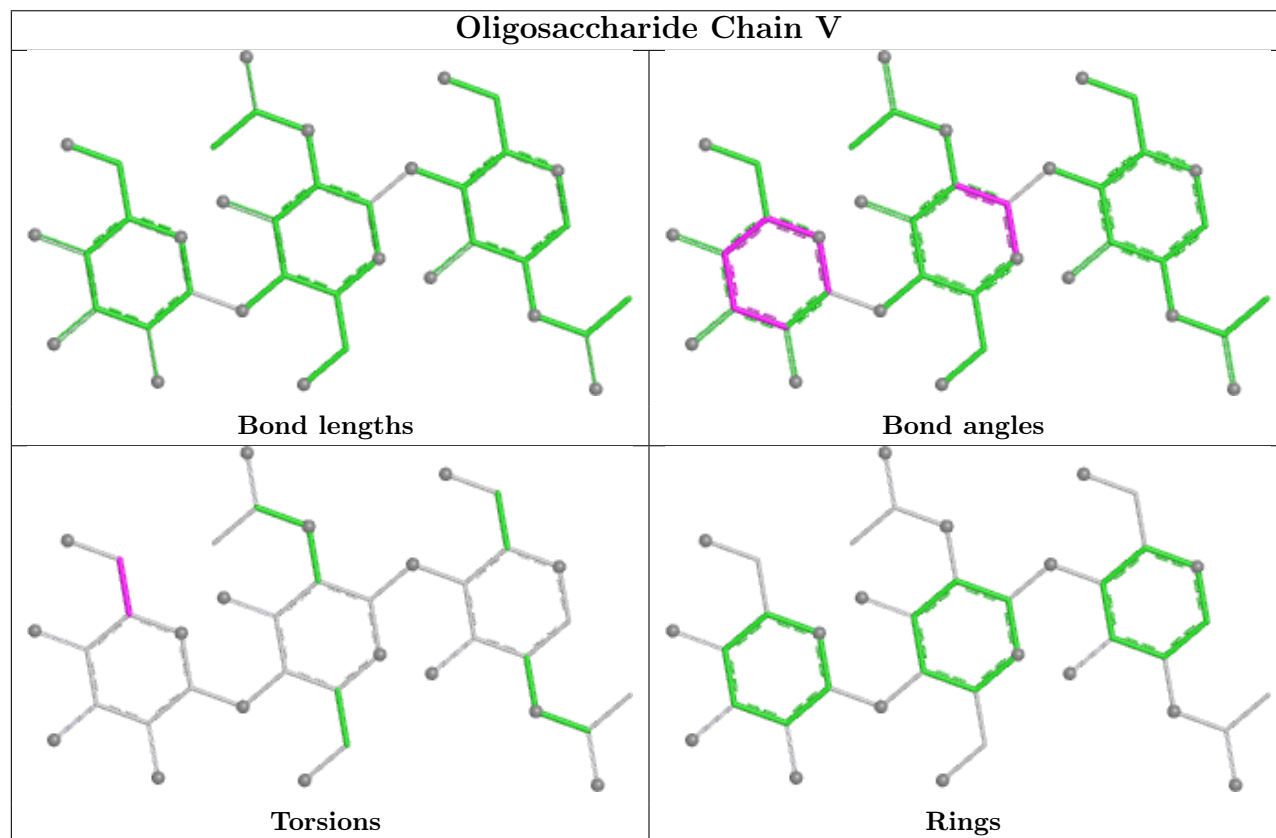
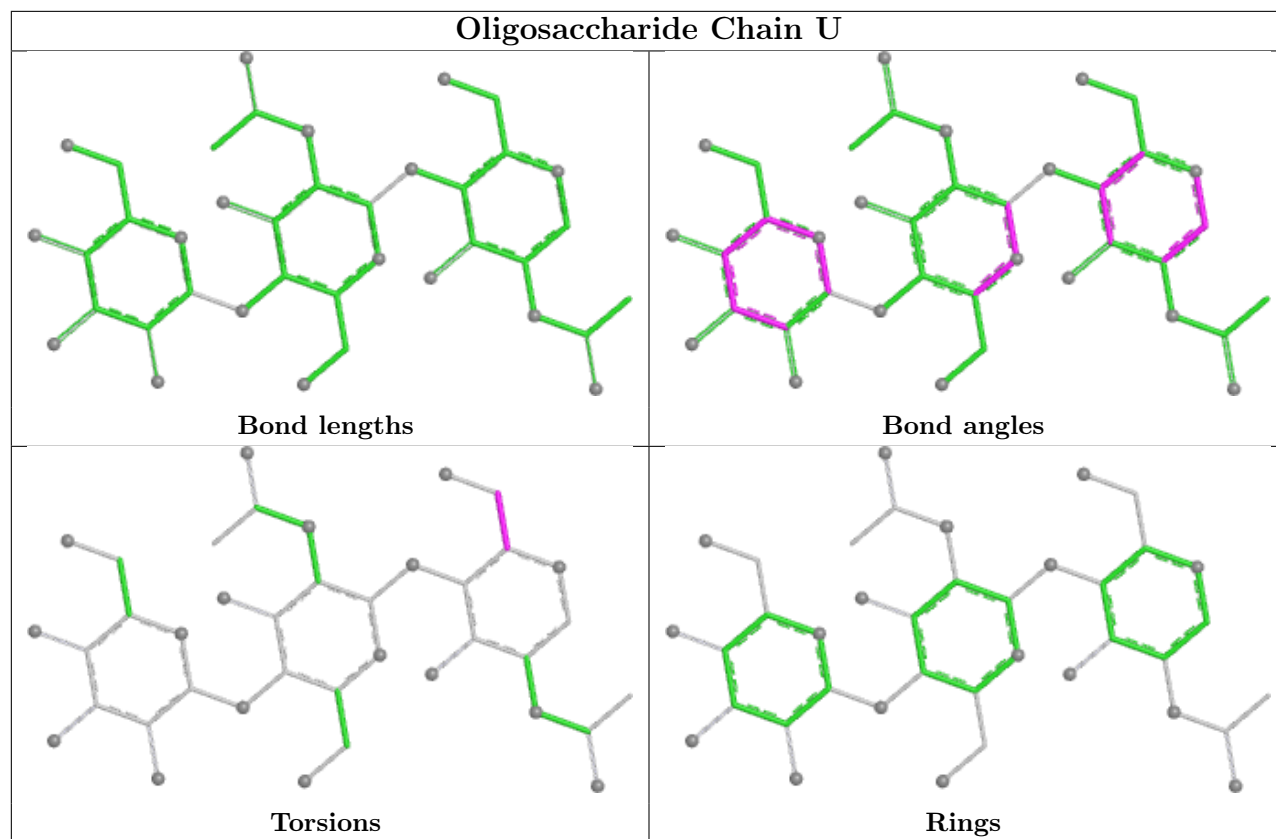


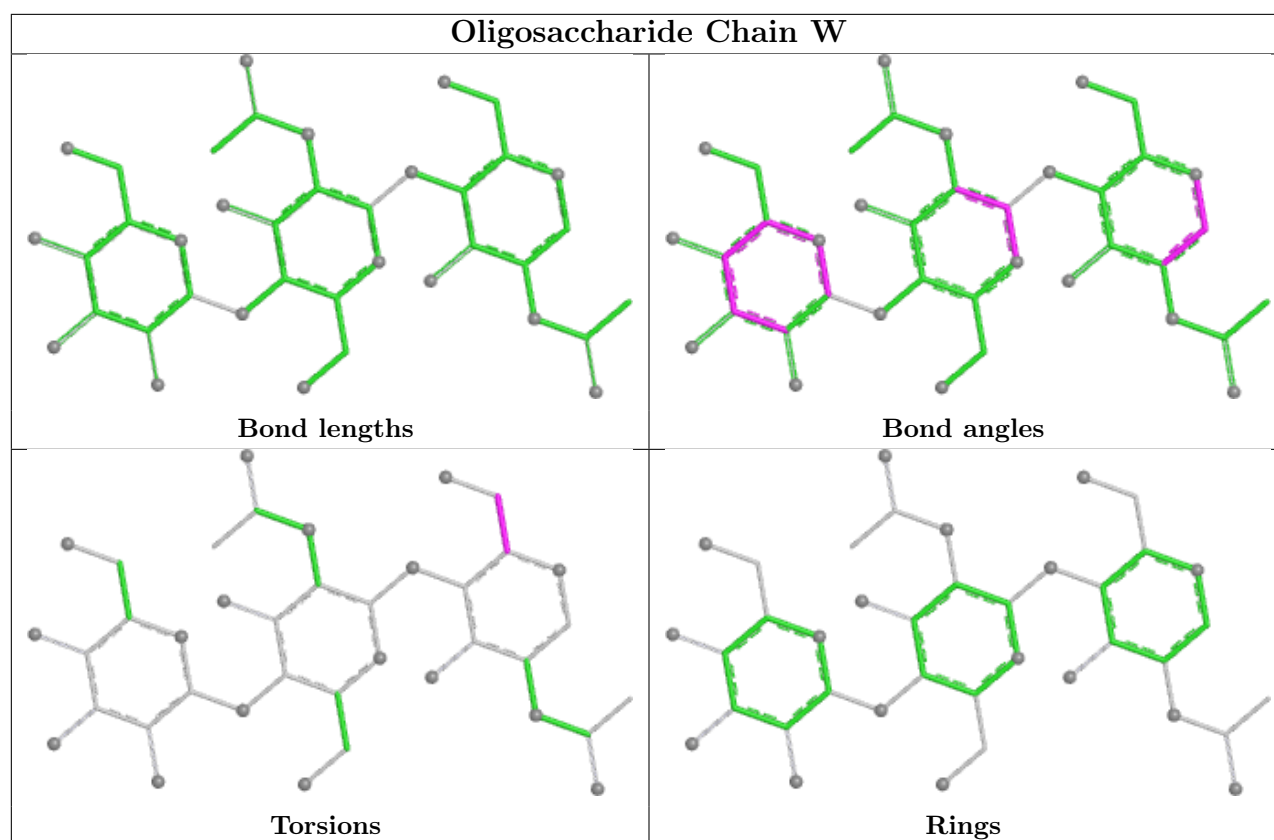












5.6 Ligand geometry [i](#)

22 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	1304	1	14,14,15	0.72	0	17,19,21	1.14	1 (5%)
4	NAG	B	1303	1	14,14,15	0.73	0	17,19,21	0.89	0
4	NAG	A	1302	1	14,14,15	0.74	0	17,19,21	0.80	0
4	NAG	C	1309	1	14,14,15	0.69	0	17,19,21	0.81	1 (5%)
4	NAG	C	1303	1	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
4	NAG	B	1301	1	14,14,15	0.70	0	17,19,21	0.85	0
4	NAG	B	1308	1	14,14,15	0.72	0	17,19,21	0.87	1 (5%)
4	NAG	B	1305	1	14,14,15	0.72	0	17,19,21	0.83	0
4	NAG	B	1304	1	14,14,15	0.75	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1302	1	14,14,15	0.73	0	17,19,21	0.80	0
4	NAG	C	1308	1	14,14,15	0.72	0	17,19,21	0.80	0
4	NAG	A	1301	1	14,14,15	0.72	0	17,19,21	0.79	0
4	NAG	B	1309	1	14,14,15	0.71	0	17,19,21	0.81	0
4	NAG	A	1304	1	14,14,15	0.70	0	17,19,21	0.88	1 (5%)
4	NAG	C	1305	1	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
4	NAG	B	1307	1	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	A	1303	1	14,14,15	0.74	0	17,19,21	0.89	0
4	NAG	B	1302	1	14,14,15	0.74	0	17,19,21	0.86	0
4	NAG	B	1306	1	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	C	1301	1	14,14,15	0.71	0	17,19,21	0.79	0
4	NAG	C	1307	1	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
4	NAG	C	1306	1	14,14,15	0.69	0	17,19,21	1.04	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1304	NAG	C2-N2-C7	3.21	127.20	122.90
4	C	1306	NAG	O5-C1-C2	-3.18	106.37	111.29
4	C	1305	NAG	O5-C1-C2	-2.77	107.00	111.29
4	C	1307	NAG	O5-C1-C2	-2.46	107.48	111.29
4	A	1304	NAG	O5-C1-C2	-2.41	107.57	111.29
4	B	1308	NAG	C2-N2-C7	2.17	125.81	122.90
4	C	1303	NAG	C1-O5-C5	2.12	115.03	112.19
4	C	1309	NAG	O5-C1-C2	-2.10	108.03	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	C	1307	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1304	NAG	C1-C2-N2-C7
4	C	1306	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1304	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1304	NAG	1	0
4	C	1309	NAG	1	0
4	B	1301	NAG	1	0
4	B	1304	NAG	1	0
4	C	1307	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

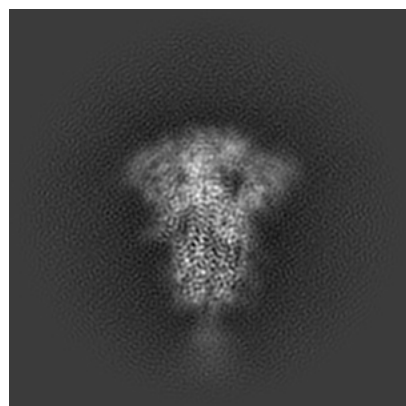
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70451. These allow visual inspection of the internal detail of the map and identification of artifacts.

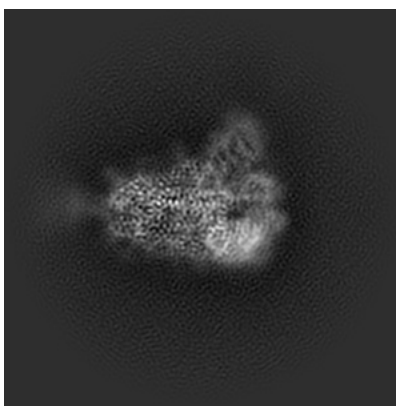
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

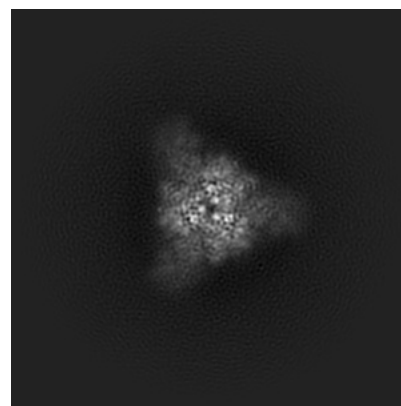
6.1.1 Primary map



X

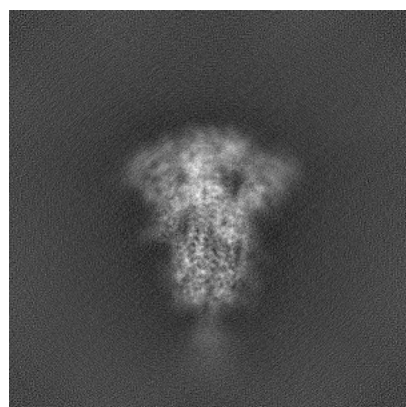


Y

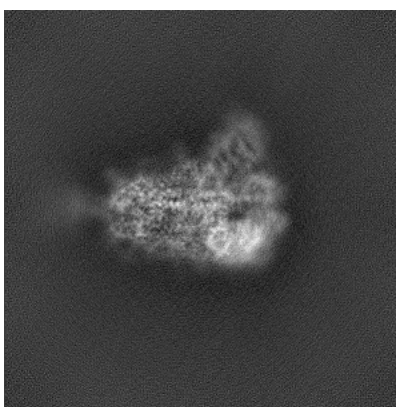


Z

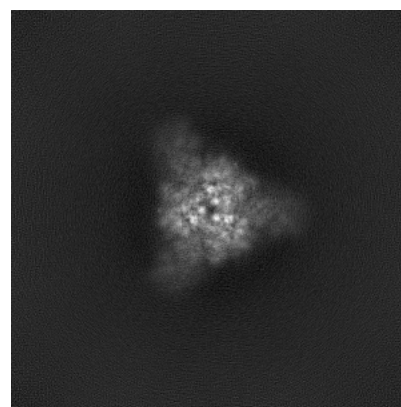
6.1.2 Raw map



X



Y

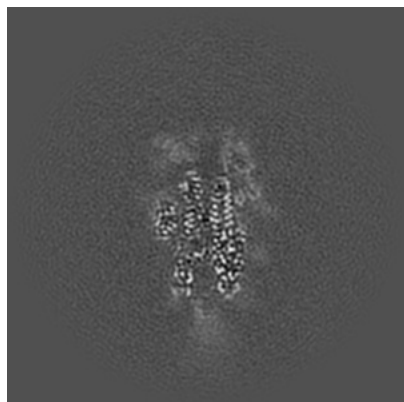


Z

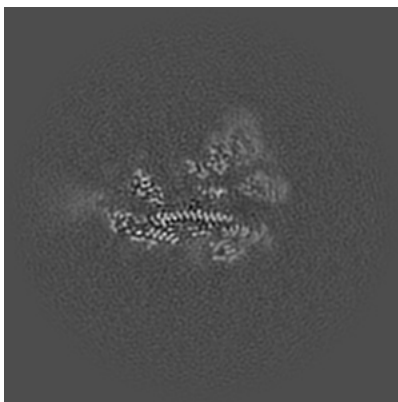
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

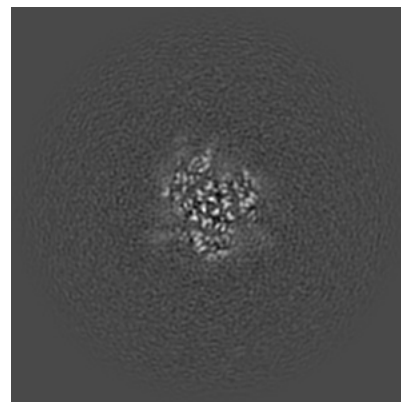
6.2.1 Primary map



X Index: 199

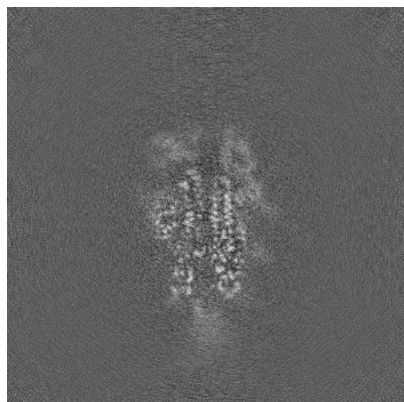


Y Index: 199

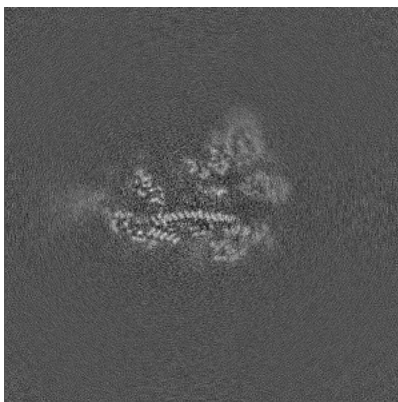


Z Index: 199

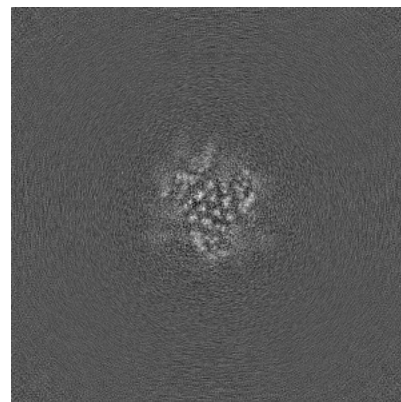
6.2.2 Raw map



X Index: 199



Y Index: 199

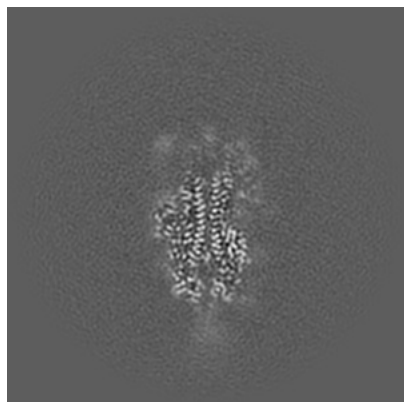


Z Index: 199

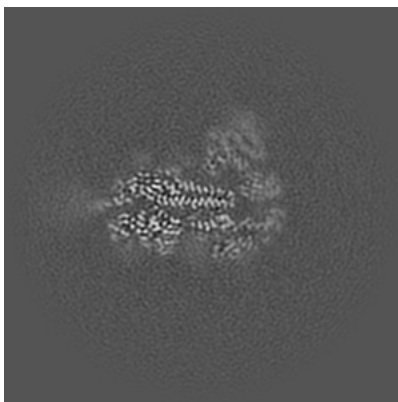
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

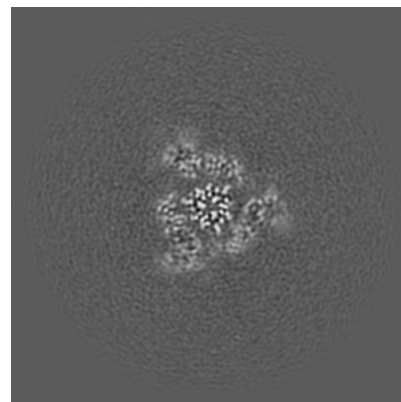
6.3.1 Primary map



X Index: 205

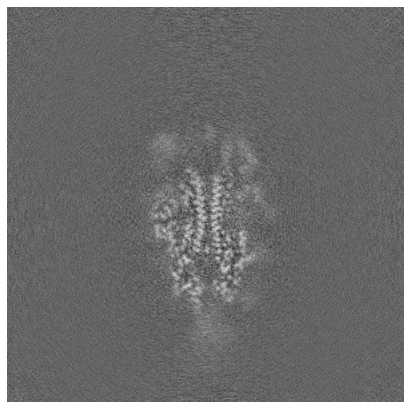


Y Index: 191

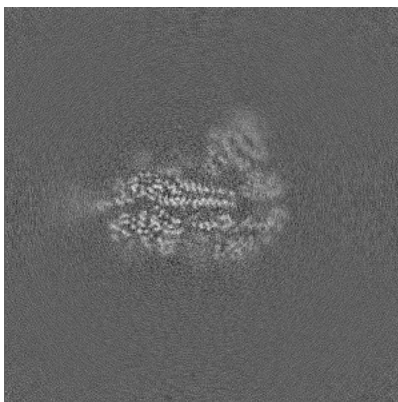


Z Index: 213

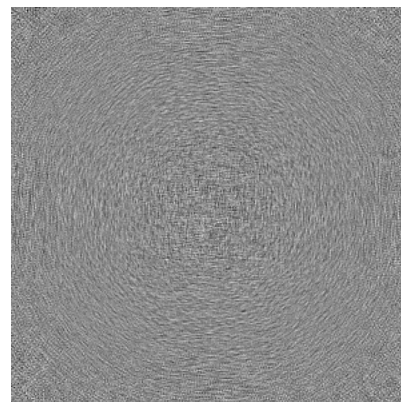
6.3.2 Raw map



X Index: 203



Y Index: 191

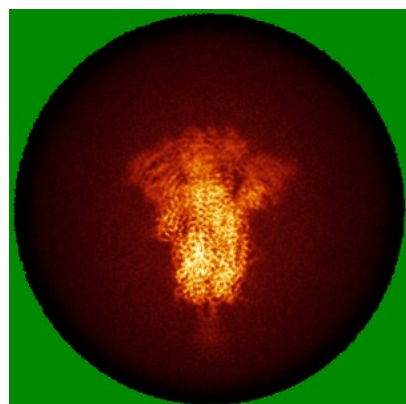


Z Index: 1

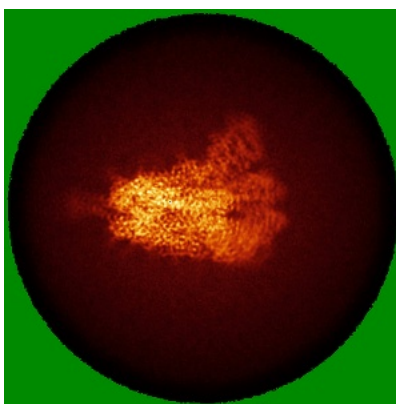
The images above show the largest variance slices of the map in three orthogonal directions.

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

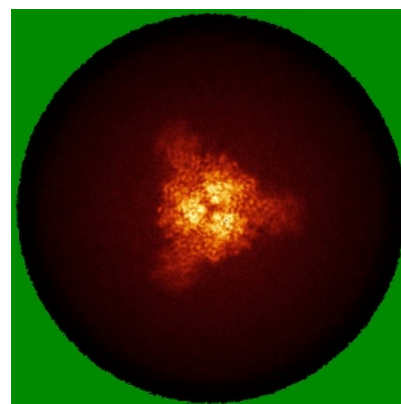
6.4.1 Primary map



X

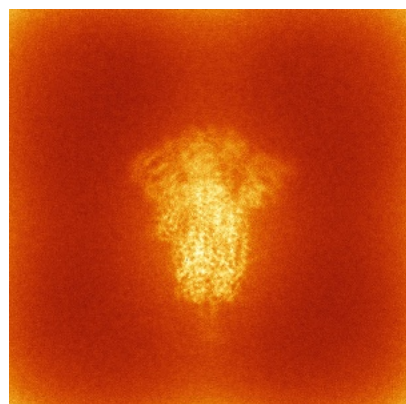


Y

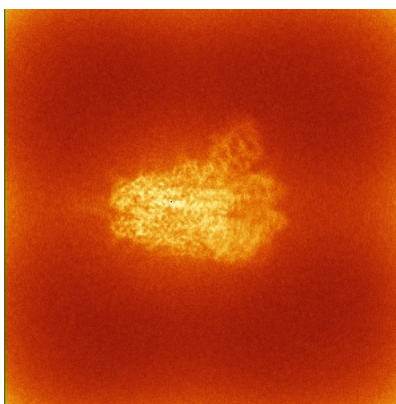


Z

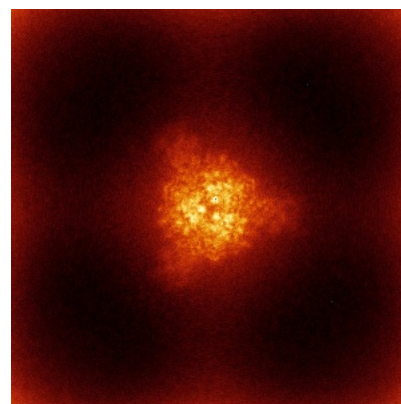
6.4.2 Raw map



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



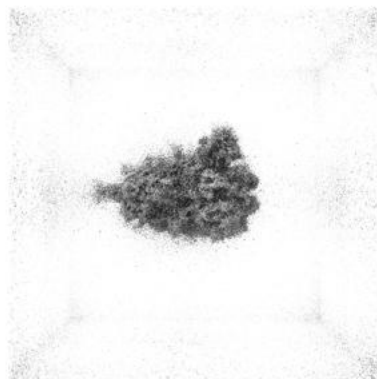
Z

The images above show the 3D surface view of the map at the recommended contour level 0.079. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

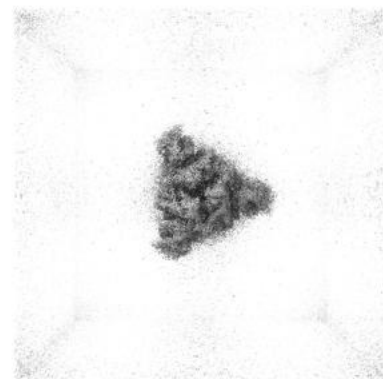
6.5.2 Raw map



X



Y



Z

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

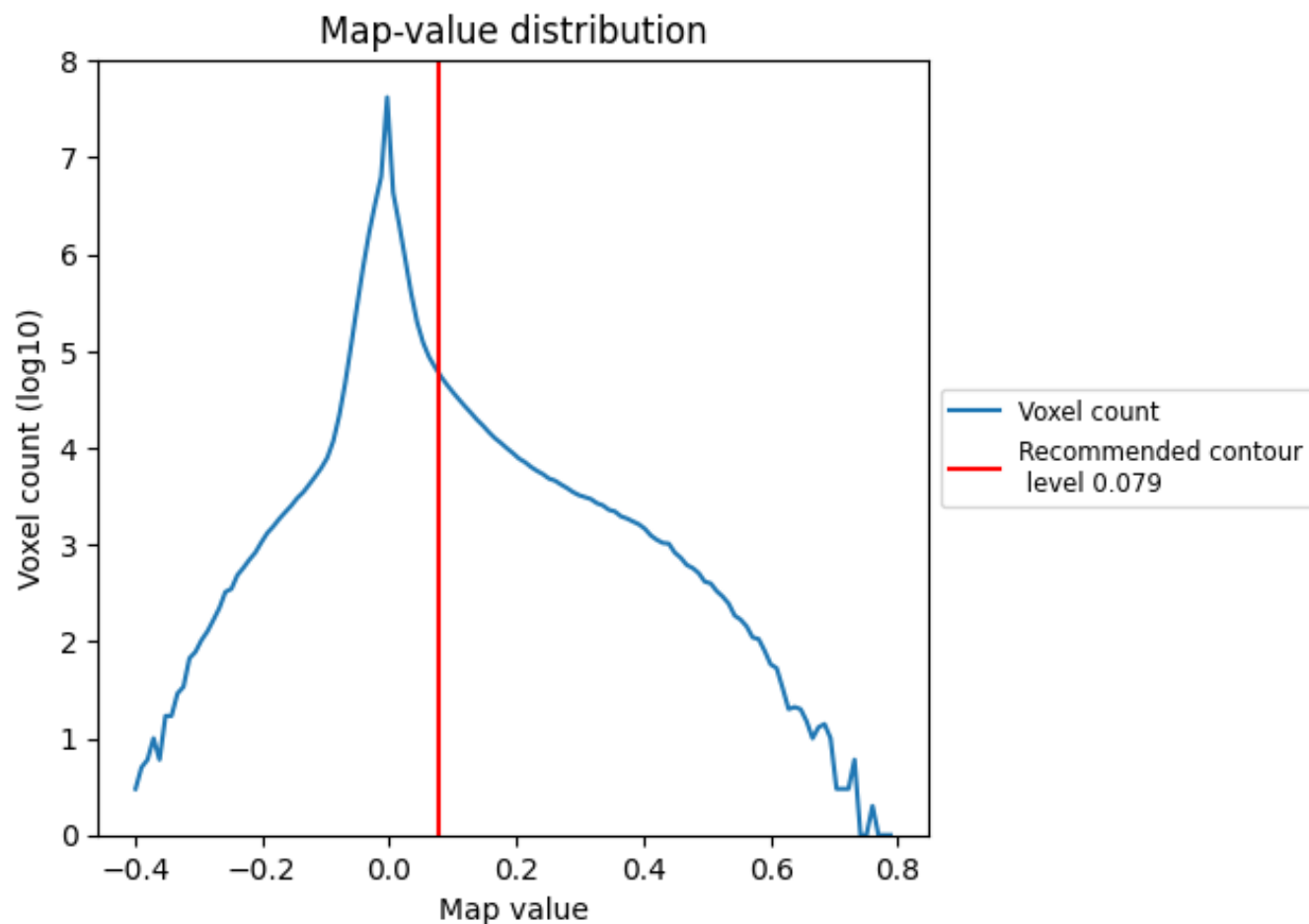
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

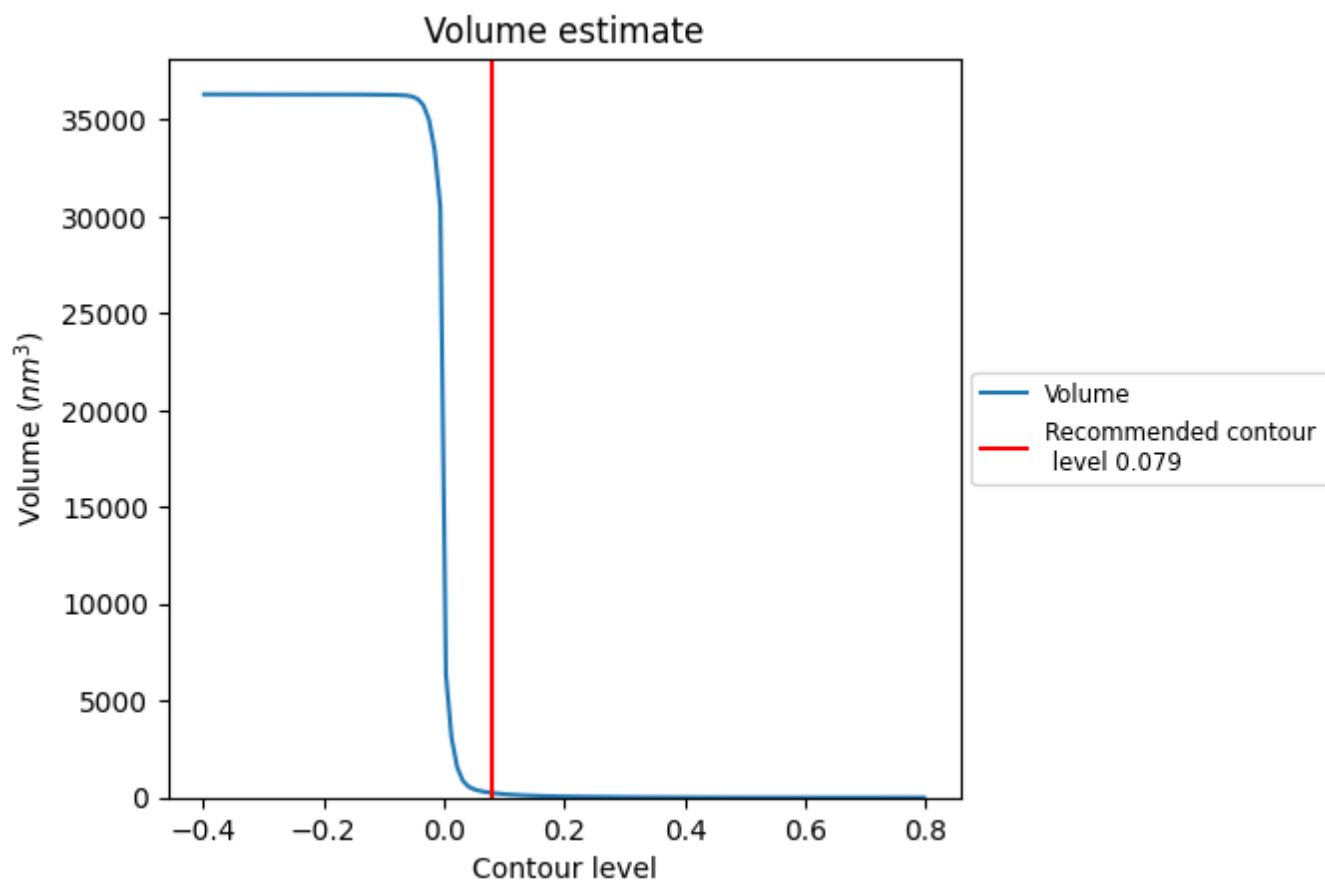
This section contains the results of statistical analysis of the map.

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.

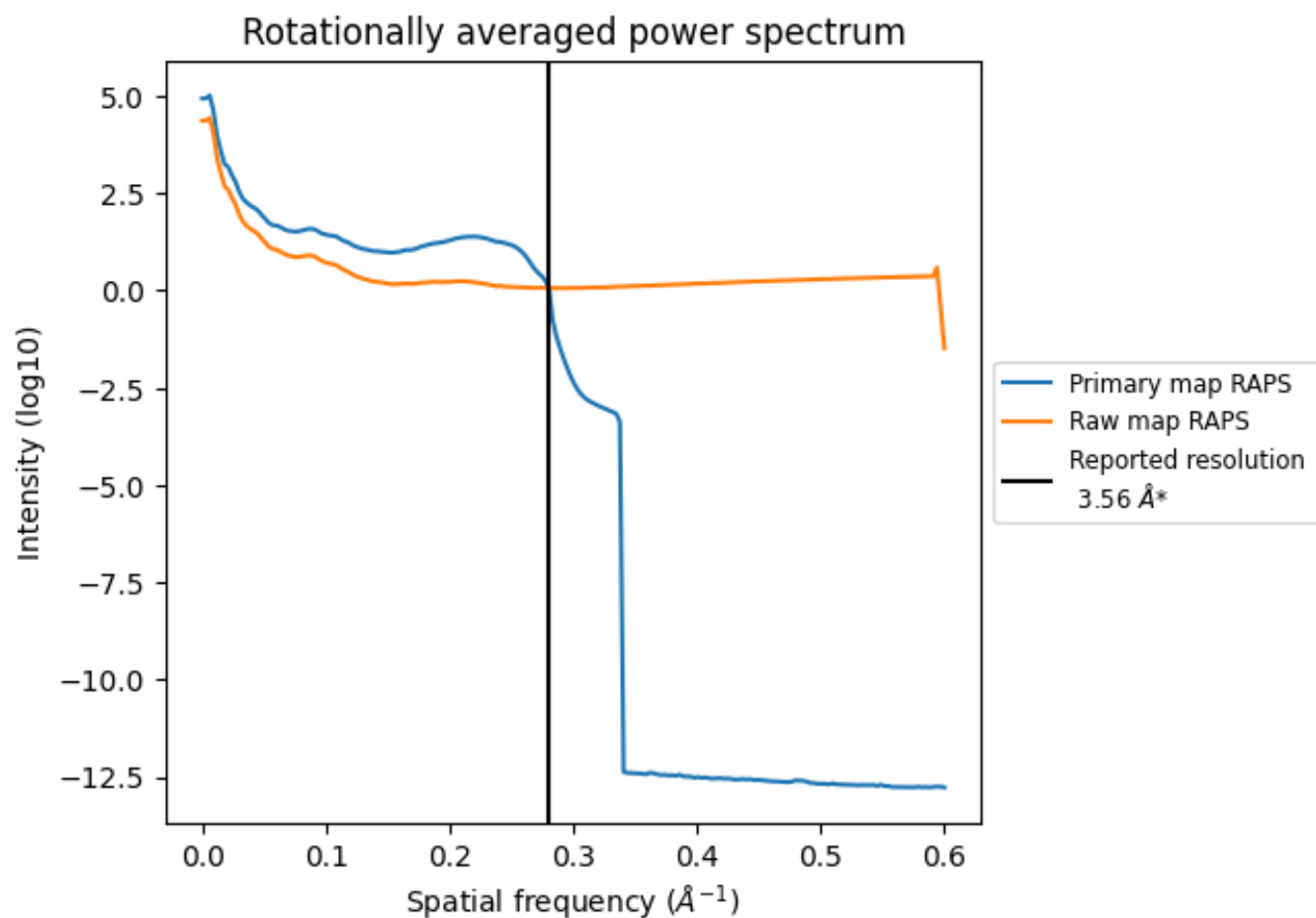
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243 nm^3 ; this corresponds to an approximate mass of 219 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 ⓘ

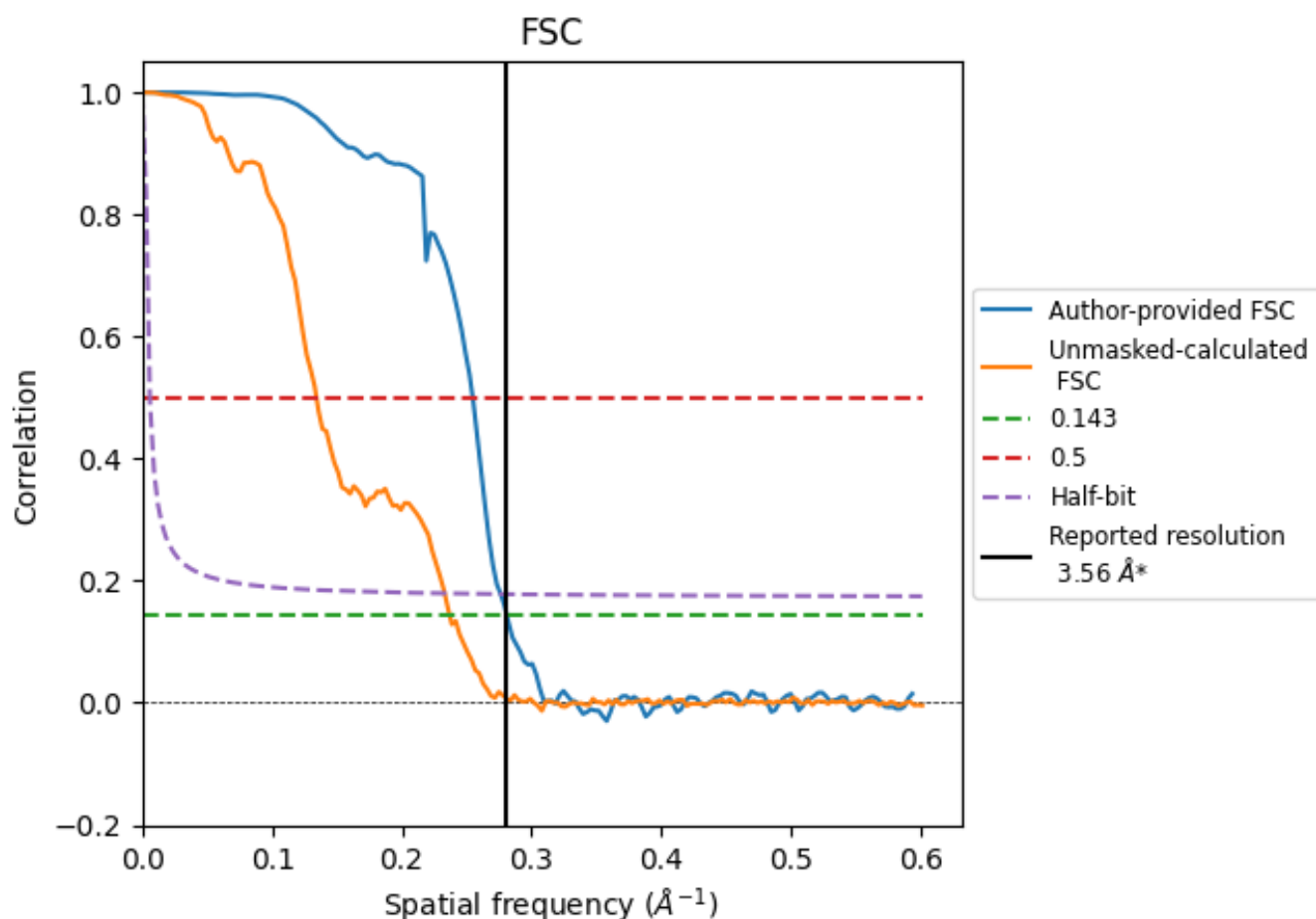


*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.281 \AA^{-1}

8.2 Resolution estimates [i](#)

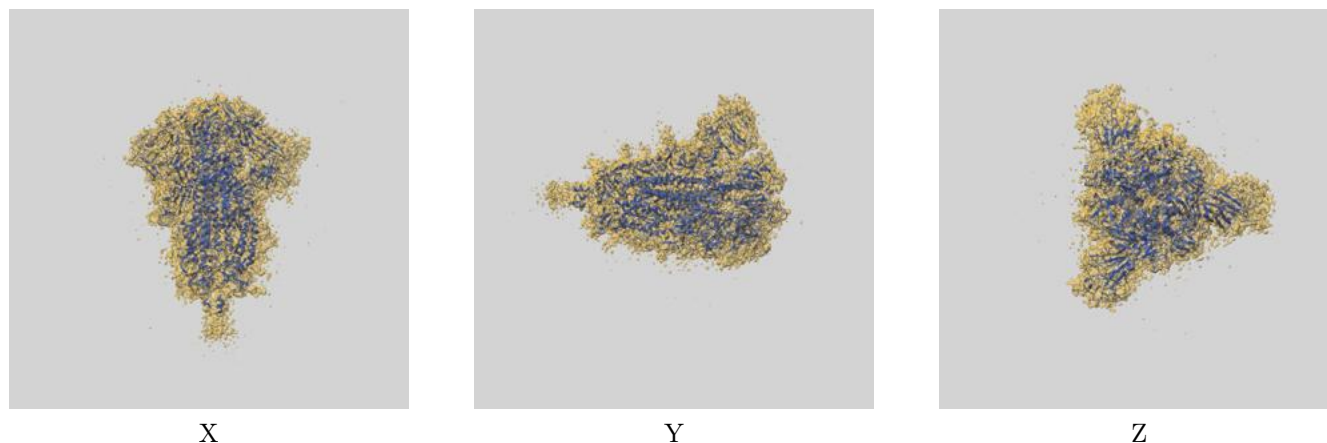
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.56	3.93	3.62
Unmasked-calculated*	4.22	7.45	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.56 by more than 10 %

9 Map-model fit [i](#)

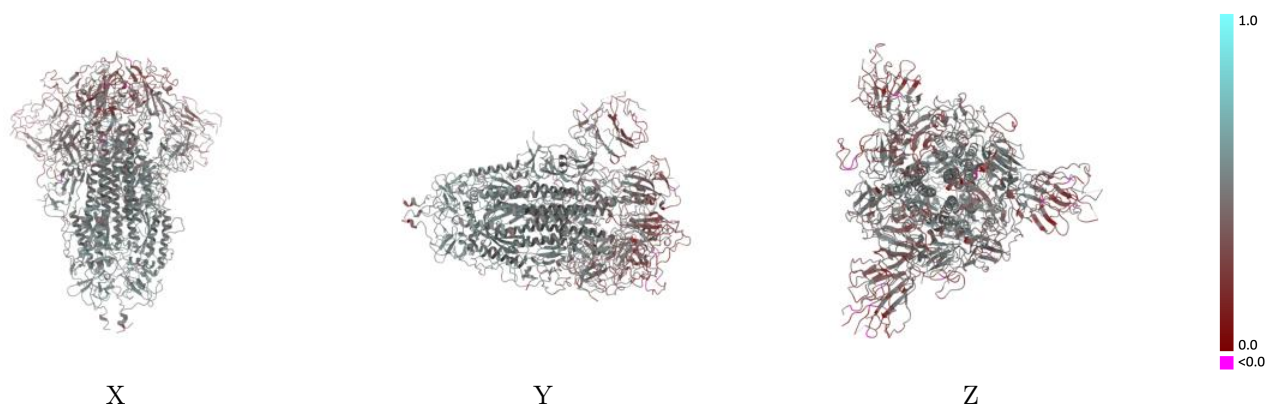
This section contains information regarding the fit between EMDB map EMD-70451 and PDB model 9OG4. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



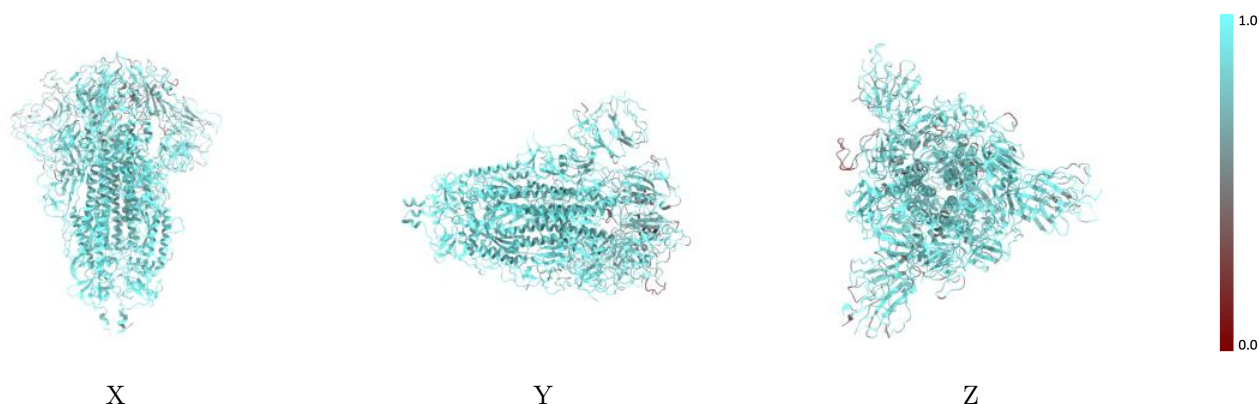
The images above show the 3D surface view of the map at the recommended contour level 0.079 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



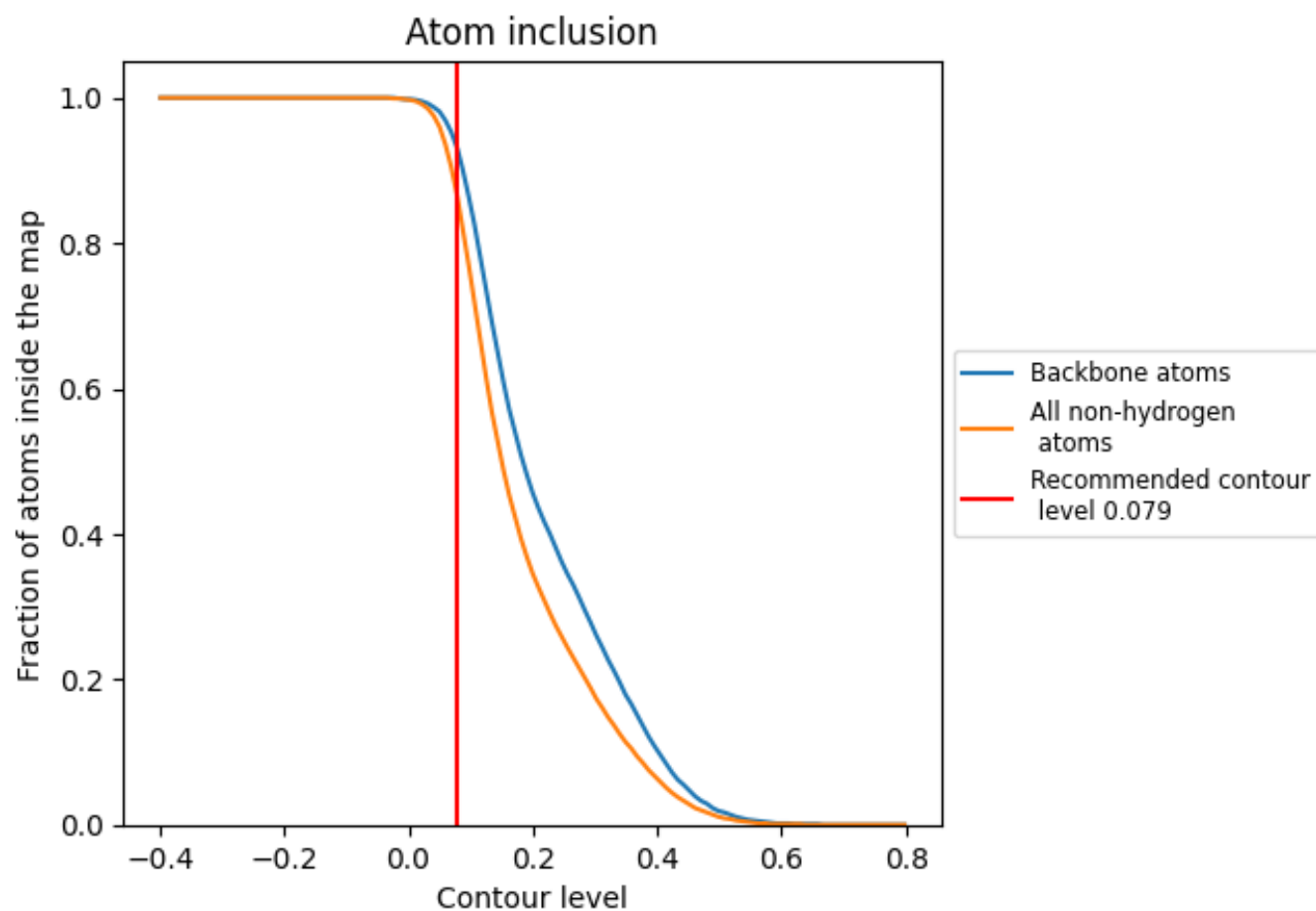
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.079).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.079) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.4410
A	 0.8550	 0.4400
B	 0.8630	 0.4370
C	 0.8790	 0.4520
D	 0.4640	 0.3220
E	 0.7140	 0.4420
F	 0.6670	 0.3810
G	 0.8930	 0.4380
H	 0.5710	 0.4030
I	 0.8210	 0.3890
J	 0.9290	 0.5160
K	 0.7860	 0.4240
L	 0.7140	 0.4500
M	 0.7860	 0.3790
N	 0.7140	 0.2540
O	 0.6790	 0.3890
P	 0.7500	 0.3910
Q	 0.7860	 0.4130
R	 0.4870	 0.3490
S	 0.6150	 0.3180
T	 0.6790	 0.3640
U	 0.6920	 0.3570
V	 0.7440	 0.3640
W	 0.6670	 0.3570

