



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 05:01 PM UTC

PDB ID : 7EDJ / pdb_00007edj
EMDB ID : EMD-31073
Title : Cryo-EM structure of SARS-CoV-2 S-UK variant (B.1.1.7) in complex with Angiotensin-converting enzyme 2 (ACE2) ectodomain
Authors : Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Wu, H.C.; Hsu, S.T.D.
Deposited on : 2021-03-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

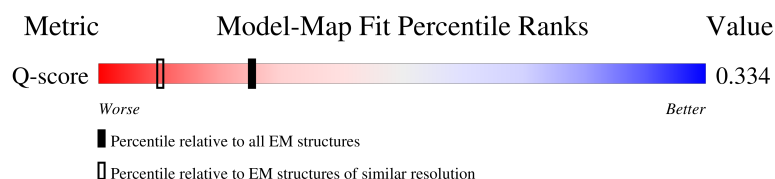
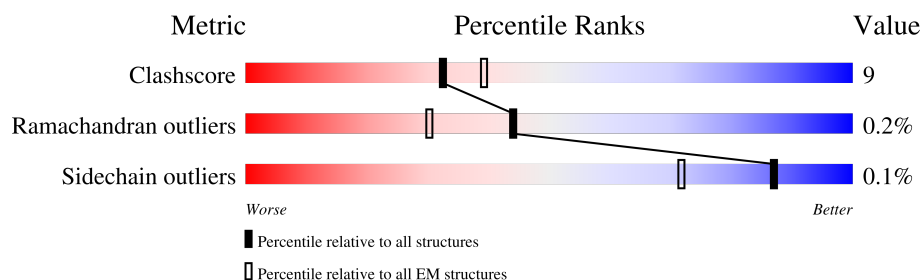
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1286	
1	B	1286	
1	C	1286	
2	I	861	

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Mol	Chain	Length	Quality of chain
2	J	861	
2	K	861	
3	D	2	
3	E	2	
3	F	2	
3	G	2	
3	H	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	
3	c	2	

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Mol	Chain	Length	Quality of chain
3	d	2	50% 100%
3	e	2	100%
3	f	2	100%
3	g	2	50% 50%
3	h	2	50% 50%
3	i	2	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39565 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	1024	Total	C	N	O	S	0	0
			7992	5104	1329	1523	36		
1	B	1016	Total	C	N	O	S	0	0
			7933	5070	1319	1508	36		
1	C	1008	Total	C	N	O	S	0	0
			7878	5037	1308	1497	36		

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P0DTC2
A	-4	GLU	-	expression tag	UNP P0DTC2
A	-3	THR	-	expression tag	UNP P0DTC2
A	-2	ASP	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	TRP	-	expression tag	UNP P0DTC2
A	4	VAL	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	TRP	-	expression tag	UNP P0DTC2
A	9	VAL	-	expression tag	UNP P0DTC2
A	10	PRO	-	expression tag	UNP P0DTC2
A	11	GLY	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	14	GLY	-	expression tag	UNP P0DTC2
A	15	ASP	-	expression tag	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	TYR	ASN	conflict	UNP P0DTC2
A	567	ASP	ALA	conflict	UNP P0DTC2
A	611	GLY	ASP	conflict	UNP P0DTC2
A	678	HIS	PRO	conflict	UNP P0DTC2
A	680	ALA	ARG	conflict	UNP P0DTC2
A	682	ALA	ARG	conflict	UNP P0DTC2
A	713	ILE	THR	conflict	UNP P0DTC2
A	979	ALA	SER	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1115	HIS	ASP	conflict	UNP P0DTC2
A	1206	GLU	-	expression tag	UNP P0DTC2
A	1207	PHE	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLN	-	expression tag	UNP P0DTC2
A	1241	ASP	-	expression tag	UNP P0DTC2
A	1242	ASN	-	expression tag	UNP P0DTC2
A	1243	SER	-	expression tag	UNP P0DTC2
A	1244	ALA	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	ILE	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	ARG	-	expression tag	UNP P0DTC2
A	1252	PRO	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLU	-	expression tag	UNP P0DTC2
A	1255	SER	-	expression tag	UNP P0DTC2
A	1256	ARG	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	PRO	-	expression tag	UNP P0DTC2
A	1259	PHE	-	expression tag	UNP P0DTC2
A	1260	GLU	-	expression tag	UNP P0DTC2
A	1261	GLN	-	expression tag	UNP P0DTC2
A	1262	LYS	-	expression tag	UNP P0DTC2
A	1263	LEU	-	expression tag	UNP P0DTC2
A	1264	ILE	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLU	-	expression tag	UNP P0DTC2
A	1268	ASP	-	expression tag	UNP P0DTC2
A	1269	LEU	-	expression tag	UNP P0DTC2
A	1270	ASN	-	expression tag	UNP P0DTC2
A	1271	MET	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	THR	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
B	-5	MET	-	initiating methionine	UNP P0DTC2
B	-4	GLU	-	expression tag	UNP P0DTC2
B	-3	THR	-	expression tag	UNP P0DTC2
B	-2	ASP	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2
B	1	LEU	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	TRP	-	expression tag	UNP P0DTC2
B	4	VAL	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	TRP	-	expression tag	UNP P0DTC2
B	9	VAL	-	expression tag	UNP P0DTC2
B	10	PRO	-	expression tag	UNP P0DTC2
B	11	GLY	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	14	GLY	-	expression tag	UNP P0DTC2
B	15	ASP	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	498	TYR	ASN	conflict	UNP P0DTC2
B	567	ASP	ALA	conflict	UNP P0DTC2
B	611	GLY	ASP	conflict	UNP P0DTC2
B	678	HIS	PRO	conflict	UNP P0DTC2
B	680	ALA	ARG	conflict	UNP P0DTC2
B	682	ALA	ARG	conflict	UNP P0DTC2
B	713	ILE	THR	conflict	UNP P0DTC2
B	979	ALA	SER	conflict	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1115	HIS	ASP	conflict	UNP P0DTC2
B	1206	GLU	-	expression tag	UNP P0DTC2
B	1207	PHE	-	expression tag	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	LYS	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	GLN	-	expression tag	UNP P0DTC2
B	1241	ASP	-	expression tag	UNP P0DTC2
B	1242	ASN	-	expression tag	UNP P0DTC2
B	1243	SER	-	expression tag	UNP P0DTC2
B	1244	ALA	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	ILE	-	expression tag	UNP P0DTC2
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	ARG	-	expression tag	UNP P0DTC2
B	1252	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLU	-	expression tag	UNP P0DTC2
B	1255	SER	-	expression tag	UNP P0DTC2
B	1256	ARG	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	PRO	-	expression tag	UNP P0DTC2
B	1259	PHE	-	expression tag	UNP P0DTC2
B	1260	GLU	-	expression tag	UNP P0DTC2
B	1261	GLN	-	expression tag	UNP P0DTC2
B	1262	LYS	-	expression tag	UNP P0DTC2
B	1263	LEU	-	expression tag	UNP P0DTC2
B	1264	ILE	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	GLU	-	expression tag	UNP P0DTC2
B	1268	ASP	-	expression tag	UNP P0DTC2
B	1269	LEU	-	expression tag	UNP P0DTC2
B	1270	ASN	-	expression tag	UNP P0DTC2
B	1271	MET	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	THR	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
B	1278	HIS	-	expression tag	UNP P0DTC2
B	1279	HIS	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
C	-5	MET	-	initiating methionine	UNP P0DTC2
C	-4	GLU	-	expression tag	UNP P0DTC2
C	-3	THR	-	expression tag	UNP P0DTC2
C	-2	ASP	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	LEU	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	TRP	-	expression tag	UNP P0DTC2
C	4	VAL	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	-	expression tag	UNP P0DTC2
C	10	PRO	-	expression tag	UNP P0DTC2
C	11	GLY	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	14	GLY	-	expression tag	UNP P0DTC2
C	15	ASP	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	498	TYR	ASN	conflict	UNP P0DTC2
C	567	ASP	ALA	conflict	UNP P0DTC2
C	611	GLY	ASP	conflict	UNP P0DTC2
C	678	HIS	PRO	conflict	UNP P0DTC2
C	680	ALA	ARG	conflict	UNP P0DTC2
C	682	ALA	ARG	conflict	UNP P0DTC2
C	713	ILE	THR	conflict	UNP P0DTC2
C	979	ALA	SER	conflict	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1115	HIS	ASP	conflict	UNP P0DTC2
C	1206	GLU	-	expression tag	UNP P0DTC2
C	1207	PHE	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	SER	-	expression tag	UNP P0DTC2
C	1210	GLY	-	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	LYS	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLN	-	expression tag	UNP P0DTC2
C	1241	ASP	-	expression tag	UNP P0DTC2
C	1242	ASN	-	expression tag	UNP P0DTC2
C	1243	SER	-	expression tag	UNP P0DTC2
C	1244	ALA	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	ILE	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	ARG	-	expression tag	UNP P0DTC2
C	1252	PRO	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLU	-	expression tag	UNP P0DTC2
C	1255	SER	-	expression tag	UNP P0DTC2
C	1256	ARG	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	PRO	-	expression tag	UNP P0DTC2
C	1259	PHE	-	expression tag	UNP P0DTC2
C	1260	GLU	-	expression tag	UNP P0DTC2
C	1261	GLN	-	expression tag	UNP P0DTC2
C	1262	LYS	-	expression tag	UNP P0DTC2
C	1263	LEU	-	expression tag	UNP P0DTC2
C	1264	ILE	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	GLU	-	expression tag	UNP P0DTC2
C	1268	ASP	-	expression tag	UNP P0DTC2

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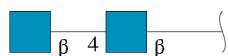
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1269	LEU	-	expression tag	UNP P0DTC2
C	1270	ASN	-	expression tag	UNP P0DTC2
C	1271	MET	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	THR	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	HIS	-	expression tag	UNP P0DTC2
C	1278	HIS	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2 (ACE2) ectodomain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		
2	J	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		
2	K	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		

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



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

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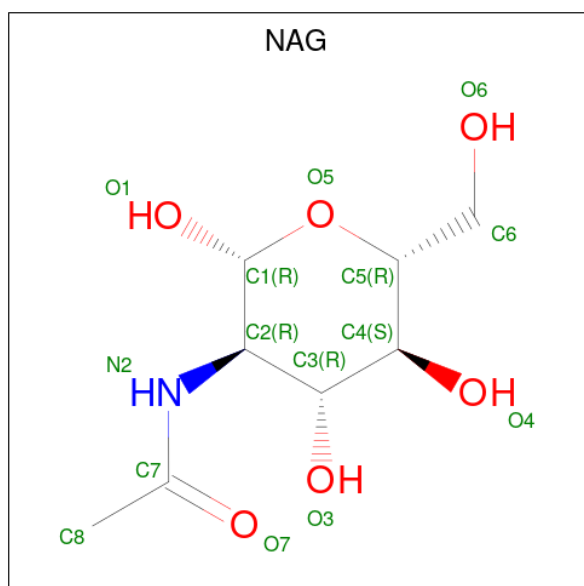
Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	B	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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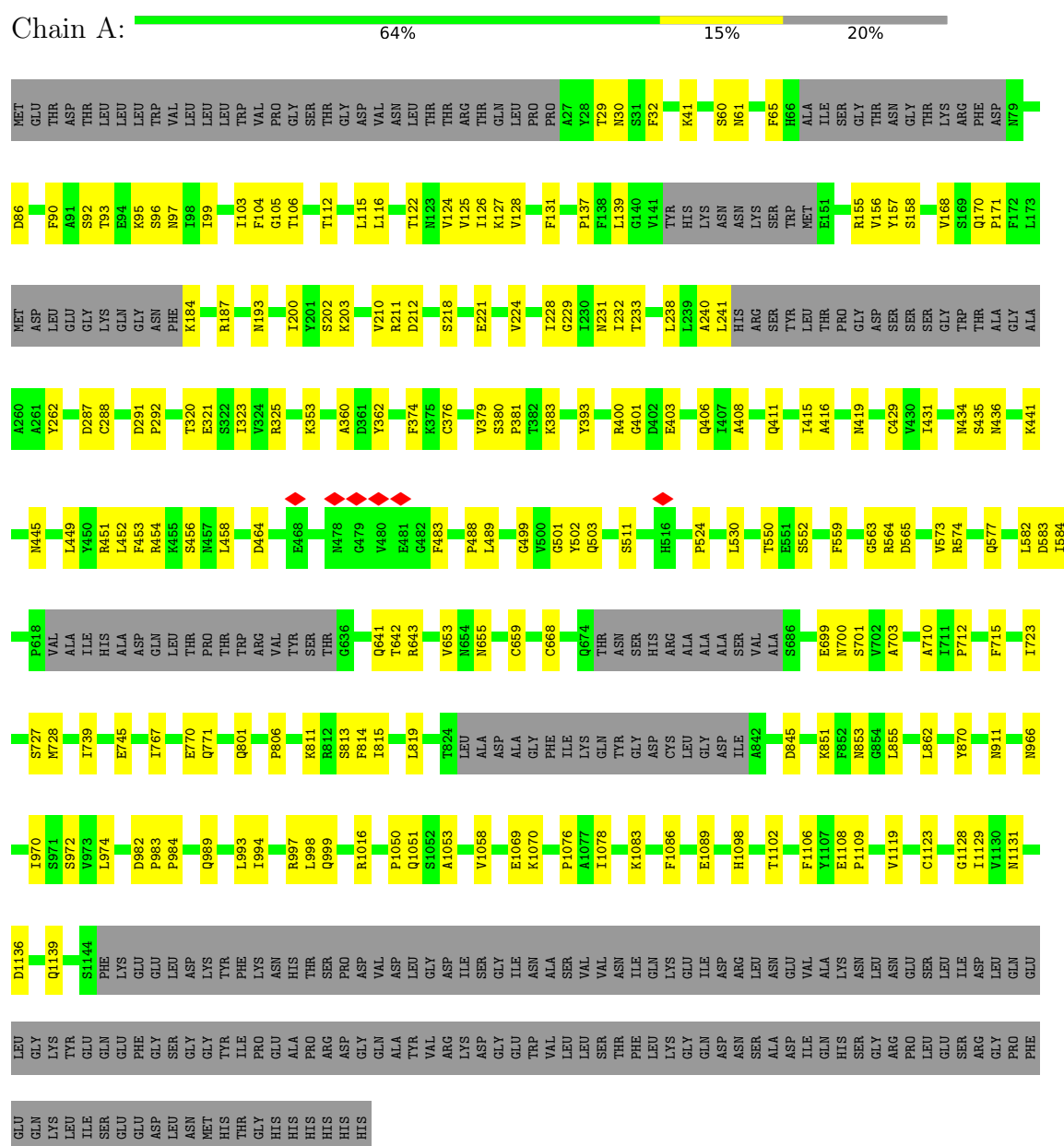
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	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	I	1	Total	C	N	O	0
			14	8	1	5	
4	I	1	Total	C	N	O	0
			14	8	1	5	
4	I	1	Total	C	N	O	0
			14	8	1	5	
4	I	1	Total	C	N	O	0
			14	8	1	5	
4	I	1	Total	C	N	O	0
			14	8	1	5	
4	I	1	Total	C	N	O	0
			14	8	1	5	
4	J	1	Total	C	N	O	0
			14	8	1	5	

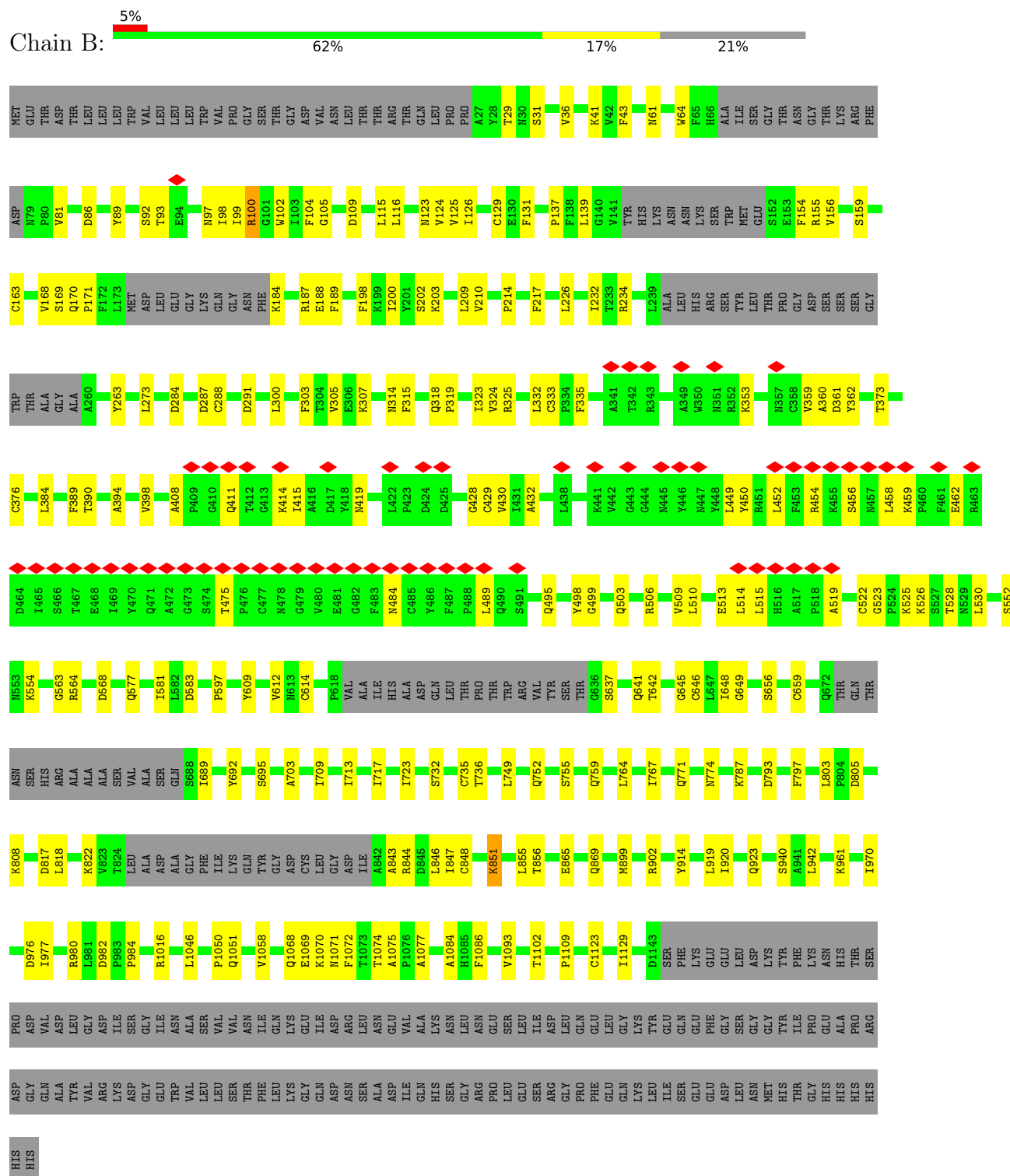
3 Residue-property plots

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

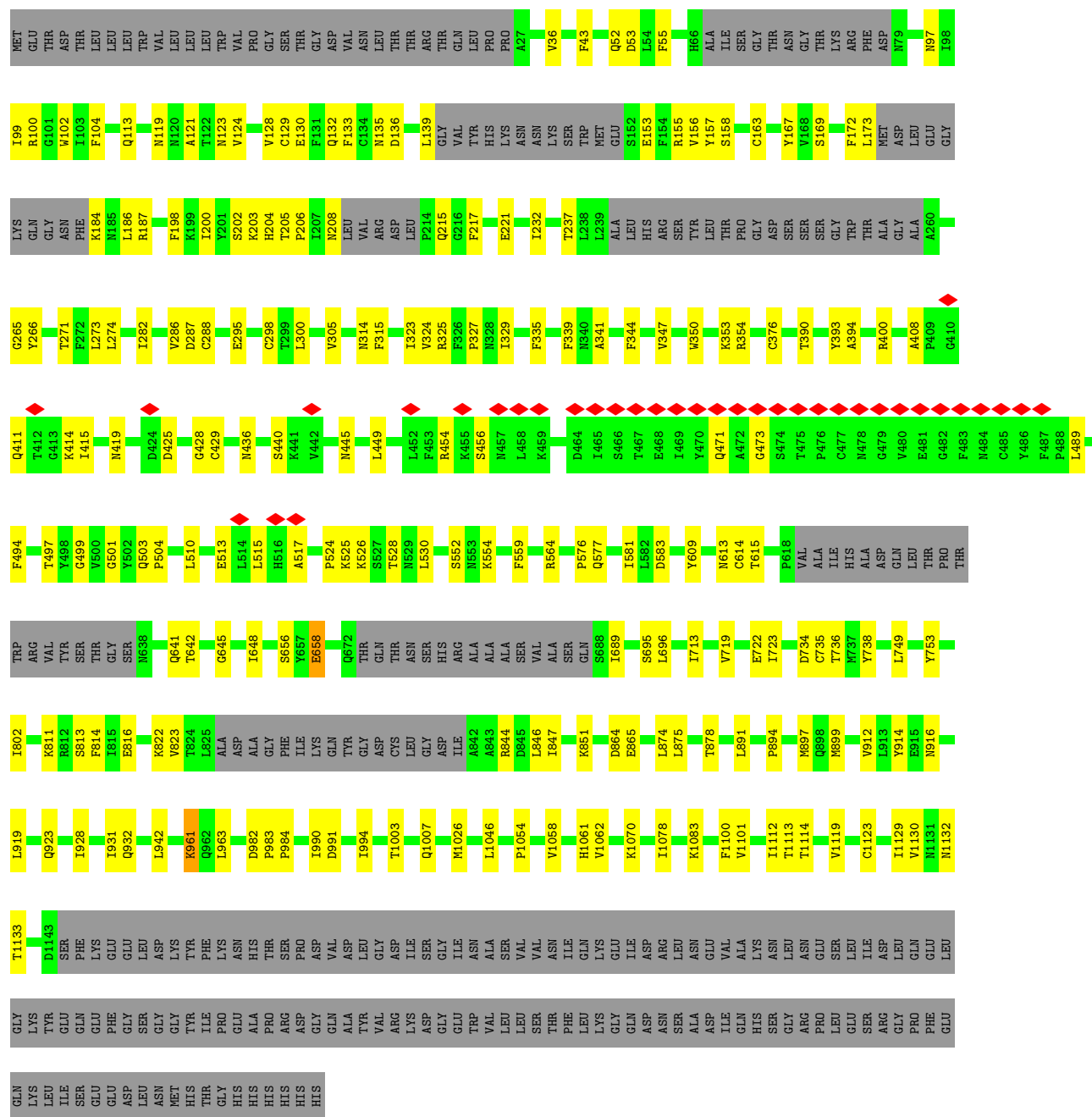


- Molecule 1: Spike glycoprotein

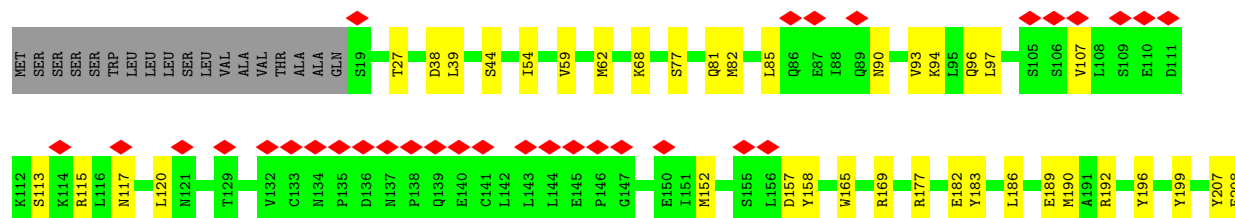


- Molecule 1: Spike glycoprotein





● Molecule 2: Angiotensin-converting enzyme 2 (ACE2) ectodomain



Chain G:  100%

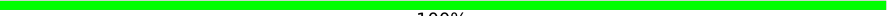


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%



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

Chain L:  100%



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

Chain M:  50% 50%



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

Chain N:  50% 100%



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

Chain O:  50% 50%



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

Chain P:  50% 50%



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

Chain Q:  100%



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

Chain R:  100%



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

Chain S:  100%



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

Chain T:  50% 50%



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

Chain U:  50% 50%



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

Chain V:  100%



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

Chain W:  100%

NAG1
NAG2

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

Chain X:  50% 50% 50%

NAG1
NAG2

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

Chain Y:  100%

NAG1
NAG2

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

Chain Z:  100%

NAG1
NAG2

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

Chain a:  50% 100%

NAG1
NAG2

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

Chain b:  100%

NAG1
NAG2

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

Chain c:  100%



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

Chain d:  50% 100%



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

Chain e:  100%



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

Chain f:  100%



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

Chain g:  50% 50% 50%



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

Chain h:  50% 50%



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

Chain i:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	460280	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 K3 (6k x 4k)	Depositor
Maximum map value	3.115	Depositor
Minimum map value	-1.813	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.27	0/8172	0.41	0/11119
1	B	0.27	0/8113	0.41	0/11039
1	C	0.27	0/8057	0.42	0/10961
2	I	0.12	0/4999	0.34	1/6792 (0.0%)
2	J	0.11	0/4999	0.31	0/6792
2	K	0.12	0/4999	0.34	0/6792
All	All	0.23	0/39339	0.38	1/53495 (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	C	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	506	VAL	N-CA-C	-7.91	106.20	113.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	614	CYS	Peptide
1	C	658	GLU	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	7992	0	7795	146	0
1	B	7933	0	7737	144	0
1	C	7878	0	7680	133	0
2	I	4862	0	4633	105	0
2	J	4862	0	4638	64	0
2	K	4862	0	4639	81	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	L	28	0	25	0	0
3	M	28	0	25	1	0
3	N	28	0	25	1	0
3	O	28	0	25	2	0
3	P	28	0	25	2	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	1	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	1	0
3	X	28	0	25	1	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	2	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	1	0
3	i	28	0	25	0	0
4	A	84	0	78	0	0
4	B	84	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	98	0	91	3	0
4	I	84	0	78	1	0
4	J	14	0	13	0	0
All	All	39565	0	38185	662	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 (662) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:814:PHE:HE2	1:C:932:GLN:HE21	1.29	0.79
1:A:1123:CYS:HB2	1:A:1129:ILE:HD13	1.67	0.77
1:C:722:GLU:OE2	1:C:1061:HIS:NE2	2.18	0.76
1:C:325:ARG:HE	1:C:577:GLN:HG3	1.50	0.76
2:K:180:TYR:OH	2:K:460:ARG:NH1	2.18	0.76
1:C:609:TYR:O	1:C:645:GLY:HA3	1.87	0.75
1:A:106:THR:HB	1:A:112:THR:HG21	1.71	0.73
1:B:851:LYS:HB2	1:B:855:LEU:HB2	1.69	0.73
1:A:851:LYS:HB2	1:A:855:LEU:HB2	1.71	0.72
1:A:29:THR:O	1:A:61:ASN:HA	1.89	0.72
1:B:105:GLY:H	1:B:232:ILE:HG23	1.53	0.72
2:I:152:MET:HE2	2:I:270:MET:H	1.57	0.70
1:A:325:ARG:HE	1:A:577:GLN:HG3	1.57	0.70
1:C:329:ILE:HG13	1:C:524:PRO:HB3	1.74	0.70
2:K:320:LEU:HD13	2:K:380:GLN:HG2	1.73	0.70
1:A:801:GLN:OE1	3:M:1:NAG:O6	2.09	0.70
1:B:755:SER:O	1:B:759:GLN:NE2	2.23	0.70
2:J:457:GLU:HG2	2:J:513:ILE:HD13	1.74	0.70
2:J:379:ILE:HG22	2:J:383:MET:HE2	1.73	0.69
1:C:325:ARG:HH21	1:C:577:GLN:HB2	1.57	0.69
2:J:373:HIS:HA	2:J:376:MET:HE2	1.75	0.69
2:I:379:ILE:HG22	2:I:383:MET:HE1	1.76	0.68
2:I:523:PHE:HB3	2:I:583:PRO:HB2	1.75	0.68
2:I:459:TRP:HB2	2:I:480:MET:HE1	1.75	0.68
1:B:353:LYS:HB3	1:B:394:ALA:HB3	1.74	0.68
1:B:641:GLN:NE2	1:B:642:THR:O	2.27	0.68
1:B:732:SER:OG	1:B:856:THR:OG1	2.11	0.68
2:I:552:GLN:NE2	2:I:556:ASN:OD1	2.27	0.68
1:A:699:GLU:OE2	1:B:787:LYS:NZ	2.26	0.68
1:A:376:CYS:HB2	1:A:429:CYS:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:GLU:OE2	1:A:1016:ARG:NE	2.27	0.67
2:J:523:PHE:HB3	2:J:583:PRO:HB2	1.75	0.67
1:A:552:SER:HB2	1:A:583:ASP:HB2	1.78	0.66
1:C:102:TRP:HB3	1:C:104:PHE:HE1	1.60	0.66
1:B:723:ILE:HG12	1:B:1058:VAL:HG22	1.77	0.66
1:A:139:LEU:HB2	1:A:240:ALA:HB2	1.77	0.66
1:A:453:PHE:HE2	2:I:27:THR:HB	1.61	0.66
2:K:331:SER:HB2	2:K:358:ILE:H	1.60	0.66
1:B:709:ILE:HD11	1:B:1093:VAL:HG12	1.76	0.66
1:C:187:ARG:HE	1:C:205:THR:HG22	1.61	0.66
2:K:85:LEU:HD11	2:K:94:LYS:HA	1.79	0.65
3:b:1:NAG:H5	3:b:2:NAG:HN2	1.61	0.65
1:B:139:LEU:HG	1:B:154:PHE:HA	1.77	0.65
2:I:96:GLN:HE21	2:I:392:LEU:HD11	1.61	0.65
1:A:105:GLY:H	1:A:232:ILE:HG23	1.60	0.65
1:C:323:ILE:HD11	1:C:530:LEU:HA	1.78	0.65
1:C:802:ILE:HD11	1:C:928:ILE:HD11	1.79	0.65
1:C:723:ILE:HG13	1:C:1058:VAL:HG22	1.79	0.64
1:A:441:LYS:NZ	1:A:445:ASN:OD1	2.30	0.64
2:J:271:TRP:NE1	2:J:502:SER:O	2.30	0.64
1:B:428:GLY:HA3	1:B:510:LEU:O	1.98	0.63
2:I:419:LYS:HD2	2:I:426:PRO:HA	1.80	0.63
1:A:454:ARG:NH1	1:A:464:ASP:OD2	2.32	0.63
1:B:61:ASN:HB3	4:B:2001:NAG:N2	2.13	0.63
1:B:300:LEU:HD12	1:B:305:VAL:HG12	1.80	0.63
1:C:735:CYS:SG	1:C:736:THR:N	2.70	0.63
2:K:37:GLU:HG2	2:K:390:PHE:HB2	1.80	0.63
2:J:119:ILE:HG22	2:J:123:MET:HE2	1.79	0.63
2:I:433:GLU:HA	2:I:436:ILE:HG22	1.80	0.63
2:I:525:PHE:HE1	2:I:573:VAL:HG11	1.64	0.63
1:A:103:ILE:HD11	1:A:238:LEU:HD23	1.81	0.62
2:I:113:SER:O	2:I:117:ASN:ND2	2.30	0.62
2:K:581:VAL:HG23	2:K:584:LEU:HD13	1.79	0.62
2:I:398:GLU:O	2:I:514:ARG:NE	2.30	0.62
1:C:133:PHE:HA	1:C:157:TYR:HA	1.81	0.62
1:A:155:ARG:NH1	1:A:156:VAL:O	2.33	0.62
1:C:414:LYS:O	1:C:419:ASN:ND2	2.33	0.62
2:I:330:ASN:O	2:I:357:ARG:NH1	2.33	0.61
2:K:263:PRO:HG2	2:K:266:LEU:HD12	1.82	0.61
2:I:344:CYS:O	2:I:361:CYS:HB2	2.01	0.61
1:A:451:ARG:HH22	1:A:454:ARG:HD3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:GLY:O	1:C:503:GLN:NE2	2.34	0.61
1:A:99:ILE:HG21	1:A:187:ARG:HH21	1.65	0.61
1:B:805:ASP:OD2	1:B:808:LYS:NZ	2.34	0.60
1:A:739:ILE:O	1:A:997:ARG:NH1	2.33	0.60
1:C:121:ALA:HB3	4:C:2002:NAG:H82	1.83	0.60
1:B:61:ASN:HB3	4:B:2001:NAG:HN2	1.66	0.60
1:C:428:GLY:HA3	1:C:510:LEU:O	2.00	0.60
1:B:129:CYS:HA	1:B:163:CYS:HB3	1.83	0.60
1:A:115:LEU:HA	1:A:128:VAL:HG12	1.84	0.59
1:B:36:VAL:HG21	1:B:217:PHE:CZ	2.37	0.59
1:B:408:ALA:HB3	1:B:411:GLN:HG3	1.84	0.59
1:B:552:SER:HB2	1:B:583:ASP:HB2	1.83	0.59
1:B:124:VAL:HG13	1:B:171:PRO:HA	1.84	0.59
1:B:376:CYS:HB2	1:B:429:CYS:HA	1.85	0.59
1:B:415:ILE:HD13	1:B:419:ASN:HD22	1.67	0.59
2:I:209:VAL:HG13	2:I:216:ASP:HA	1.83	0.59
1:B:389:PHE:HE1	1:B:514:LEU:HG	1.67	0.59
2:J:133:CYS:HA	2:J:141:CYS:HA	1.83	0.59
1:C:324:VAL:O	1:C:528:THR:OG1	2.21	0.59
1:B:99:ILE:HG23	1:B:100:ARG:HG3	1.84	0.59
1:B:99:ILE:HG13	1:B:100:ARG:H	1.67	0.59
1:C:641:GLN:NE2	1:C:642:THR:O	2.33	0.59
2:I:545:SER:HB3	4:I:1006:NAG:H82	1.85	0.59
1:A:806:PRO:HA	1:A:811:LYS:HD3	1.85	0.58
1:B:1102:THR:HG22	1:B:1109:PRO:HA	1.84	0.58
1:B:92:SER:OG	1:B:93:THR:N	2.36	0.58
1:A:408:ALA:HB3	1:A:411:GLN:HG3	1.85	0.58
1:B:449:LEU:HD23	1:B:489:LEU:HB3	1.84	0.58
1:B:125:VAL:HG12	1:B:168:VAL:HG22	1.84	0.58
1:C:274:LEU:HD22	1:C:282:ILE:HD13	1.85	0.58
2:K:326:GLY:O	2:K:330:ASN:ND2	2.37	0.58
1:A:92:SER:OG	1:A:93:THR:N	2.37	0.58
1:A:400:ARG:NH2	1:A:403:GLU:OE1	2.37	0.58
2:K:428:PHE:CE2	2:K:430:GLU:HB3	2.39	0.57
4:C:2003:NAG:H83	4:C:2003:NAG:H3	1.86	0.57
2:K:90:ASN:HB3	2:K:93:VAL:HG22	1.84	0.57
2:I:428:PHE:CE2	2:I:430:GLU:HB3	2.40	0.57
2:J:460:ARG:NH1	2:J:505:HIS:O	2.32	0.57
2:K:249:MET:HE1	2:K:258:PRO:HD3	1.87	0.57
1:A:483:PHE:HZ	2:I:82:MET:HE3	1.70	0.57
1:A:106:THR:OG1	1:A:231:ASN:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HH12	1:A:454:ARG:HH11	1.50	0.57
1:A:723:ILE:HG13	1:A:1058:VAL:HG22	1.87	0.57
1:C:104:PHE:HD2	1:C:232:ILE:HD11	1.70	0.57
2:J:331:SER:HB2	2:J:358:ILE:H	1.69	0.57
2:K:123:MET:HE3	2:K:176:LEU:HD12	1.87	0.57
2:K:590:PRO:HA	2:K:593:THR:HG22	1.87	0.57
1:C:390:THR:HG21	1:C:517:ALA:HB3	1.87	0.56
2:K:235:PRO:O	2:K:239:HIS:ND1	2.34	0.56
2:I:394:ASN:HB2	2:I:562:LYS:HE3	1.87	0.56
2:J:54:ILE:HD12	2:J:341:LYS:HG3	1.87	0.56
1:A:90:PHE:HD1	1:A:187:ARG:HH12	1.53	0.56
1:A:184:LYS:HE3	1:A:210:VAL:HG12	1.86	0.56
1:A:1083:LYS:HD2	1:A:1119:VAL:HG21	1.88	0.56
1:C:471:GLN:NE2	1:C:473:GLY:O	2.32	0.56
2:I:314:PHE:HE2	2:I:408:MET:HG3	1.70	0.56
2:I:567:THR:HB	2:I:577:LYS:HD3	1.86	0.56
2:J:113:SER:O	2:J:117:ASN:ND2	2.38	0.56
1:B:414:LYS:O	1:B:419:ASN:ND2	2.38	0.56
1:B:976:ASP:O	1:B:980:ARG:HB2	2.06	0.56
1:C:347:VAL:HG21	1:C:415:ILE:HD12	1.86	0.56
2:K:419:LYS:HD2	2:K:426:PRO:HA	1.88	0.56
1:A:703:ALA:HB2	3:N:2:NAG:H3	1.87	0.56
1:C:445:ASN:HB2	1:C:494:PHE:HB2	1.88	0.56
2:I:248:LEU:HD12	2:I:262:LEU:HD11	1.87	0.56
1:C:719:VAL:HG22	1:C:1062:VAL:HG22	1.88	0.56
1:C:552:SER:HB2	1:C:583:ASP:HB2	1.88	0.56
1:B:865:GLU:OE1	1:B:869:GLN:NE2	2.39	0.55
1:B:817:ASP:OD1	1:B:818:LEU:N	2.39	0.55
2:I:85:LEU:HD11	2:I:94:LYS:HA	1.87	0.55
1:A:127:LYS:HZ2	1:A:131:PHE:HZ	1.55	0.55
1:C:734:ASP:OD1	1:C:735:CYS:N	2.38	0.55
2:I:177:ARG:NH1	2:I:495:GLU:O	2.32	0.55
2:I:249:MET:HE1	2:I:258:PRO:HG3	1.87	0.55
2:K:293:VAL:HG11	2:K:424:LEU:HD21	1.87	0.55
2:K:343:VAL:HG12	2:K:345:HIS:H	1.71	0.55
1:A:287:ASP:OD1	1:A:288:CYS:N	2.40	0.55
2:I:208:GLU:OE2	2:I:219:ARG:NH1	2.38	0.55
2:K:271:TRP:NE1	2:K:502:SER:O	2.40	0.55
1:A:563:GLY:HA2	1:B:43:PHE:HB3	1.89	0.55
2:I:380:GLN:HA	2:I:383:MET:HE2	1.88	0.55
2:J:428:PHE:CE2	2:J:430:GLU:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:TYR:HE2	1:B:452:LEU:HD13	1.70	0.55
1:B:774:ASN:OD1	1:B:1016:ARG:NH1	2.39	0.55
1:B:1069:GLU:HG2	1:C:891:LEU:HD22	1.88	0.55
2:J:119:ILE:HD12	2:J:179:LEU:HD22	1.87	0.55
2:K:133:CYS:HA	2:K:140:GLU:O	2.06	0.55
1:A:325:ARG:HH12	1:A:530:LEU:HB2	1.72	0.55
2:I:402:GLU:HG3	2:I:514:ARG:HH12	1.72	0.55
3:T:2:NAG:H83	3:T:2:NAG:H3	1.88	0.55
1:C:990:ILE:O	1:C:994:ILE:HG12	2.06	0.55
2:J:248:LEU:HD21	2:J:278:LEU:HD11	1.88	0.55
1:C:123:ASN:HB2	4:C:2002:NAG:H5	1.88	0.54
1:A:1050:PRO:O	1:A:1051:GLN:NE2	2.25	0.54
1:B:209:LEU:HD12	1:B:214:PRO:HB3	1.89	0.54
2:I:115:ARG:HH12	2:I:186:LEU:HD13	1.71	0.54
1:B:324:VAL:O	1:B:528:THR:OG1	2.25	0.54
1:C:102:TRP:HB3	1:C:104:PHE:CE1	2.40	0.54
1:B:767:ILE:O	1:B:771:GLN:HG2	2.07	0.54
1:B:1070:LYS:HG2	1:B:1071:ASN:H	1.72	0.54
1:A:41:LYS:HD2	1:C:559:PHE:O	2.07	0.54
1:C:52:GLN:NE2	1:C:271:THR:OG1	2.40	0.54
2:J:115:ARG:NH1	2:J:182:GLU:OE2	2.41	0.54
2:K:133:CYS:HA	2:K:141:CYS:HA	1.90	0.54
2:K:113:SER:O	2:K:117:ASN:ND2	2.41	0.54
1:A:106:THR:HA	1:A:233:THR:HG22	1.89	0.54
1:A:320:THR:OG1	1:A:321:GLU:OE1	2.25	0.54
1:B:81:VAL:HG11	1:B:234:ARG:HE	1.73	0.54
2:I:478:TRP:NE1	2:I:499:ASP:OD2	2.41	0.54
2:I:402:GLU:HG2	2:I:514:ARG:HH22	1.73	0.53
2:K:223:ILE:HB	2:K:461:TRP:HZ3	1.72	0.53
1:C:376:CYS:HB2	1:C:429:CYS:HA	1.91	0.53
2:I:517:THR:HB	2:I:521:TYR:CZ	2.43	0.53
1:A:452:LEU:N	1:A:488:PRO:O	2.40	0.53
1:A:643:ARG:NH1	1:B:844:ARG:O	2.41	0.53
1:A:1131:ASN:HD21	3:P:1:NAG:H62	1.73	0.53
1:B:284:ASP:OD1	1:B:284:ASP:N	2.40	0.53
1:B:970:ILE:HG12	1:B:977:ILE:HD12	1.90	0.53
2:J:90:ASN:HB3	2:J:93:VAL:HG22	1.89	0.53
1:A:380:SER:H	1:A:383:LYS:HE2	1.73	0.53
1:B:291:ASP:OD1	1:B:291:ASP:N	2.41	0.53
1:C:408:ALA:HB3	1:C:411:GLN:HG3	1.90	0.53
1:C:1101:VAL:HG13	1:C:1112:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:271:TRP:NE1	2:I:502:SER:O	2.39	0.53
1:A:415:ILE:HD13	1:A:419:ASN:HD22	1.72	0.53
1:B:123:ASN:HB3	1:B:168:VAL:HG13	1.90	0.53
1:C:202:SER:OG	1:C:203:LYS:N	2.41	0.53
1:B:976:ASP:OD1	1:B:977:ILE:N	2.41	0.53
1:C:119:ASN:ND2	1:C:173:LEU:HB3	2.24	0.53
2:K:29:LEU:HD11	2:K:97:LEU:HD13	1.90	0.53
2:K:145:GLU:HB2	2:K:146:PRO:HD2	1.90	0.53
1:A:124:VAL:O	1:A:126:ILE:HG13	2.08	0.53
1:B:398:VAL:HG22	1:B:506:ARG:HG2	1.91	0.53
1:C:577:GLN:HB3	3:b:2:NAG:H81	1.91	0.53
2:I:554:LEU:O	2:I:558:LEU:HG	2.09	0.53
1:A:643:ARG:NH2	1:B:843:ALA:O	2.41	0.53
1:B:982:ASP:HB2	1:B:984:PRO:HD2	1.91	0.53
1:C:300:LEU:HD22	1:C:305:VAL:HG12	1.90	0.53
1:A:1098:HIS:CD2	3:O:1:NAG:H5	2.44	0.52
1:B:430:VAL:HG22	1:B:509:VAL:HG22	1.91	0.52
1:C:287:ASP:OD1	1:C:288:CYS:N	2.38	0.52
2:K:85:LEU:HD13	2:K:97:LEU:HD23	1.90	0.52
2:K:209:VAL:HG21	2:K:565:PRO:HB3	1.91	0.52
2:K:582:ARG:HG3	2:K:583:PRO:HD3	1.90	0.52
1:B:415:ILE:HA	1:B:419:ASN:HB2	1.92	0.52
1:B:373:THR:HB	1:B:432:ALA:HB3	1.91	0.52
1:C:874:LEU:HD13	1:C:1026:MET:HE2	1.91	0.52
2:I:573:VAL:HG13	2:I:574:VAL:HG13	1.91	0.52
2:J:108:LEU:HD11	2:J:190:MET:HB2	1.91	0.52
1:C:822:LYS:HD2	1:C:942:LEU:HD13	1.92	0.52
2:I:505:HIS:HB2	2:I:512:PHE:CZ	2.44	0.52
1:C:347:VAL:HG21	1:C:415:ILE:HG23	1.91	0.52
2:K:53:ASN:ND2	2:K:58:ASN:OD1	2.43	0.52
2:K:132:VAL:O	2:K:141:CYS:HA	2.10	0.52
1:C:184:LYS:HG3	1:C:208:ASN:HB2	1.92	0.52
1:C:139:LEU:HD22	1:C:153:GLU:HG3	1.91	0.52
1:A:813:SER:O	1:A:815:ILE:N	2.43	0.51
1:B:184:LYS:HD2	1:B:210:VAL:HG12	1.91	0.51
3:H:1:NAG:O4	3:H:1:NAG:O7	2.27	0.51
1:B:523:GLY:O	1:B:525:LYS:NZ	2.38	0.51
1:A:325:ARG:HH21	1:A:577:GLN:HB2	1.74	0.51
1:C:1132:ASN:OD1	1:C:1133:THR:N	2.44	0.51
2:I:460:ARG:HA	2:I:463:VAL:HG12	1.92	0.51
1:B:86:ASP:OD1	1:B:86:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:GLY:O	1:B:503:GLN:NE2	2.44	0.51
2:I:365:THR:HG22	2:I:367:ASP:H	1.75	0.51
2:I:450:LEU:O	2:I:453:THR:OG1	2.27	0.51
1:C:202:SER:OG	1:C:204:HIS:N	2.39	0.51
1:A:400:ARG:HG3	1:A:502:TYR:HA	1.93	0.51
1:C:315:PHE:CE1	1:C:609:TYR:HD1	2.29	0.51
2:K:293:VAL:HG23	2:K:366:MET:HE1	1.91	0.51
1:C:1100:PHE:HZ	3:h:1:NAG:H62	1.76	0.51
2:J:455:MET:HE3	2:J:481:LYS:HA	1.92	0.51
1:C:104:PHE:HB3	1:C:232:ILE:HD11	1.93	0.51
2:J:261:CYS:HB3	2:J:606:TRP:HB3	1.93	0.51
1:A:845:ASP:OD1	1:A:845:ASP:N	2.44	0.51
2:I:315:PHE:HE1	2:I:376:MET:HE2	1.75	0.50
2:J:343:VAL:HG12	2:J:345:HIS:H	1.76	0.50
2:I:189:GLU:HA	2:I:192:ARG:HE	1.77	0.50
1:A:499:GLY:O	1:A:503:GLN:NE2	2.45	0.50
3:W:1:NAG:O3	3:W:2:NAG:O5	2.27	0.50
1:A:228:ILE:HG13	1:A:229:GLY:N	2.27	0.50
1:B:169:SER:OG	1:B:170:GLN:N	2.44	0.50
1:C:609:TYR:O	1:C:645:GLY:CA	2.56	0.50
1:C:124:VAL:HG11	1:C:172:PHE:CE2	2.47	0.50
1:C:864:ASP:OD1	1:C:865:GLU:N	2.45	0.50
2:I:408:MET:O	2:I:412:ALA:CB	2.60	0.50
2:J:244:VAL:HG21	2:J:275:TRP:HZ3	1.75	0.50
2:K:482:ARG:HH21	2:K:488:VAL:HB	1.76	0.50
1:A:291:ASP:OD1	1:A:291:ASP:N	2.45	0.50
2:J:172:VAL:O	2:J:176:LEU:HD23	2.12	0.50
1:C:203:LYS:O	1:C:206:PRO:HD3	2.12	0.50
2:J:183:TYR:OH	2:J:509:ASP:OD1	2.29	0.50
2:K:119:ILE:HD12	2:K:179:LEU:HD22	1.94	0.50
1:C:613:ASN:O	1:C:615:THR:N	2.42	0.49
1:C:753:TYR:OH	1:C:991:ASP:OD1	2.30	0.49
1:A:966:ASN:OD1	1:A:972:SER:OG	2.25	0.49
1:C:325:ARG:NH1	1:C:530:LEU:HB2	2.28	0.49
1:C:325:ARG:HH12	1:C:530:LEU:HB2	1.77	0.49
1:A:374:PHE:HE2	1:A:381:PRO:HB3	1.78	0.49
1:B:29:THR:O	1:B:61:ASN:HA	2.13	0.49
1:C:273:LEU:HB3	1:C:286:VAL:HG22	1.95	0.49
2:K:366:MET:HE2	2:K:423:LEU:HD21	1.94	0.49
1:C:167:TYR:CE1	1:C:169:SER:HB2	2.47	0.49
2:I:429:GLN:N	2:I:429:GLN:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PHE:HB2	1:B:41:LYS:HZ3	1.78	0.49
1:B:325:ARG:HH12	1:B:530:LEU:HB2	1.77	0.49
2:K:122:THR:HA	2:K:125:THR:HG22	1.95	0.49
2:K:267:LEU:HD23	2:K:275:TRP:HE1	1.77	0.49
1:C:129:CYS:HB2	1:C:163:CYS:HA	1.94	0.49
2:I:404:VAL:HA	2:I:407:ILE:HD12	1.95	0.49
1:C:97:ASN:O	1:C:100:ARG:NH1	2.46	0.49
1:C:658:GLU:CD	1:C:658:GLU:H	2.20	0.49
2:I:505:HIS:HB3	2:I:510:TYR:HB2	1.95	0.49
2:I:408:MET:O	2:I:412:ALA:HB3	2.13	0.49
1:B:273:LEU:HD23	1:B:303:PHE:HE1	1.78	0.48
2:I:207:TYR:HH	2:I:521:TYR:HH	1.57	0.48
1:A:221:GLU:OE1	1:A:221:GLU:N	2.46	0.48
1:A:453:PHE:CE2	2:I:27:THR:HB	2.46	0.48
1:B:64:TRP:HD1	1:B:263:TYR:CE2	2.32	0.48
1:C:823:VAL:HG21	1:C:1054:PRO:HG2	1.94	0.48
2:I:560:LEU:HD13	2:I:564:GLU:HG3	1.95	0.48
2:K:565:PRO:HD2	2:K:568:LEU:HD23	1.94	0.48
1:C:1083:LYS:HE2	1:C:1119:VAL:HG21	1.95	0.48
2:K:62:MET:HE2	2:K:62:MET:N	2.27	0.48
1:B:97:ASN:HB3	1:B:100:ARG:HH12	1.77	0.48
1:A:103:ILE:HD11	1:A:238:LEU:HB3	1.94	0.48
2:I:482:ARG:HH22	2:I:610:TRP:H	1.62	0.48
1:A:745:GLU:H	1:A:745:GLU:CD	2.22	0.48
1:B:315:PHE:HZ	1:B:612:VAL:HG11	1.78	0.48
2:I:152:MET:HG3	2:I:270:MET:HB2	1.95	0.48
1:A:993:LEU:O	1:A:997:ARG:HG2	2.14	0.48
1:B:390:THR:HG22	1:B:519:ALA:HA	1.96	0.48
1:C:203:LYS:HG3	1:C:206:PRO:HG3	1.95	0.48
2:J:29:LEU:HD11	2:J:97:LEU:HD13	1.95	0.48
1:B:139:LEU:HD11	1:B:155:ARG:H	1.78	0.48
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.48	0.48
1:C:982:ASP:HB2	1:C:984:PRO:HD2	1.95	0.48
1:B:1070:LYS:HD3	1:B:1072:PHE:CZ	2.49	0.48
2:J:408:MET:O	2:J:412:ALA:CB	2.61	0.47
1:A:30:ASN:HA	1:A:60:SER:O	2.15	0.47
1:A:1098:HIS:HD2	3:O:1:NAG:H5	1.78	0.47
1:B:525:LYS:O	1:B:526:LYS:NZ	2.32	0.47
1:C:128:VAL:HG12	1:C:128:VAL:O	2.14	0.47
2:K:204:ARG:HD3	2:K:461:TRP:CH2	2.49	0.47
1:A:712:PRO:HA	1:A:1069:GLU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:85:LEU:HD11	2:J:94:LYS:HA	1.96	0.47
2:K:292:ASP:OD1	2:K:292:ASP:N	2.46	0.47
1:A:559:PHE:O	1:B:41:LYS:NZ	2.43	0.47
1:A:767:ILE:O	1:A:771:GLN:HG2	2.14	0.47
1:A:982:ASP:HB2	1:A:984:PRO:HD2	1.97	0.47
1:B:131:PHE:HA	1:B:159:SER:O	2.13	0.47
1:B:333:CYS:N	1:B:359:VAL:O	2.34	0.47
2:J:152:MET:HG2	2:J:161:ARG:HH21	1.79	0.47
2:K:294:THR:O	2:K:297:MET:HG3	2.14	0.47
1:A:86:ASP:N	1:A:86:ASP:OD1	2.46	0.47
1:A:92:SER:HB3	1:A:187:ARG:CZ	2.44	0.47
1:B:564:ARG:NH1	1:B:568:ASP:HB3	2.30	0.47
1:B:793:ASP:OD1	1:B:793:ASP:N	2.45	0.47
1:C:135:ASN:OD1	1:C:136:ASP:N	2.47	0.47
1:C:497:THR:O	2:K:41:TYR:OH	2.26	0.47
1:C:656:SER:HB3	1:C:695:SER:HB2	1.97	0.47
2:I:346:PRO:HA	2:I:359:LEU:O	2.15	0.47
1:A:870:TYR:CZ	1:C:696:LEU:HD22	2.50	0.47
1:B:89:TYR:OH	1:B:188:GLU:OE2	2.22	0.47
1:B:919:LEU:O	1:B:923:GLN:HG3	2.15	0.47
1:B:822:LYS:HD2	1:B:942:LEU:HD13	1.97	0.47
1:C:449:LEU:HD23	1:C:489:LEU:HB3	1.97	0.47
2:J:62:MET:SD	2:J:63:ASN:N	2.88	0.47
2:J:589:GLU:HB3	2:J:590:PRO:HD3	1.97	0.47
1:A:434:ASN:OD1	1:A:436:ASN:N	2.45	0.47
2:I:90:ASN:HB3	2:I:93:VAL:HG22	1.96	0.47
2:K:187:LYS:HD2	2:K:199:TYR:CZ	2.49	0.47
2:K:535:HIS:NE2	2:K:541:LYS:O	2.48	0.47
1:A:727:SER:OG	1:A:728:MET:N	2.48	0.46
1:A:1102:THR:HG22	1:A:1109:PRO:HA	1.97	0.46
1:A:653:VAL:HG12	1:A:655:ASN:H	1.80	0.46
1:C:295:GLU:HA	1:C:298:CYS:HB2	1.97	0.46
2:I:403:ALA:O	2:I:407:ILE:HG13	2.15	0.46
2:I:535:HIS:NE2	2:I:541:LYS:O	2.47	0.46
2:J:371:THR:O	2:J:375:GLU:HG2	2.14	0.46
1:B:659:CYS:HB3	1:B:692:TYR:CE1	2.50	0.46
2:I:581:VAL:HG23	2:I:584:LEU:HD13	1.97	0.46
2:J:192:ARG:NE	2:J:197:GLU:O	2.48	0.46
2:K:256:ILE:HG12	2:K:263:PRO:HD3	1.97	0.46
1:A:200:ILE:CG2	1:A:224:VAL:HB	2.46	0.46
1:B:851:LYS:HA	1:B:851:LYS:HD3	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:189:GLU:O	2:I:192:ARG:HG2	2.15	0.46
2:I:482:ARG:O	2:I:606:TRP:NE1	2.49	0.46
2:K:385:TYR:OH	2:K:401:HIS:NE2	2.40	0.46
1:C:265:GLY:C	1:C:266:TYR:HD1	2.24	0.46
2:I:590:PRO:HA	2:I:593:THR:HG22	1.98	0.46
2:J:432:ASN:O	2:J:436:ILE:HG13	2.14	0.46
1:B:902:ARG:NH1	1:B:1046:LEU:O	2.46	0.46
1:C:335:PHE:HD2	1:C:339:PHE:HE2	1.64	0.46
2:J:162:LEU:HD13	2:J:490:PRO:HB2	1.97	0.46
2:K:186:LEU:O	2:K:190:MET:HG2	2.16	0.46
1:A:96:SER:O	1:A:96:SER:OG	2.34	0.46
2:K:347:THR:OG1	2:K:359:LEU:HB3	2.16	0.46
1:A:137:PRO:HB3	1:A:157:TYR:HA	1.97	0.46
1:A:1086:PHE:HE2	1:B:914:TYR:HD2	1.63	0.46
2:I:169:ARG:NH1	2:I:502:SER:OG	2.49	0.46
2:I:192:ARG:HA	2:I:196:TYR:O	2.15	0.46
2:I:260:GLY:HA3	2:I:610:TRP:HB3	1.98	0.46
2:I:268:GLY:O	2:I:277:ASN:ND2	2.48	0.46
2:J:356:PHE:CZ	2:J:383:MET:HG2	2.51	0.46
1:A:360:ALA:HB1	1:A:362:TYR:CE1	2.51	0.46
1:A:853:ASN:O	1:A:855:LEU:HG	2.16	0.46
1:C:1003:THR:O	1:C:1007:GLN:HG2	2.15	0.46
1:A:360:ALA:O	1:A:524:PRO:HD3	2.16	0.46
1:B:659:CYS:HB3	1:B:692:TYR:HE1	1.81	0.46
2:I:182:GLU:HG2	2:I:186:LEU:HD12	1.97	0.46
2:K:187:LYS:HD3	2:K:190:MET:HE3	1.98	0.46
2:K:307:ILE:HG23	2:K:369:PHE:CD1	2.51	0.46
1:A:999:GLN:HA	1:A:999:GLN:OE1	2.15	0.45
1:C:186:LEU:O	1:C:206:PRO:HD2	2.16	0.45
2:I:39:LEU:HD22	2:I:68:LYS:HD3	1.98	0.45
2:I:44:SER:HB3	2:I:351:LEU:HD22	1.97	0.45
1:A:1108:GLU:OE1	1:A:1108:GLU:N	2.50	0.45
1:B:307:LYS:HG3	1:B:597:PRO:HA	1.98	0.45
2:J:460:ARG:HA	2:J:463:VAL:HG12	1.99	0.45
2:I:441:LYS:HA	2:I:444:LEU:HD12	1.99	0.45
2:K:208:GLU:OE2	2:K:219:ARG:NH1	2.49	0.45
1:B:287:ASP:OD1	1:B:288:CYS:N	2.45	0.45
1:B:563:GLY:HA2	1:C:43:PHE:HB3	1.97	0.45
2:K:84:PRO:O	2:K:86:GLN:N	2.47	0.45
1:A:583:ASP:OD1	1:A:584:ILE:N	2.49	0.45
1:B:1084:ALA:HB2	1:B:1123:CYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:77:SER:O	2:I:81:GLN:NE2	2.45	0.45
2:I:248:LEU:HD11	2:I:278:LEU:HD11	1.98	0.45
1:B:332:LEU:HA	1:B:359:VAL:HB	1.98	0.45
1:B:735:CYS:SG	1:B:736:THR:N	2.90	0.45
1:C:738:TYR:CE1	1:C:963:LEU:HD12	2.52	0.45
1:C:341:ALA:HB3	1:C:344:PHE:CE1	2.51	0.45
1:C:961:LYS:HB2	1:C:961:LYS:NZ	2.31	0.45
2:J:581:VAL:O	2:J:581:VAL:HG13	2.17	0.45
1:A:125:VAL:HG22	1:A:168:VAL:HG22	1.99	0.45
1:A:454:ARG:NH1	1:A:458:LEU:HD21	2.31	0.45
1:B:137:PRO:HB2	1:B:156:VAL:HG22	1.99	0.45
1:A:65:PHE:HB2	1:A:262:TYR:O	2.17	0.45
1:A:115:LEU:HD23	1:A:116:LEU:N	2.31	0.45
1:A:211:ARG:HD3	1:A:212:ASP:HB2	1.98	0.45
1:B:325:ARG:NH1	1:B:530:LEU:HB2	2.31	0.45
1:C:354:ARG:HG2	1:C:393:TYR:CE1	2.52	0.45
1:C:813:SER:OG	1:C:816:GLU:HG3	2.16	0.45
1:A:104:PHE:HB3	1:A:232:ILE:HD13	1.99	0.45
1:A:187:ARG:O	1:A:187:ARG:HG3	2.17	0.44
1:B:554:LYS:HB2	1:B:581:ILE:HG21	1.99	0.44
2:I:446:ILE:HD13	2:I:523:PHE:HZ	1.82	0.44
2:J:38:ASP:O	2:J:42:GLN:OE1	2.35	0.44
1:A:451:ARG:HH12	1:A:454:ARG:NH1	2.15	0.44
1:A:994:ILE:O	1:A:998:LEU:HD23	2.16	0.44
1:C:415:ILE:HD13	1:C:419:ASN:HD22	1.81	0.44
2:I:581:VAL:O	2:I:581:VAL:HG13	2.16	0.44
2:J:315:PHE:CE2	2:J:408:MET:HE3	2.52	0.44
1:A:380:SER:HB3	1:A:383:LYS:HG2	1.99	0.44
1:A:564:ARG:HG3	1:A:565:ASP:H	1.83	0.44
1:C:186:LEU:C	1:C:187:ARG:HD2	2.42	0.44
2:I:158:TYR:CE1	2:I:266:LEU:HD11	2.52	0.44
2:I:482:ARG:NH2	2:I:607:SER:O	2.50	0.44
3:F:1:NAG:H4	3:F:2:NAG:H83	1.99	0.44
1:A:393:TYR:HB2	1:A:511:SER:OG	2.17	0.44
1:C:983:PRO:N	1:C:984:PRO:HD2	2.31	0.44
2:K:374:HIS:HE1	2:K:406:GLU:HG2	1.82	0.44
1:A:710:ALA:HA	1:A:1070:LYS:O	2.18	0.44
1:A:1086:PHE:HE2	1:B:914:TYR:CD2	2.36	0.44
1:B:115:LEU:O	1:B:116:LEU:HD12	2.18	0.44
1:B:198:PHE:CD2	1:B:200:ILE:HD11	2.52	0.44
2:I:215:TYR:CD1	2:I:577:LYS:HE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ASN:HD21	1:A:232:ILE:HD12	1.83	0.44
1:B:1050:PRO:O	1:B:1051:GLN:NE2	2.28	0.44
1:A:819:LEU:HD23	1:A:1053:ALA:HB2	1.99	0.44
1:A:911:ASN:OD1	1:A:911:ASN:N	2.51	0.44
1:A:982:ASP:OD1	1:A:982:ASP:N	2.51	0.44
1:B:325:ARG:NE	1:B:577:GLN:HG3	2.33	0.44
1:B:609:TYR:HE1	1:B:648:ILE:HD12	1.82	0.44
1:C:1123:CYS:HB2	1:C:1129:ILE:HG21	1.99	0.44
2:K:120:LEU:HD23	2:K:120:LEU:HA	1.88	0.44
1:A:353:LYS:HE2	1:A:353:LYS:HB3	1.84	0.44
1:A:573:VAL:HG12	1:A:574:ARG:N	2.33	0.44
1:A:1136:ASP:HB3	1:A:1139:GLN:HG2	1.99	0.44
1:B:458:LEU:HD22	1:B:462:GLU:HB3	2.00	0.44
1:C:425:ASP:OD1	1:C:425:ASP:N	2.50	0.44
2:I:407:ILE:HD11	2:I:525:PHE:CD2	2.53	0.44
2:K:187:LYS:HD2	2:K:199:TYR:CE1	2.53	0.44
1:B:109:ASP:OD1	1:B:109:ASP:N	2.51	0.44
1:B:323:ILE:HD12	1:B:530:LEU:HA	1.99	0.44
1:C:894:PRO:HG2	1:C:897:MET:HG3	2.00	0.44
1:A:97:ASN:OD1	1:A:99:ILE:HG12	2.18	0.43
1:A:449:LEU:HD13	1:A:489:LEU:HD23	2.00	0.43
1:A:550:THR:O	1:A:582:LEU:HD12	2.18	0.43
1:B:335:PHE:HE2	1:B:361:ASP:H	1.66	0.43
1:B:713:ILE:HG12	1:B:1068:GLN:O	2.18	0.43
1:B:749:LEU:O	1:B:752:GLN:HG2	2.18	0.43
1:C:525:LYS:O	1:C:526:LYS:HE2	2.18	0.43
2:J:78:THR:O	2:J:81:GLN:NE2	2.51	0.43
2:K:38:ASP:OD1	2:K:39:LEU:N	2.51	0.43
2:K:307:ILE:HG23	2:K:369:PHE:HD1	1.83	0.43
2:K:379:ILE:HG22	2:K:383:MET:HE3	1.98	0.43
1:A:983:PRO:N	1:A:984:PRO:HD2	2.33	0.43
1:B:522:CYS:HB3	1:B:525:LYS:HZ1	1.83	0.43
1:B:1074:THR:OG1	1:B:1075:ALA:N	2.51	0.43
1:C:525:LYS:HB3	1:C:526:LYS:HG2	2.01	0.43
2:I:245:ARG:O	2:I:249:MET:HG3	2.19	0.43
2:I:249:MET:HG2	2:I:256:ILE:HB	2.00	0.43
2:K:56:GLU:O	2:K:59:VAL:HG12	2.18	0.43
1:B:475:THR:HB	1:B:484:ASN:HB2	2.00	0.43
1:C:198:PHE:CE2	1:C:200:ILE:HD11	2.53	0.43
2:I:165:TRP:HD1	2:I:270:MET:HG2	1.83	0.43
2:I:517:THR:HB	2:I:521:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:97:LEU:HD12	2:J:100:LEU:HD12	2.00	0.43
2:K:215:TYR:CE2	2:K:568:LEU:HD13	2.53	0.43
1:B:637:SER:HB2	1:B:649:GLY:HA2	2.01	0.43
1:B:817:ASP:OD1	1:B:818:LEU:HD12	2.18	0.43
2:J:293:VAL:O	2:J:297:MET:HG3	2.19	0.43
2:K:61:ASN:HB2	2:K:62:MET:HE2	2.01	0.43
2:K:201:ASP:OD1	2:K:204:ARG:NH2	2.42	0.43
1:A:126:ILE:HG22	1:A:126:ILE:O	2.18	0.43
1:A:406:GLN:HB3	1:A:416:ALA:HB2	2.00	0.43
1:B:115:LEU:HD12	1:B:115:LEU:H	1.84	0.43
1:B:202:SER:OG	1:B:203:LYS:N	2.52	0.43
2:I:107:VAL:HG12	2:I:190:MET:HE1	2.01	0.43
2:I:565:PRO:HD2	2:I:568:LEU:HD23	2.01	0.43
2:J:310:GLU:HA	2:J:313:LYS:HE2	1.99	0.43
1:A:30:ASN:HD21	1:A:32:PHE:HE1	1.66	0.43
1:A:95:LYS:HA	1:A:95:LYS:HD3	1.77	0.43
1:B:703:ALA:HB2	3:X:2:NAG:H82	2.00	0.43
1:C:400:ARG:NH1	1:C:501:GLY:O	2.51	0.43
2:J:428:PHE:HE2	2:J:430:GLU:HB3	1.81	0.43
2:K:199:TYR:OH	2:K:509:ASP:OD2	2.30	0.43
1:A:155:ARG:HD2	1:A:156:VAL:N	2.33	0.43
1:B:846:LEU:C	1:B:848:CYS:H	2.25	0.43
2:J:188:ASN:O	2:J:192:ARG:HG2	2.18	0.43
1:B:609:TYR:O	1:B:645:GLY:HA3	2.19	0.43
1:C:899:MET:HE1	1:C:1046:LEU:HD13	2.00	0.43
2:I:38:ASP:OD1	2:I:39:LEU:N	2.52	0.43
2:J:307:ILE:HG23	2:J:369:PHE:CD1	2.54	0.43
2:K:378:HIS:CE1	2:K:401:HIS:HB3	2.54	0.43
1:A:99:ILE:HD13	1:A:187:ARG:NE	2.33	0.43
1:A:137:PRO:HG3	1:A:158:SER:H	1.83	0.43
1:A:401:GLY:HA3	1:A:501:GLY:O	2.18	0.43
1:A:700:ASN:OD1	1:A:701:SER:N	2.52	0.43
3:P:1:NAG:O4	3:P:2:NAG:O7	2.37	0.43
1:C:454:ARG:HG3	1:C:456:SER:H	1.84	0.43
1:C:513:GLU:HG3	1:C:515:LEU:HD22	2.00	0.43
1:B:98:ILE:HG22	1:B:98:ILE:O	2.19	0.42
1:C:36:VAL:HG21	1:C:217:PHE:CZ	2.54	0.42
1:C:928:ILE:O	1:C:931:ILE:HG22	2.19	0.42
2:I:378:HIS:CE1	2:I:401:HIS:HB3	2.54	0.42
2:K:343:VAL:HB	2:K:359:LEU:HD21	2.01	0.42
1:A:641:GLN:NE2	1:A:642:THR:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ARG:O	1:C:157:TYR:N	2.53	0.42
1:C:353:LYS:HB3	1:C:394:ALA:HB3	2.01	0.42
1:C:749:LEU:HA	1:C:749:LEU:HD23	1.86	0.42
2:J:311:ALA:HB1	2:J:373:HIS:CE1	2.54	0.42
2:K:455:MET:HE1	2:K:477:TRP:CZ2	2.54	0.42
1:A:659:CYS:HB2	1:A:668:CYS:HB3	1.55	0.42
1:B:102:TRP:HB3	1:B:104:PHE:CE1	2.54	0.42
1:B:656:SER:HB3	1:B:695:SER:HB2	2.02	0.42
1:C:445:ASN:H	1:C:494:PHE:H	1.66	0.42
2:K:135:PRO:HD3	2:K:163:TRP:CZ2	2.53	0.42
1:A:325:ARG:NH1	1:A:530:LEU:HB2	2.34	0.42
1:A:441:LYS:NZ	1:A:445:ASN:HA	2.34	0.42
1:A:1089:GLU:HA	1:A:1089:GLU:OE2	2.19	0.42
1:B:454:ARG:HG3	1:B:456:SER:H	1.84	0.42
1:C:99:ILE:HD11	1:C:237:THR:OG1	2.20	0.42
2:J:172:VAL:HA	2:J:175:GLN:NE2	2.35	0.42
2:K:294:THR:O	2:K:298:VAL:HG23	2.18	0.42
1:A:203:LYS:HE2	1:A:218:SER:OG	2.20	0.42
1:A:715:PHE:HD1	1:A:1106:PHE:HE1	1.68	0.42
2:I:318:VAL:HG23	2:I:320:LEU:HG	2.01	0.42
2:K:365:THR:HG22	2:K:367:ASP:H	1.83	0.42
1:A:184:LYS:HA	1:A:184:LYS:HD3	1.90	0.42
2:I:85:LEU:HD13	2:I:97:LEU:HD23	2.01	0.42
2:K:134:ASN:HA	2:K:163:TRP:CZ2	2.54	0.42
1:A:1076:PRO:HD2	1:A:1128:GLY:O	2.19	0.42
1:B:314:ASN:ND2	1:C:734:ASP:OD2	2.53	0.42
1:B:513:GLU:HG3	1:B:515:LEU:HD22	2.02	0.42
1:B:982:ASP:OD1	1:B:982:ASP:N	2.51	0.42
1:C:347:VAL:O	1:C:350:TRP:HD1	2.02	0.42
1:C:912:VAL:O	1:C:916:ASN:ND2	2.53	0.42
2:I:325:GLN:OE1	2:I:326:GLY:N	2.50	0.42
2:J:245:ARG:O	2:J:249:MET:HG2	2.20	0.42
1:B:360:ALA:HB1	1:B:362:TYR:CZ	2.55	0.42
1:C:104:PHE:CD2	1:C:232:ILE:HD11	2.51	0.42
1:C:129:CYS:CB	1:C:163:CYS:HA	2.49	0.42
2:K:523:PHE:HB3	2:K:583:PRO:HG2	2.01	0.42
1:C:113:GLN:HA	1:C:130:GLU:HG3	2.02	0.42
1:C:436:ASN:O	1:C:440:SER:HB2	2.20	0.42
1:C:554:LYS:HB2	1:C:581:ILE:HG21	2.01	0.42
2:I:221:GLN:O	2:I:224:GLU:HG3	2.20	0.42
1:A:122:THR:O	1:A:171:PRO:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ARG:HG2	1:B:189:PHE:CE1	2.55	0.42
2:I:120:LEU:HD21	2:I:183:TYR:CE1	2.55	0.42
2:I:165:TRP:CD1	2:I:270:MET:HG2	2.54	0.42
2:I:396:ALA:HB3	2:I:400:PHE:CE2	2.55	0.42
1:B:899:MET:HE3	1:B:899:MET:HB3	1.76	0.41
2:I:199:TYR:HD2	2:I:464:PHE:CE2	2.38	0.41
2:J:564:GLU:HB3	2:J:568:LEU:HD23	2.02	0.41
2:K:525:PHE:CZ	2:K:557:MET:HE1	2.54	0.41
1:A:241:LEU:H	1:A:241:LEU:HD23	1.86	0.41
2:I:59:VAL:HA	2:I:62:MET:HE2	2.02	0.41
2:I:209:VAL:HB	2:I:566:TRP:CH2	2.54	0.41
2:K:108:LEU:HD11	2:K:190:MET:HB3	2.00	0.41
2:K:374:HIS:CE1	2:K:406:GLU:HG2	2.55	0.41
1:C:327:PRO:HA	1:C:576:PRO:O	2.20	0.41
2:I:54:ILE:HD11	2:I:343:VAL:HG23	2.01	0.41
2:I:589:GLU:HB3	2:I:590:PRO:HD3	2.02	0.41
2:J:68:LYS:HB3	2:J:68:LYS:HE3	1.78	0.41
1:A:323:ILE:HD11	1:A:530:LEU:HD12	2.01	0.41
1:A:454:ARG:HG3	1:A:456:SER:H	1.86	0.41
1:B:717:ILE:HD12	1:B:920:ILE:HG23	2.02	0.41
1:C:847:ILE:HG22	1:C:847:ILE:O	2.19	0.41
2:I:581:VAL:HG22	2:I:584:LEU:HB2	2.02	0.41
2:K:346:PRO:HA	2:K:359:LEU:O	2.20	0.41
1:A:379:VAL:HG23	1:A:383:LYS:HE3	2.03	0.41
1:B:315:PHE:CZ	1:B:612:VAL:HG11	2.55	0.41
2:I:158:TYR:HE1	2:I:266:LEU:HD11	1.85	0.41
2:I:455:MET:SD	2:I:455:MET:N	2.90	0.41
2:J:377:GLY:HA3	2:J:408:MET:HE1	2.03	0.41
1:A:434:ASN:OD1	1:A:435:SER:N	2.53	0.41
1:B:31:SER:O	1:B:31:SER:OG	2.34	0.41
1:B:564:ARG:HH11	1:B:568:ASP:HB3	1.85	0.41
1:C:132:GLN:O	1:C:158:SER:N	2.46	0.41
1:C:713:ILE:HD11	1:C:1070:LYS:HD3	2.03	0.41
2:I:248:LEU:HD23	2:I:248:LEU:HA	1.91	0.41
2:I:275:TRP:N	2:I:275:TRP:CD1	2.89	0.41
2:I:477:TRP:O	2:I:480:MET:HG2	2.20	0.41
2:J:56:GLU:O	2:J:59:VAL:HG12	2.21	0.41
2:K:162:LEU:HD11	2:K:490:PRO:HB2	2.03	0.41
1:A:103:ILE:CD1	1:A:238:LEU:HD23	2.49	0.41
1:A:202:SER:OG	1:A:203:LYS:N	2.54	0.41
1:A:291:ASP:HB2	1:A:292:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:CYS:HB2	1:B:1129:ILE:HG21	2.01	0.41
1:C:341:ALA:HB3	1:C:344:PHE:HE1	1.83	0.41
1:C:494:PHE:CZ	1:C:504:PRO:HB3	2.55	0.41
1:C:919:LEU:O	1:C:923:GLN:HG3	2.20	0.41
2:J:347:THR:OG1	2:J:359:LEU:HB3	2.21	0.41
2:K:70:SER:O	2:K:74:LYS:HG3	2.21	0.41
1:B:126:ILE:HD13	1:B:226:LEU:HD11	2.02	0.41
1:B:495:GLN:HG3	1:B:498:TYR:OH	2.21	0.41
1:B:817:ASP:OD1	1:B:817:ASP:C	2.62	0.41
1:B:1077:ALA:HB3	1:B:1129:ILE:HG22	2.03	0.41
1:C:139:LEU:H	1:C:139:LEU:HD23	1.86	0.41
1:C:314:ASN:OD1	1:C:314:ASN:N	2.54	0.41
1:C:875:LEU:HA	1:C:878:THR:HG22	2.01	0.41
2:J:169:ARG:HH22	2:J:271:TRP:HD1	1.68	0.41
2:K:137:ASN:OD1	2:K:140:GLU:HB2	2.21	0.41
2:K:221:GLN:O	2:K:224:GLU:HG3	2.21	0.41
1:A:451:ARG:NH2	1:A:454:ARG:HD3	2.32	0.41
1:A:974:LEU:HA	1:A:974:LEU:HD12	1.89	0.41
1:B:318:GLN:OE1	1:B:319:PRO:HD2	2.21	0.41
1:C:609:TYR:HE2	1:C:648:ILE:HD12	1.86	0.41
2:J:115:ARG:O	2:J:119:ILE:HG12	2.21	0.41
2:J:162:LEU:HD11	2:J:491:VAL:HG13	2.02	0.41
1:A:157:TYR:O	1:A:157:TYR:CG	2.73	0.41
1:A:862:LEU:HD23	1:A:862:LEU:HA	1.98	0.41
1:B:415:ILE:HD13	1:B:419:ASN:ND2	2.35	0.41
1:B:1086:PHE:HE2	1:C:914:TYR:CD2	2.39	0.41
1:C:221:GLU:N	1:C:221:GLU:OE1	2.54	0.41
2:J:79:LEU:O	2:J:82:MET:HG2	2.21	0.41
1:B:459:LYS:HG2	1:B:462:GLU:OE1	2.21	0.40
1:B:940:SER:O	1:B:940:SER:OG	2.32	0.40
1:C:811:LYS:HA	1:C:811:LYS:HD2	1.87	0.40
1:C:844:ARG:O	1:C:846:LEU:N	2.52	0.40
1:C:1113:THR:HG22	1:C:1114:THR:H	1.86	0.40
2:J:132:VAL:O	2:J:141:CYS:HA	2.21	0.40
1:A:1078:ILE:O	1:A:1078:ILE:HG13	2.22	0.40
1:B:362:TYR:CD2	1:B:384:LEU:HB3	2.56	0.40
1:B:614:CYS:HB2	1:B:646:CYS:HB3	1.79	0.40
1:B:797:PHE:N	1:B:797:PHE:CD1	2.88	0.40
1:C:564:ARG:HA	1:C:564:ARG:HD3	1.90	0.40
2:J:145:GLU:HB2	2:J:146:PRO:HD2	2.02	0.40
2:J:244:VAL:HG21	2:J:275:TRP:CZ3	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PHE:HD1	1:A:431:ILE:HG12	1.87	0.40
2:I:477:TRP:HA	2:I:480:MET:HE2	2.03	0.40
2:J:528:ALA:HB1	2:J:573:VAL:O	2.22	0.40
2:J:568:LEU:HA	2:J:577:LYS:NZ	2.37	0.40
2:K:332:MET:HE2	2:K:359:LEU:HG	2.03	0.40
2:K:565:PRO:O	2:K:569:ALA:N	2.48	0.40
1:A:970:ILE:HG13	1:A:989:GLN:OE1	2.21	0.40
1:B:803:LEU:HD23	1:B:803:LEU:HA	1.95	0.40
1:C:1078:ILE:HG12	1:C:1130:VAL:HG23	2.03	0.40
2:I:157:ASP:OD1	2:I:158:TYR:N	2.55	0.40
2:I:248:LEU:HD21	2:I:278:LEU:HD11	2.04	0.40
2:K:71:ALA:O	2:K:75:GLU:HG2	2.21	0.40
1:B:102:TRP:HB3	1:B:104:PHE:HE1	1.86	0.40
1:B:764:LEU:HD23	1:B:764:LEU:HA	1.86	0.40
2:I:557:MET:HE2	2:I:557:MET:HB3	1.83	0.40
2:J:237:TYR:CE1	2:J:451:PRO:HG2	2.57	0.40
2:J:365:THR:HG22	2:J:367:ASP:H	1.85	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	1008/1286 (78%)	908 (90%)	98 (10%)	2 (0%)	43	71
1	B	1000/1286 (78%)	913 (91%)	84 (8%)	3 (0%)	36	65
1	C	990/1286 (77%)	898 (91%)	89 (9%)	3 (0%)	36	65
2	I	594/861 (69%)	556 (94%)	38 (6%)	0	100	100
2	J	594/861 (69%)	559 (94%)	35 (6%)	0	100	100
2	K	594/861 (69%)	558 (94%)	36 (6%)	0	100	100
All	All	4780/6441 (74%)	4392 (92%)	380 (8%)	8 (0%)	44	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	814	PHE
1	B	847	ILE
1	C	156	VAL
1	B	100	ARG
1	B	689	ILE
1	C	215	GLN
1	C	689	ILE
1	A	170	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	893/1115 (80%)	893 (100%)	0	100	100
1	B	886/1115 (80%)	884 (100%)	2 (0%)	87	88
1	C	880/1115 (79%)	878 (100%)	2 (0%)	87	88
2	I	526/752 (70%)	526 (100%)	0	100	100
2	J	526/752 (70%)	526 (100%)	0	100	100
2	K	526/752 (70%)	526 (100%)	0	100	100
All	All	4237/5601 (76%)	4233 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	851	LYS
1	B	961	LYS
1	C	851	LYS
1	C	961	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	419	ASN
1	A	537	ASN
1	A	577	GLN
1	A	652	HIS
1	A	951	GLN
1	A	952	ASN
1	B	97	ASN
1	B	419	ASN
1	B	561	GLN
1	B	577	GLN
1	B	962	GLN
1	B	1008	GLN
1	C	52	GLN
1	C	236	GLN
1	C	268	GLN
1	C	419	ASN
1	C	577	GLN
1	C	748	ASN
1	C	904	ASN
1	C	1085	HIS
2	I	58	ASN
2	I	96	GLN
2	J	34	HIS
2	J	81	GLN
2	J	330	ASN
2	J	401	HIS
2	J	417	HIS
2	K	33	ASN
2	K	53	ASN
2	K	96	GLN
2	K	374	HIS
2	K	540	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

58 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	D	1	1,3	14,14,15	0.31	0	17,19,21	0.48	0
3	NAG	D	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	E	1	1,3	14,14,15	0.43	0	17,19,21	0.58	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.52	0
3	NAG	F	1	1,3	14,14,15	0.19	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.61	0	17,19,21	0.47	0
3	NAG	G	1	1,3	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	H	1	1,3	14,14,15	0.94	1 (7%)	17,19,21	1.48	3 (17%)
3	NAG	H	2	3	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	L	1	1,3	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	M	1	1,3	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	M	2	3	14,14,15	0.27	0	17,19,21	0.41	0
3	NAG	N	1	1,3	14,14,15	0.21	0	17,19,21	1.21	2 (11%)
3	NAG	N	2	3	14,14,15	0.42	0	17,19,21	0.52	0
3	NAG	O	1	1,3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	O	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	P	1	1,3	14,14,15	0.39	0	17,19,21	1.27	1 (5%)
3	NAG	P	2	3	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	Q	1	1,3	14,14,15	0.33	0	17,19,21	0.52	0
3	NAG	Q	2	3	14,14,15	0.26	0	17,19,21	0.62	0
3	NAG	R	1	1,3	14,14,15	0.32	0	17,19,21	0.59	0
3	NAG	R	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	S	1	1,3	14,14,15	0.17	0	17,19,21	0.46	0
3	NAG	S	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	T	1	1,3	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	T	2	3	14,14,15	0.46	0	17,19,21	1.33	2 (11%)
3	NAG	U	1	1,3	14,14,15	0.73	1 (7%)	17,19,21	1.27	1 (5%)
3	NAG	U	2	3	14,14,15	0.21	0	17,19,21	0.51	0
3	NAG	V	1	1,3	14,14,15	0.28	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	V	2	3	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	W	1	1,3	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	W	2	3	14,14,15	0.36	0	17,19,21	0.58	0
3	NAG	X	1	1,3	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	X	2	3	14,14,15	0.29	0	17,19,21	0.41	0
3	NAG	Y	1	1,3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	Y	2	3	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	Z	1	1,3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	Z	2	3	14,14,15	0.29	0	17,19,21	0.54	0
3	NAG	a	1	1,3	14,14,15	0.35	0	17,19,21	0.47	0
3	NAG	a	2	3	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	b	1	1,3	14,14,15	0.29	0	17,19,21	1.19	2 (11%)
3	NAG	b	2	3	14,14,15	0.35	0	17,19,21	0.61	1 (5%)
3	NAG	c	1	1,3	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	c	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	d	1	1,3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	d	2	3	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	e	1	1,3	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	e	2	3	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	f	1	1,3	14,14,15	0.29	0	17,19,21	0.45	0
3	NAG	f	2	3	14,14,15	0.22	0	17,19,21	0.50	0
3	NAG	g	1	1,3	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
3	NAG	g	2	3	14,14,15	0.30	0	17,19,21	0.45	0
3	NAG	h	1	1,3	14,14,15	0.34	0	17,19,21	0.38	0
3	NAG	h	2	3	14,14,15	0.23	0	17,19,21	0.51	0
3	NAG	i	1	1,3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	i	2	3	14,14,15	0.28	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	4/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	c	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	0/6/23/26	0/1/1/1
3	NAG	e	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	e	2	3	-	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	-	2/6/23/26	0/1/1/1
3	NAG	g	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	i	2	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	C1-C2	3.11	1.56	1.52
3	U	1	NAG	O5-C1	2.27	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1	NAG	C1-O5-C5	4.96	118.84	112.19
3	P	1	NAG	C1-O5-C5	4.76	118.56	112.19
3	H	1	NAG	C1-O5-C5	4.69	118.47	112.19
3	T	2	NAG	C2-N2-C7	4.59	129.04	122.90
3	N	1	NAG	C1-O5-C5	3.78	117.25	112.19
3	b	1	NAG	C1-O5-C5	3.53	116.92	112.19
3	b	1	NAG	O4-C4-C5	2.62	115.79	109.32
3	g	1	NAG	C1-O5-C5	2.62	115.70	112.19
3	N	1	NAG	O4-C4-C5	2.42	115.29	109.32
3	T	2	NAG	C1-C2-N2	2.16	113.84	110.43
3	H	1	NAG	C1-C2-N2	2.14	113.81	110.43
3	H	1	NAG	C2-N2-C7	2.14	125.77	122.90
3	b	2	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C1-C2-N2-C7
3	N	2	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	i	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	i	1	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	a	1	NAG	C8-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2
3	U	2	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	f	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	Q	2	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
3	Z	2	NAG	C1-C2-N2-C7

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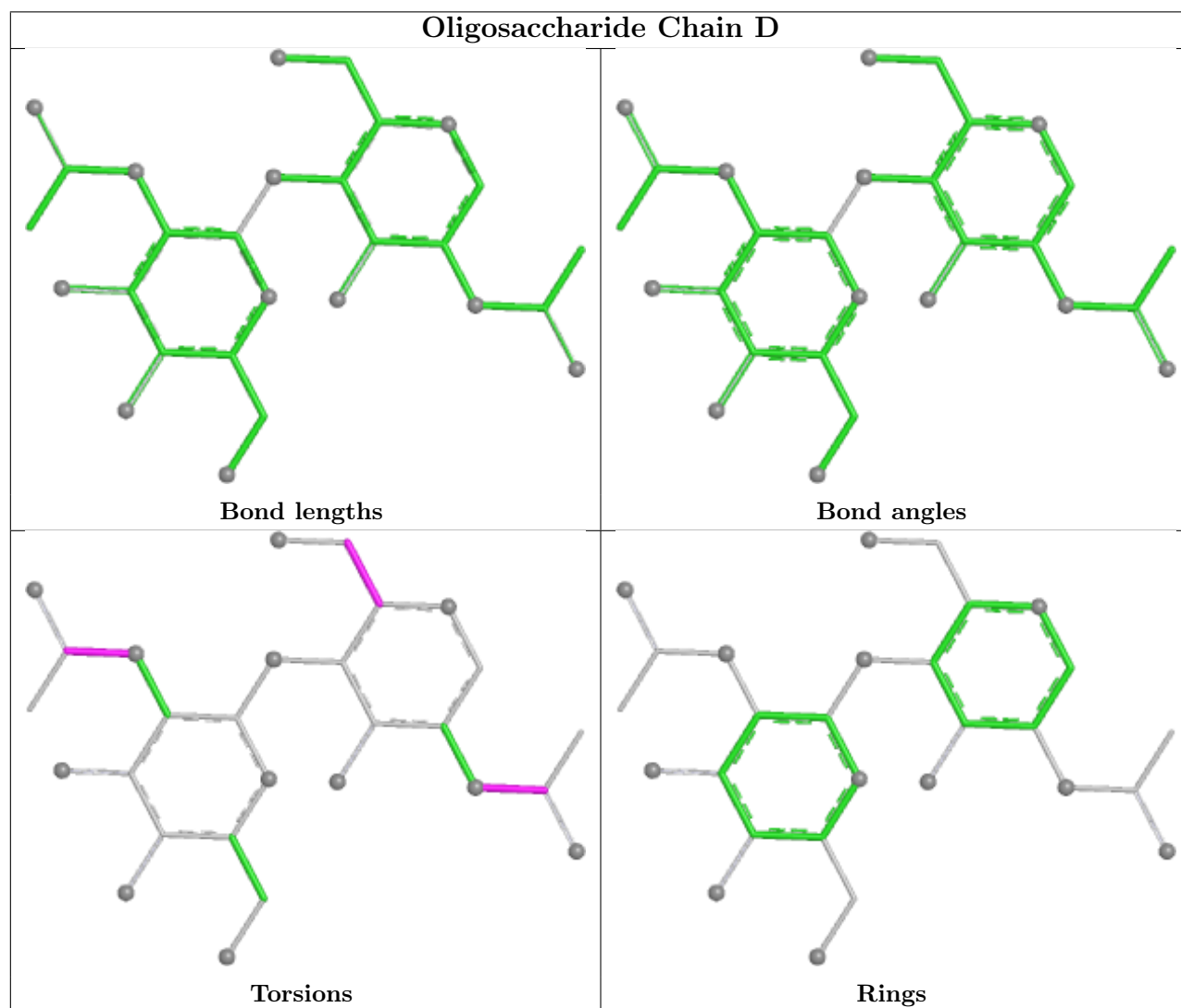
Mol	Chain	Res	Type	Atoms
3	h	2	NAG	C1-C2-N2-C7
3	i	1	NAG	C1-C2-N2-C7
3	f	1	NAG	O5-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	Z	2	NAG	C3-C2-N2-C7
3	i	2	NAG	C3-C2-N2-C7
3	f	2	NAG	C4-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	T	2	NAG	C1-C2-N2-C7
3	i	2	NAG	C1-C2-N2-C7
3	Q	2	NAG	C3-C2-N2-C7
3	R	1	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
3	h	2	NAG	C3-C2-N2-C7
3	i	1	NAG	C3-C2-N2-C7
3	L	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6

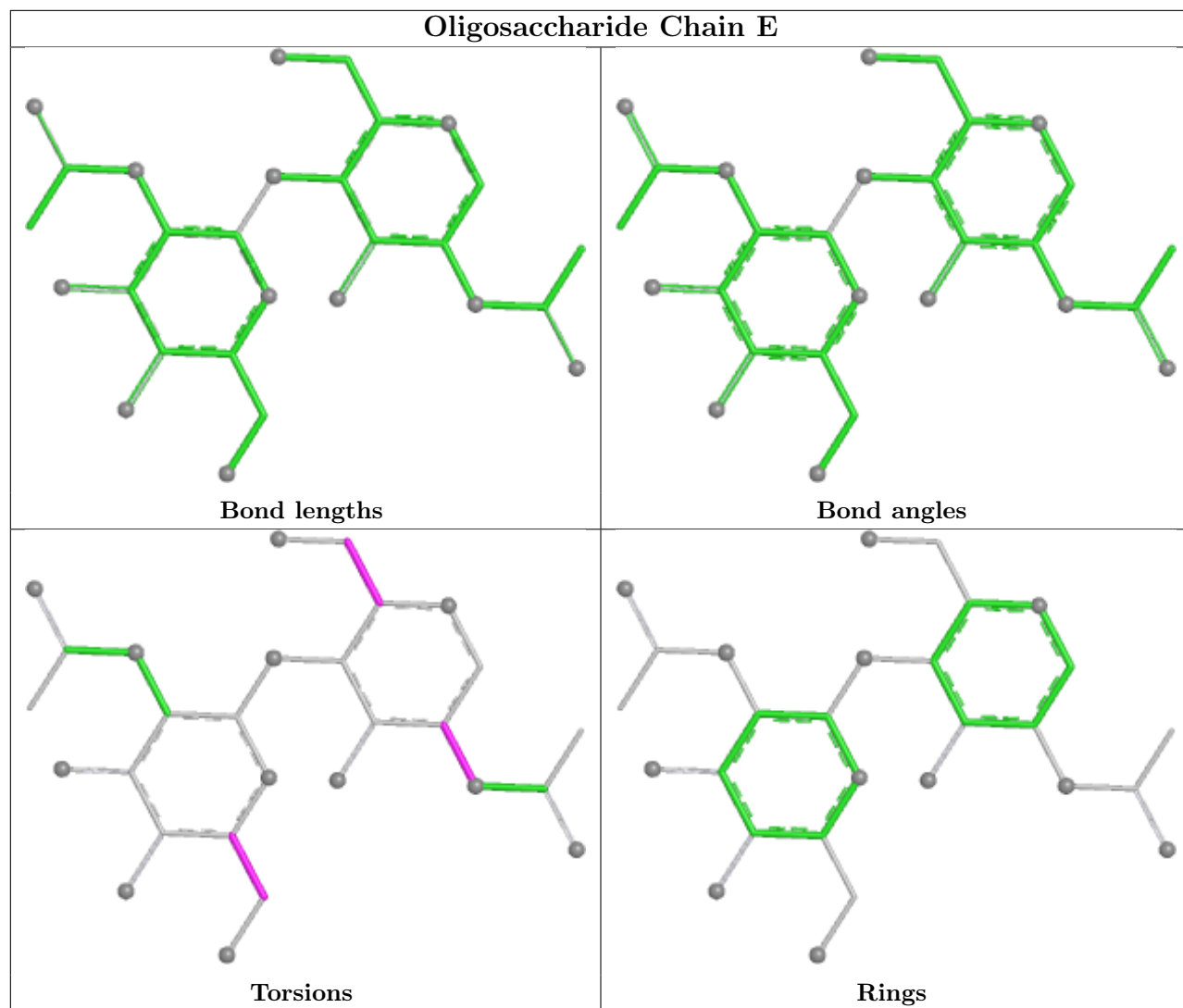
There are no ring outliers.

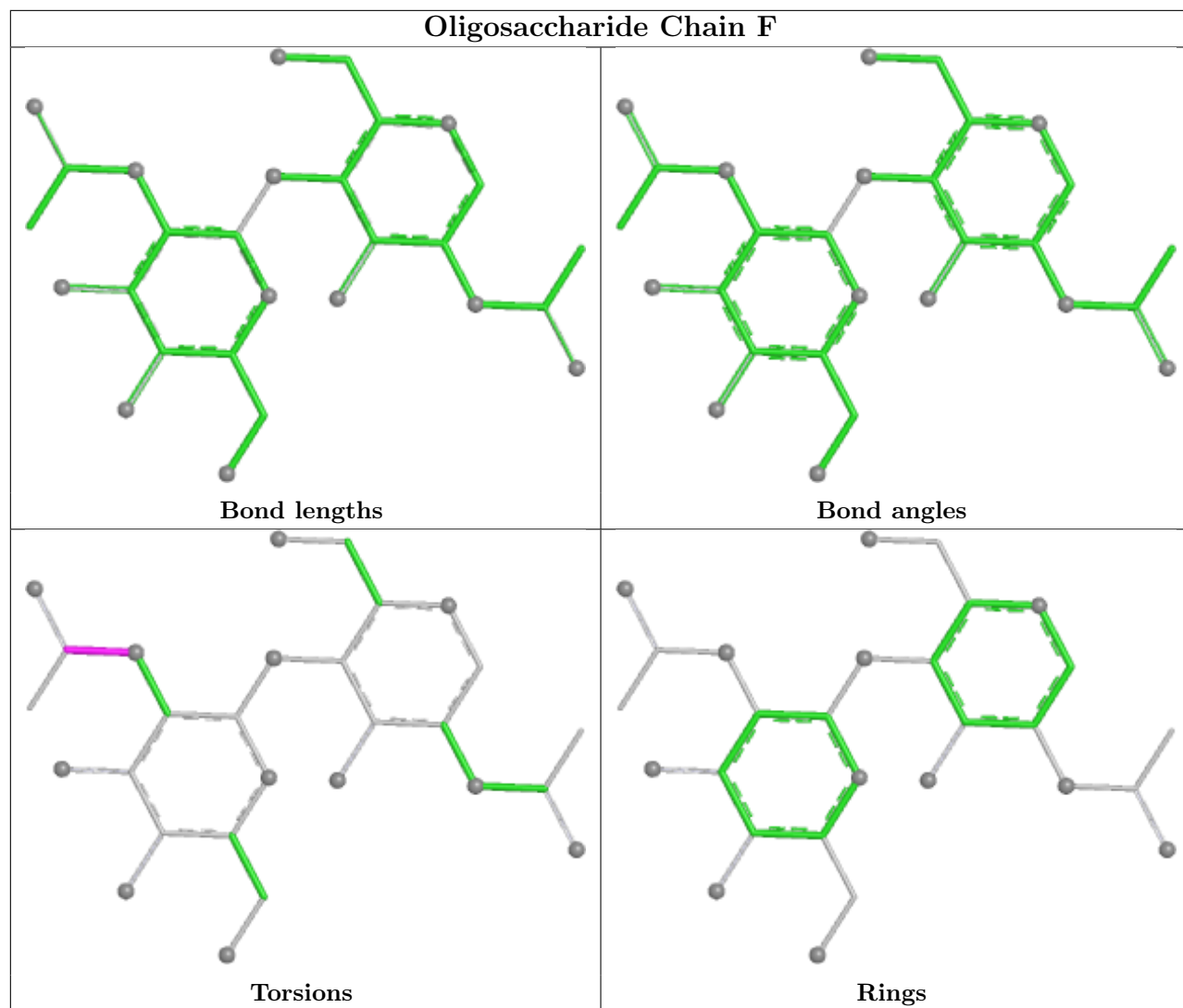
15 monomers are involved in 14 short contacts:

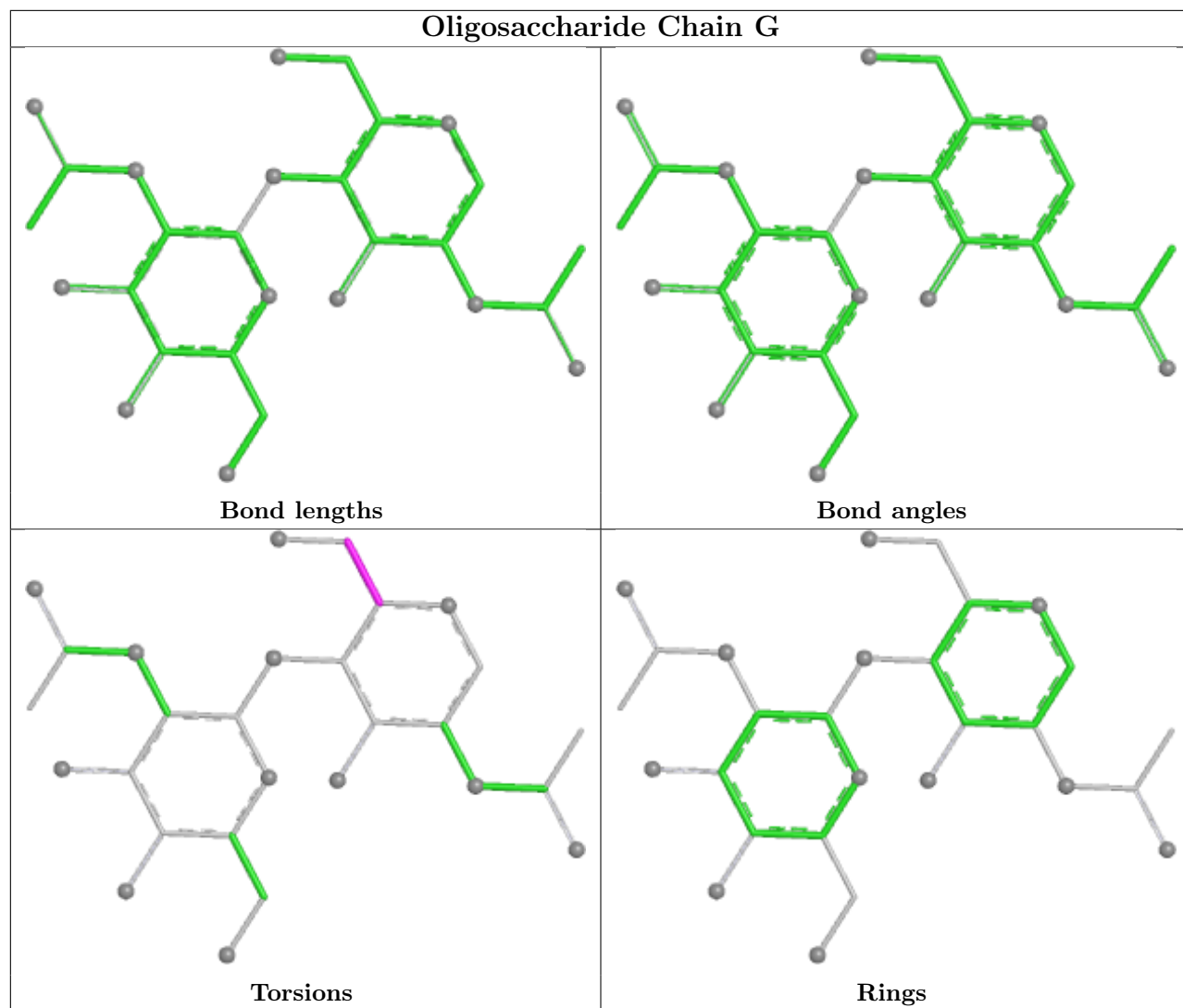
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
3	W	2	NAG	1	0
3	X	2	NAG	1	0
3	b	1	NAG	1	0
3	O	1	NAG	2	0
3	F	1	NAG	1	0
3	h	1	NAG	1	0
3	M	1	NAG	1	0
3	N	2	NAG	1	0
3	T	2	NAG	1	0
3	W	1	NAG	1	0
3	H	1	NAG	1	0
3	b	2	NAG	2	0
3	P	1	NAG	2	0
3	P	2	NAG	1	0

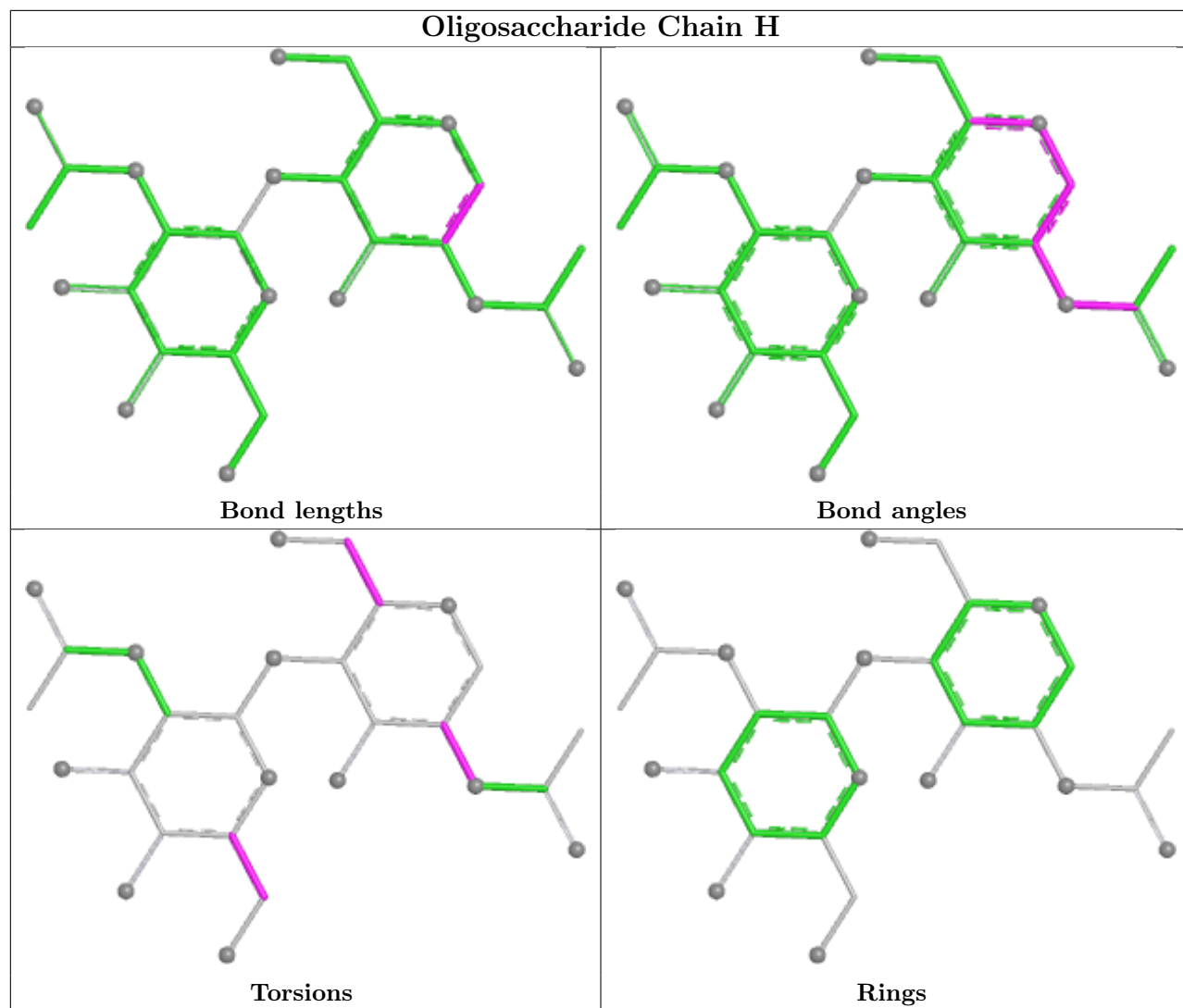
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

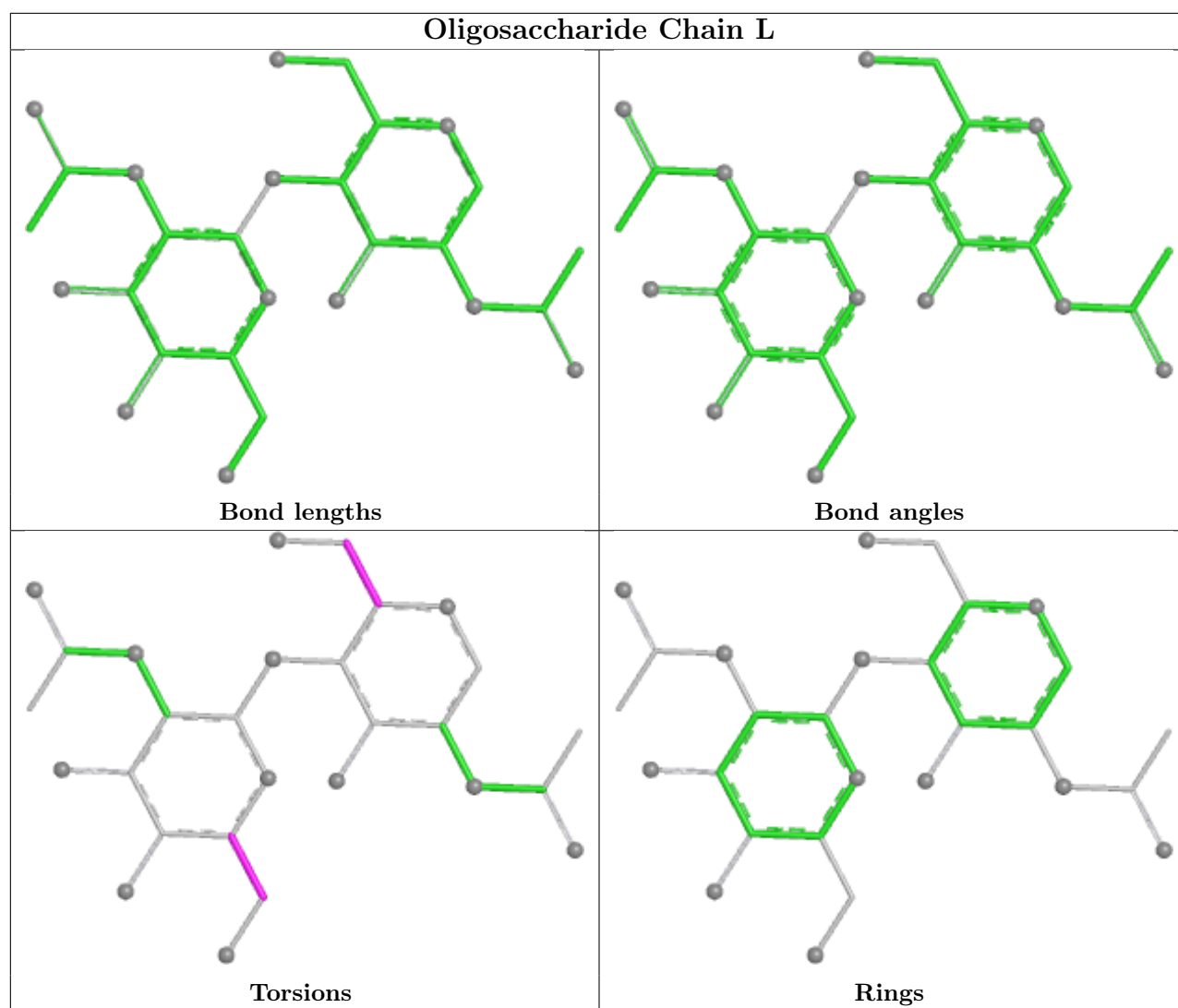


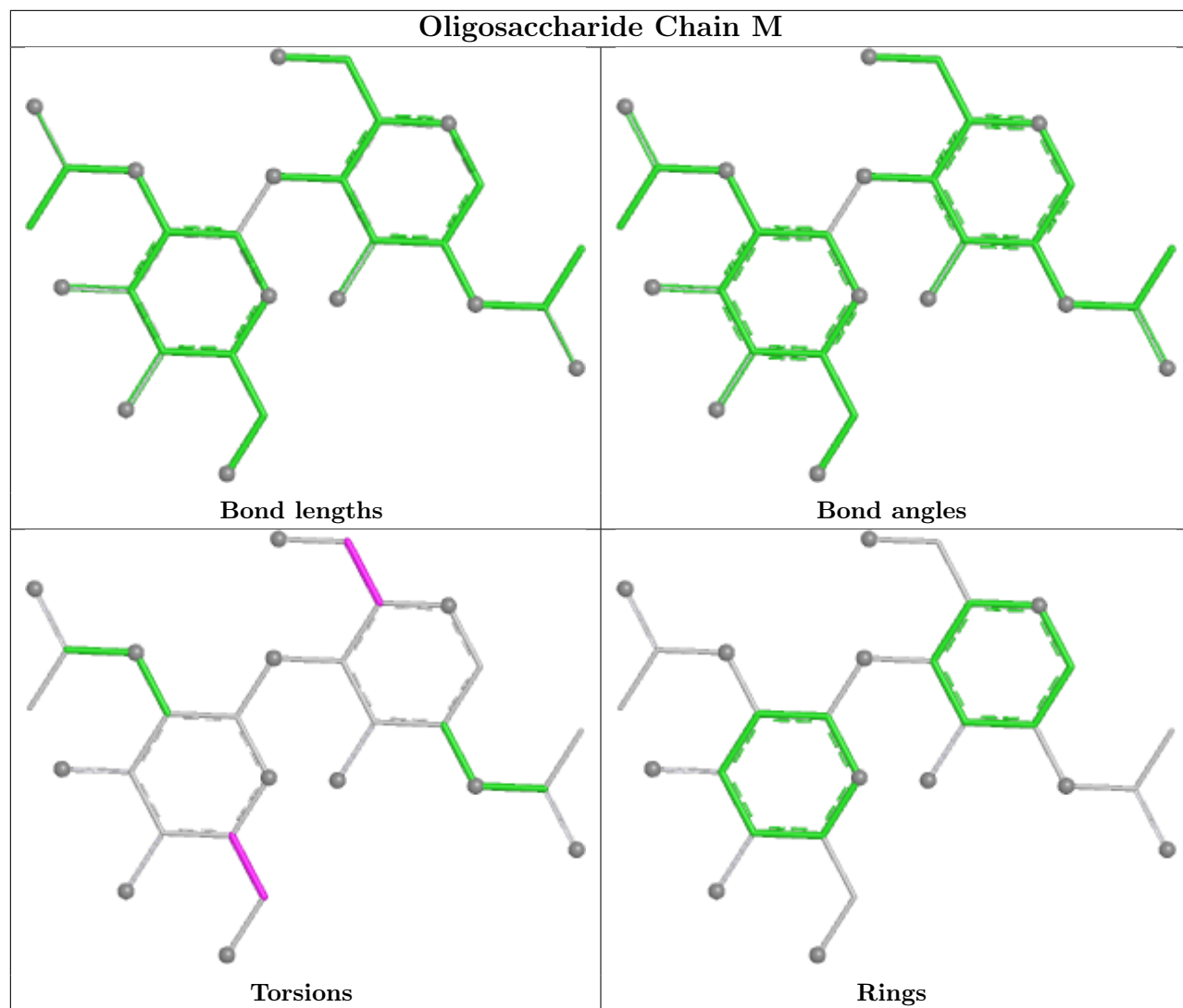


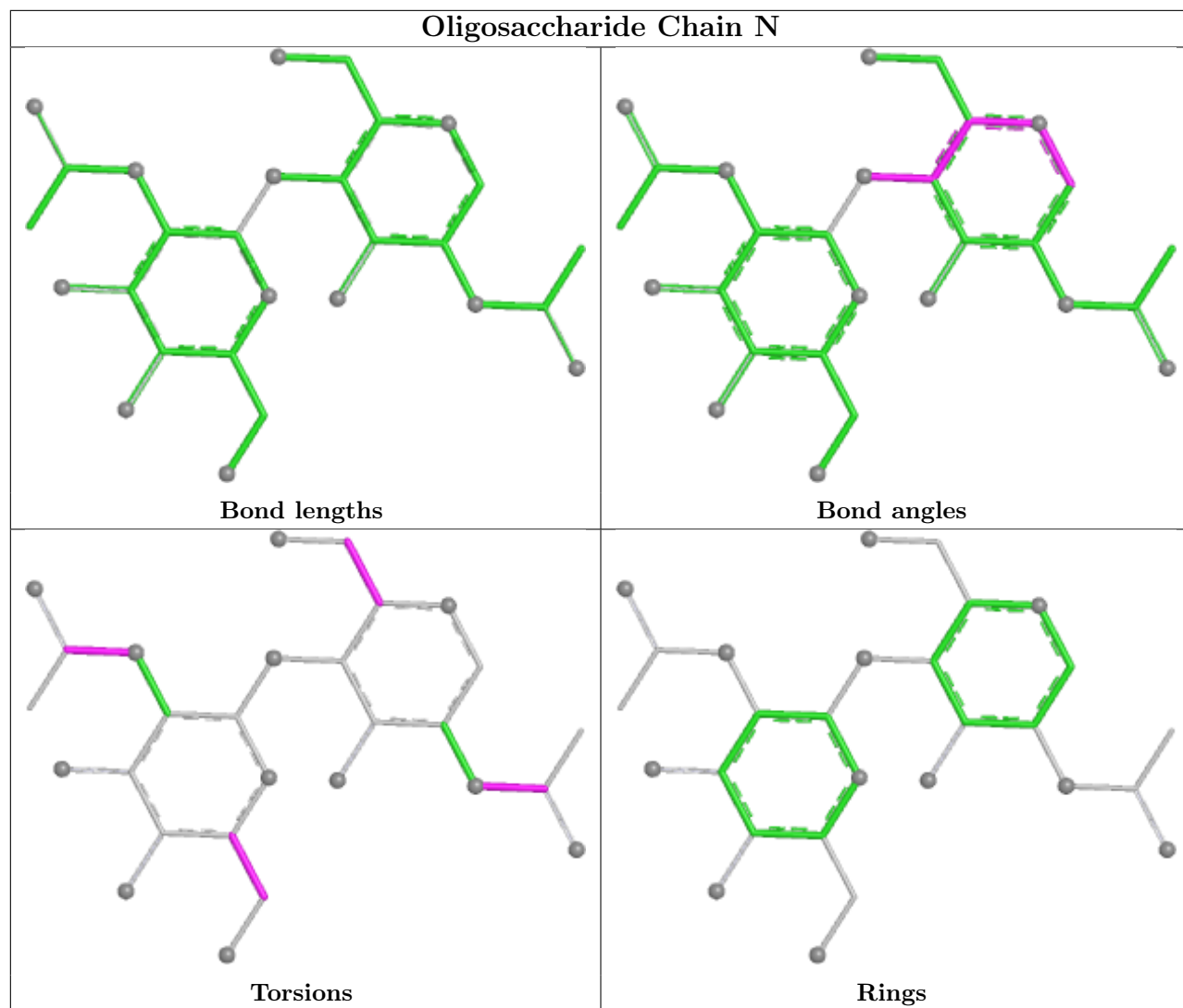


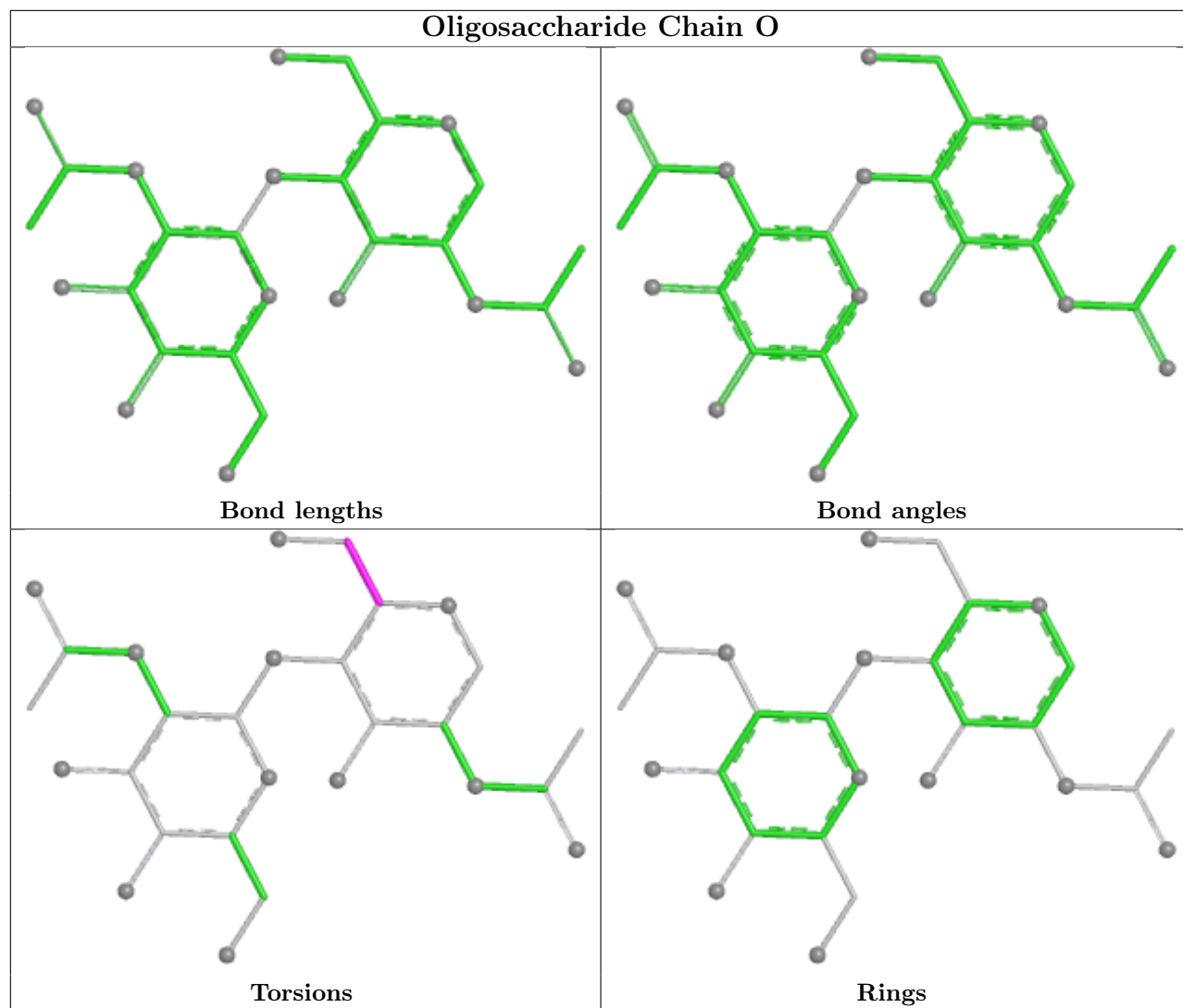


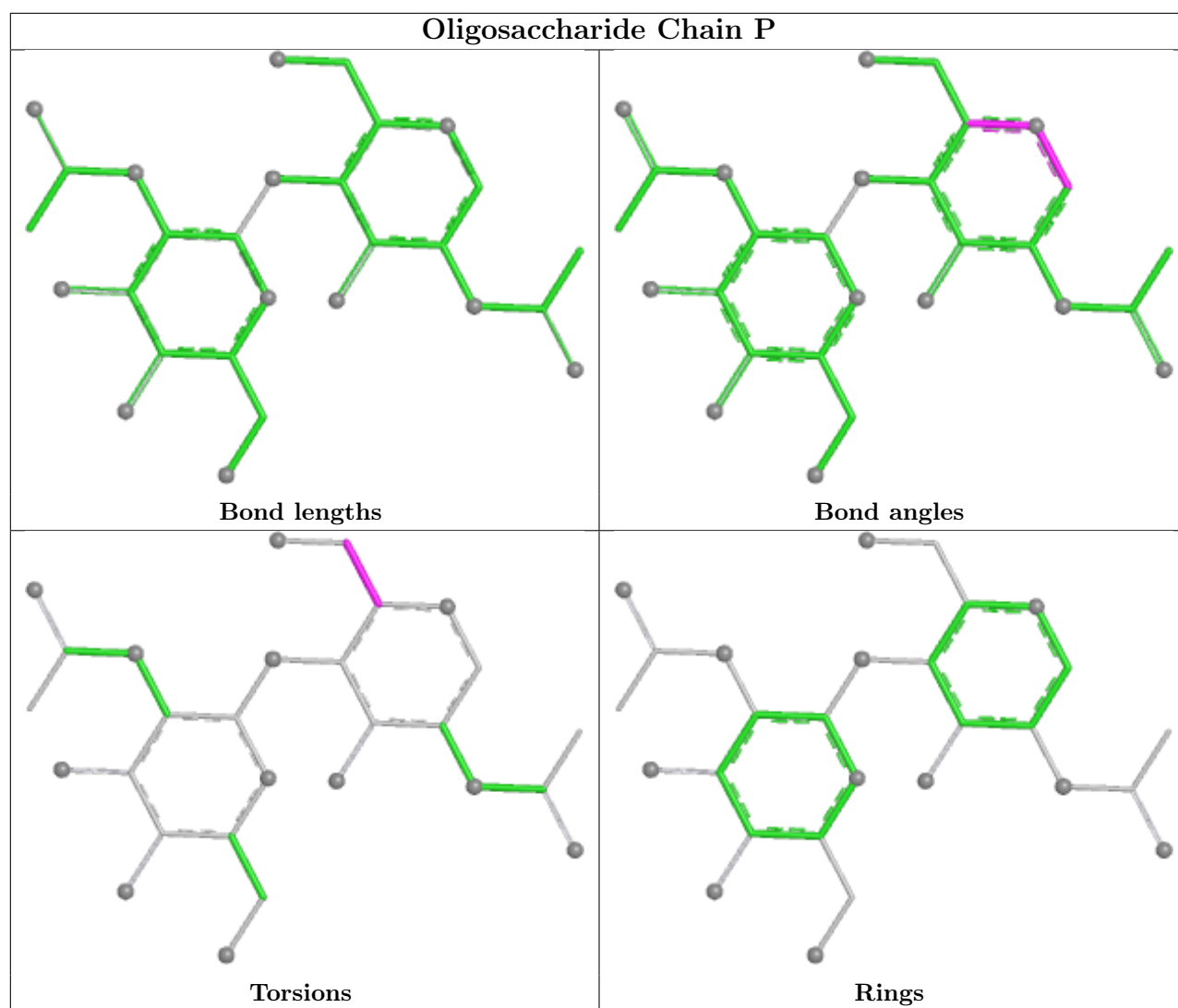


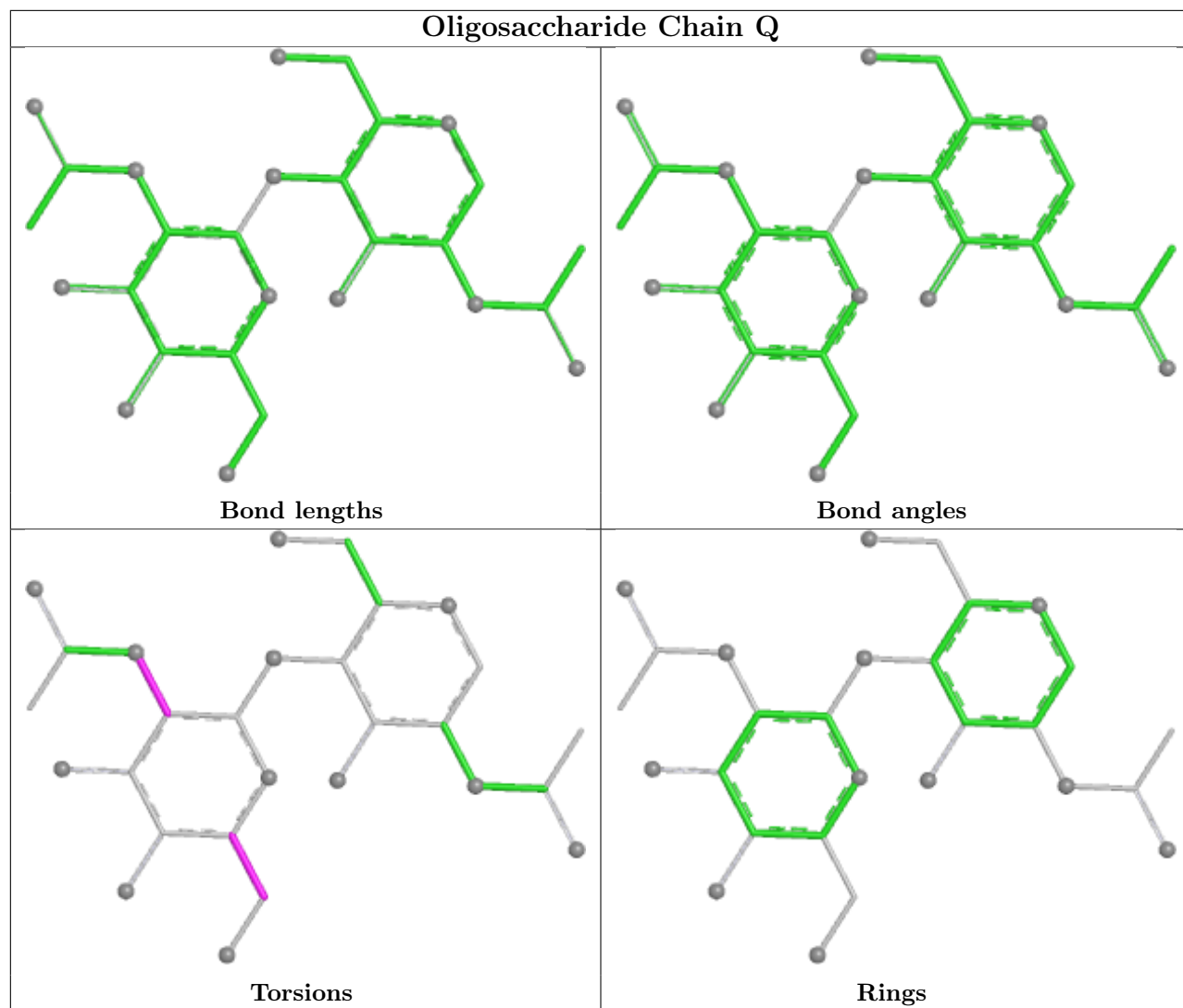


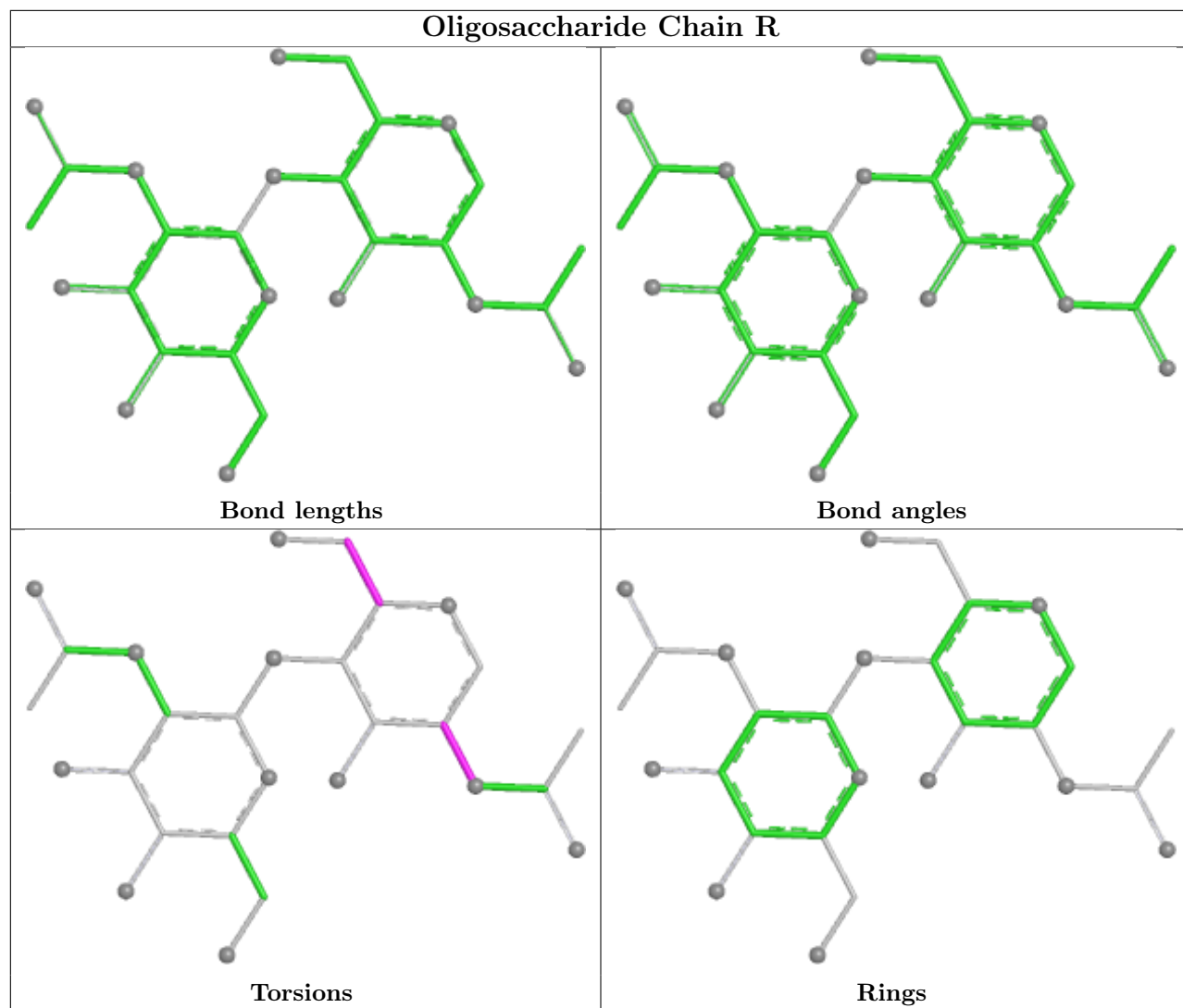


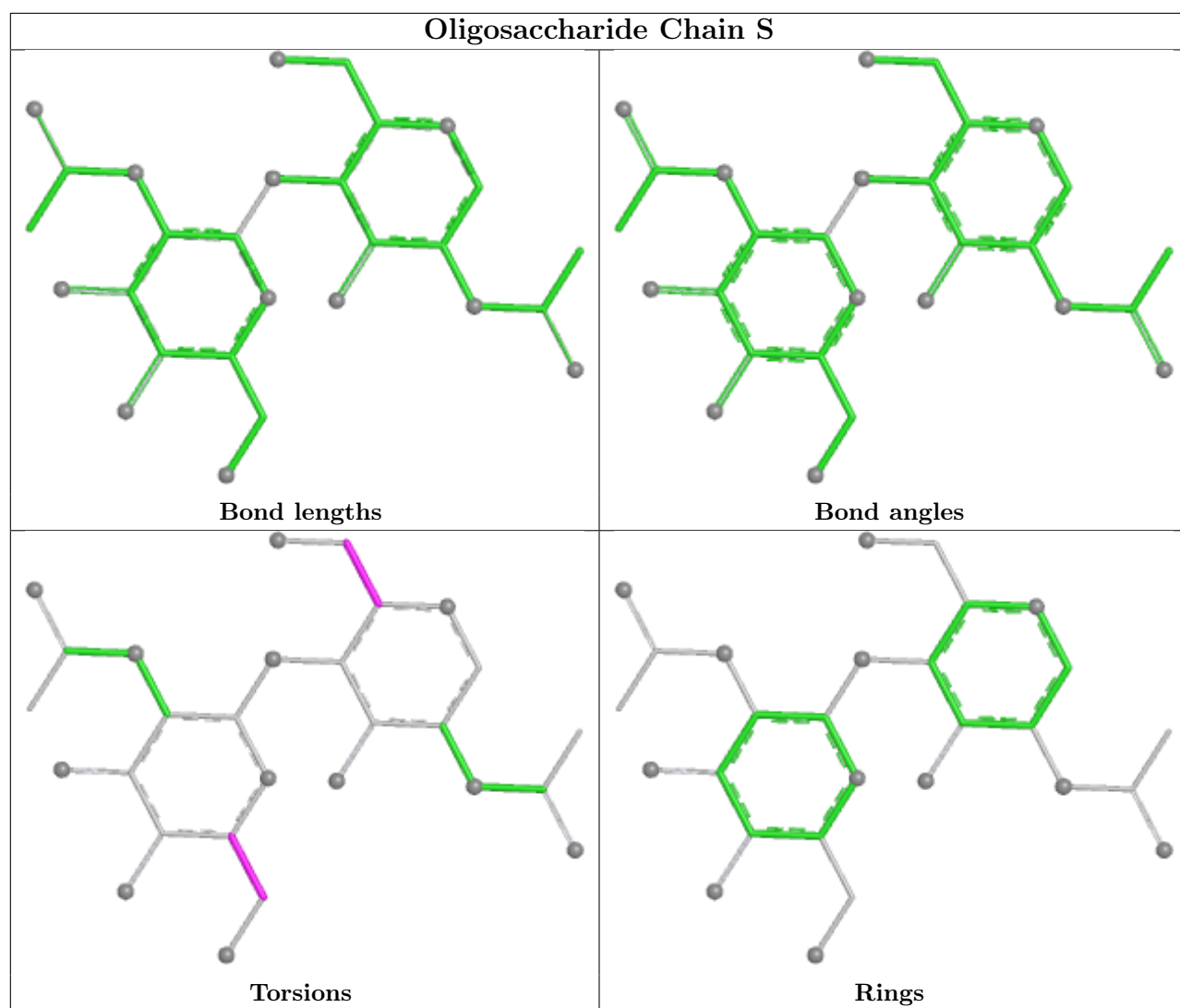


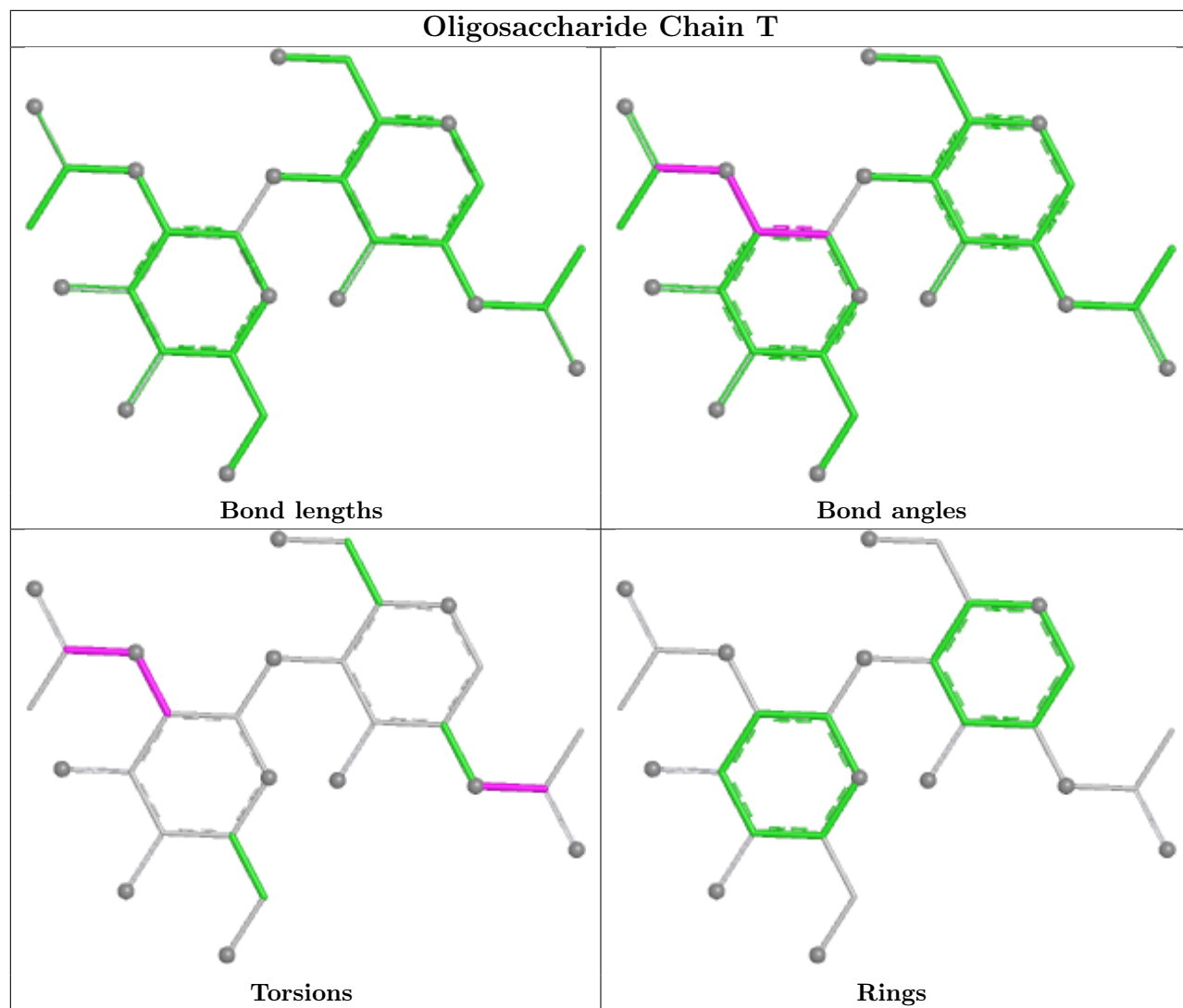


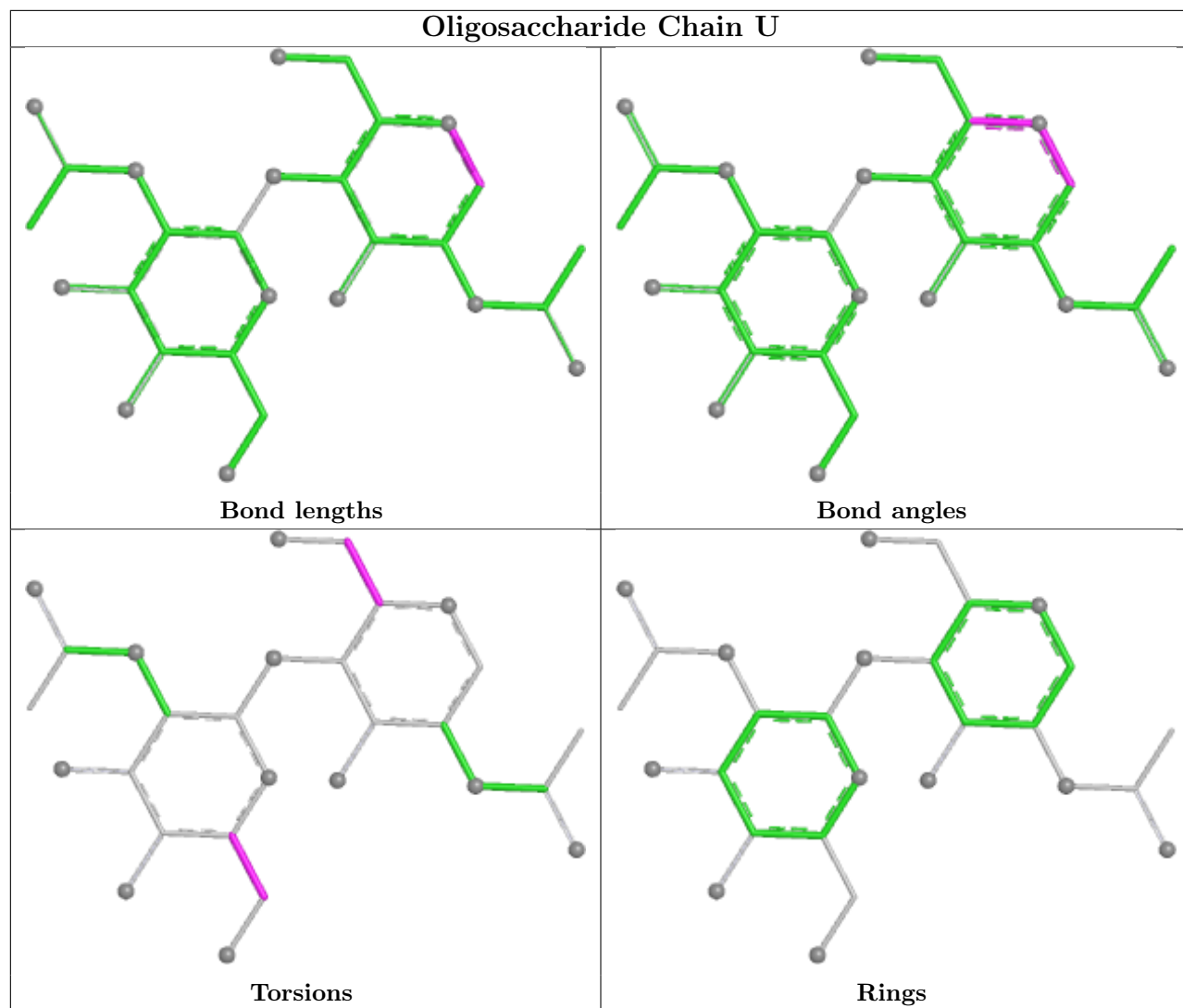


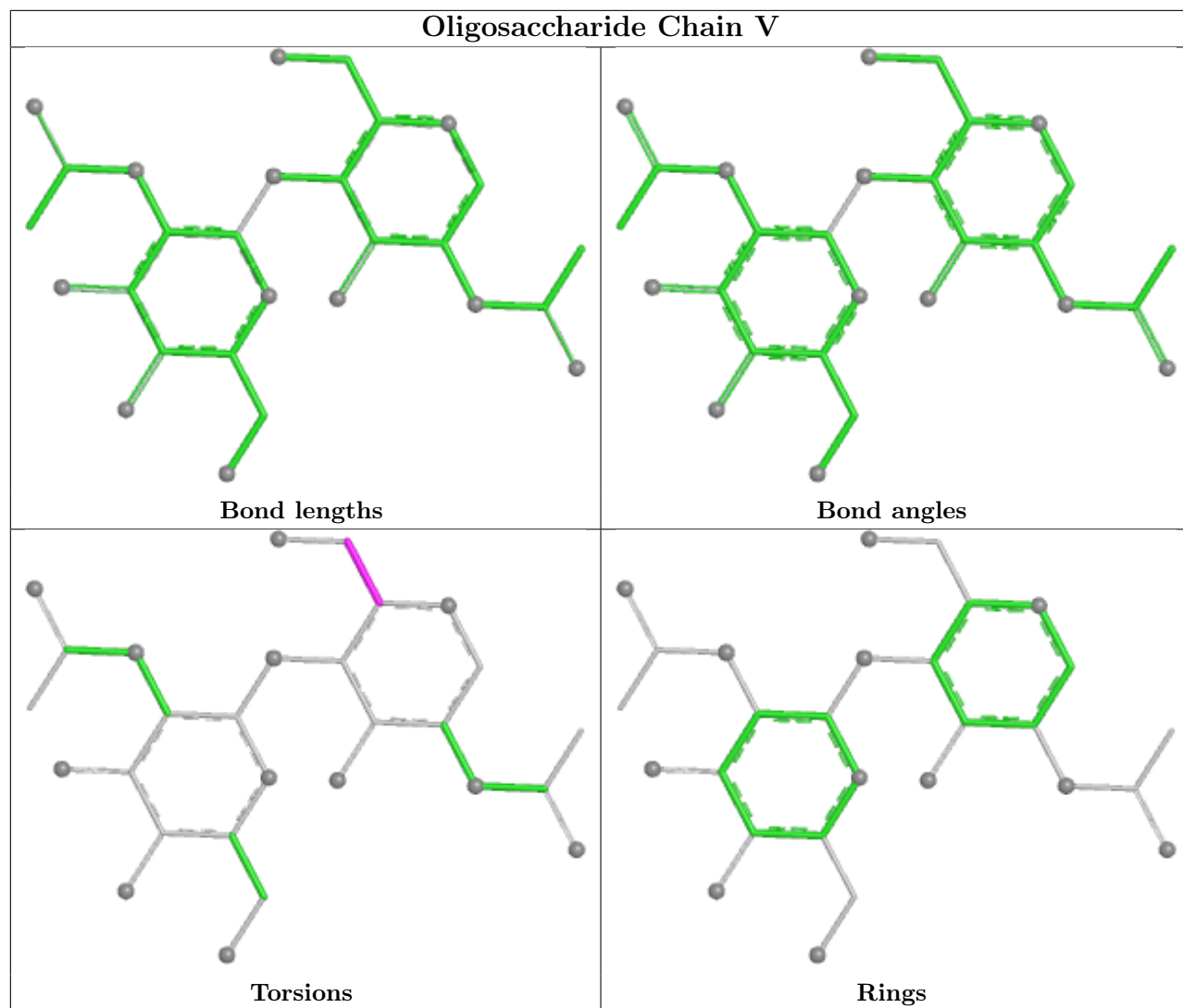


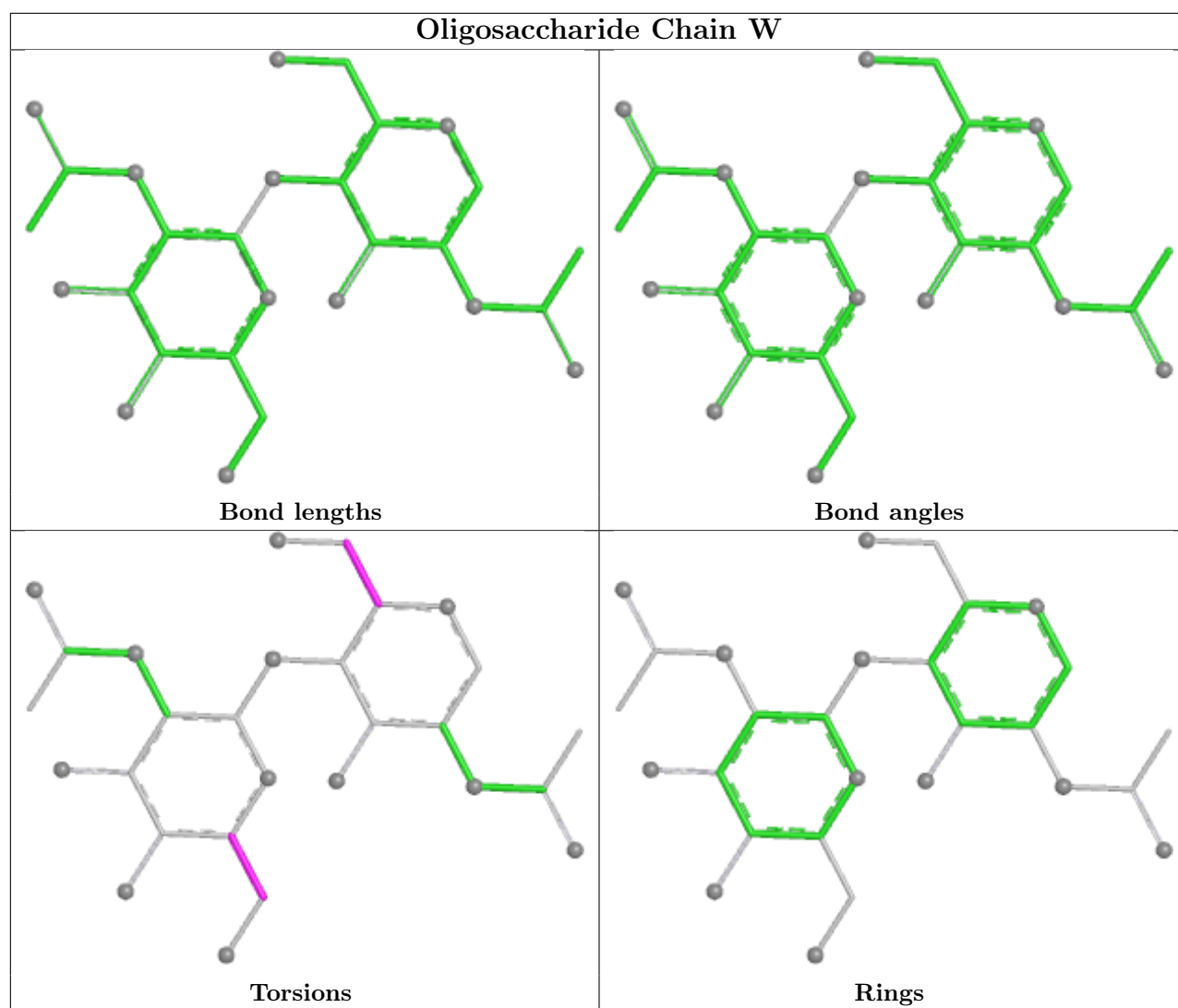


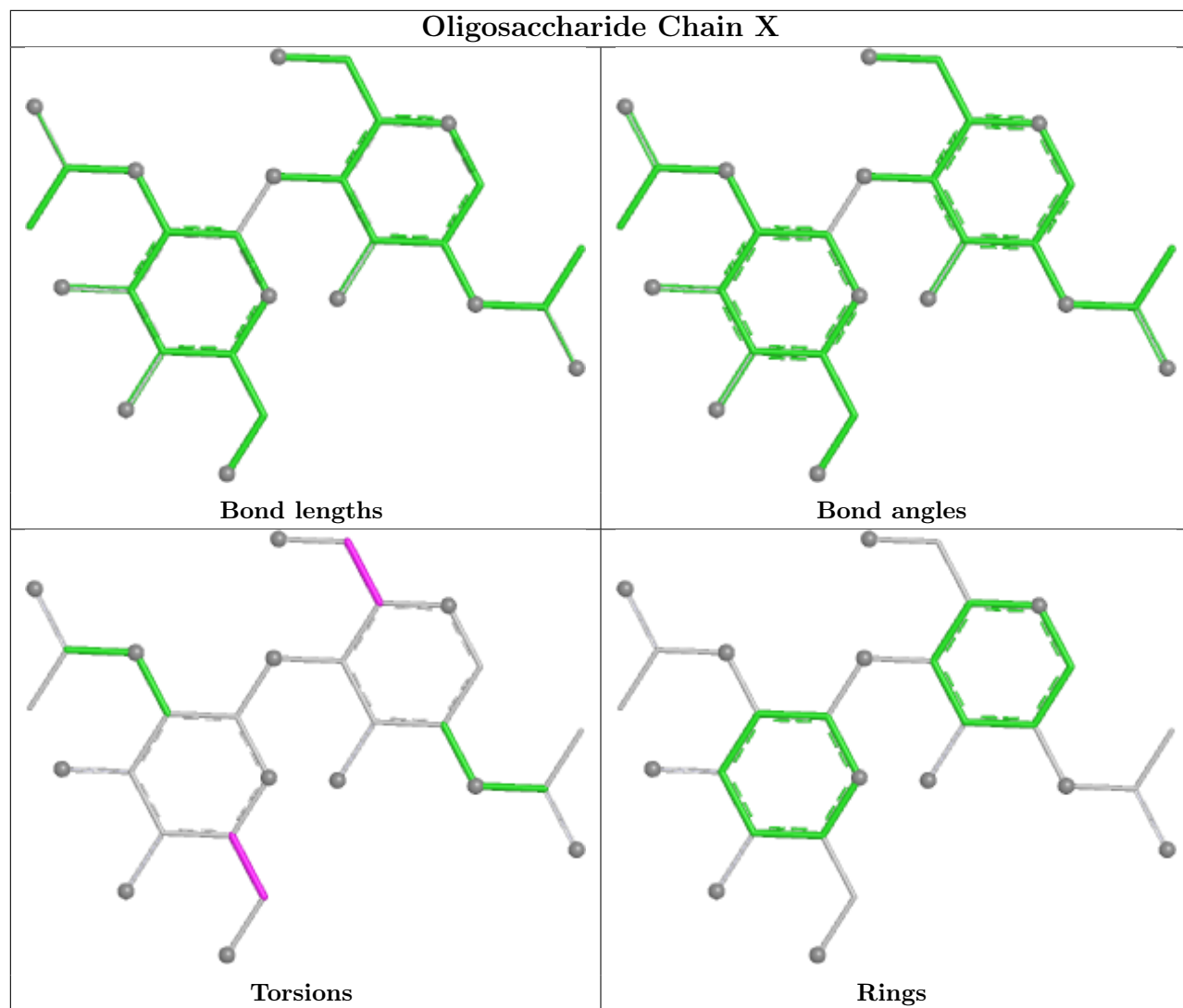


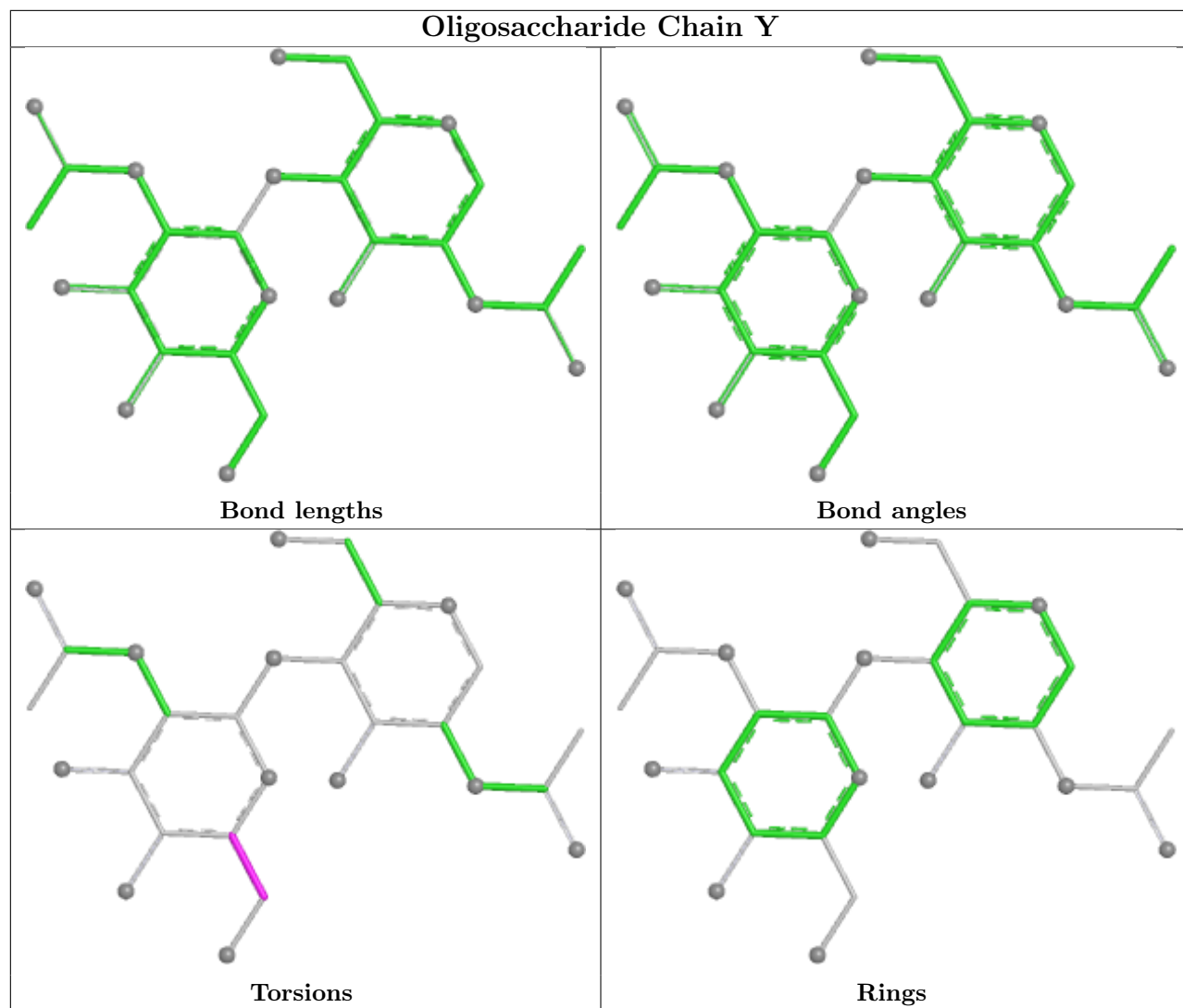


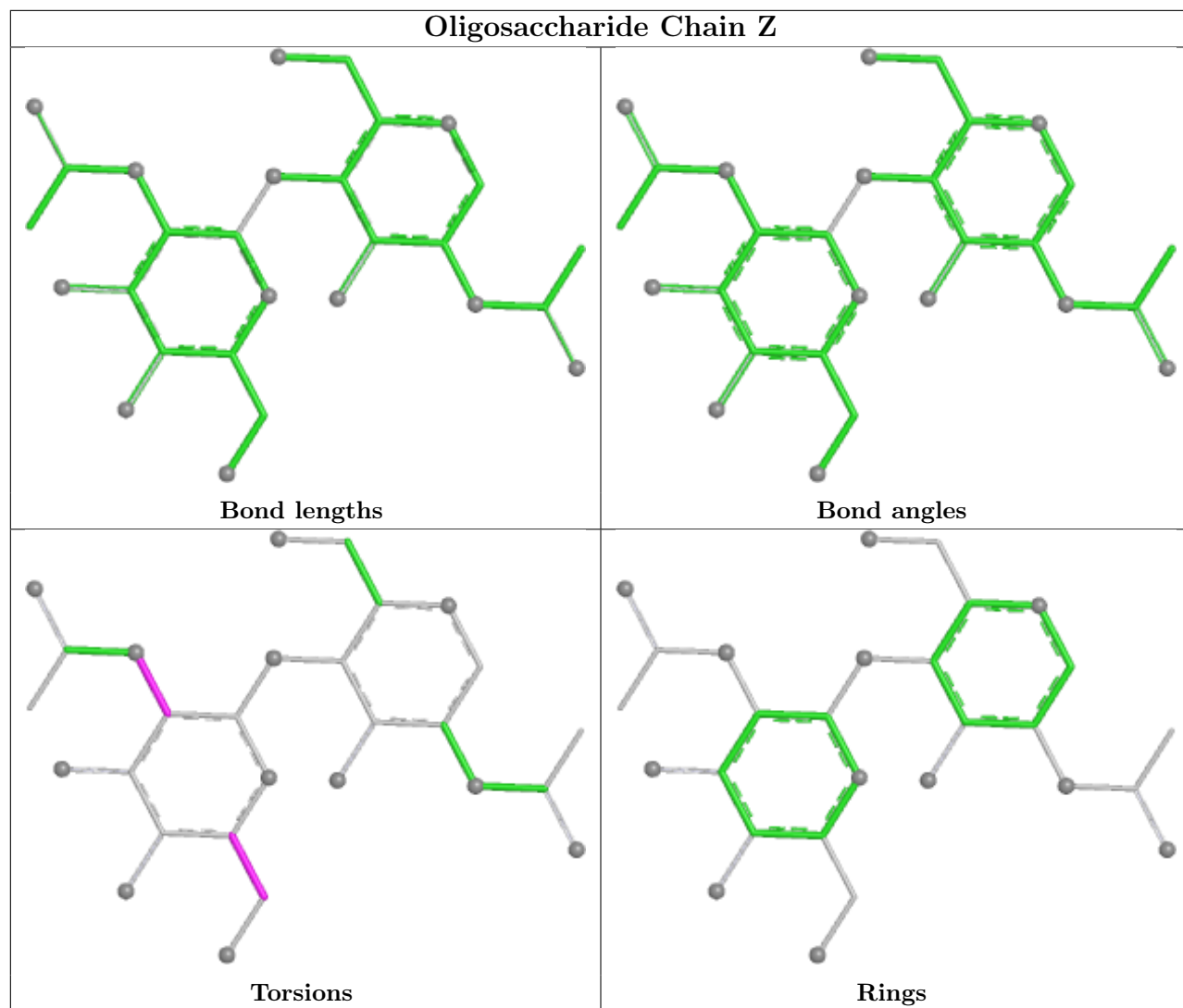


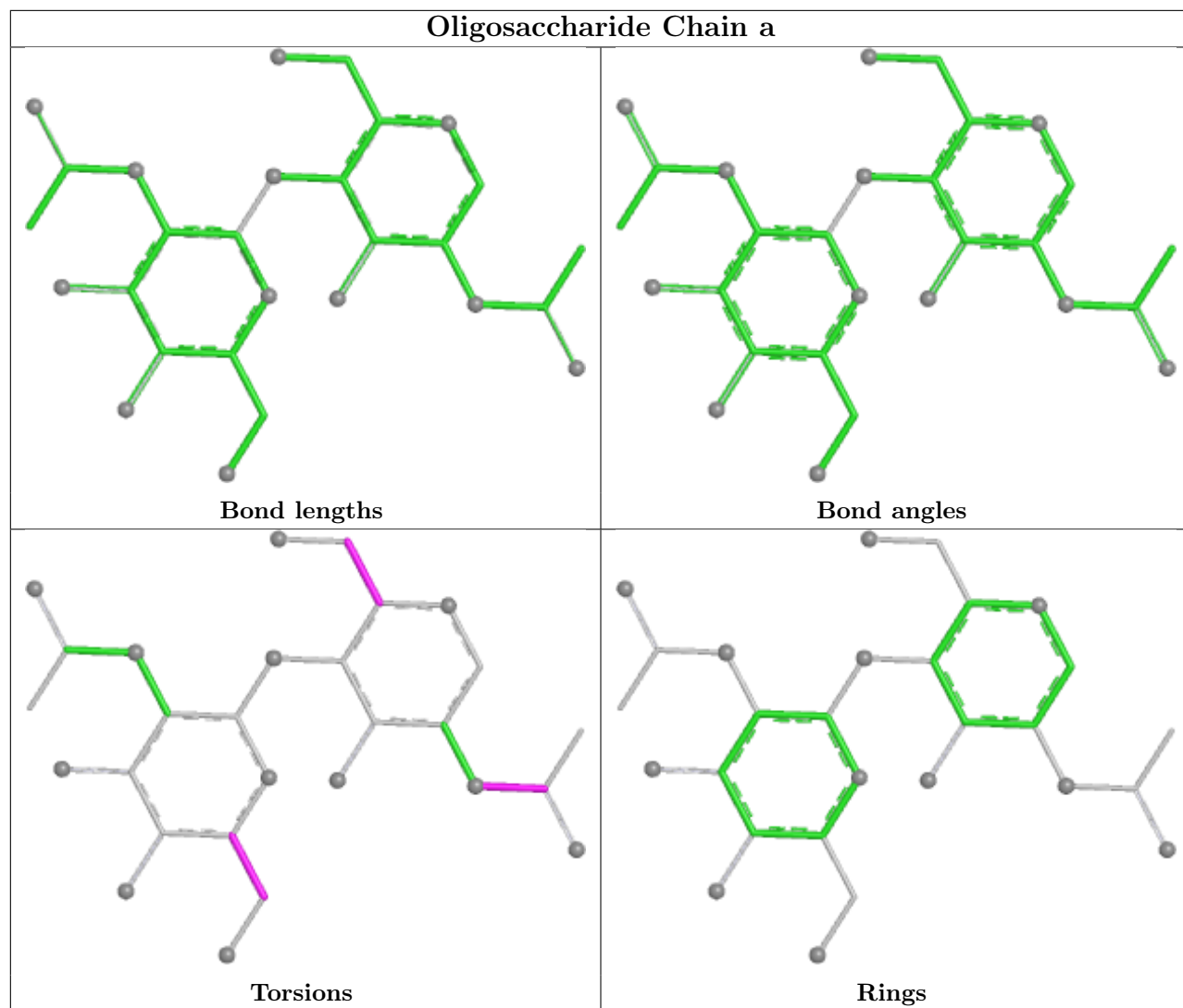


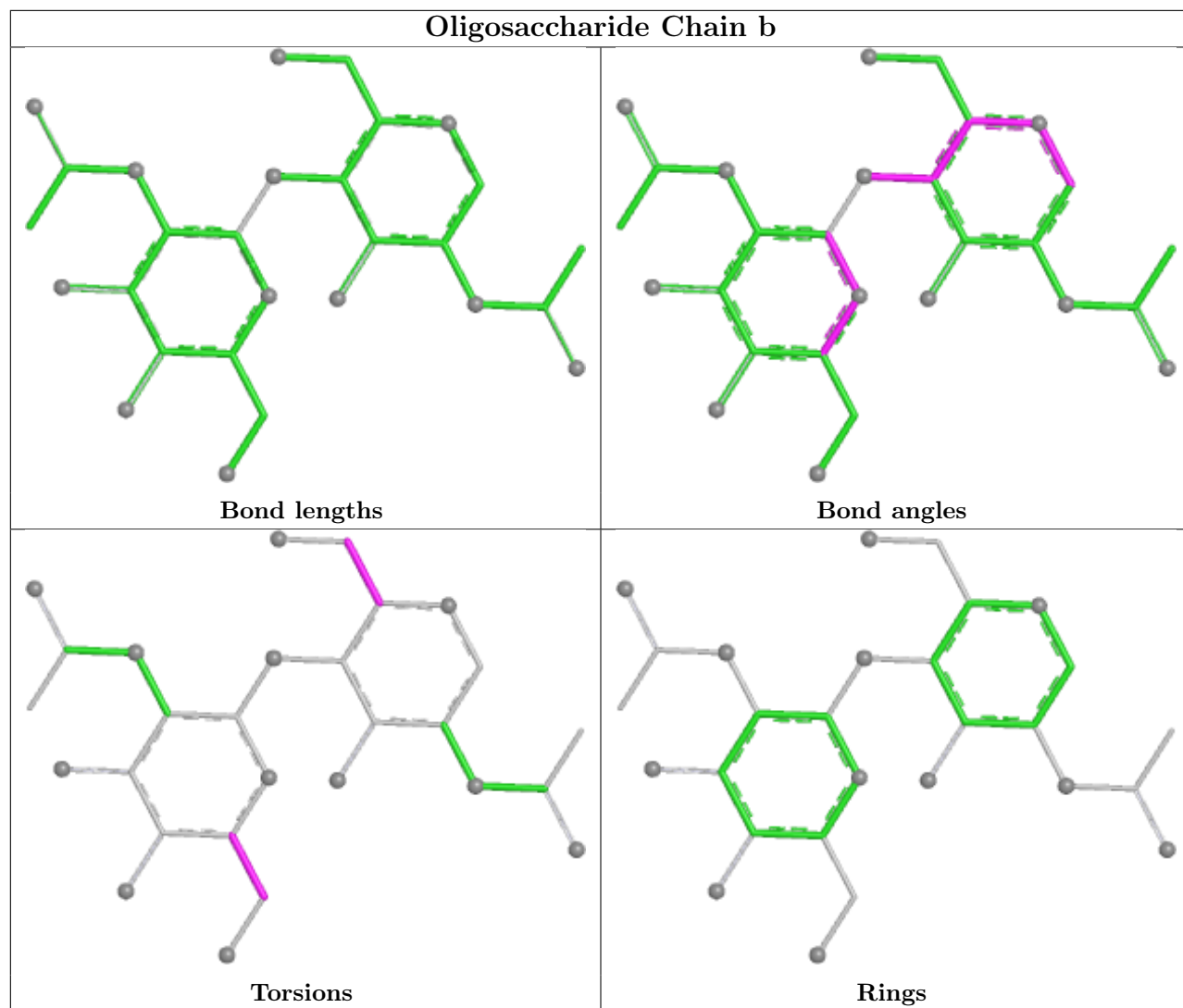


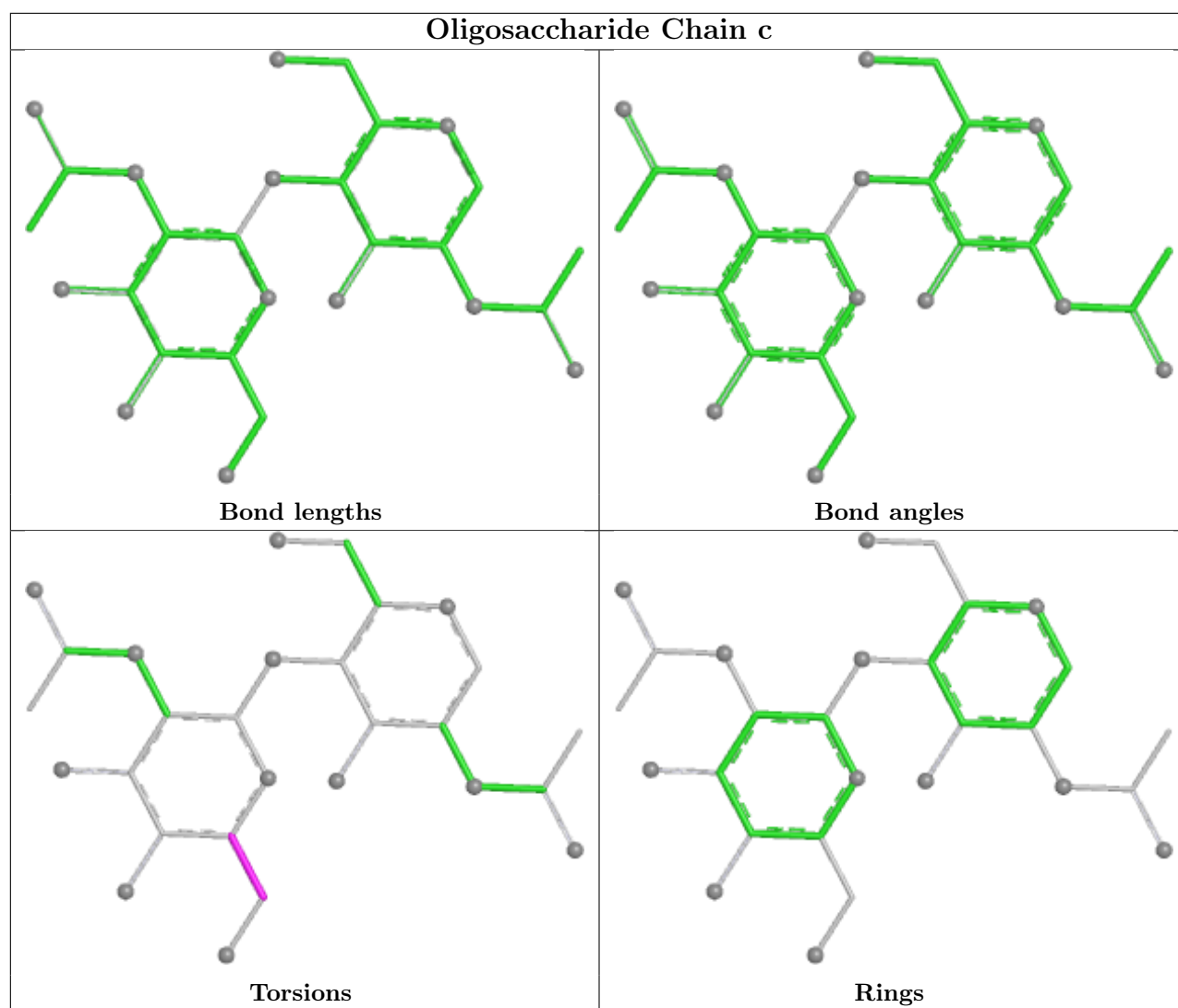


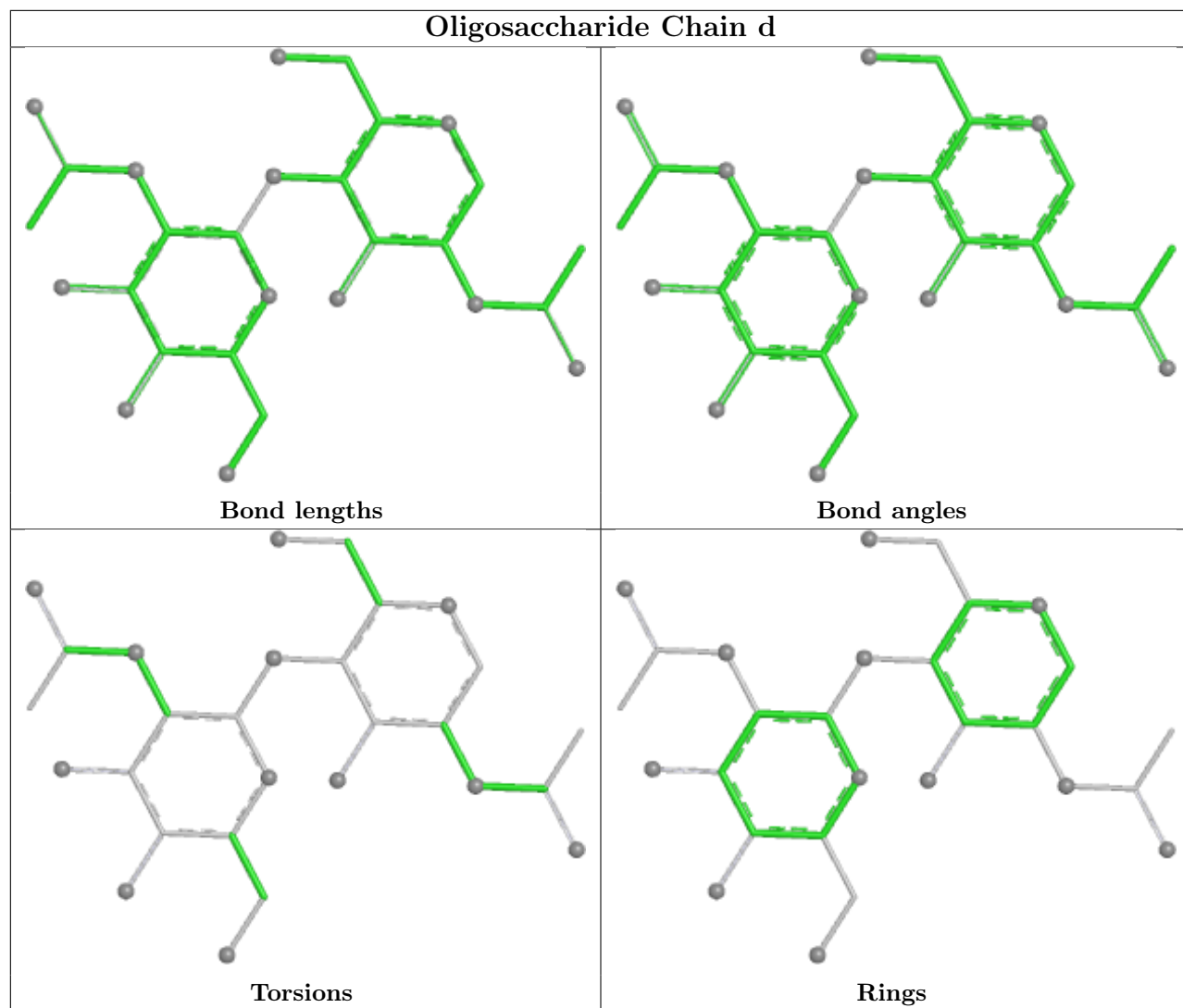


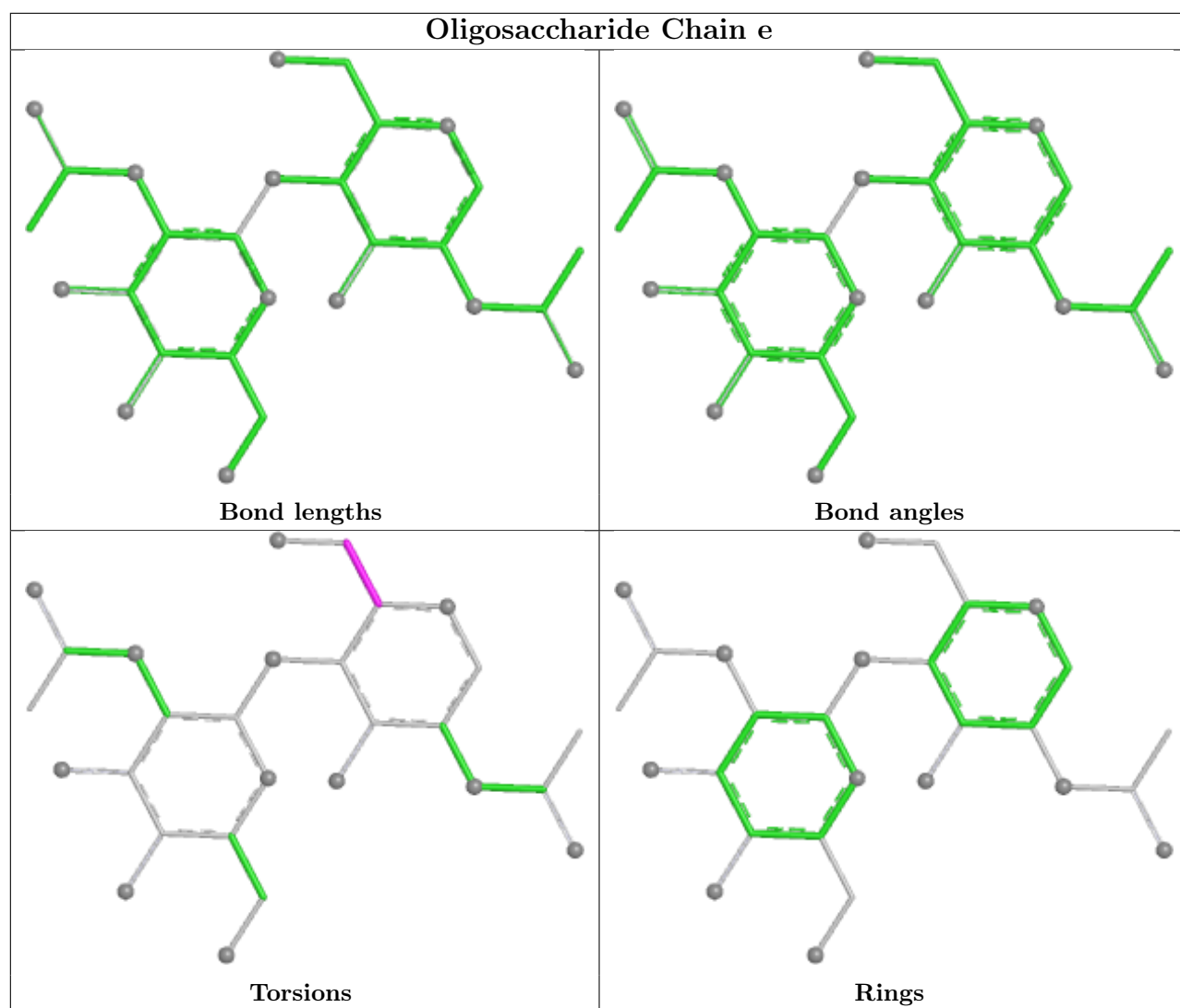


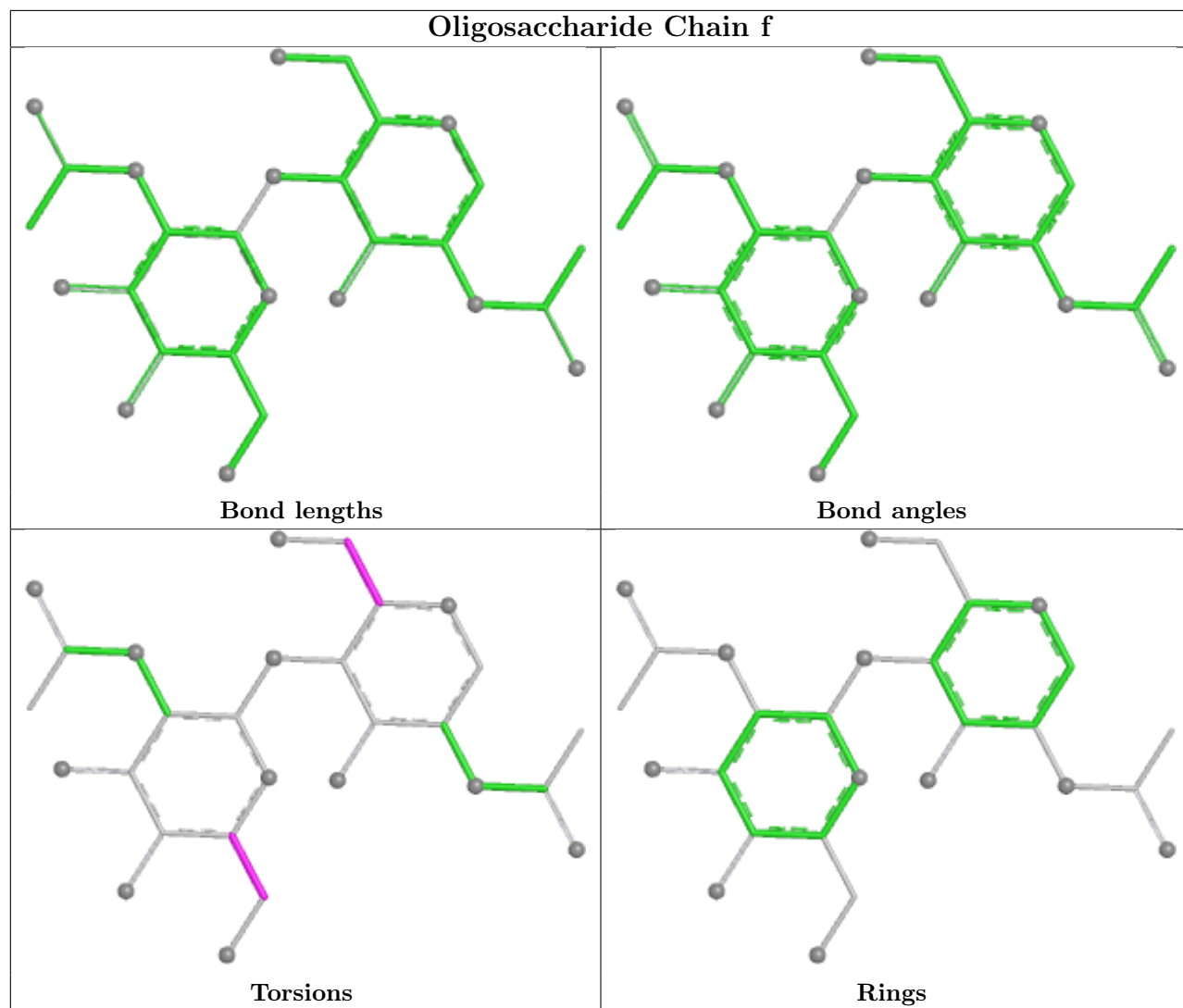


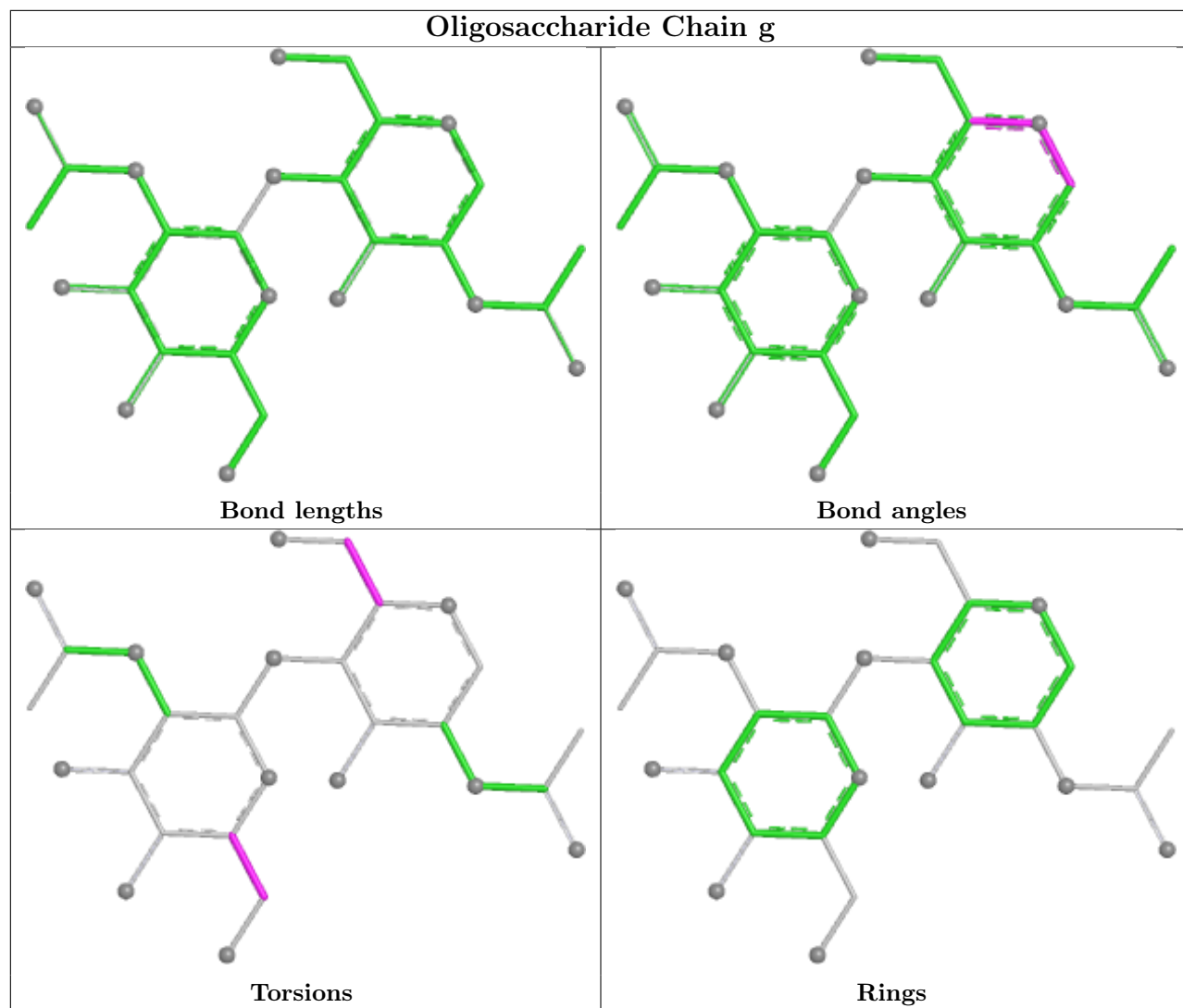


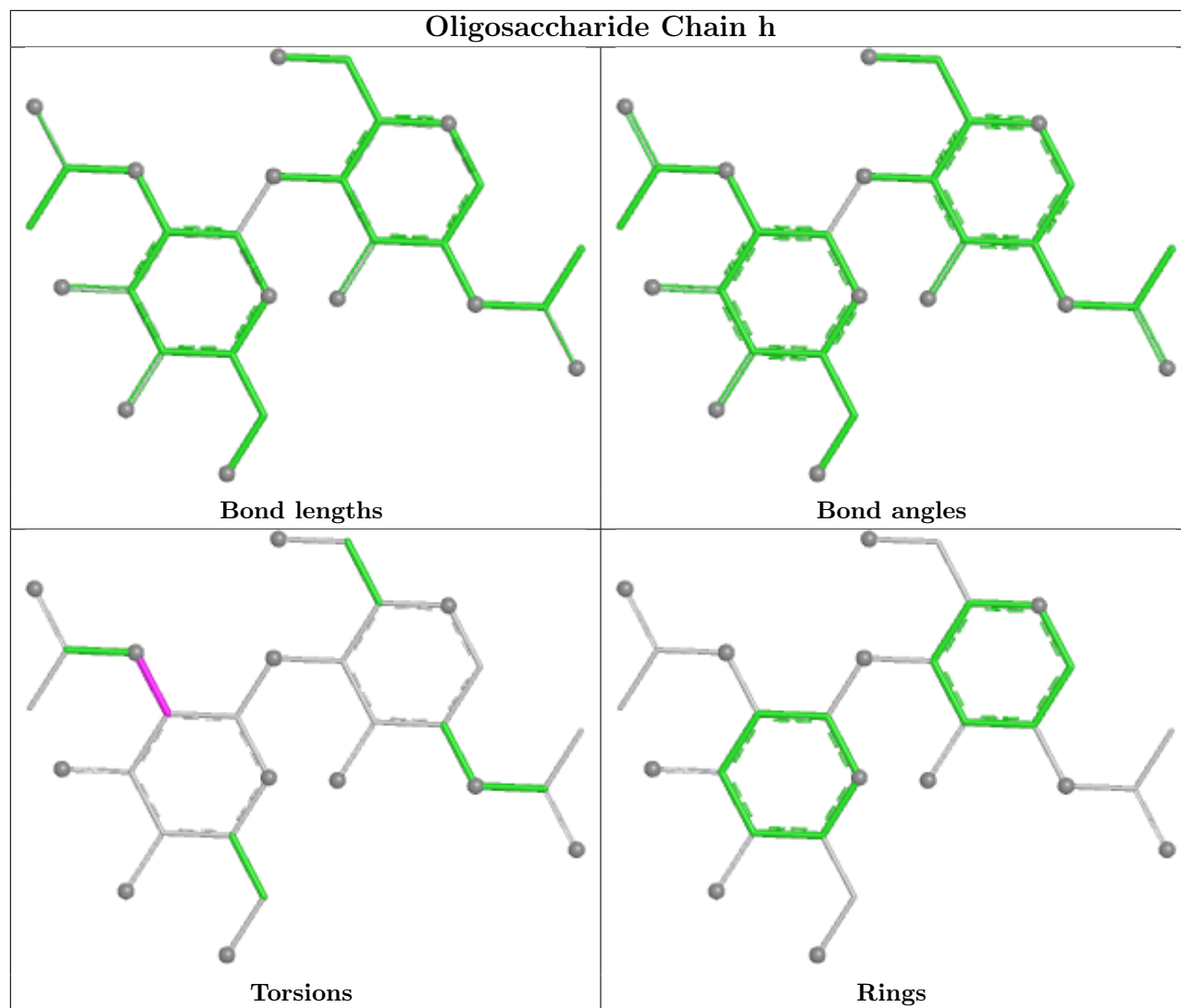


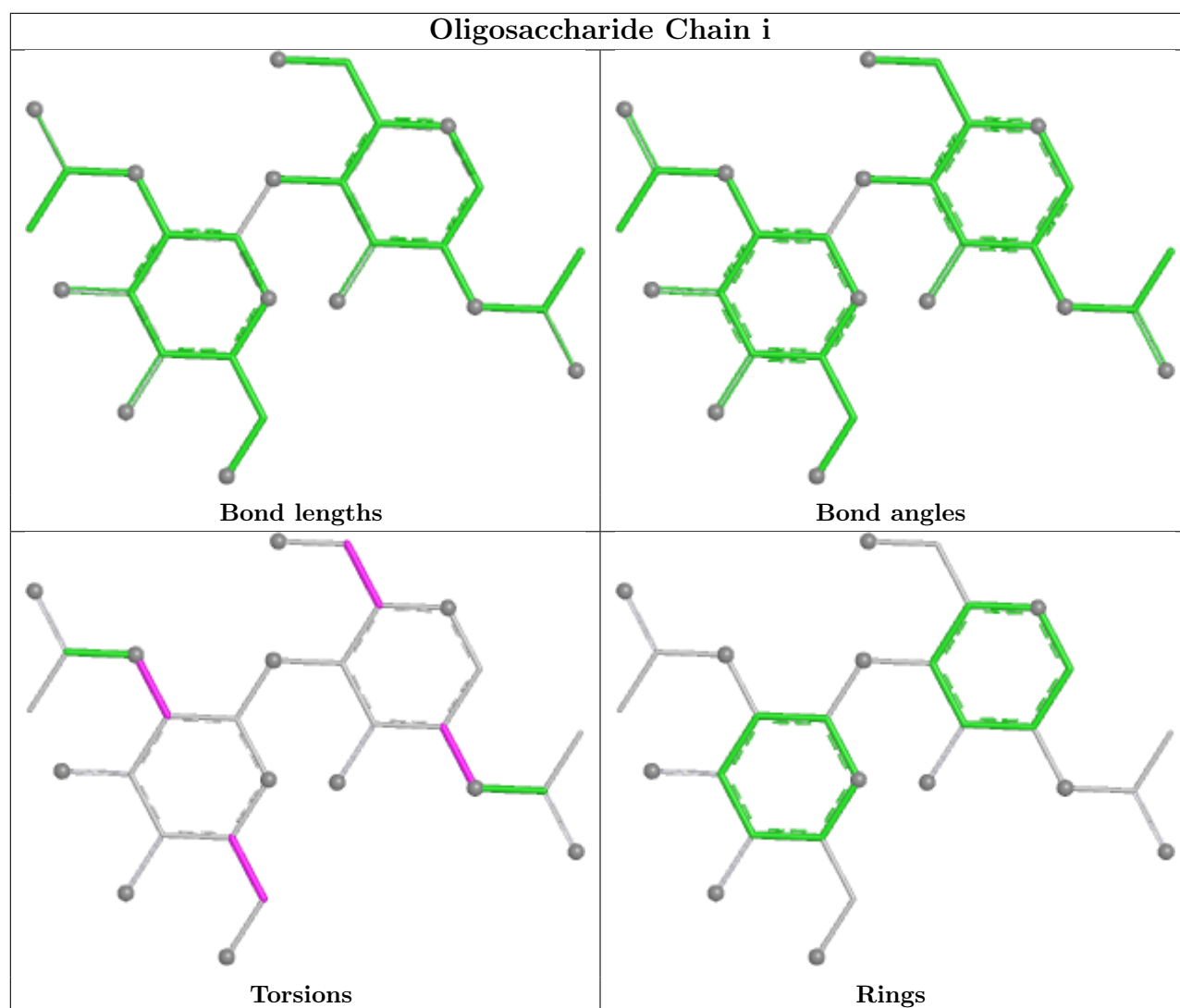












5.6 Ligand geometry [i](#)

26 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	2004	1	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	C	2007	1	14,14,15	0.30	0	17,19,21	0.49	0
4	NAG	C	2006	1	14,14,15	0.22	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	2006	1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	A	2002	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	C	2001	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	A	2005	1	14,14,15	0.19	0	17,19,21	0.42	0
4	NAG	I	1006	2	14,14,15	0.18	0	17,19,21	0.50	0
4	NAG	A	2001	1	14,14,15	0.51	0	17,19,21	0.65	0
4	NAG	B	2001	1	14,14,15	0.49	0	17,19,21	0.65	0
4	NAG	B	2005	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	C	2005	1	14,14,15	0.30	0	17,19,21	0.37	0
4	NAG	I	1002	2	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	C	2003	1	14,14,15	0.49	0	17,19,21	1.29	1 (5%)
4	NAG	B	2002	1	14,14,15	0.47	0	17,19,21	0.72	1 (5%)
4	NAG	A	2006	1	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	A	2003	-	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	I	1003	2	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	B	2004	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	I	1004	2	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	A	2004	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	I	1005	2	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	I	1001	2	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	2003	1	14,14,15	0.16	0	17,19,21	0.50	0
4	NAG	J	1001	2	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	C	2002	1	14,14,15	0.18	0	17,19,21	0.62	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	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	I	1006	2	-	0/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	I	1002	2	-	2/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	5/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2003	-	-	1/6/23/26	0/1/1/1
4	NAG	I	1003	2	-	2/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	I	1004	2	-	2/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	I	1005	2	-	0/6/23/26	0/1/1/1
4	NAG	I	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	J	1001	2	-	2/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2003	NAG	C2-N2-C7	4.54	128.98	122.90
4	B	2002	NAG	C1-O5-C5	2.31	115.28	112.19

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2001	NAG	O5-C5-C6-O6
4	B	2002	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	C	2001	NAG	C4-C5-C6-O6
4	I	1004	NAG	C4-C5-C6-O6
4	C	2005	NAG	O5-C5-C6-O6
4	C	2007	NAG	O5-C5-C6-O6
4	A	2001	NAG	O5-C5-C6-O6
4	B	2002	NAG	O5-C5-C6-O6
4	A	2001	NAG	C4-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	B	2006	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	2001	NAG	C4-C5-C6-O6
4	I	1004	NAG	O5-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	B	2006	NAG	C4-C5-C6-O6
4	C	2007	NAG	C4-C5-C6-O6
4	B	2001	NAG	C8-C7-N2-C2
4	B	2001	NAG	O7-C7-N2-C2
4	B	2003	NAG	C8-C7-N2-C2
4	B	2003	NAG	O7-C7-N2-C2
4	C	2003	NAG	C8-C7-N2-C2
4	C	2003	NAG	O7-C7-N2-C2
4	I	1003	NAG	C8-C7-N2-C2
4	I	1003	NAG	O7-C7-N2-C2
4	B	2005	NAG	O5-C5-C6-O6
4	C	2005	NAG	C4-C5-C6-O6
4	C	2002	NAG	C4-C5-C6-O6
4	C	2002	NAG	O5-C5-C6-O6
4	A	2006	NAG	O5-C5-C6-O6
4	A	2005	NAG	C4-C5-C6-O6
4	C	2006	NAG	C4-C5-C6-O6
4	A	2003	NAG	O5-C5-C6-O6
4	C	2006	NAG	O5-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	A	2005	NAG	O5-C5-C6-O6
4	A	2006	NAG	C1-C2-N2-C7
4	J	1001	NAG	C1-C2-N2-C7
4	I	1002	NAG	C4-C5-C6-O6
4	B	2002	NAG	C3-C2-N2-C7
4	B	2002	NAG	C1-C2-N2-C7
4	C	2003	NAG	C1-C2-N2-C7
4	A	2006	NAG	C3-C2-N2-C7
4	C	2003	NAG	C3-C2-N2-C7
4	J	1001	NAG	C3-C2-N2-C7
4	I	1002	NAG	O5-C5-C6-O6
4	A	2006	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1006	NAG	1	0
4	B	2001	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2003	NAG	1	0
4	C	2002	NAG	2	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.

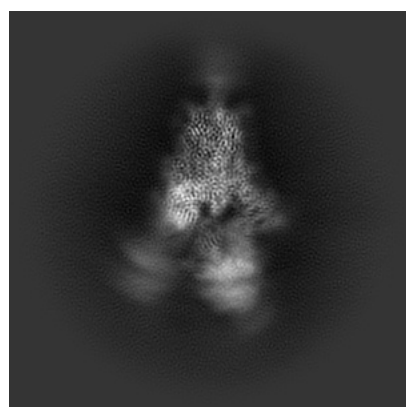
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31073. These allow visual inspection of the internal detail of the map and identification of artifacts.

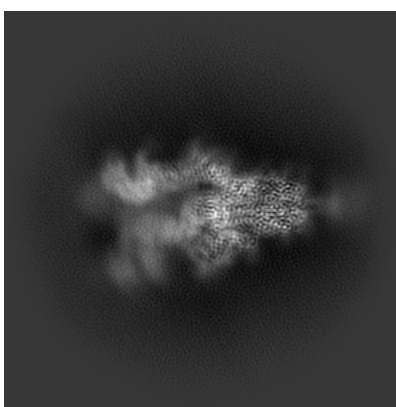
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

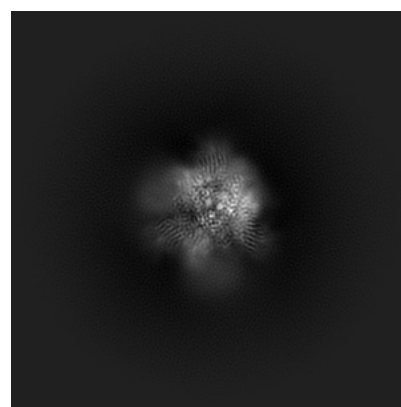
6.1.1 Primary map



X



Y

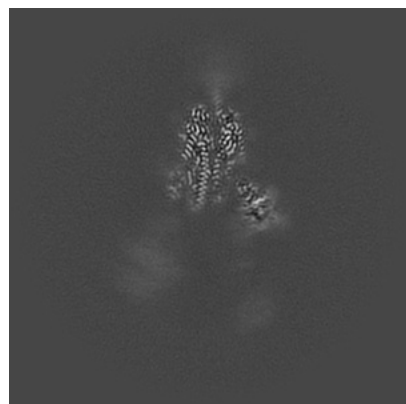


Z

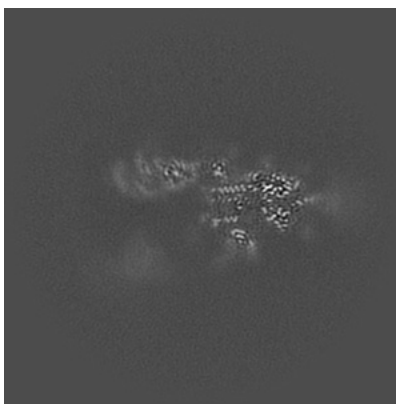
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

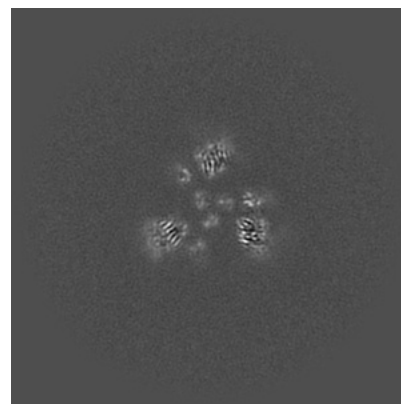
6.2.1 Primary map



X Index: 192



Y Index: 192

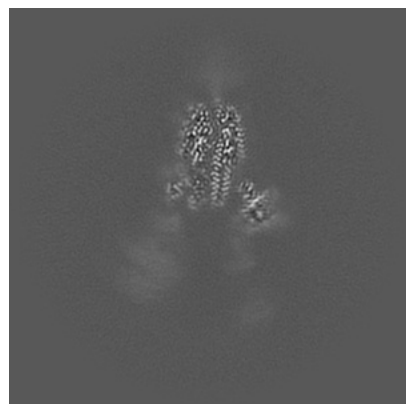


Z Index: 192

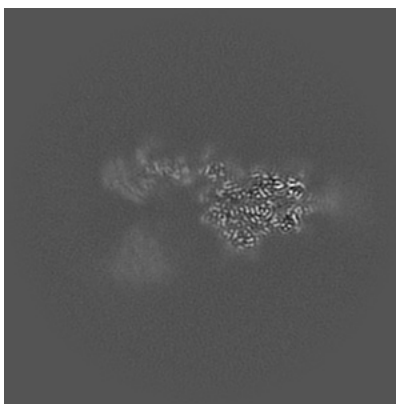
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

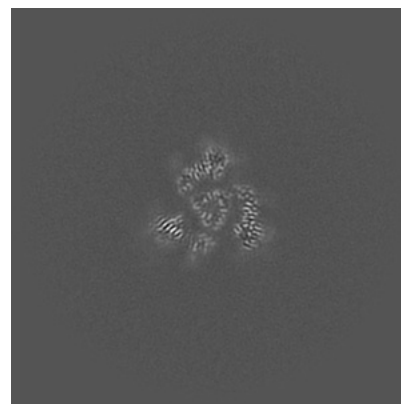
6.3.1 Primary map



X Index: 188



Y Index: 201

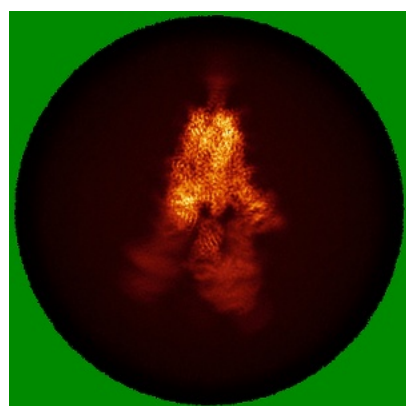


Z Index: 203

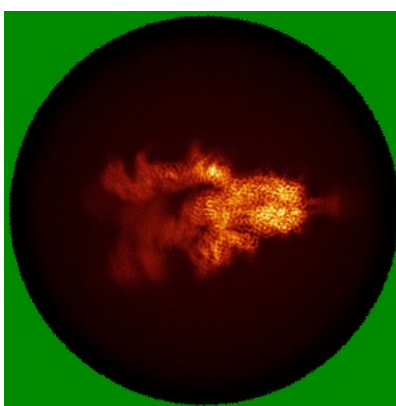
The images above show the largest variance slices of the map in three orthogonal directions.

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

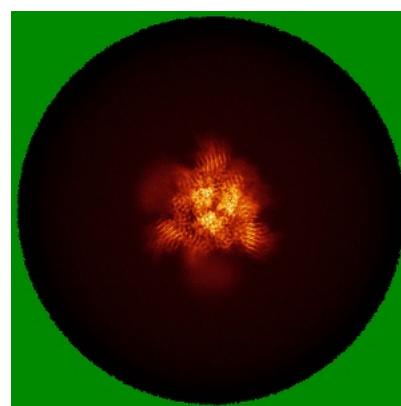
6.4.1 Primary map



X



Y

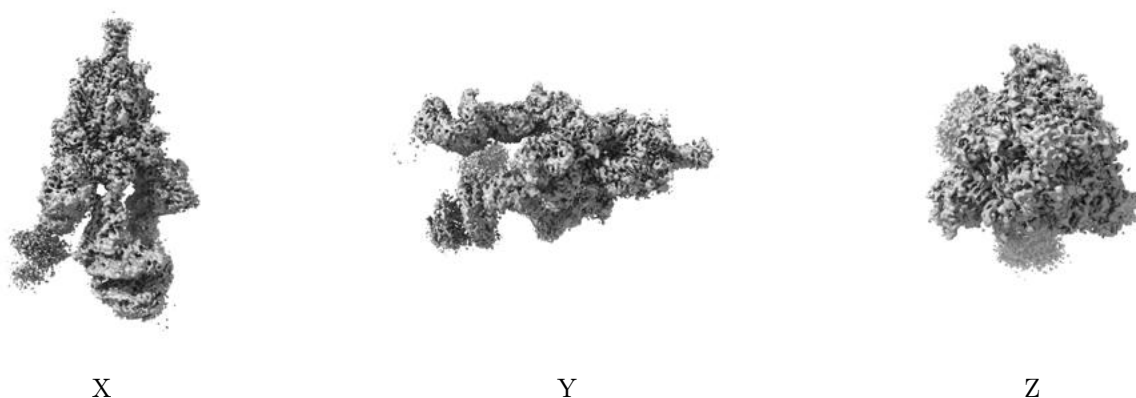


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

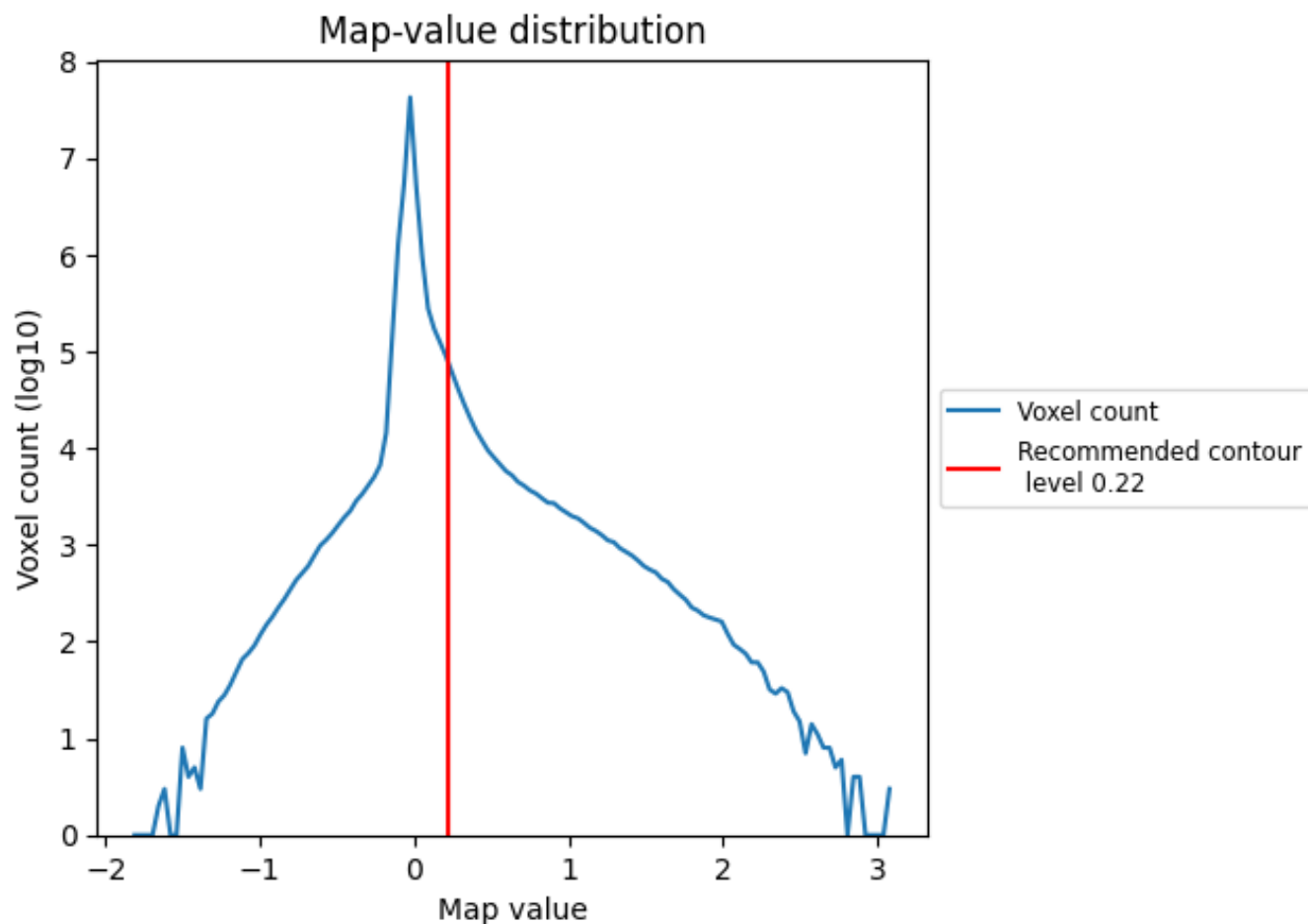
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

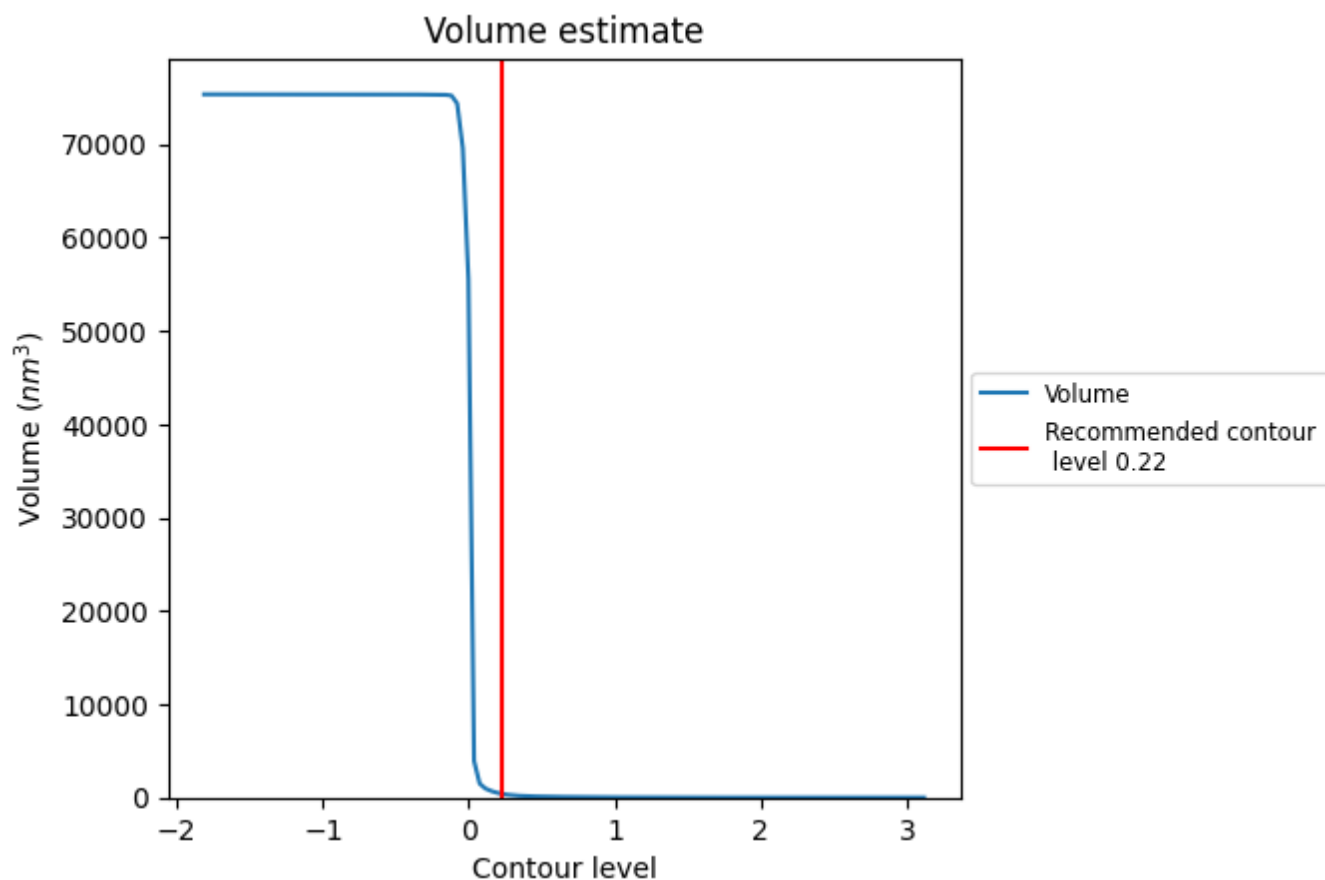
This section contains the results of statistical analysis of the map.

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.

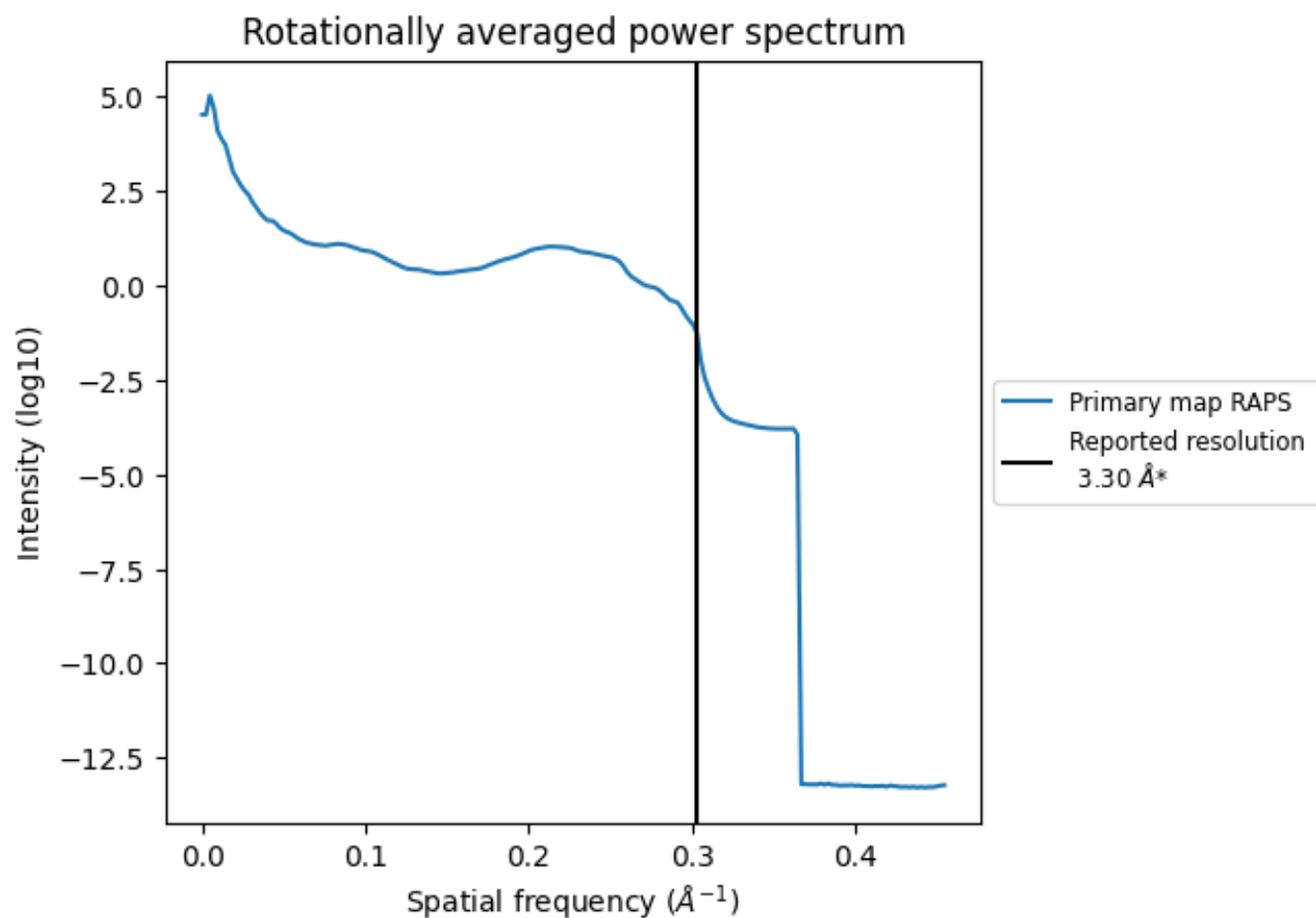
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 420 nm³; this corresponds to an approximate mass of 379 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 $\text{\AA}^{-1}$

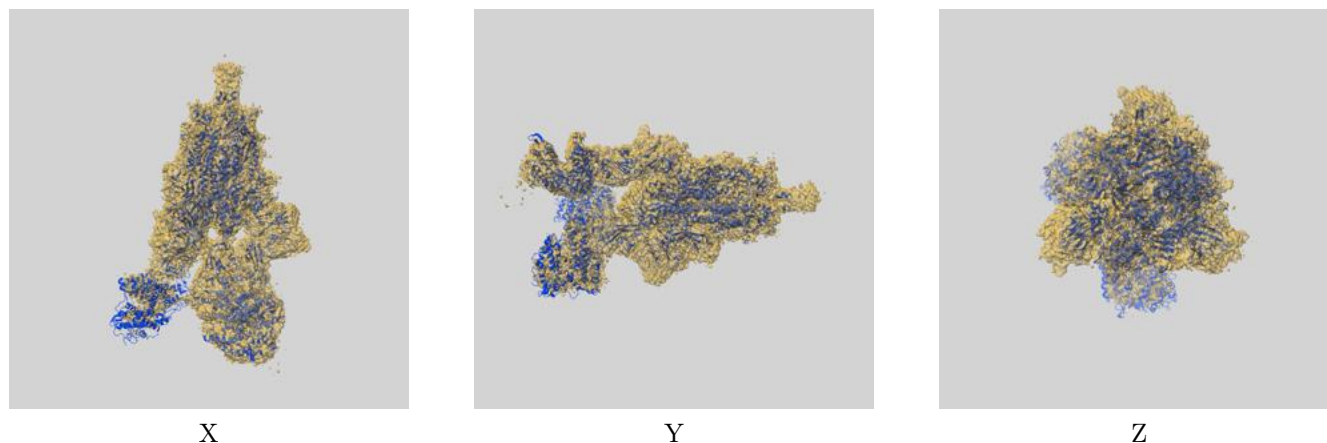
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

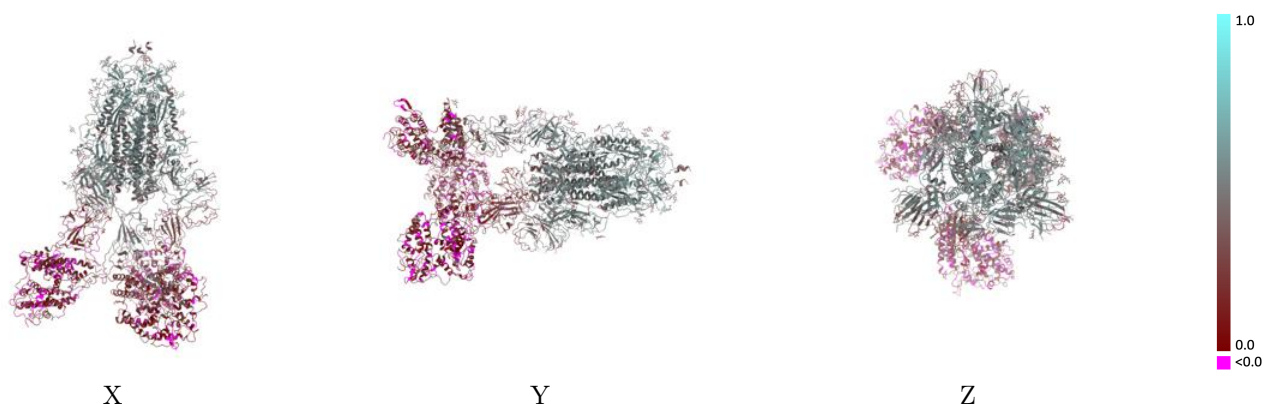
This section contains information regarding the fit between EMDB map EMD-31073 and PDB model 7EDJ. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



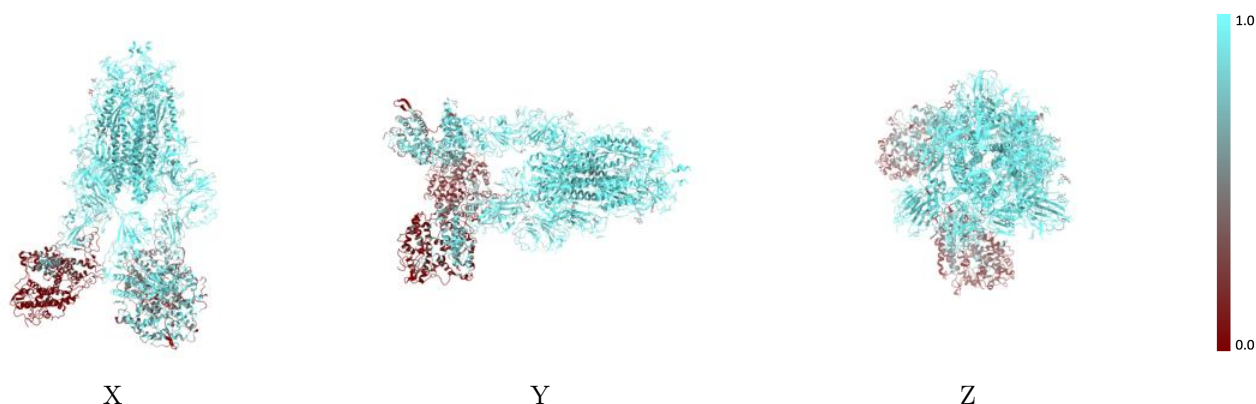
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



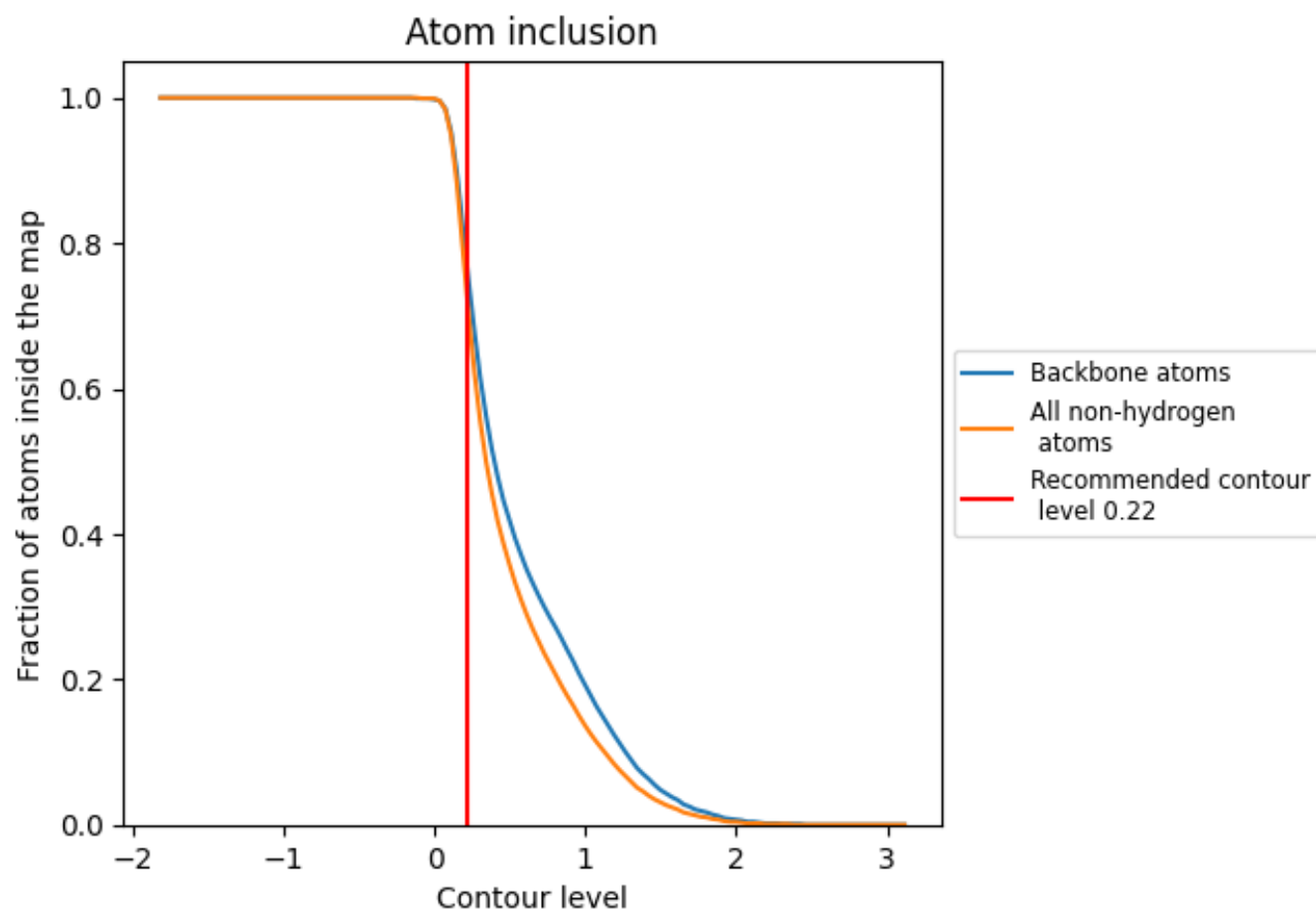
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.3340
A	 0.9480	 0.4750
B	 0.8830	 0.4290
C	 0.9090	 0.4360
D	 0.6430	 0.2970
E	 0.8570	 0.3910
F	 0.9290	 0.3900
G	 0.8570	 0.3710
H	 0.7860	 0.3550
I	 0.7320	 0.2030
J	 0.1340	 0.1140
K	 0.3190	 0.1180
L	 0.9290	 0.5060
M	 0.8570	 0.4040
N	 0.6070	 0.3450
O	 0.9640	 0.5090
P	 0.8570	 0.3030
Q	 0.7860	 0.2250
R	 0.6430	 0.3740
S	 0.8210	 0.4310
T	 0.9290	 0.4350
U	 0.6790	 0.3880
V	 0.8570	 0.4750
W	 0.9290	 0.3960
X	 0.5710	 0.3960
Y	 0.9290	 0.4360
Z	 0.8570	 0.4680
a	 0.5360	 0.2540
b	 0.7500	 0.2650
c	 0.8570	 0.3790
d	 0.6070	 0.3770
e	 0.7140	 0.4620
f	 0.9290	 0.4480
g	 0.6790	 0.3890
h	 0.8930	 0.4510
i	 0.8210	 0.3870

