



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:11 PM UTC

PDB ID : 6ZP5 / pdb_00006zp5
EMDB ID : EMD-11336
Title : SARS-CoV-2 spike in prefusion state (flexibility analysis, 1-up closed conformation)
Authors : Martinez, M.; Marabini, R.; Carazo, J.M.
Deposited on : 2020-07-08
Resolution : 3.10 Å(reported)
Based on initial model : 6ZOW

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

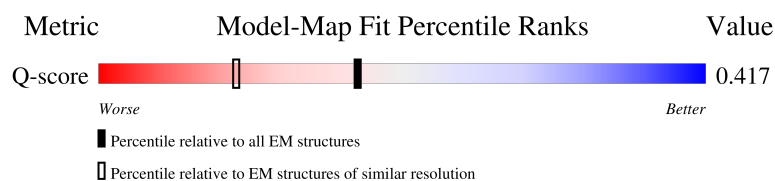
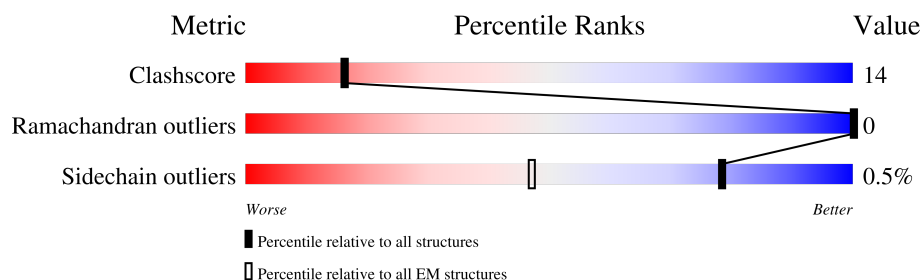
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



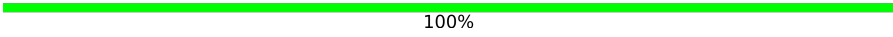
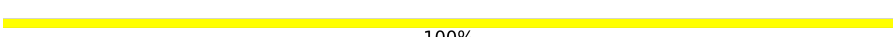
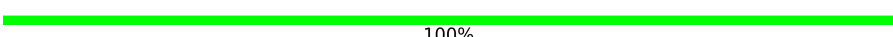
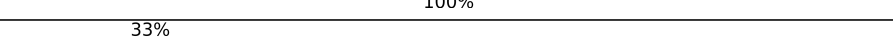
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1288	 5% 58% 18% 23%
1	B	1288	 52% 22% 27%
1	C	1288	 50% 23% 28%
2	D	2	 50% 100%

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 50%50%
2	I	2	 100%
2	J	2	 50%50%
2	K	2	 100%
2	L	2	 100%
2	M	2	 50%50%
2	P	2	 100%
2	S	2	 50%50%
2	T	2	 50%50%
2	V	2	 50%50%
2	X	2	 50%50%
2	Z	2	 50%50%
2	c	2	 50%50%
2	d	2	 50%50%
3	E	4	 75%25%
3	F	4	 75%25%
3	R	4	 50%50%
3	U	4	 50%50%
4	N	3	 67%33%
4	O	3	 33%67%33%
4	W	3	 33%67%33%
4	Y	3	 100%
4	a	3	 33%67%
4	b	3	 67%33%

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Mol	Chain	Length	Quality of chain
5	Q	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	O	1	-	-	X	-
4	NAG	W	2	X	-	-	-
6	NAG	A	1304	-	-	X	-
6	NAG	C	1302	X	-	-	-
8	DMS	A	1309	-	-	X	-
8	DMS	A	1310	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23615 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	988	Total	C	N	O	S	0	0
			7709	4918	1282	1475	34		
1	B	943	Total	C	N	O	S	0	0
			7367	4704	1223	1408	32		
1	C	930	Total	C	N	O	S	0	0
			7243	4621	1203	1387	32		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	655	GLY	ARG	engineered mutation	UNP P0DTC2
A	656	SER	ARG	engineered mutation	UNP P0DTC2
A	658	SER	ARG	engineered mutation	UNP P0DTC2
A	959	PRO	LYS	engineered mutation	UNP P0DTC2
A	960	PRO	VAL	engineered mutation	UNP P0DTC2
A	1182	GLY	-	expression tag	UNP P0DTC2
A	1183	SER	-	expression tag	UNP P0DTC2
A	1184	GLY	-	expression tag	UNP P0DTC2
A	1185	TYR	-	expression tag	UNP P0DTC2
A	1186	ILE	-	expression tag	UNP P0DTC2
A	1187	PRO	-	expression tag	UNP P0DTC2
A	1188	GLU	-	expression tag	UNP P0DTC2
A	1189	ALA	-	expression tag	UNP P0DTC2
A	1190	PRO	-	expression tag	UNP P0DTC2
A	1191	ARG	-	expression tag	UNP P0DTC2
A	1192	ASP	-	expression tag	UNP P0DTC2
A	1193	GLY	-	expression tag	UNP P0DTC2
A	1194	GLN	-	expression tag	UNP P0DTC2
A	1195	ALA	-	expression tag	UNP P0DTC2
A	1196	TYR	-	expression tag	UNP P0DTC2
A	1197	VAL	-	expression tag	UNP P0DTC2
A	1198	ARG	-	expression tag	UNP P0DTC2
A	1199	LYS	-	expression tag	UNP P0DTC2
A	1200	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1201	GLY	-	expression tag	UNP P0DTC2
A	1202	GLU	-	expression tag	UNP P0DTC2
A	1203	TRP	-	expression tag	UNP P0DTC2
A	1204	VAL	-	expression tag	UNP P0DTC2
A	1205	LEU	-	expression tag	UNP P0DTC2
A	1206	LEU	-	expression tag	UNP P0DTC2
A	1207	SER	-	expression tag	UNP P0DTC2
A	1208	THR	-	expression tag	UNP P0DTC2
A	1209	PHE	-	expression tag	UNP P0DTC2
A	1210	LEU	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	ARG	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	VAL	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	PHE	-	expression tag	UNP P0DTC2
A	1219	GLN	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	HIS	-	expression tag	UNP P0DTC2
A	1224	HIS	-	expression tag	UNP P0DTC2
A	1225	HIS	-	expression tag	UNP P0DTC2
A	1226	HIS	-	expression tag	UNP P0DTC2
A	1227	HIS	-	expression tag	UNP P0DTC2
A	1228	HIS	-	expression tag	UNP P0DTC2
A	1229	HIS	-	expression tag	UNP P0DTC2
A	1230	HIS	-	expression tag	UNP P0DTC2
A	1231	SER	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	HIS	-	expression tag	UNP P0DTC2
A	1236	PRO	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	PHE	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	LYS	-	expression tag	UNP P0DTC2
A	1241	GLY	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	SER	-	expression tag	UNP P0DTC2
A	1245	GLY	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	SER	-	expression tag	UNP P0DTC2
A	1253	ALA	-	expression tag	UNP P0DTC2
A	1254	TRP	-	expression tag	UNP P0DTC2
A	1255	SER	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	PRO	-	expression tag	UNP P0DTC2
A	1258	GLN	-	expression tag	UNP P0DTC2
A	1259	PHE	-	expression tag	UNP P0DTC2
A	1260	GLU	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
B	509F	GLY	ARG	engineered mutation	UNP P0DTC2
B	509G	SER	ARG	engineered mutation	UNP P0DTC2
B	509I	SER	ARG	engineered mutation	UNP P0DTC2
B	783	PRO	LYS	engineered mutation	UNP P0DTC2
B	784	PRO	VAL	engineered mutation	UNP P0DTC2
B	1006	GLY	-	expression tag	UNP P0DTC2
B	1007	SER	-	expression tag	UNP P0DTC2
B	1008	GLY	-	expression tag	UNP P0DTC2
B	1009	TYR	-	expression tag	UNP P0DTC2
B	1010	ILE	-	expression tag	UNP P0DTC2
B	1011	PRO	-	expression tag	UNP P0DTC2
B	1012	GLU	-	expression tag	UNP P0DTC2
B	1013	ALA	-	expression tag	UNP P0DTC2
B	1014	PRO	-	expression tag	UNP P0DTC2
B	1015	ARG	-	expression tag	UNP P0DTC2
B	1016	ASP	-	expression tag	UNP P0DTC2
B	1017	GLY	-	expression tag	UNP P0DTC2
B	1018	GLN	-	expression tag	UNP P0DTC2
B	1019	ALA	-	expression tag	UNP P0DTC2
B	1020	TYR	-	expression tag	UNP P0DTC2
B	1021	VAL	-	expression tag	UNP P0DTC2
B	1022	ARG	-	expression tag	UNP P0DTC2
B	1023	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1024	ASP	-	expression tag	UNP P0DTC2
B	1025	GLY	-	expression tag	UNP P0DTC2
B	1026	GLU	-	expression tag	UNP P0DTC2
B	1027	TRP	-	expression tag	UNP P0DTC2
B	1028	VAL	-	expression tag	UNP P0DTC2
B	1029	LEU	-	expression tag	UNP P0DTC2
B	1030	LEU	-	expression tag	UNP P0DTC2
B	1031	SER	-	expression tag	UNP P0DTC2
B	1032	THR	-	expression tag	UNP P0DTC2
B	1033	PHE	-	expression tag	UNP P0DTC2
B	1034	LEU	-	expression tag	UNP P0DTC2
B	1035	GLY	-	expression tag	UNP P0DTC2
B	1036	ARG	-	expression tag	UNP P0DTC2
B	1037	SER	-	expression tag	UNP P0DTC2
B	1038	LEU	-	expression tag	UNP P0DTC2
B	1039	GLU	-	expression tag	UNP P0DTC2
B	1040	VAL	-	expression tag	UNP P0DTC2
B	1041	LEU	-	expression tag	UNP P0DTC2
B	1042	PHE	-	expression tag	UNP P0DTC2
B	1043	GLN	-	expression tag	UNP P0DTC2
B	1044	GLY	-	expression tag	UNP P0DTC2
B	1045	PRO	-	expression tag	UNP P0DTC2
B	1046	GLY	-	expression tag	UNP P0DTC2
B	1047	HIS	-	expression tag	UNP P0DTC2
B	1048	HIS	-	expression tag	UNP P0DTC2
B	1049	HIS	-	expression tag	UNP P0DTC2
B	1050	HIS	-	expression tag	UNP P0DTC2
B	1051	HIS	-	expression tag	UNP P0DTC2
B	1052	HIS	-	expression tag	UNP P0DTC2
B	1053	HIS	-	expression tag	UNP P0DTC2
B	1054	HIS	-	expression tag	UNP P0DTC2
B	1055	SER	-	expression tag	UNP P0DTC2
B	1056	ALA	-	expression tag	UNP P0DTC2
B	1057	TRP	-	expression tag	UNP P0DTC2
B	1058	SER	-	expression tag	UNP P0DTC2
B	1059	HIS	-	expression tag	UNP P0DTC2
B	1060	PRO	-	expression tag	UNP P0DTC2
B	1061	GLN	-	expression tag	UNP P0DTC2
B	1062	PHE	-	expression tag	UNP P0DTC2
B	1063	GLU	-	expression tag	UNP P0DTC2
B	1064	LYS	-	expression tag	UNP P0DTC2
B	1065	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1066	GLY	-	expression tag	UNP P0DTC2
B	1067	GLY	-	expression tag	UNP P0DTC2
B	1068	SER	-	expression tag	UNP P0DTC2
B	1069	GLY	-	expression tag	UNP P0DTC2
B	1070	GLY	-	expression tag	UNP P0DTC2
B	1071	GLY	-	expression tag	UNP P0DTC2
B	1072	GLY	-	expression tag	UNP P0DTC2
B	1073	SER	-	expression tag	UNP P0DTC2
B	1074	GLY	-	expression tag	UNP P0DTC2
B	1075	GLY	-	expression tag	UNP P0DTC2
B	1076	SER	-	expression tag	UNP P0DTC2
B	1077	ALA	-	expression tag	UNP P0DTC2
B	1078	TRP	-	expression tag	UNP P0DTC2
B	1079	SER	-	expression tag	UNP P0DTC2
B	1080	HIS	-	expression tag	UNP P0DTC2
B	1081	PRO	-	expression tag	UNP P0DTC2
B	1082	GLN	-	expression tag	UNP P0DTC2
B	1083	PHE	-	expression tag	UNP P0DTC2
B	1084	GLU	-	expression tag	UNP P0DTC2
B	1085	LYS	-	expression tag	UNP P0DTC2
C	656	GLY	ARG	engineered mutation	UNP P0DTC2
C	657	SER	ARG	engineered mutation	UNP P0DTC2
C	659	SER	ARG	engineered mutation	UNP P0DTC2
C	960	PRO	LYS	engineered mutation	UNP P0DTC2
C	961	PRO	VAL	engineered mutation	UNP P0DTC2
C	1183	GLY	-	expression tag	UNP P0DTC2
C	1184	SER	-	expression tag	UNP P0DTC2
C	1185	GLY	-	expression tag	UNP P0DTC2
C	1186	TYR	-	expression tag	UNP P0DTC2
C	1187	ILE	-	expression tag	UNP P0DTC2
C	1188	PRO	-	expression tag	UNP P0DTC2
C	1189	GLU	-	expression tag	UNP P0DTC2
C	1190	ALA	-	expression tag	UNP P0DTC2
C	1191	PRO	-	expression tag	UNP P0DTC2
C	1192	ARG	-	expression tag	UNP P0DTC2
C	1193	ASP	-	expression tag	UNP P0DTC2
C	1194	GLY	-	expression tag	UNP P0DTC2
C	1195	GLN	-	expression tag	UNP P0DTC2
C	1196	ALA	-	expression tag	UNP P0DTC2
C	1197	TYR	-	expression tag	UNP P0DTC2
C	1198	VAL	-	expression tag	UNP P0DTC2
C	1199	ARG	-	expression tag	UNP P0DTC2

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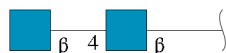
Chain	Residue	Modelled	Actual	Comment	Reference
C	1200	LYS	-	expression tag	UNP P0DTC2
C	1201	ASP	-	expression tag	UNP P0DTC2
C	1202	GLY	-	expression tag	UNP P0DTC2
C	1203	GLU	-	expression tag	UNP P0DTC2
C	1204	TRP	-	expression tag	UNP P0DTC2
C	1205	VAL	-	expression tag	UNP P0DTC2
C	1206	LEU	-	expression tag	UNP P0DTC2
C	1207	LEU	-	expression tag	UNP P0DTC2
C	1208	SER	-	expression tag	UNP P0DTC2
C	1209	THR	-	expression tag	UNP P0DTC2
C	1210	PHE	-	expression tag	UNP P0DTC2
C	1211	LEU	-	expression tag	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	ARG	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	LEU	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	VAL	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	PHE	-	expression tag	UNP P0DTC2
C	1220	GLN	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	PRO	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	HIS	-	expression tag	UNP P0DTC2
C	1225	HIS	-	expression tag	UNP P0DTC2
C	1226	HIS	-	expression tag	UNP P0DTC2
C	1227	HIS	-	expression tag	UNP P0DTC2
C	1228	HIS	-	expression tag	UNP P0DTC2
C	1229	HIS	-	expression tag	UNP P0DTC2
C	1230	HIS	-	expression tag	UNP P0DTC2
C	1231	HIS	-	expression tag	UNP P0DTC2
C	1232	SER	-	expression tag	UNP P0DTC2
C	1233	ALA	-	expression tag	UNP P0DTC2
C	1234	TRP	-	expression tag	UNP P0DTC2
C	1235	SER	-	expression tag	UNP P0DTC2
C	1236	HIS	-	expression tag	UNP P0DTC2
C	1237	PRO	-	expression tag	UNP P0DTC2
C	1238	GLN	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	SER	-	expression tag	UNP P0DTC2
C	1254	ALA	-	expression tag	UNP P0DTC2
C	1255	TRP	-	expression tag	UNP P0DTC2
C	1256	SER	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	PRO	-	expression tag	UNP P0DTC2
C	1259	GLN	-	expression tag	UNP P0DTC2
C	1260	PHE	-	expression tag	UNP P0DTC2
C	1261	GLU	-	expression tag	UNP P0DTC2
C	1262	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.



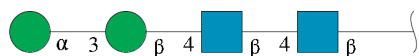
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			30	16	2	12		
2	G	2	Total	C	N	O	0	0
			30	16	2	12		
2	H	2	Total	C	N	O	0	0
			30	16	2	12		
2	I	2	Total	C	N	O	0	0
			30	16	2	12		
2	J	2	Total	C	N	O	0	0
			30	16	2	12		
2	K	2	Total	C	N	O	0	0
			30	16	2	12		

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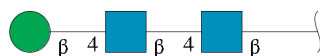
Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	2	Total	C	N	O	0	0
			30	16	2	12		
2	M	2	Total	C	N	O	0	0
			30	16	2	12		
2	P	2	Total	C	N	O	0	0
			30	16	2	12		
2	S	2	Total	C	N	O	0	0
			30	16	2	12		
2	T	2	Total	C	N	O	0	0
			30	16	2	12		
2	V	2	Total	C	N	O	0	0
			30	16	2	12		
2	X	2	Total	C	N	O	0	0
			30	16	2	12		
2	Z	2	Total	C	N	O	0	0
			30	16	2	12		
2	c	2	Total	C	N	O	0	0
			30	16	2	12		
2	d	2	Total	C	N	O	0	0
			30	16	2	12		

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



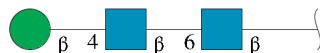
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	4	Total	C	N	O	0	0
			54	28	2	24		
3	F	4	Total	C	N	O	0	0
			54	28	2	24		
3	R	4	Total	C	N	O	0	0
			54	28	2	24		
3	U	4	Total	C	N	O	0	0
			54	28	2	24		

- Molecule 4 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
4	N	3	Total	C	N	O	0	0
			42	22	2	18		
4	O	3	Total	C	N	O	0	0
			42	22	2	18		
4	W	3	Total	C	N	O	0	0
			42	22	2	18		
4	Y	3	Total	C	N	O	0	0
			42	22	2	18		
4	a	3	Total	C	N	O	0	0
			42	22	2	18		
4	b	3	Total	C	N	O	0	0
			42	22	2	18		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	Q	3	Total	C	N	O	0	0
			42	22	2	18		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



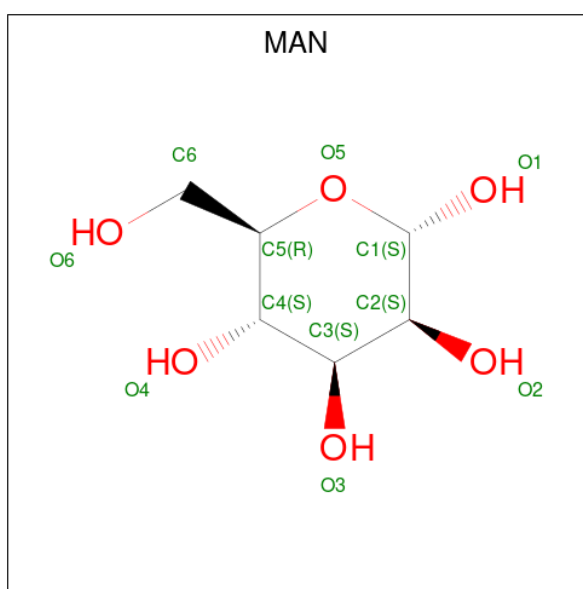
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			15	8	1	6	
6	A	1	Total	C	N	O	0
			15	8	1	6	
6	A	1	Total	C	N	O	0
			15	8	1	6	
6	A	1	Total	C	N	O	0
			15	8	1	6	
6	A	1	Total	C	N	O	0
			15	8	1	6	
6	A	1	Total	C	N	O	0
			15	8	1	6	
6	B	1	Total	C	N	O	0
			15	8	1	6	
6	B	1	Total	C	N	O	0
			15	8	1	6	
6	B	1	Total	C	N	O	0
			15	8	1	6	
6	B	1	Total	C	N	O	0
			15	8	1	6	
6	B	1	Total	C	N	O	0
			15	8	1	6	
6	B	1	Total	C	N	O	0
			15	8	1	6	

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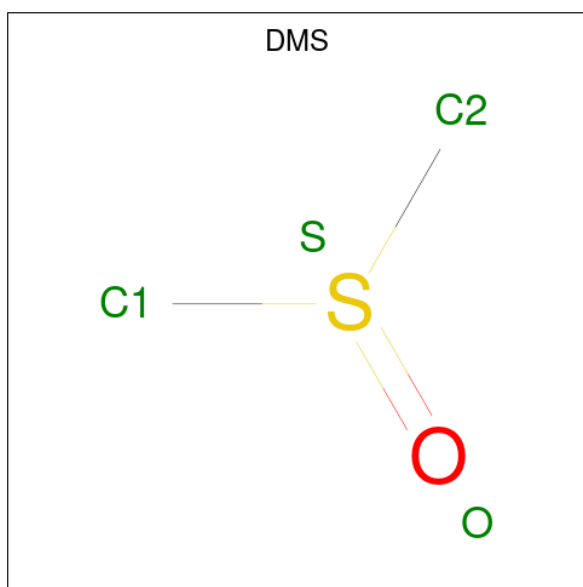
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			15	8	1	6	
6	C	1	Total	C	N	O	0
			15	8	1	6	
6	C	1	Total	C	N	O	0
			15	8	1	6	
6	C	1	Total	C	N	O	0
			15	8	1	6	

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).

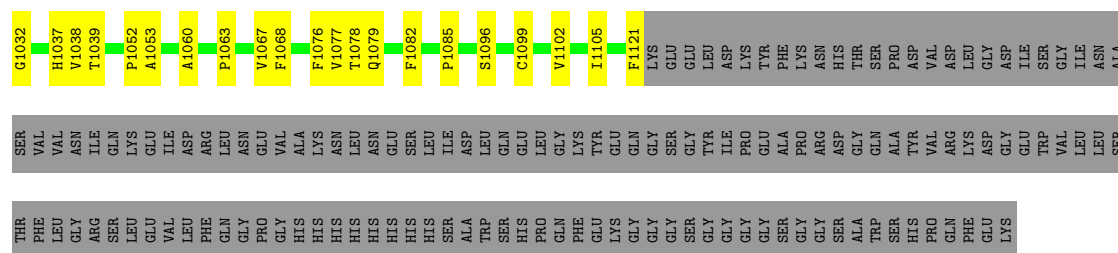


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			12	6	6	
7	C	1	Total	C	O	0
			12	6	6	

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).

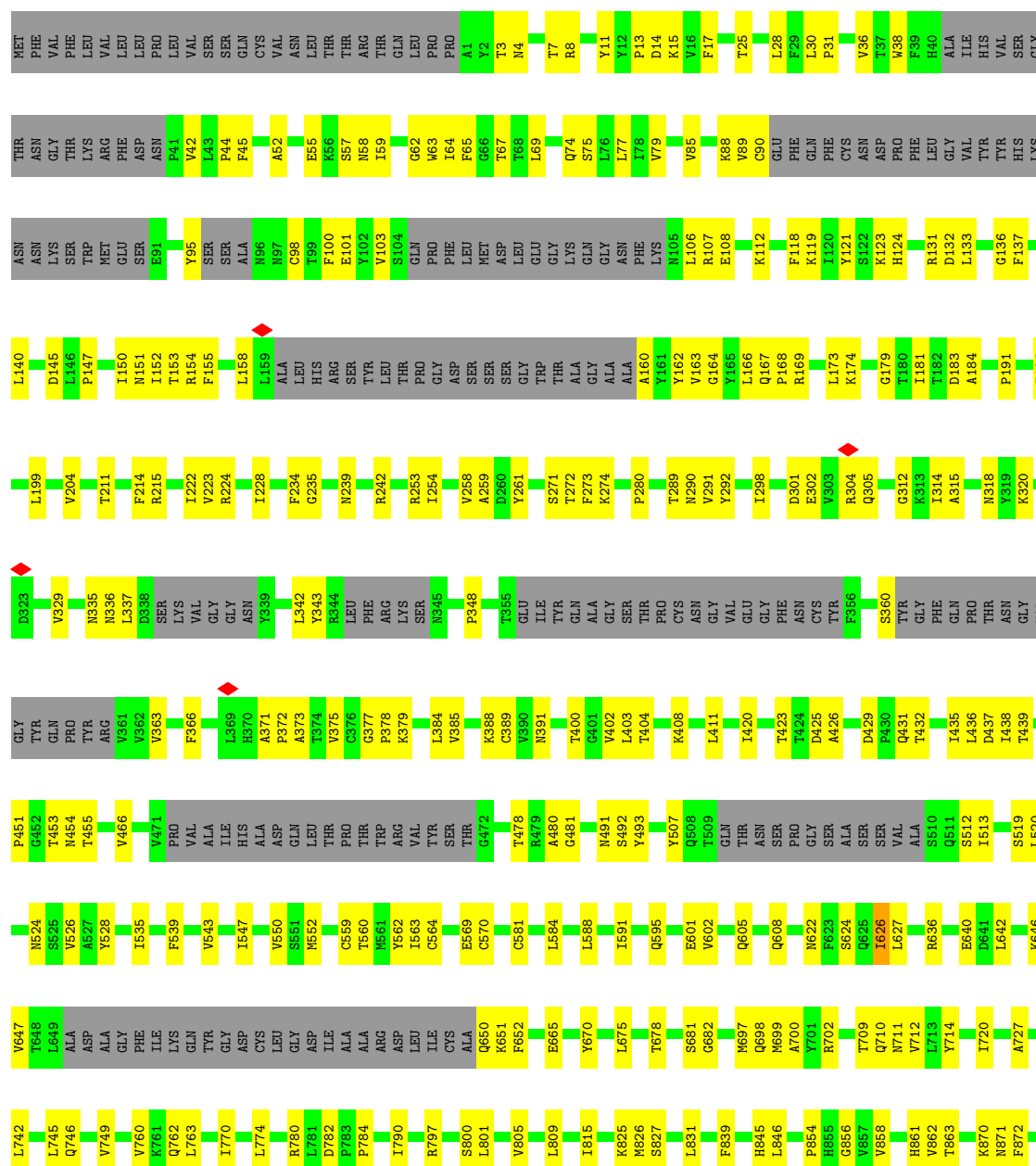


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	S	0
			4	2	1	1	
8	A	1	Total	C	O	S	0
			4	2	1	1	
8	A	1	Total	C	O	S	0
			4	2	1	1	

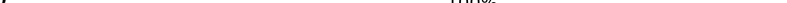


Molecule 1: Spike glycoprotein

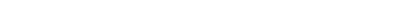
Chain B: 52% 22% 27%



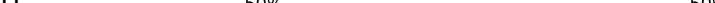
SER
HIS
PRO
GLN
PHE
GLU
LYS

- Chain D:  50% 100%

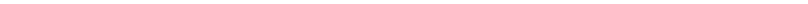


- Chain G:  50% 50%

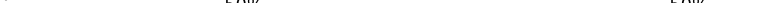


- Chain H:  50% 50%



- Chain I:  100%



- Chain J: 

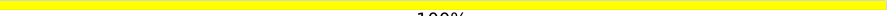


- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Chain K:  100%

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 M:  50% 50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain S:  50% 50%

MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain V:  50% 50%

MAG1
MAG2

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

Chain X:  50% 50%



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

Chain Z:  50% 50%



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

Chain c:  50% 50%



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

Chain d:  50% 50%



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

Chain E:  75% 25%



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

Chain F:  75% 25%



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

Chain R:  50% 50%



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

Chain U:  50% 50%



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

Chain N:  67% 33%



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

Chain O:  33% 67% 33%



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

Chain W:  33% 67% 33%



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

Chain Y:  100%



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

Chain a:  33% 33% 67%



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

Chain b: 67% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 33% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	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 ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.655	Depositor
Minimum map value	-0.621	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	452.30396, 452.30396, 452.30396	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0469999, 1.0469999, 1.0469999	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, MAN, BMA, DMS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	1/7877 (0.0%)	0.42	1/10717 (0.0%)
1	B	0.26	0/7522	0.41	0/10229
1	C	0.27	0/7395	0.46	0/10059
All	All	0.34	1/22794 (0.0%)	0.43	1/31005 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	LEU	C-N	31.90	1.99	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	LEU	O-C-N	-22.41	90.99	122.81

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	7709	0	7525	210	0
1	B	7367	0	7208	228	0
1	C	7243	0	7100	249	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	30	0	27	0	0
2	G	30	0	27	2	0
2	H	30	0	27	2	0
2	I	30	0	27	0	0
2	J	30	0	27	1	0
2	K	30	0	27	0	0
2	L	30	0	27	1	0
2	M	30	0	27	2	0
2	P	30	0	26	0	0
2	S	30	0	27	2	0
2	T	30	0	25	4	0
2	V	30	0	27	6	0
2	X	30	0	27	4	0
2	Z	30	0	26	1	0
2	c	30	0	27	1	0
2	d	30	0	27	1	0
3	E	54	0	47	0	0
3	F	54	0	47	0	0
3	R	54	0	47	0	0
3	U	54	0	47	5	0
4	N	42	0	37	2	0
4	O	42	0	38	8	0
4	W	42	0	37	5	0
4	Y	42	0	37	0	0
4	a	42	0	37	3	0
4	b	42	0	36	4	0
5	Q	42	0	37	4	0
6	A	90	0	86	10	0
6	B	120	0	111	5	0
6	C	60	0	55	8	0
7	A	12	0	12	0	0
7	C	12	0	12	5	0
8	A	12	0	18	17	0
All	All	23615	0	23002	663	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 14.

All (663) 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:871:ASN:HD21	4:O:1:NAG:C1	1.03	1.60
1:A:95:ASN:HD21	6:A:1304:NAG:C1	0.97	1.52
1:B:871:ASN:CG	4:O:1:NAG:O1	1.70	1.34
1:A:308:LEU:C	1:A:309:CYS:N	1.99	1.19
1:A:377:GLY:O	8:A:1309:DMS:H13	1.44	1.16
1:A:355:VAL:CG2	8:A:1310:DMS:H22	1.73	1.16
1:A:95:ASN:CG	6:A:1304:NAG:O1	1.87	1.15
1:B:871:ASN:CG	4:O:1:NAG:HO1	1.47	1.15
1:A:355:VAL:HG22	8:A:1310:DMS:H22	1.20	1.14
1:A:95:ASN:HD21	6:A:1304:NAG:H1	1.16	1.08
1:A:95:ASN:ND2	6:A:1304:NAG:C1	1.73	1.02
1:C:1077:PHE:HZ	2:V:1:NAG:H62	1.25	1.00
4:W:1:NAG:O3	4:W:2:NAG:O1	1.80	1.00
1:A:95:ASN:CG	6:A:1304:NAG:HO1	1.71	0.94
1:A:330:ARG:CZ	6:C:1305:NAG:O6	2.16	0.93
1:B:455:THR:HA	6:B:1107:NAG:H82	1.47	0.93
1:B:871:ASN:ND2	4:O:1:NAG:C1	1.81	0.91
1:C:778:GLN:NE2	2:X:1:NAG:H62	1.87	0.90
1:C:306:ILE:HD11	6:C:1303:NAG:H81	1.54	0.89
1:C:31:PRO:HA	1:C:247:ARG:HH12	1.33	0.89
1:C:1077:PHE:CZ	2:V:1:NAG:H62	2.07	0.89
1:B:204:VAL:HG22	1:B:453:THR:HG23	1.53	0.88
1:B:107:ARG:HH11	1:B:124:HIS:HB3	1.39	0.87
1:A:330:ARG:HH12	1:C:141:THR:HG23	1.37	0.87
1:A:355:VAL:CG2	8:A:1310:DMS:C2	2.53	0.87
4:W:1:NAG:C3	4:W:2:NAG:O1	2.21	0.85
1:A:377:GLY:C	8:A:1309:DMS:H22	2.05	0.81
1:A:713:MET:SD	1:B:215:ARG:NH1	2.52	0.81
1:A:846:TYR:CZ	1:B:520:LEU:HD12	2.16	0.81
1:A:1121:PHE:HZ	1:B:942:LEU:HG	1.46	0.80
1:A:355:VAL:HG23	8:A:1310:DMS:C2	2.11	0.80
1:C:706:THR:OG1	1:C:929:ASN:ND2	2.15	0.79
1:B:11:TYR:HA	1:B:140:LEU:H	1.45	0.79
1:C:369:VAL:HG12	1:C:489:PHE:HB3	1.64	0.79
1:A:428:LEU:HD11	1:A:466:GLN:HG3	1.66	0.78
1:A:873:MET:HE1	1:B:891:VAL:HG23	1.66	0.78
1:B:62:GLY:HA3	1:B:158:LEU:HD22	1.66	0.77
1:C:800:VAL:HG21	1:C:1031:PRO:HG3	1.65	0.77
1:A:1102:VAL:HG13	1:C:891:TYR:HB3	1.66	0.76
1:C:696:VAL:HG12	1:C:1039:VAL:HG22	1.68	0.76
1:C:101:VAL:HG12	1:C:145:VAL:HG22	1.69	0.75
1:A:536:GLN:O	1:A:550:ARG:NH2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:THR:OG1	1:B:151:ASN:O	2.03	0.75
1:C:313:GLY:HA2	4:b:1:NAG:O7	1.86	0.75
1:A:672:LEU:HD12	1:C:847:TYR:CZ	2.21	0.74
1:A:856:THR:HG23	1:B:528:TYR:HB2	1.67	0.74
1:C:376:ILE:HG22	1:C:484:VAL:HG11	1.69	0.74
1:C:533:PHE:HB2	1:C:558:ILE:HD13	1.69	0.74
1:B:44:PRO:HA	1:B:153:THR:O	1.88	0.73
1:A:531:LYS:HE3	4:a:1:NAG:H83	1.71	0.73
1:C:383:GLN:HB3	1:C:393:ALA:HB2	1.69	0.73
1:B:329:VAL:HG22	1:B:363:VAL:HG22	1.70	0.73
1:C:351:PHE:HE2	1:C:358:PRO:HB3	1.54	0.72
1:C:1072:ASN:ND2	2:V:1:NAG:C2	1.81	0.72
1:C:680:ALA:CB	4:W:1:NAG:H5	2.20	0.72
1:B:77:LEU:HD22	1:B:95:TYR:CE2	2.25	0.72
1:C:778:GLN:HE22	2:X:1:NAG:H62	1.53	0.72
1:A:709:VAL:HG11	1:A:977:LEU:HD11	1.71	0.71
1:C:726:LEU:HD21	1:C:964:GLU:HG2	1.73	0.71
1:B:88:LYS:HD3	1:B:89:VAL:H	1.56	0.71
1:C:306:ILE:CD1	6:C:1303:NAG:H81	2.21	0.71
1:A:355:VAL:HG23	8:A:1310:DMS:H22	1.63	0.70
1:B:871:ASN:HD21	4:O:1:NAG:C2	1.99	0.70
1:B:235:GLY:O	1:B:239:ASN:HB2	1.89	0.70
1:C:712:CYS:O	1:C:715:TYR:N	2.24	0.70
1:A:81:THR:OG1	1:A:207:ASN:O	2.09	0.70
1:A:831:LEU:HD21	1:A:935:LEU:HD23	1.74	0.70
1:A:856:THR:HG21	1:B:526:VAL:HB	1.74	0.69
1:C:13:PRO:HG3	1:C:25:THR:HG21	1.74	0.69
1:A:477:GLY:HA2	8:A:1309:DMS:H23	1.72	0.69
1:B:782:ASP:HB3	1:B:784:PRO:HD2	1.75	0.69
1:C:142:PHE:CZ	1:C:144:TYR:HB2	2.28	0.69
1:C:947:ILE:HG22	1:C:954:ILE:HD13	1.74	0.69
1:A:798:LYS:HB3	1:A:918:LEU:HD12	1.74	0.68
1:A:736:LEU:HD22	1:A:981:VAL:HG11	1.75	0.68
1:A:576:ASN:HB2	6:A:1302:NAG:O5	1.93	0.68
1:B:543:VAL:HG12	1:B:862:VAL:HG22	1.75	0.67
1:B:543:VAL:HG22	1:B:727:ALA:HB1	1.75	0.67
1:B:228:ILE:HG13	1:B:258:VAL:HG23	1.74	0.67
1:C:313:GLY:HA2	4:b:1:NAG:C7	2.24	0.67
1:B:700:ALA:HB1	1:B:710:GLN:HB2	1.76	0.67
1:B:8:ARG:HD2	1:B:108:GLU:OE1	1.95	0.67
1:C:301:VAL:HG12	1:C:516:ASN:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:SER:O	1:C:33:PHE:HA	1.95	0.67
1:C:60:PHE:HB3	1:C:210:THR:HA	1.77	0.66
1:A:337:ASP:OD1	1:A:500:PRO:HG3	1.95	0.66
1:A:95:ASN:ND2	6:A:1304:NAG:O1	0.58	0.66
1:B:318:ASN:HD21	1:B:343:TYR:HB2	1.61	0.66
1:B:901:VAL:HG23	1:B:912:ILE:HG12	1.77	0.66
1:C:305:ASN:HB3	6:C:1303:NAG:N2	2.11	0.66
1:B:651:LYS:HD2	1:B:760:VAL:HG11	1.76	0.66
1:B:90:CYS:HB3	1:B:98:CYS:HA	1.76	0.66
1:C:649:GLN:HG2	1:C:667:ILE:HD13	1.77	0.65
5:Q:1:NAG:H3	5:Q:1:NAG:H83	1.78	0.65
1:C:247:ARG:HD2	1:C:266:ALA:HB3	1.76	0.65
1:B:404:THR:OG1	1:B:437:ASP:OD1	2.14	0.65
1:B:11:TYR:HB3	1:B:140:LEU:HB2	1.79	0.65
1:B:11:TYR:OH	1:B:112:LYS:NZ	2.19	0.65
1:A:921:LEU:HD23	1:A:1030:PRO:HG2	1.78	0.65
1:C:492:LEU:HD22	1:C:539:PHE:HZ	1.62	0.65
1:C:541:ARG:NH1	1:C:545:ASP:OD1	2.30	0.65
1:C:339:TYR:HD2	1:C:361:LEU:HB3	1.62	0.65
1:C:435:LEU:HD12	1:C:439:GLU:HG2	1.78	0.64
1:C:1079:THR:HG22	1:C:1086:PRO:HA	1.80	0.64
1:B:626:ILE:HG22	1:B:675:LEU:HD11	1.79	0.64
1:C:313:GLY:CA	4:b:1:NAG:O7	2.45	0.64
1:C:1072:ASN:ND2	2:V:1:NAG:N2	2.40	0.64
1:A:874:GLN:HE21	1:A:878:ARG:HE	1.46	0.64
1:C:1056:CYS:HB2	1:C:1106:ILE:HD12	1.79	0.64
1:B:77:LEU:HD22	1:B:95:TYR:CZ	2.32	0.64
1:C:650:THR:HG22	1:C:664:GLN:HB3	1.81	0.63
1:A:377:GLY:C	8:A:1309:DMS:H13	2.20	0.63
1:C:188:ARG:HH12	1:C:238:ALA:HB3	1.61	0.63
1:C:358:PRO:HA	1:C:361:LEU:HD13	1.79	0.63
1:A:677:SER:HB3	1:C:764:LYS:HB2	1.80	0.63
1:A:528:SER:HB3	1:A:559:ASP:HB2	1.80	0.63
1:A:1121:PHE:HZ	1:B:942:LEU:CG	2.10	0.63
1:C:494:ALA:HB1	1:C:495:PRO:HD2	1.81	0.62
1:A:531:LYS:HE3	4:a:1:NAG:C8	2.30	0.62
1:A:695:VAL:HG12	1:A:1038:VAL:HG22	1.81	0.62
1:A:330:ARG:NE	6:C:1305:NAG:O6	2.31	0.62
1:B:403:LEU:HB3	1:B:436:LEU:HD13	1.81	0.62
1:C:32:PHE:HE1	1:C:249:PHE:CE2	2.18	0.62
1:C:1078:VAL:HG23	1:C:1089:ILE:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD13	1:A:204:ILE:HD13	1.82	0.62
1:C:696:VAL:HG22	1:C:904:ALA:HB1	1.80	0.62
4:N:2:NAG:H83	4:N:2:NAG:H3	1.82	0.62
1:A:1121:PHE:CZ	1:B:942:LEU:HG	2.33	0.61
1:A:376:ARG:NH1	1:A:378:ASP:OD1	2.34	0.61
1:A:1026:PRO:O	1:A:1027:GLN:NE2	2.28	0.61
1:C:282:VAL:HG22	1:C:576:THR:HG23	1.82	0.61
1:C:680:ALA:HB2	4:W:1:NAG:H5	1.82	0.61
1:A:695:VAL:HG22	1:A:903:ALA:HB1	1.81	0.61
1:B:291:VAL:HG23	1:B:375:VAL:HG11	1.83	0.60
1:B:547:ILE:HG13	1:B:858:VAL:HG22	1.83	0.60
1:A:38:PHE:O	1:A:237:ALA:HA	2.00	0.60
1:A:831:LEU:HD23	1:A:932:LEU:HD22	1.84	0.60
1:B:273:PHE:HE2	1:B:280:PRO:HB3	1.67	0.60
1:C:327:TRP:O	1:C:440:ARG:NE	2.26	0.60
1:A:173:TYR:OH	1:B:290:ASN:ND2	2.35	0.60
1:B:52:ALA:HB1	1:B:106:LEU:HD11	1.82	0.60
1:C:93:ILE:HG12	1:C:102:ILE:HG12	1.83	0.60
1:C:703:VAL:HG22	1:C:1033:GLY:HA2	1.84	0.59
1:B:38:TRP:HE1	1:B:160:ALA:HB1	1.66	0.59
1:B:408:LYS:NZ	1:B:425:ASP:OD2	2.35	0.59
1:C:327:TRP:H	1:C:327:TRP:CD1	2.21	0.59
1:C:1027:PRO:O	1:C:1028:GLN:NE2	2.35	0.59
1:C:302:ARG:NH1	1:C:554:GLN:OE1	2.36	0.59
1:A:1096:SER:HB2	1:C:888:ASN:HD22	1.67	0.59
1:B:15:LYS:O	1:C:537:GLN:HA	2.01	0.59
1:B:62:GLY:C	1:B:158:LEU:HD13	2.28	0.59
1:C:507:LEU:HD11	1:C:559:LEU:HD11	1.85	0.59
1:C:514:ASN:HB3	1:C:523:THR:HG22	1.85	0.59
1:A:709:VAL:HG22	1:A:831:LEU:HG	1.84	0.59
1:A:86:LYS:HG3	1:A:87:THR:HG23	1.85	0.58
1:A:685:ILE:HG13	1:C:870:ILE:HG13	1.85	0.58
1:B:147:PRO:HB2	1:C:370:TYR:OH	2.02	0.58
1:C:293:ARG:HD3	1:C:566:PHE:HB2	1.83	0.58
5:Q:1:NAG:O4	5:Q:2:NAG:N2	2.36	0.58
1:A:246:ARG:HH22	1:A:263:ASP:HB2	1.68	0.58
1:C:80:PHE:HB2	1:C:91:LEU:HB3	1.85	0.58
1:A:377:GLY:CA	8:A:1309:DMS:H22	2.34	0.58
1:C:577:ASN:OD1	1:C:578:THR:N	2.37	0.58
1:C:1076:TRP:HB2	1:C:1109:ASN:ND2	2.18	0.58
4:b:1:NAG:H3	4:b:1:NAG:H83	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:SER:CB	1:C:888:ASN:HD22	2.16	0.58
1:C:80:PHE:HB2	1:C:91:LEU:HD22	1.86	0.58
2:S:1:NAG:H3	2:S:1:NAG:H83	1.86	0.58
1:A:254:GLU:OE1	2:J:1:NAG:O6	2.21	0.58
1:A:477:GLY:HA2	8:A:1309:DMS:C2	2.33	0.58
1:A:851:LEU:HA	1:A:854:THR:HG22	1.86	0.57
1:B:7:THR:OG1	1:B:136:GLY:O	2.22	0.57
1:B:101:GLU:OE2	1:B:103:VAL:HG23	2.04	0.57
1:C:689:PRO:HA	1:C:1046:GLU:HA	1.86	0.57
1:A:308:LEU:O	1:A:309:CYS:N	2.36	0.57
1:A:846:TYR:CE1	1:B:520:LEU:HD12	2.38	0.57
1:A:868:GLN:HB3	1:B:526:VAL:HG12	1.87	0.57
1:B:224:ARG:HH21	1:B:431:GLN:HE21	1.53	0.57
1:A:377:GLY:HA3	8:A:1309:DMS:H22	1.87	0.57
2:M:2:NAG:H3	2:M:2:NAG:H83	1.85	0.57
7:C:1304:MAN:O1	3:U:3:BMA:H4	2.05	0.57
1:A:7:ARG:HG3	1:A:189:LEU:HD12	1.85	0.57
1:C:5:SER:O	1:C:33:PHE:CA	2.52	0.57
1:C:80:PHE:CD2	1:C:209:ILE:HG21	2.39	0.57
1:A:272:THR:HA	1:A:275:THR:HG22	1.86	0.57
1:A:672:LEU:HD21	1:C:843:MET:HG2	1.87	0.57
1:B:774:LEU:HD11	1:B:790:ILE:HG12	1.87	0.57
1:C:324:VAL:HG21	1:C:376:ILE:HD13	1.87	0.57
1:A:330:ARG:NH1	1:C:141:THR:HG23	2.14	0.57
1:A:2:THR:HG21	1:A:188:ASP:HB2	1.86	0.56
1:B:845:HIS:HA	1:B:863:THR:HG22	1.87	0.56
1:A:531:LYS:HG2	4:a:1:NAG:H82	1.86	0.56
1:B:137:PHE:HE2	1:B:181:ILE:HG22	1.69	0.56
1:B:191:PRO:O	1:B:195:THR:HG23	2.05	0.56
1:B:234:PHE:CE2	1:B:259:ALA:HB1	2.40	0.56
1:B:543:VAL:HA	1:B:861:HIS:O	2.05	0.56
1:A:889:LEU:HD12	1:A:896:ILE:HD12	1.86	0.56
1:B:647:VAL:CG2	1:B:854:PRO:HG2	2.35	0.56
1:C:38:TRP:HE1	1:C:238:ALA:HB1	1.70	0.56
1:A:37:TRP:HE1	1:A:237:ALA:HB1	1.69	0.56
1:C:80:PHE:HD2	1:C:209:ILE:HG21	1.70	0.56
1:C:939:GLN:O	1:C:942:SER:OG	2.19	0.56
1:C:247:ARG:NH1	1:C:264:ASP:OD2	2.39	0.56
1:A:1052:PRO:HB3	1:C:891:TYR:CZ	2.41	0.56
1:A:337:ASP:HA	1:A:500:PRO:HD3	1.86	0.56
6:A:1305:NAG:H83	6:A:1305:NAG:H3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ILE:HB	1:B:302:GLU:HB2	1.88	0.56
1:A:168:LYS:HD2	1:A:175:LYS:HD2	1.89	0.55
1:B:454:ASN:OD1	6:B:1107:NAG:H2	2.06	0.55
1:B:714:TYR:HB3	1:C:1103:VAL:HG23	1.88	0.55
1:C:210:THR:O	1:C:211:ARG:NE	2.39	0.55
1:C:633:SER:HB2	1:C:672:SER:HB3	1.87	0.55
1:C:1030:ALA:HB1	1:C:1031:PRO:HD2	1.89	0.55
1:C:650:THR:HA	1:C:664:GLN:HA	1.88	0.55
2:G:2:NAG:H3	2:G:2:NAG:H3	1.88	0.55
1:B:31:PRO:HG3	1:B:167:GLN:HB2	1.88	0.55
1:B:45:PHE:CZ	1:B:152:ILE:HD11	2.42	0.55
1:C:77:GLY:HA3	1:C:94:VAL:HA	1.86	0.55
1:A:784:LYS:HD2	1:A:785:PRO:HD2	1.87	0.55
1:B:222:ILE:HD11	1:B:385:VAL:HG12	1.89	0.55
1:C:531:LYS:O	1:C:558:ILE:HD11	2.07	0.55
1:A:364:CYS:SG	1:A:498:CYS:HB3	2.47	0.55
1:B:112:LYS:HG3	1:B:119:LYS:HB2	1.89	0.55
1:C:324:VAL:HA	1:C:374:PHE:HB2	1.88	0.55
1:B:242:ARG:NH1	1:B:242:ARG:HA	2.22	0.55
1:B:780:ARG:O	1:C:356:VAL:HA	2.07	0.55
1:C:958:LEU:HD13	1:C:962:GLU:HG3	1.89	0.55
2:T:1:NAG:H3	2:T:1:NAG:H3	1.89	0.55
1:C:91:LEU:CD2	1:C:93:ILE:HG13	2.37	0.54
1:C:517:PHE:HE2	1:C:552:ASP:HB3	1.72	0.54
1:C:569:VAL:HG12	1:C:586:TYR:CD1	2.43	0.54
2:V:2:NAG:H2	2:V:2:NAG:H1	1.89	0.54
1:C:407:VAL:HG23	1:C:486:VAL:HG22	1.89	0.54
1:C:710:VAL:HG21	1:C:978:LEU:HD11	1.89	0.54
1:A:680:TYR:HB2	1:C:857:THR:HG23	1.89	0.54
1:B:591:ILE:HD11	1:B:809:LEU:HD23	1.90	0.54
1:C:689:PRO:HG2	1:C:1082:ASN:O	2.08	0.54
7:C:1304:MAN:O1	3:U:3:BMA:C4	2.56	0.54
1:A:631:ASN:ND2	1:A:633:TYR:OH	2.41	0.54
1:A:676:ASN:ND2	1:C:761:GLN:HE21	2.05	0.54
1:C:26:GLN:HG2	1:C:248:THR:HG22	1.90	0.54
1:B:478:THR:OG1	1:B:481:GLY:O	2.12	0.54
2:Z:1:NAG:H3	2:Z:1:NAG:H3	1.88	0.54
1:A:95:ASN:ND2	6:A:1304:NAG:HO1	0.67	0.54
1:A:699:ILE:HD13	1:A:918:LEU:HD23	1.90	0.54
6:B:1103:NAG:H82	6:B:1103:NAG:H1	1.90	0.54
1:B:825:LYS:NZ	1:B:839:PHE:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1103:NAG:H83	6:B:1103:NAG:H3	1.90	0.53
1:C:251:LEU:HD22	1:C:259:ILE:HD13	1.89	0.53
1:A:16:PHE:CZ	1:A:18:SER:HB2	2.43	0.53
1:C:68:SER:HB2	1:C:70:GLU:OE2	2.09	0.53
2:V:2:NAG:H83	2:V:2:NAG:H3	1.90	0.53
1:A:678:VAL:HG13	1:C:857:THR:HG21	1.90	0.53
2:T:1:NAG:O3	2:T:2:NAG:H2	2.08	0.53
1:A:950:LEU:HD11	1:A:966:ILE:HG12	1.91	0.53
1:C:261:ASP:OD1	1:C:262:ALA:N	2.41	0.53
1:B:535:ILE:HD12	1:B:893:VAL:HG11	1.91	0.53
1:A:958:ASP:HB3	1:A:960:PRO:HD2	1.90	0.53
1:A:502:LYS:HD2	1:A:503:SER:H	1.74	0.53
1:C:332:ILE:HB	1:C:369:VAL:HG23	1.91	0.53
1:C:775:ASN:ND2	2:X:1:NAG:C2	2.36	0.53
1:B:871:ASN:ND2	4:O:1:NAG:C2	2.67	0.52
1:A:300:VAL:HG12	1:A:515:ASN:HB3	1.92	0.52
1:C:80:PHE:HB3	1:C:209:ILE:HG21	1.91	0.52
1:A:541:ASP:OD2	1:A:542:ILE:N	2.42	0.52
1:C:80:PHE:HB3	1:C:209:ILE:HD13	1.90	0.52
1:C:744:ILE:O	1:C:748:GLN:HG2	2.10	0.52
2:G:2:NAG:H82	2:G:2:NAG:H1	1.91	0.52
4:W:1:NAG:H4	4:W:2:NAG:H83	1.91	0.52
1:B:709:THR:CG2	1:B:903:GLN:HE22	2.22	0.52
1:C:91:LEU:HD21	1:C:93:ILE:HG13	1.92	0.52
1:A:695:VAL:HA	1:A:1037:HIS:O	2.09	0.52
1:B:88:LYS:HG3	1:B:90:CYS:H	1.73	0.52
2:S:1:NAG:H82	2:S:1:NAG:H1	1.90	0.52
1:A:672:LEU:HD12	1:C:847:TYR:CE1	2.44	0.52
1:C:376:ILE:HG12	1:C:380:GLU:OE1	2.10	0.52
1:C:515:PHE:CZ	1:C:561:ILE:HD13	2.44	0.52
1:B:312:GLY:H	1:B:315:ALA:HB3	1.73	0.52
1:A:857:SER:O	1:A:860:THR:HG22	2.10	0.52
1:C:5:SER:O	1:C:33:PHE:N	2.43	0.52
1:A:2:THR:HG21	1:A:188:ASP:CB	2.40	0.52
1:B:426:ALA:HB1	1:B:435:ILE:HD11	1.91	0.52
1:B:871:ASN:ND2	4:O:1:NAG:O1	0.41	0.52
1:C:4:ASN:HA	1:C:35:ASN:HA	1.92	0.52
1:C:168:PHE:CD1	1:C:177:ILE:HG12	2.45	0.52
1:B:584:LEU:HD22	1:B:805:VAL:HG21	1.92	0.51
1:C:60:PHE:HB3	1:C:209:ILE:O	2.10	0.51
1:A:1076:PHE:CZ	2:H:1:NAG:H61	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:GLY:HA2	1:B:698:GLN:CD	2.34	0.51
1:C:516:ASN:HA	1:C:520:LEU:O	2.11	0.51
1:A:613:SER:OG	1:A:614:ASN:N	2.44	0.51
1:A:779:LEU:HD23	1:A:851:LEU:HD11	1.92	0.51
1:C:66:PHE:O	1:C:166:PHE:HB2	2.10	0.51
1:C:70:GLU:OE2	1:C:75:ILE:HD12	2.10	0.51
1:A:335:VAL:HG22	1:A:498:CYS:SG	2.50	0.51
1:B:665:GLU:N	1:B:665:GLU:OE1	2.44	0.51
1:C:90:SER:OG	1:C:105:CYS:O	2.27	0.51
1:B:320:LYS:HD2	1:B:348:PRO:HG3	1.92	0.51
1:B:77:LEU:HD22	1:B:95:TYR:OH	2.10	0.51
6:A:1305:NAG:H82	6:A:1305:NAG:H1	1.92	0.51
1:A:535:PHE:CD2	1:C:198:GLU:HG2	2.46	0.51
1:A:162:LEU:HD11	1:A:183:ILE:HG12	1.93	0.51
1:A:775:PHE:HD1	1:A:778:ILE:HD11	1.76	0.51
1:C:5:SER:HB2	1:C:36:VAL:HG13	1.93	0.51
1:A:272:THR:HG21	1:A:570:VAL:CG2	2.41	0.50
1:B:711:ASN:OD1	1:B:712:VAL:N	2.44	0.50
1:C:696:VAL:HA	1:C:1038:HIS:O	2.10	0.50
1:B:608:GLN:NE2	1:C:677:ASN:HD21	2.09	0.50
1:C:370:TYR:O	1:C:487:LEU:HA	2.11	0.50
1:C:694:ILE:HD13	1:C:897:ILE:HG23	1.94	0.50
1:A:1063:PRO:HG2	1:C:887:GLN:HE22	1.75	0.50
1:B:298:ILE:HD12	1:B:302:GLU:HB2	1.94	0.50
1:A:680:TYR:CD1	1:C:857:THR:HG23	2.46	0.50
1:B:391:ASN:ND2	1:B:400:THR:HG22	2.26	0.50
1:B:88:LYS:HD2	1:B:98:CYS:HB3	1.94	0.50
1:A:649:THR:HA	1:A:663:GLN:H	1.76	0.50
1:A:1079:GLN:HE21	1:A:1082:PHE:HB3	1.76	0.50
1:B:88:LYS:HE2	1:B:101:GLU:HB2	1.94	0.50
1:C:65:TYR:HD1	1:C:167:VAL:HG22	1.76	0.50
1:B:272:THR:HB	1:B:274:LYS:NZ	2.27	0.49
1:B:682:GLY:HA2	1:B:698:GLN:NE2	2.27	0.49
7:C:1304:MAN:O1	3:U:3:BMA:O4	2.28	0.49
1:A:26:ASP:OD2	1:A:27:LEU:N	2.45	0.49
1:B:88:LYS:HD3	1:B:89:VAL:N	2.26	0.49
1:C:22:LEU:HD23	1:C:252:LYS:HA	1.94	0.49
1:B:55:GLU:HG3	1:B:59:ILE:HG22	1.93	0.49
1:C:104:VAL:HG11	1:C:141:THR:HB	1.93	0.49
1:A:680:TYR:OH	1:C:872:PHE:N	2.42	0.49
1:B:36:VAL:HG12	1:B:164:GLY:HA3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:VAL:HG13	1:C:564:CYS:HB3	1.94	0.49
1:A:101:ILE:HD13	1:A:143:TYR:HD2	1.77	0.49
1:B:760:VAL:HG12	1:C:544:ALA:HB2	1.95	0.49
1:B:132:ASP:OD1	1:B:133:LEU:N	2.44	0.49
2:M:2:NAG:H82	2:M:2:NAG:H1	1.95	0.49
1:B:13:PRO:HG3	1:B:25:THR:HG21	1.94	0.49
1:B:402:VAL:HG12	1:B:439:THR:O	2.12	0.49
1:B:878:ILE:HD11	1:B:912:ILE:HG21	1.94	0.49
1:C:636:CYS:HA	1:C:669:TYR:OH	2.12	0.49
1:C:844:ILE:O	1:C:848:THR:HG23	2.13	0.49
1:A:163:ARG:HE	1:A:180:HIS:HE1	1.60	0.49
1:A:187:ARG:HG3	1:A:188:ASP:OD1	2.12	0.49
1:A:535:PHE:HD2	1:C:198:GLU:OE2	1.96	0.49
1:A:1021:HIS:HA	1:A:1039:THR:HG22	1.95	0.49
1:B:199:LEU:HD12	1:B:204:VAL:HG12	1.95	0.49
1:B:314:ILE:HA	1:B:318:ASN:HB2	1.94	0.49
1:B:335:ASN:OD1	1:B:336:ASN:N	2.46	0.49
1:B:342:LEU:HD13	1:B:360:SER:HB2	1.94	0.49
1:C:5:SER:HB3	1:C:34:SER:O	2.13	0.49
1:C:316:PHE:CE1	1:C:485:VAL:HG11	2.47	0.49
1:A:799:VAL:HG21	1:A:1030:PRO:HG3	1.95	0.48
1:B:301:ASP:OD1	1:B:301:ASP:N	2.45	0.48
1:C:165:GLU:HB3	1:C:180:LYS:HB3	1.95	0.48
4:N:2:NAG:H82	4:N:2:NAG:H1	1.94	0.48
1:B:312:GLY:N	1:B:315:ALA:HB3	2.29	0.48
1:A:378:ASP:N	8:A:1309:DMS:H22	2.27	0.48
1:B:64:ILE:HG13	1:B:158:LEU:HD11	1.95	0.48
1:B:173:LEU:HD23	1:B:181:ILE:HD13	1.95	0.48
1:B:378:PRO:O	1:B:379:LYS:HD2	2.12	0.48
1:B:552:MET:HG3	1:B:815:ILE:HG13	1.95	0.48
1:A:289:SER:OG	1:A:290:ASN:N	2.46	0.48
1:A:470:PHE:CE2	1:A:480:PRO:HB3	2.48	0.48
1:B:318:ASN:ND2	1:B:343:TYR:HB2	2.29	0.48
1:B:702:ARG:NH1	1:B:846:LEU:O	2.38	0.48
1:C:168:PHE:HD1	1:C:177:ILE:HG12	1.79	0.48
1:C:1024:MET:HE2	1:C:1026:PHE:CE1	2.48	0.48
1:A:685:ILE:HA	1:C:869:GLN:O	2.14	0.48
1:B:123:LYS:HB3	1:B:140:LEU:HD23	1.95	0.48
1:A:308:LEU:HD12	1:A:335:VAL:O	2.13	0.48
1:A:676:ASN:ND2	1:C:761:GLN:NE2	2.62	0.48
1:A:826:GLN:H	1:A:826:GLN:CD	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LYS:HD2	1:B:90:CYS:SG	2.53	0.48
1:B:3:THR:HG22	1:B:4:ASN:H	1.78	0.48
1:B:591:ILE:O	1:B:595:GLN:HG2	2.14	0.48
1:A:1060:ALA:HB2	1:A:1099:CYS:HB3	1.95	0.48
1:B:451:PRO:HB3	1:B:507:TYR:HB2	1.95	0.48
1:C:726:LEU:O	1:C:729:GLN:HG2	2.13	0.47
1:A:533:LEU:H	1:A:536:GLN:NE2	2.12	0.47
1:B:183:ASP:OD1	1:B:184:ALA:N	2.47	0.47
1:B:254:ILE:HB	1:B:291:VAL:HB	1.96	0.47
1:C:495:PRO:HB3	1:C:538:GLN:NE2	2.29	0.47
1:C:31:PRO:HG3	1:C:247:ARG:HH22	1.79	0.47
1:A:187:ARG:O	1:A:187:ARG:HD3	2.14	0.47
1:A:693:ILE:HD11	1:A:900:PHE:HB2	1.97	0.47
1:C:1076:TRP:CZ2	1:C:1107:VAL:HG21	2.49	0.47
1:B:681:SER:O	1:B:681:SER:OG	2.29	0.47
1:C:577:ASN:OD1	6:C:1302:NAG:H2	2.11	0.47
1:C:631:ASN:ND2	2:d:1:NAG:O7	2.47	0.47
1:B:302:GLU:HA	1:B:305:GLN:HB2	1.96	0.47
1:B:371:ALA:HB1	1:B:372:PRO:HD2	1.95	0.47
1:B:762:GLN:HG3	1:B:800:SER:HB2	1.97	0.47
1:C:335:CYS:SG	1:C:336:VAL:N	2.87	0.47
1:A:538:PHE:O	1:C:16:VAL:HA	2.14	0.47
1:A:762:TYR:HA	1:B:524:ASN:O	2.15	0.47
1:C:59:PRO:HA	1:C:210:THR:O	2.15	0.47
1:C:335:CYS:O	1:C:498:VAL:HA	2.14	0.47
1:C:348:PHE:HA	1:C:410:TRP:HB3	1.95	0.47
1:C:392:ILE:HG23	1:C:396:ASN:HD22	1.80	0.47
1:C:722:GLU:HG2	1:C:723:CYS:N	2.30	0.47
1:B:107:ARG:NH1	1:B:124:HIS:HB3	2.19	0.47
1:B:214:PHE:HZ	1:B:466:VAL:HG21	1.79	0.47
1:B:420:ILE:O	1:B:423:THR:OG1	2.32	0.47
1:B:560:THR:O	1:B:564:CYS:HB2	2.15	0.47
1:B:887:PRO:HD3	1:B:892:PHE:CE2	2.49	0.47
1:C:434:ASN:OD1	1:C:435:LEU:N	2.47	0.47
1:C:869:GLN:OE1	1:C:869:GLN:N	2.41	0.47
1:A:355:VAL:HG22	1:A:360:LEU:HD23	1.96	0.47
1:B:642:LEU:O	1:B:646:LYS:HG2	2.14	0.47
1:C:293:ARG:HD3	1:C:566:PHE:CB	2.45	0.47
1:C:367:THR:O	1:C:497:THR:OG1	2.23	0.47
1:A:528:SER:OG	1:A:557:ILE:HG12	2.15	0.46
1:A:1078:THR:HG22	1:A:1085:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:LYS:HE2	1:B:872:PHE:CZ	2.50	0.46
1:C:31:PRO:HA	1:C:247:ARG:NH1	2.14	0.46
1:C:344:ASN:OD1	1:C:345:SER:N	2.48	0.46
1:A:6:THR:OG1	1:A:192:GLY:O	2.34	0.46
1:A:592:GLU:N	1:A:592:GLU:OE1	2.48	0.46
1:C:1:ALA:O	1:C:38:TRP:HB3	2.16	0.46
1:A:842:MET:HB3	1:B:520:LEU:HD11	1.96	0.46
1:A:1076:PHE:HZ	2:H:1:NAG:H61	1.80	0.46
1:C:215:LEU:HD23	1:C:215:LEU:H	1.80	0.46
5:Q:1:NAG:H82	5:Q:1:NAG:H1	1.96	0.46
1:B:167:GLN:OE1	1:B:168:PRO:HD2	2.16	0.46
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.80	0.46
1:B:584:LEU:HD13	1:B:801:LEU:HG	1.97	0.46
1:B:923:CYS:HB2	1:B:929:ILE:HD13	1.98	0.46
1:C:520:LEU:HD11	1:C:539:PHE:CD1	2.50	0.46
1:A:355:VAL:HA	8:A:1310:DMS:O	2.16	0.46
1:A:377:GLY:O	8:A:1309:DMS:C1	2.38	0.46
1:A:681:SER:HB3	1:A:684:SER:HB3	1.98	0.46
1:A:1029:ALA:HB1	1:A:1030:PRO:HD2	1.96	0.46
1:B:892:PHE:CE1	1:B:901:VAL:HG22	2.50	0.46
1:C:691:ASN:OD1	1:C:692:PHE:N	2.45	0.46
1:C:1076:TRP:HB2	1:C:1109:ASN:HD22	1.78	0.46
1:B:569:GLU:H	1:B:569:GLU:CD	2.24	0.46
1:C:332:ILE:HB	1:C:369:VAL:CG2	2.45	0.46
7:C:1304:MAN:HO1	3:U:3:BMA:C4	2.28	0.46
1:A:26:ASP:HB3	1:A:28:PHE:CE1	2.51	0.46
1:A:267:ASP:OD1	1:A:267:ASP:N	2.49	0.46
1:B:622:ASN:OD1	1:B:624:SER:HB3	2.16	0.46
1:A:355:VAL:HG23	8:A:1310:DMS:H23	1.95	0.46
1:B:651:LYS:HE2	1:B:760:VAL:HG21	1.98	0.46
1:C:328:ASN:OD1	1:C:373:SER:HB3	2.16	0.46
1:C:877:ALA:HB1	1:C:887:GLN:HB2	1.98	0.46
1:A:691:PHE:HE2	1:A:896:ILE:HG12	1.81	0.45
1:B:8:ARG:HD2	1:B:108:GLU:CD	2.40	0.45
1:B:608:GLN:HB2	1:C:675:ALA:O	2.16	0.45
1:B:782:ASP:N	1:C:357:SER:HB2	2.31	0.45
1:C:356:VAL:HG12	1:C:361:LEU:HD12	1.96	0.45
1:A:296:THR:C	1:A:297:GLU:HG3	2.41	0.45
1:C:283:GLU:H	1:C:283:GLU:CD	2.23	0.45
1:C:701:LEU:HD11	1:C:1002:LYS:HD3	1.98	0.45
1:A:471:GLN:H	1:A:474:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ARG:O	1:B:162:TYR:OH	2.34	0.45
1:B:261:TYR:OH	1:B:366:PHE:HE1	1.99	0.45
1:B:670:TYR:CZ	1:C:673:LEU:HD12	2.51	0.45
1:A:272:THR:HG21	1:A:570:VAL:HG21	1.99	0.45
1:A:303:PRO:HB3	1:A:552:PRO:HB2	1.98	0.45
1:A:352:CYS:HA	1:A:405:CYS:HA	1.97	0.45
1:B:112:LYS:HE3	1:B:121:TYR:CE1	2.51	0.45
1:B:403:LEU:HD23	1:B:438:ILE:HG12	1.98	0.45
1:B:627:LEU:HD23	1:B:675:LEU:HD22	1.98	0.45
1:C:436:LYS:HB2	1:C:437:PRO:HD2	1.99	0.45
1:A:921:LEU:HD21	1:A:1029:ALA:HB1	1.98	0.45
1:A:1014:ASP:HB2	1:C:1004:SER:OG	2.17	0.45
1:C:205:ILE:HG22	1:C:207:ILE:HG23	1.99	0.45
1:A:676:ASN:CG	1:C:761:GLN:HE21	2.23	0.45
1:B:559:CYS:HB3	1:B:581:CYS:HB3	1.74	0.45
1:C:36:VAL:HB	1:C:241:VAL:O	2.16	0.45
1:A:37:TRP:NE1	1:A:237:ALA:HB1	2.32	0.45
1:A:204:ILE:HG13	1:A:205:GLY:N	2.31	0.45
1:A:364:CYS:SG	1:A:498:CYS:CB	3.04	0.45
1:C:380:GLU:HA	1:C:383:GLN:HE21	1.82	0.45
1:A:79:PHE:HD1	1:A:211:PHE:HB2	1.81	0.45
1:A:104:CYS:HB3	1:A:139:CYS:HA	1.98	0.45
1:A:680:TYR:HE1	1:C:870:ILE:O	1.99	0.45
1:B:11:TYR:OH	1:B:28:LEU:O	2.32	0.45
1:B:174:LYS:HE3	1:B:174:LYS:HB2	1.74	0.45
1:B:770:ILE:HD12	1:B:780:ARG:NH2	2.32	0.45
1:B:871:ASN:ND2	4:O:1:NAG:HO1	0.67	0.45
1:A:365:PHE:CD1	1:A:488:PHE:HB3	2.52	0.44
1:B:44:PRO:O	1:B:155:PHE:HE1	2.00	0.44
1:A:578:SER:OG	1:A:579:ASN:N	2.51	0.44
1:B:222:ILE:HD13	1:B:384:LEU:HA	1.99	0.44
1:C:57:VAL:HA	1:C:213:GLN:NE2	2.32	0.44
1:C:490:GLU:OE2	1:C:493:HIS:HB2	2.17	0.44
1:B:42:VAL:HB	1:B:154:ARG:NE	2.33	0.44
1:C:951:LEU:HA	1:C:954:ILE:HG22	1.99	0.44
1:A:293:VAL:HG12	1:A:564:SER:O	2.18	0.44
1:A:184:ASN:O	1:A:185:LEU:HD22	2.18	0.44
1:A:524:VAL:HG13	1:A:563:CYS:HB3	2.00	0.44
1:B:17:PHE:O	1:C:540:GLY:HA2	2.18	0.44
1:B:746:GLN:HA	1:B:749:VAL:HG12	2.00	0.44
1:B:826:MET:HE2	1:B:826:MET:HB2	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLN:CD	1:C:192:GLN:H	2.26	0.44
2:L:1:NAG:H4	2:L:2:NAG:H2	1.74	0.44
1:A:248:PHE:CE1	1:A:263:ASP:HB3	2.52	0.44
1:B:85:VAL:O	1:B:103:VAL:HA	2.18	0.44
1:B:223:VAL:O	1:B:224:ARG:HD2	2.18	0.44
1:C:211:ARG:HB3	1:C:213:GLN:OE1	2.16	0.44
1:B:563:ILE:HG22	1:B:797:ARG:HB3	1.99	0.44
1:C:177:ILE:O	1:C:200:LEU:HB3	2.18	0.44
1:A:38:PHE:CZ	1:A:57:LEU:HD21	2.53	0.44
1:B:14:ASP:OD1	1:B:15:LYS:N	2.45	0.44
1:B:17:PHE:HA	1:C:537:GLN:OE1	2.18	0.44
1:B:36:VAL:HA	1:B:163:VAL:O	2.17	0.44
1:C:165:GLU:O	1:C:179:SER:HA	2.18	0.44
1:A:946:ILE:HG13	1:A:956:ARG:HH22	1.83	0.44
1:B:454:ASN:OD1	6:B:1107:NAG:C2	2.58	0.44
1:C:180:LYS:HA	1:C:180:LYS:HD2	1.81	0.44
1:A:79:PHE:CD1	1:A:211:PHE:HB2	2.52	0.43
1:B:147:PRO:CB	1:C:370:TYR:OH	2.66	0.43
1:B:745:LEU:HD21	1:B:856:GLY:HA3	2.00	0.43
1:A:79:PHE:HD2	1:A:90:LEU:HD23	1.82	0.43
1:A:539:GLY:HA2	1:C:17:PHE:H	1.82	0.43
1:B:426:ALA:HA	1:B:437:ASP:HA	2.00	0.43
1:B:697:MET:HE1	1:C:1068:VAL:HG23	1.99	0.43
1:A:1068:PHE:CE1	1:A:1077:VAL:HG22	2.54	0.43
1:B:570:CYS:HB2	1:B:774:LEU:HD21	1.99	0.43
1:C:210:THR:HG22	1:C:211:ARG:HH21	1.82	0.43
2:T:1:NAG:H61	2:T:2:NAG:C1	2.41	0.43
1:A:858:GLY:HA2	1:A:874:GLN:NE2	2.33	0.43
1:B:57:SER:OG	1:B:58:ASN:N	2.50	0.43
1:B:131:ARG:C	1:B:131:ARG:HD3	2.43	0.43
1:B:224:ARG:NH1	1:B:384:LEU:HD23	2.33	0.43
1:B:550:VAL:HG12	1:B:856:GLY:HA2	2.01	0.43
1:C:492:LEU:HD22	1:C:539:PHE:CZ	2.47	0.43
1:B:601:GLU:O	1:B:605:GLN:NE2	2.47	0.43
1:C:292:PHE:C	1:C:293:ARG:HG2	2.43	0.43
1:C:550:VAL:O	1:C:558:ILE:HA	2.18	0.43
1:C:775:ASN:ND2	2:X:1:NAG:N2	2.67	0.43
1:C:1064:PRO:HD3	1:C:1069:PHE:CE2	2.53	0.43
1:A:301:ARG:HD3	1:A:516:PHE:CE1	2.53	0.43
1:B:271:SER:OG	1:B:272:THR:HG23	2.19	0.43
1:B:336:ASN:OD1	1:B:337:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:TYR:HD2	1:C:202:ASP:HB3	1.83	0.43
7:C:1304:MAN:H3	3:U:3:BMA:O6	2.19	0.43
1:A:878:ARG:HD3	1:A:1022:LEU:O	2.18	0.43
1:C:382:ARG:HB3	1:C:382:ARG:NH1	2.34	0.43
1:C:712:CYS:O	1:C:713:THR:C	2.61	0.43
2:c:1:NAG:O6	2:c:2:NAG:H82	2.18	0.43
1:A:702:VAL:HG22	1:A:1032:GLY:HA2	2.01	0.43
1:A:170:ILE:HG13	1:A:170:ILE:O	2.19	0.43
1:A:1053:ALA:HB3	1:A:1105:ILE:HG22	2.01	0.43
1:B:234:PHE:HE1	1:B:254:ILE:HG21	1.84	0.43
1:B:259:ALA:O	1:B:377:GLY:HA2	2.18	0.43
1:B:491:ASN:ND2	1:B:493:TYR:OH	2.45	0.43
1:B:74:GLN:HB2	1:B:150:ILE:HD13	2.01	0.43
1:C:896:LEU:O	1:C:900:GLN:HG3	2.19	0.43
1:C:1046:GLU:CD	1:C:1046:GLU:H	2.27	0.43
1:A:31:PHE:HB2	1:A:263:ASP:OD2	2.19	0.42
1:A:163:ARG:HE	1:A:180:HIS:CE1	2.37	0.42
1:A:952:ASP:O	1:A:956:ARG:HG2	2.19	0.42
1:B:112:LYS:HE3	1:B:121:TYR:HE1	1.84	0.42
1:A:326:TRP:O	1:A:439:ARG:NH2	2.52	0.42
1:C:341:VAL:HG23	1:C:342:LEU:HD12	2.01	0.42
1:C:574:PRO:HB3	1:C:648:TYR:HB2	2.01	0.42
1:C:832:LEU:HD13	1:C:933:LEU:HD22	2.01	0.42
1:A:30:PRO:HB3	1:A:246:ARG:HE	1.84	0.42
1:A:530:LYS:O	1:A:557:ILE:HD13	2.19	0.42
1:B:63:TRP:N	1:B:158:LEU:HD13	2.34	0.42
1:B:242:ARG:HA	1:B:242:ARG:CZ	2.50	0.42
1:C:324:VAL:HG11	1:C:376:ILE:HD13	2.01	0.42
1:C:441:ASP:OD1	1:C:443:SER:OG	2.33	0.42
1:C:951:LEU:HD11	1:C:967:ILE:HG12	2.01	0.42
1:A:170:ILE:HD11	1:A:175:LYS:HE3	2.00	0.42
1:B:552:MET:HB2	1:B:595:GLN:NE2	2.34	0.42
1:C:310:CYS:N	1:C:335:CYS:SG	2.91	0.42
1:A:301:ARG:HH21	1:A:553:GLN:HB2	1.83	0.42
1:A:1011:LYS:HB3	1:A:1011:LYS:HE3	1.72	0.42
1:B:8:ARG:CZ	1:B:108:GLU:OE2	2.68	0.42
1:B:492:SER:HB3	1:B:519:SER:HB3	2.00	0.42
1:B:512:SER:OG	1:B:513:ILE:N	2.52	0.42
1:C:72:SER:OG	1:C:74:ILE:HG13	2.20	0.42
1:C:314:GLU:H	1:C:314:GLU:CD	2.26	0.42
1:A:184:ASN:OD1	1:A:185:LEU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:PHE:CE2	1:C:358:PRO:HB3	2.45	0.42
1:C:923:GLN:NE2	1:C:927:ASN:OD1	2.53	0.42
1:A:477:GLY:CA	8:A:1309:DMS:H23	2.45	0.42
1:B:30:LEU:HB2	1:B:166:LEU:CD2	2.49	0.42
1:B:153:THR:HG1	2:T:1:NAG:HO6	1.68	0.42
1:B:304:ARG:HD2	1:B:304:ARG:O	2.20	0.42
1:B:650:GLN:HB3	1:B:652:PHE:HE1	1.84	0.42
1:C:203:LEU:HD12	1:C:205:ILE:HD11	2.02	0.42
1:C:351:PHE:HD1	1:C:408:ILE:HG13	1.85	0.42
1:C:950:VAL:HG13	1:C:953:ASP:HB3	2.02	0.42
1:A:76:GLY:O	1:A:214:LEU:HG	2.20	0.42
1:A:330:ARG:NH1	6:C:1305:NAG:O6	2.52	0.42
1:A:540:ARG:HD3	1:A:544:ASP:HA	2.01	0.42
1:A:765:PRO:HG3	1:B:528:TYR:HB3	2.02	0.42
1:B:539:PHE:HE1	1:B:720:ILE:HG12	1.84	0.42
1:B:699:MET:HE3	1:B:846:LEU:HD13	2.02	0.42
1:B:253:ARG:HH21	1:B:292:TYR:HE2	1.67	0.42
1:B:411:LEU:HD23	1:B:411:LEU:HA	1.86	0.42
1:B:827:SER:O	1:B:831:LEU:HB2	2.19	0.42
1:C:533:PHE:CG	1:C:558:ILE:HG21	2.54	0.42
1:C:639:PRO:HA	1:C:645:CYS:SG	2.59	0.42
1:C:710:VAL:HG22	1:C:741:LEU:HD12	2.02	0.42
5:Q:2:NAG:H3	5:Q:3:BMA:H1	1.85	0.42
1:B:89:VAL:HG12	1:B:89:VAL:O	2.20	0.41
1:B:214:PHE:CZ	1:B:466:VAL:HG21	2.55	0.41
1:B:388:LYS:HD3	1:B:389:CYS:N	2.35	0.41
1:C:351:PHE:CD1	1:C:408:ILE:HG13	2.55	0.41
1:A:932:LEU:HD23	1:A:932:LEU:HA	1.87	0.41
1:B:646:LYS:HB2	1:B:742:LEU:HD12	2.02	0.41
1:C:300:ILE:HG23	1:C:513:VAL:HG11	2.02	0.41
1:B:305:GLN:OE1	1:B:312:GLY:HA3	2.20	0.41
1:B:550:VAL:HG23	1:B:602:VAL:HG21	2.03	0.41
1:B:675:LEU:HA	1:B:678:THR:HG22	2.02	0.41
1:C:504:SER:OG	1:C:554:GLN:NE2	2.51	0.41
1:C:741:LEU:HD23	1:C:741:LEU:HA	1.84	0.41
1:A:573:PRO:HB3	1:A:647:TYR:HB2	2.01	0.41
1:B:118:PHE:O	1:B:145:ASP:HA	2.19	0.41
1:B:636:ARG:HG2	1:B:640:GLU:HB2	2.01	0.41
1:C:640:ILE:HD11	1:C:646:ALA:HB2	2.02	0.41
1:A:704:MET:HB3	1:A:928:ASN:HD21	1.85	0.41
1:B:588:LEU:HD23	1:B:588:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:GLU:CD	1:C:493:HIS:HB2	2.45	0.41
1:B:137:PHE:CE2	1:B:181:ILE:HG22	2.53	0.41
1:B:894:SER:HB2	1:B:899:TRP:CD2	2.56	0.41
1:B:195:THR:HG22	1:B:211:THR:HG21	2.03	0.41
1:B:289:THR:HA	1:B:373:ALA:HA	2.03	0.41
1:C:174:TYR:CD2	1:C:202:ASP:HB3	2.54	0.41
1:C:380:GLU:HA	1:C:383:GLN:NE2	2.36	0.41
1:A:54:ASN:ND2	1:A:238:TYR:HE1	2.19	0.41
1:A:787:LYS:HD3	1:A:787:LYS:N	2.36	0.41
1:B:77:LEU:HG	1:B:79:VAL:HG23	2.01	0.41
1:B:646:LYS:HD2	1:B:646:LYS:HA	1.74	0.41
1:C:64:VAL:HG11	1:C:212:PHE:CZ	2.56	0.41
1:C:277:LEU:HD23	1:C:282:VAL:HG12	2.03	0.41
1:C:710:VAL:CG1	1:C:832:LEU:HD22	2.51	0.41
1:C:765:THR:OG1	1:C:766:PRO:HD2	2.21	0.41
1:A:281:VAL:H	1:A:575:THR:HG23	1.86	0.41
1:A:784:LYS:HD3	1:A:793:ASP:OD2	2.20	0.41
1:A:921:LEU:O	1:A:924:VAL:HG22	2.20	0.41
1:B:17:PHE:CE1	1:B:179:GLY:HA3	2.56	0.41
1:B:89:VAL:HG23	1:B:100:PHE:O	2.21	0.41
1:C:203:LEU:HA	1:C:204:PRO:HD3	1.80	0.41
1:C:705:MET:HB3	1:C:992:ILE:HD13	2.03	0.41
1:A:957:LEU:HD23	1:A:957:LEU:HA	1.90	0.41
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.92	0.41
1:C:800:VAL:CG2	1:C:1031:PRO:HG3	2.45	0.41
1:A:186:VAL:HG11	1:A:190:PRO:HD3	2.04	0.40
1:A:576:ASN:OD1	1:A:577:THR:N	2.54	0.40
1:A:714:TYR:CE2	1:A:977:LEU:HD13	2.55	0.40
1:A:835:PRO:HG3	1:B:480:ALA:HA	2.02	0.40
1:B:429:ASP:OD2	1:B:432:THR:HB	2.21	0.40
1:A:843:ILE:O	1:A:847:THR:HG23	2.22	0.40
1:A:1001:LYS:O	1:A:1005:CYS:HB2	2.21	0.40
1:B:38:TRP:HE1	1:B:160:ALA:CB	2.32	0.40
1:B:65:PHE:O	1:B:75:SER:HA	2.20	0.40
1:A:13:ASP:OD1	1:A:14:LYS:N	2.54	0.40
1:A:693:ILE:HD13	1:A:896:ILE:HG23	2.03	0.40
1:B:17:PHE:HB2	1:C:537:GLN:CD	2.46	0.40
1:C:139:ASN:ND2	6:C:1305:NAG:O5	2.23	0.40
1:C:268:ASP:OD1	1:C:269:PRO:HD2	2.21	0.40
1:C:1080:GLN:HG3	1:C:1083:PHE:O	2.21	0.40
1:A:78:ILE:HG22	1:A:91:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1067:VAL:HG11	1:C:878:TYR:OH	2.21	0.40
1:B:562:TYR:CE2	1:B:763:LEU:HD11	2.57	0.40
1:C:858:SER:HA	1:C:869:GLN:HA	2.04	0.40
1:A:1052:PRO:HB3	1:C:891:TYR:CE1	2.56	0.40
1:B:153:THR:O	1:B:153:THR:HG22	2.22	0.40
1:C:277:LEU:HD12	1:C:277:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	968/1288 (75%)	924 (96%)	44 (4%)	0	100	100
1	B	917/1288 (71%)	903 (98%)	14 (2%)	0	100	100
1	C	908/1288 (70%)	882 (97%)	26 (3%)	0	100	100
All	All	2793/3864 (72%)	2709 (97%)	84 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	865/1113 (78%)	856 (99%)	9 (1%)	68	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	829/1113 (74%)	828 (100%)	1 (0%)	88	90
1	C	816/1113 (73%)	813 (100%)	3 (0%)	84	86
All	All	2510/3339 (75%)	2497 (100%)	13 (0%)	78	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	LEU
1	A	349	THR
1	A	360	LEU
1	A	378	ASP
1	A	413	ASN
1	A	450	SER
1	A	453	CYS
1	A	476	VAL
1	A	490	LEU
1	B	626	ILE
1	C	96	ASN
1	C	576	THR
1	C	591	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	54	ASN
1	A	95	ASN
1	A	180	HIS
1	A	423	ASN
1	A	536	GLN
1	A	537	GLN
1	A	617	GLN
1	A	628	HIS
1	A	631	ASN
1	A	663	GLN
1	A	724	ASN
1	A	874	GLN
1	A	938	GLN
1	A	984	GLN
1	A	1009	GLN

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Mol	Chain	Res	Type
1	A	1031	HIS
1	A	1056	HIS
1	A	1061	HIS
1	A	1074	HIS
1	A	1108	ASN
1	B	105	ASN
1	B	128	ASN
1	B	239	ASN
1	B	290	ASN
1	B	333	ASN
1	B	391	ASN
1	B	431	GLN
1	B	477	GLN
1	B	490	ASN
1	B	572	ASN
1	B	583	GLN
1	B	650	GLN
1	B	710	GLN
1	B	751	GLN
1	B	833	GLN
1	B	871	ASN
1	B	898	HIS
1	B	903	GLN
1	C	40	HIS
1	C	139	ASN
1	C	192	GLN
1	C	295	GLN
1	C	317	ASN
1	C	537	GLN
1	C	677	ASN
1	C	725	ASN
1	C	758	GLN
1	C	761	GLN
1	C	775	ASN
1	C	887	GLN
1	C	909	GLN
1	C	923	GLN
1	C	929	ASN
1	C	943	ASN
1	C	1048	ASN
1	C	1057	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 ⓘ

69 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	15,15,15	0.33	0	21,21,21	0.14	0
2	NAG	D	2	2	15,15,15	0.35	0	21,21,21	0.11	0
3	NAG	E	1	3,1	15,15,15	0.35	0	21,21,21	0.16	0
3	NAG	E	2	3	15,15,15	0.33	0	21,21,21	0.28	0
3	BMA	E	3	3	12,12,12	0.52	0	17,17,17	0.74	0
3	MAN	E	4	3	12,12,12	0.65	0	17,17,17	1.26	1 (5%)
3	NAG	F	1	3,1	15,15,15	0.36	0	21,21,21	0.18	0
3	NAG	F	2	3	15,15,15	0.40	0	21,21,21	0.59	0
3	BMA	F	3	3	12,12,12	0.56	0	17,17,17	0.67	0
3	MAN	F	4	3	12,12,12	0.61	0	17,17,17	1.17	2 (11%)
2	NAG	G	1	2,1	15,15,15	0.34	0	21,21,21	0.19	0
2	NAG	G	2	2	15,15,15	0.49	0	21,21,21	0.91	2 (9%)
2	NAG	H	1	2,1	15,15,15	0.34	0	21,21,21	0.28	0
2	NAG	H	2	2	15,15,15	0.36	0	21,21,21	0.27	0
2	NAG	I	1	2,1	15,15,15	0.32	0	21,21,21	0.12	0
2	NAG	I	2	2	15,15,15	0.33	0	21,21,21	0.11	0
2	NAG	J	1	2,1	15,15,15	0.35	0	21,21,21	0.33	0
2	NAG	J	2	2	15,15,15	0.36	0	21,21,21	0.13	0
2	NAG	K	1	2,1	15,15,15	0.34	0	21,21,21	0.28	0
2	NAG	K	2	2	15,15,15	0.33	0	21,21,21	0.14	0
2	NAG	L	1	2,1	15,15,15	0.34	0	21,21,21	0.27	0
2	NAG	L	2	2	15,15,15	0.59	0	21,21,21	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	M	1	2,1	15,15,15	0.58	0	21,21,21	0.50	0
2	NAG	M	2	2	15,15,15	0.61	0	21,21,21	0.99	2 (9%)
4	NAG	N	1	4,1	15,15,15	0.35	0	21,21,21	0.15	0
4	NAG	N	2	4	15,15,15	0.44	0	21,21,21	0.91	2 (9%)
4	BMA	N	3	4	12,12,12	0.51	0	17,17,17	0.70	0
4	NAG	O	1	4	15,15,15	0.41	0	21,21,21	0.40	0
4	NAG	O	2	4	15,15,15	0.33	0	21,21,21	0.26	0
4	BMA	O	3	4	12,12,12	0.62	0	17,17,17	0.64	0
2	NAG	P	1	2	15,15,15	0.44	0	21,21,21	0.50	0
2	NAG	P	2	2	15,15,15	0.38	0	21,21,21	0.28	0
5	NAG	Q	1	5	15,15,15	0.43	0	21,21,21	0.97	2 (9%)
5	NAG	Q	2	5	15,15,15	0.52	0	21,21,21	0.62	0
5	BMA	Q	3	5	12,12,12	1.26	2 (16%)	17,17,17	0.71	0
3	NAG	R	1	3,1	15,15,15	0.35	0	21,21,21	0.22	0
3	NAG	R	2	3	15,15,15	0.34	0	21,21,21	0.39	0
3	BMA	R	3	3	12,12,12	0.82	1 (8%)	17,17,17	0.88	1 (5%)
3	MAN	R	4	3	12,12,12	0.59	0	17,17,17	0.89	1 (5%)
2	NAG	S	1	2	15,15,15	0.85	1 (6%)	21,21,21	1.65	5 (23%)
2	NAG	S	2	2	15,15,15	0.48	0	21,21,21	0.32	0
2	NAG	T	1	2	15,15,15	0.42	0	21,21,21	0.96	2 (9%)
2	NAG	T	2	2	15,15,15	0.55	0	21,21,21	0.31	0
3	NAG	U	1	3	15,15,15	0.36	0	21,21,21	0.18	0
3	NAG	U	2	3	15,15,15	0.34	0	21,21,21	0.20	0
3	BMA	U	3	3	12,12,12	0.51	0	17,17,17	0.56	0
3	MAN	U	4	3	12,12,12	0.83	1 (8%)	17,17,17	1.54	2 (11%)
2	NAG	V	1	2	15,15,15	0.34	0	21,21,21	0.23	0
2	NAG	V	2	2	15,15,15	0.50	0	21,21,21	0.91	2 (9%)
4	NAG	W	1	4	15,15,15	0.41	0	21,21,21	0.47	0
4	NAG	W	2	4	15,15,15	0.55	0	21,21,21	1.83	1 (4%)
4	BMA	W	3	4	12,12,12	0.67	0	17,17,17	0.85	1 (5%)
2	NAG	X	1	2	15,15,15	0.33	0	21,21,21	0.19	0
2	NAG	X	2	2	15,15,15	0.43	0	21,21,21	0.25	0
4	NAG	Y	1	4,1	15,15,15	0.33	0	21,21,21	0.17	0
4	NAG	Y	2	4	15,15,15	0.33	0	21,21,21	0.24	0
4	BMA	Y	3	4	12,12,12	0.63	0	17,17,17	0.65	0
2	NAG	Z	1	2	15,15,15	0.42	0	21,21,21	0.92	2 (9%)
2	NAG	Z	2	2	15,15,15	0.34	0	21,21,21	0.18	0
4	NAG	a	1	4,1	15,15,15	0.41	0	21,21,21	0.85	0
4	NAG	a	2	4	15,15,15	0.43	0	21,21,21	0.32	0
4	BMA	a	3	4	12,12,12	0.59	0	17,17,17	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	b	1	4	15,15,15	0.48	0	21,21,21	0.95	2 (9%)
4	NAG	b	2	4	15,15,15	0.32	0	21,21,21	0.33	0
4	BMA	b	3	4	12,12,12	0.63	0	17,17,17	0.70	0
2	NAG	c	1	2	15,15,15	0.42	0	21,21,21	0.81	1 (4%)
2	NAG	c	2	2	15,15,15	0.39	0	21,21,21	0.33	0
2	NAG	d	1	2	15,15,15	0.36	0	21,21,21	0.29	0
2	NAG	d	2	2	15,15,15	0.44	0	21,21,21	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	1/6/26/26	0/1/1/1
2	NAG	D	2	2	-	0/6/26/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/26/26	0/1/1/1
3	NAG	E	2	3	-	0/6/26/26	0/1/1/1
3	BMA	E	3	3	-	0/2/22/22	0/1/1/1
3	MAN	E	4	3	-	0/2/22/22	0/1/1/1
3	NAG	F	1	3,1	-	1/6/26/26	0/1/1/1
3	NAG	F	2	3	-	4/6/26/26	0/1/1/1
3	BMA	F	3	3	-	1/2/22/22	0/1/1/1
3	MAN	F	4	3	-	0/2/22/22	0/1/1/1
2	NAG	G	1	2,1	-	0/6/26/26	0/1/1/1
2	NAG	G	2	2	-	4/6/26/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	H	2	2	-	2/6/26/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	I	2	2	-	0/6/26/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	J	2	2	-	2/6/26/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	K	2	2	-	2/6/26/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/26/26	0/1/1/1
2	NAG	L	2	2	-	1/6/26/26	0/1/1/1
2	NAG	M	1	2,1	-	4/6/26/26	0/1/1/1
2	NAG	M	2	2	-	4/6/26/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	N	2	4	-	4/6/26/26	0/1/1/1
4	BMA	N	3	4	-	2/2/22/22	0/1/1/1
4	NAG	O	1	4	-	4/6/26/26	0/1/1/1
4	NAG	O	2	4	-	0/6/26/26	0/1/1/1
4	BMA	O	3	4	-	0/2/22/22	0/1/1/1
2	NAG	P	1	2	-	2/6/26/26	0/1/1/1
2	NAG	P	2	2	-	2/6/26/26	0/1/1/1
5	NAG	Q	1	5	-	6/6/26/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/26/26	0/1/1/1
5	BMA	Q	3	5	-	0/2/22/22	0/1/1/1
3	NAG	R	1	3,1	-	0/6/26/26	0/1/1/1
3	NAG	R	2	3	-	0/6/26/26	0/1/1/1
3	BMA	R	3	3	-	1/2/22/22	0/1/1/1
3	MAN	R	4	3	-	1/2/22/22	0/1/1/1
2	NAG	S	1	2	-	5/6/26/26	0/1/1/1
2	NAG	S	2	2	-	2/6/26/26	0/1/1/1
2	NAG	T	1	2	-	6/6/26/26	0/1/1/1
2	NAG	T	2	2	-	1/6/26/26	0/1/1/1
3	NAG	U	1	3	-	2/6/26/26	0/1/1/1
3	NAG	U	2	3	-	0/6/26/26	0/1/1/1
3	BMA	U	3	3	-	2/2/22/22	0/1/1/1
3	MAN	U	4	3	-	0/2/22/22	0/1/1/1
2	NAG	V	1	2	-	2/6/26/26	0/1/1/1
2	NAG	V	2	2	-	6/6/26/26	0/1/1/1
4	NAG	W	1	4	-	0/6/26/26	0/1/1/1
4	NAG	W	2	4	1/1/6/7	4/6/26/26	0/1/1/1
4	BMA	W	3	4	-	2/2/22/22	0/1/1/1
2	NAG	X	1	2	-	2/6/26/26	0/1/1/1
2	NAG	X	2	2	-	4/6/26/26	0/1/1/1
4	NAG	Y	1	4,1	-	0/6/26/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/26/26	0/1/1/1
4	BMA	Y	3	4	-	1/2/22/22	0/1/1/1
2	NAG	Z	1	2	-	4/6/26/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/26/26	0/1/1/1
4	NAG	a	1	4,1	-	3/6/26/26	0/1/1/1
4	NAG	a	2	4	-	4/6/26/26	0/1/1/1
4	BMA	a	3	4	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	b	1	4	-	5/6/26/26	0/1/1/1
4	NAG	b	2	4	-	0/6/26/26	0/1/1/1
4	BMA	b	3	4	-	0/2/22/22	0/1/1/1
2	NAG	c	1	2	-	4/6/26/26	0/1/1/1
2	NAG	c	2	2	-	1/6/26/26	0/1/1/1
2	NAG	d	1	2	-	0/6/26/26	0/1/1/1
2	NAG	d	2	2	-	3/6/26/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	3	BMA	C4-C5	2.98	1.59	1.53
2	S	1	NAG	O5-C1	-2.81	1.36	1.42
3	R	3	BMA	C1-C2	2.22	1.57	1.52
5	Q	3	BMA	O5-C1	2.08	1.48	1.42
3	U	4	MAN	C1-C2	2.02	1.57	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	2	NAG	O1-C1-O5	8.29	135.04	110.41
3	U	4	MAN	O1-C1-O5	-5.06	95.38	110.41
2	S	1	NAG	C3-C4-C5	4.27	117.97	110.23
3	E	4	MAN	O1-C1-O5	-4.16	98.05	110.41
3	F	4	MAN	O1-C1-O5	-3.85	98.97	110.41
2	S	1	NAG	C4-C3-C2	3.45	115.43	110.40
5	Q	1	NAG	C1-C2-N2	3.08	114.30	110.73
2	M	2	NAG	C1-C2-N2	2.97	114.17	110.73
4	b	1	NAG	C1-C2-N2	2.94	114.13	110.73
2	G	2	NAG	C1-C2-N2	2.83	114.01	110.73
2	V	2	NAG	C1-C2-N2	2.74	113.91	110.73
2	Z	1	NAG	C2-N2-C7	2.69	129.40	123.11
2	Z	1	NAG	C1-C2-N2	2.69	113.84	110.73
2	T	1	NAG	C1-C2-N2	2.64	113.78	110.73
2	c	1	NAG	C1-O5-C5	2.63	118.75	113.65
2	V	2	NAG	C2-N2-C7	2.58	129.14	123.11
2	M	2	NAG	C2-N2-C7	2.57	129.12	123.11
4	b	1	NAG	C2-N2-C7	2.57	129.12	123.11
3	R	4	MAN	O1-C1-O5	-2.55	102.83	110.41
4	N	2	NAG	C2-N2-C7	2.50	128.95	123.11
2	T	1	NAG	C2-N2-C7	2.48	128.91	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	2	NAG	C1-C2-N2	2.48	113.60	110.73
2	G	2	NAG	C2-N2-C7	2.47	128.90	123.11
5	Q	1	NAG	C2-N2-C7	2.46	128.88	123.11
4	W	3	BMA	O1-C1-O5	2.46	117.71	110.41
2	S	1	NAG	C2-N2-C7	2.43	128.80	123.11
3	U	4	MAN	C1-O5-C5	2.43	118.35	113.65
4	a	3	BMA	O1-C1-O5	2.30	117.26	110.41
2	S	1	NAG	C1-C2-N2	2.17	113.24	110.73
3	R	3	BMA	O1-C1-O5	2.14	116.76	110.41
2	S	1	NAG	O5-C5-C4	2.12	113.53	109.70
3	F	4	MAN	O2-C2-C3	-2.01	105.63	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	W	2	NAG	C1

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	1	NAG	C1-C2-N2-C7
2	d	2	NAG	C1-C2-N2-C7
4	O	1	NAG	C1-C2-N2-C7
3	F	2	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	c	1	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
3	U	3	BMA	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	S	1	NAG	C8-C7-N2-C2
2	S	1	NAG	O7-C7-N2-C2
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2
2	V	2	NAG	C8-C7-N2-C2
2	V	2	NAG	O7-C7-N2-C2
2	Z	1	NAG	C8-C7-N2-C2
2	Z	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2
4	b	1	NAG	C8-C7-N2-C2
4	b	1	NAG	O7-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
4	W	3	BMA	O5-C5-C6-O6
3	U	3	BMA	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	X	1	NAG	C1-C2-N2-C7
2	I	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	L	1	NAG	C4-C5-C6-O6
3	R	4	MAN	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
4	Y	3	BMA	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	R	3	BMA	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C3-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7
2	X	2	NAG	C3-C2-N2-C7
2	c	1	NAG	C3-C2-N2-C7
5	Q	1	NAG	C3-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
2	M	1	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
4	b	1	NAG	C3-C2-N2-C7
3	U	1	NAG	O5-C5-C6-O6
4	W	3	BMA	C4-C5-C6-O6
2	Z	1	NAG	C3-C2-N2-C7
2	J	2	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7
2	S	1	NAG	C3-C2-N2-C7
2	P	2	NAG	C1-C2-N2-C7
2	T	1	NAG	C1-C2-N2-C7
2	V	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
4	a	1	NAG	C1-C2-N2-C7
4	N	3	BMA	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	T	1	NAG	C3-C2-N2-C7
2	V	2	NAG	C3-C2-N2-C7
5	Q	1	NAG	C4-C5-C6-O6
4	O	1	NAG	C3-C2-N2-C7
2	d	2	NAG	C3-C2-N2-C7
2	c	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	X	2	NAG	C1-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7
4	a	1	NAG	C3-C2-N2-C7
2	V	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C1-C2-N2-C7
2	S	1	NAG	C1-C2-N2-C7
2	Z	1	NAG	C1-C2-N2-C7
2	c	1	NAG	C1-C2-N2-C7
4	N	2	NAG	C1-C2-N2-C7
4	b	1	NAG	C1-C2-N2-C7
5	Q	1	NAG	C1-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
2	V	1	NAG	C3-C2-N2-C7
2	X	1	NAG	C3-C2-N2-C7
2	S	2	NAG	O5-C5-C6-O6

There are no ring outliers.

26 monomers are involved in 58 short contacts:

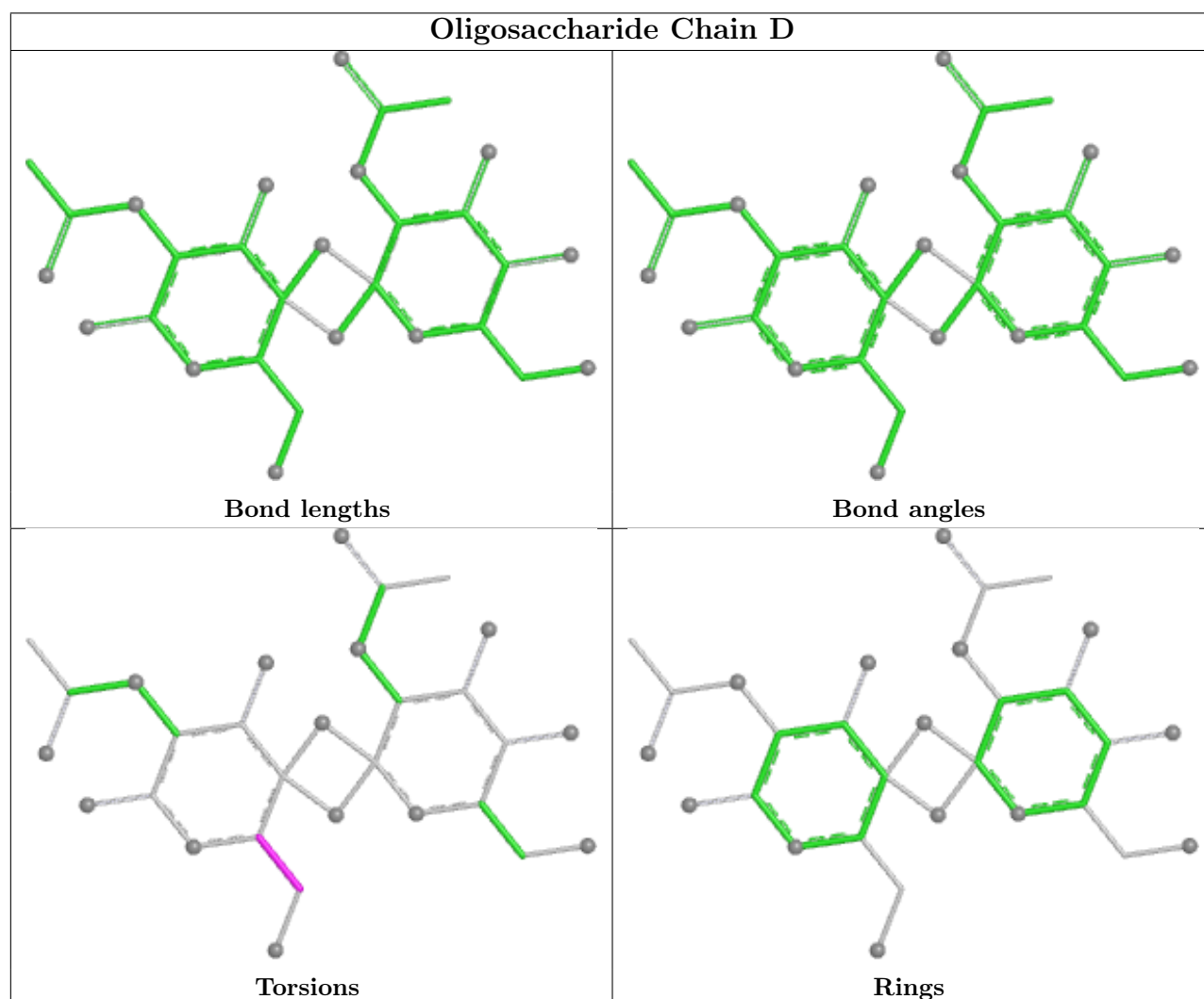
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	c	2	NAG	1	0
5	Q	2	NAG	2	0
2	d	1	NAG	1	0
2	T	2	NAG	2	0
2	L	1	NAG	1	0
4	W	1	NAG	5	0
4	O	1	NAG	8	0
4	b	1	NAG	4	0
2	G	2	NAG	2	0
4	N	2	NAG	2	0
2	J	1	NAG	1	0
2	M	2	NAG	2	0
2	c	1	NAG	1	0
2	L	2	NAG	1	0

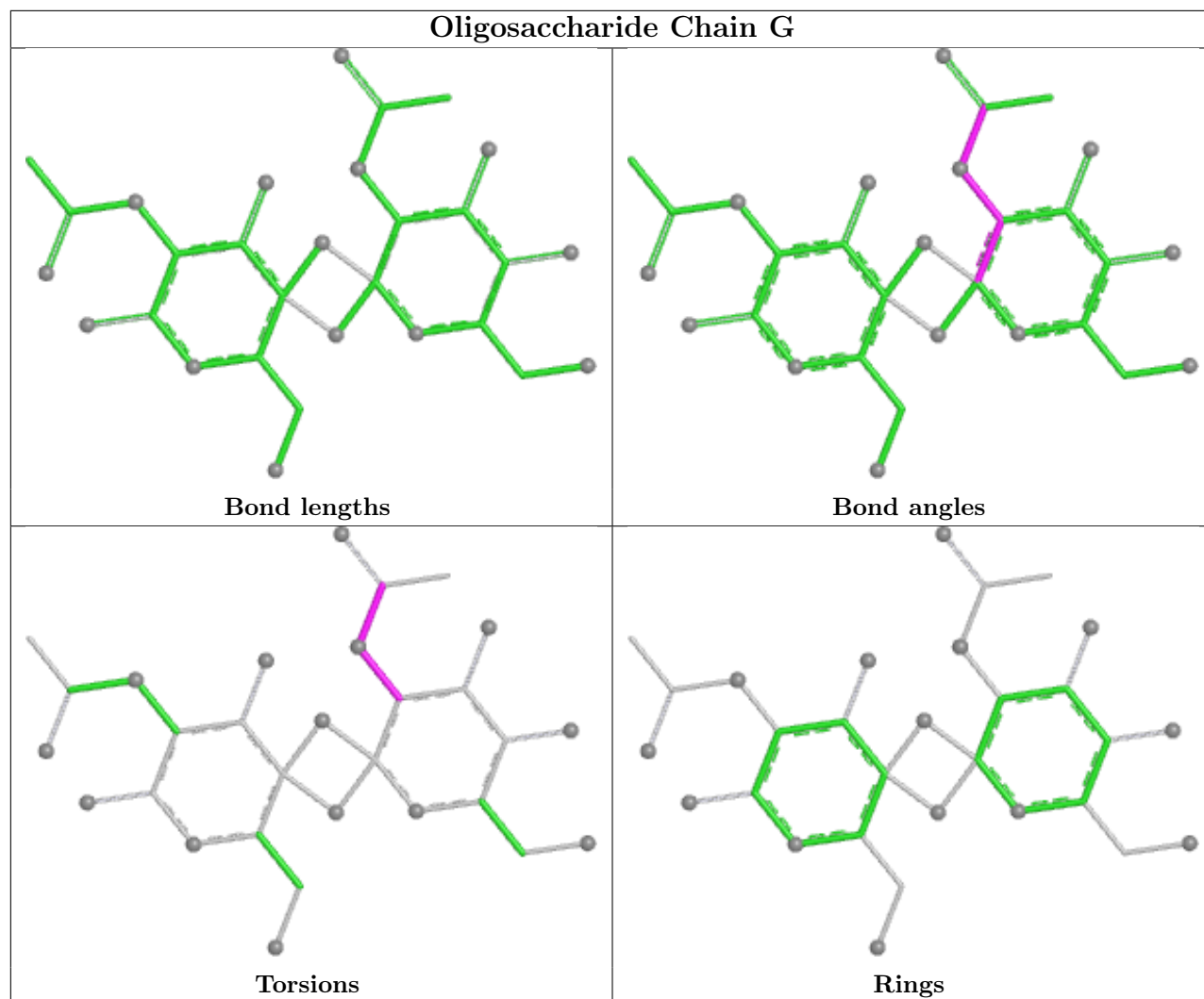
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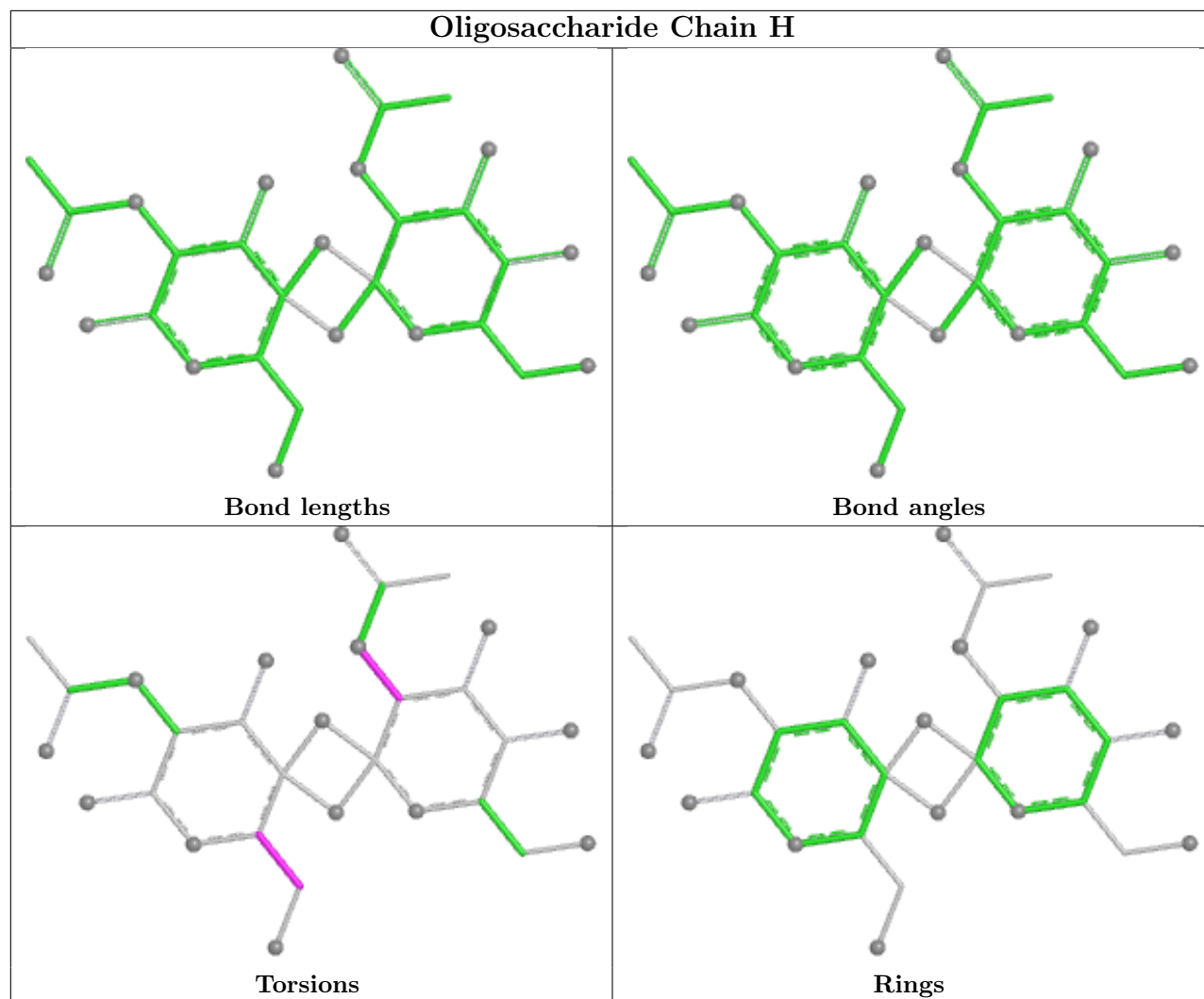
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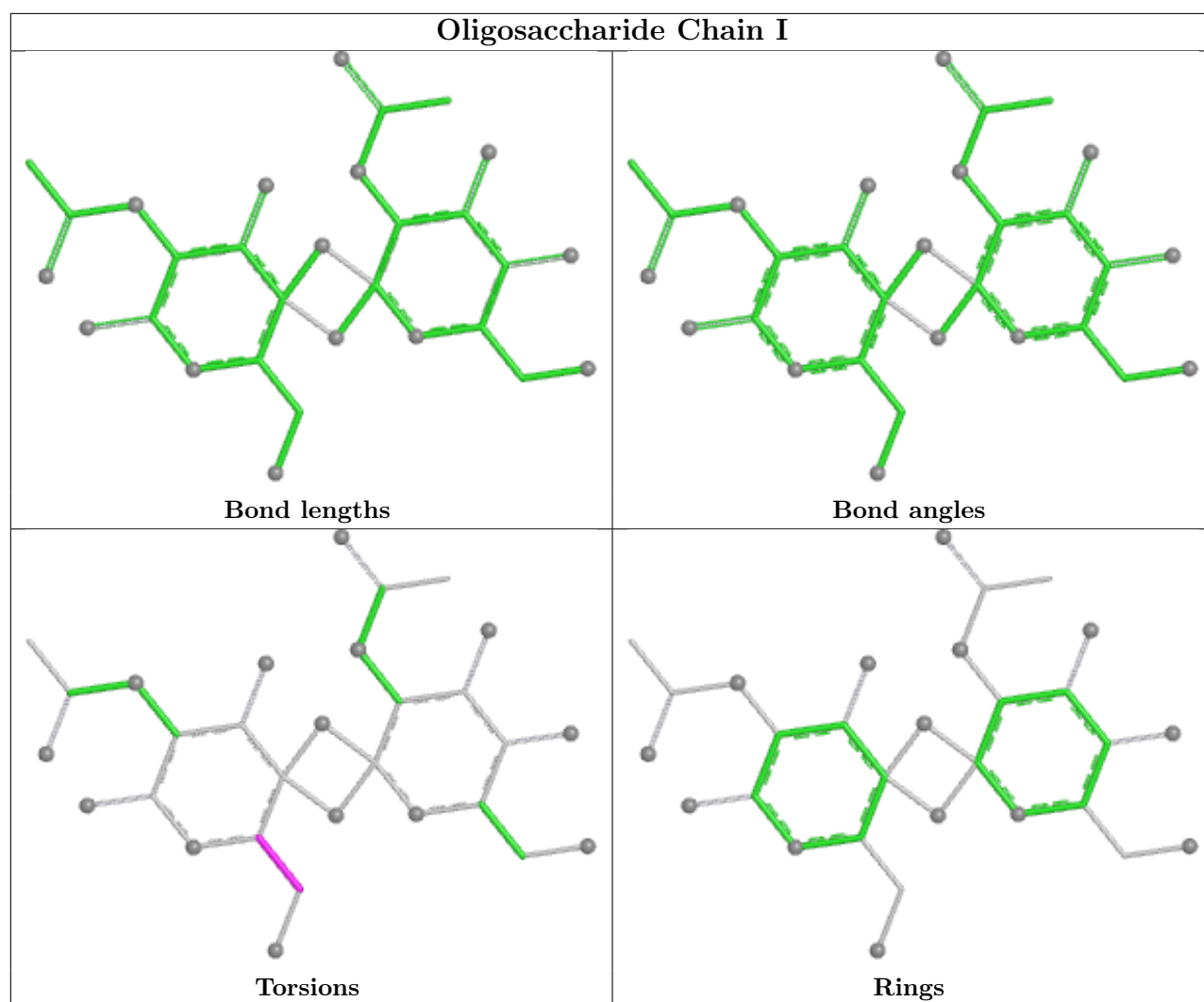
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	3	BMA	1	0
4	a	1	NAG	3	0
4	W	2	NAG	3	0
2	H	1	NAG	2	0
2	Z	1	NAG	1	0
3	U	3	BMA	5	0
5	Q	1	NAG	3	0
2	X	1	NAG	4	0
2	S	1	NAG	2	0
2	T	1	NAG	4	0
2	V	2	NAG	2	0
2	V	1	NAG	4	0

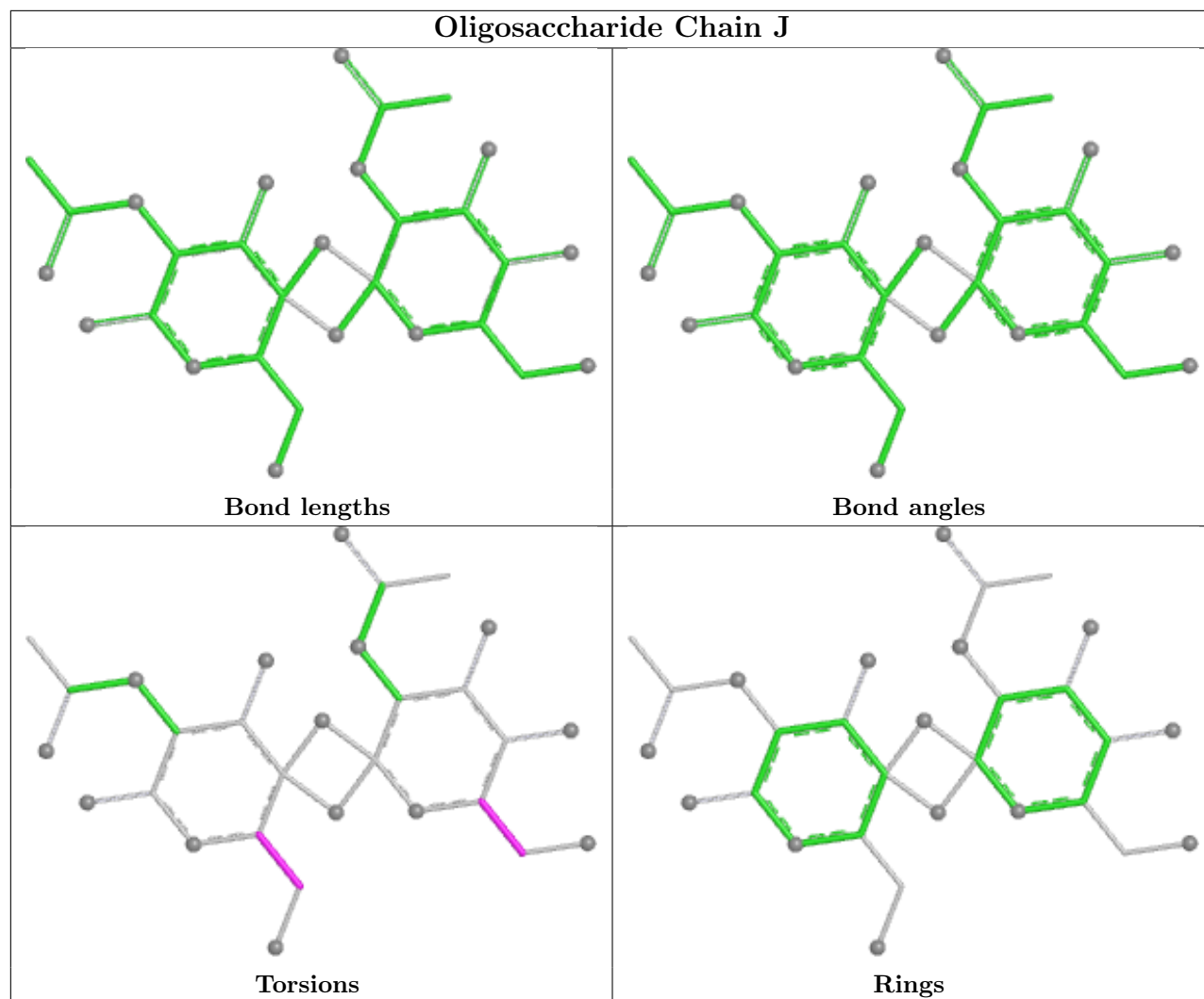
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

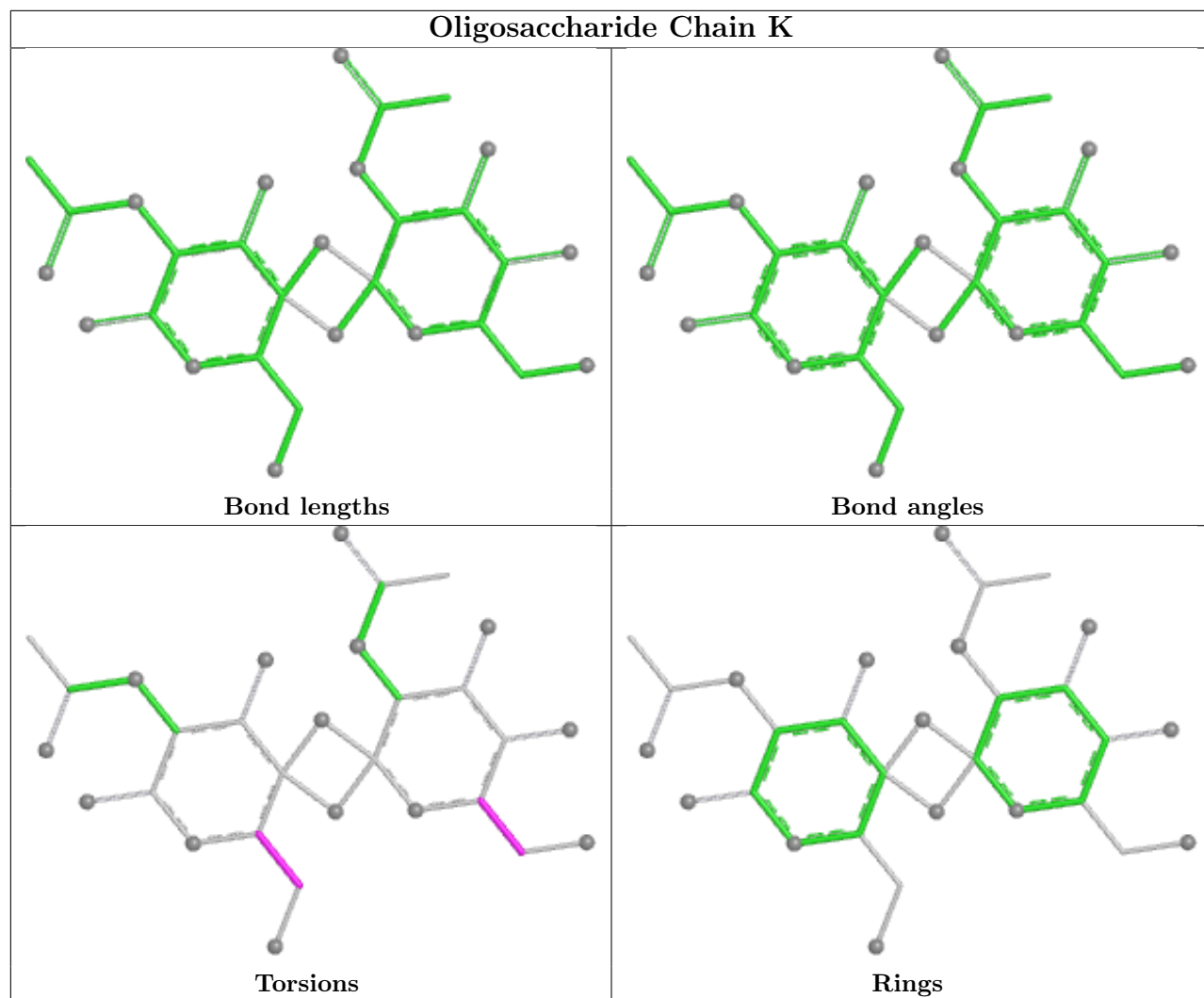


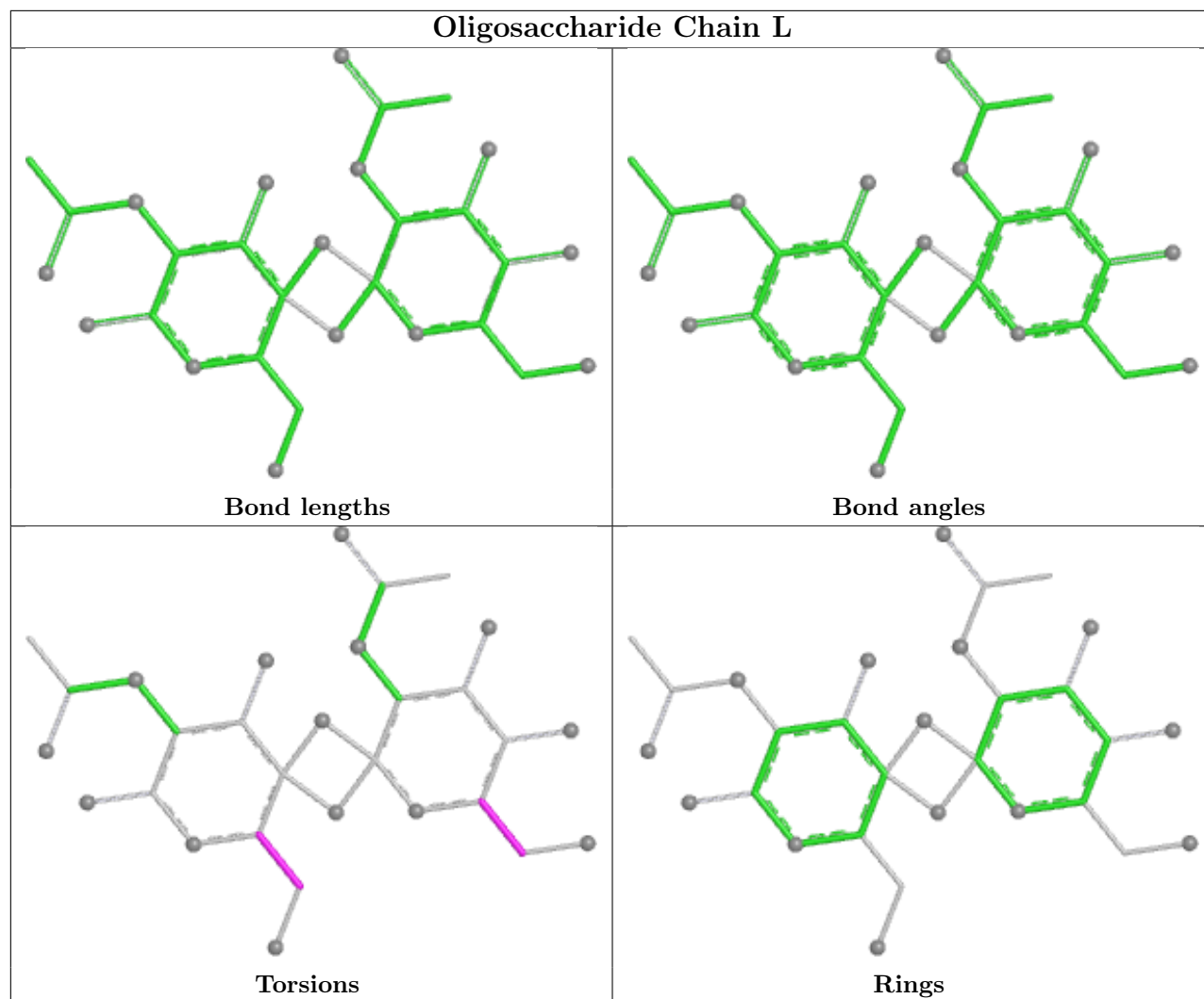


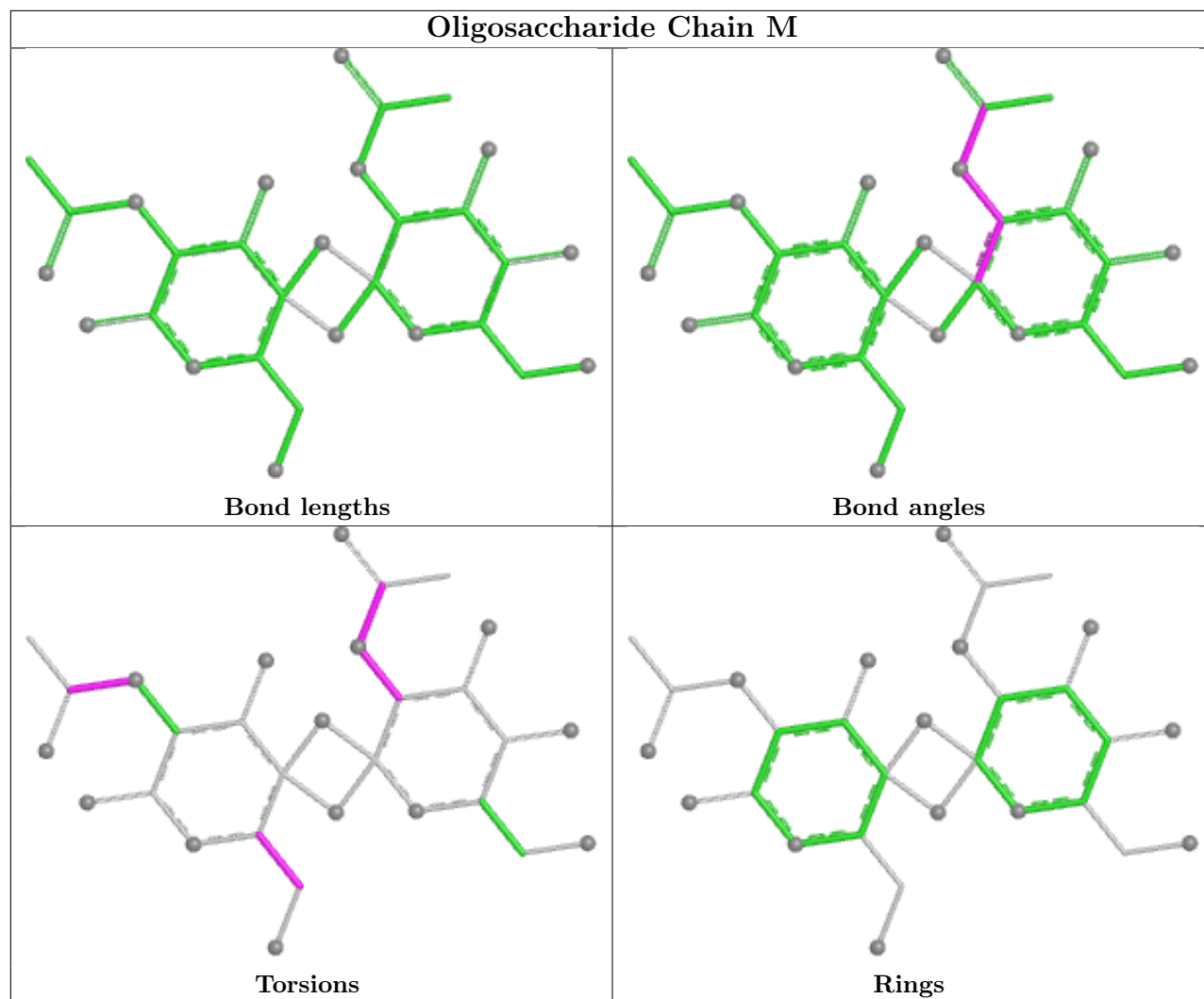


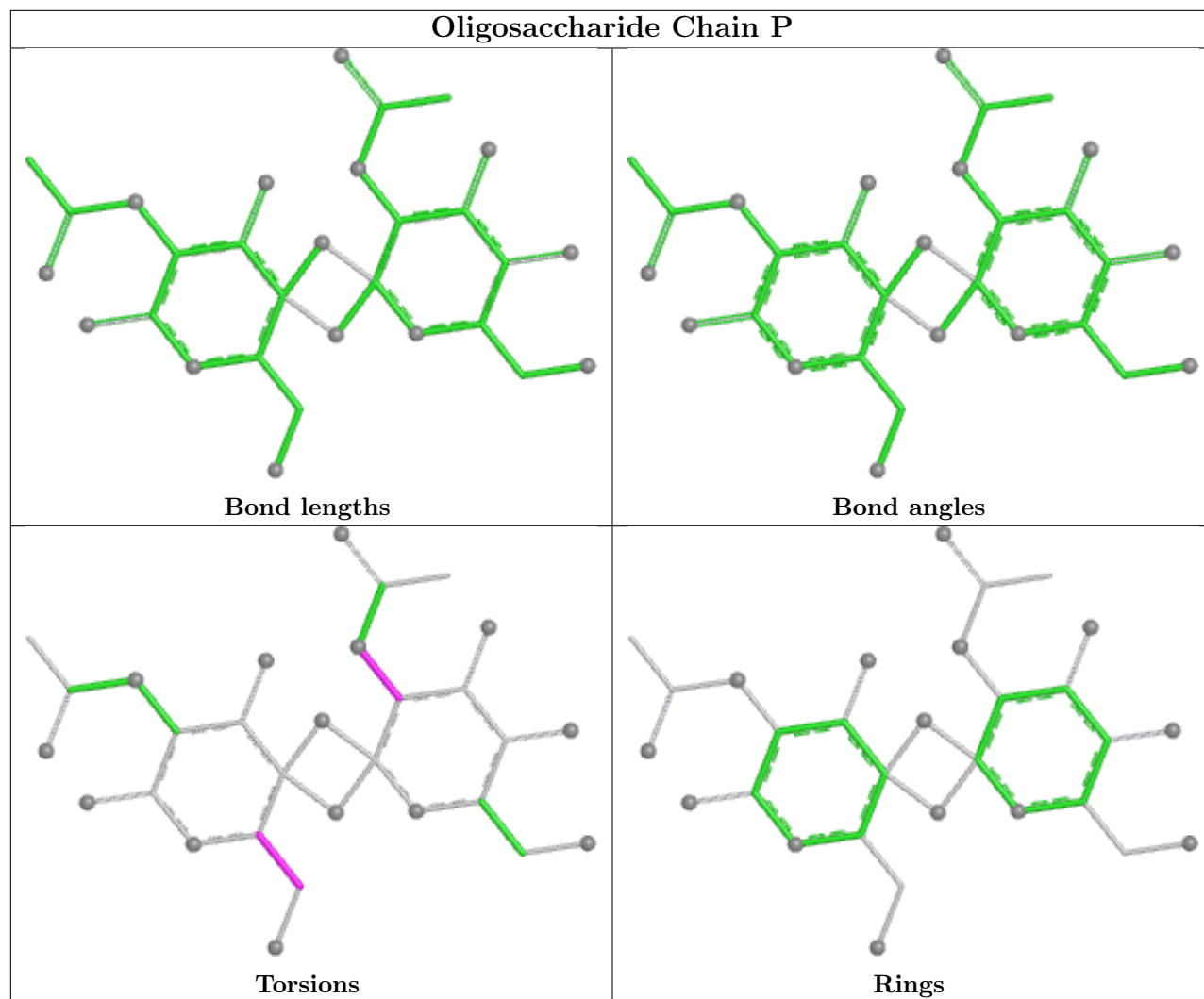


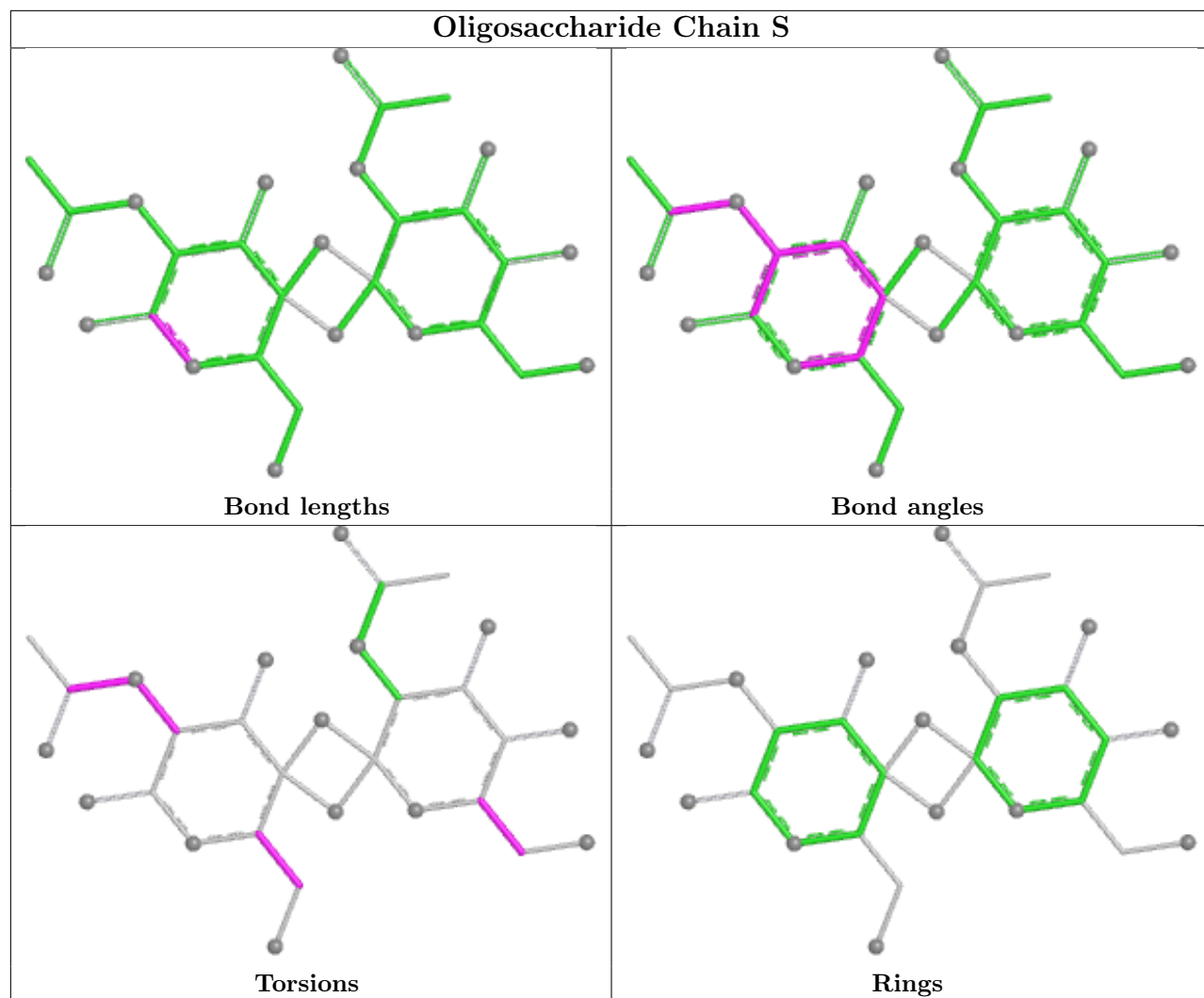


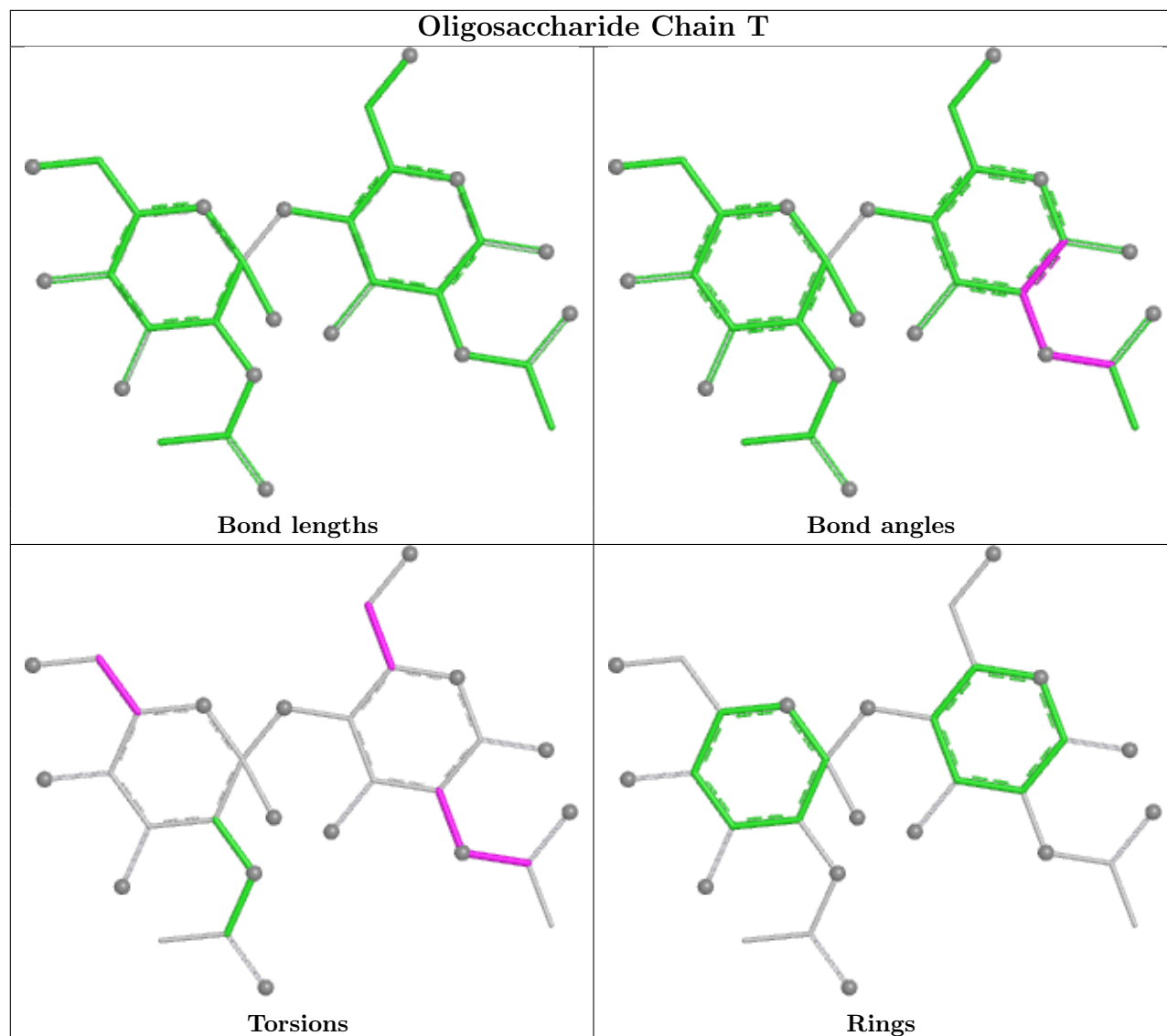


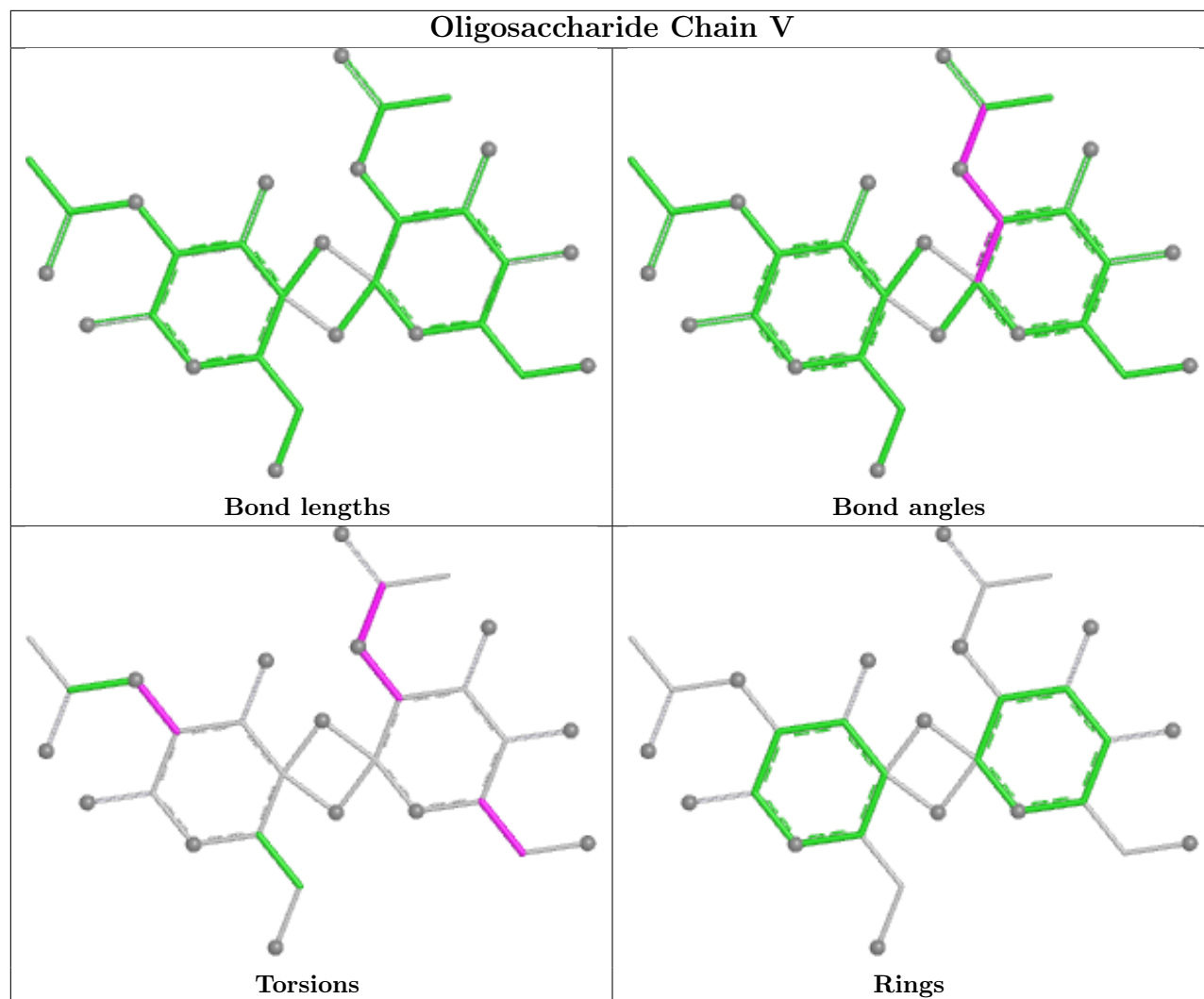


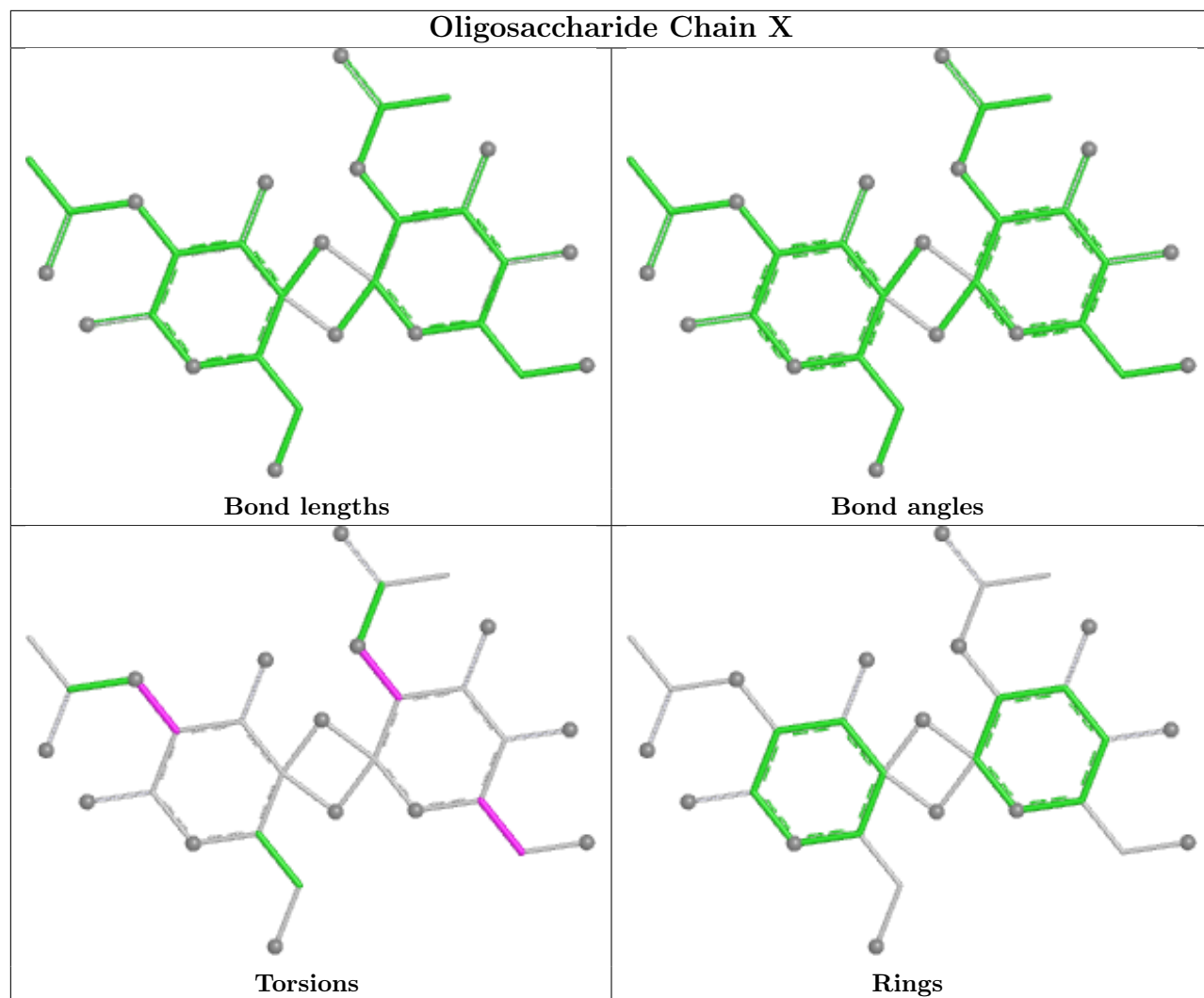


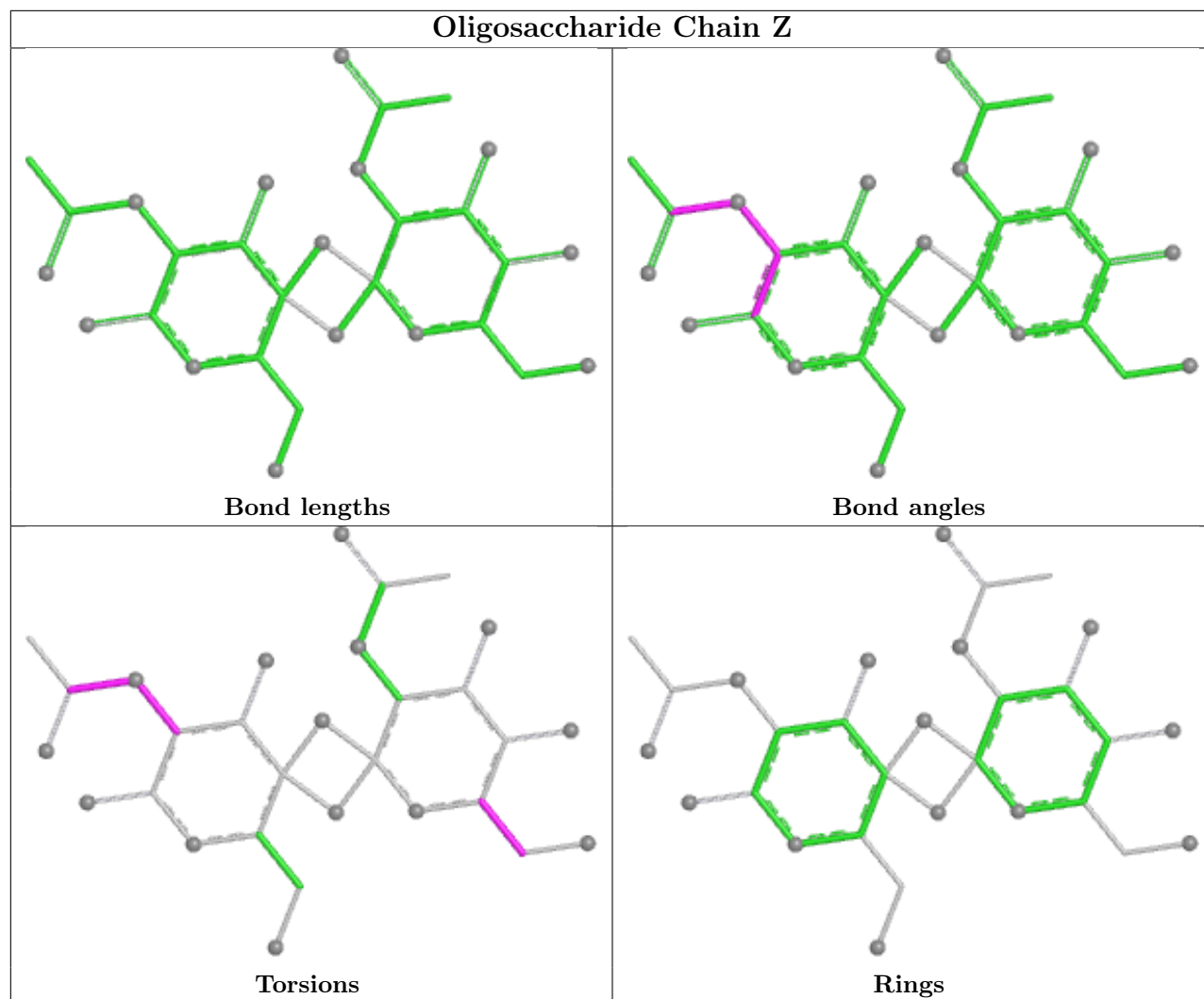


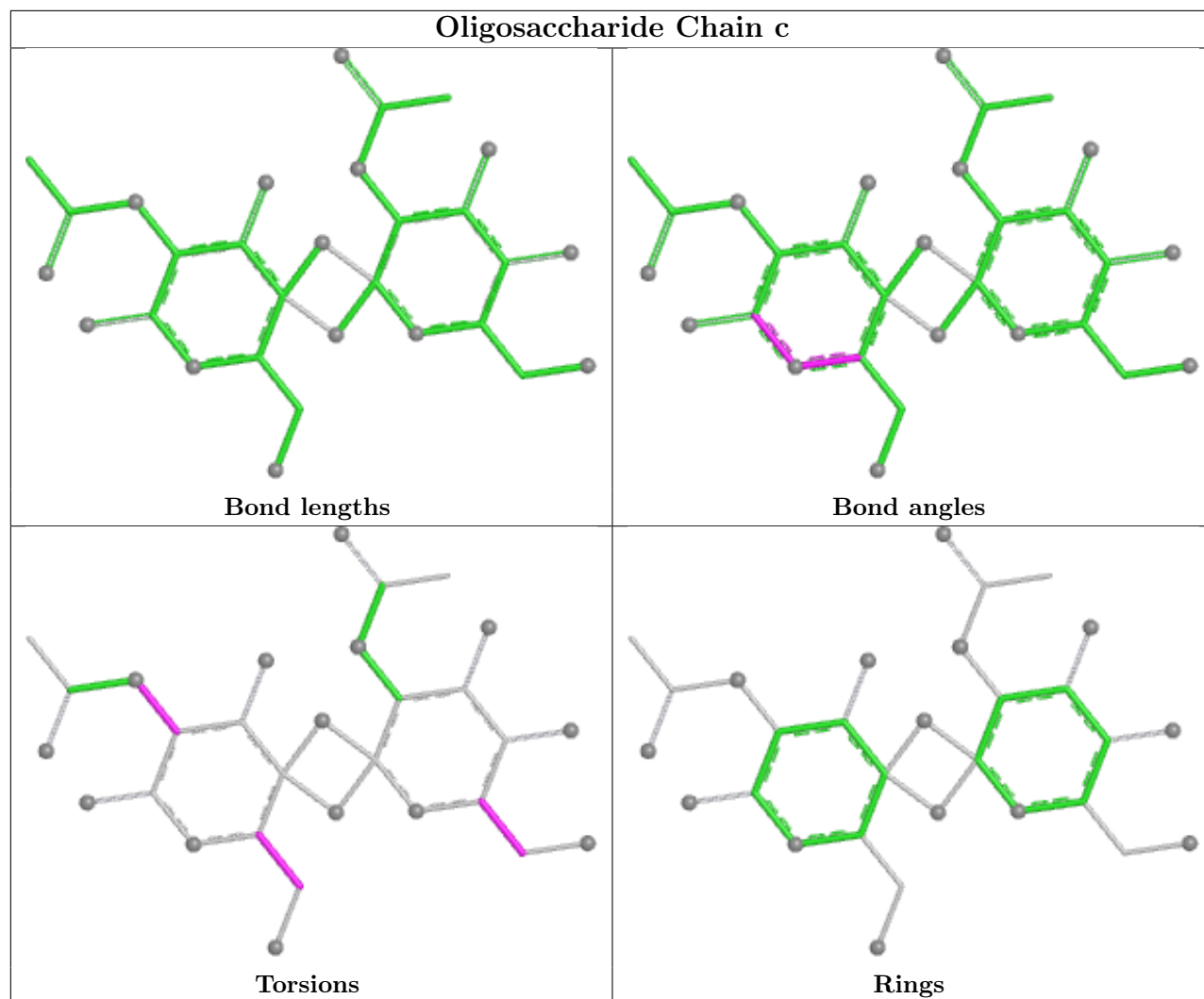


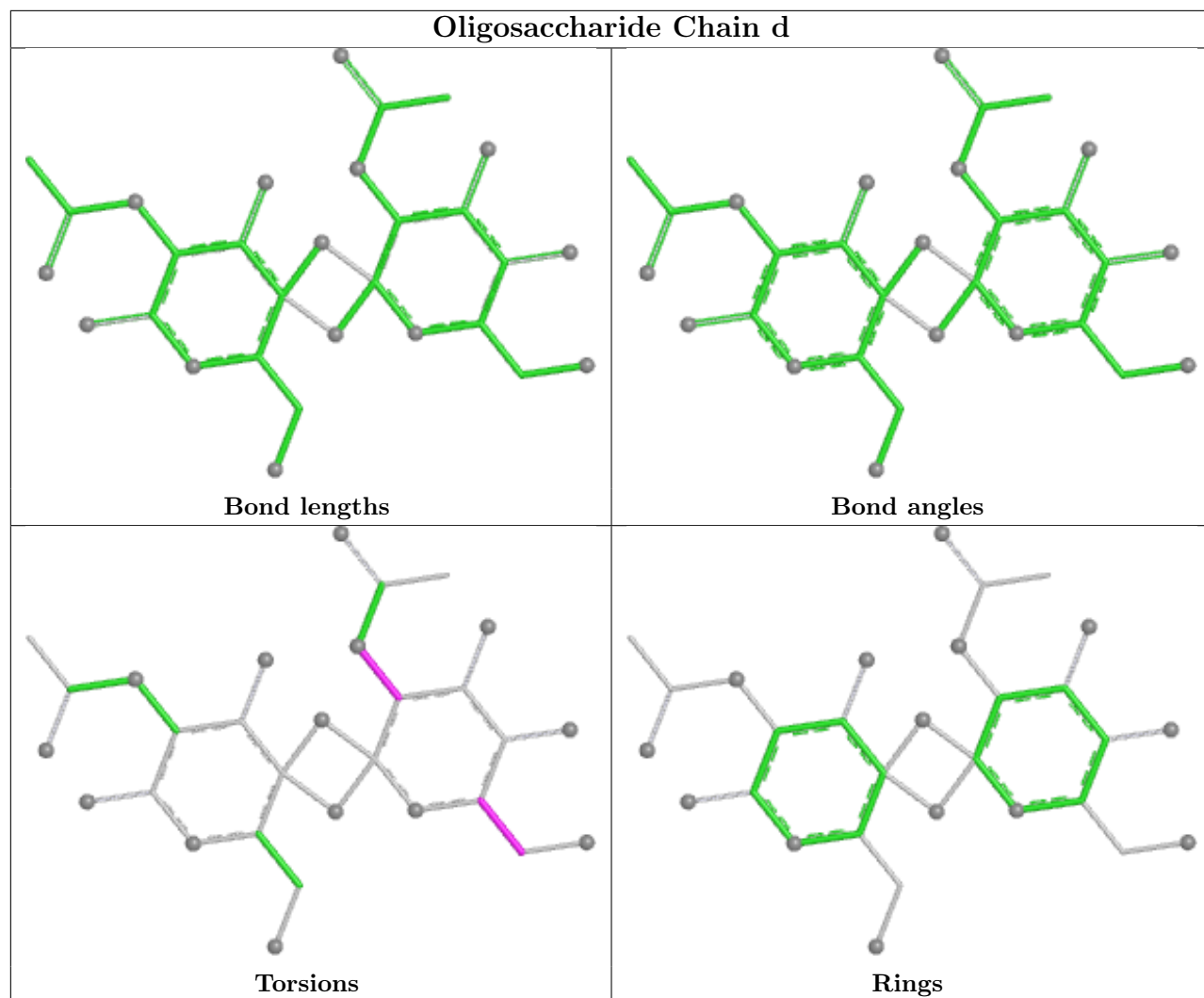


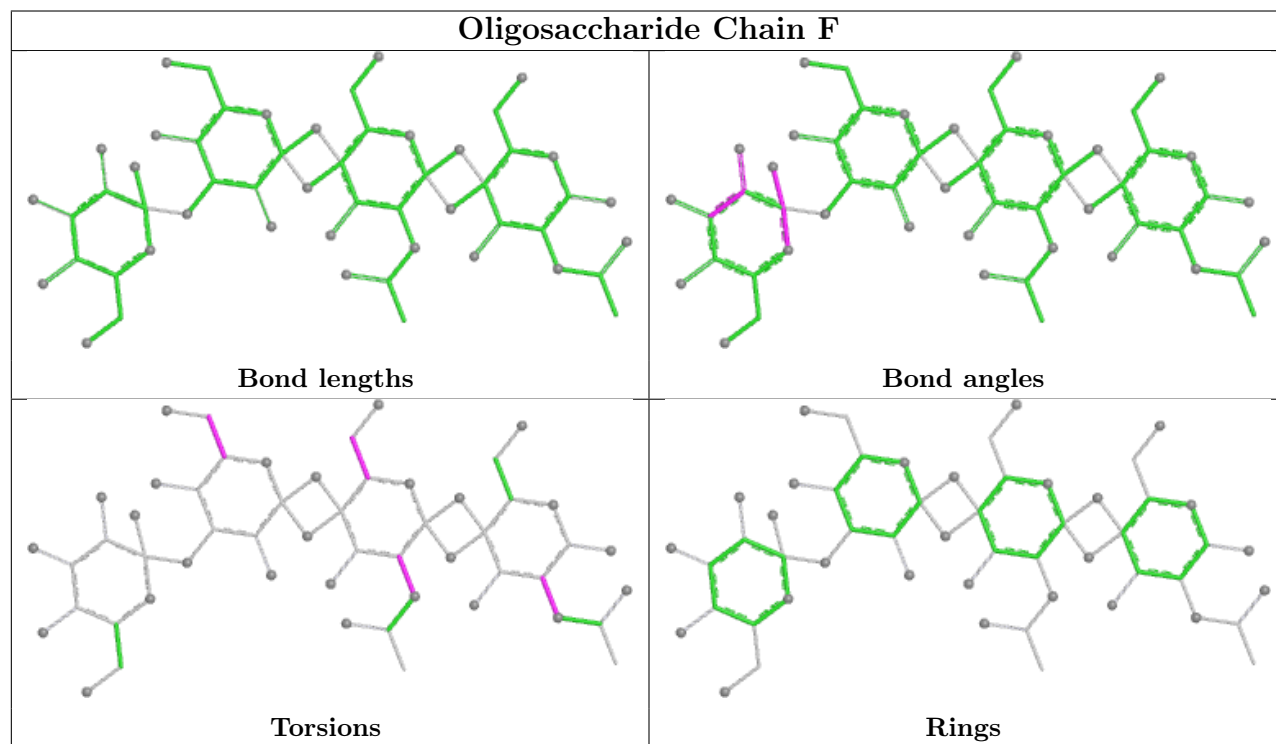
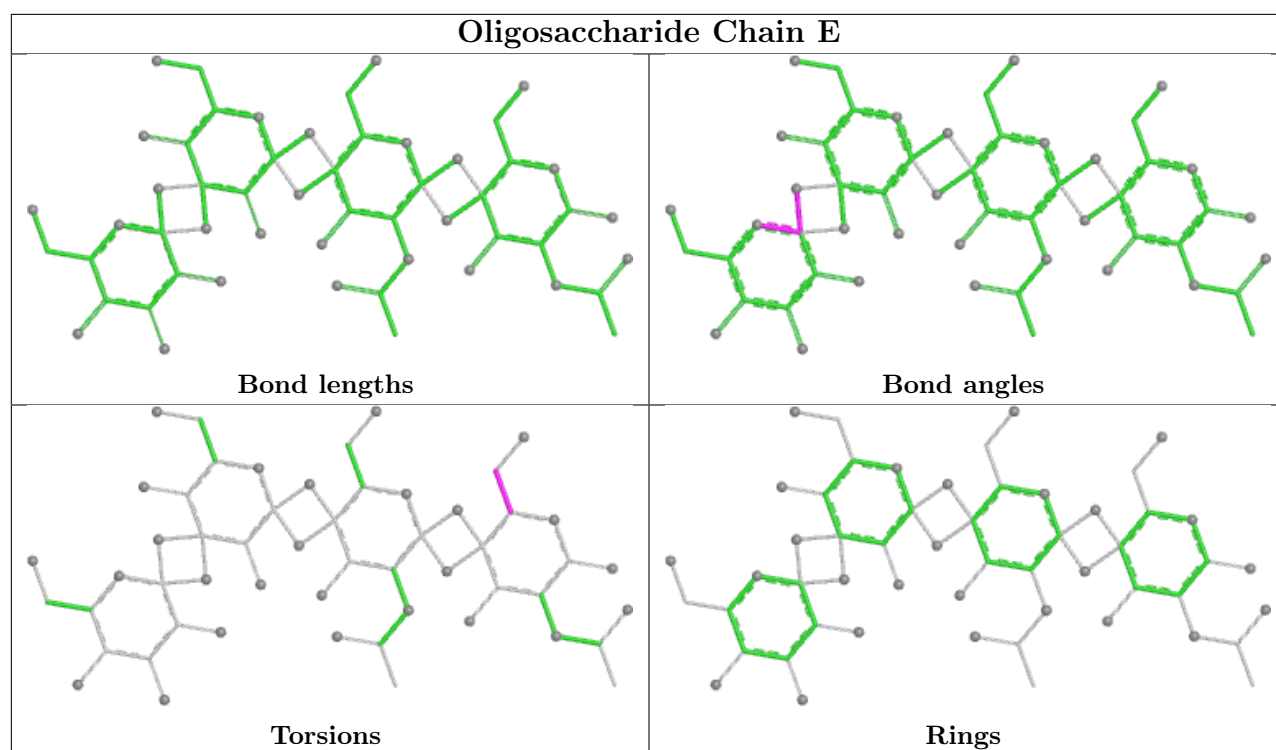


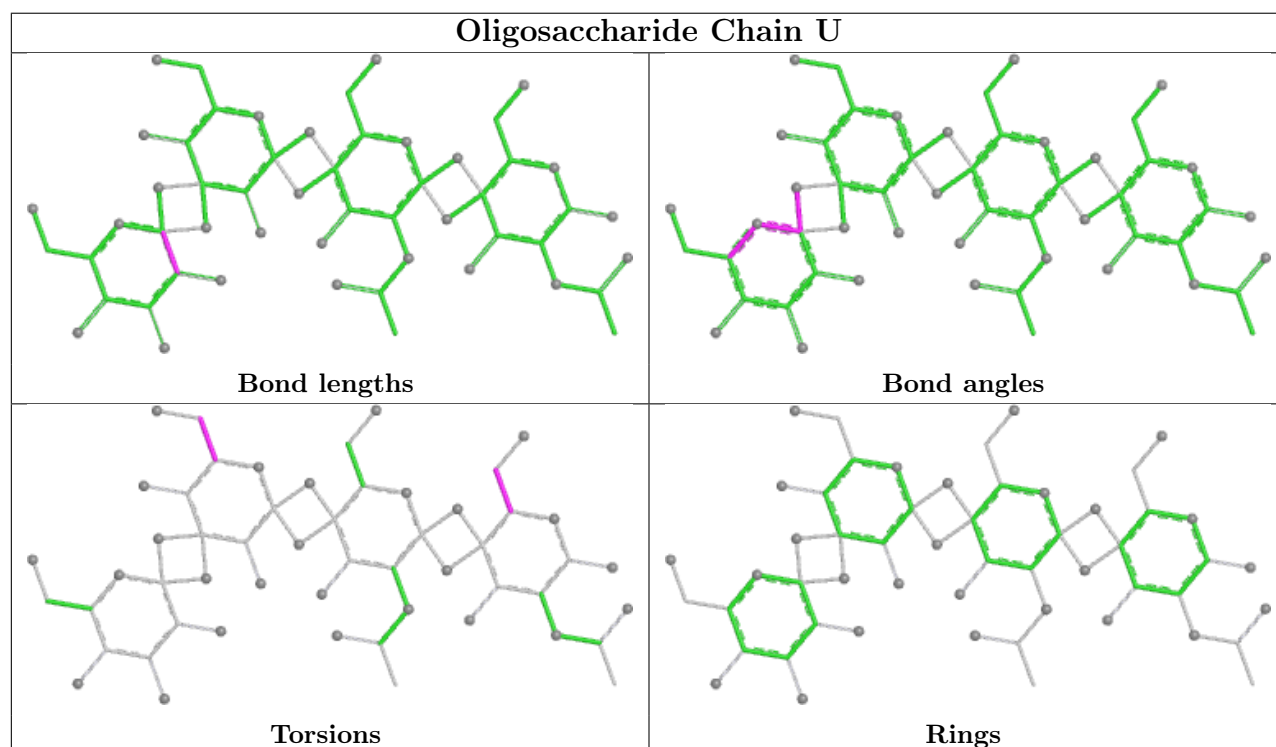
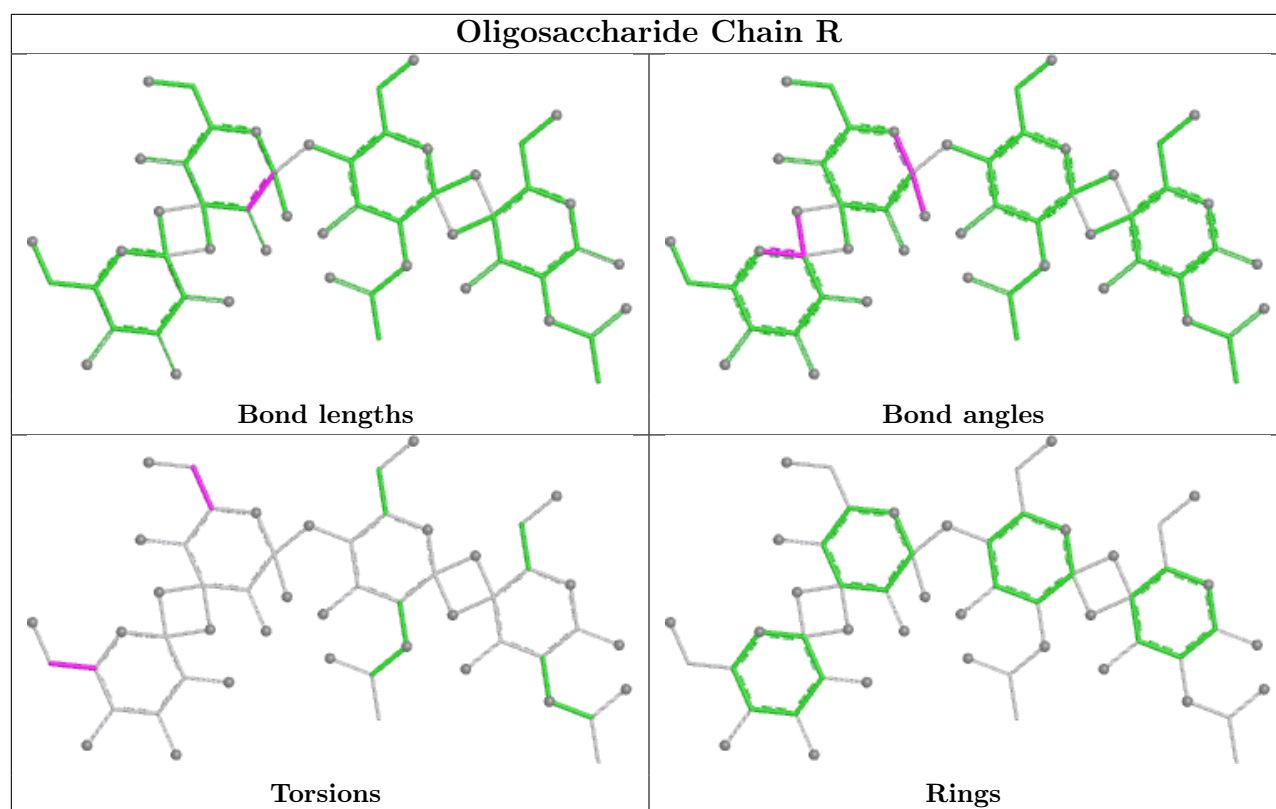


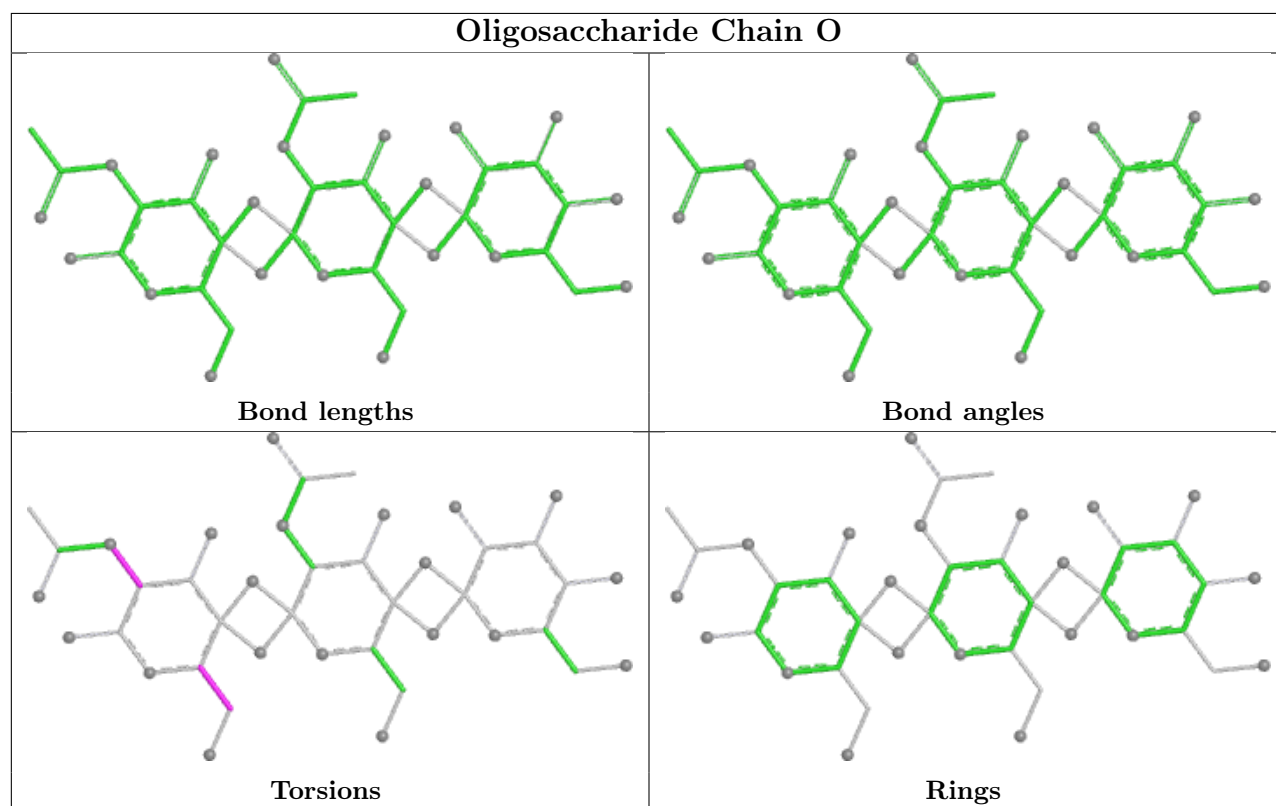
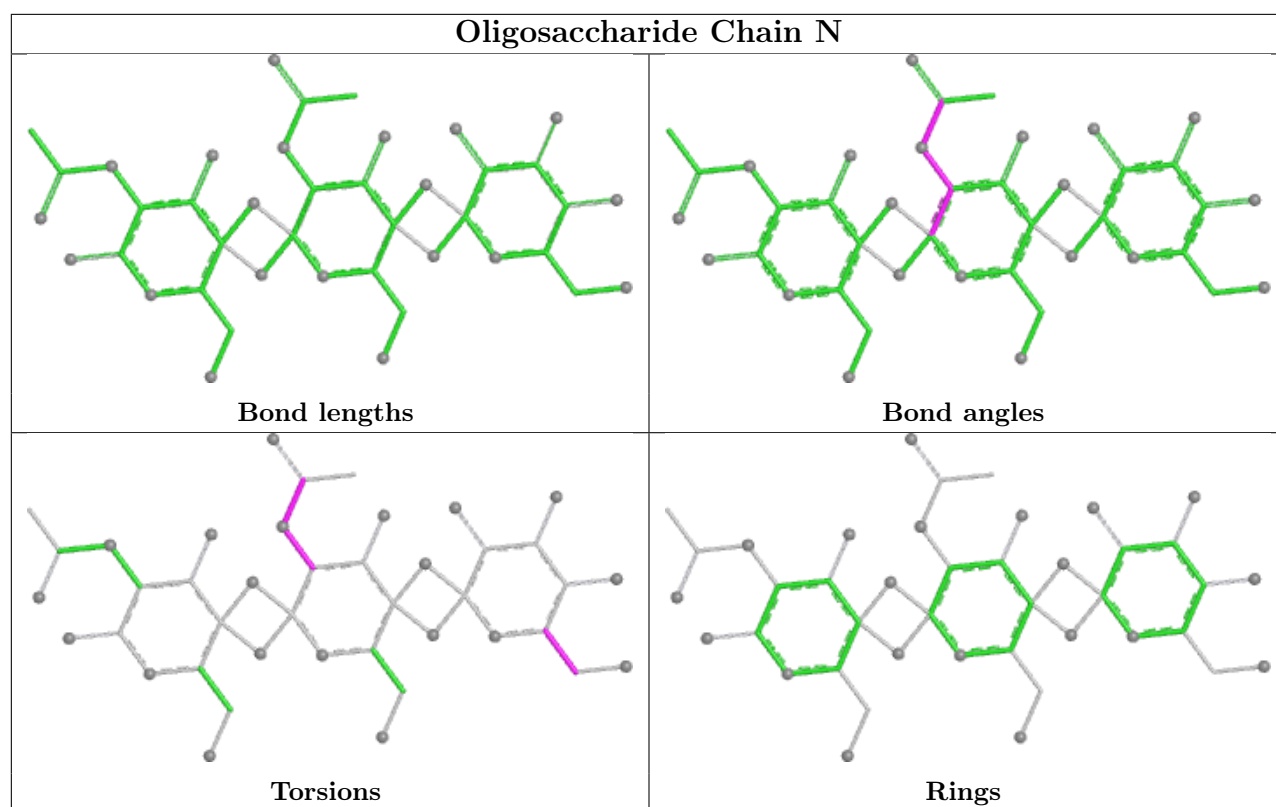




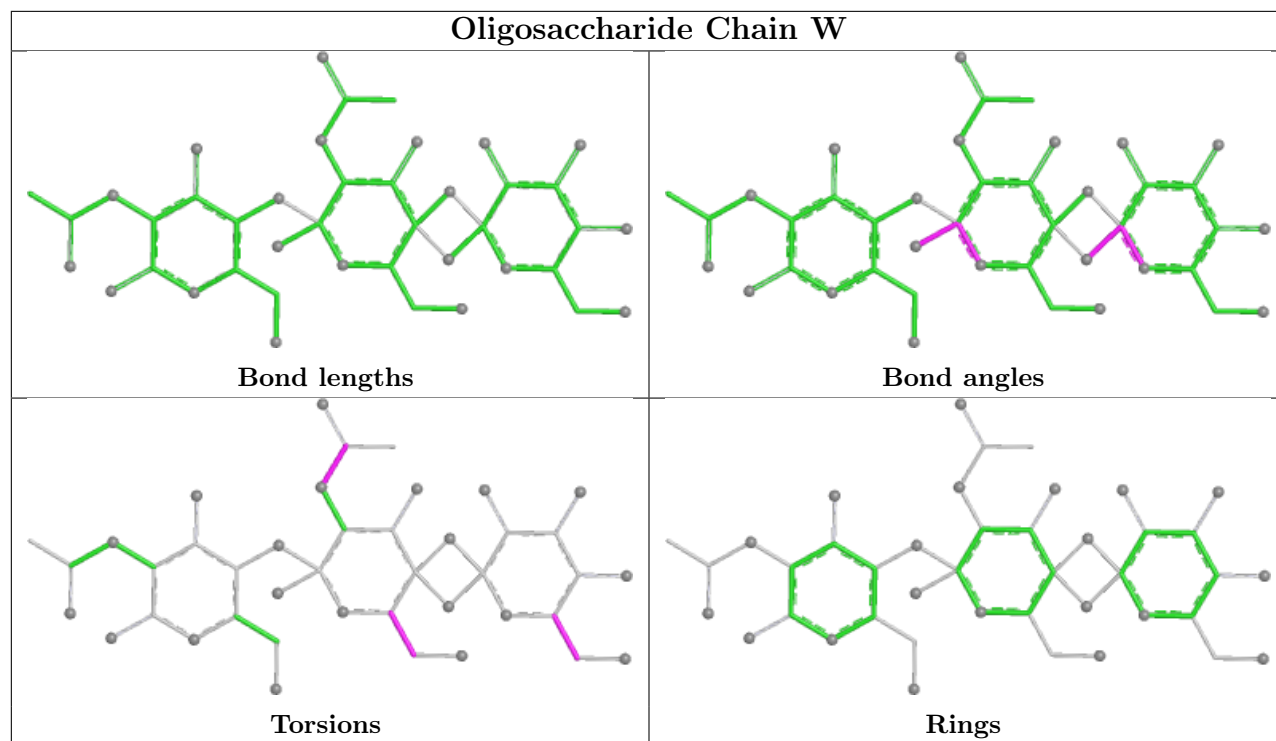




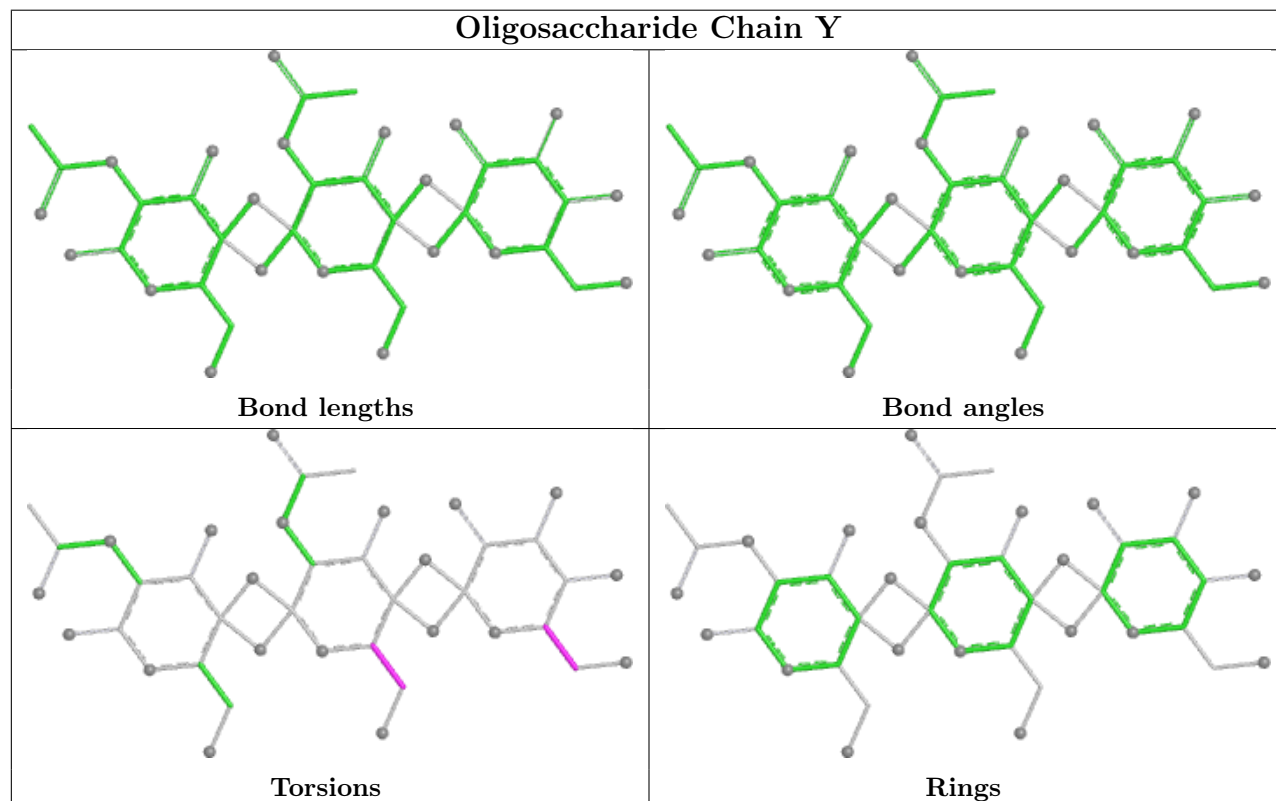


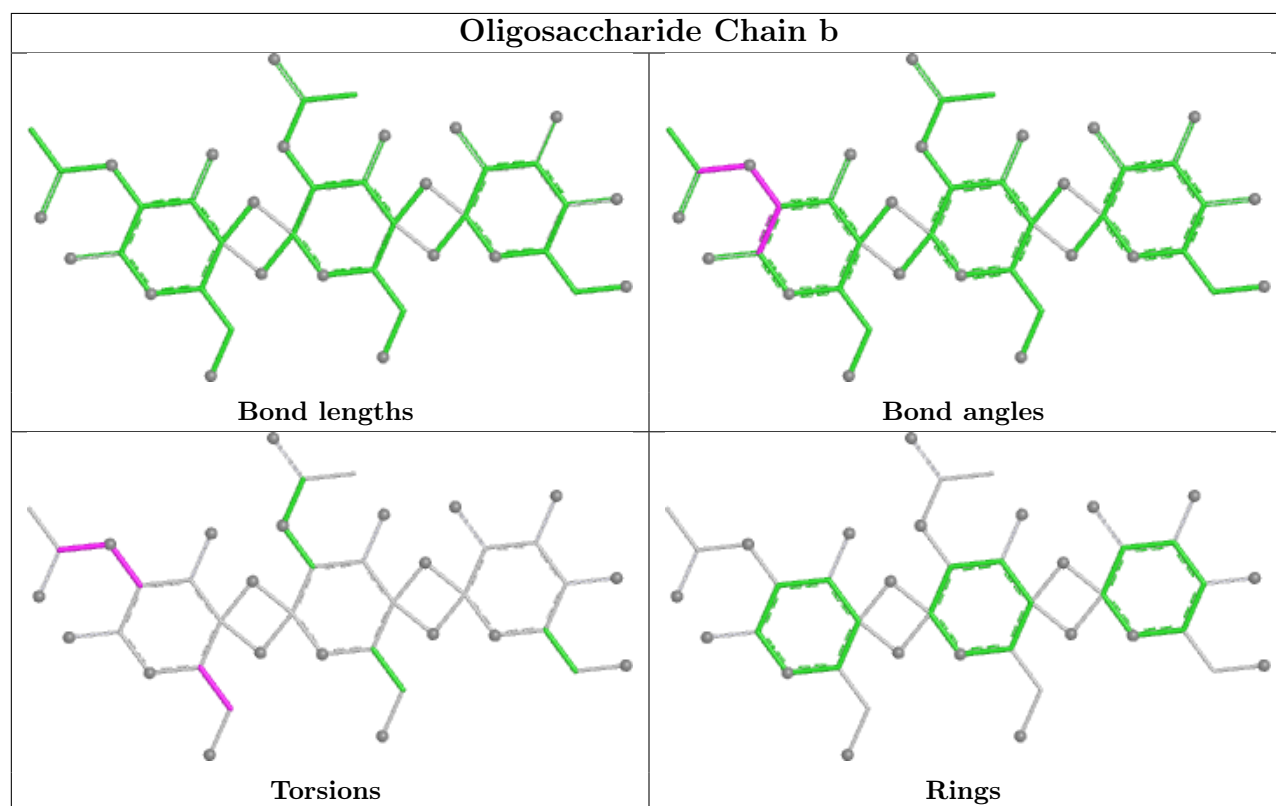
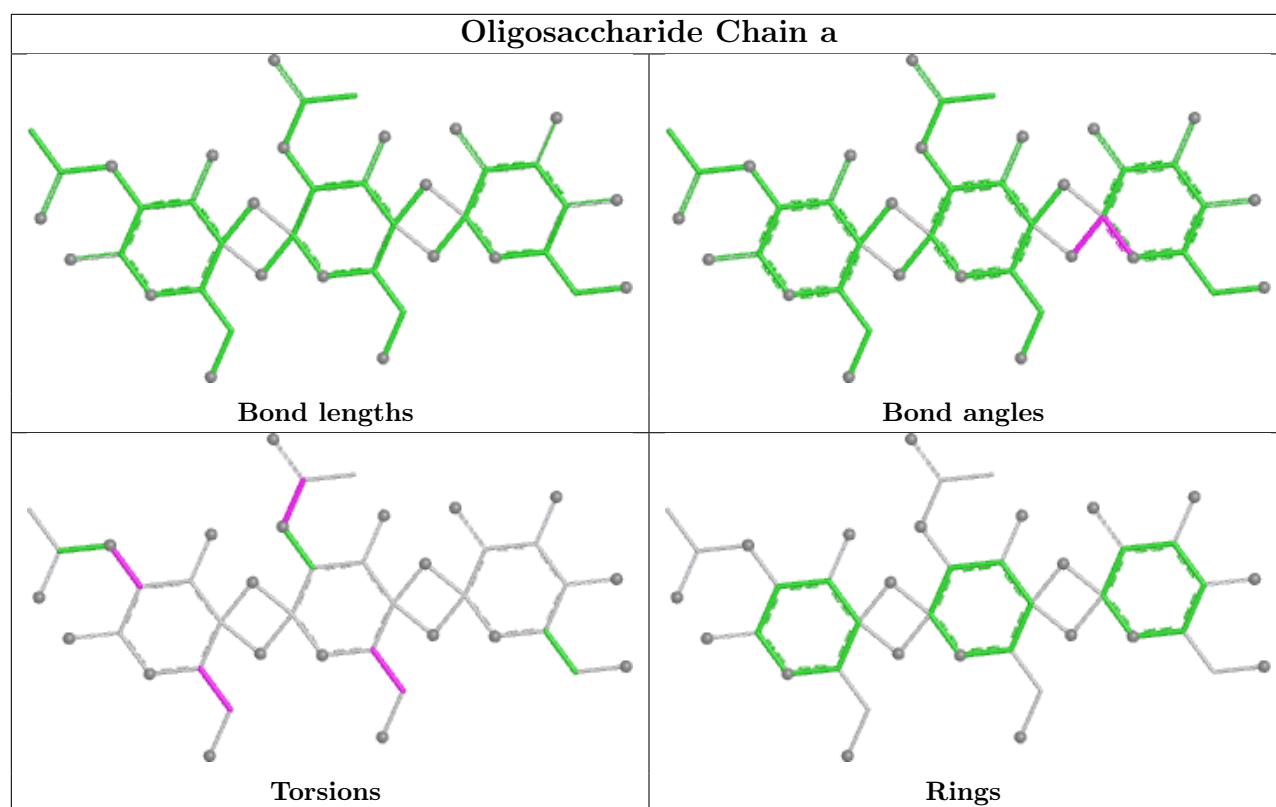


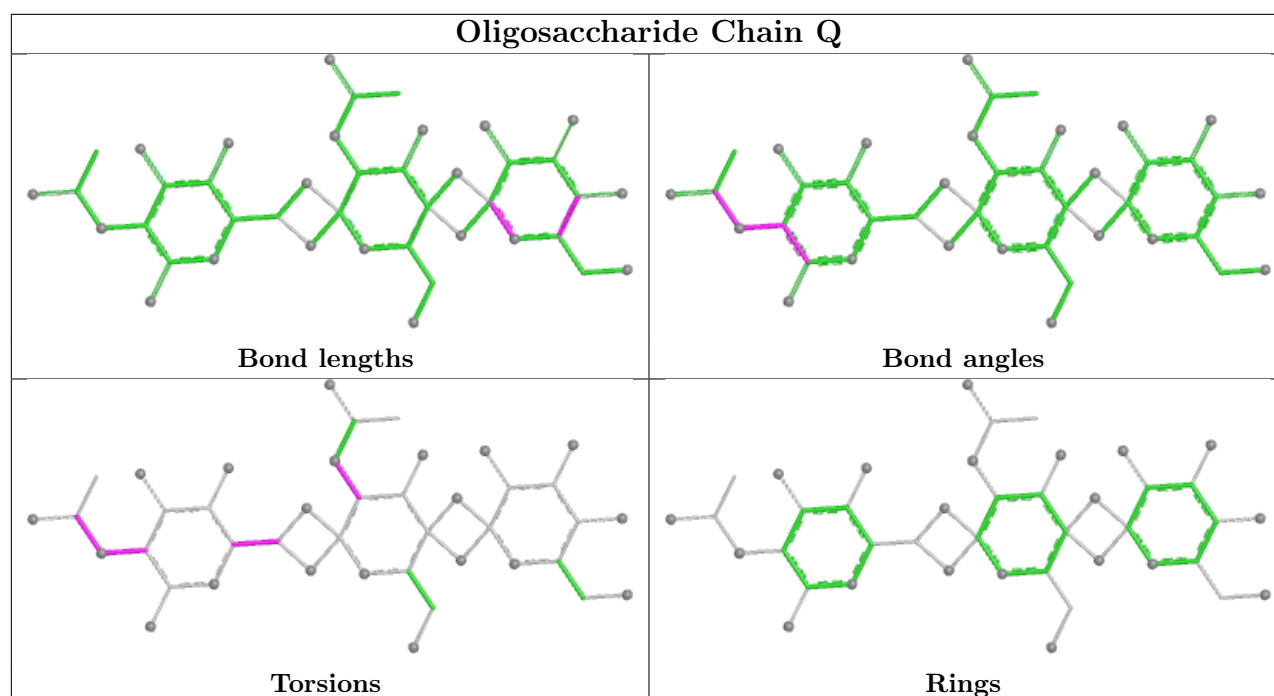
Oligosaccharide Chain W



Oligosaccharide Chain Y







5.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
7	MAN	A	1307	-	12,12,12	0.57	0	17,17,17	1.33	2 (11%)
6	NAG	B	1104	-	15,15,15	0.49	0	21,21,21	0.34	0
8	DMS	A	1308	-	3,3,3	0.67	0	3,3,3	0.50	0
6	NAG	B	1105	-	15,15,15	0.36	0	21,21,21	0.13	0
6	NAG	A	1302	1	15,15,15	0.35	0	21,21,21	0.16	0
6	NAG	B	1106	1	15,15,15	0.51	0	21,21,21	0.42	0
6	NAG	C	1301	-	15,15,15	0.35	0	21,21,21	0.11	0
6	NAG	C	1305	-	15,15,15	0.49	0	21,21,21	0.30	0
8	DMS	A	1309	-	3,3,3	0.68	0	3,3,3	0.52	0
6	NAG	A	1305	-	15,15,15	0.43	0	21,21,21	0.91	2 (9%)
6	NAG	A	1304	-	15,15,15	0.33	0	21,21,21	0.13	0
6	NAG	A	1301	1	15,15,15	0.74	1 (6%)	21,21,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	DMS	A	1310	-	3,3,3	0.67	0	3,3,3	1.15	0
7	MAN	C	1304	-	12,12,12	0.59	0	17,17,17	1.32	1 (5%)
6	NAG	B	1107	1	15,15,15	0.63	0	21,21,21	0.25	0
6	NAG	A	1303	1	15,15,15	0.33	0	21,21,21	0.11	0
6	NAG	B	1108	1	15,15,15	0.33	0	21,21,21	0.25	0
6	NAG	A	1306	1	15,15,15	0.33	0	21,21,21	0.16	0
6	NAG	C	1303	1	15,15,15	0.92	1 (6%)	21,21,21	0.49	0
6	NAG	B	1101	1	15,15,15	0.34	0	21,21,21	0.42	0
6	NAG	C	1302	-	15,15,15	0.74	1 (6%)	21,21,21	0.45	0
6	NAG	B	1103	-	15,15,15	0.42	0	21,21,21	0.92	2 (9%)
6	NAG	B	1102	1	15,15,15	0.43	0	21,21,21	0.29	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
7	MAN	A	1307	-	-	0/2/22/22	0/1/1/1
6	NAG	B	1104	-	-	3/6/26/26	0/1/1/1
6	NAG	B	1105	-	-	0/6/26/26	0/1/1/1
6	NAG	A	1302	1	-	0/6/26/26	0/1/1/1
6	NAG	B	1106	1	-	0/6/26/26	0/1/1/1
6	NAG	C	1301	-	-	2/6/26/26	0/1/1/1
6	NAG	C	1305	-	-	0/6/26/26	0/1/1/1
6	NAG	A	1304	-	-	2/6/26/26	0/1/1/1
6	NAG	A	1305	-	-	5/6/26/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/26/26	0/1/1/1
7	MAN	C	1304	-	-	0/2/22/22	0/1/1/1
6	NAG	B	1107	1	-	2/6/26/26	0/1/1/1
6	NAG	A	1303	1	-	2/6/26/26	0/1/1/1
6	NAG	B	1108	1	-	3/6/26/26	0/1/1/1
6	NAG	A	1306	1	-	2/6/26/26	0/1/1/1
6	NAG	C	1303	1	-	2/6/26/26	0/1/1/1
6	NAG	B	1101	1	-	4/6/26/26	0/1/1/1
6	NAG	C	1302	-	1/1/6/7	2/6/26/26	0/1/1/1
6	NAG	B	1103	-	-	6/6/26/26	0/1/1/1
6	NAG	B	1102	1	-	4/6/26/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1303	NAG	C1-C2	2.94	1.56	1.52
6	A	1301	NAG	C1-C2	2.41	1.55	1.52
6	C	1302	NAG	O5-C1	2.12	1.48	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1307	MAN	O1-C1-O5	-4.41	97.32	110.41
7	C	1304	MAN	O1-C1-O5	-4.39	97.36	110.41
6	B	1103	NAG	C1-C2-N2	2.82	114.00	110.73
6	A	1305	NAG	C1-C2-N2	2.78	113.95	110.73
6	A	1305	NAG	C2-N2-C7	2.63	129.25	123.11
6	B	1103	NAG	C2-N2-C7	2.50	128.96	123.11
7	A	1307	MAN	O2-C2-C3	-2.08	105.47	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	1302	NAG	C1

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1102	NAG	C1-C2-N2-C7
6	A	1306	NAG	O5-C5-C6-O6
6	C	1303	NAG	O5-C5-C6-O6
6	A	1303	NAG	O5-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6
6	C	1303	NAG	C4-C5-C6-O6
6	A	1304	NAG	C4-C5-C6-O6
6	B	1103	NAG	C4-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	B	1101	NAG	C4-C5-C6-O6
6	A	1301	NAG	C8-C7-N2-C2
6	A	1301	NAG	O7-C7-N2-C2
6	A	1305	NAG	C8-C7-N2-C2
6	A	1305	NAG	O7-C7-N2-C2
6	B	1103	NAG	C8-C7-N2-C2
6	B	1103	NAG	O7-C7-N2-C2
6	C	1302	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	1108	NAG	O5-C5-C6-O6
6	B	1103	NAG	O5-C5-C6-O6
6	A	1305	NAG	O5-C5-C6-O6
6	B	1101	NAG	O5-C5-C6-O6
6	C	1302	NAG	O5-C5-C6-O6
6	B	1104	NAG	O5-C5-C6-O6
6	B	1108	NAG	C3-C2-N2-C7
6	B	1102	NAG	C4-C5-C6-O6
6	B	1104	NAG	C3-C2-N2-C7
6	B	1102	NAG	O5-C5-C6-O6
6	B	1101	NAG	C1-C2-N2-C7
6	A	1305	NAG	C3-C2-N2-C7
6	B	1103	NAG	C1-C2-N2-C7
6	B	1107	NAG	C1-C2-N2-C7
6	B	1103	NAG	C3-C2-N2-C7
6	B	1101	NAG	C3-C2-N2-C7
6	A	1305	NAG	C1-C2-N2-C7
6	C	1301	NAG	C1-C2-N2-C7
6	B	1102	NAG	C3-C2-N2-C7
6	C	1301	NAG	O5-C5-C6-O6
6	B	1107	NAG	C3-C2-N2-C7
6	B	1104	NAG	C1-C2-N2-C7
6	B	1108	NAG	C1-C2-N2-C7

There are no ring outliers.

11 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1302	NAG	1	0
6	C	1305	NAG	4	0
8	A	1309	DMS	10	0
6	A	1305	NAG	2	0
6	A	1304	NAG	7	0
8	A	1310	DMS	7	0
7	C	1304	MAN	5	0
6	B	1107	NAG	3	0
6	C	1303	NAG	3	0
6	C	1302	NAG	1	0
6	B	1103	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	498:CYS	C	499:GLY	N	2.83
1	A	308:LEU	C	309:CYS	N	1.99

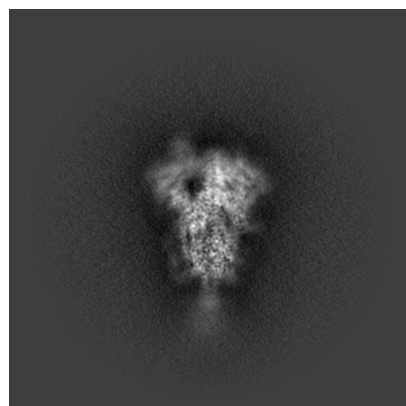
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11336. These allow visual inspection of the internal detail of the map and identification of artifacts.

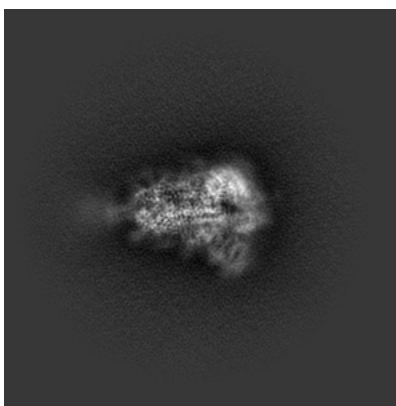
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

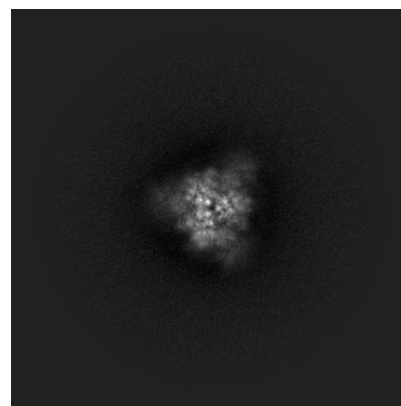
6.1.1 Primary map



X

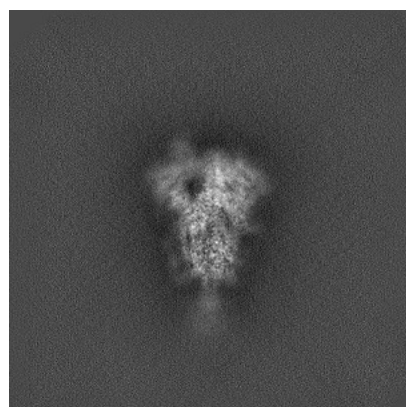


Y

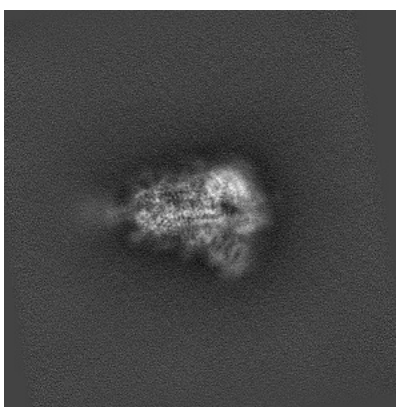


Z

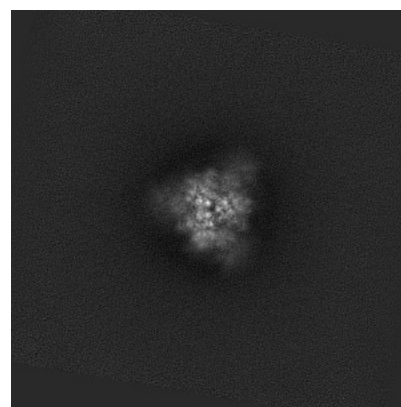
6.1.2 Raw map



X



Y

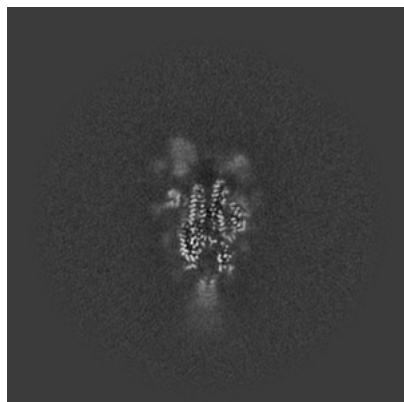


Z

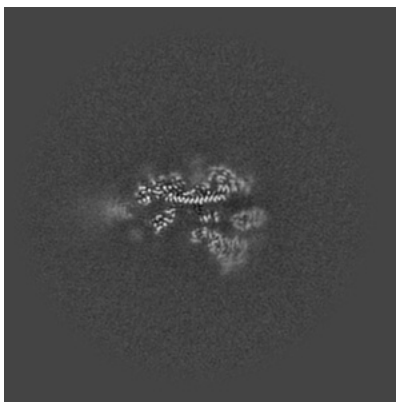
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

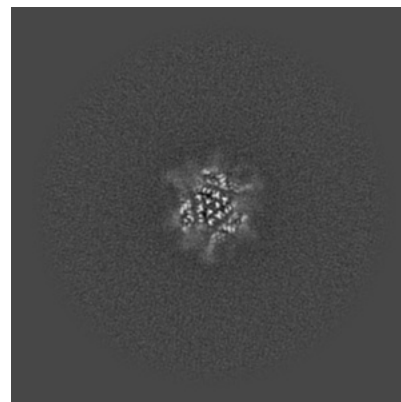
6.2.1 Primary map



X Index: 216

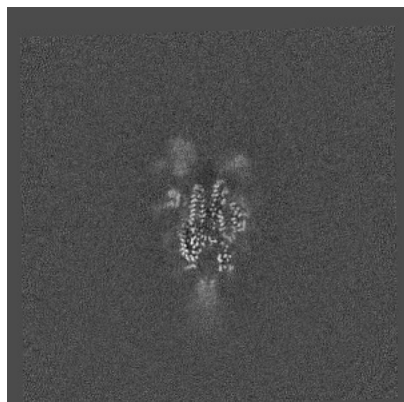


Y Index: 216

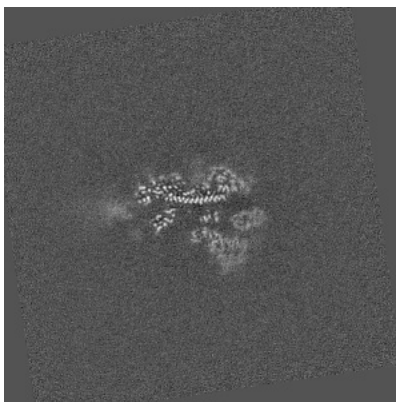


Z Index: 216

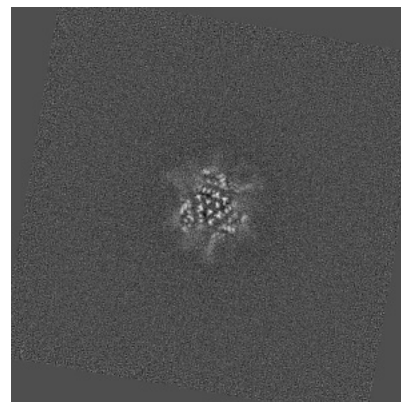
6.2.2 Raw map



X Index: 216



Y Index: 216

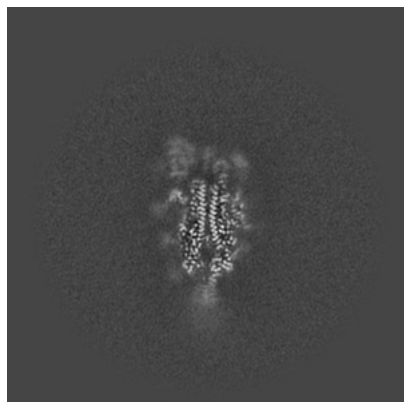


Z Index: 216

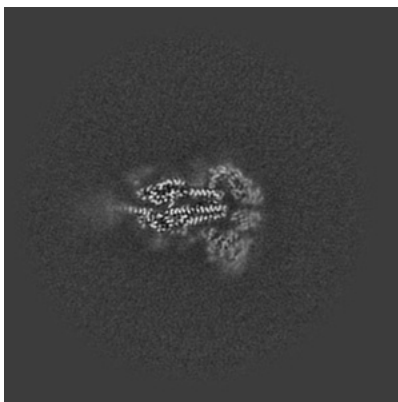
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

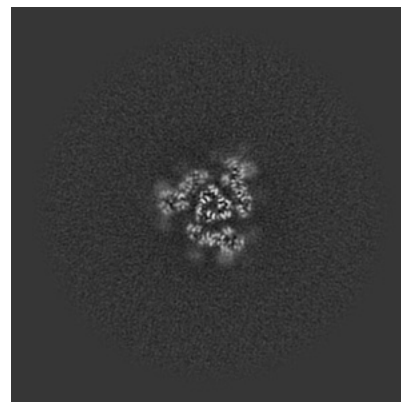
6.3.1 Primary map



X Index: 212

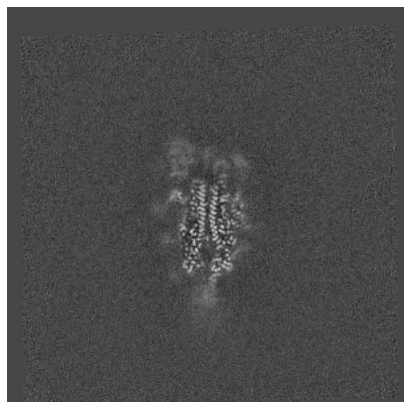


Y Index: 224

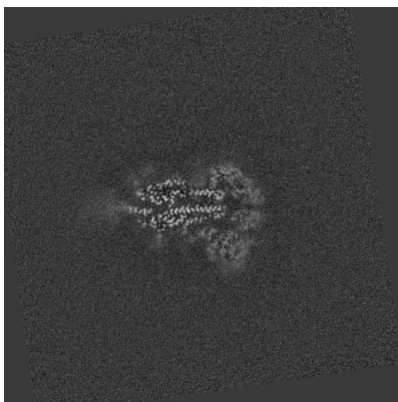


Z Index: 231

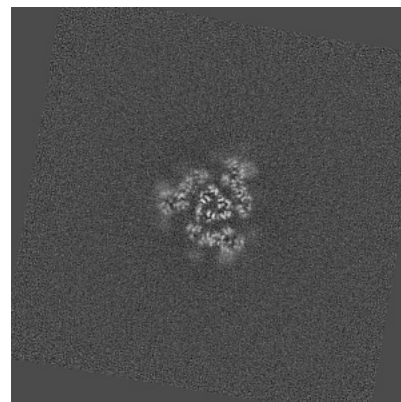
6.3.2 Raw map



X Index: 212



Y Index: 223

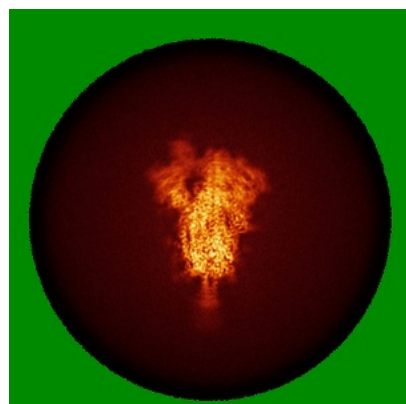


Z Index: 231

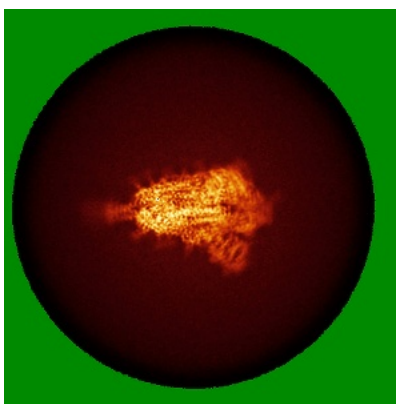
The images above show the largest variance slices of the map in three orthogonal directions.

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

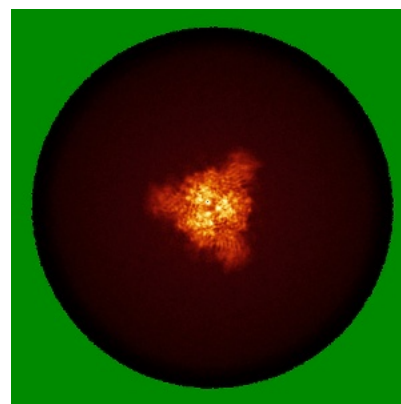
6.4.1 Primary map



X

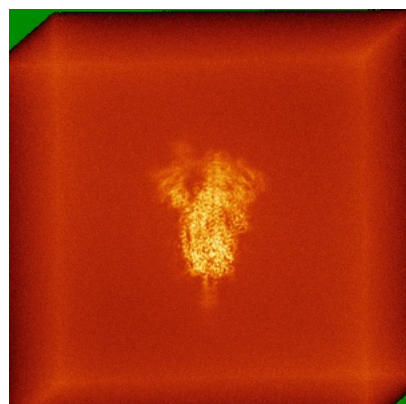


Y

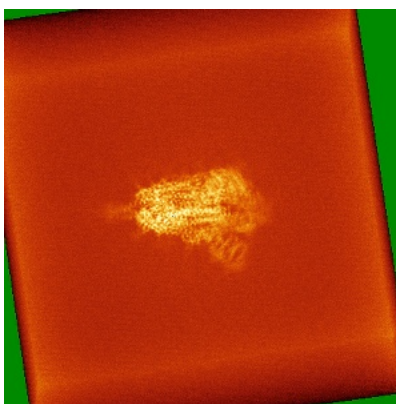


Z

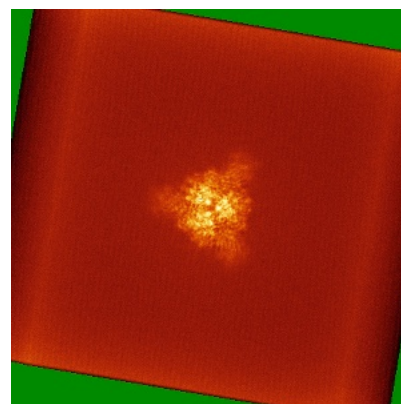
6.4.2 Raw map



X



Y

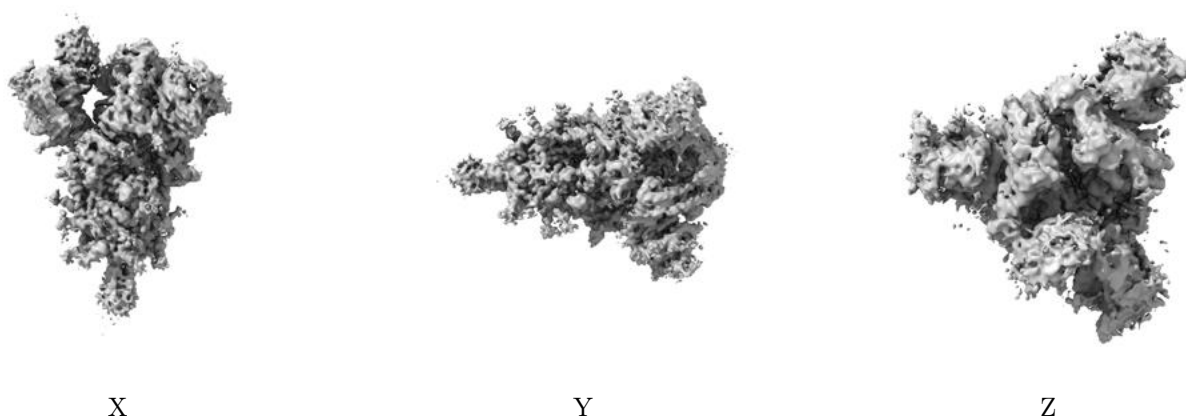


Z

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.

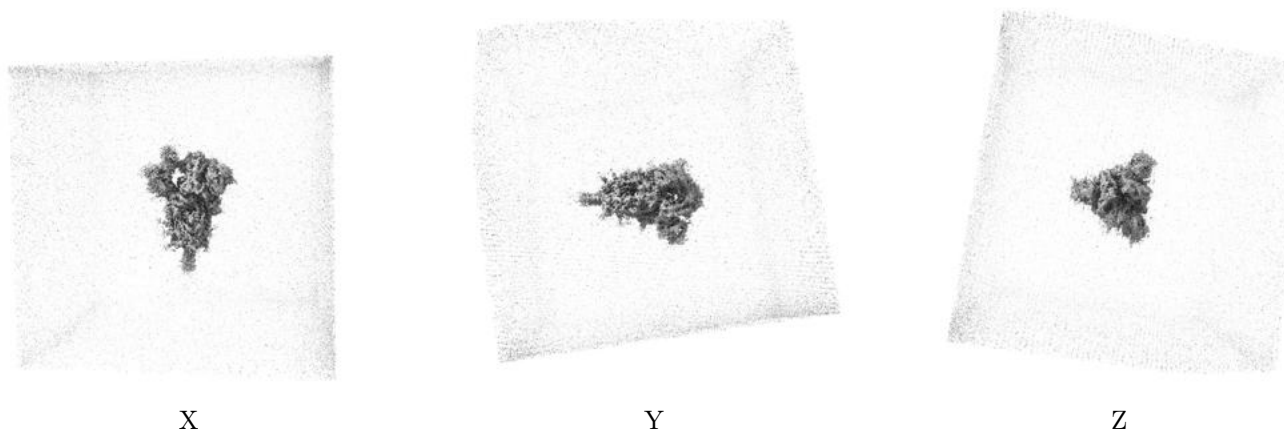
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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



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.

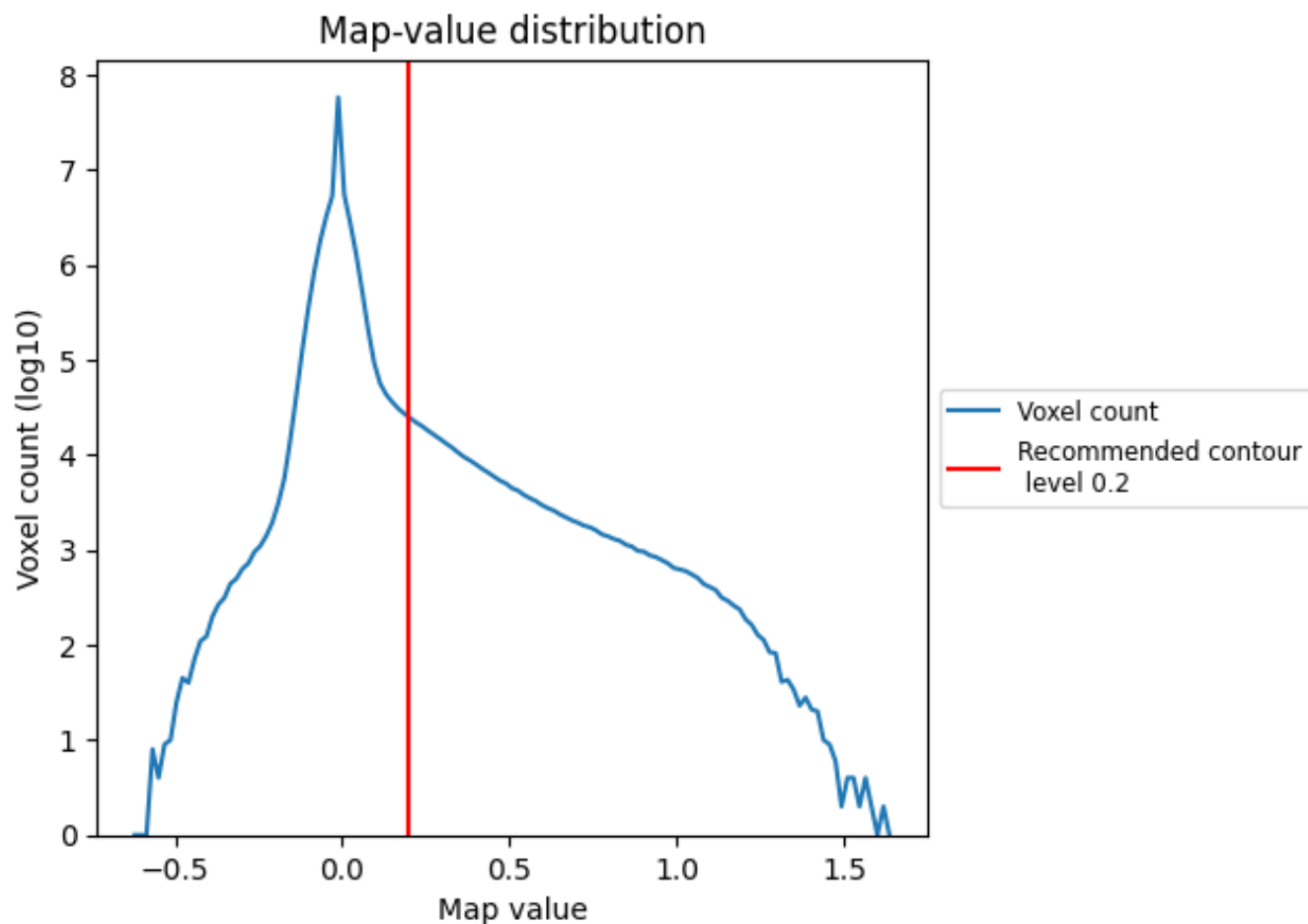
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

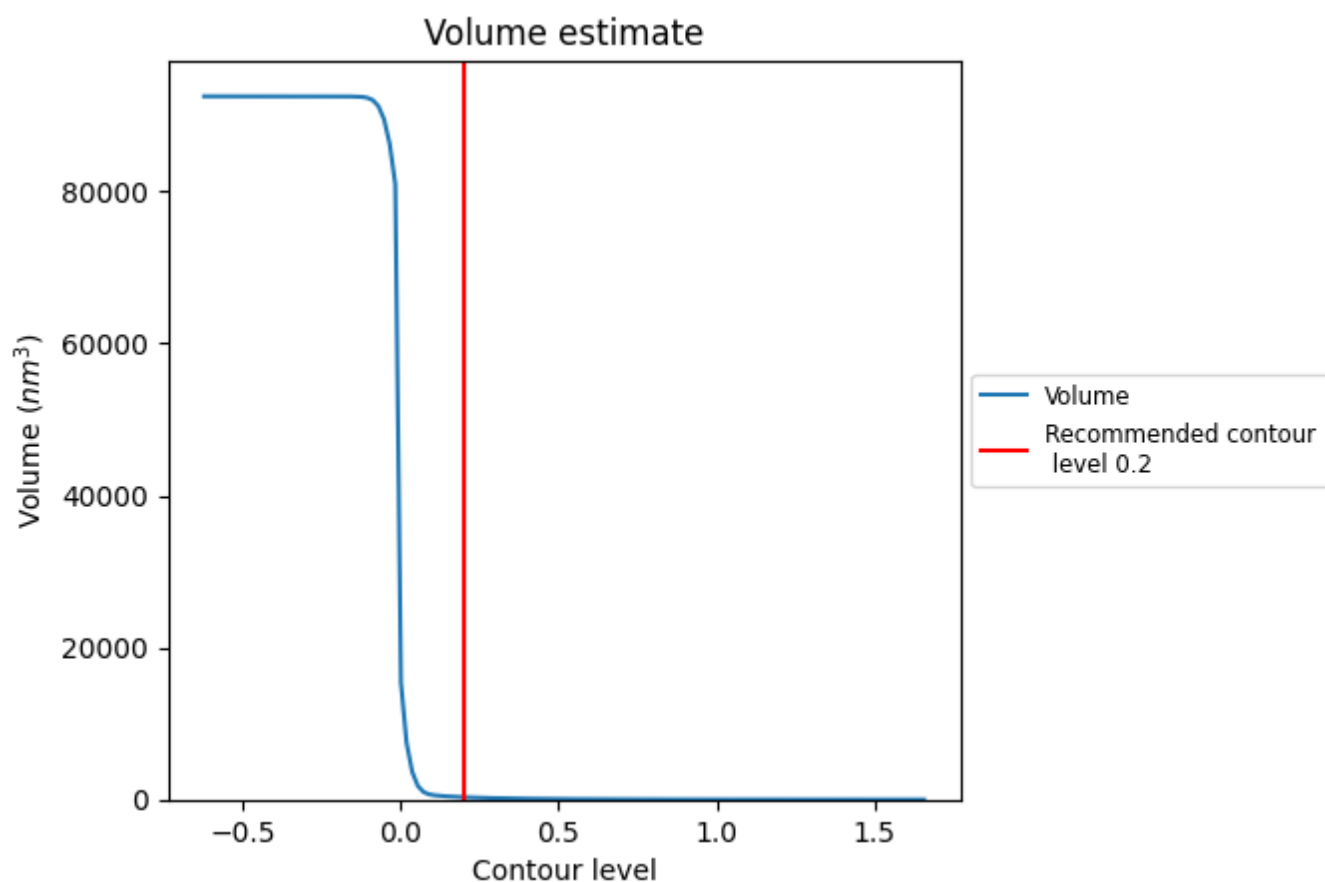
This section contains the results of statistical analysis of the map.

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.

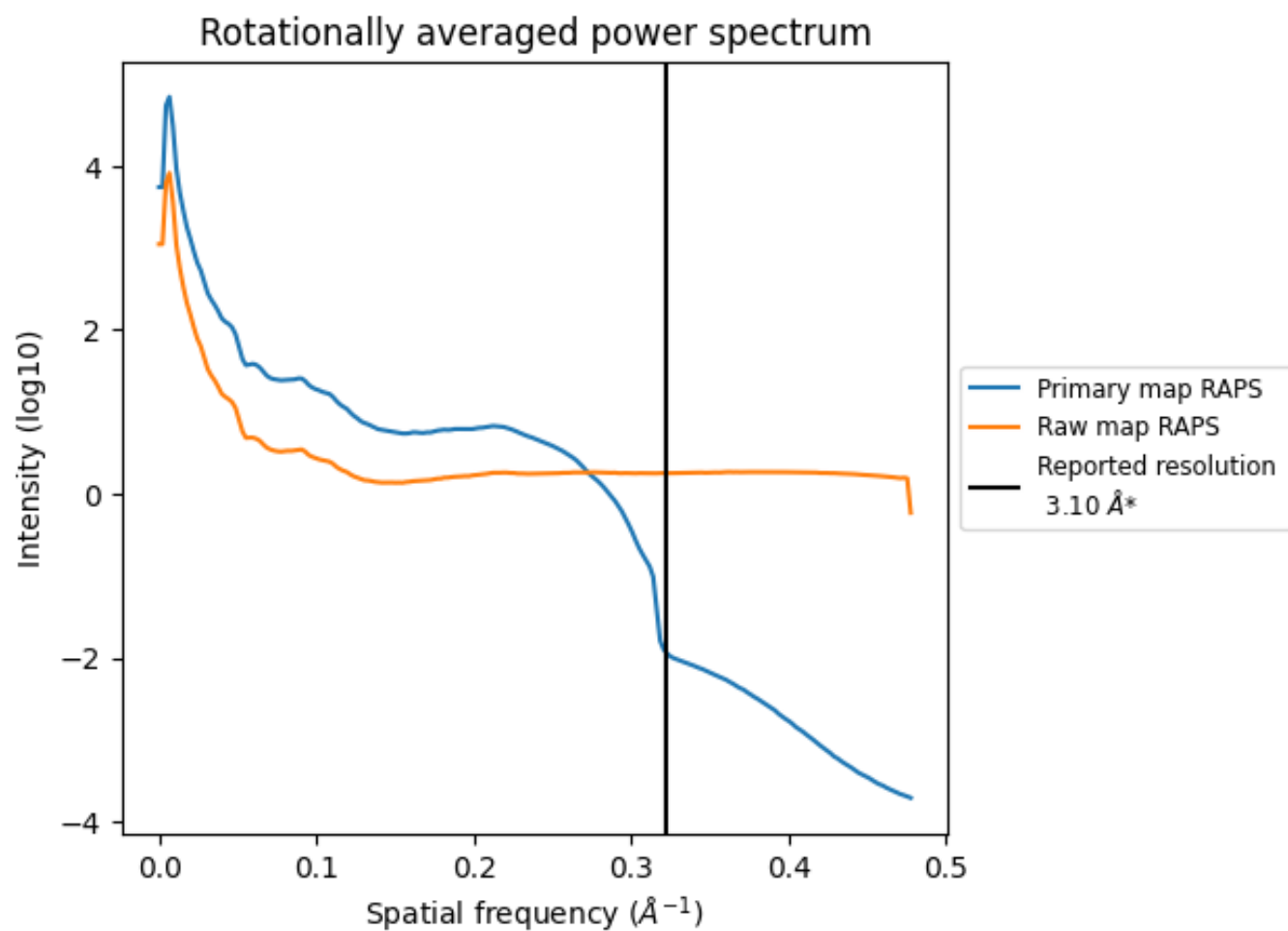
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 313 nm^3 ; this corresponds to an approximate mass of 283 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 ⓘ

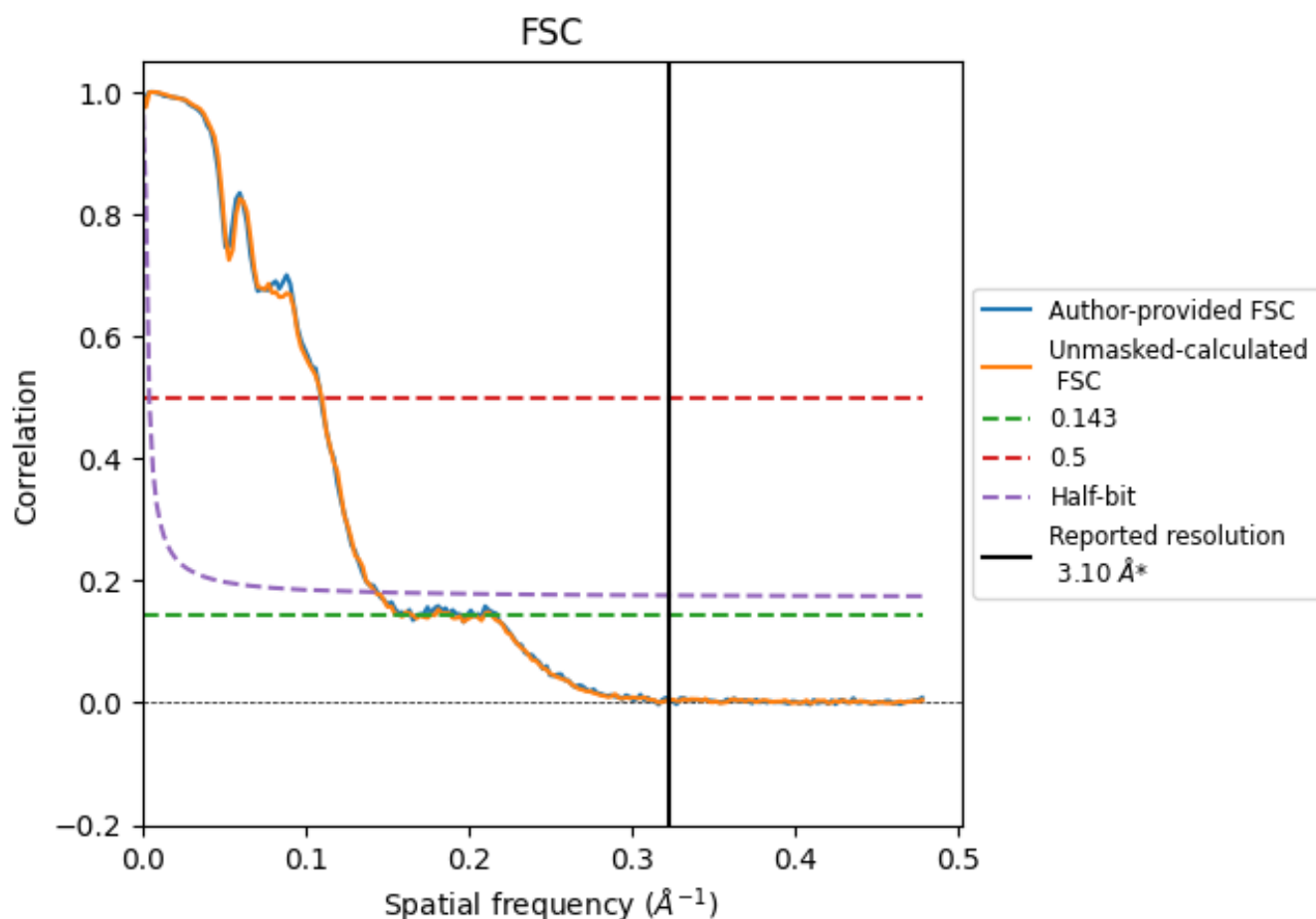


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	6.07	9.15	6.94
Unmasked-calculated*	6.34	9.10	7.00

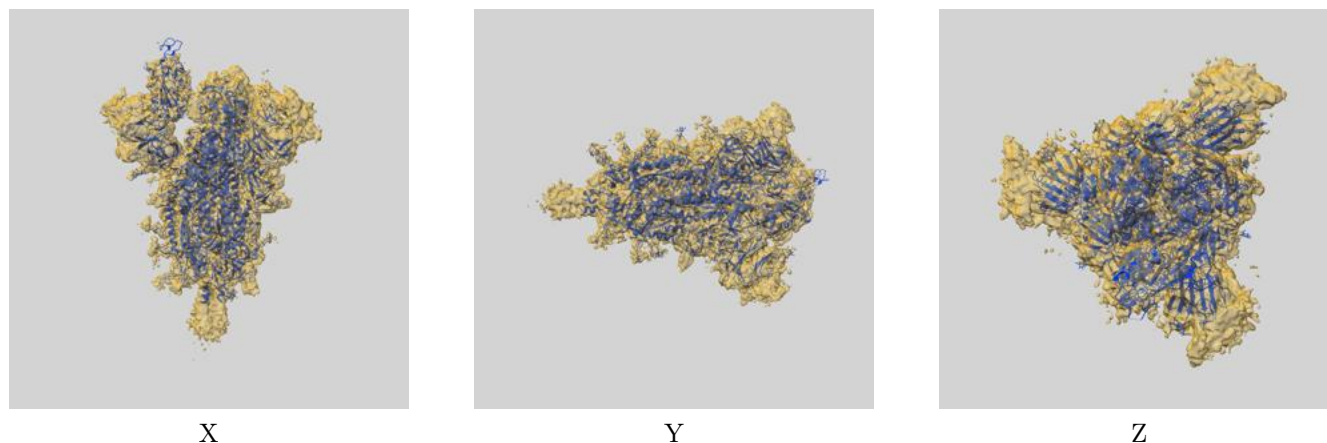
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.07 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.34 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

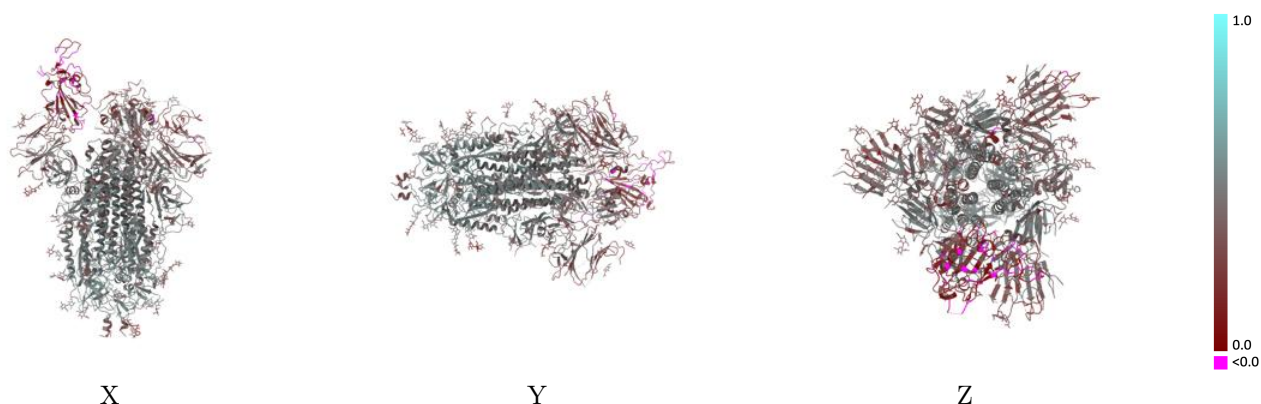
This section contains information regarding the fit between EMDB map EMD-11336 and PDB model 6ZP5. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.2 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](#)

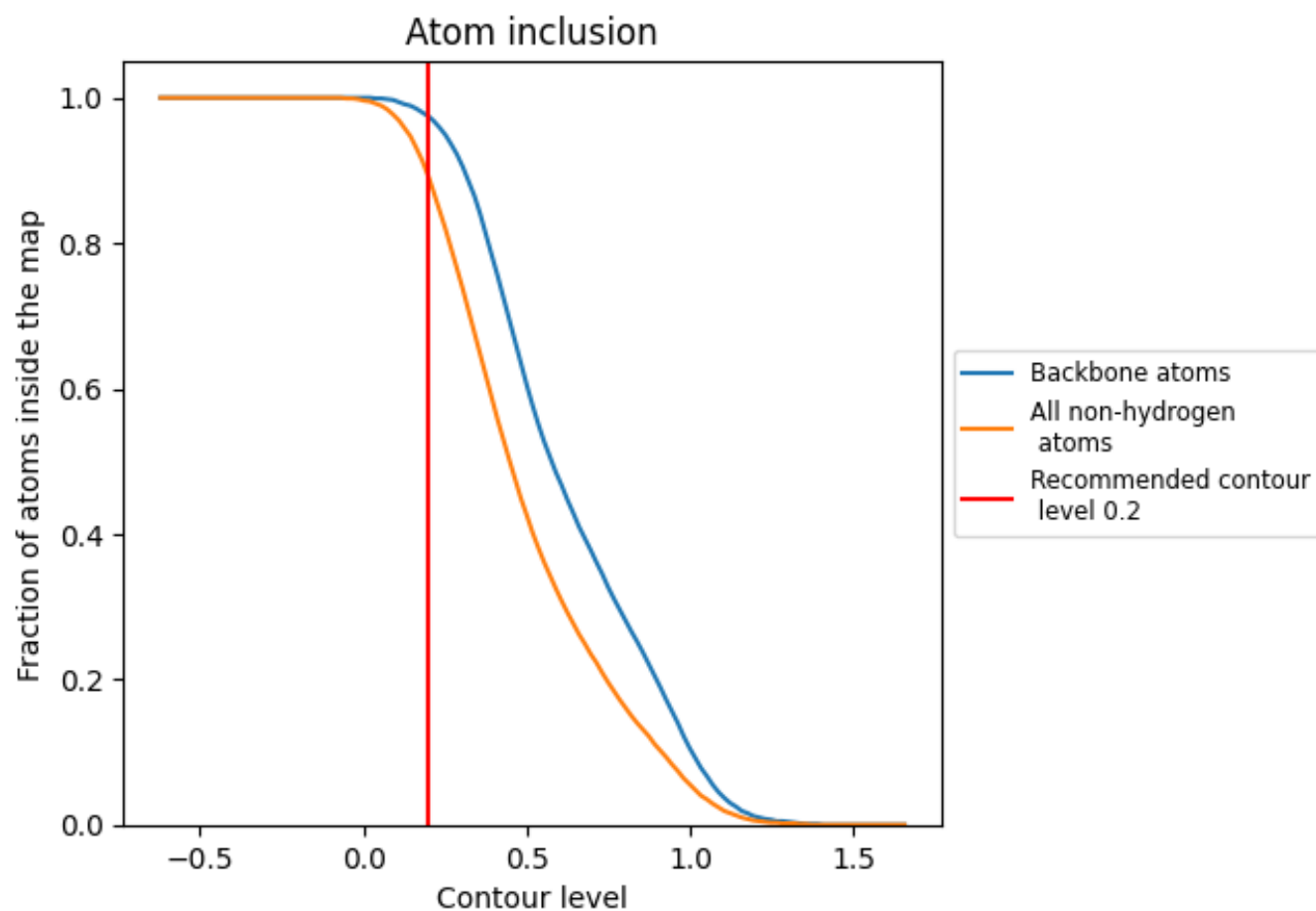


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.4170
A	 0.8570	 0.3960
B	 0.9100	 0.4270
C	 0.9210	 0.4370
D	 0.4670	 0.2950
E	 0.9070	 0.4320
F	 0.7410	 0.3080
G	 0.8000	 0.4620
H	 0.9330	 0.4330
I	 0.9330	 0.4210
J	 0.5000	 0.2630
K	 0.8670	 0.3340
L	 0.7330	 0.2970
M	 0.8670	 0.4230
N	 0.9290	 0.3710
O	 0.6190	 0.3230
P	 0.9670	 0.4170
Q	 0.9520	 0.3850
R	 0.9070	 0.4180
S	 0.6670	 0.2840
T	 0.7330	 0.1980
U	 0.7590	 0.3200
V	 0.9330	 0.4130
W	 0.4760	 0.3130
X	 0.8670	 0.3650
Y	 0.9290	 0.4750
Z	 0.8330	 0.4100
a	 0.5000	 0.1940
b	 0.8090	 0.3060
c	 0.7000	 0.3490
d	 0.3670	 0.3010

