



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 12:22 PM JST

PDB ID : 7Y7J  
EMDB ID : EMD-33667  
Title : SARS-CoV-2 S trimer in complex with 1F Fab  
Authors : Zhao, S.; Liu, F.; Yang, X.; Zhong, G.  
Deposited on : 2022-06-22  
Resolution : 3.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

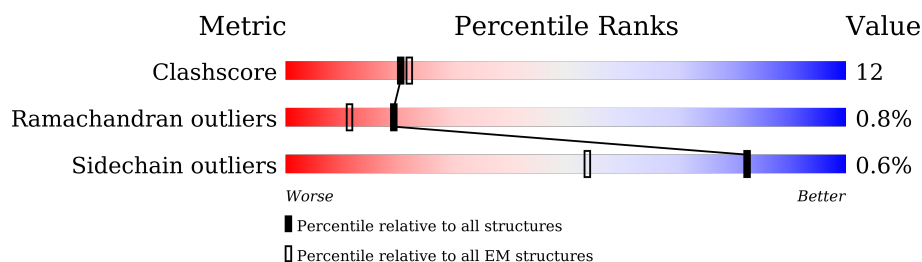
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	61% 16% • 22%
1	B	1288	59% 16% 24%
1	C	1288	59% 16% 24%
2	E	132	37% 71% 27% ••
3	D	111	46% 71% 27% •
4	F	2	100%
4	G	2	100%
4	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	I	2	 100%
4	J	2	 100%
4	K	2	 100%
4	L	2	 50%  50%
4	N	2	 100%
4	O	2	 50%  50%
4	P	2	 100%
4	Q	2	 50%  50%
4	R	2	 100%
4	S	2	 100%
4	T	2	 100%
4	U	2	 50%  50%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23742 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	1002	Total	C	N	O	S	0	0
			7245	4587	1218	1407	33		
1	B	973	Total	C	N	O	S	0	0
			7086	4507	1195	1352	32		
1	C	973	Total	C	N	O	S	0	0
			6908	4367	1165	1349	27		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called 1F VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	132	Total	C	N	O	S	0	0
			960	601	159	198	2		

- Molecule 3 is a protein called 1F VL.

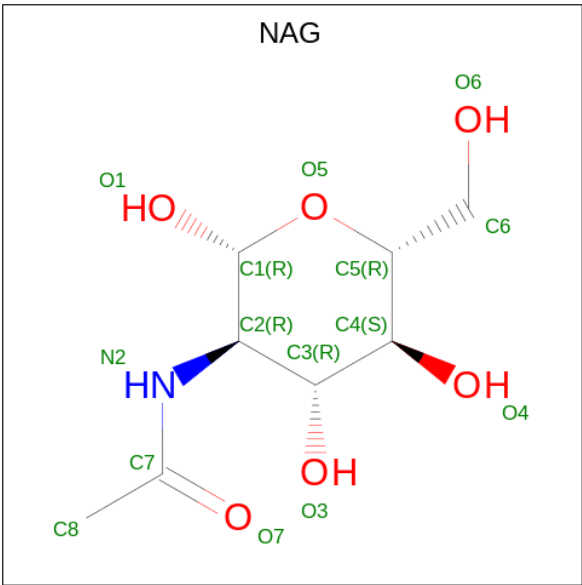
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	111	Total	C	N	O	S	0	0
			759	463	137	157	2		

- Molecule 4 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
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

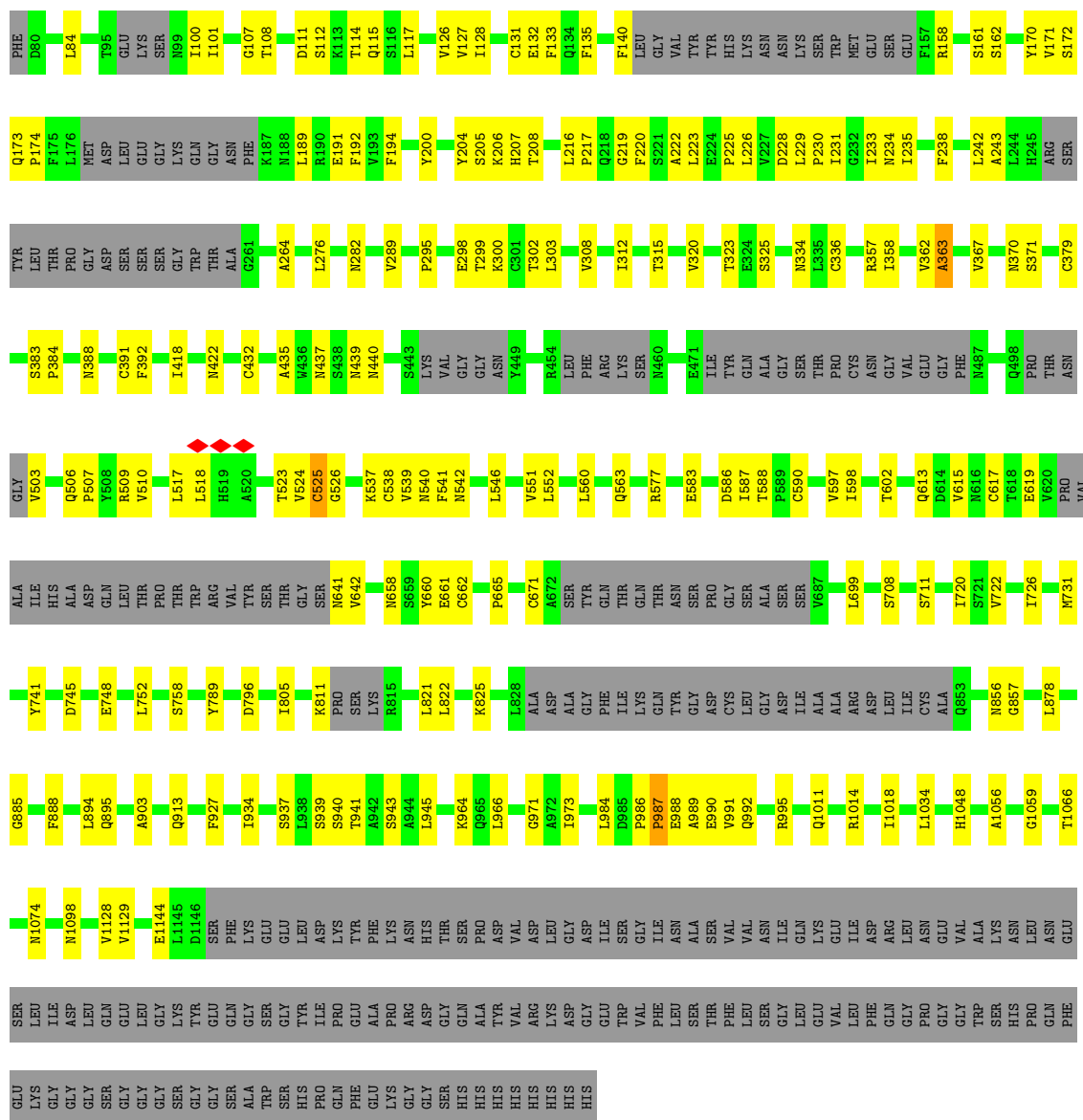
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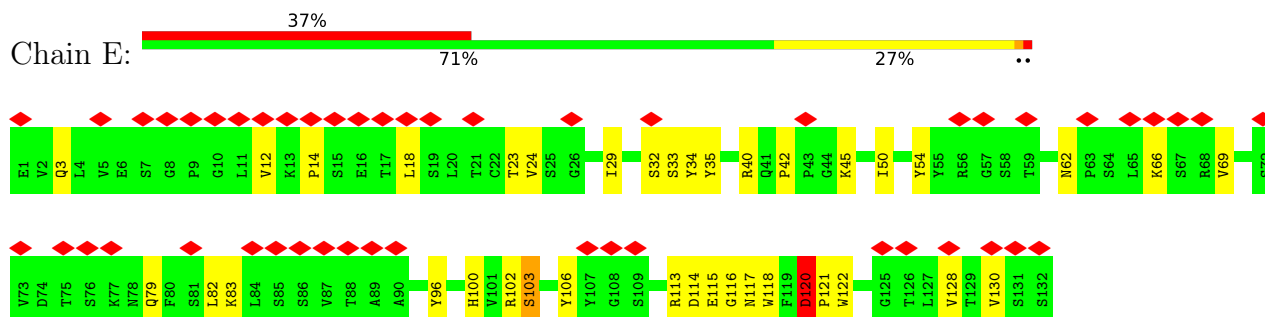
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5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







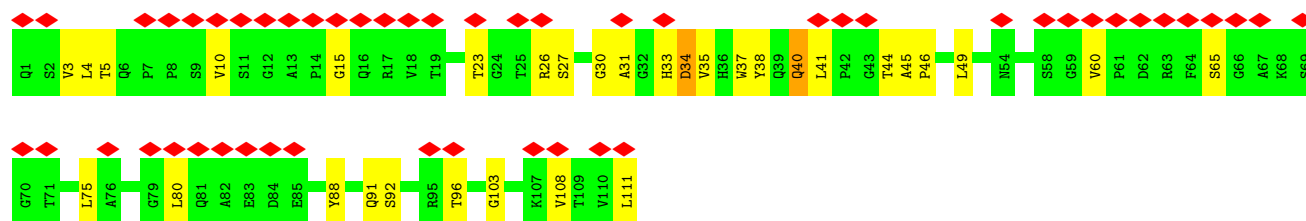
• Molecule 2: 1F VH



• Molecule 3: 1F VL







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

Chain F:  100%



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

Chain G:  100%



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

Chain H:  50% 50%



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

Chain I:  100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  50% 50%



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

Chain N:  100%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  100%



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

Chain T:  100%



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

Chain U:  50% 50%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61103	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 ( $e^-/\text{\AA}^2$ )	60.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.178	Depositor
Minimum map value	-0.412	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	367.36, 367.36, 367.36	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/7386	0.58	0/10098
1	B	0.41	0/7230	0.57	0/9880
1	C	0.39	0/7031	0.56	0/9627
2	E	0.30	0/982	0.64	0/1340
3	D	0.28	0/774	0.58	0/1059
All	All	0.39	0/23403	0.57	0/32004

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7245	0	6614	167	0
1	B	7086	0	6486	174	0
1	C	6908	0	6245	146	0
2	E	960	0	885	47	0
3	D	759	0	672	28	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	N	28	0	25	2	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	1	0
4	R	28	0	25	2	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	1	0
5	A	112	0	104	2	0
5	B	126	0	117	2	0
5	C	126	0	117	1	0
All	All	23742	0	21615	538	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 12.

All (538) 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)
2:E:122:TRP:CD1	3:D:46:PRO:HD2	1.79	1.16
2:E:120:ASP:CG	2:E:121:PRO:HD3	1.68	1.11
2:E:120:ASP:OD2	2:E:121:PRO:HD3	1.51	1.10
2:E:96:TYR:CB	2:E:122:TRP:CZ3	2.36	1.08
2:E:96:TYR:CB	2:E:122:TRP:HZ3	1.66	1.08
2:E:96:TYR:HB2	2:E:122:TRP:HZ3	1.16	1.07
2:E:120:ASP:OD2	2:E:121:PRO:CD	2.01	1.07
2:E:96:TYR:HB2	2:E:122:TRP:CZ3	1.94	1.00
3:D:40:GLN:HB3	3:D:46:PRO:HA	1.45	0.98
1:C:551:VAL:HG22	1:C:588:THR:O	1.68	0.92
2:E:35:TYR:HB2	2:E:100:HIS:HB3	1.50	0.91
1:A:707:TYR:CE1	1:B:797:PHE:CE1	2.59	0.90
1:B:616:ASN:HA	1:B:644:GLN:HE22	1.37	0.89
1:A:707:TYR:CE1	1:B:797:PHE:HE1	1.92	0.88
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.37	0.87
1:A:476:GLY:HA3	1:A:487:ASN:HB3	1.55	0.87
2:E:120:ASP:OD2	2:E:121:PRO:HD2	1.75	0.86
1:A:478:THR:HB	1:A:479:PRO:HD2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:122:TRP:HB2	3:D:45:ALA:CB	2.07	0.84
3:D:40:GLN:CB	3:D:46:PRO:HA	2.06	0.84
1:B:616:ASN:HA	1:B:644:GLN:NE2	1.95	0.81
2:E:120:ASP:CB	2:E:121:PRO:HD3	2.10	0.80
1:B:392:PHE:O	1:B:524:VAL:HG12	1.82	0.79
1:C:303:LEU:HD23	1:C:308:VAL:HG12	1.65	0.79
1:A:560:LEU:HB2	1:A:563:GLN:HE22	1.49	0.78
2:E:96:TYR:CG	2:E:122:TRP:CZ3	2.70	0.78
3:D:38:TYR:CE2	3:D:91:GLN:NE2	2.51	0.78
1:B:392:PHE:CE2	1:B:515:PHE:CE2	2.71	0.78
2:E:96:TYR:CG	2:E:122:TRP:HZ3	2.02	0.77
1:A:83:VAL:HA	1:A:239:GLN:HB2	1.65	0.77
1:B:550:GLY:HA2	1:B:590:CYS:SG	2.25	0.76
1:B:551:VAL:HG13	1:B:588:THR:OG1	1.85	0.76
2:E:96:TYR:HB3	2:E:122:TRP:CE3	2.21	0.76
1:C:542:ASN:HA	1:C:546:LEU:O	1.87	0.75
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.69	0.75
1:B:392:PHE:CE1	1:B:515:PHE:CD2	2.75	0.74
2:E:42:PRO:HG2	2:E:45:LYS:HB2	1.70	0.73
1:A:484:GLU:HG3	1:A:489:TYR:HA	1.68	0.73
1:A:197:ILE:HD11	1:A:202:LYS:HD2	1.69	0.73
2:E:96:TYR:HB3	2:E:122:TRP:CZ3	2.22	0.73
1:B:392:PHE:CZ	1:B:515:PHE:CD2	2.77	0.72
1:A:707:TYR:HH	1:B:797:PHE:HD1	1.37	0.70
1:A:353:TRP:NE1	1:A:465:GLU:O	2.22	0.70
1:A:490:PHE:CG	1:A:491:PRO:HD2	2.25	0.70
2:E:122:TRP:HB2	3:D:45:ALA:HB2	1.73	0.69
1:B:392:PHE:CD1	1:B:515:PHE:HD2	2.10	0.68
1:B:722:VAL:HG12	1:B:1065:VAL:HG22	1.74	0.68
1:C:748:GLU:N	1:C:748:GLU:OE2	2.27	0.68
1:C:811:LYS:O	1:C:811:LYS:HG3	1.94	0.67
2:E:96:TYR:CB	2:E:122:TRP:CE3	2.77	0.67
1:C:31:SER:O	1:C:59:PHE:N	2.27	0.66
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.61	0.66
1:C:731:MET:HE3	1:C:1018:ILE:HD12	1.77	0.65
1:A:987:PRO:O	1:A:990:GLU:HG3	1.96	0.65
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.32	0.65
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.78	0.65
1:B:1105:THR:HG22	1:B:1112:PRO:HA	1.78	0.65
1:C:388:ASN:O	1:C:526:GLY:HA3	1.96	0.65
1:C:437:ASN:HD21	1:C:506:GLN:HG2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:SER:HB3	2:E:102:ARG:HH22	1.62	0.65
1:B:34:ARG:NH2	1:B:217:PRO:O	2.29	0.64
1:B:977:LEU:HD12	1:B:980:ILE:HD11	1.79	0.64
1:B:217:PRO:HG3	1:B:266:TYR:HE2	1.61	0.64
1:C:805:ILE:HD12	1:C:878:LEU:HD21	1.79	0.64
1:C:334:ASN:O	1:C:362:VAL:N	2.26	0.64
1:A:308:VAL:N	1:A:602:THR:OG1	2.31	0.63
1:A:707:TYR:CE1	1:B:797:PHE:CD1	2.87	0.63
1:B:586:ASP:OD1	1:B:587:ILE:N	2.32	0.63
1:A:493:GLN:HE21	2:E:32:SER:HB3	1.63	0.63
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.81	0.63
1:B:325:SER:HA	1:B:540:ASN:O	1.98	0.63
1:C:658:ASN:ND2	1:C:660:TYR:OH	2.32	0.63
1:A:455:LEU:HB2	1:A:492:LEU:HB2	1.81	0.63
1:B:392:PHE:CG	1:B:515:PHE:HD2	2.17	0.63
1:B:821:LEU:HD11	1:B:939:SER:HB3	1.80	0.62
1:B:741:TYR:CE1	1:B:966:LEU:HD11	2.34	0.62
1:A:65:PHE:O	1:A:264:ALA:HA	2.00	0.62
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.81	0.62
1:A:811:LYS:O	1:A:811:LYS:HG3	1.99	0.62
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.81	0.61
3:D:38:TYR:CD2	3:D:91:GLN:NE2	2.68	0.61
1:B:392:PHE:CD1	1:B:515:PHE:CD2	2.88	0.61
1:B:867:ASP:OD1	1:B:868:GLU:N	2.34	0.61
2:E:33:SER:HB2	2:E:102:ARG:HG3	1.83	0.61
1:A:353:TRP:HZ3	1:A:355:ARG:HB2	1.66	0.61
1:B:280:ASN:OD1	1:B:281:GLU:N	2.32	0.60
1:B:392:PHE:HB2	1:B:524:VAL:HG13	1.84	0.60
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.28	0.60
1:A:83:VAL:HB	1:A:237:ARG:HD3	1.82	0.60
1:A:586:ASP:OD1	1:A:587:ILE:N	2.34	0.60
1:A:619:GLU:OE1	1:A:619:GLU:N	2.34	0.59
1:A:707:TYR:HB2	1:B:883:THR:CG2	2.32	0.59
3:D:27:SER:OG	3:D:96:THR:N	2.33	0.59
1:C:726:ILE:HD13	1:C:945:LEU:HD23	1.85	0.59
1:C:888:PHE:CZ	1:C:1034:LEU:HG	2.37	0.59
1:B:66:HIS:CD2	1:B:264:ALA:HB2	2.38	0.59
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.38	0.59
2:E:113:ARG:O	2:E:115:GLU:N	2.36	0.59
1:B:190:ARG:HE	1:B:207:HIS:CE1	2.20	0.59
1:B:392:PHE:CE2	1:B:515:PHE:CD2	2.90	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:122:TRP:CD1	3:D:46:PRO:CD	2.72	0.58
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.66	0.58
1:A:707:TYR:OH	1:B:797:PHE:HD1	1.85	0.58
1:A:367:VAL:O	1:A:371:SER:HB2	2.03	0.58
1:B:658:ASN:ND2	1:B:660:TYR:OH	2.36	0.58
1:C:619:GLU:N	1:C:619:GLU:OE1	2.37	0.58
4:U:1:NAG:H83	4:U:1:NAG:H3	1.85	0.58
1:A:166:CYS:HB3	1:A:169:GLU:OE1	2.03	0.58
1:A:741:TYR:CE1	1:A:966:LEU:HD11	2.39	0.58
1:C:108:THR:OG1	1:C:234:ASN:O	2.21	0.58
1:A:53:ASP:OD1	1:A:54:LEU:N	2.32	0.58
5:A:1308:NAG:H83	5:A:1308:NAG:H3	1.85	0.58
1:B:189:LEU:HB3	1:B:208:THR:O	2.03	0.58
1:B:532:ASN:OD1	1:B:533:LEU:N	2.37	0.58
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.39	0.58
1:B:66:HIS:HD2	1:B:264:ALA:HB2	1.68	0.58
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.86	0.58
3:D:35:VAL:HG22	3:D:92:SER:HB2	1.86	0.57
1:A:34:ARG:NH2	1:A:218:GLN:O	2.36	0.57
1:C:895:GLN:OE1	1:C:895:GLN:N	2.29	0.57
1:A:1090:PRO:HD3	1:A:1095:PHE:HE1	1.70	0.57
1:C:111:ASP:OD1	1:C:135:PHE:N	2.38	0.57
1:C:191:GLU:N	1:C:191:GLU:OE1	2.37	0.57
1:C:295:PRO:O	1:C:299:THR:HG23	2.05	0.57
1:C:821:LEU:O	1:C:825:LYS:HG2	2.05	0.57
1:B:64:TRP:CD1	1:B:266:TYR:HE1	2.22	0.57
1:A:873:TYR:CZ	1:C:699:LEU:HD12	2.40	0.56
1:A:658:ASN:ND2	1:A:660:TYR:OH	2.38	0.56
5:B:1309:NAG:H83	5:B:1309:NAG:H3	1.87	0.56
1:A:604:THR:HA	5:A:1301:NAG:H82	1.87	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.56
1:B:172:SER:OG	1:B:173:GLN:N	2.38	0.56
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.38	0.56
1:A:971:GLY:HA3	1:A:995:ARG:HH21	1.70	0.56
1:B:965:GLN:HE22	1:C:758:SER:H	1.53	0.56
1:A:108:THR:HA	1:A:236:THR:HG22	1.88	0.56
1:A:379:CYS:SG	1:A:384:PRO:HB3	2.46	0.56
1:C:115:GLN:HA	1:C:132:GLU:HG3	1.88	0.56
4:R:2:NAG:H3	4:R:2:NAG:H83	1.88	0.56
1:A:391:CYS:HA	1:A:524:VAL:O	2.06	0.56
1:B:330:PRO:HD3	1:B:544:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PHE:CZ	1:B:578:ASP:HA	2.41	0.56
1:B:613:GLN:O	1:B:615:VAL:HG22	2.06	0.56
1:A:172:SER:OG	1:A:173:GLN:N	2.40	0.55
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.88	0.55
1:C:741:TYR:CE1	1:C:966:LEU:HD11	2.40	0.55
1:C:133:PHE:HA	1:C:162:SER:O	2.07	0.55
1:C:112:SER:HA	1:C:132:GLU:HB3	1.88	0.55
1:C:988:GLU:O	1:C:991:VAL:HG12	2.06	0.55
2:E:96:TYR:CG	2:E:122:TRP:CE3	2.94	0.55
1:A:53:ASP:HB3	1:A:55:PHE:CE1	2.41	0.55
1:C:299:THR:HG22	1:C:315:THR:HG21	1.89	0.55
1:C:987:PRO:O	1:C:990:GLU:HG3	2.07	0.55
1:B:319:ARG:NH2	1:C:745:ASP:OD2	2.40	0.55
1:B:748:GLU:H	1:B:748:GLU:CD	2.10	0.55
1:A:965:GLN:NE2	1:B:758:SER:OG	2.40	0.55
4:H:2:NAG:H3	4:H:2:NAG:H83	1.89	0.55
1:B:377:PHE:HD1	1:B:434:ILE:HG12	1.71	0.54
1:B:521:PRO:HB3	1:B:564:GLN:HE21	1.71	0.54
5:C:1303:NAG:H83	5:C:1303:NAG:H3	1.88	0.54
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.90	0.54
1:A:439:ASN:HA	1:A:507:PRO:HG2	1.90	0.54
1:C:435:ALA:HB2	1:C:510:VAL:HG22	1.90	0.54
1:A:365:TYR:CD2	1:A:388:ASN:HB3	2.42	0.54
2:E:120:ASP:OD2	2:E:120:ASP:N	2.38	0.54
1:A:748:GLU:O	1:A:752:LEU:HD12	2.07	0.54
1:A:1056:ALA:HB3	1:A:1059:GLY:O	2.08	0.54
1:B:452:LEU:HD23	1:B:494:SER:HB2	1.90	0.54
1:B:716:THR:O	1:B:1109:PHE:CE1	2.61	0.54
1:C:661:GLU:OE1	1:C:662:CYS:N	2.41	0.54
1:A:218:GLN:HG2	1:A:219:GLY:H	1.72	0.54
1:B:392:PHE:HB2	1:B:524:VAL:CG1	2.37	0.54
1:A:455:LEU:HB3	1:A:492:LEU:N	2.23	0.53
1:C:101:ILE:HD12	1:C:101:ILE:H	1.72	0.53
1:A:903:ALA:HB2	1:A:916:LEU:HD22	1.90	0.53
1:B:130:VAL:HG12	1:B:168:PHE:HB3	1.91	0.53
1:A:451:TYR:O	1:A:495:TYR:N	2.40	0.53
1:B:431:GLY:HA3	1:B:515:PHE:CD1	2.42	0.53
1:C:552:LEU:HA	1:C:586:ASP:O	2.09	0.53
1:B:336:CYS:SG	1:B:337:PRO:HD2	2.49	0.53
1:C:140:PHE:HA	1:C:243:ALA:HA	1.90	0.53
1:C:206:LYS:NZ	1:C:207:HIS:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:ASP:OD1	1:A:796:ASP:N	2.42	0.53
1:B:318:PHE:CZ	1:B:615:VAL:HG21	2.44	0.53
1:C:973:ILE:N	1:C:992:GLN:OE1	2.35	0.53
2:E:120:ASP:CB	2:E:121:PRO:CD	2.82	0.53
1:C:127:VAL:HG12	1:C:171:VAL:HG22	1.91	0.52
1:C:299:THR:CG2	1:C:597:VAL:HG21	2.40	0.52
3:D:5:THR:HB	3:D:23:THR:HB	1.91	0.52
1:A:36:VAL:HG23	1:A:222:ALA:HA	1.92	0.52
1:C:33:THR:OG1	1:C:219:GLY:O	2.27	0.52
1:C:117:LEU:HD11	1:C:231:ILE:HG21	1.92	0.52
1:A:709:ASN:OD1	1:A:709:ASN:N	2.41	0.52
1:A:977:LEU:HD12	1:A:980:ILE:HD11	1.92	0.52
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.32	0.52
1:C:388:ASN:O	1:C:526:GLY:CA	2.57	0.52
1:C:577:ARG:HA	1:C:583:GLU:O	2.10	0.52
1:C:299:THR:HG21	1:C:597:VAL:HG21	1.91	0.52
2:E:12:VAL:HG21	2:E:18:LEU:HD13	1.91	0.52
1:B:204:TYR:HD1	1:B:225:PRO:HA	1.73	0.52
1:C:140:PHE:O	1:C:158:ARG:N	2.37	0.52
1:C:517:LEU:HG	1:C:518:LEU:HD23	1.92	0.51
3:D:37:TRP:CE2	3:D:75:LEU:HB2	2.46	0.51
1:A:228:ASP:OD1	1:A:229:LEU:N	2.43	0.51
1:A:645:THR:OG1	1:A:648:GLY:O	2.23	0.51
1:B:204:TYR:CE1	1:B:225:PRO:HB3	2.46	0.51
2:E:122:TRP:HB2	3:D:45:ALA:CA	2.39	0.51
1:B:394:ASN:HB3	1:B:396:TYR:CE2	2.45	0.51
1:A:57:PRO:HA	1:A:273:ARG:HH21	1.75	0.51
1:B:375:SER:OG	1:B:436:TRP:HA	2.10	0.51
5:B:1304:NAG:H83	5:B:1304:NAG:H3	1.92	0.51
1:A:616:ASN:OD1	1:A:618:THR:HG23	2.10	0.51
1:B:521:PRO:HB3	1:B:564:GLN:NE2	2.26	0.51
1:C:722:VAL:O	1:C:934:ILE:HD11	2.10	0.51
1:A:477:SER:OG	1:A:478:THR:HG23	2.10	0.51
1:A:502:GLY:O	1:A:506:GLN:HG3	2.11	0.51
1:B:217:PRO:HG3	1:B:266:TYR:CE2	2.45	0.51
1:B:973:ILE:N	1:B:992:GLN:OE1	2.33	0.51
4:N:1:NAG:H61	4:N:2:NAG:C7	2.41	0.51
1:A:200:TYR:HB3	1:A:228:ASP:OD1	2.10	0.51
1:A:276:LEU:HB3	1:A:289:VAL:HG23	1.92	0.51
1:C:172:SER:OG	1:C:173:GLN:N	2.43	0.51
2:E:122:TRP:HB2	3:D:45:ALA:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:HB2	1:A:563:GLN:NE2	2.22	0.50
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.46	0.50
1:B:922:LEU:HD11	1:B:926:GLN:HE21	1.75	0.50
1:C:388:ASN:O	1:C:526:GLY:N	2.44	0.50
3:D:40:GLN:OE1	3:D:46:PRO:HB3	2.11	0.50
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.44	0.50
1:B:190:ARG:HE	1:B:207:HIS:HE1	1.59	0.50
3:D:38:TYR:O	3:D:88:TYR:HA	2.11	0.50
1:A:551:VAL:HG12	1:A:588:THR:O	2.11	0.50
1:A:566:GLY:HA3	1:B:43:PHE:HB3	1.93	0.50
1:B:787:GLN:N	1:B:787:GLN:OE1	2.45	0.50
1:A:498:GLN:HB2	1:A:501:ASN:ND2	2.27	0.50
1:B:299:THR:HG22	1:B:315:THR:HG21	1.94	0.50
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.94	0.50
1:B:108:THR:OG1	1:B:234:ASN:O	2.30	0.50
1:A:205:SER:OG	1:A:206:LYS:N	2.44	0.49
1:B:773:GLU:OE2	1:B:1019:ARG:HD3	2.12	0.49
1:C:541:PHE:CZ	1:C:587:ILE:HD13	2.46	0.49
2:E:62:ASN:O	2:E:66:LYS:N	2.45	0.49
1:A:369:TYR:CE1	1:A:384:PRO:HB2	2.47	0.49
1:C:720:ILE:HD11	1:C:927:PHE:HB2	1.93	0.49
1:C:943:SER:O	1:C:943:SER:OG	2.28	0.49
1:A:362:VAL:HG13	1:A:526:GLY:O	2.12	0.49
1:A:707:TYR:CZ	1:B:797:PHE:CD1	3.00	0.49
2:E:18:LEU:O	2:E:83:LYS:HA	2.12	0.49
1:B:44:ARG:O	1:B:283:GLY:HA2	2.12	0.49
1:C:1056:ALA:HB3	1:C:1059:GLY:O	2.12	0.49
1:C:205:SER:OG	1:C:206:LYS:N	2.46	0.49
2:E:35:TYR:CZ	2:E:54:TYR:HE2	2.31	0.49
1:C:276:LEU:HB3	1:C:289:VAL:CG2	2.42	0.48
2:E:3:GLN:O	2:E:24:VAL:HA	2.13	0.48
1:C:64:TRP:NE1	1:C:264:ALA:HB1	2.28	0.48
3:D:40:GLN:HG3	3:D:44:THR:O	2.13	0.48
1:C:418:ILE:HG23	1:C:422:ASN:HB2	1.95	0.48
1:C:439:ASN:OD1	1:C:440:ASN:N	2.45	0.48
3:D:33:HIS:O	3:D:34:ASP:O	2.31	0.48
1:B:106:PHE:HD2	1:B:235:ILE:HG21	1.78	0.48
1:B:552:LEU:HD22	1:B:587:ILE:HG12	1.95	0.48
1:C:796:ASP:OD1	1:C:796:ASP:N	2.44	0.48
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.94	0.48
3:D:40:GLN:CG	3:D:46:PRO:HA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.49	0.48
1:A:1092:GLU:O	1:A:1092:GLU:HG2	2.14	0.48
1:B:431:GLY:HA3	1:B:515:PHE:HD1	1.78	0.48
1:C:856:ASN:OD1	1:C:856:ASN:N	2.47	0.48
1:C:1011:GLN:OE1	1:C:1014:ARG:NH1	2.46	0.48
1:B:439:ASN:HB3	1:B:507:PRO:HD2	1.96	0.48
1:B:748:GLU:OE1	1:B:748:GLU:N	2.30	0.48
1:B:392:PHE:O	1:B:524:VAL:CG1	2.57	0.48
1:C:298:GLU:O	1:C:302:THR:HG23	2.13	0.48
1:C:370:ASN:OD1	1:C:371:SER:N	2.46	0.48
1:A:431:GLY:HA2	1:A:515:PHE:CE2	2.48	0.48
1:A:462:LYS:N	1:A:465:GLU:OE2	2.47	0.48
1:A:707:TYR:CD1	1:B:797:PHE:HE1	2.31	0.48
1:A:906:PHE:HD2	1:A:916:LEU:HB2	1.78	0.48
1:B:308:VAL:N	1:B:602:THR:OG1	2.46	0.48
1:B:276:LEU:HB3	1:B:289:VAL:HB	1.95	0.48
1:C:53:ASP:HB2	1:C:55:PHE:CE2	2.48	0.48
1:A:466:ARG:O	1:A:468:ILE:N	2.47	0.47
1:B:299:THR:CG2	1:B:597:VAL:HG21	2.44	0.47
1:C:524:VAL:O	1:C:524:VAL:HG12	2.12	0.47
2:E:102:ARG:HG2	2:E:103:SER:H	1.79	0.47
1:A:276:LEU:HB3	1:A:289:VAL:CG2	2.44	0.47
1:A:105:ILE:HG12	1:A:118:LEU:HG	1.96	0.47
1:A:199:GLY:HA2	1:A:232:GLY:HA2	1.96	0.47
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.96	0.47
1:A:758:SER:O	1:A:762:GLN:HG3	2.14	0.47
1:B:569:ILE:HD11	1:C:964:LYS:HD3	1.95	0.47
1:A:351:TYR:O	1:A:467:ASP:N	2.43	0.47
1:A:984:LEU:HD22	1:A:988:GLU:HG3	1.95	0.47
1:B:111:ASP:OD1	1:B:112:SER:N	2.43	0.47
1:C:276:LEU:HB3	1:C:289:VAL:HG22	1.96	0.47
1:C:336:CYS:SG	1:C:358:ILE:HG23	2.55	0.47
1:B:551:VAL:HG12	1:B:588:THR:O	2.15	0.47
1:C:192:PHE:HB3	1:C:194:PHE:CE1	2.50	0.47
2:E:40:ARG:CB	2:E:50:ILE:HD11	2.45	0.47
1:B:31:SER:O	1:B:59:PHE:N	2.48	0.47
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.79	0.47
1:C:665:PRO:HA	1:C:671:CYS:SG	2.55	0.47
1:A:542:ASN:HA	1:A:546:LEU:O	2.14	0.47
1:B:316:SER:O	1:B:595:VAL:HG12	2.15	0.47
1:B:392:PHE:CD2	1:B:515:PHE:CD2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:SER:O	3:D:75:LEU:HD12	2.15	0.47
1:A:887:THR:O	1:A:889:GLY:N	2.48	0.47
1:B:392:PHE:CZ	1:B:515:PHE:CE2	3.00	0.47
1:B:886:TRP:HH2	1:B:904:TYR:CD2	2.33	0.47
1:B:971:GLY:HA3	1:B:995:ARG:NH2	2.30	0.47
1:B:1056:ALA:HB3	1:B:1059:GLY:O	2.14	0.47
1:C:1074:ASN:OD1	4:R:1:NAG:H2	2.14	0.47
1:A:114:THR:HG22	1:A:233:ILE:HD11	1.96	0.47
2:E:103:SER:HB2	2:E:106:TYR:CE1	2.49	0.47
1:A:335:LEU:HA	1:A:362:VAL:H	1.80	0.46
1:B:392:PHE:CG	1:B:515:PHE:CD2	3.03	0.46
1:B:192:PHE:HE1	1:B:205:SER:HG	1.62	0.46
1:B:449:TYR:HA	1:B:495:TYR:O	2.16	0.46
1:C:189:LEU:HG	1:C:208:THR:O	2.15	0.46
1:B:1140:PRO:O	1:B:1144:GLU:HG2	2.16	0.46
1:A:493:GLN:HB3	1:A:494:SER:H	1.55	0.46
1:B:645:THR:HG22	1:B:648:GLY:O	2.15	0.46
1:C:708:SER:HB2	1:C:711:SER:HB3	1.96	0.46
1:A:105:ILE:HG22	1:A:110:LEU:HD22	1.98	0.46
1:A:555:SER:HB3	1:A:586:ASP:N	2.30	0.46
1:C:40:ASP:OD1	1:C:41:LYS:N	2.48	0.46
1:A:707:TYR:CZ	1:B:797:PHE:HD1	2.33	0.46
1:B:388:ASN:O	1:B:526:GLY:HA3	2.16	0.46
1:C:191:GLU:CG	1:C:206:LYS:HB3	2.45	0.46
1:C:228:ASP:OD1	1:C:229:LEU:N	2.49	0.46
1:C:308:VAL:N	1:C:602:THR:OG1	2.38	0.46
1:A:29:THR:O	1:A:61:ASN:HA	2.15	0.46
1:B:111:ASP:HA	1:B:134:GLN:HA	1.98	0.46
1:C:133:PHE:HD2	1:C:161:SER:N	2.13	0.46
1:C:312:ILE:HD12	1:C:598:ILE:HD11	1.97	0.46
1:A:1090:PRO:HG2	1:B:913:GLN:HE22	1.81	0.46
1:B:473:TYR:N	1:B:489:TYR:O	2.30	0.46
1:C:191:GLU:HG3	1:C:223:LEU:HD11	1.97	0.46
1:C:439:ASN:HB3	1:C:506:GLN:CD	2.36	0.46
1:C:523:THR:O	1:C:523:THR:HG22	2.16	0.46
1:A:980:ILE:HG13	1:A:981:LEU:N	2.32	0.46
1:C:128:ILE:HD13	1:C:170:TYR:HD2	1.81	0.46
1:B:1072:GLU:HG3	1:C:894:LEU:HD22	1.97	0.45
1:C:107:GLY:N	1:C:235:ILE:HG23	2.30	0.45
1:A:497:PHE:CD2	1:A:507:PRO:HB3	2.51	0.45
1:A:565:PHE:HE1	1:A:567:ARG:HH21	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLY:HA2	1:B:194:PHE:O	2.16	0.45
1:B:552:LEU:CD2	1:B:587:ILE:HG12	2.46	0.45
1:C:323:THR:O	1:C:539:VAL:HG13	2.15	0.45
1:C:641:ASN:OD1	1:C:642:VAL:N	2.43	0.45
1:C:984:LEU:HD23	1:C:984:LEU:HA	1.67	0.45
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.64	0.45
1:A:1043:CYS:HB3	1:A:1064:HIS:CE1	2.51	0.45
1:B:204:TYR:HE1	1:B:225:PRO:HB3	1.80	0.45
1:B:354:ASN:OD1	1:B:355:ARG:N	2.49	0.45
1:B:528:LYS:HD2	1:B:528:LYS:HA	1.80	0.45
1:B:977:LEU:HD11	1:B:993:ILE:HG12	1.98	0.45
1:C:939:SER:OG	1:C:940:SER:N	2.49	0.45
1:A:335:LEU:HA	1:A:362:VAL:HB	1.98	0.45
1:B:176:LEU:HA	1:B:190:ARG:NH2	2.32	0.45
1:A:707:TYR:CD2	1:B:883:THR:HG23	2.51	0.45
1:A:1139:ASP:OD1	1:A:1139:ASP:N	2.49	0.45
1:B:897:PRO:HG2	1:B:900:MET:SD	2.57	0.45
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.51	0.45
2:E:103:SER:H	2:E:106:TYR:HE1	1.63	0.45
1:A:62:VAL:HG13	1:A:267:VAL:O	2.16	0.45
1:B:319:ARG:HG2	1:B:592:PHE:HB2	1.98	0.45
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.98	0.45
1:C:538:CYS:HB2	1:C:590:CYS:HB3	1.71	0.45
1:B:619:GLU:H	1:B:619:GLU:HG3	1.52	0.45
1:A:1086:LYS:HE3	1:A:1086:LYS:HB2	1.72	0.45
1:B:374:PHE:HD1	1:B:436:TRP:CE3	2.34	0.45
1:A:92:PHE:HZ	1:A:101:ILE:HD13	1.82	0.44
1:A:114:THR:N	1:A:132:GLU:OE2	2.50	0.44
1:A:233:ILE:HG12	1:A:234:ASN:N	2.32	0.44
1:C:379:CYS:HA	1:C:432:CYS:HA	1.98	0.44
1:C:392:PHE:O	1:C:523:THR:N	2.50	0.44
4:N:1:NAG:H61	4:N:2:NAG:N2	2.32	0.44
1:A:327:VAL:HB	1:A:531:THR:HG23	2.00	0.44
1:A:752:LEU:HD21	1:A:990:GLU:HB2	1.98	0.44
1:C:38:TYR:HE1	1:C:222:ALA:HB1	1.83	0.44
1:A:708:SER:HB3	1:A:709:ASN:H	1.56	0.44
1:A:895:GLN:O	1:A:895:GLN:HG2	2.17	0.44
1:A:1004:LEU:HD12	1:A:1004:LEU:HA	1.81	0.44
1:B:115:GLN:N	1:B:132:GLU:HG2	2.32	0.44
2:E:69:VAL:HG13	2:E:82:LEU:HD11	2.00	0.44
3:D:4:LEU:HB2	3:D:103:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5:THR:O	3:D:23:THR:N	2.33	0.44
1:A:689:SER:O	1:A:690:GLN:NE2	2.50	0.44
1:B:380:TYR:HB2	1:B:430:THR:O	2.18	0.44
1:C:991:VAL:O	1:C:995:ARG:HG3	2.17	0.44
1:C:1098:ASN:ND2	4:Q:1:NAG:O7	2.50	0.44
1:A:94:SER:OG	1:A:95:THR:N	2.50	0.44
1:A:353:TRP:CZ3	1:A:355:ARG:HB2	2.48	0.44
1:A:650:LEU:HD12	1:A:650:LEU:HA	1.82	0.44
1:A:421:TYR:O	1:A:454:ARG:HB3	2.17	0.44
1:A:1090:PRO:CD	1:A:1095:PHE:HE1	2.30	0.44
1:B:1129:VAL:O	1:B:1132:ILE:HG12	2.18	0.44
1:A:748:GLU:O	1:A:751:ASN:HB2	2.18	0.44
1:C:539:VAL:HG12	1:C:540:ASN:N	2.33	0.44
2:E:14:PRO:HG3	2:E:130:VAL:HG12	1.99	0.44
1:A:131:CYS:HA	1:A:166:CYS:HA	1.99	0.43
1:B:205:SER:OG	1:B:206:LYS:N	2.51	0.43
1:B:374:PHE:HA	1:B:436:TRP:HB3	2.00	0.43
1:C:189:LEU:HD12	1:C:191:GLU:OE1	2.18	0.43
1:C:320:VAL:CG1	1:C:590:CYS:HB2	2.48	0.43
1:C:506:GLN:HG3	1:C:507:PRO:HD2	1.99	0.43
1:A:984:LEU:HB3	1:A:988:GLU:HG2	1.99	0.43
1:A:33:THR:OG1	1:A:219:GLY:O	2.35	0.43
1:A:917:TYR:HB3	1:C:1129:VAL:CG2	2.47	0.43
1:C:131:CYS:HB2	1:C:133:PHE:CE1	2.54	0.43
1:A:348:ALA:O	1:A:400:PHE:HA	2.18	0.43
1:B:85:PRO:O	1:B:238:PHE:HE1	2.01	0.43
1:B:980:ILE:HG13	1:B:981:LEU:N	2.32	0.43
1:B:592:PHE:HZ	1:C:857:GLY:H	1.67	0.43
1:A:722:VAL:HA	1:A:1064:HIS:O	2.17	0.43
1:B:767:LEU:HA	1:B:770:ILE:HG12	2.01	0.43
1:B:856:ASN:C	1:B:858:LEU:H	2.21	0.43
1:A:948:LEU:O	1:A:951:VAL:HG12	2.19	0.43
1:A:985:ASP:N	1:C:383:SER:OG	2.52	0.43
1:B:282:ASN:HB2	1:B:284:THR:HG22	2.01	0.43
1:B:532:ASN:OD1	1:B:533:LEU:HD23	2.18	0.43
1:C:503:VAL:HA	1:C:506:GLN:HB2	2.01	0.43
1:B:299:THR:HG21	1:B:597:VAL:HG21	2.01	0.43
1:B:353:TRP:NE1	1:B:466:ARG:HG2	2.34	0.43
1:C:200:TYR:HE1	1:C:230:PRO:HB3	1.84	0.43
1:C:206:LYS:HA	1:C:206:LYS:HD2	1.78	0.43
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:VAL:O	3:D:108:VAL:HA	2.18	0.43
1:A:28:TYR:HA	1:A:62:VAL:O	2.18	0.43
1:A:100:ILE:HD11	1:A:243:ALA:O	2.19	0.43
1:A:100:ILE:HG13	1:A:242:LEU:HG	2.00	0.43
1:A:617:CYS:HB2	1:A:649:CYS:HB3	1.90	0.43
1:B:36:VAL:HG21	1:B:220:PHE:HE1	1.83	0.43
1:B:299:THR:O	1:B:302:THR:OG1	2.27	0.43
1:B:392:PHE:CD2	1:B:515:PHE:CE2	3.06	0.43
1:C:133:PHE:HD2	1:C:161:SER:H	1.65	0.43
1:A:1141:LEU:O	1:A:1145:LEU:HG	2.19	0.43
1:B:118:LEU:O	1:B:120:VAL:HG23	2.19	0.43
1:C:435:ALA:HA	1:C:509:ARG:O	2.19	0.43
2:E:23:THR:HA	2:E:79:GLN:HG2	2.01	0.43
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.86	0.42
1:A:729:VAL:HG22	1:A:1059:GLY:HA2	2.01	0.42
1:C:613:GLN:O	1:C:615:VAL:HG23	2.18	0.42
1:A:94:SER:O	1:A:189:LEU:HD12	2.19	0.42
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.18	0.42
2:E:18:LEU:HD22	2:E:128:VAL:HG11	2.01	0.42
1:A:396:TYR:O	1:A:513:LEU:HA	2.18	0.42
1:B:44:ARG:HD2	1:B:279:TYR:CE2	2.54	0.42
1:B:759:PHE:HD2	1:B:1001:LEU:HD11	1.85	0.42
1:C:84:LEU:N	1:C:238:PHE:O	2.33	0.42
1:A:204:TYR:HA	1:A:225:PRO:HA	2.00	0.42
1:C:100:ILE:O	1:C:242:LEU:HD21	2.19	0.42
2:E:115:GLU:O	2:E:117:ASN:N	2.53	0.42
3:D:49:LEU:HA	3:D:60:VAL:HG21	2.02	0.42
1:B:193:VAL:HB	1:B:204:TYR:HB2	2.02	0.42
1:B:617:CYS:CB	1:B:642:VAL:HG23	2.49	0.42
1:B:709:ASN:OD1	1:B:709:ASN:N	2.47	0.42
1:C:114:THR:HG22	1:C:115:GLN:N	2.35	0.42
2:E:122:TRP:CG	3:D:46:PRO:HD2	2.45	0.42
1:B:319:ARG:HG2	1:B:592:PHE:CB	2.49	0.42
1:C:299:THR:OG1	1:C:300:LYS:N	2.52	0.42
1:A:32:PHE:CG	1:A:218:GLN:HG3	2.55	0.42
1:B:52:GLN:HA	1:B:274:THR:HA	2.00	0.42
1:B:376:THR:O	1:B:434:ILE:HA	2.20	0.42
1:B:973:ILE:HD11	1:B:983:ARG:HH12	1.84	0.42
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.20	0.42
1:B:560:LEU:HB2	1:B:563:GLN:OE1	2.20	0.42
1:C:537:LYS:O	1:C:539:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:TYR:CD1	2:E:100:HIS:CD2	3.08	0.42
1:A:34:ARG:HH21	1:A:217:PRO:C	2.22	0.42
1:B:392:PHE:CE2	1:B:515:PHE:HE2	2.32	0.42
1:C:325:SER:HA	1:C:540:ASN:OD1	2.19	0.42
1:C:560:LEU:HB2	1:C:563:GLN:OE1	2.19	0.42
1:A:118:LEU:HD22	1:A:133:PHE:CE2	2.55	0.41
1:A:906:PHE:HD1	1:A:906:PHE:HA	1.69	0.41
1:B:716:THR:HB	1:B:1071:GLN:O	2.20	0.41
1:A:767:LEU:HA	1:A:767:LEU:HD23	1.85	0.41
1:A:988:GLU:HG2	1:A:989:ALA:N	2.35	0.41
1:B:50:SER:O	1:B:50:SER:OG	2.38	0.41
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.68	0.41
1:C:748:GLU:O	1:C:752:LEU:HD13	2.20	0.41
1:C:964:LYS:HA	1:C:964:LYS:HD2	1.81	0.41
1:B:34:ARG:HD3	1:B:34:ARG:HA	1.93	0.41
1:B:308:VAL:HG22	1:B:602:THR:OG1	2.20	0.41
1:C:822:LEU:HD22	1:C:945:LEU:HD11	2.02	0.41
1:C:242:LEU:HA	1:C:242:LEU:HD23	1.86	0.41
1:C:367:VAL:O	1:C:371:SER:HB3	2.21	0.41
1:A:393:THR:N	1:A:516:GLU:O	2.52	0.41
1:A:699:LEU:HD12	1:B:873:TYR:OH	2.20	0.41
1:B:106:PHE:CD2	1:B:235:ILE:HG21	2.55	0.41
1:C:379:CYS:SG	1:C:384:PRO:HG3	2.60	0.41
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.55	0.41
1:A:359:SER:HA	1:A:524:VAL:HG22	2.03	0.41
1:B:30:ASN:HB3	1:B:32:PHE:HE1	1.85	0.41
1:B:1055:SER:OG	1:B:1056:ALA:N	2.53	0.41
4:O:1:NAG:HO3	4:O:1:NAG:C7	2.28	0.41
1:A:63:THR:O	1:A:266:TYR:HA	2.20	0.41
1:A:455:LEU:H	1:A:491:PRO:HB2	1.85	0.41
1:A:762:GLN:HG3	1:A:762:GLN:H	1.65	0.41
1:C:204:TYR:CE2	1:C:225:PRO:HB3	2.55	0.41
3:D:15:GLY:N	3:D:80:LEU:O	2.37	0.41
1:A:29:THR:HG22	1:A:30:ASN:N	2.36	0.41
1:A:34:ARG:NH2	1:A:217:PRO:O	2.52	0.41
1:A:498:GLN:HB2	1:A:501:ASN:HD21	1.86	0.41
1:A:1140:PRO:HB2	1:A:1144:GLU:OE2	2.21	0.41
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.86	0.41
1:B:531:THR:OG1	1:B:532:ASN:N	2.51	0.41
1:C:334:ASN:H	1:C:362:VAL:HG23	1.85	0.41
1:C:937:SER:O	1:C:941:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LYS:HG2	1:B:207:HIS:H	1.85	0.41
1:C:903:ALA:HB1	1:C:913:GLN:HB2	2.03	0.41
1:C:1144:GLU:N	1:C:1144:GLU:OE2	2.53	0.41
2:E:29:ILE:HA	2:E:34:TYR:CD2	2.56	0.41
1:A:615:VAL:HG12	1:A:616:ASN:N	2.36	0.40
1:A:886:TRP:H	1:A:886:TRP:HE3	1.65	0.40
1:A:1119:ASN:OD1	1:A:1120:THR:HG23	2.21	0.40
1:A:1141:LEU:HA	1:A:1144:GLU:OE1	2.21	0.40
1:B:115:GLN:HA	1:B:132:GLU:HG2	2.01	0.40
1:B:1126:CYS:SG	1:B:1132:ILE:HD12	2.61	0.40
1:C:233:ILE:HG12	1:C:234:ASN:N	2.36	0.40
1:C:986:PRO:HA	1:C:989:ALA:HB3	2.04	0.40
1:B:276:LEU:O	1:B:288:ALA:HA	2.20	0.40
1:B:402:ILE:HG13	1:B:403:ARG:O	2.20	0.40
1:B:703:ASN:O	1:C:789:TYR:HA	2.21	0.40
1:C:363:ALA:HB3	1:C:525:CYS:C	2.42	0.40
3:D:26:ARG:O	3:D:31:ALA:N	2.40	0.40
1:A:917:TYR:HB3	1:C:1129:VAL:HG21	2.02	0.40
1:B:906:PHE:O	1:B:909:ILE:HG12	2.20	0.40
1:C:885:GLY:O	1:C:888:PHE:HD1	2.03	0.40
1:A:192:PHE:CD2	1:A:205:SER:HB2	2.57	0.40
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.56	0.40
1:B:308:VAL:N	1:B:602:THR:HG1	2.19	0.40
1:C:357:ARG:HD2	1:C:358:ILE:N	2.36	0.40
1:C:418:ILE:H	1:C:418:ILE:HD12	1.86	0.40
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.83	0.40
1:B:318:PHE:CZ	1:B:615:VAL:HG11	2.56	0.40
2:E:113:ARG:HH12	3:D:34:ASP:HB2	1.86	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	980/1288 (76%)	903 (92%)	67 (7%)	10 (1%)	13	44
1	B	945/1288 (73%)	900 (95%)	42 (4%)	3 (0%)	37	69
1	C	945/1288 (73%)	895 (95%)	47 (5%)	3 (0%)	37	69
2	E	130/132 (98%)	113 (87%)	12 (9%)	5 (4%)	2	21
3	D	109/111 (98%)	101 (93%)	5 (5%)	3 (3%)	4	27
All	All	3109/4107 (76%)	2912 (94%)	173 (6%)	24 (1%)	19	49

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	PRO
1	A	467	ASP
1	A	477	SER
3	D	3	VAL
3	D	34	ASP
1	A	464	PHE
1	B	164	ASN
1	B	543	PHE
1	C	363	ALA
1	C	1128	VAL
2	E	114	ASP
1	A	337	PRO
1	A	491	PRO
2	E	120	ASP
1	A	493	GLN
1	A	744	GLY
1	B	166	CYS
2	E	103	SER
2	E	118	TRP
1	A	527	PRO
2	E	116	GLY
1	C	987	PRO
3	D	30	GLY
1	A	462	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	728/1112 (66%)	726 (100%)	2 (0%)	91	92
1	B	713/1112 (64%)	709 (99%)	4 (1%)	84	88
1	C	680/1112 (61%)	677 (100%)	3 (0%)	89	91
2	E	100/113 (88%)	99 (99%)	1 (1%)	73	80
3	D	71/90 (79%)	68 (96%)	3 (4%)	25	49
All	All	2292/3539 (65%)	2279 (99%)	13 (1%)	82	88

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

Mol	Chain	Res	Type
1	A	708	SER
1	A	906	PHE
1	B	165	ASN
1	B	615	VAL
1	B	619	GLU
1	B	708	SER
1	C	282	ASN
1	C	525	CYS
1	C	617	CYS
2	E	120	ASP
3	D	40	GLN
3	D	41	LEU
3	D	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	HIS
1	A	317	ASN
1	A	493	GLN
1	A	498	GLN
1	A	501	ASN
1	A	542	ASN
1	A	563	GLN
1	A	644	GLN
1	A	755	GLN
1	A	787	GLN

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Mol	Chain	Res	Type
1	A	901	GLN
1	A	907	ASN
1	A	965	GLN
1	B	66	HIS
1	B	207	HIS
1	B	564	GLN
1	B	644	GLN
1	B	658	ASN
1	B	762	GLN
1	B	901	GLN
1	B	913	GLN
1	B	954	GLN
1	B	955	ASN
1	B	965	GLN
1	C	66	HIS
1	C	536	ASN
1	C	606	ASN
1	C	644	GLN
1	C	658	ASN
1	C	755	GLN
1	C	955	ASN
1	C	965	GLN
1	C	1101	HIS
1	C	1113	GLN
3	D	33	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

30 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	F	1	1,4	14,14,15	0.33	0	17,19,21	0.39	0
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.63	0
4	NAG	G	1	1,4	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	G	2	4	14,14,15	0.15	0	17,19,21	0.58	0
4	NAG	H	1	1,4	14,14,15	0.21	0	17,19,21	0.52	0
4	NAG	H	2	4	14,14,15	0.30	0	17,19,21	1.31	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.19	0	17,19,21	0.52	0
4	NAG	I	2	4	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	J	1	1,4	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	J	2	4	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	K	1	1,4	14,14,15	0.18	0	17,19,21	0.49	0
4	NAG	K	2	4	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	L	1	1,4	14,14,15	0.57	1 (7%)	17,19,21	0.54	0
4	NAG	L	2	4	14,14,15	0.17	0	17,19,21	0.59	0
4	NAG	N	1	1,4	14,14,15	0.41	0	17,19,21	0.49	0
4	NAG	N	2	4	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	O	1	1,4	14,14,15	0.25	0	17,19,21	0.64	0
4	NAG	O	2	4	14,14,15	0.18	0	17,19,21	0.53	0
4	NAG	P	1	1,4	14,14,15	0.30	0	17,19,21	0.50	0
4	NAG	P	2	4	14,14,15	0.29	0	17,19,21	0.64	0
4	NAG	Q	1	1,4	14,14,15	0.16	0	17,19,21	0.59	0
4	NAG	Q	2	4	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	R	1	1,4	14,14,15	0.50	0	17,19,21	0.65	1 (5%)
4	NAG	R	2	4	14,14,15	0.40	0	17,19,21	1.27	1 (5%)
4	NAG	S	1	1,4	14,14,15	0.24	0	17,19,21	0.55	0
4	NAG	S	2	4	14,14,15	0.16	0	17,19,21	0.59	0
4	NAG	T	1	1,4	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	T	2	4	14,14,15	0.30	0	17,19,21	0.65	0
4	NAG	U	1	1,4	14,14,15	0.24	0	17,19,21	1.29	1 (5%)
4	NAG	U	2	4	14,14,15	0.16	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	5/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	5/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	3/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1	NAG	O5-C1	-2.08	1.40	1.43

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2	NAG	C2-N2-C7	4.38	129.15	122.90
4	R	2	NAG	C2-N2-C7	4.31	129.03	122.90
4	U	1	NAG	C2-N2-C7	4.24	128.95	122.90
4	R	1	NAG	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	T	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	G	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C1-C2-N2-C7
4	O	1	NAG	C1-C2-N2-C7

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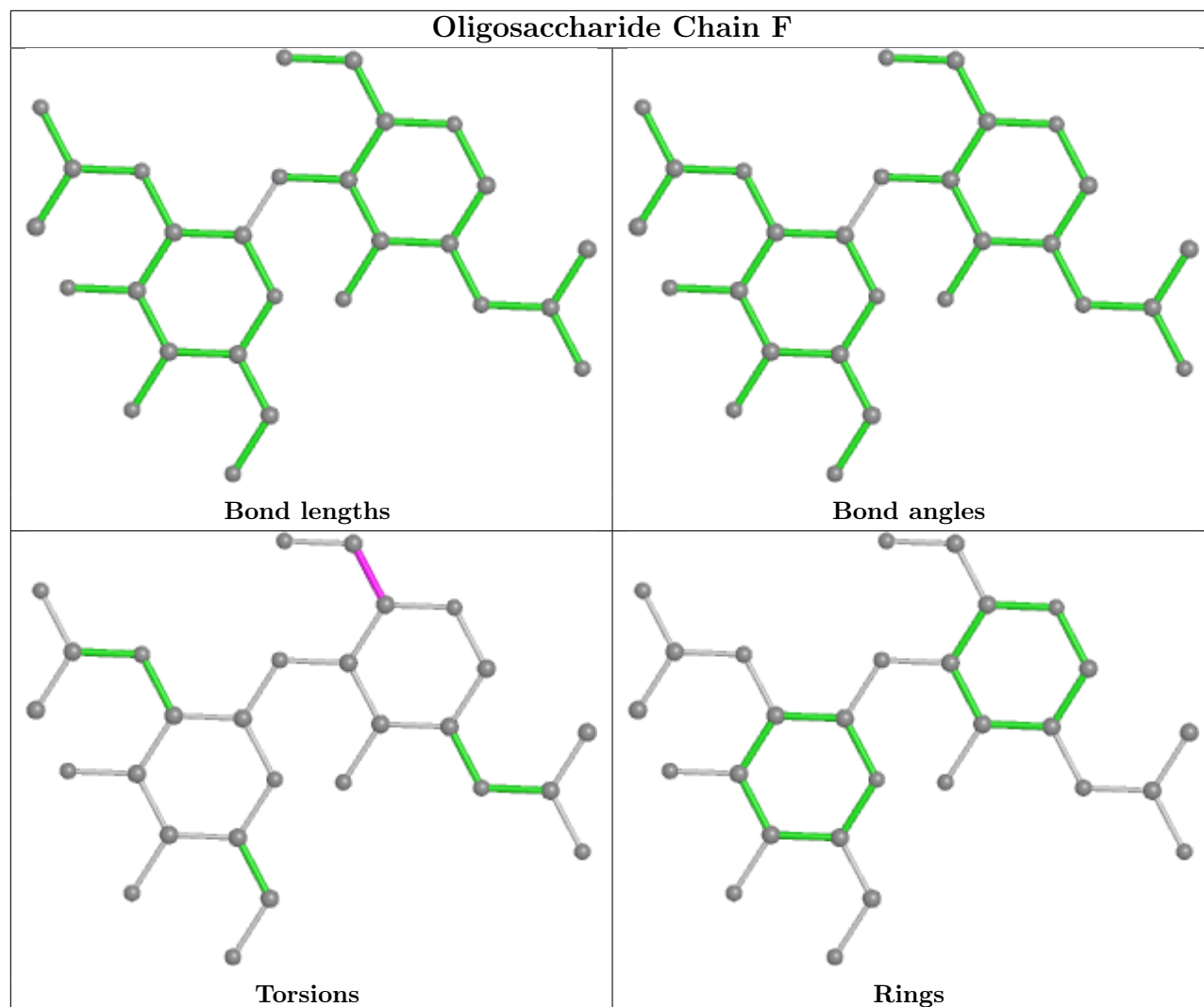
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	U	1	NAG	C3-C2-N2-C7
4	H	2	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	L	1	NAG	C3-C2-N2-C7
4	O	1	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7

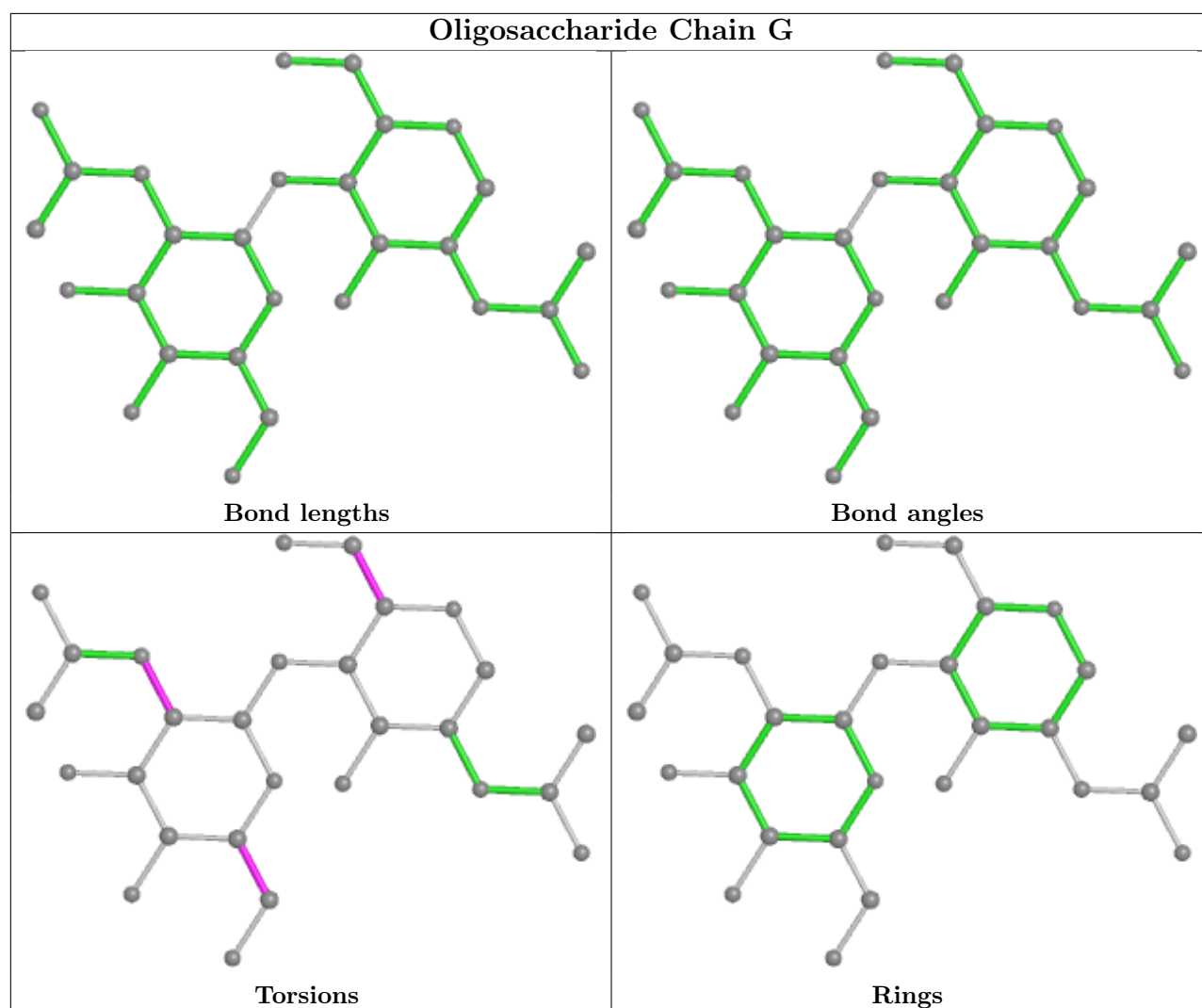
There are no ring outliers.

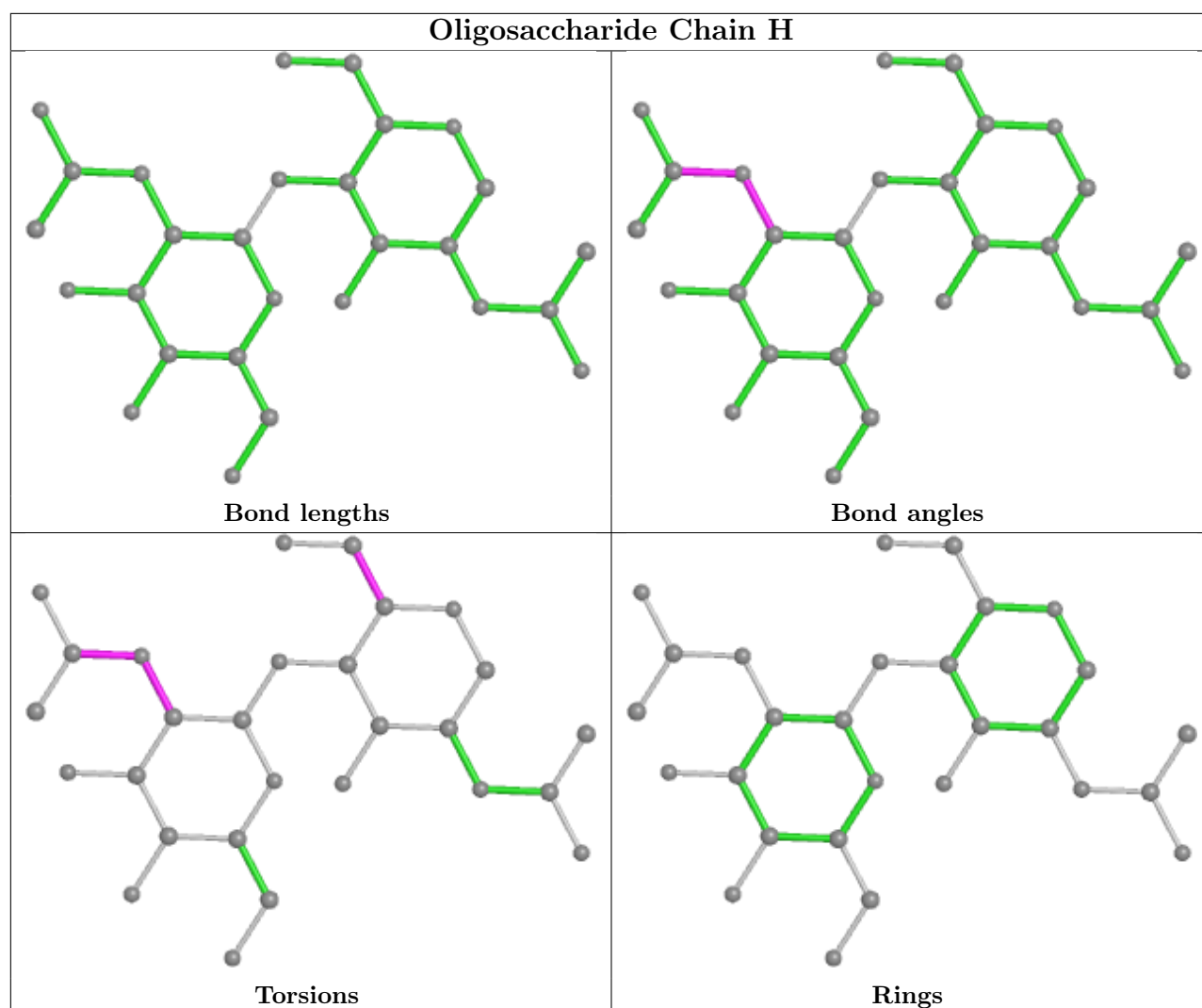
8 monomers are involved in 8 short contacts:

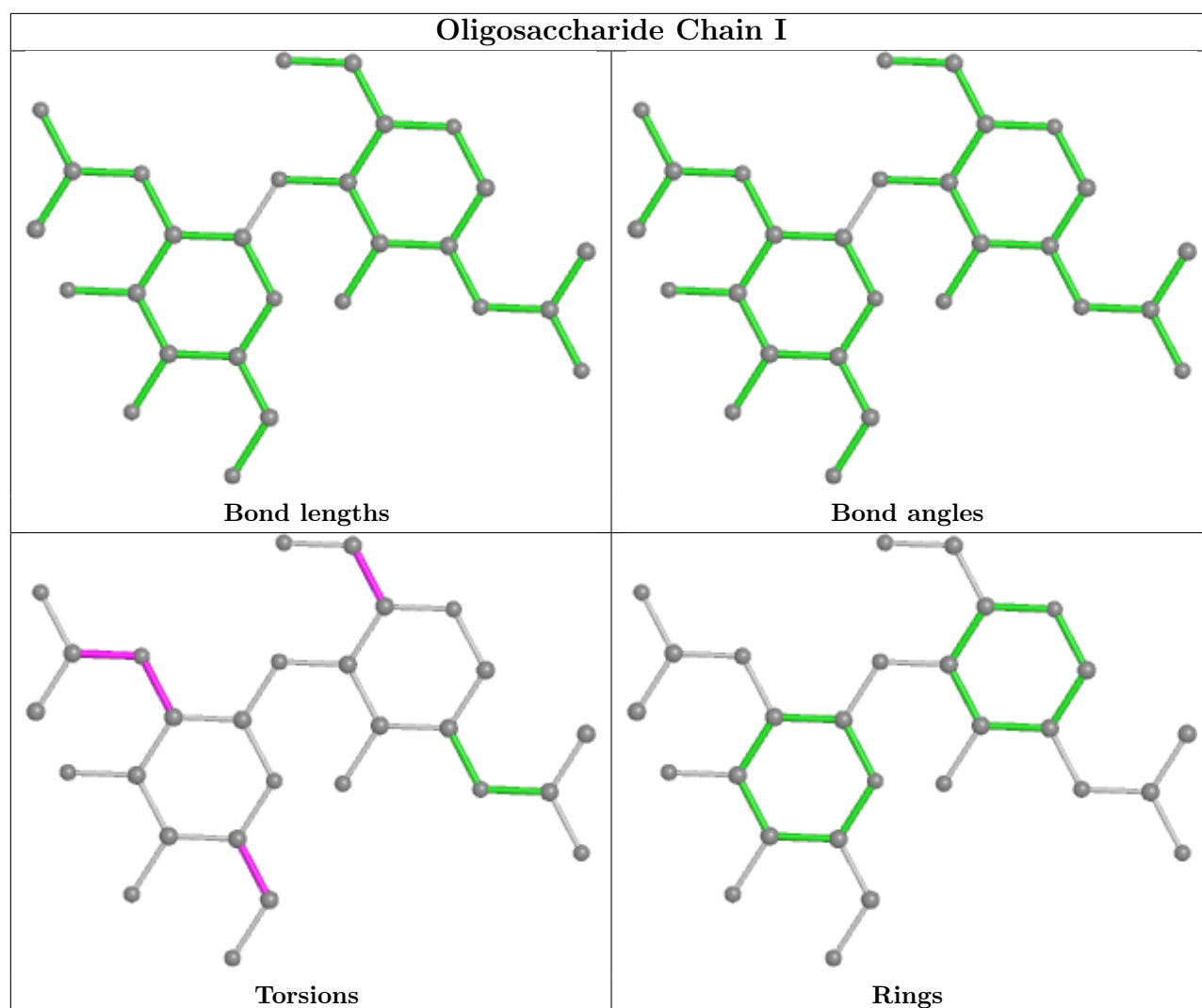
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	1	NAG	1	0
4	U	1	NAG	1	0
4	O	1	NAG	1	0
4	N	1	NAG	2	0
4	N	2	NAG	2	0
4	H	2	NAG	1	0
4	R	2	NAG	1	0
4	R	1	NAG	1	0

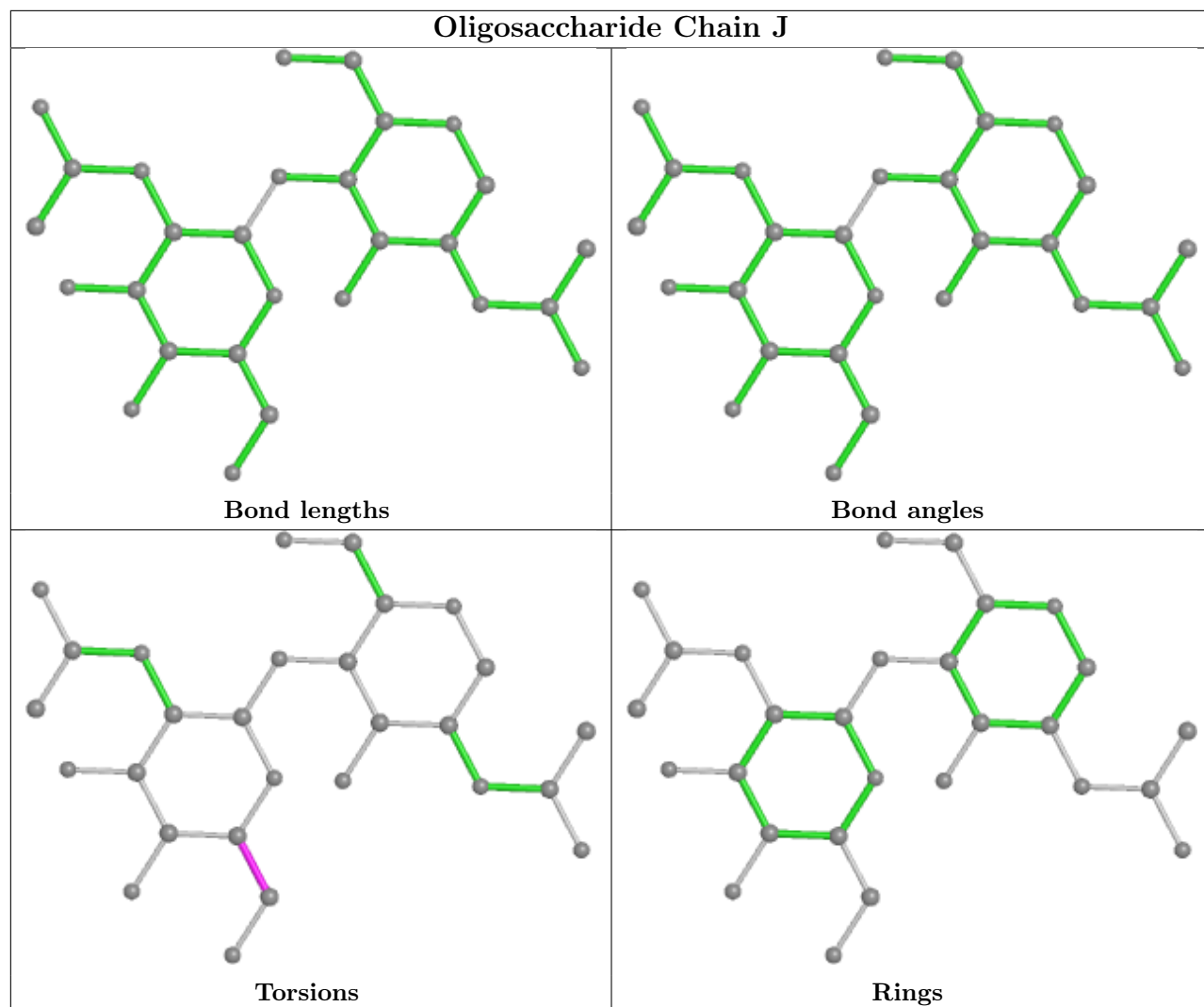
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

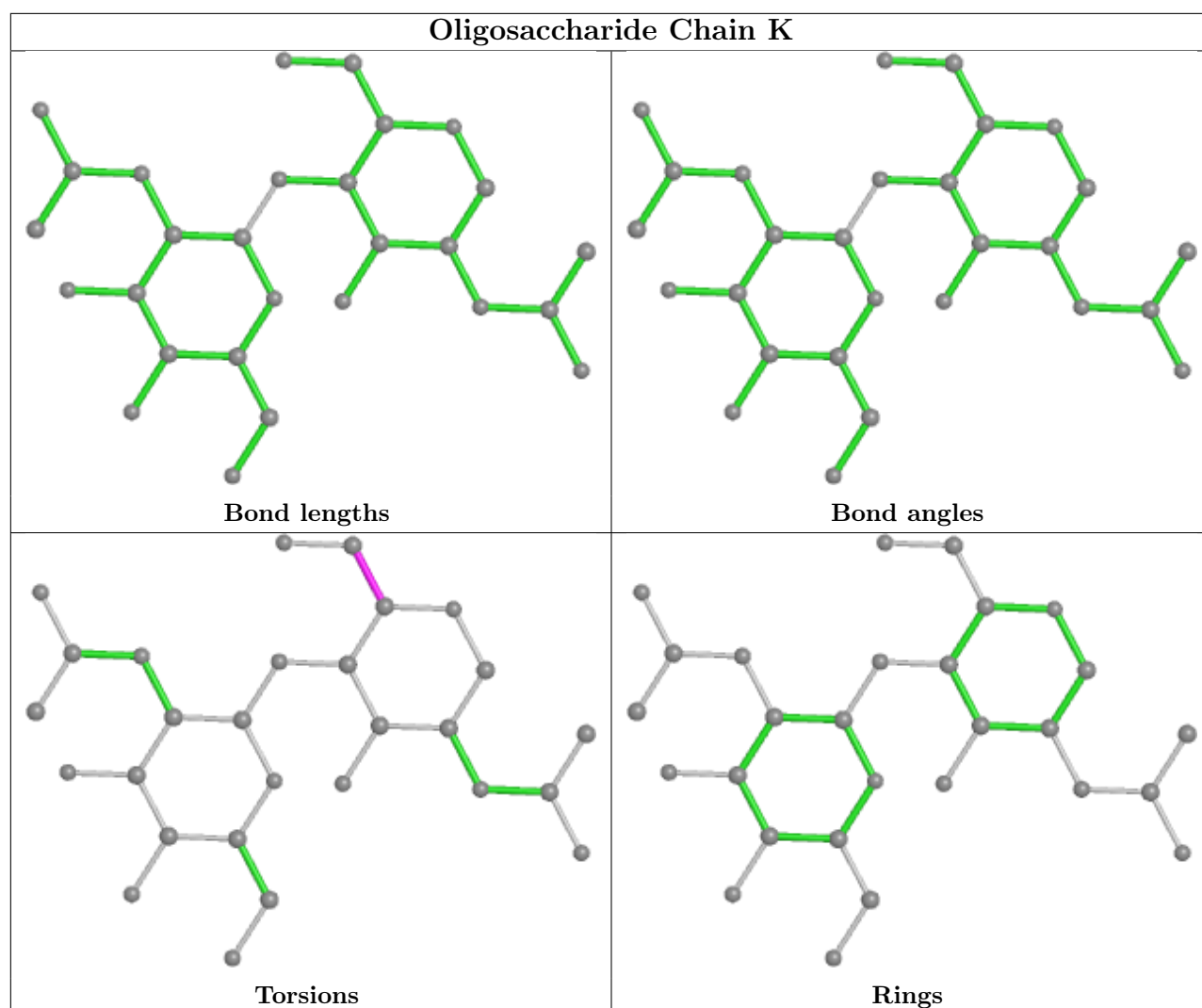




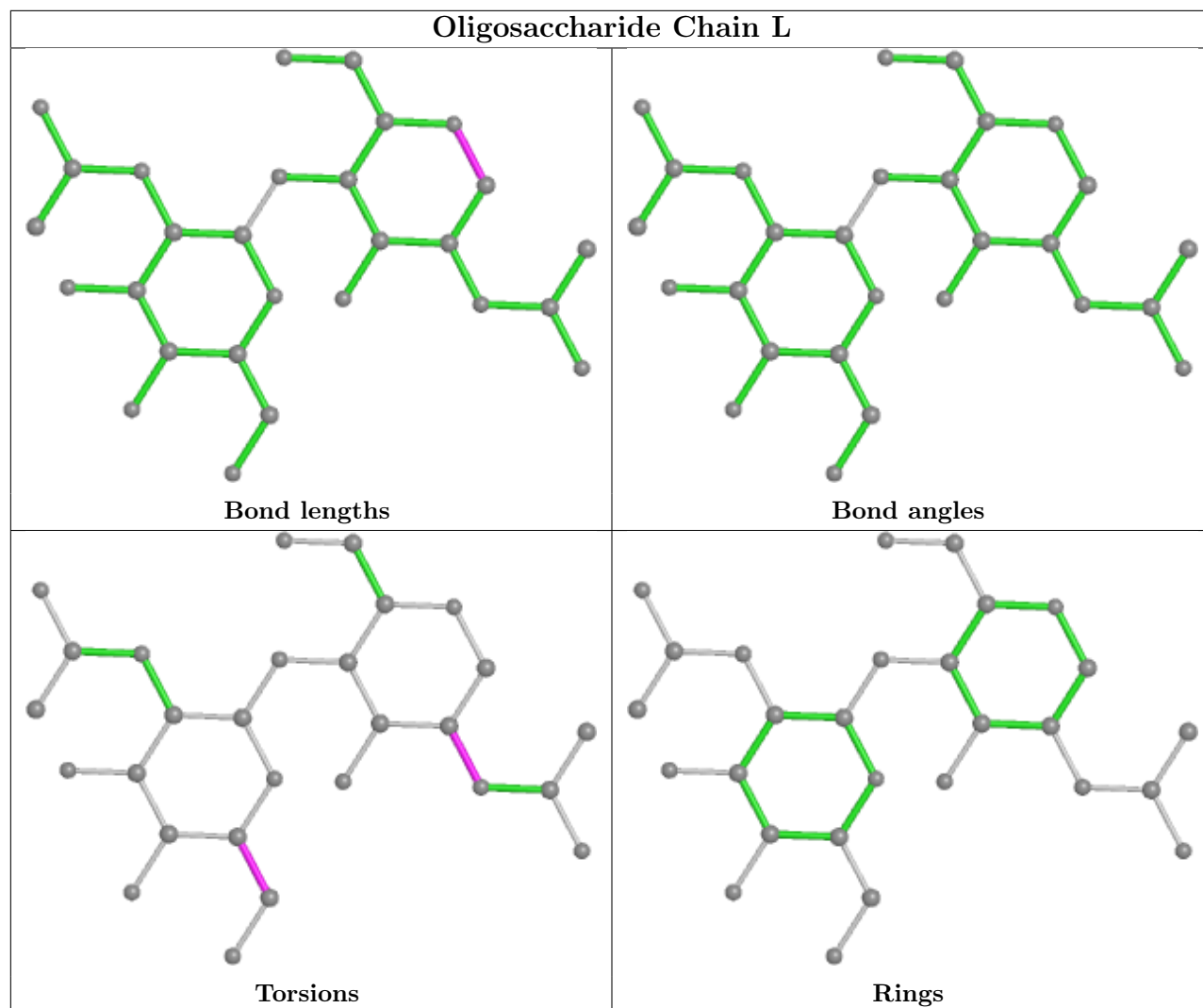


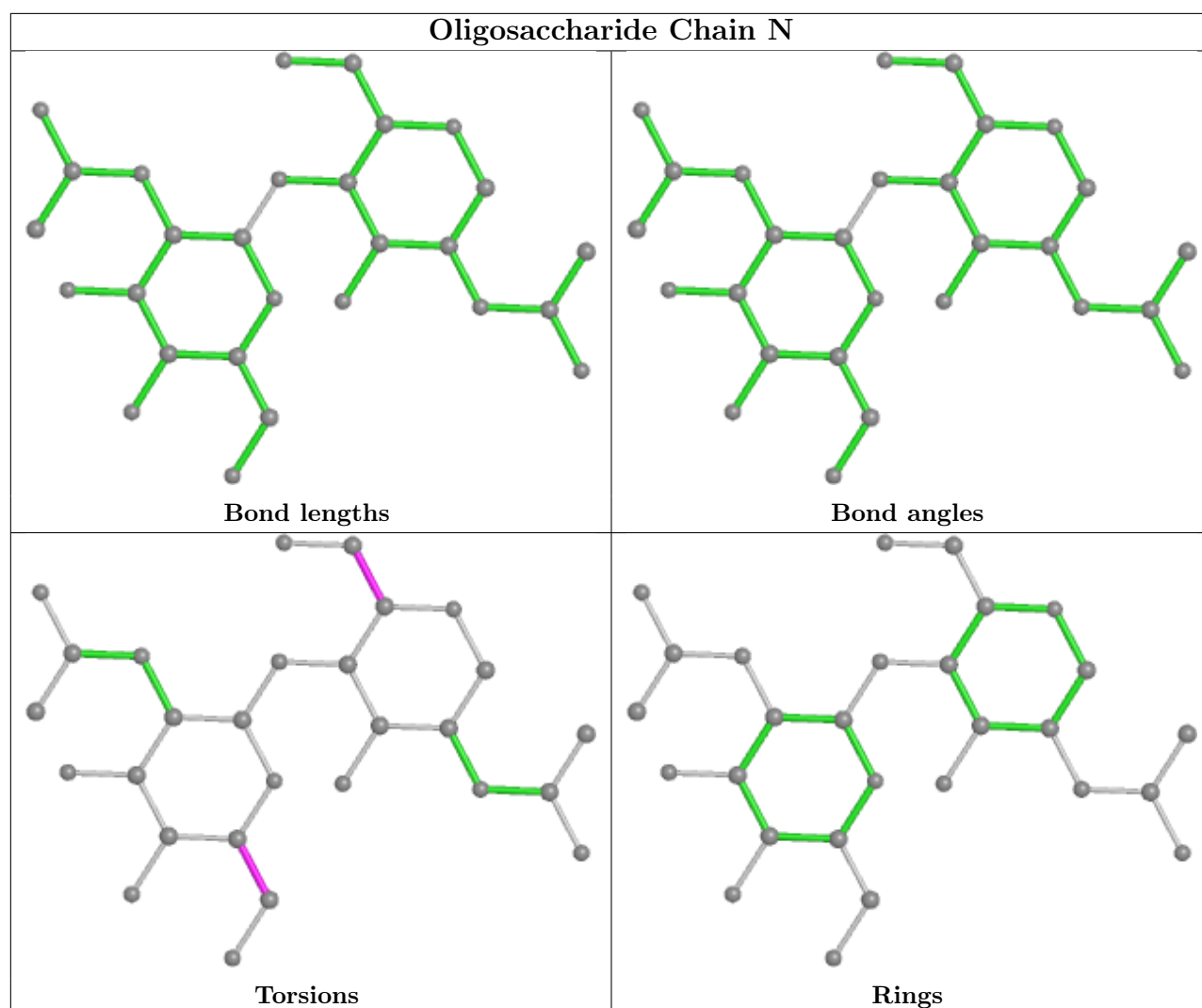


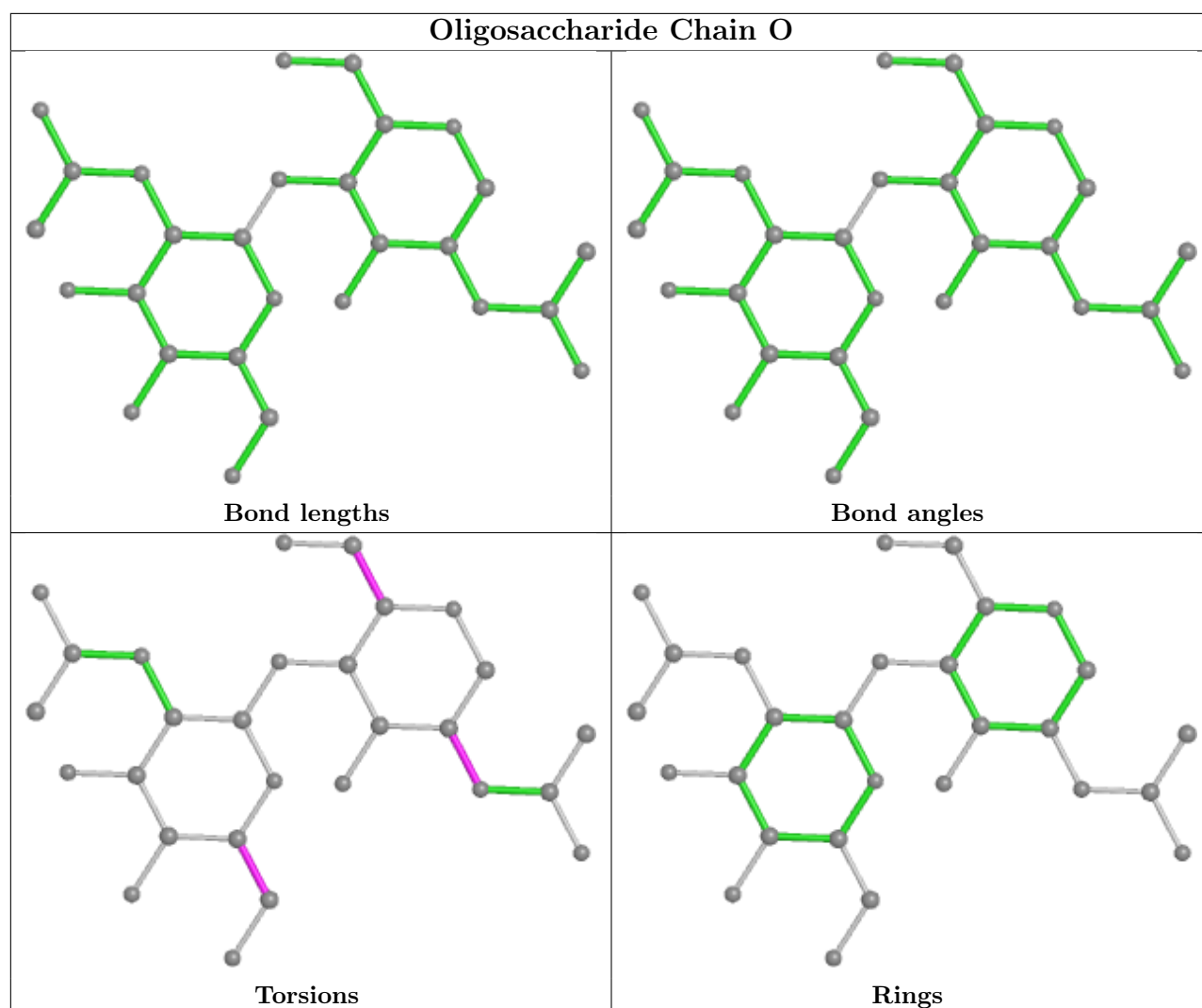


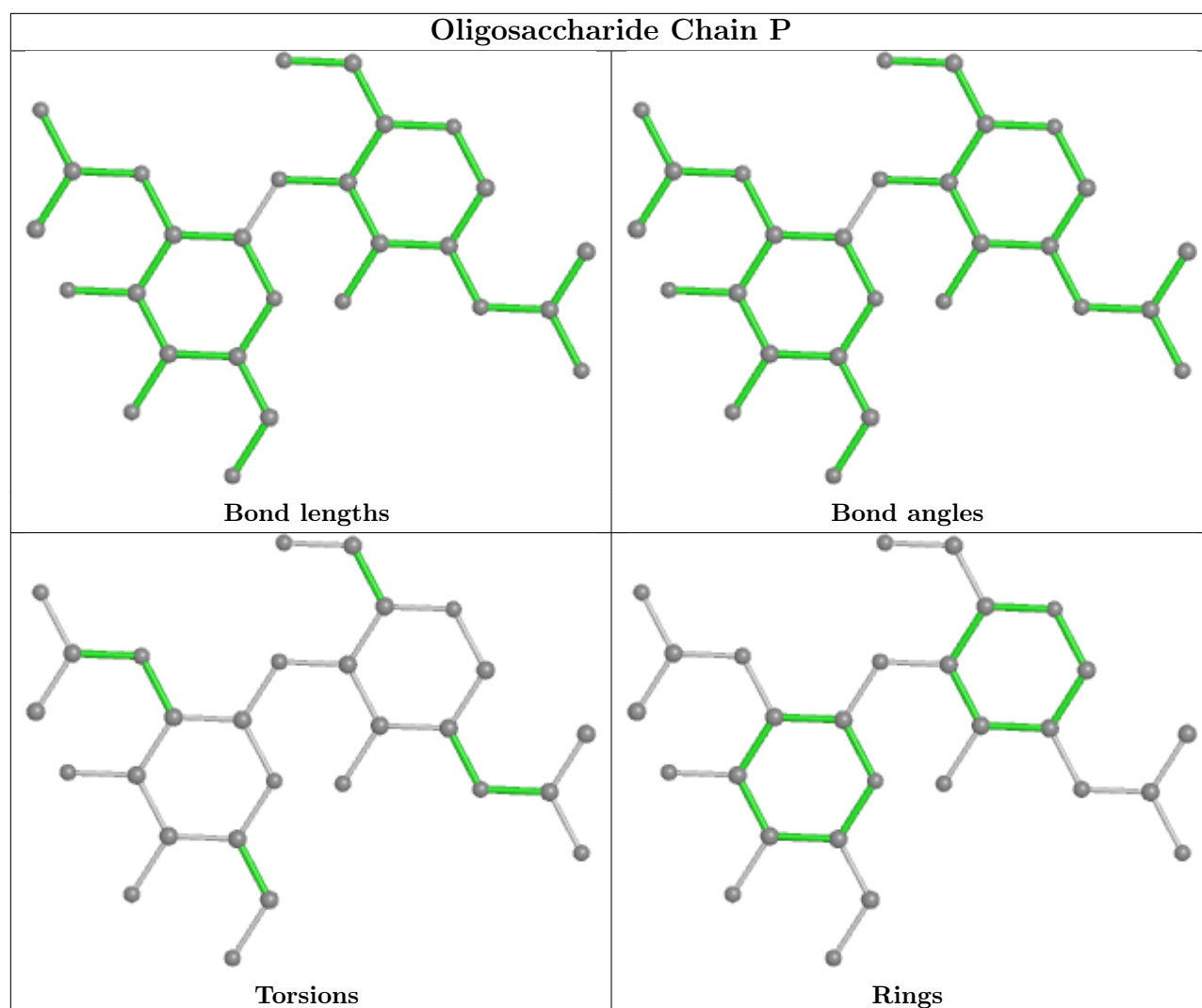


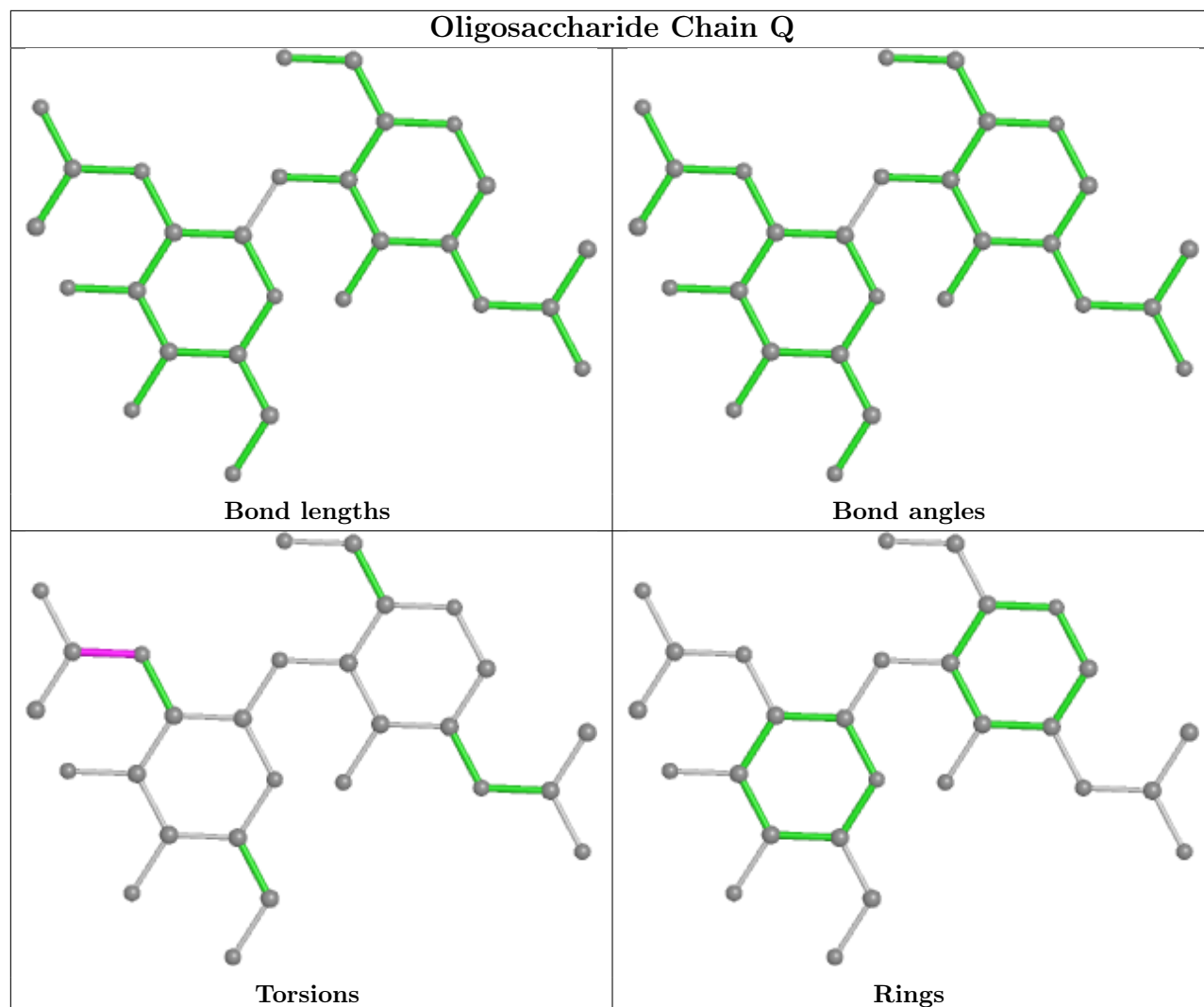


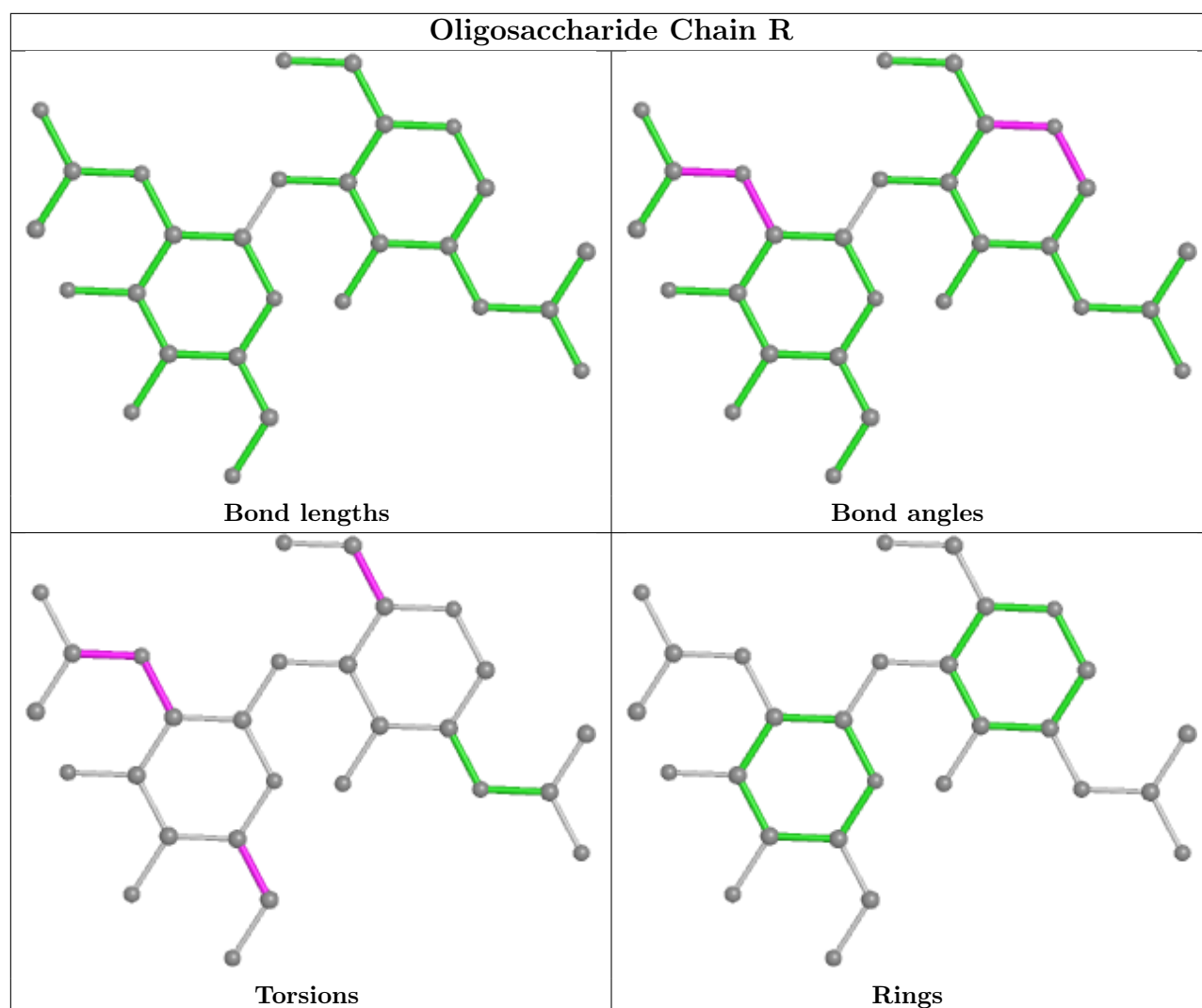


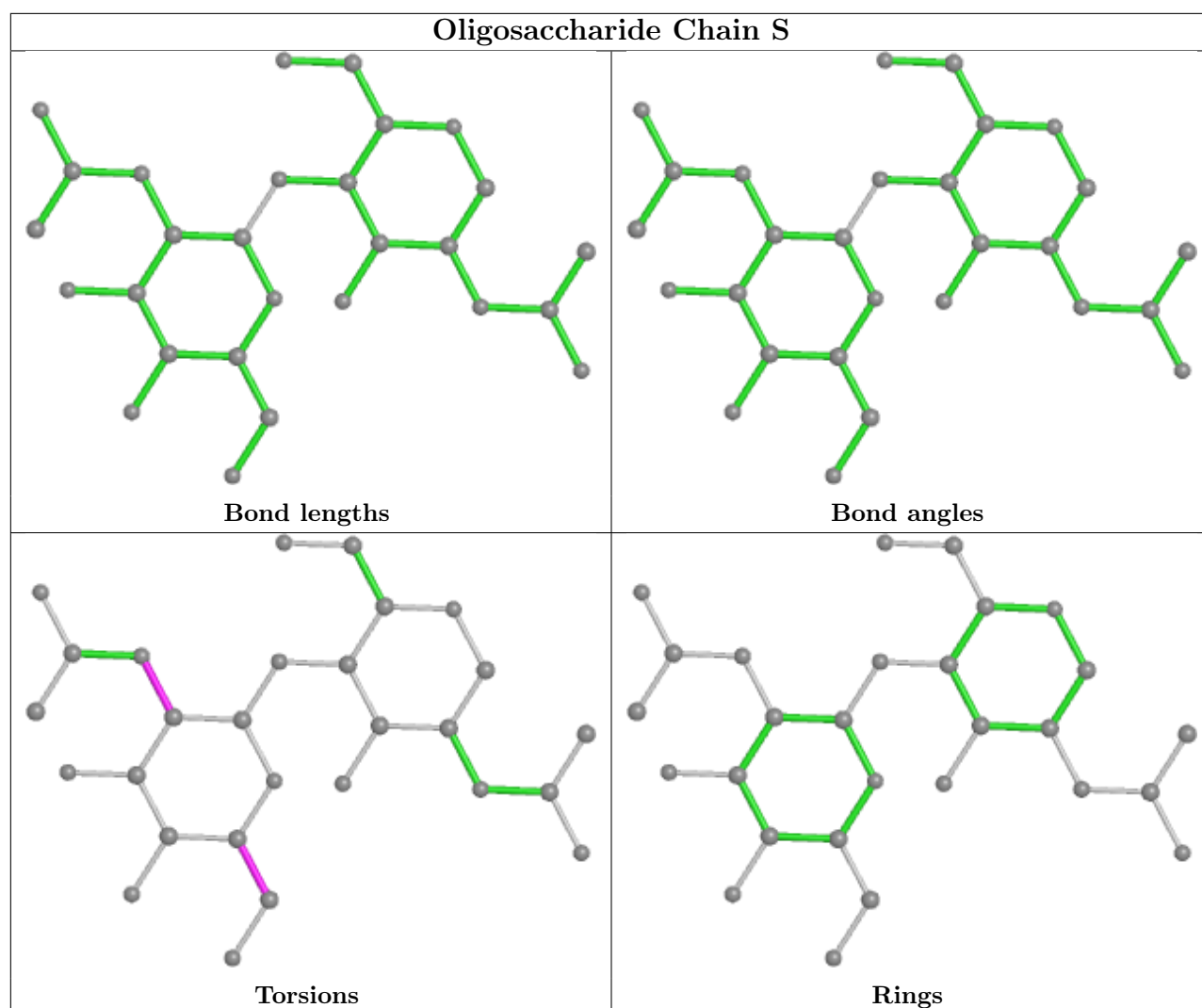


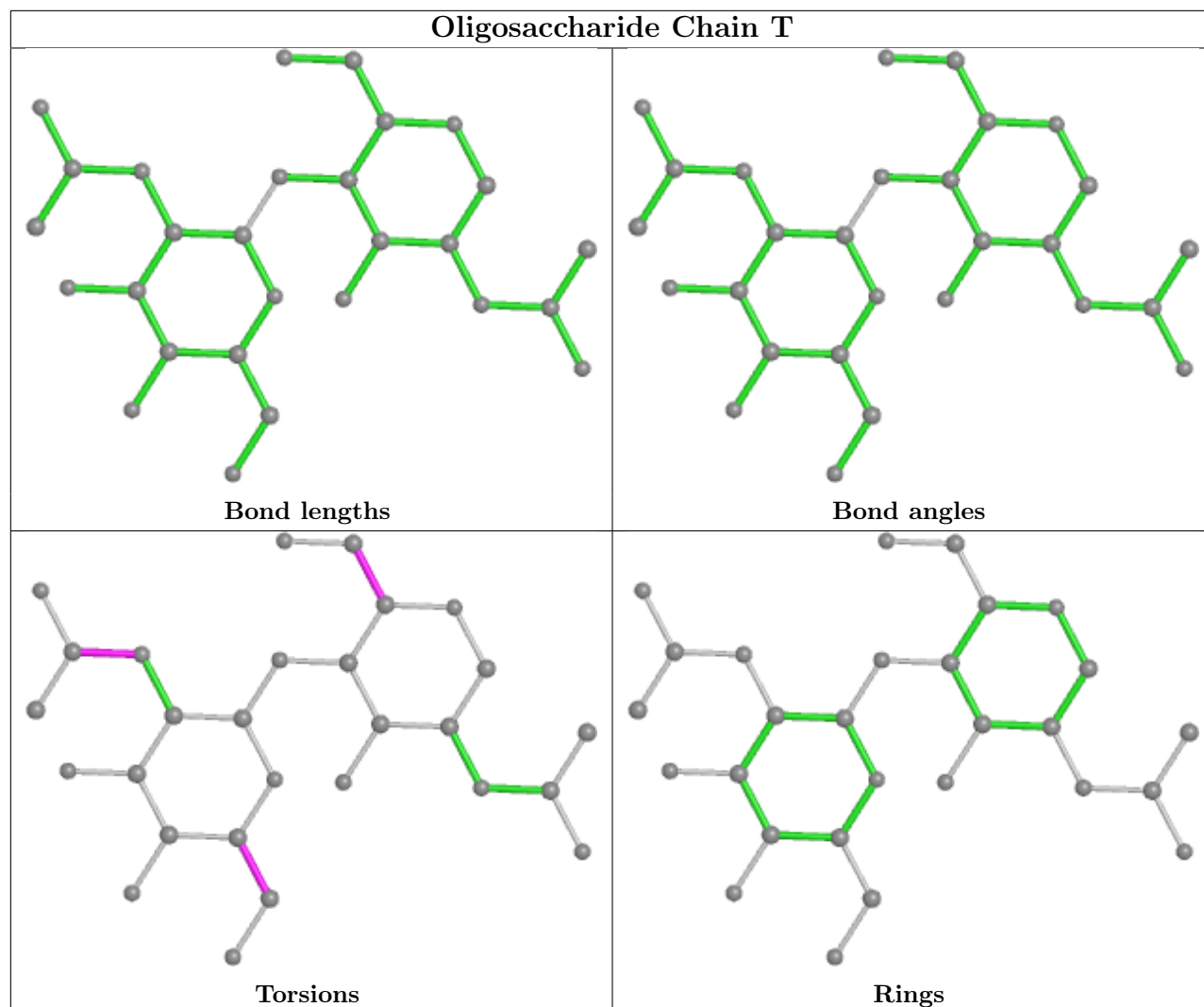




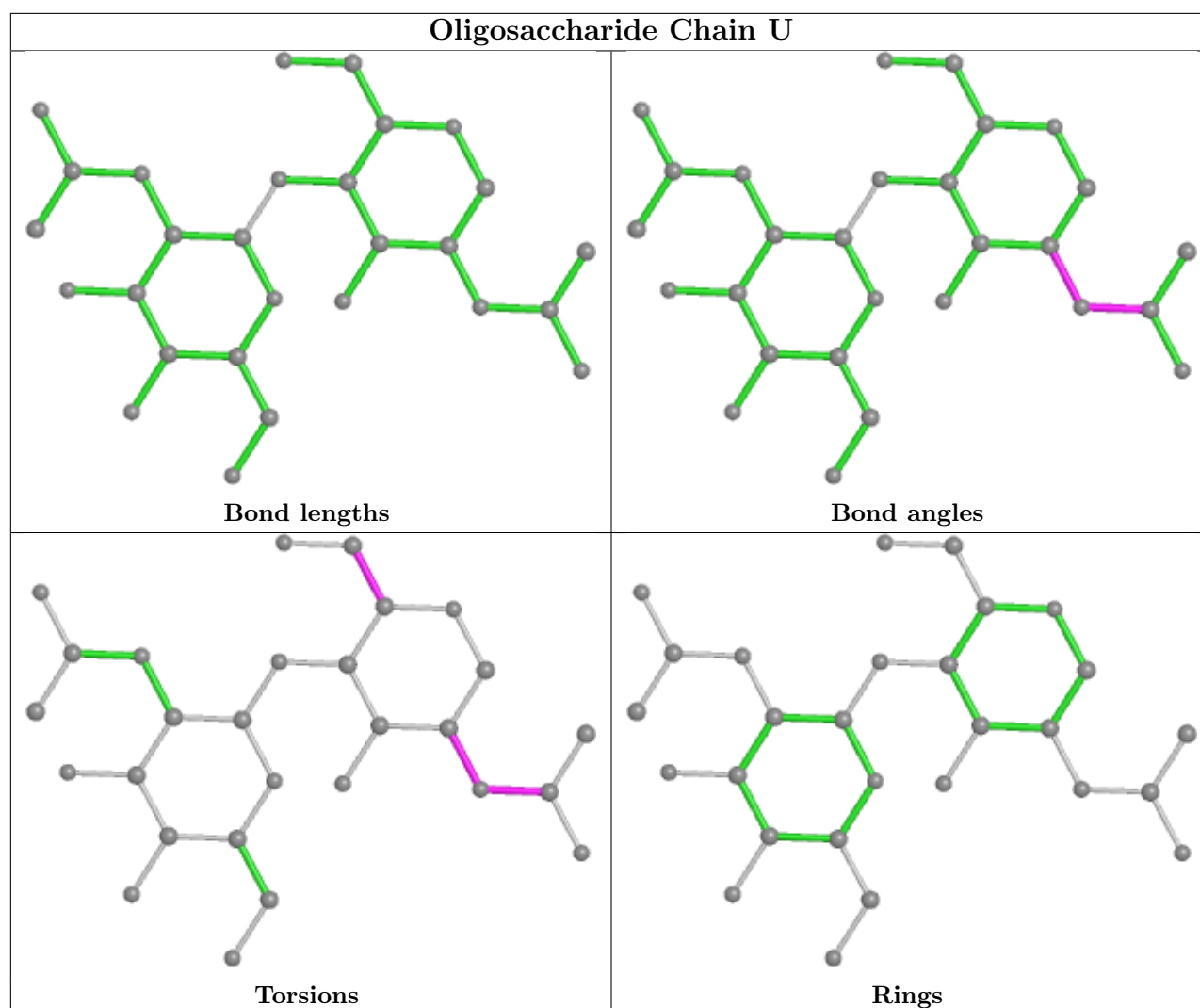












## 5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	B	1306	1	14,14,15	0.25	0	17,19,21	0.51	0
5	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.50	0
5	NAG	C	1305	1	14,14,15	0.35	0	17,19,21	0.57	0
5	NAG	B	1303	1	14,14,15	0.30	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	1301	1	14,14,15	0.32	0	17,19,21	0.71	0
5	NAG	C	1308	1	14,14,15	0.72	1 (7%)	17,19,21	0.60	0
5	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	A	1306	1	14,14,15	2.07	1 (7%)	17,19,21	2.09	1 (5%)
5	NAG	A	1307	1	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	1.36	2 (11%)
5	NAG	A	1304	1	14,14,15	0.31	0	17,19,21	0.57	0
5	NAG	B	1302	1	14,14,15	0.27	0	17,19,21	0.67	0
5	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.51	0
5	NAG	B	1308	1	14,14,15	0.40	0	17,19,21	0.62	0
5	NAG	C	1303	1	14,14,15	0.43	0	17,19,21	1.26	1 (5%)
5	NAG	C	1307	1	14,14,15	0.41	0	17,19,21	0.44	0
5	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	A	1308	1	14,14,15	0.53	0	17,19,21	1.22	1 (5%)
5	NAG	B	1305	1	14,14,15	0.38	0	17,19,21	0.42	0
5	NAG	B	1309	1	14,14,15	0.47	0	17,19,21	1.28	1 (5%)
5	NAG	A	1305	1	14,14,15	0.21	0	17,19,21	0.48	0
5	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.60	1 (5%)
5	NAG	A	1301	1	14,14,15	0.17	0	17,19,21	0.70	1 (5%)
5	NAG	C	1309	1	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	A	1303	1	14,14,15	0.25	0	17,19,21	0.53	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
5	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	5/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1306	NAG	C1-C2	7.68	1.63	1.52
5	C	1308	NAG	O5-C1	-2.05	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1306	NAG	O5-C1-C2	-8.33	98.14	111.29
5	B	1304	NAG	C2-N2-C7	4.42	129.20	122.90
5	B	1309	NAG	C2-N2-C7	4.33	129.07	122.90
5	A	1308	NAG	C2-N2-C7	4.28	129.00	122.90
5	C	1303	NAG	C2-N2-C7	4.23	128.92	122.90
5	A	1301	NAG	C1-O5-C5	2.26	115.25	112.19
5	B	1304	NAG	C4-C3-C2	-2.06	108.00	111.02
5	C	1304	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1306	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	A	1308	NAG	C8-C7-N2-C2
5	A	1308	NAG	O7-C7-N2-C2
5	B	1304	NAG	C8-C7-N2-C2
5	B	1304	NAG	O7-C7-N2-C2
5	B	1309	NAG	C8-C7-N2-C2
5	B	1309	NAG	O7-C7-N2-C2
5	C	1303	NAG	C8-C7-N2-C2
5	C	1303	NAG	O7-C7-N2-C2
5	B	1307	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1301	NAG	C3-C2-N2-C7
5	B	1302	NAG	C3-C2-N2-C7
5	B	1306	NAG	C3-C2-N2-C7
5	B	1307	NAG	C3-C2-N2-C7
5	C	1307	NAG	C3-C2-N2-C7
5	B	1302	NAG	O5-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1301	NAG	C1-C2-N2-C7
5	B	1305	NAG	C4-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	A	1308	NAG	C3-C2-N2-C7
5	B	1304	NAG	C3-C2-N2-C7
5	B	1309	NAG	C3-C2-N2-C7
5	C	1302	NAG	C3-C2-N2-C7
5	C	1303	NAG	C3-C2-N2-C7
5	C	1302	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1304	NAG	1	0
5	C	1303	NAG	1	0
5	A	1308	NAG	1	0
5	B	1309	NAG	1	0
5	A	1301	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

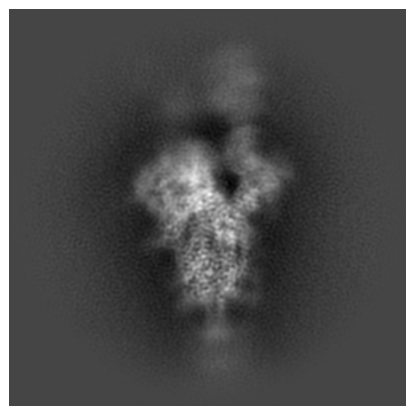
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33667. These allow visual inspection of the internal detail of the map and identification of artifacts.

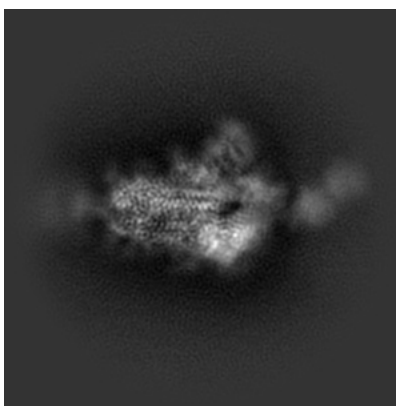
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

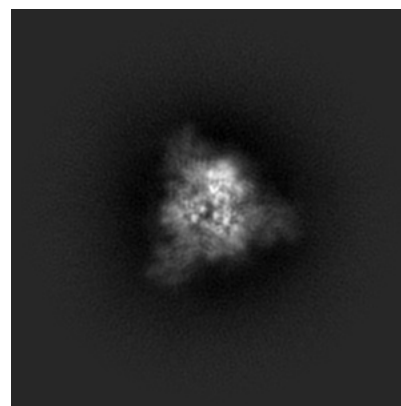
#### 6.1.1 Primary map



X

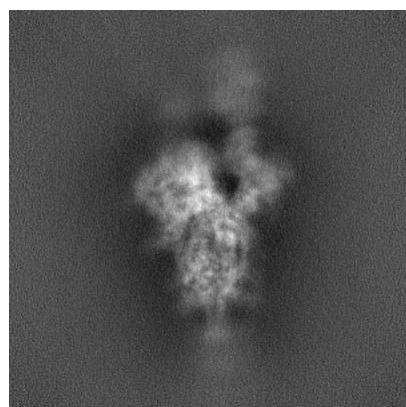


Y

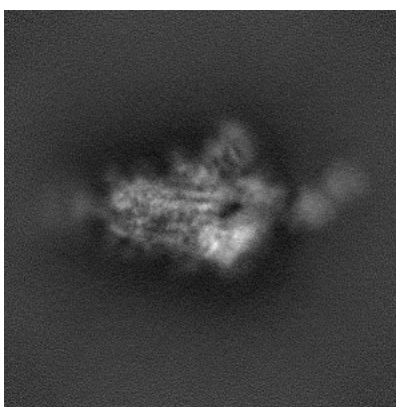


Z

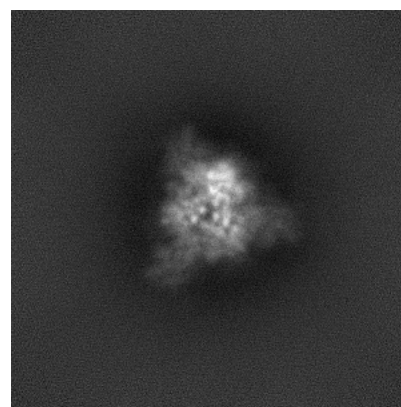
#### 6.1.2 Raw map



X



Y



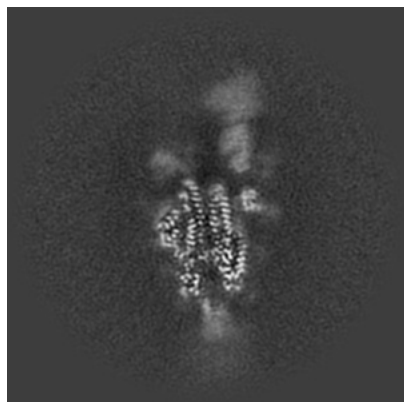
Z

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

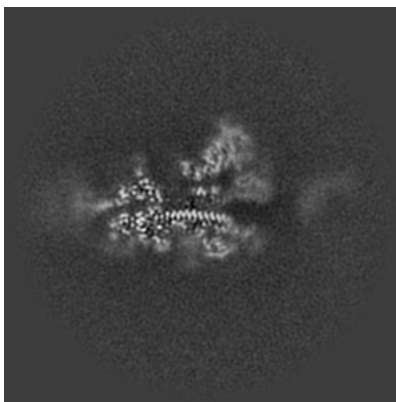


## 6.2 Central slices [i](#)

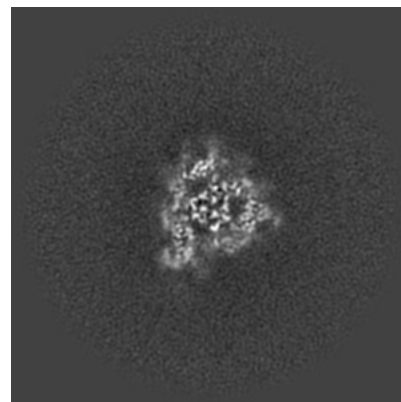
### 6.2.1 Primary map



X Index: 224

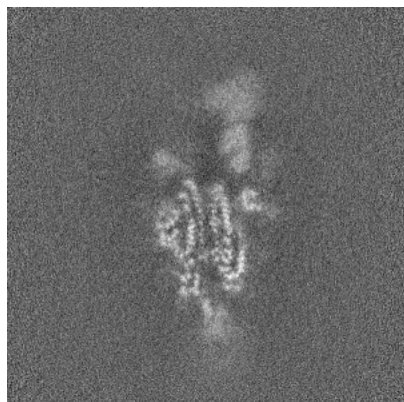


Y Index: 224

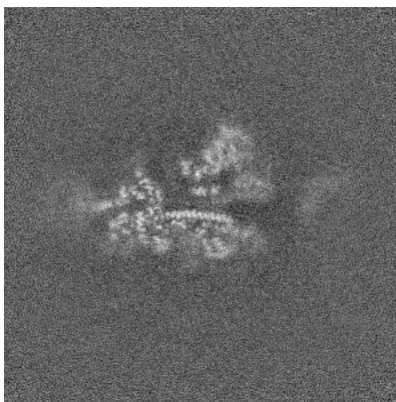


Z Index: 224

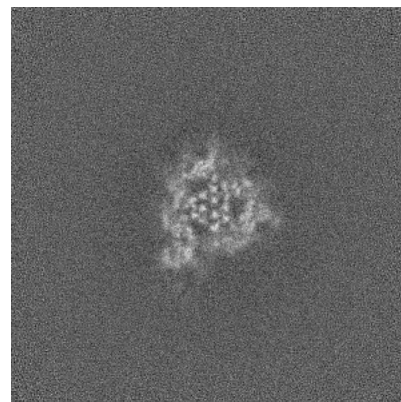
### 6.2.2 Raw map



X Index: 224



Y Index: 224

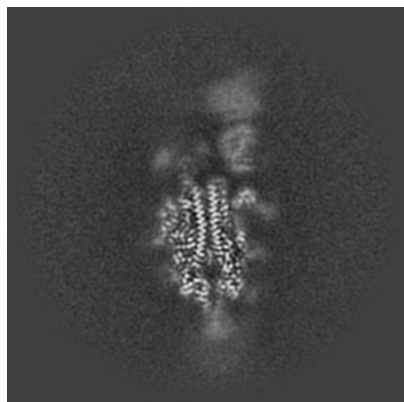


Z Index: 224

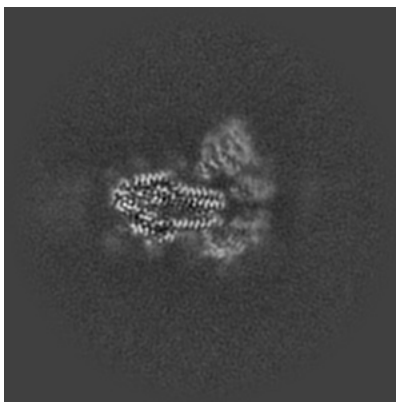
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

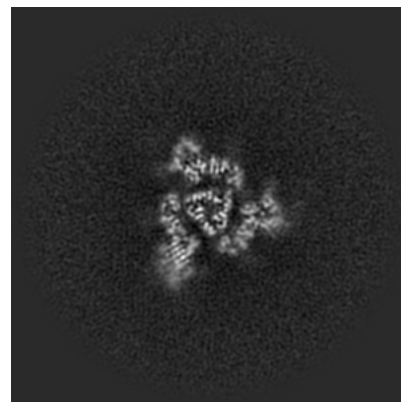
### 6.3.1 Primary map



X Index: 229

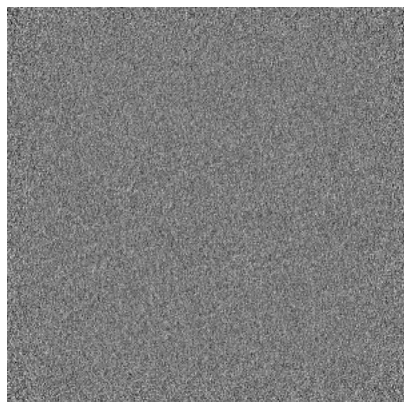


Y Index: 212

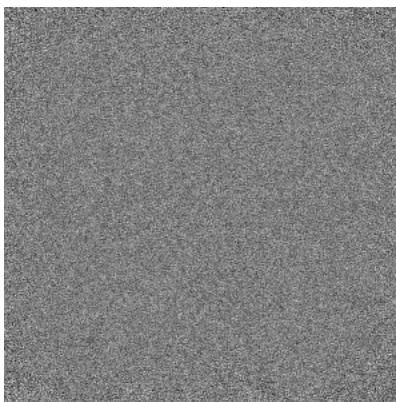


Z Index: 236

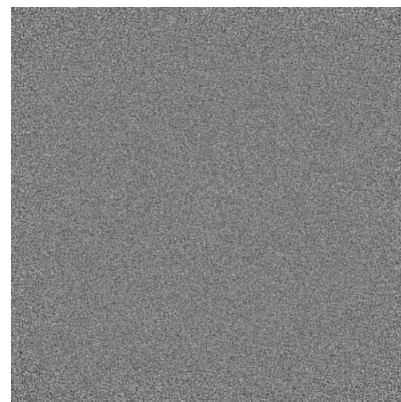
### 6.3.2 Raw map



X Index: 0



Y Index: 0



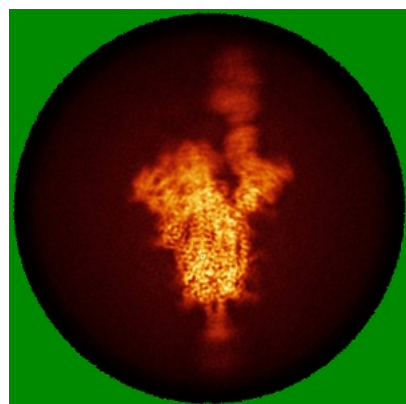
Z Index: 0

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

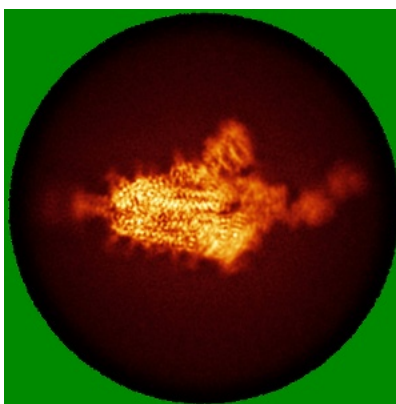


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

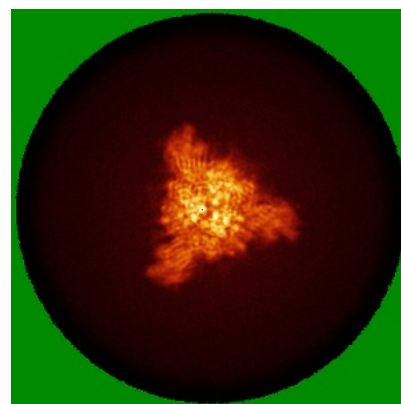
### 6.4.1 Primary map



X

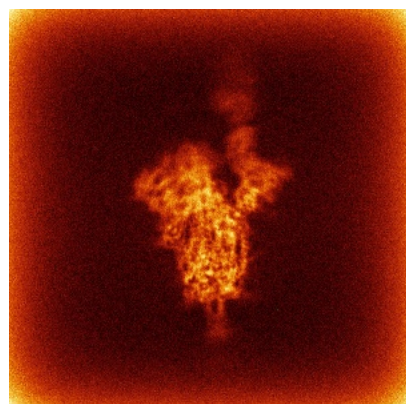


Y

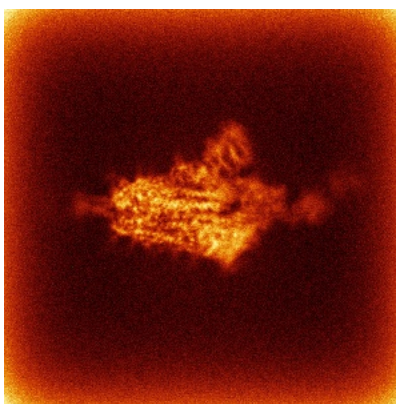


Z

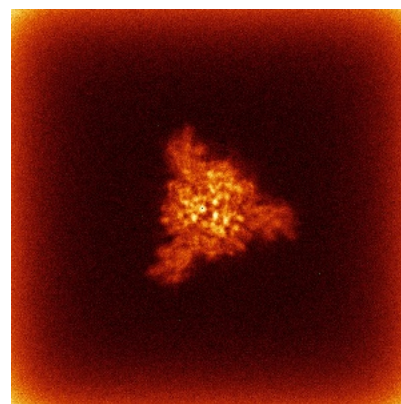
### 6.4.2 Raw map



X



Y

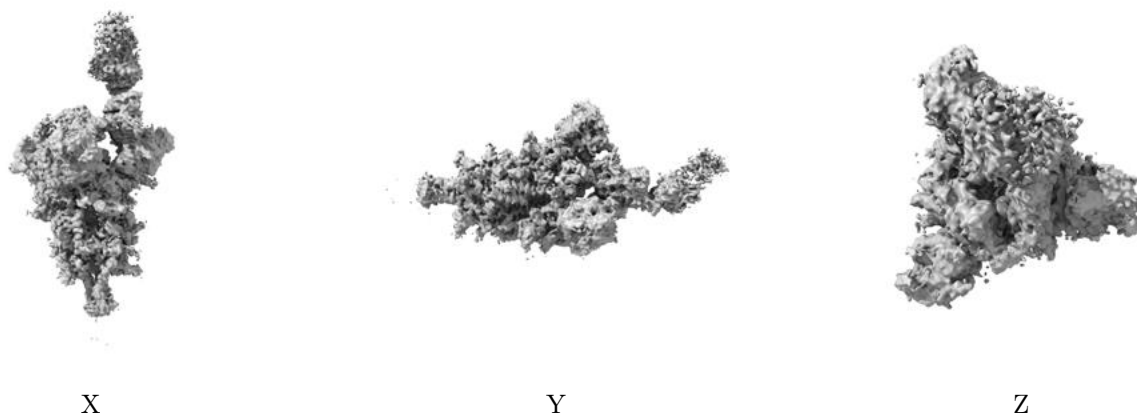


Z

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.

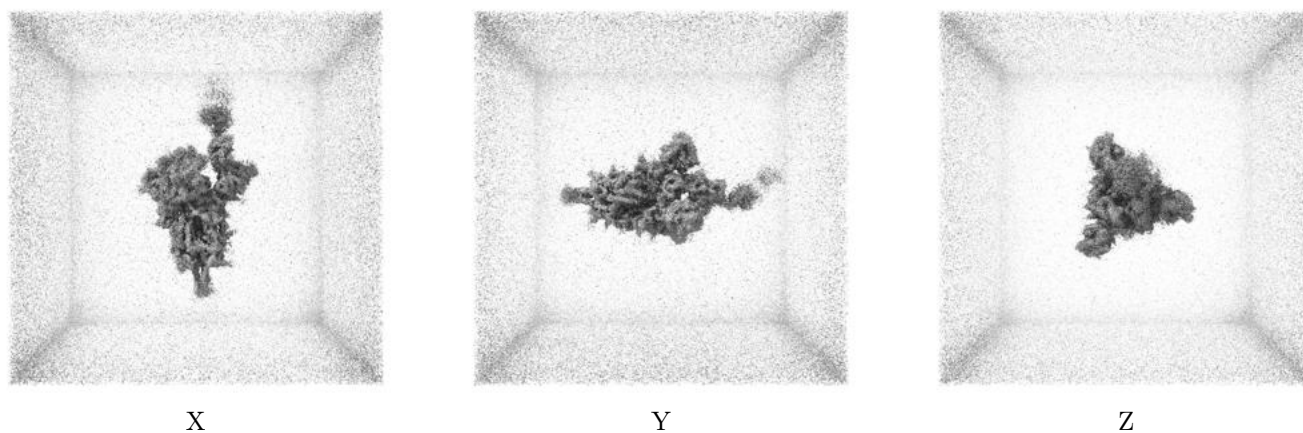
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

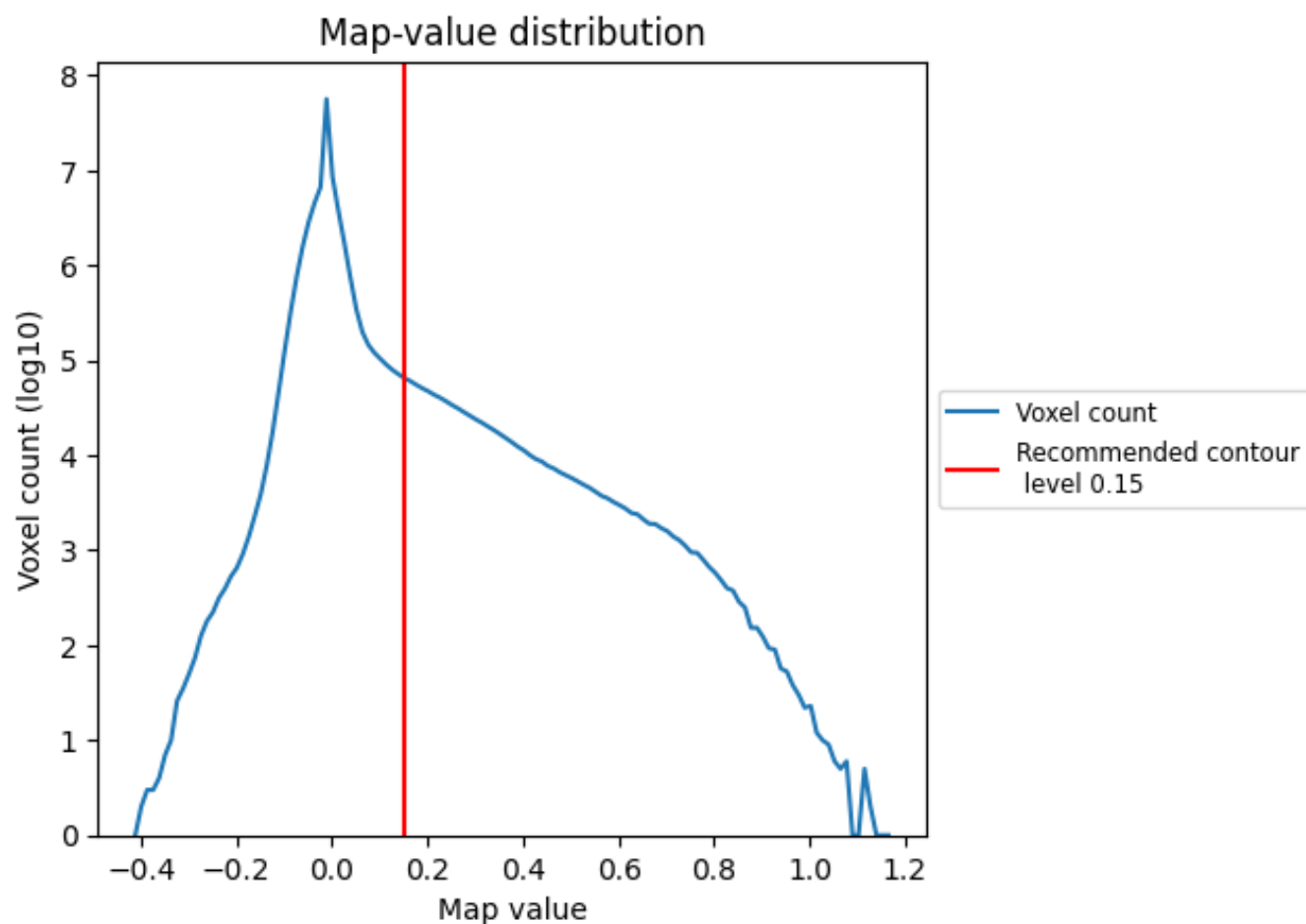
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

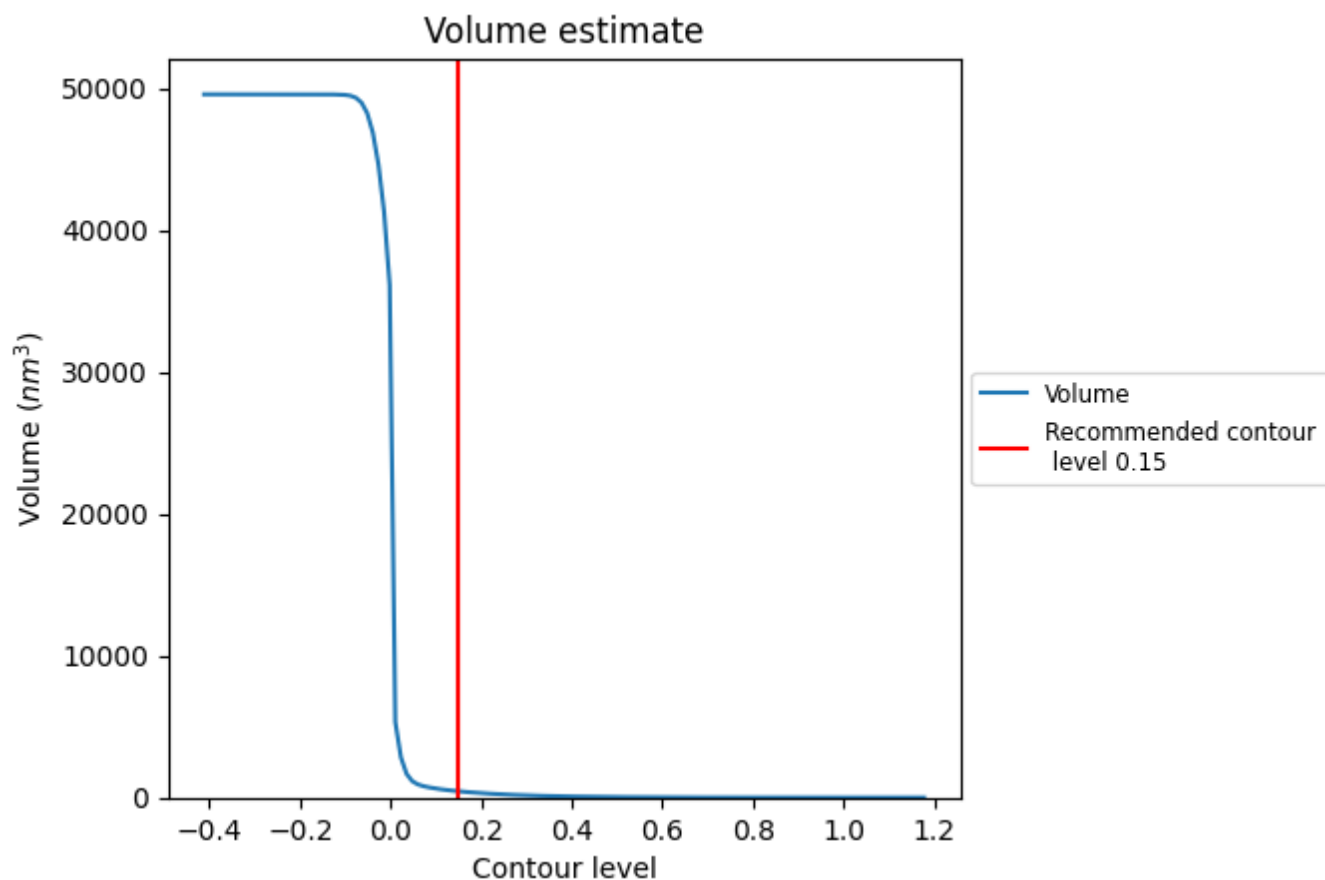
This section contains the results of statistical analysis of the map.

### 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.

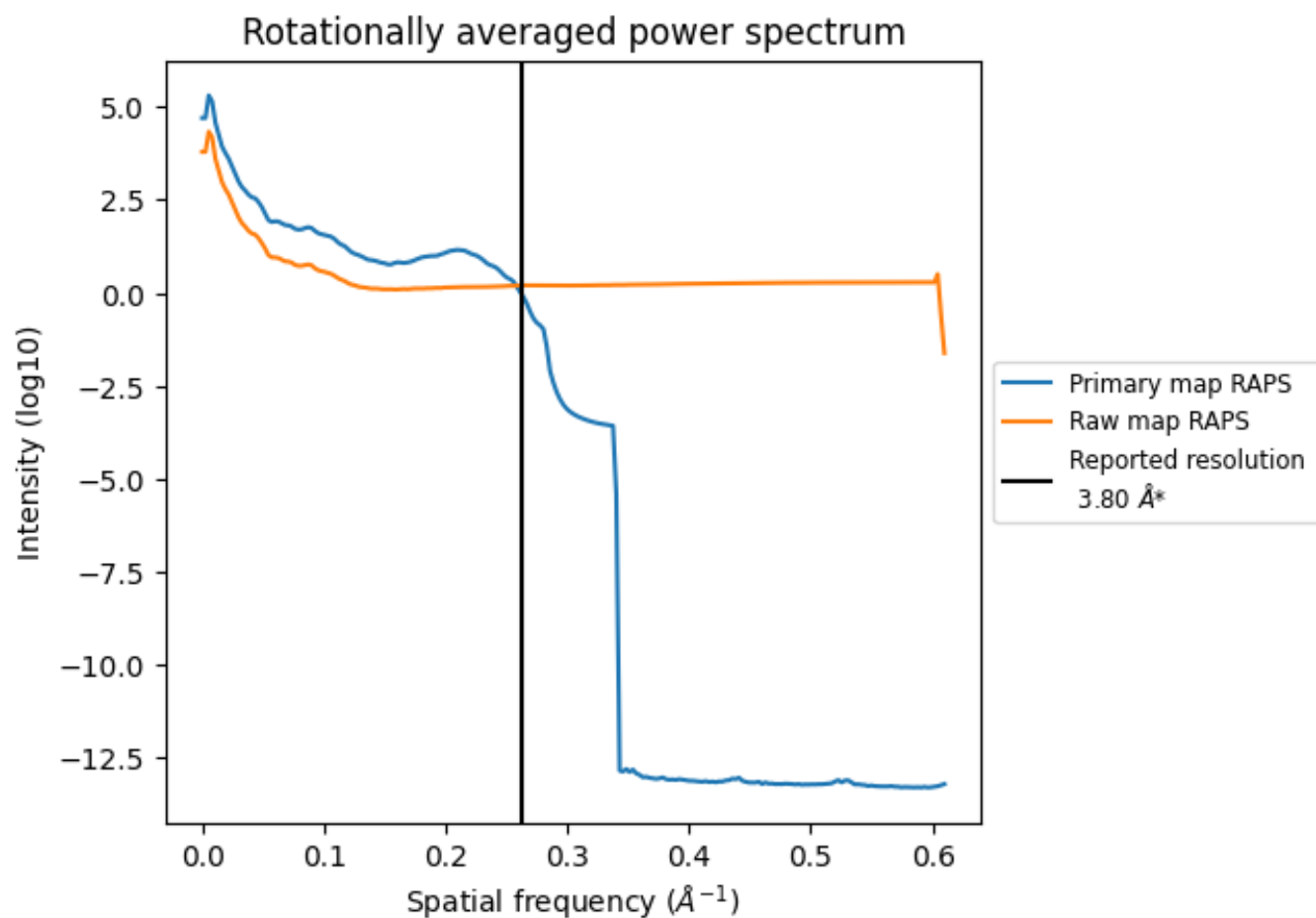
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 443  $\text{nm}^3$ ; this corresponds to an approximate mass of 400 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 ⓘ

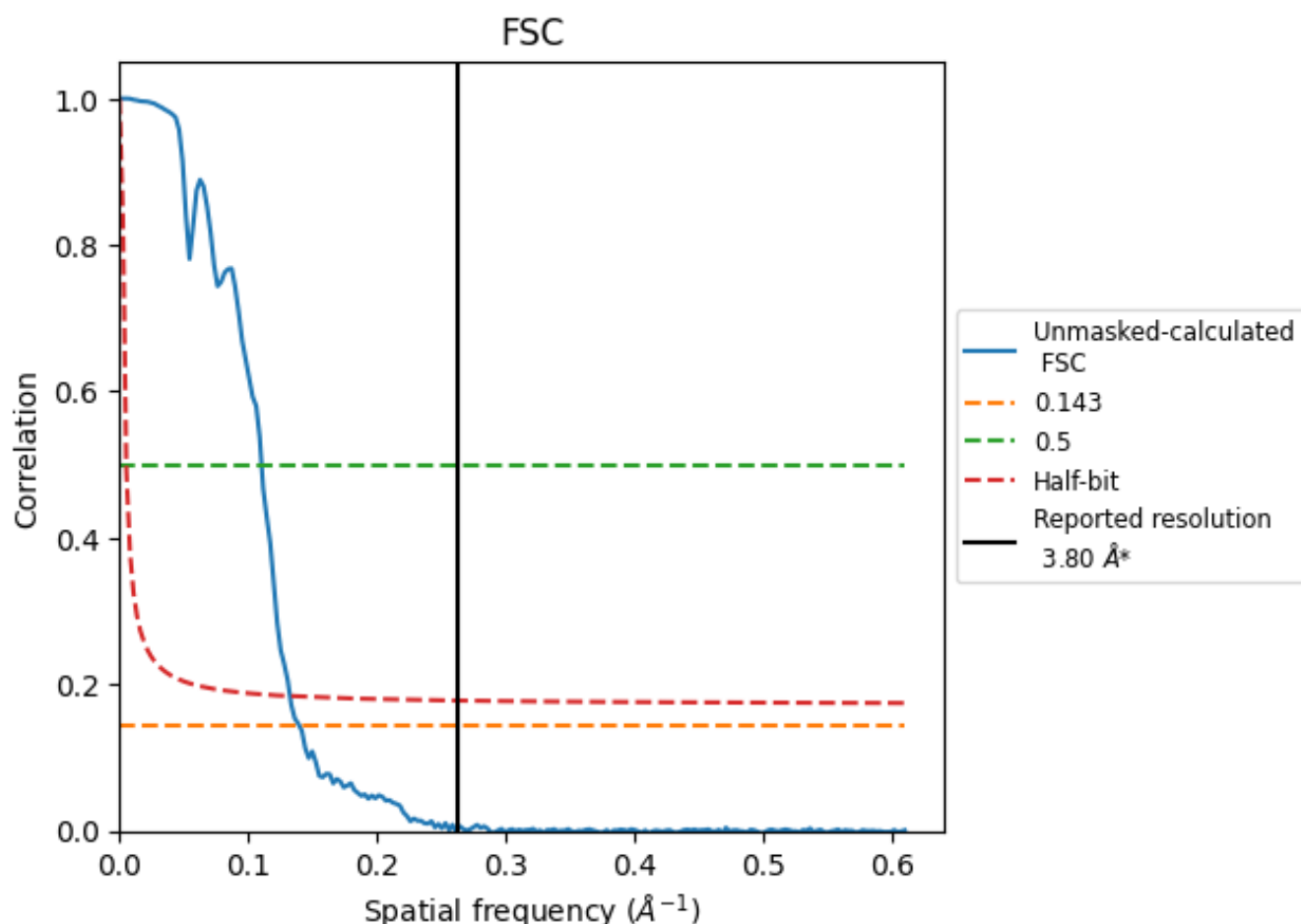


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

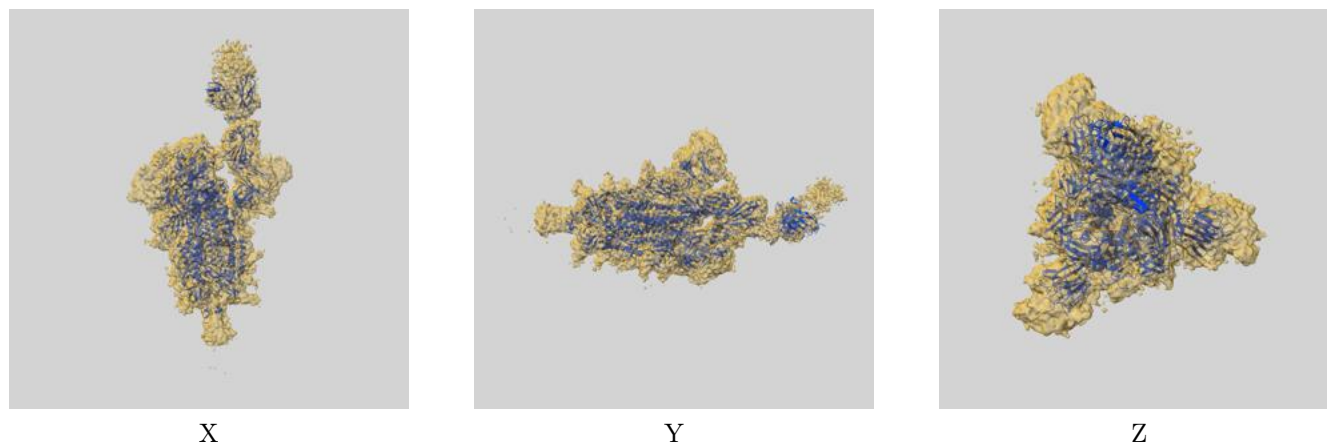
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.16	9.07	7.55

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.16 differs from the reported value 3.8 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33667 and PDB model 7Y7J. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

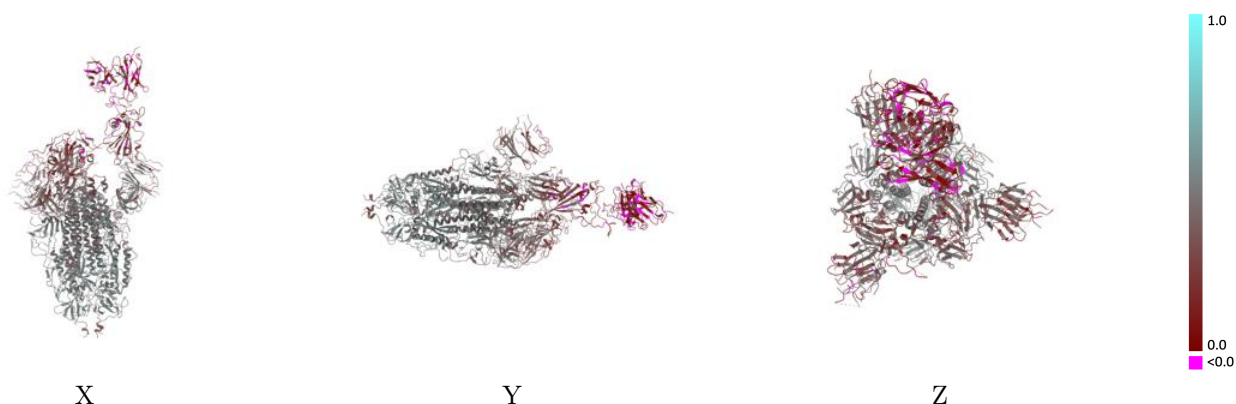
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

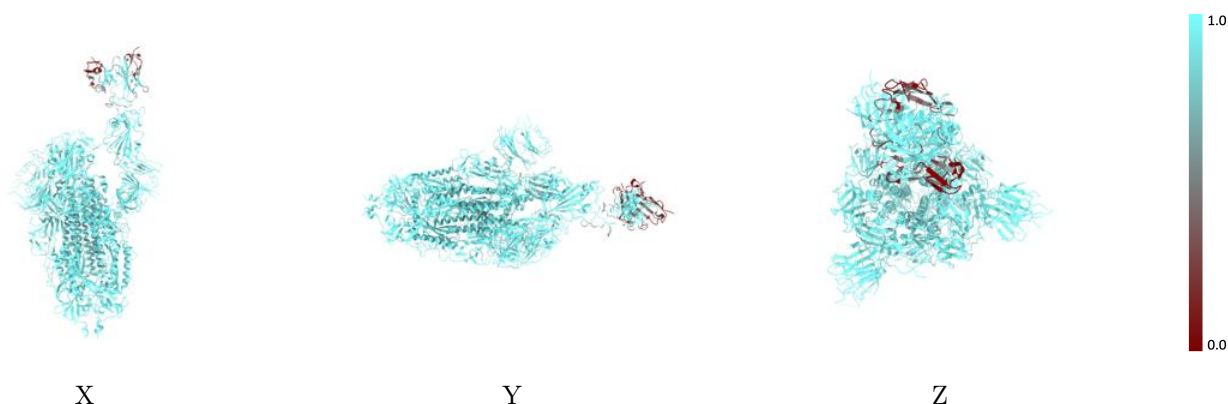


## 9.2 Q-score mapped to coordinate model [i](#)



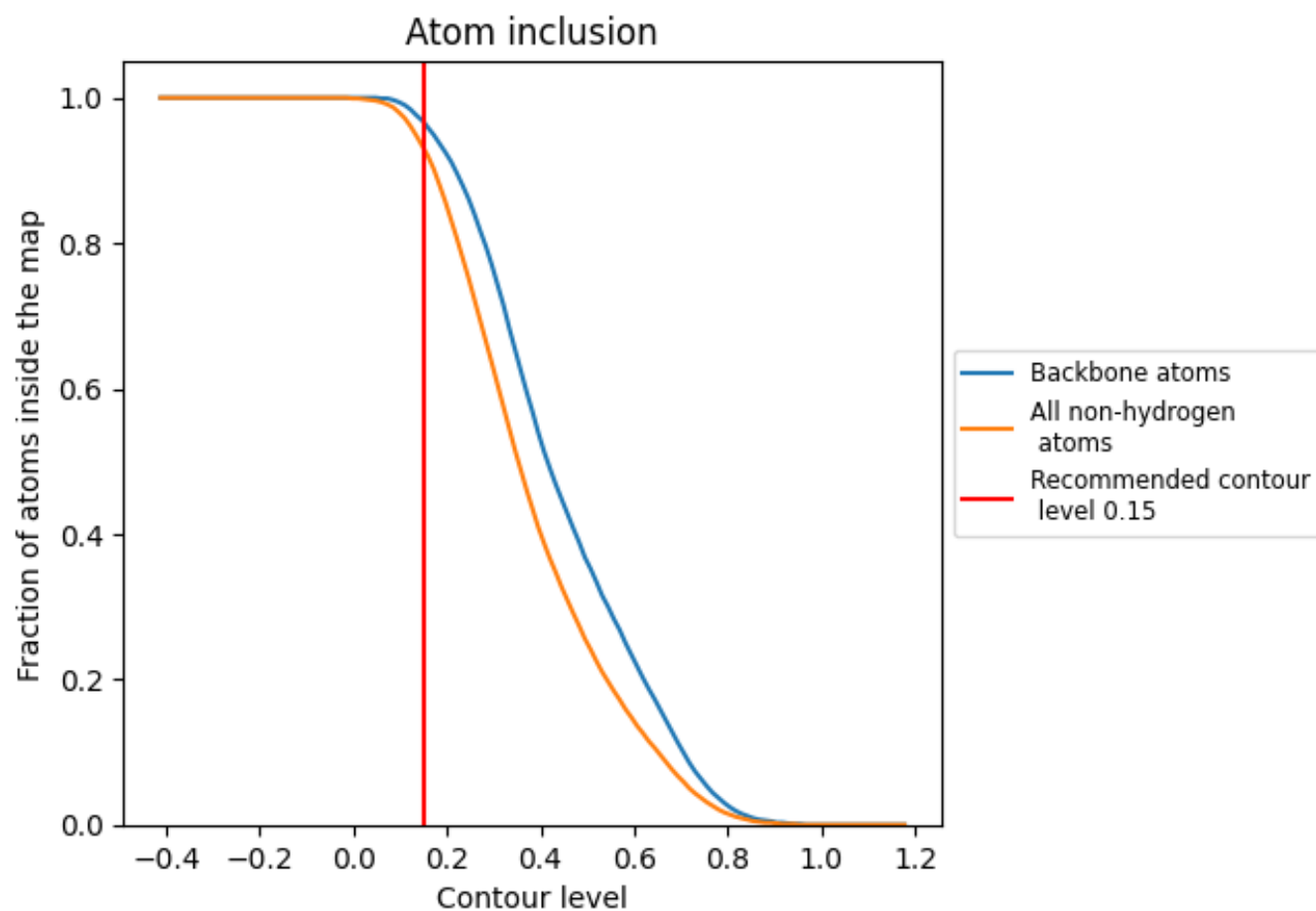
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).











































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9310	 0.3830
A	 0.9530	 0.3940
B	 0.9640	 0.4190
C	 0.9570	 0.4030
D	 0.5620	 0.1020
E	 0.6220	 0.1030
F	 0.9640	 0.4800
G	 0.9290	 0.4110
H	 0.8210	 0.4200
I	 0.8930	 0.3400
J	 0.9640	 0.4490
K	 0.8930	 0.3520
L	 1.0000	 0.4450
N	 1.0000	 0.4420
O	 0.8930	 0.3550
P	 0.8570	 0.2790
Q	 1.0000	 0.4150
R	 0.7140	 0.2160
S	 0.9640	 0.4330
T	 0.9290	 0.4210
U	 0.9290	 0.4110

