



## Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 03:41 PM JST

PDB ID : 7DF4  
EMDB ID : EMD-30661  
Title : SARS-CoV-2 S-ACE2 complex  
Authors : Cong, X.; Yao, C.  
Deposited on : 2020-11-06  
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

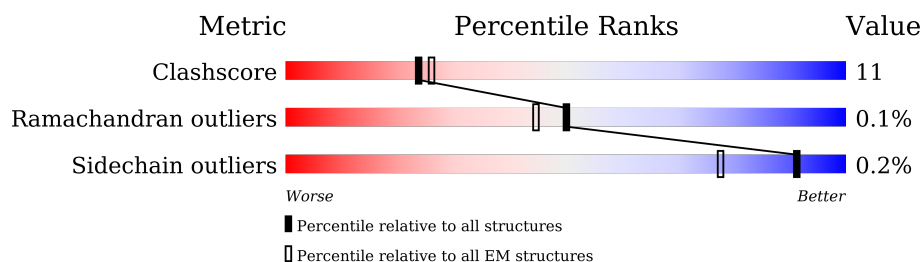
# 1 Overall quality at a glance

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	625	<div> <div>79%</div> <div>67%</div> <div>28%</div> <div>.</div> </div>
2	B	1261	<div> <div>19%</div> <div>64%</div> <div>20%</div> <div>15%</div> </div>
2	C	1261	<div> <div>14%</div> <div>64%</div> <div>21%</div> <div>16%</div> </div>
2	D	1261	<div> <div>17%</div> <div>62%</div> <div>22%</div> <div>15%</div> </div>
3	E	2	<div> <div>100%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>
3	G	2	<div> <div>50%</div> <div>50%</div> </div>
3	H	2	<div> <div>50%</div> <div>100%</div> </div>

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

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30920 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q9BYF1
A	1	HIS	-	expression tag	UNP Q9BYF1
A	2	SER	-	expression tag	UNP Q9BYF1
A	3	SER	-	expression tag	UNP Q9BYF1
A	4	ALA	-	expression tag	UNP Q9BYF1
A	5	LEU	-	expression tag	UNP Q9BYF1
A	6	LEU	-	expression tag	UNP Q9BYF1
A	7	CYS	-	expression tag	UNP Q9BYF1
A	8	CYS	-	expression tag	UNP Q9BYF1
A	9	LEU	-	expression tag	UNP Q9BYF1
A	10	VAL	-	expression tag	UNP Q9BYF1
A	11	LEU	-	expression tag	UNP Q9BYF1
A	12	LEU	-	expression tag	UNP Q9BYF1
A	13	THR	-	expression tag	UNP Q9BYF1
A	14	GLY	-	expression tag	UNP Q9BYF1
A	15	VAL	-	expression tag	UNP Q9BYF1
A	16	ARG	-	expression tag	UNP Q9BYF1
A	616	HIS	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
A	624	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1065	Total 8332	C 5316	N 1392	O 1586	S 38	0	0
2	B	1068	Total 8355	C 5328	N 1396	O 1592	S 39	0	0
2	D	1068	Total 8355	C 5328	N 1396	O 1592	S 39	0	0

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLU	-	expression tag	UNP P0DTC2
C	1239	ASN	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	TYR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	TYR	-	expression tag	UNP P0DTC2
C	1247	LYS	-	expression tag	UNP P0DTC2
C	1248	ASP	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	ASP	-	expression tag	UNP P0DTC2
C	1251	ASP	-	expression tag	UNP P0DTC2
C	1252	LYS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLU	-	expression tag	UNP P0DTC2
B	1239	ASN	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	TYR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	TYR	-	expression tag	UNP P0DTC2
B	1247	LYS	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	ASP	-	expression tag	UNP P0DTC2
B	1251	ASP	-	expression tag	UNP P0DTC2
B	1252	LYS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
D	682	GLY	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	683	SER	ARG	engineered mutation	UNP P0DTC2
D	685	SER	ARG	engineered mutation	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLU	-	expression tag	UNP P0DTC2
D	1239	ASN	-	expression tag	UNP P0DTC2
D	1240	LEU	-	expression tag	UNP P0DTC2
D	1241	TYR	-	expression tag	UNP P0DTC2
D	1242	PHE	-	expression tag	UNP P0DTC2
D	1243	GLN	-	expression tag	UNP P0DTC2
D	1244	GLY	-	expression tag	UNP P0DTC2
D	1245	ASP	-	expression tag	UNP P0DTC2
D	1246	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1247	LYS	-	expression tag	UNP P0DTC2
D	1248	ASP	-	expression tag	UNP P0DTC2
D	1249	ASP	-	expression tag	UNP P0DTC2
D	1250	ASP	-	expression tag	UNP P0DTC2
D	1251	ASP	-	expression tag	UNP P0DTC2
D	1252	LYS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	HIS	-	expression tag	UNP P0DTC2
D	1259	HIS	-	expression tag	UNP P0DTC2
D	1260	HIS	-	expression tag	UNP P0DTC2
D	1261	HIS	-	expression tag	UNP P0DTC2

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



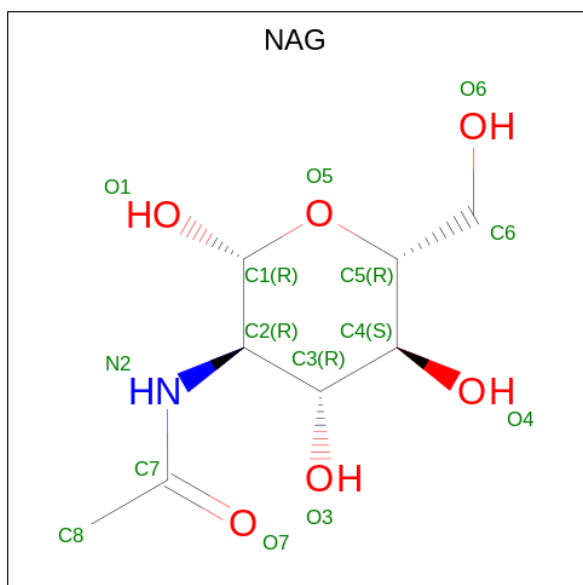
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

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

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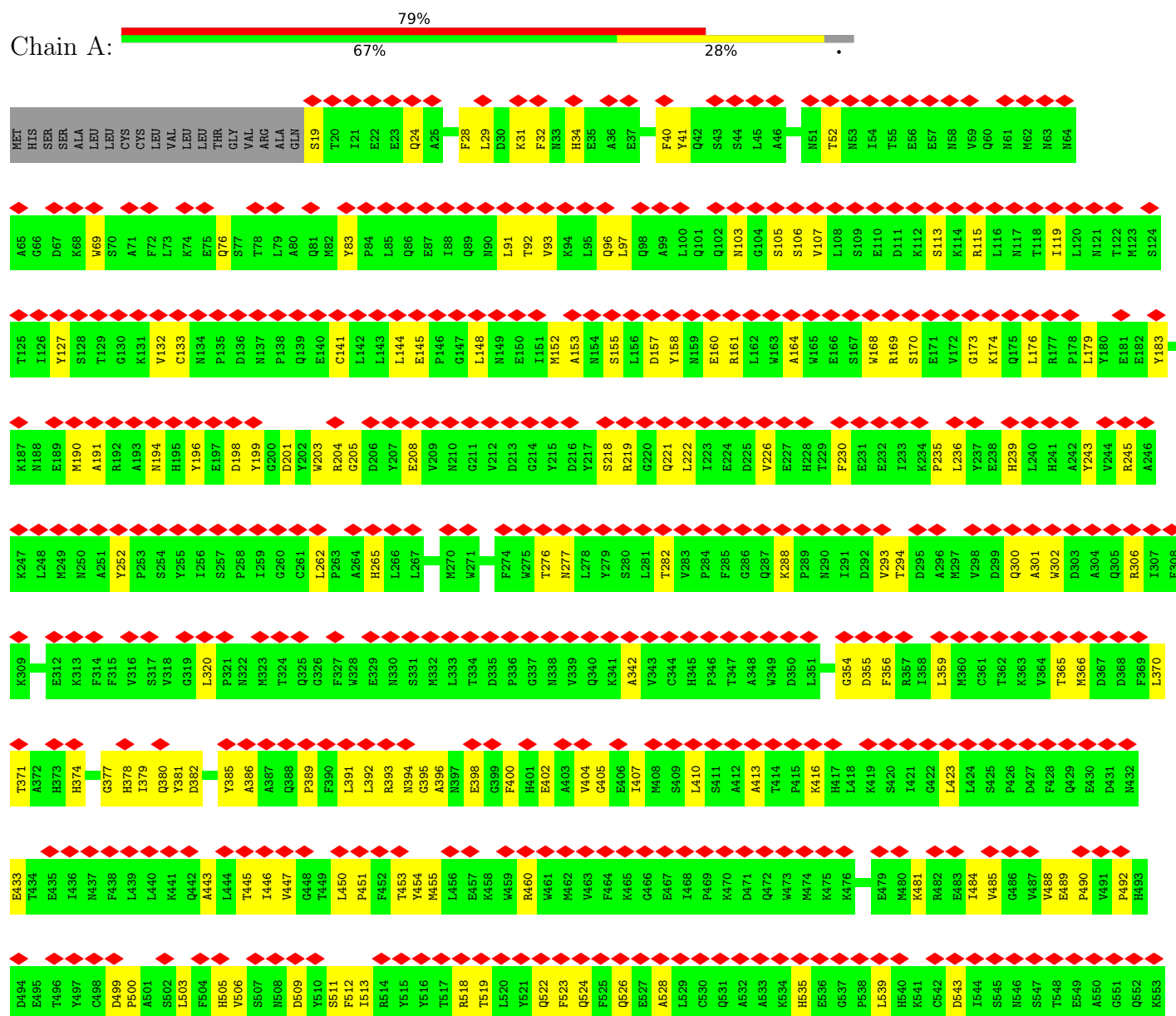
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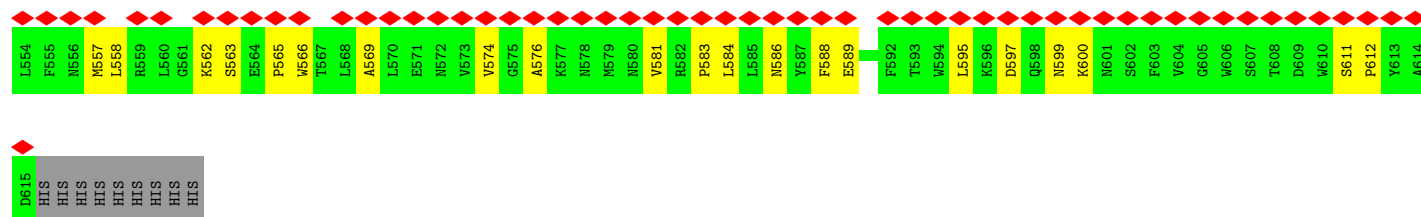
Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4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

### 3 Residue-property plots

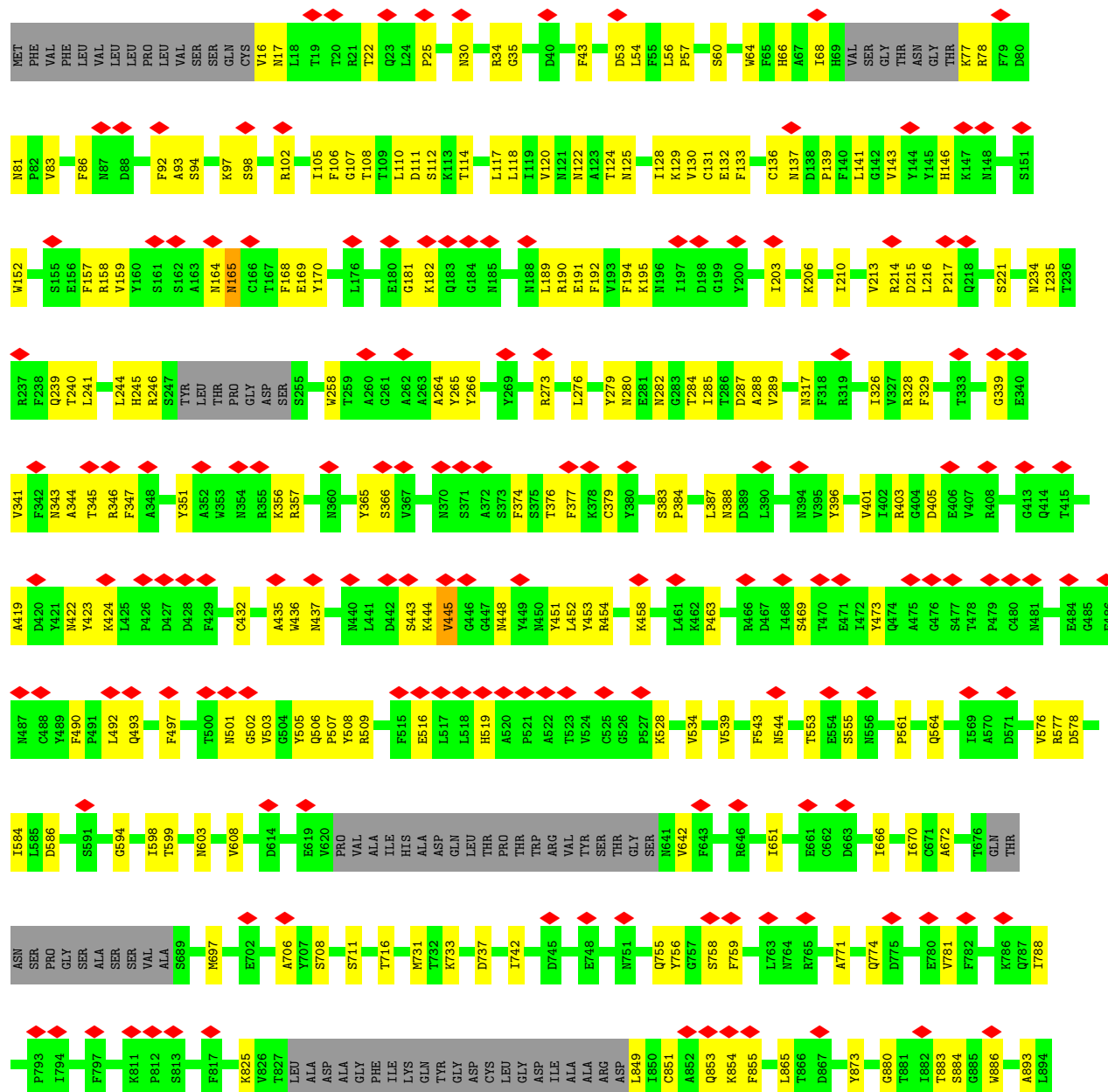
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

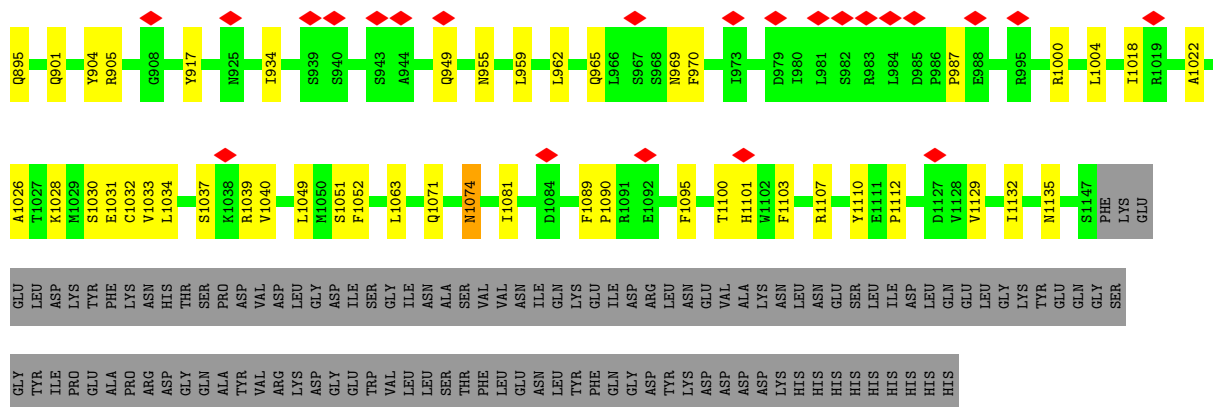
#### • Molecule 1: Angiotensin-converting enzyme 2



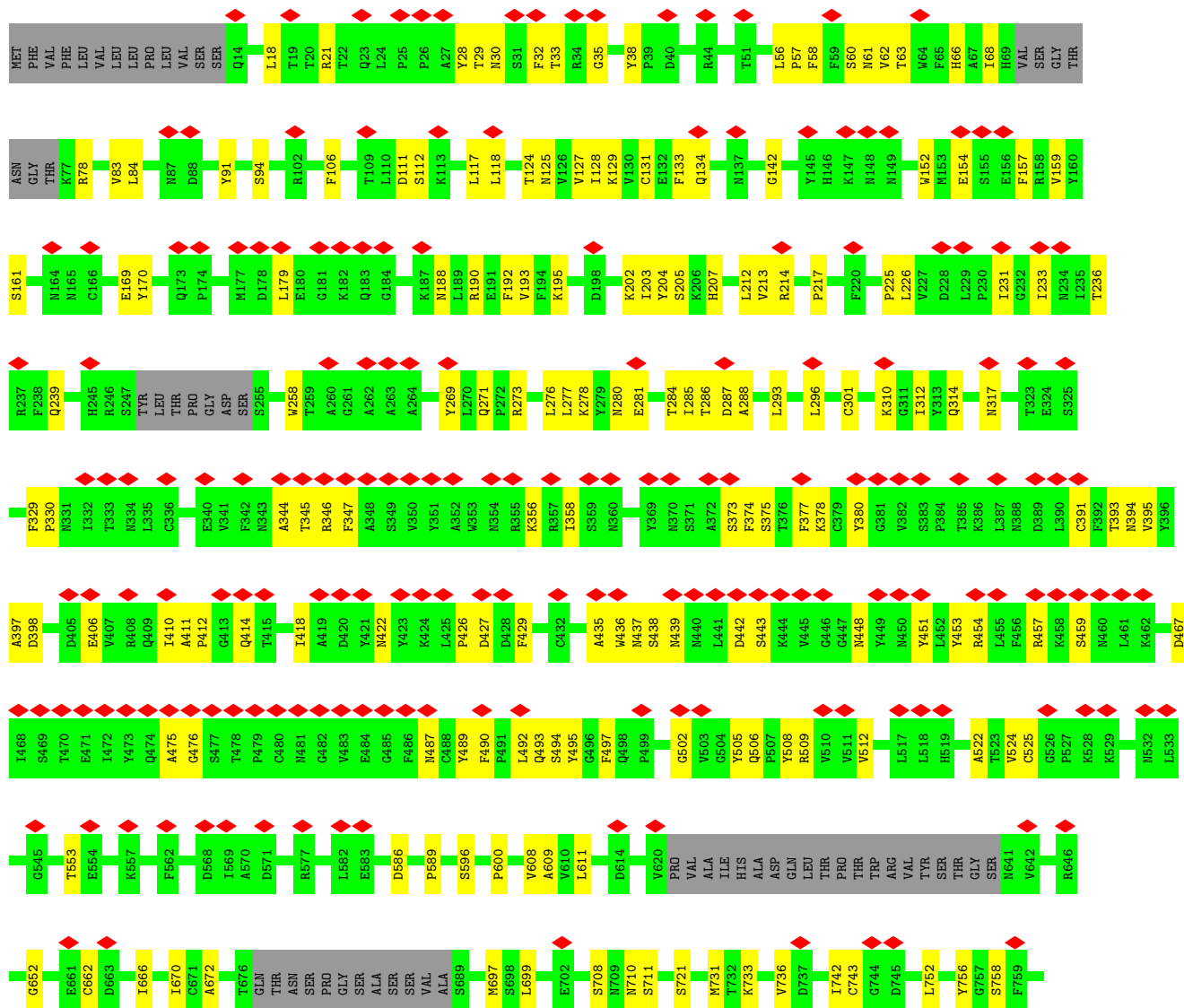


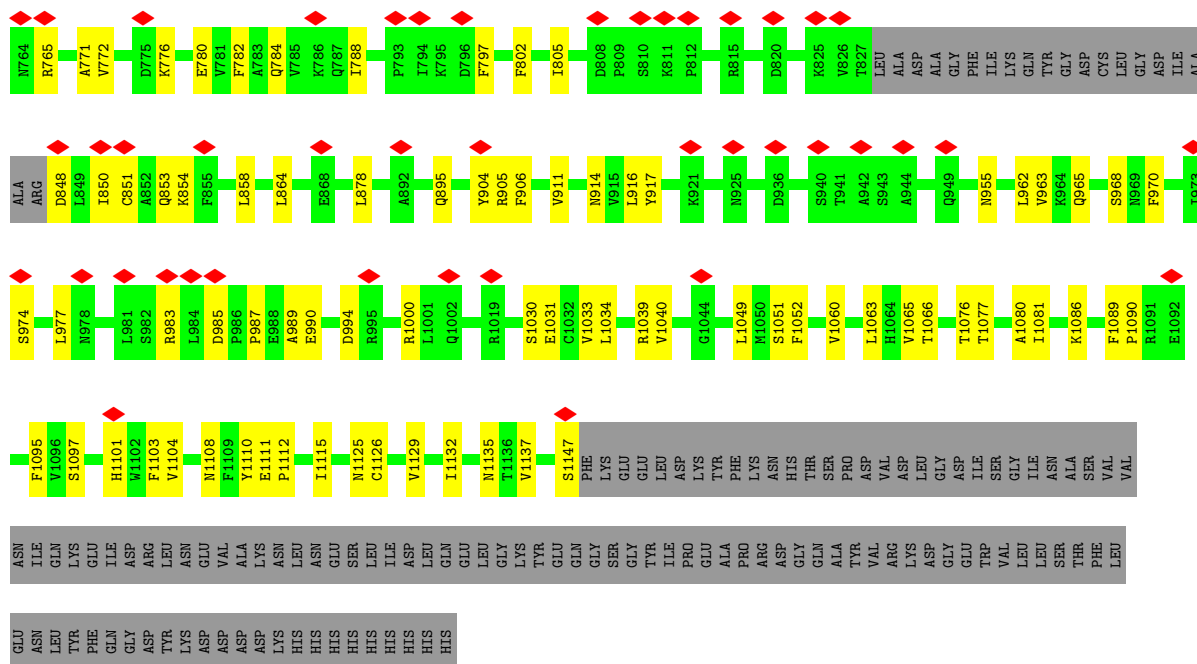
• Molecule 2: Spike glycoprotein



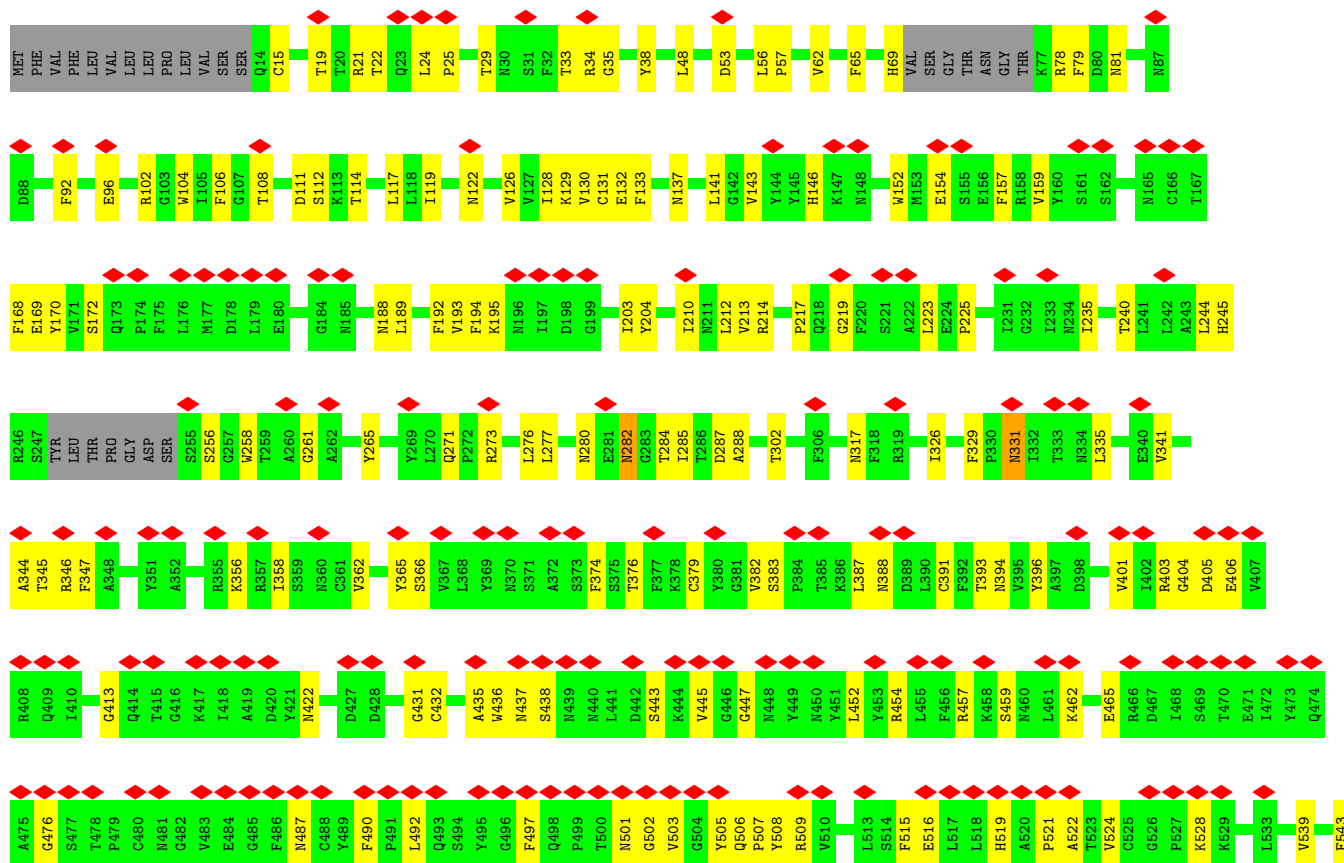


• Molecule 2: Spike glycoprotein

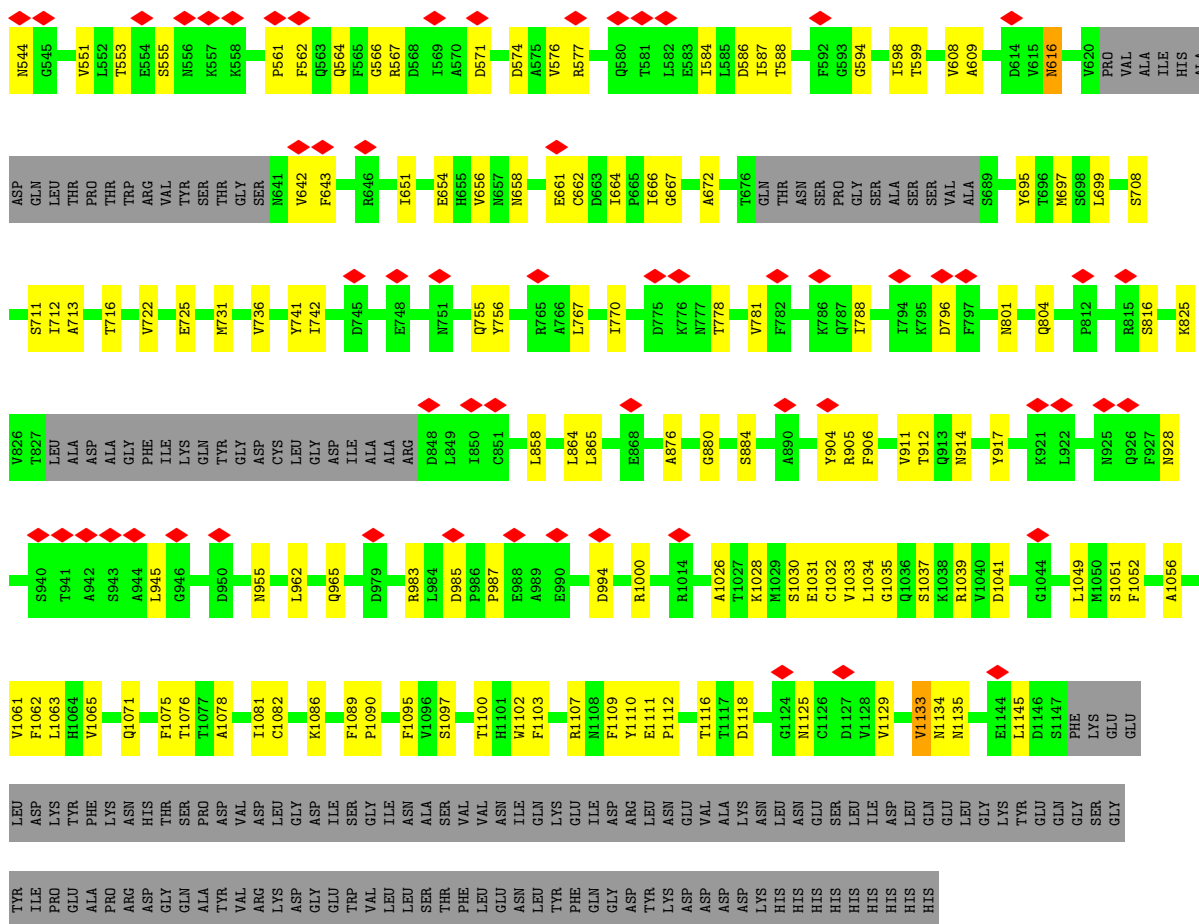




• Molecule 2: Spike glycoprotein







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

Chain E: 100%

MAG1  
MAG2

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

Chain F: 50%

MAG1  
MAG2

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

Chain G: 50%

MAG1  
MAG2

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



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



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



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



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



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



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



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



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



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



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



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



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





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

Chain U:  100%



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

Chain V:  50%  
 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68987	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.715	Depositor
Minimum map value	-1.345	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.767	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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	0.23	0/5007	0.37	0/6803
2	B	0.25	0/8547	0.42	0/11629
2	C	0.26	1/8524 (0.0%)	0.42	0/11598
2	D	0.27	2/8547 (0.0%)	0.42	0/11629
All	All	0.25	3/30625 (0.0%)	0.41	0/41659

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	271	GLN	C-N	6.79	1.47	1.34
2	C	25	PRO	C-N	5.93	1.45	1.34
2	D	25	PRO	C-N	5.47	1.44	1.34

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	4870	0	4643	114	0
2	B	8355	0	8132	181	0
2	C	8332	0	8115	189	0
2	D	8355	0	8130	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	3	0
3	F	28	0	25	3	0
3	G	28	0	25	3	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
3	K	28	0	25	0	0
3	L	28	0	25	2	0
3	M	28	0	25	1	0
3	N	28	0	24	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	3	0
3	R	28	0	25	0	0
3	S	28	0	25	4	0
3	T	28	0	25	1	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
4	B	168	0	156	8	0
4	C	154	0	143	13	0
4	D	182	0	168	4	0
All	All	30920	0	29936	652	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 11.

All (652) 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:D:1102:TRP:CD1	2:D:1135:ASN:ND2	2.32	0.98
2:B:281:GLU:HB2	4:B:1306:NAG:H82	1.50	0.93
2:D:122:ASN:OD1	2:D:154:GLU:HG2	1.74	0.86
2:D:122:ASN:O	2:D:154:GLU:OE2	1.95	0.85
2:D:1102:TRP:HB2	2:D:1135:ASN:ND2	1.92	0.84
2:D:1081:ILE:CG2	2:D:1135:ASN:HB3	2.09	0.82
2:D:1081:ILE:HG23	2:D:1135:ASN:HB3	1.59	0.82
2:C:136:CYS:SG	2:C:139:PRO:HA	2.20	0.81
2:C:343:ASN:OD1	2:C:343:ASN:O	2.00	0.80
2:C:136:CYS:SG	2:C:139:PRO:CA	2.71	0.79
2:B:127:VAL:HG22	4:B:1310:NAG:H62	1.65	0.79
1:A:356:PHE:HB3	1:A:379:ILE:HD12	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:ALA:HB3	2:D:347:PHE:HE1	1.48	0.78
3:T:1:NAG:H61	3:T:2:NAG:HN2	1.50	0.77
2:B:1103:PHE:HZ	3:M:1:NAG:H62	1.50	0.76
2:C:137:ASN:HB2	4:C:1311:NAG:H83	1.67	0.75
1:A:524:GLN:HB3	1:A:574:VAL:HG11	1.69	0.75
2:C:1132:ILE:O	3:E:1:NAG:H81	1.87	0.74
2:C:157:PHE:HZ	4:C:1309:NAG:C1	2.00	0.74
2:C:1052:PHE:HB2	2:C:1063:LEU:HB2	1.68	0.74
2:C:849:LEU:HD23	2:C:851:CYS:H	1.53	0.73
1:A:204:ARG:HG2	1:A:222:LEU:HD23	1.70	0.73
2:D:1102:TRP:HB2	2:D:1135:ASN:HD21	1.52	0.73
2:B:28:TYR:HB3	2:B:61:ASN:HB3	1.72	0.72
2:C:93:ALA:HB3	2:C:266:TYR:HB2	1.71	0.72
2:B:758:SER:OG	2:D:965:GLN:NE2	2.23	0.72
2:C:136:CYS:SG	2:C:158:ARG:O	2.41	0.71
2:C:758:SER:OG	2:B:965:GLN:NE2	2.23	0.71
2:C:351:TYR:HA	2:C:422:ASN:HD21	1.54	0.71
2:C:603:ASN:OD1	2:C:603:ASN:O	2.09	0.71
4:C:1311:NAG:O7	4:C:1311:NAG:O3	2.05	0.70
2:C:136:CYS:HB2	2:C:159:VAL:O	1.91	0.70
2:D:555:SER:HB2	2:D:586:ASP:HB2	1.74	0.70
2:B:596:SER:HB2	2:B:611:LEU:HB3	1.73	0.70
4:C:1307:NAG:O7	4:C:1307:NAG:O3	2.05	0.69
1:A:377:GLY:HA3	1:A:405:GLY:HA2	1.73	0.69
2:D:344:ALA:HB3	2:D:347:PHE:CE1	2.27	0.69
1:A:52:THR:HG22	1:A:359:LEU:HD13	1.73	0.69
2:C:129:LYS:HG2	2:C:169:GLU:HG3	1.75	0.69
2:D:1102:TRP:CG	2:D:1135:ASN:ND2	2.61	0.68
2:C:706:ALA:HB2	3:G:2:NAG:O6	1.94	0.68
2:B:398:ASP:HB3	2:B:512:VAL:HB	1.76	0.67
2:D:1102:TRP:HD1	2:D:1135:ASN:ND2	1.90	0.67
2:C:555:SER:HB2	2:C:586:ASP:HB2	1.77	0.67
2:D:212:LEU:HD22	2:D:217:PRO:HD3	1.75	0.67
2:D:331:ASN:OD1	2:D:331:ASN:N	2.26	0.67
2:D:403:ARG:NH2	2:D:406:GLU:OE2	2.27	0.67
1:A:276:THR:HG1	1:A:445:THR:HG1	1.41	0.67
2:D:1081:ILE:HG23	2:D:1135:ASN:CB	2.25	0.67
1:A:152:MET:O	1:A:161:ARG:NH1	2.28	0.66
2:B:1031:GLU:OE2	2:D:1039:ARG:NE	2.28	0.66
2:C:564:GLN:HG3	2:C:577:ARG:HB3	1.78	0.65
2:C:157:PHE:CZ	4:C:1309:NAG:C1	2.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:544:ASN:HD22	2:C:564:GLN:HE22	1.43	0.65
2:D:106:PHE:HB2	2:D:117:LEU:HB3	1.78	0.65
1:A:103:ASN:HB2	1:A:107:VAL:HG13	1.79	0.64
2:B:373:SER:HB2	4:B:1304:NAG:H81	1.79	0.64
2:C:97:LYS:HB3	2:C:182:LYS:HB2	1.79	0.64
2:C:143:VAL:HG11	2:C:152:TRP:HA	1.80	0.64
2:D:33:THR:OG1	2:D:219:GLY:O	2.15	0.64
2:C:280:ASN:HD21	2:C:284:THR:HB	1.63	0.64
1:A:523:PHE:HB3	1:A:583:PRO:HB2	1.78	0.64
2:C:666:ILE:HD11	2:C:672:ALA:HB2	1.79	0.64
2:B:457:ARG:NH1	2:B:459:SER:OG	2.31	0.64
2:C:851:CYS:HA	2:C:854:LYS:HE3	1.80	0.63
1:A:451:PRO:HB2	1:A:485:VAL:HG12	1.79	0.63
2:B:742:ILE:O	2:B:1000:ARG:NH1	2.31	0.62
2:D:781:VAL:HG22	2:D:1026:ALA:HB2	1.81	0.62
2:C:57:PRO:HG3	2:C:273:ARG:HG3	1.82	0.62
1:A:190:MET:O	1:A:194:ASN:ND2	2.32	0.62
2:C:357:ARG:HG3	2:C:396:TYR:HE1	1.64	0.62
2:B:60:SER:HA	4:B:1311:NAG:H82	1.82	0.62
2:C:132:GLU:CD	2:C:165:ASN:OD1	2.37	0.62
2:C:108:THR:HB	2:C:114:THR:HG21	1.81	0.62
1:A:103:ASN:HB3	1:A:106:SER:HB2	1.81	0.62
2:D:1102:TRP:CB	2:D:1135:ASN:ND2	2.62	0.62
2:B:1030:SER:HB3	2:D:1041:ASP:HB3	1.82	0.61
1:A:503:LEU:HD23	1:A:506:VAL:HG23	1.82	0.61
2:B:29:THR:O	2:B:62:VAL:HG22	2.01	0.61
2:C:108:THR:OG1	2:C:234:ASN:O	2.18	0.61
2:C:895:GLN:NE2	2:B:711:SER:OG	2.34	0.61
2:B:32:PHE:CD2	2:B:33:THR:HG23	2.36	0.60
2:D:157:PHE:CE1	4:D:1311:NAG:H83	2.35	0.60
2:B:280:ASN:HD21	2:B:284:THR:HB	1.67	0.60
2:C:34:ARG:HH12	2:C:216:LEU:HD13	1.66	0.60
2:C:401:VAL:HG22	2:C:509:ARG:HG2	1.84	0.60
2:B:905:ARG:NH1	2:B:1049:LEU:O	2.34	0.60
2:D:24:LEU:HD12	2:D:78:ARG:HD2	1.84	0.60
2:D:277:LEU:HD22	2:D:285:ILE:HD13	1.84	0.60
2:C:365:TYR:HD2	2:C:387:LEU:HB3	1.67	0.60
2:B:780:GLU:O	2:B:784:GLN:NE2	2.35	0.60
2:B:356:LYS:HB2	2:B:397:ALA:HB3	1.84	0.60
2:B:974:SER:OG	2:B:983:ARG:NH2	2.35	0.60
2:C:443:SER:HA	2:C:497:PHE:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:ALA:HB3	2:B:347:PHE:HE1	1.67	0.59
2:D:561:PRO:O	2:D:577:ARG:NH1	2.36	0.59
2:C:81:ASN:ND2	2:C:240:THR:O	2.33	0.59
2:D:345:THR:HG22	2:D:346:ARG:HG2	1.83	0.59
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.84	0.59
2:D:756:TYR:OH	2:D:994:ASP:OD1	2.20	0.59
2:B:106:PHE:HB2	2:B:117:LEU:HB3	1.84	0.59
2:D:57:PRO:HG3	2:D:273:ARG:HG3	1.84	0.59
2:B:1086:LYS:HA	2:B:1125:ASN:HA	1.86	0.58
2:B:236:THR:HG21	4:B:1307:NAG:H5	1.85	0.58
3:Q:1:NAG:O7	3:Q:1:NAG:O3	2.17	0.58
1:A:370:LEU:HD21	1:A:413:ALA:HB2	1.85	0.58
2:B:374:PHE:HA	2:B:436:TRP:HB2	1.86	0.58
1:A:394:ASN:OD1	1:A:395:GLY:N	2.36	0.58
2:B:1104:VAL:HG23	2:B:1115:ILE:HG12	1.85	0.58
2:C:708:SER:HB3	2:C:711:SER:HB2	1.85	0.58
3:S:1:NAG:H82	3:S:1:NAG:O3	2.04	0.58
3:F:1:NAG:O3	3:F:1:NAG:H82	2.04	0.57
1:A:342:ALA:HB1	1:A:359:LEU:HD11	1.85	0.57
2:C:377:PHE:HE2	2:C:384:PRO:HB3	1.69	0.57
2:B:296:LEU:HB2	2:B:608:VAL:HG21	1.86	0.57
2:C:213:VAL:HG12	2:C:214:ARG:HG2	1.86	0.57
2:B:914:ASN:ND2	2:B:1111:GLU:OE1	2.36	0.57
2:C:825:LYS:O	2:C:949:GLN:NE2	2.37	0.57
2:D:143:VAL:HG11	2:D:152:TRP:HA	1.86	0.57
1:A:443:ALA:O	1:A:447:VAL:N	2.36	0.57
2:B:154:GLU:OE2	4:B:1310:NAG:O7	2.23	0.57
2:B:358:ILE:HG22	2:B:524:VAL:HG21	1.85	0.57
1:A:132:VAL:HG11	1:A:164:ALA:HA	1.87	0.57
2:D:374:PHE:HA	2:D:436:TRP:HB3	1.85	0.57
1:A:381:TYR:HB2	1:A:404:VAL:HG11	1.87	0.57
2:C:106:PHE:HB2	2:C:117:LEU:HB3	1.87	0.57
2:D:736:VAL:HG22	2:D:858:LEU:HG	1.86	0.57
1:A:96:GLN:HE21	1:A:392:LEU:HG	1.70	0.57
1:A:557:MET:HG3	1:A:569:ALA:HB1	1.87	0.56
2:D:401:VAL:HG22	2:D:509:ARG:HG2	1.87	0.56
3:E:2:NAG:O7	3:E:2:NAG:H3	2.04	0.56
2:D:119:ILE:HG12	2:D:128:ILE:HG12	1.88	0.56
2:D:341:VAL:HG21	2:D:358:ILE:HD11	1.87	0.56
2:C:83:VAL:HG22	2:C:239:GLN:HG2	1.87	0.56
2:C:102:ARG:HG2	2:C:141:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ASN:O	2:B:443:SER:OG	2.22	0.56
2:C:503:VAL:HG22	2:D:503:VAL:HG11	1.88	0.56
2:C:1132:ILE:O	3:E:1:NAG:C8	2.54	0.56
2:C:345:THR:HG22	2:C:346:ARG:HG2	1.86	0.56
2:B:736:VAL:HG22	2:B:858:LEU:HG	1.88	0.56
2:C:53:ASP:OD2	2:C:195:LYS:NZ	2.38	0.56
2:B:393:THR:HA	2:B:522:ALA:HA	1.88	0.56
2:B:756:TYR:OH	2:B:994:ASP:OD1	2.24	0.56
1:A:201:ASP:HA	1:A:204:ARG:HB2	1.87	0.56
2:C:1040:VAL:HG21	2:D:1035:GLY:HA3	1.87	0.56
2:D:564:GLN:HG3	2:D:577:ARG:HB3	1.88	0.56
2:D:825:LYS:HB2	2:D:945:LEU:HD12	1.86	0.56
2:B:378:LYS:HE2	2:B:380:TYR:HE1	1.71	0.55
1:A:595:LEU:O	1:A:599:ASN:ND2	2.34	0.55
2:B:710:ASN:O	2:B:1077:THR:HG22	2.06	0.55
2:C:755:GLN:O	2:B:968:SER:OG	2.24	0.55
2:B:128:ILE:HB	2:B:170:TYR:HB3	1.88	0.55
2:D:193:VAL:HG23	2:D:223:LEU:HD22	1.88	0.55
2:C:706:ALA:HB2	3:G:2:NAG:C6	2.36	0.55
2:D:1030:SER:HA	2:D:1034:LEU:HD12	1.87	0.55
2:B:853:GLN:HG2	2:B:963:VAL:HG21	1.88	0.55
2:B:35:GLY:HA3	2:B:56:LEU:HB3	1.88	0.55
2:B:277:LEU:HD22	2:B:285:ILE:HD13	1.87	0.55
2:D:129:LYS:HG2	2:D:169:GLU:HG3	1.89	0.55
2:B:788:ILE:HD11	2:D:699:LEU:HB2	1.87	0.55
1:A:518:ARG:NH1	1:A:522:GLN:OE1	2.40	0.55
2:C:376:THR:HB	2:C:435:ALA:HB3	1.89	0.55
2:D:551:VAL:N	2:D:588:THR:O	2.33	0.55
2:D:317:ASN:HA	2:D:594:GLY:HA2	1.89	0.54
2:B:708:SER:HB3	2:B:711:SER:HB3	1.89	0.54
2:D:708:SER:HB3	2:D:711:SER:HB3	1.89	0.54
2:D:712:ILE:HG22	2:D:1075:PHE:O	2.06	0.54
2:C:855:PHE:HB3	2:B:589:PRO:HG2	1.89	0.54
2:D:53:ASP:OD2	2:D:195:LYS:NZ	2.37	0.54
1:A:34:HIS:CD2	2:B:493:GLN:HB3	2.42	0.54
4:C:1311:NAG:HO3	4:C:1311:NAG:C7	2.10	0.54
2:D:567:ARG:NH1	2:D:571:ASP:O	2.37	0.54
2:C:905:ARG:NH1	2:C:1049:LEU:O	2.40	0.54
2:C:326:ILE:HD12	2:C:539:VAL:HG21	1.89	0.54
1:A:407:ILE:O	1:A:526:GLN:NE2	2.41	0.54
2:C:130:VAL:HB	2:C:168:PHE:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:CYS:O	4:D:1313:NAG:H82	2.07	0.54
2:C:598:ILE:HD13	2:C:666:ILE:HG12	1.89	0.54
2:B:287:ASP:OD1	2:B:288:ALA:N	2.41	0.54
2:D:796:ASP:HB2	3:J:1:NAG:O6	2.08	0.54
1:A:245:ARG:HA	1:A:262:LEU:HD21	1.90	0.54
2:C:22:THR:OG1	2:C:77:LYS:O	2.21	0.54
2:C:1089:PHE:HZ	2:C:1129:VAL:HG21	1.72	0.54
2:D:92:PHE:HB2	2:D:192:PHE:HB2	1.90	0.54
2:C:122:ASN:OD1	2:C:157:PHE:CE1	2.60	0.54
2:D:19:THR:HG23	2:D:256:SER:HB2	1.88	0.54
2:C:553:THR:O	2:C:586:ASP:N	2.40	0.53
2:B:895:GLN:NE2	2:D:711:SER:OG	2.41	0.53
2:D:858:LEU:HD21	2:D:962:LEU:HD23	1.90	0.53
1:A:235:PRO:O	1:A:239:HIS:ND1	2.35	0.53
2:C:781:VAL:HG22	2:C:1026:ALA:HB2	1.90	0.53
2:C:452:LEU:HD13	2:C:492:LEU:HD21	1.90	0.53
2:C:716:THR:N	2:C:1071:GLN:O	2.36	0.53
2:C:452:LEU:HB3	2:C:492:LEU:HD11	1.91	0.53
2:C:543:PHE:HD2	2:C:576:VAL:HG21	1.73	0.53
2:C:731:MET:HG3	2:C:955:ASN:HD21	1.73	0.53
2:D:244:LEU:HB3	2:D:258:TRP:HB3	1.91	0.53
2:B:106:PHE:O	2:B:117:LEU:N	2.39	0.53
2:B:733:LYS:HE3	2:B:771:ALA:HB1	1.89	0.53
2:D:880:GLY:O	2:D:884:SER:N	2.40	0.53
1:A:410:LEU:HB2	1:A:526:GLN:HE21	1.73	0.53
1:A:450:LEU:HD21	1:A:519:THR:HB	1.89	0.53
2:B:411:ALA:HB3	2:B:414:GLN:HG3	1.90	0.53
2:B:662:CYS:HB2	2:B:697:MET:HG3	1.91	0.53
2:D:555:SER:HB3	2:D:584:ILE:HG22	1.91	0.53
2:D:666:ILE:HD11	2:D:672:ALA:HB2	1.91	0.53
2:B:203:ILE:HG23	2:B:226:LEU:HB3	1.89	0.53
2:D:731:MET:HG3	2:D:955:ASN:HD21	1.74	0.53
2:C:157:PHE:CZ	4:C:1309:NAG:N2	2.78	0.52
2:C:379:CYS:HA	2:C:432:CYS:HA	1.90	0.52
2:C:555:SER:HB3	2:C:584:ILE:HG22	1.89	0.52
2:D:447:GLY:HA2	2:D:497:PHE:H	1.74	0.52
2:C:66:HIS:HA	2:C:264:ALA:HA	1.91	0.52
2:B:152:TRP:HB3	2:B:179:LEU:HB2	1.91	0.52
2:D:106:PHE:O	2:D:117:LEU:N	2.40	0.52
2:D:1086:LYS:HA	2:D:1125:ASN:HA	1.91	0.52
2:C:122:ASN:OD1	2:C:157:PHE:CZ	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:SER:N	2:B:475:ALA:O	2.43	0.52
2:B:314:GLN:NE2	2:B:317:ASN:OD1	2.39	0.52
2:B:731:MET:HG3	2:B:955:ASN:HD21	1.73	0.52
2:B:985:ASP:O	2:B:989:ALA:N	2.39	0.52
2:D:662:CYS:HB2	2:D:697:MET:HG3	1.92	0.52
2:C:136:CYS:HB3	2:C:139:PRO:HB3	1.92	0.52
2:D:566:GLY:O	2:D:574:ASP:N	2.38	0.52
2:C:880:GLY:O	2:C:884:SER:N	2.43	0.51
1:A:378:HIS:HE1	1:A:402:GLU:HA	1.75	0.51
1:A:393:ARG:NH2	2:B:505:TYR:OH	2.43	0.51
1:A:396:ALA:HA	1:A:562:LYS:HB3	1.91	0.51
2:C:102:ARG:HB3	2:C:241:LEU:HB3	1.92	0.51
2:C:287:ASP:OD1	2:C:288:ALA:N	2.42	0.51
2:B:502:GLY:O	2:B:506:GLN:HG3	2.11	0.51
1:A:450:LEU:HB2	1:A:451:PRO:HD3	1.91	0.51
2:C:244:LEU:HB3	2:C:258:TRP:HB3	1.92	0.51
2:B:212:LEU:HD22	2:B:217:PRO:HD3	1.93	0.51
2:D:326:ILE:HD12	2:D:539:VAL:HG21	1.91	0.51
2:D:1076:THR:HB	2:D:1097:SER:HB3	1.92	0.51
1:A:302:TRP:HA	1:A:306:ARG:HE	1.74	0.51
1:A:597:ASP:HA	1:A:600:LYS:HE3	1.93	0.51
2:C:1100:THR:HG21	3:F:1:NAG:H3	1.92	0.51
2:C:16:VAL:HA	4:C:1311:NAG:C7	2.41	0.51
2:B:406:GLU:HB3	2:B:418:ILE:HG13	1.92	0.51
2:B:192:PHE:HE1	2:B:205:SER:HG	1.59	0.51
1:A:243:TYR:HE2	1:A:282:THR:HB	1.76	0.51
2:B:127:VAL:HG22	4:B:1310:NAG:C6	2.39	0.51
2:B:553:THR:O	2:B:586:ASP:N	2.43	0.51
2:D:287:ASP:OD1	2:D:288:ALA:N	2.44	0.51
2:C:102:ARG:HG3	2:C:120:VAL:HG23	1.93	0.50
2:C:194:PHE:HE1	2:C:203:ILE:HG23	1.76	0.50
2:C:339:GLY:HA2	2:C:343:ASN:HB3	1.93	0.50
3:Q:1:NAG:HO3	3:Q:1:NAG:C7	2.21	0.50
1:A:34:HIS:NE2	2:B:494:SER:O	2.42	0.50
1:A:169:ARG:HA	1:A:173:GLY:H	1.76	0.50
1:A:236:LEU:HD21	1:A:588:PHE:HD2	1.76	0.50
2:B:490:PHE:CE2	2:B:492:LEU:HB2	2.47	0.50
2:C:111:ASP:OD1	2:C:112:SER:N	2.42	0.50
2:B:345:THR:HG22	2:B:346:ARG:HG2	1.93	0.50
2:B:58:PHE:HB2	2:B:293:LEU:HD22	1.93	0.50
2:B:380:TYR:OH	2:B:410:ILE:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1081:ILE:HG23	2:B:1135:ASN:HB3	1.92	0.50
2:D:131:CYS:HB2	2:D:133:PHE:CE1	2.47	0.50
1:A:92:THR:HB	1:A:392:LEU:HD11	1.94	0.50
2:B:131:CYS:HB2	2:B:133:PHE:CE1	2.47	0.50
2:B:1052:PHE:HB2	2:B:1063:LEU:HB2	1.93	0.50
2:D:1081:ILE:HG21	2:D:1135:ASN:HB3	1.91	0.50
2:D:403:ARG:NE	2:D:405:ASP:OD1	2.41	0.50
1:A:488:VAL:HG21	1:A:611:SER:HA	1.93	0.50
2:B:111:ASP:OD1	2:B:112:SER:N	2.41	0.50
2:D:65:PHE:HB2	2:D:265:TYR:O	2.12	0.50
2:C:43:PHE:CZ	2:C:282:ASN:O	2.64	0.49
2:C:1039:ARG:HD2	2:D:1039:ARG:HD2	1.94	0.49
2:B:310:LYS:HG3	2:B:600:PRO:HA	1.92	0.49
2:B:710:ASN:C	2:B:1077:THR:HG22	2.31	0.49
2:D:1100:THR:HG21	3:S:1:NAG:H3	1.94	0.49
4:C:1307:NAG:HO3	4:C:1307:NAG:C7	2.16	0.49
2:B:188:ASN:HB3	2:B:207:HIS:HE1	1.77	0.49
2:B:418:ILE:HA	2:B:422:ASN:HD22	1.77	0.49
2:D:366:SER:OG	2:D:388:ASN:ND2	2.45	0.49
2:D:1052:PHE:HB2	2:D:1063:LEU:HB2	1.94	0.49
1:A:41:TYR:HE1	1:A:355:ASP:HB3	1.77	0.49
2:C:965:GLN:HB3	2:C:970:PHE:HZ	1.77	0.49
2:B:437:ASN:HA	2:B:508:TYR:HD1	1.78	0.49
2:D:111:ASP:OD1	2:D:112:SER:N	2.41	0.49
2:C:451:TYR:HD2	2:C:497:PHE:HE2	1.60	0.49
2:C:490:PHE:CE2	2:C:492:LEU:HB3	2.47	0.49
2:B:312:ILE:HD11	2:B:596:SER:HB3	1.95	0.49
1:A:199:TYR:OH	1:A:509:ASP:OD1	2.27	0.49
1:A:301:ALA:O	1:A:306:ARG:NH2	2.46	0.49
2:C:136:CYS:SG	2:C:139:PRO:N	2.85	0.49
2:B:864:LEU:HA	2:D:667:GLY:HA2	1.95	0.49
2:D:376:THR:HB	2:D:435:ALA:HB3	1.94	0.49
2:B:375:SER:N	2:B:435:ALA:O	2.42	0.49
2:D:126:VAL:HB	2:D:172:SER:HB3	1.95	0.49
2:C:516:GLU:HB3	2:C:519:HIS:HD2	1.78	0.49
2:B:157:PHE:CZ	2:B:159:VAL:HB	2.48	0.49
2:D:35:GLY:HA3	2:D:56:LEU:HB3	1.95	0.49
2:C:344:ALA:HB3	2:C:347:PHE:HE1	1.78	0.49
2:D:544:ASN:HD22	2:D:564:GLN:HE22	1.61	0.49
2:D:1082:CYS:HB3	2:D:1134:ASN:HA	1.95	0.49
1:A:574:VAL:HG23	1:A:576:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:666:ILE:HD12	2:C:670:ILE:HG22	1.95	0.49
2:C:1129:VAL:HG13	2:D:917:TYR:HB3	1.94	0.49
2:D:282:ASN:N	2:D:282:ASN:OD1	2.45	0.49
2:D:767:LEU:HD23	2:D:770:ILE:HD12	1.93	0.49
1:A:389:PRO:O	1:A:393:ARG:HG3	2.13	0.48
2:C:92:PHE:HB2	2:C:192:PHE:HB2	1.95	0.48
2:B:347:PHE:HE2	2:B:509:ARG:HB3	1.77	0.48
1:A:24:GLN:HE21	2:B:476:GLY:HA3	1.76	0.48
2:B:1081:ILE:HG12	2:B:1095:PHE:CE2	2.47	0.48
2:D:108:THR:HB	2:D:114:THR:HG21	1.95	0.48
2:D:521:PRO:HA	2:D:544:ASN:HD21	1.78	0.48
1:A:535:HIS:NE2	1:A:543:ASP:O	2.46	0.48
2:C:34:ARG:NH2	2:C:217:PRO:O	2.46	0.48
2:C:64:TRP:CD1	2:C:266:TYR:HE1	2.32	0.48
2:D:742:ILE:O	2:D:1000:ARG:NH1	2.39	0.48
2:D:788:ILE:HG23	2:D:876:ALA:HB2	1.94	0.48
2:C:136:CYS:SG	2:C:139:PRO:HB3	2.53	0.48
2:D:457:ARG:NH1	2:D:459:SER:OG	2.47	0.48
2:D:1056:ALA:HB2	2:D:1061:VAL:HG23	1.95	0.48
2:B:708:SER:HA	3:Q:1:NAG:H82	1.95	0.48
2:D:329:PHE:HE2	2:D:528:LYS:HB2	1.79	0.48
2:C:35:GLY:HA3	2:C:56:LEU:HB3	1.96	0.48
2:B:63:THR:HG21	2:B:84:LEU:HD21	1.95	0.48
1:A:294:THR:HG23	1:A:365:THR:HA	1.96	0.48
2:B:129:LYS:HG2	2:B:169:GLU:HA	1.96	0.48
2:D:34:ARG:HH22	2:D:217:PRO:HD2	1.78	0.48
2:B:276:LEU:HD11	2:B:301:CYS:HA	1.95	0.48
2:D:280:ASN:HD21	2:D:284:THR:HB	1.78	0.48
1:A:28:PHE:HZ	1:A:76:GLN:HB3	1.79	0.48
2:C:341:VAL:HG22	2:C:356:LYS:HD3	1.95	0.48
2:C:865:LEU:HD13	2:C:873:TYR:HE2	1.78	0.48
2:D:29:THR:O	2:D:62:VAL:HG22	2.14	0.48
2:B:1080:ALA:HB2	2:B:1089:PHE:HE1	1.78	0.47
2:D:543:PHE:HD2	2:D:576:VAL:HG21	1.79	0.47
2:D:146:HIS:NE2	2:D:245:HIS:HB2	2.30	0.47
1:A:198:ASP:OD1	1:A:201:ASP:N	2.45	0.47
1:A:586:ASN:HA	1:A:589:GLU:HB2	1.96	0.47
2:C:128:ILE:O	2:C:170:TYR:N	2.44	0.47
2:B:708:SER:HB3	2:B:711:SER:CB	2.43	0.47
2:B:752:LEU:HD11	2:B:990:GLU:HG2	1.96	0.47
2:C:1030:SER:HA	2:C:1034:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:443:SER:HA	2:D:497:PHE:HB3	1.97	0.47
2:D:905:ARG:NH1	2:D:1049:LEU:O	2.47	0.47
1:A:183:TYR:OH	1:A:460:ARG:NH2	2.47	0.47
1:A:382:ASP:HA	1:A:385:TYR:CE2	2.48	0.47
2:B:448:ASN:HB3	2:B:497:PHE:HB2	1.96	0.47
2:D:157:PHE:CE1	4:D:1311:NAG:C8	2.97	0.47
2:D:490:PHE:CE2	2:D:492:LEU:HB3	2.49	0.47
1:A:265:HIS:ND1	1:A:490:PRO:HG3	2.30	0.47
1:A:453:THR:HG22	1:A:513:ILE:HD12	1.97	0.47
2:C:742:ILE:O	2:C:1000:ARG:NH1	2.42	0.47
2:D:476:GLY:H	2:D:487:ASN:HB3	1.79	0.47
2:C:374:PHE:HA	2:C:436:TRP:HB3	1.96	0.47
2:B:391:CYS:HA	2:B:525:CYS:HA	1.97	0.47
2:D:599:THR:HB	2:D:608:VAL:HG12	1.97	0.47
2:D:616:ASN:OD1	2:D:616:ASN:N	2.46	0.47
2:D:1102:TRP:CE2	2:D:1133:VAL:HG21	2.50	0.47
1:A:32:PHE:HE2	1:A:391:LEU:HD21	1.79	0.47
2:C:106:PHE:HB3	2:C:235:ILE:HD13	1.97	0.47
2:C:132:GLU:HB2	2:C:164:ASN:HB2	1.97	0.47
2:C:403:ARG:NE	2:C:405:ASP:OD1	2.46	0.47
2:B:225:PRO:HB2	2:D:562:PHE:HD2	1.80	0.47
2:C:86:PHE:HZ	2:C:195:LYS:HA	1.80	0.46
2:C:788:ILE:HD11	2:B:699:LEU:HB2	1.96	0.46
2:B:118:LEU:HB2	2:B:133:PHE:CE2	2.50	0.46
3:L:1:NAG:H62	3:L:2:NAG:N2	2.30	0.46
1:A:161:ARG:NE	1:A:265:HIS:O	2.40	0.46
1:A:293:VAL:HG22	1:A:366:MET:HG3	1.97	0.46
2:C:131:CYS:HB2	2:C:133:PHE:CE1	2.50	0.46
2:C:561:PRO:O	2:C:577:ARG:NH1	2.46	0.46
2:C:1107:ARG:CZ	2:D:904:TYR:HB2	2.45	0.46
1:A:170:SER:HA	1:A:174:LYS:HD3	1.98	0.46
1:A:354:GLY:HA3	2:B:502:GLY:HA3	1.97	0.46
2:B:124:THR:HB	4:B:1310:NAG:C1	2.45	0.46
1:A:157:ASP:OD1	1:A:158:TYR:N	2.49	0.46
2:B:454:ARG:NH2	2:B:467:ASP:O	2.46	0.46
1:A:503:LEU:HG	1:A:505:HIS:H	1.81	0.46
2:C:136:CYS:CB	2:C:159:VAL:O	2.63	0.46
1:A:288:LYS:HG3	1:A:433:GLU:HB3	1.96	0.46
2:B:906:PHE:HB3	2:B:911:VAL:HB	1.97	0.46
2:D:379:CYS:HA	2:D:432:CYS:HA	1.98	0.46
2:C:366:SER:HB3	2:C:388:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:721:SER:O	2:B:1066:THR:OG1	2.30	0.46
2:D:438:SER:HB3	2:D:509:ARG:HG3	1.96	0.46
2:D:551:VAL:HB	2:D:588:THR:HB	1.97	0.46
2:C:136:CYS:SG	2:C:139:PRO:CB	3.04	0.46
2:C:1103:PHE:CD2	2:C:1112:PRO:HB3	2.51	0.46
2:B:329:PHE:HB3	2:B:330:PRO:HD2	1.97	0.46
2:B:438:SER:HB3	2:B:509:ARG:HG3	1.98	0.46
2:B:1089:PHE:HZ	2:B:1129:VAL:HG21	1.81	0.46
1:A:31:LYS:HE3	2:B:493:GLN:HE22	1.81	0.46
2:D:38:TYR:HE1	2:D:285:ILE:HG13	1.82	0.46
2:B:134:GLN:HB3	2:B:161:SER:H	1.81	0.45
2:D:393:THR:HA	2:D:522:ALA:HA	1.98	0.45
2:D:452:LEU:HD13	2:D:492:LEU:HD11	1.97	0.45
1:A:392:LEU:HD22	1:A:563:SER:HA	1.99	0.45
2:C:383:SER:N	2:D:983:ARG:O	2.49	0.45
2:D:48:LEU:HB3	2:D:276:LEU:HD11	1.98	0.45
2:C:105:ILE:HD11	2:C:159:VAL:HG13	1.99	0.45
2:C:128:ILE:HB	2:C:170:TYR:HB3	1.97	0.45
2:C:1110:TYR:CZ	2:C:1112:PRO:HG3	2.51	0.45
2:D:722:VAL:HG22	2:D:1065:VAL:HG22	1.99	0.45
1:A:526:GLN:HG3	1:A:539:LEU:HD11	1.99	0.45
2:D:81:ASN:ND2	2:D:240:THR:O	2.44	0.45
2:D:422:ASN:HB3	2:D:454:ARG:HB3	1.99	0.45
2:B:1076:THR:HB	2:B:1097:SER:HB3	1.98	0.45
2:D:194:PHE:HE1	2:D:203:ILE:HG23	1.81	0.45
1:A:83:TYR:OH	2:B:487:ASN:OD1	2.26	0.45
2:C:497:PHE:CE1	2:C:507:PRO:HB3	2.51	0.45
2:D:462:LYS:HB2	2:D:465:GLU:HG3	1.97	0.45
2:C:276:LEU:HB3	2:C:289:VAL:HB	1.99	0.45
2:B:57:PRO:HG3	2:B:273:ARG:HG3	1.98	0.45
2:B:213:VAL:HG12	2:B:214:ARG:HG2	1.99	0.45
2:D:1103:PHE:HZ	3:S:1:NAG:HO6	1.63	0.45
1:A:230:PHE:CZ	1:A:484:ILE:HG23	2.52	0.45
2:C:419:ALA:HA	2:C:423:TYR:O	2.16	0.45
2:C:448:ASN:HB3	2:C:497:PHE:HD2	1.82	0.45
2:B:358:ILE:HB	2:B:395:VAL:HB	1.99	0.45
2:D:725:GLU:HB2	2:D:1062:PHE:HB2	1.99	0.45
2:D:1028:LYS:O	2:D:1032:CYS:N	2.41	0.45
2:B:442:ASP:HB3	2:B:451:TYR:HE2	1.79	0.45
3:L:1:NAG:H62	3:L:2:NAG:H82	1.97	0.45
2:C:737:ASP:CG	2:B:317:ASN:HD22	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:TYR:HD1	2:B:193:VAL:HG22	1.82	0.45
2:B:269:TYR:HD1	2:B:271:GLN:HE21	1.65	0.45
1:A:416:LYS:HD3	1:A:543:ASP:HB3	1.98	0.44
2:C:98:SER:HB3	2:C:181:GLY:HA2	1.98	0.44
2:D:130:VAL:HB	2:D:168:PHE:HB3	1.98	0.44
2:D:656:VAL:HG12	2:D:658:ASN:H	1.83	0.44
1:A:203:TRP:HZ3	1:A:398:GLU:HG3	1.81	0.44
2:C:93:ALA:HA	2:C:191:GLU:HA	1.99	0.44
2:C:157:PHE:HE2	4:C:1309:NAG:H3	1.82	0.44
2:C:454:ARG:NH2	2:C:469:SER:O	2.48	0.44
2:C:1018:ILE:O	2:C:1022:ALA:N	2.44	0.44
2:B:666:ILE:HD11	2:B:672:ALA:HB2	1.98	0.44
2:B:772:VAL:HG12	2:B:776:LYS:HE3	1.99	0.44
1:A:489:GLU:HG3	1:A:492:PRO:HA	1.99	0.44
2:C:246:ARG:HG2	2:C:258:TRP:CE3	2.53	0.44
2:D:1082:CYS:O	2:D:1134:ASN:HA	2.17	0.44
2:C:544:ASN:ND2	2:C:564:GLN:HE22	2.10	0.44
2:C:706:ALA:HB2	3:G:2:NAG:H62	1.99	0.44
4:C:1302:NAG:O7	4:C:1302:NAG:O3	2.33	0.44
2:B:917:TYR:HB3	2:D:1129:VAL:HG13	1.99	0.44
2:D:106:PHE:HB3	2:D:235:ILE:HD13	2.00	0.44
2:D:501:ASN:HB3	2:D:505:TYR:HB2	1.97	0.44
1:A:105:SER:HB2	1:A:113:SER:HB2	2.00	0.44
1:A:378:HIS:CE1	1:A:402:GLU:HA	2.53	0.44
1:A:389:PRO:HD2	1:A:392:LEU:HD12	2.00	0.44
2:C:43:PHE:HZ	2:C:282:ASN:O	1.98	0.44
2:C:458:LYS:HA	2:C:473:TYR:HE1	1.82	0.44
2:B:18:LEU:HD12	2:B:21:ARG:HD2	2.00	0.44
2:B:743:CYS:HA	2:B:977:LEU:HD11	1.99	0.44
2:B:1115:ILE:HG22	2:B:1137:VAL:HG13	1.99	0.44
2:B:983:ARG:O	2:D:383:SER:N	2.51	0.44
2:D:437:ASN:HA	2:D:508:TYR:HD1	1.83	0.44
2:D:661:GLU:O	2:D:695:TYR:OH	2.30	0.44
1:A:300:GLN:HG3	1:A:423:LEU:HD23	1.99	0.44
2:B:94:SER:N	2:B:190:ARG:O	2.50	0.44
2:B:985:ASP:HB3	2:B:987:PRO:HD2	2.00	0.44
2:D:204:TYR:HD1	2:D:225:PRO:HA	1.82	0.44
2:D:213:VAL:HG12	2:D:214:ARG:HG2	2.00	0.44
2:D:716:THR:N	2:D:1071:GLN:O	2.45	0.44
2:D:804:GLN:O	2:D:816:SER:HB2	2.18	0.44
2:C:206:LYS:HD3	2:C:221:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:666:ILE:HD12	2:B:670:ILE:HG22	2.00	0.44
2:D:21:ARG:HB3	2:D:79:PHE:HB3	2.00	0.44
2:D:985:ASP:HB3	2:D:987:PRO:HD2	2.00	0.44
1:A:157:ASP:HB3	1:A:160:GLU:HB3	2.00	0.43
2:C:94:SER:HA	2:C:265:TYR:HA	1.99	0.43
2:C:329:PHE:HE2	2:C:528:LYS:HB3	1.83	0.43
2:C:962:LEU:HD11	2:C:1004:LEU:HD23	2.00	0.43
2:C:987:PRO:HG3	2:D:413:GLY:HA3	1.98	0.43
2:B:38:TYR:HE1	2:B:285:ILE:HG13	1.83	0.43
2:B:142:GLY:HA3	2:B:258:TRP:HZ3	1.82	0.43
2:B:765:ARG:NH2	2:D:302:THR:O	2.51	0.43
2:D:598:ILE:HG23	2:D:664:ILE:HG21	2.00	0.43
1:A:29:LEU:HD11	1:A:97:LEU:HG	2.00	0.43
1:A:381:TYR:HD1	1:A:558:LEU:HD22	1.82	0.43
2:C:708:SER:HB3	2:C:711:SER:CB	2.48	0.43
2:C:917:TYR:HB3	2:B:1129:VAL:HG13	1.99	0.43
2:B:374:PHE:CE1	2:B:377:PHE:HB2	2.53	0.43
2:B:412:PRO:HB3	2:B:427:ASP:HA	1.99	0.43
1:A:158:TYR:HB2	1:A:252:TYR:CZ	2.53	0.43
1:A:294:THR:OG1	1:A:366:MET:N	2.50	0.43
2:B:393:THR:HG22	2:B:394:ASN:ND2	2.33	0.43
2:D:1090:PRO:HG3	2:D:1095:PHE:CE1	2.53	0.43
1:A:386:ALA:O	2:B:505:TYR:OH	2.36	0.43
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.81	0.43
2:C:756:TYR:HB3	2:C:759:PHE:CD2	2.54	0.43
2:B:66:HIS:CE1	2:B:78:ARG:HE	2.36	0.43
2:B:124:THR:HG22	2:B:125:ASN:ND2	2.34	0.43
2:B:904:TYR:HB2	2:D:1107:ARG:CZ	2.49	0.43
2:D:104:TRP:HE1	2:D:240:THR:HG1	1.64	0.43
2:D:598:ILE:HB	2:D:609:ALA:HB3	2.00	0.43
2:B:195:LYS:HG3	2:B:202:LYS:HB2	2.01	0.43
2:B:345:THR:O	2:B:509:ARG:NH2	2.51	0.43
2:D:335:LEU:HD23	2:D:362:VAL:HB	2.01	0.43
2:D:643:PHE:HE2	2:D:654:GLU:HA	1.84	0.43
1:A:176:LEU:HD23	1:A:179:LEU:HD12	2.00	0.43
1:A:528:ALA:HB2	1:A:574:VAL:HG12	2.01	0.43
2:C:94:SER:N	2:C:190:ARG:O	2.52	0.43
2:D:15:CYS:HA	2:D:137:ASN:HB2	2.00	0.43
2:D:778:THR:HB	2:D:865:LEU:HD12	1.99	0.43
1:A:153:ALA:HB1	1:A:277:ASN:ND2	2.34	0.43
2:B:848:ASP:HB2	2:B:851:CYS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:THR:HG22	2:D:78:ARG:HA	2.01	0.43
2:D:69:HIS:CE1	2:D:261:GLY:HA2	2.54	0.43
2:D:403:ARG:HD2	2:D:505:TYR:HD1	1.84	0.43
2:D:1033:VAL:HA	2:D:1051:SER:HB3	2.00	0.43
3:F:1:NAG:H82	3:F:1:NAG:C3	2.49	0.43
2:C:501:ASN:HB3	2:C:505:TYR:HB2	2.00	0.43
2:D:404:GLY:HA2	2:D:508:TYR:CD2	2.54	0.43
2:C:502:GLY:O	2:C:506:GLN:HG3	2.18	0.42
2:B:66:HIS:HD2	2:B:68:ILE:HG23	1.83	0.42
2:D:642:VAL:HA	2:D:651:ILE:HG22	2.00	0.42
2:C:30:ASN:HA	2:C:60:SER:O	2.18	0.42
2:C:106:PHE:HD2	2:C:117:LEU:HD23	1.85	0.42
2:C:107:GLY:H	2:C:235:ILE:HG23	1.83	0.42
2:C:437:ASN:HA	2:C:508:TYR:HD1	1.84	0.42
2:C:883:THR:O	2:C:901:GLN:NE2	2.52	0.42
2:B:1103:PHE:CD2	2:B:1112:PRO:HB3	2.54	0.42
2:D:128:ILE:O	2:D:170:TYR:N	2.51	0.42
1:A:40:PHE:HB2	1:A:69:TRP:NE1	2.34	0.42
1:A:91:LEU:HD21	1:A:565:PRO:HD3	2.00	0.42
1:A:519:THR:HA	1:A:522:GLN:HG2	2.00	0.42
2:D:394:ASN:HB3	2:D:396:TYR:CZ	2.55	0.42
2:D:801:ASN:N	2:D:928:ASN:OD1	2.45	0.42
2:D:497:PHE:CE1	2:D:507:PRO:HB3	2.54	0.42
2:D:906:PHE:HB3	2:D:911:VAL:HB	2.02	0.42
2:D:1081:ILE:HG12	2:D:1095:PHE:CE2	2.55	0.42
2:C:733:LYS:HE3	2:C:771:ALA:HB1	2.01	0.42
2:B:231:ILE:HG22	2:B:233:ILE:HG12	2.00	0.42
2:B:378:LYS:HE2	2:B:380:TYR:CE1	2.52	0.42
2:D:102:ARG:NE	2:D:141:LEU:HD12	2.34	0.42
1:A:29:LEU:HD12	1:A:93:VAL:HG13	2.01	0.42
1:A:455:MET:SD	1:A:481:LYS:HA	2.60	0.42
1:A:499:ASP:HB3	1:A:500:PRO:HD3	2.02	0.42
2:C:599:THR:HB	2:C:608:VAL:HG12	2.02	0.42
2:B:278:LYS:O	2:B:286:THR:N	2.35	0.42
2:B:426:PRO:HG2	2:B:429:PHE:HB2	2.00	0.42
2:B:858:LEU:HD21	2:B:962:LEU:HD23	2.01	0.42
2:B:965:GLN:HB3	2:B:970:PHE:HZ	1.85	0.42
2:B:1147:SER:HB3	2:D:1145:LEU:HD13	2.02	0.42
2:D:1078:ALA:CB	2:D:1133:VAL:HG13	2.49	0.42
1:A:127:TYR:OH	1:A:145:GLU:OE2	2.24	0.42
1:A:133:CYS:HA	1:A:141:CYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:HD13	1:A:380:GLN:HG2	2.02	0.42
2:C:118:LEU:HB2	2:C:133:PHE:CE2	2.55	0.42
2:C:934:ILE:HD13	2:C:1063:LEU:HD22	2.02	0.42
2:B:30:ASN:OD1	2:B:61:ASN:OD1	2.38	0.42
2:B:83:VAL:HG22	2:B:239:GLN:HE21	1.84	0.42
2:D:34:ARG:NH2	2:D:217:PRO:HD2	2.35	0.42
2:D:914:ASN:ND2	2:D:1111:GLU:OE1	2.52	0.42
1:A:371:THR:HA	1:A:374:HIS:HB3	2.02	0.42
1:A:396:ALA:HB1	1:A:566:TRP:HB3	2.01	0.42
1:A:453:THR:HA	1:A:512:PHE:HE2	1.84	0.42
2:C:853:GLN:HE22	2:C:959:LEU:HD13	1.84	0.42
2:C:969:ASN:HB2	2:D:755:GLN:HB3	2.01	0.42
2:D:465:GLU:OE1	2:D:465:GLU:HA	2.20	0.42
2:D:586:ASP:OD1	2:D:587:ILE:N	2.53	0.42
2:C:1030:SER:HB3	2:B:1040:VAL:O	2.20	0.42
2:B:204:TYR:HD1	2:B:225:PRO:HA	1.85	0.42
2:B:797:PHE:CE2	2:B:802:PHE:HB2	2.55	0.42
1:A:581:VAL:HG13	1:A:584:LEU:HD23	2.01	0.42
2:C:642:VAL:HG13	2:C:651:ILE:HG22	2.02	0.41
2:B:895:GLN:HG2	2:D:713:ALA:HB2	2.01	0.41
2:D:157:PHE:CZ	2:D:159:VAL:HB	2.55	0.41
2:D:1110:TYR:CZ	2:D:1112:PRO:HG3	2.55	0.41
1:A:155:SER:O	1:A:161:ARG:HD2	2.20	0.41
2:C:68:ILE:HD11	2:C:78:ARG:HG3	2.01	0.41
2:C:886:TRP:CD1	2:C:904:TYR:CZ	3.08	0.41
2:B:29:THR:O	2:B:62:VAL:N	2.51	0.41
2:B:142:GLY:HA3	2:B:258:TRP:CZ3	2.55	0.41
2:D:341:VAL:HG22	2:D:356:LYS:HD3	2.01	0.41
2:D:516:GLU:HB3	2:D:519:HIS:HD2	1.85	0.41
2:D:1116:THR:HG23	2:D:1118:ASP:H	1.85	0.41
1:A:191:ALA:HB1	1:A:196:TYR:HB2	2.02	0.41
2:C:157:PHE:CE2	4:C:1309:NAG:H3	2.55	0.41
2:C:424:LYS:HG2	2:C:463:PRO:HG3	2.02	0.41
2:D:502:GLY:O	2:D:506:GLN:HG3	2.20	0.41
1:A:203:TRP:CZ3	1:A:511:SER:HB2	2.55	0.41
2:C:697:MET:HE1	2:D:864:LEU:HG	2.01	0.41
2:C:884:SER:OG	2:C:893:ALA:HB1	2.19	0.41
2:C:1031:GLU:HB2	2:B:1039:ARG:HG3	2.02	0.41
2:B:983:ARG:HB3	2:D:382:VAL:HG12	2.01	0.41
2:D:96:GLU:HB2	2:D:188:ASN:HB2	2.01	0.41
2:D:132:GLU:OE2	4:D:1309:NAG:O7	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:365:TYR:HD2	2:D:387:LEU:HB3	1.84	0.41
1:A:115:ARG:O	1:A:119:ILE:HG12	2.20	0.41
2:C:1089:PHE:CZ	2:C:1129:VAL:HG21	2.54	0.41
1:A:132:VAL:HG23	1:A:168:TRP:HE3	1.84	0.41
1:A:205:GLY:HA2	1:A:208:GLU:HB2	2.03	0.41
1:A:218:SER:HB3	1:A:221:GLN:HB2	2.03	0.41
2:B:850:ILE:O	2:B:854:LYS:N	2.45	0.41
2:C:165:ASN:OD1	2:C:165:ASN:N	2.52	0.41
2:C:189:LEU:HB2	2:C:210:ILE:HD13	2.03	0.41
2:C:326:ILE:HD11	2:C:534:VAL:HB	2.02	0.41
2:C:444:LYS:HG2	2:C:445:VAL:HG23	2.03	0.41
2:C:1028:LYS:O	2:C:1032:CYS:N	2.48	0.41
2:C:1081:ILE:HG23	2:C:1135:ASN:HB3	2.02	0.41
2:B:1090:PRO:HD3	2:B:1095:PHE:CZ	2.55	0.41
2:D:912:THR:H	2:D:1109:PHE:HE2	1.69	0.41
1:A:396:ALA:HB3	1:A:400:PHE:CD2	2.55	0.41
2:C:1074:ASN:OD1	2:C:1074:ASN:N	2.52	0.41
2:C:1090:PRO:HG3	2:C:1095:PHE:CE1	2.55	0.41
2:B:437:ASN:HA	2:B:508:TYR:CD1	2.54	0.41
2:B:453:TYR:HB3	2:B:495:TYR:CE2	2.56	0.41
2:B:911:VAL:HG22	2:B:1108:ASN:HB2	2.03	0.41
1:A:226:VAL:HG23	1:A:454:TYR:HE1	1.86	0.41
1:A:490:PRO:HA	1:A:612:PRO:HG2	2.02	0.41
2:C:16:VAL:N	4:C:1311:NAG:H82	2.35	0.41
2:C:105:ILE:HG22	2:C:110:LEU:HD22	2.02	0.41
2:C:1031:GLU:HG2	2:C:1037:SER:HB2	2.03	0.41
2:B:1033:VAL:HA	2:B:1051:SER:HB3	2.03	0.41
2:D:365:TYR:CD2	2:D:387:LEU:HB3	2.56	0.41
2:D:741:TYR:OH	2:D:962:LEU:O	2.26	0.41
2:C:53:ASP:OD1	2:C:54:LEU:N	2.46	0.41
2:C:124:THR:HG22	2:C:125:ASN:ND2	2.35	0.41
2:C:901:GLN:HA	2:C:904:TYR:HE2	1.86	0.41
2:B:609:ALA:HA	2:B:652:GLY:HA3	2.03	0.41
2:D:431:GLY:HA2	2:D:515:PHE:HE2	1.85	0.41
1:A:208:GLU:OE2	1:A:219:ARG:NH1	2.54	0.40
2:C:328:ARG:NH2	2:C:578:ASP:OD2	2.45	0.40
2:C:1033:VAL:HA	2:C:1051:SER:HB3	2.03	0.40
2:B:190:ARG:HH11	2:B:192:PHE:HZ	1.68	0.40
2:B:782:PHE:HE1	2:B:1060:VAL:HB	1.85	0.40
2:B:1101:HIS:CE1	2:B:1135:ASN:HD21	2.39	0.40
2:B:1110:TYR:CZ	2:B:1112:PRO:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1126:CYS:HA	2:B:1132:ILE:HD13	2.02	0.40
2:D:708:SER:HB3	2:D:711:SER:CB	2.50	0.40
1:A:28:PHE:HD1	2:B:489:TYR:HH	1.67	0.40
2:C:279:TYR:HE1	2:C:285:ILE:HG12	1.87	0.40
2:B:106:PHE:HD2	2:B:117:LEU:HD23	1.85	0.40
2:B:453:TYR:CZ	2:B:493:GLN:HB2	2.56	0.40
2:B:1049:LEU:HD12	2:B:1065:VAL:HG12	2.03	0.40
2:D:189:LEU:HB2	2:D:210:ILE:HD13	2.03	0.40
2:D:1031:GLU:HG2	2:D:1037:SER:HB2	2.02	0.40
3:S:1:NAG:H82	3:S:1:NAG:C3	2.51	0.40
2:C:146:HIS:NE2	2:C:245:HIS:HB2	2.36	0.40
2:C:317:ASN:HA	2:C:594:GLY:HA2	2.03	0.40
2:C:731:MET:N	2:C:774:GLN:OE1	2.51	0.40
2:B:805:ILE:HB	2:B:878:LEU:HD11	2.03	0.40
2:B:906:PHE:CE2	2:B:916:LEU:HB2	2.57	0.40
2:C:215:ASP:O	2:C:266:TYR:OH	2.39	0.40
2:D:117:LEU:HD11	2:D:128:ILE:HG23	2.04	0.40
2:D:391:CYS:HB2	2:D:524:VAL:O	2.21	0.40
2:C:453:TYR:CZ	2:C:493:GLN:HB2	2.57	0.40
2:C:1101:HIS:CE1	2:C:1135:ASN:HD21	2.39	0.40
2:B:1030:SER:O	2:B:1034:LEU:HB3	2.21	0.40
2:B:1076:THR:O	2:B:1097:SER:N	2.54	0.40
2:D:106:PHE:HD2	2:D:117:LEU:HD23	1.87	0.40
2:D:553:THR:O	2:D:586:ASP:N	2.44	0.40
2:D:1089:PHE:CZ	2:D:1129:VAL:HG21	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	595/625 (95%)	588 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1056/1261 (84%)	1014 (96%)	42 (4%)	0	100	100
2	C	1053/1261 (84%)	995 (94%)	57 (5%)	1 (0%)	48	79
2	D	1056/1261 (84%)	1003 (95%)	52 (5%)	1 (0%)	48	79
All	All	3760/4408 (85%)	3600 (96%)	158 (4%)	2 (0%)	50	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	445	VAL
2	D	445	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	527/552 (96%)	527 (100%)	0	100	100
2	B	934/1099 (85%)	934 (100%)	0	100	100
2	C	931/1099 (85%)	928 (100%)	3 (0%)	91	92
2	D	934/1099 (85%)	930 (100%)	4 (0%)	89	91
All	All	3326/3849 (86%)	3319 (100%)	7 (0%)	91	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	17	ASN
2	C	165	ASN
2	C	1074	ASN
2	D	282	ASN
2	D	331	ASN
2	D	616	ASN
2	D	1133	VAL

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	24	GLN
1	A	300	GLN
1	A	378	HIS
1	A	380	GLN
1	A	401	HIS
1	A	526	GLN
2	C	188	ASN
2	C	409	GLN
2	C	422	ASN
2	C	498	GLN
2	C	519	HIS
2	C	564	GLN
2	C	856	ASN
2	C	895	GLN
2	C	955	ASN
2	C	1101	HIS
2	B	125	ASN
2	B	207	HIS
2	B	239	GLN
2	B	394	ASN
2	B	895	GLN
2	B	920	GLN
2	B	955	ASN
2	B	965	GLN
2	B	1101	HIS
2	D	69	HIS
2	D	188	ASN
2	D	481	ASN
2	D	498	GLN
2	D	519	HIS
2	D	564	GLN
2	D	901	GLN
2	D	913	GLN
2	D	955	ASN
2	D	965	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	E	1	2,3	14,14,15	0.34	0	17,19,21	1.14	1 (5%)
3	NAG	E	2	3	14,14,15	0.27	0	17,19,21	0.90	1 (5%)
3	NAG	F	1	2,3	14,14,15	2.04	1 (7%)	17,19,21	2.67	5 (29%)
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	0.57	0
3	NAG	G	1	2,3	14,14,15	0.27	0	17,19,21	0.67	0
3	NAG	G	2	3	14,14,15	0.27	0	17,19,21	0.61	0
3	NAG	H	1	2,3	14,14,15	0.28	0	17,19,21	0.61	0
3	NAG	H	2	3	14,14,15	0.25	0	17,19,21	0.67	0
3	NAG	I	1	2,3	14,14,15	0.28	0	17,19,21	0.69	0
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.72	0
3	NAG	J	1	2,3	14,14,15	0.48	0	17,19,21	0.98	1 (5%)
3	NAG	J	2	3	14,14,15	0.30	0	17,19,21	0.64	0
3	NAG	K	1	2,3	14,14,15	0.27	0	17,19,21	0.64	0
3	NAG	K	2	3	14,14,15	0.28	0	17,19,21	0.70	0
3	NAG	L	1	2,3	14,14,15	0.28	0	17,19,21	0.63	0
3	NAG	L	2	3	14,14,15	0.27	0	17,19,21	0.67	0
3	NAG	M	1	2,3	14,14,15	0.28	0	17,19,21	0.65	0
3	NAG	M	2	3	14,14,15	0.28	0	17,19,21	0.69	0
3	NAG	N	1	2,3	14,14,15	0.31	0	17,19,21	0.72	0
3	NAG	N	2	3	14,14,15	0.27	0	17,19,21	0.72	0
3	NAG	O	1	2,3	14,14,15	0.28	0	17,19,21	0.79	0
3	NAG	O	2	3	14,14,15	0.28	0	17,19,21	0.78	0
3	NAG	P	1	2,3	14,14,15	0.27	0	17,19,21	0.68	0
3	NAG	P	2	3	14,14,15	0.27	0	17,19,21	0.71	0
3	NAG	Q	1	2,3	14,14,15	0.27	0	17,19,21	0.74	0
3	NAG	Q	2	3	14,14,15	0.39	0	17,19,21	2.38	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	R	1	2,3	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
3	NAG	R	2	3	14,14,15	0.38	0	17,19,21	0.69	0
3	NAG	S	1	2,3	14,14,15	2.07	1 (7%)	17,19,21	2.51	5 (29%)
3	NAG	S	2	3	14,14,15	0.26	0	17,19,21	0.70	0
3	NAG	T	1	2,3	14,14,15	0.27	0	17,19,21	0.63	0
3	NAG	T	2	3	14,14,15	0.25	0	17,19,21	0.70	0
3	NAG	U	1	2,3	14,14,15	0.27	0	17,19,21	0.72	0
3	NAG	U	2	3	14,14,15	0.25	0	17,19,21	0.71	0
3	NAG	V	1	2,3	14,14,15	0.28	0	17,19,21	0.63	0
3	NAG	V	2	3	14,14,15	0.27	0	17,19,21	0.66	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	P	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Q	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	5/6/23/26	0/1/1/1
3	NAG	U	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	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)
3	S	1	NAG	C1-C2	7.69	1.63	1.52
3	F	1	NAG	C1-C2	7.48	1.63	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	2	NAG	O5-C5-C6	8.39	120.35	107.20
3	F	1	NAG	O5-C1-C2	-8.16	98.41	111.29
3	S	1	NAG	O5-C1-C2	-7.89	98.84	111.29
3	F	1	NAG	C1-O5-C5	4.10	117.75	112.19
3	F	1	NAG	O4-C4-C3	3.50	118.45	110.35
3	S	1	NAG	C1-O5-C5	3.38	116.77	112.19
3	F	1	NAG	C4-C3-C2	-3.25	106.25	111.02
3	S	1	NAG	C4-C3-C2	-3.13	106.43	111.02
3	R	1	NAG	C1-O5-C5	3.08	116.36	112.19
3	J	1	NAG	O4-C4-C3	3.07	117.45	110.35
3	R	1	NAG	O4-C4-C3	-2.94	103.56	110.35
3	S	1	NAG	C1-C2-N2	2.89	115.43	110.49
3	E	1	NAG	C1-O5-C5	2.80	115.98	112.19
3	Q	2	NAG	C4-C3-C2	2.73	115.02	111.02
3	Q	2	NAG	O3-C3-C4	2.51	116.15	110.35
3	S	1	NAG	C2-N2-C7	2.50	126.47	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-C2-N2	2.45	114.67	110.49
3	Q	2	NAG	O4-C4-C5	2.04	114.37	109.30
3	E	2	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	Q	1	NAG	C3-C2-N2-C7
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	T	2	NAG	C8-C7-N2-C2
3	T	2	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	R	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
3	U	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	R	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O7-C7-N2-C2
3	O	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C1-C2-N2-C7
3	P	1	NAG	C1-C2-N2-C7
3	H	1	NAG	O5-C5-C6-O6
3	T	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
3	N	1	NAG	C1-C2-N2-C7
3	K	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
3	U	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	S	1	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
3	V	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C1-C2-N2-C7
3	E	1	NAG	C8-C7-N2-C2
3	V	2	NAG	O5-C5-C6-O6
3	M	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C3-C2-N2-C7
3	J	1	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	O	2	NAG	C3-C2-N2-C7
3	E	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	V	1	NAG	C4-C5-C6-O6
3	T	1	NAG	O7-C7-N2-C2
3	I	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C8-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	H	1	NAG	C3-C2-N2-C7
3	N	1	NAG	C3-C2-N2-C7

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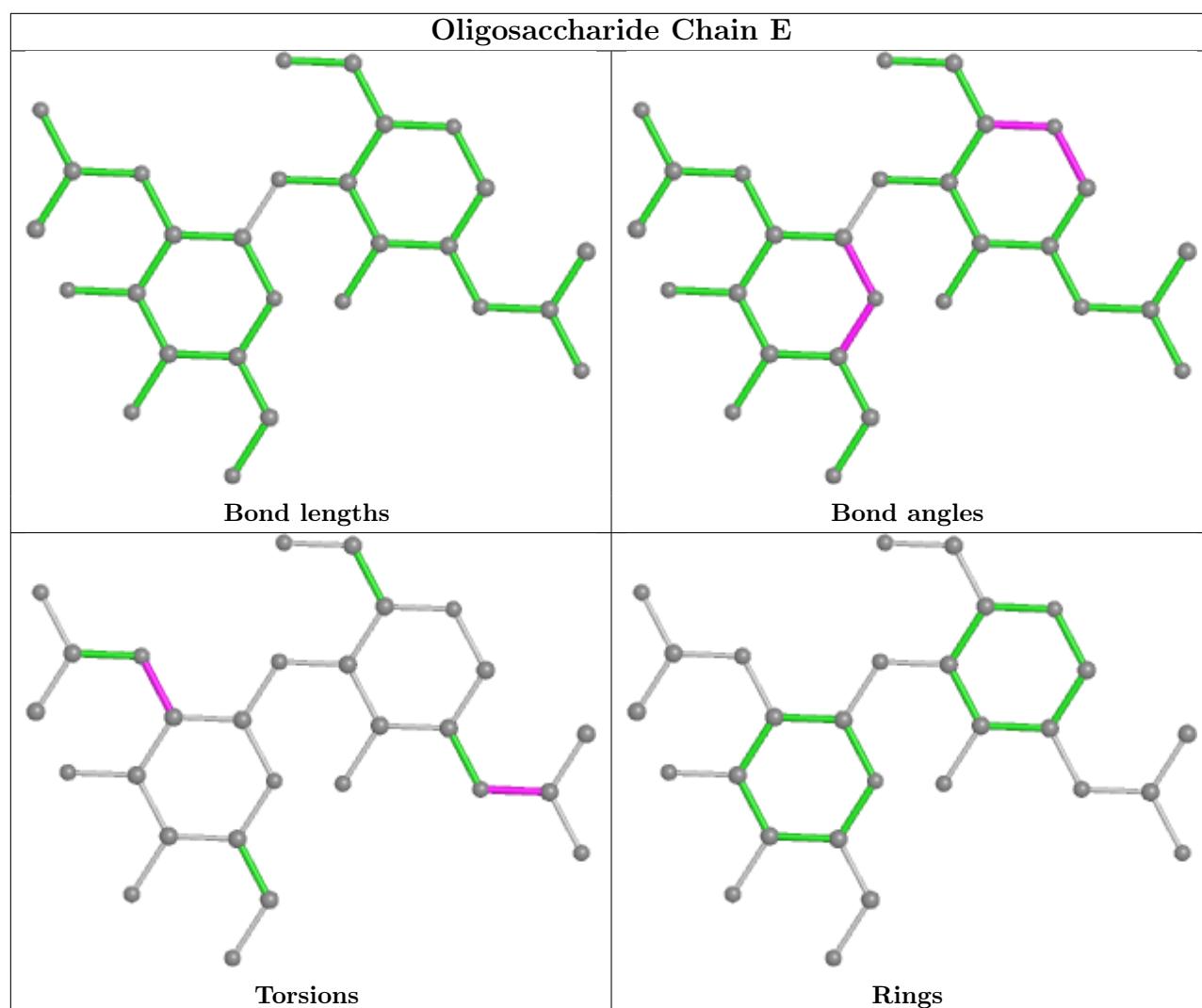
Mol	Chain	Res	Type	Atoms
3	U	1	NAG	C3-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7

There are no ring outliers.

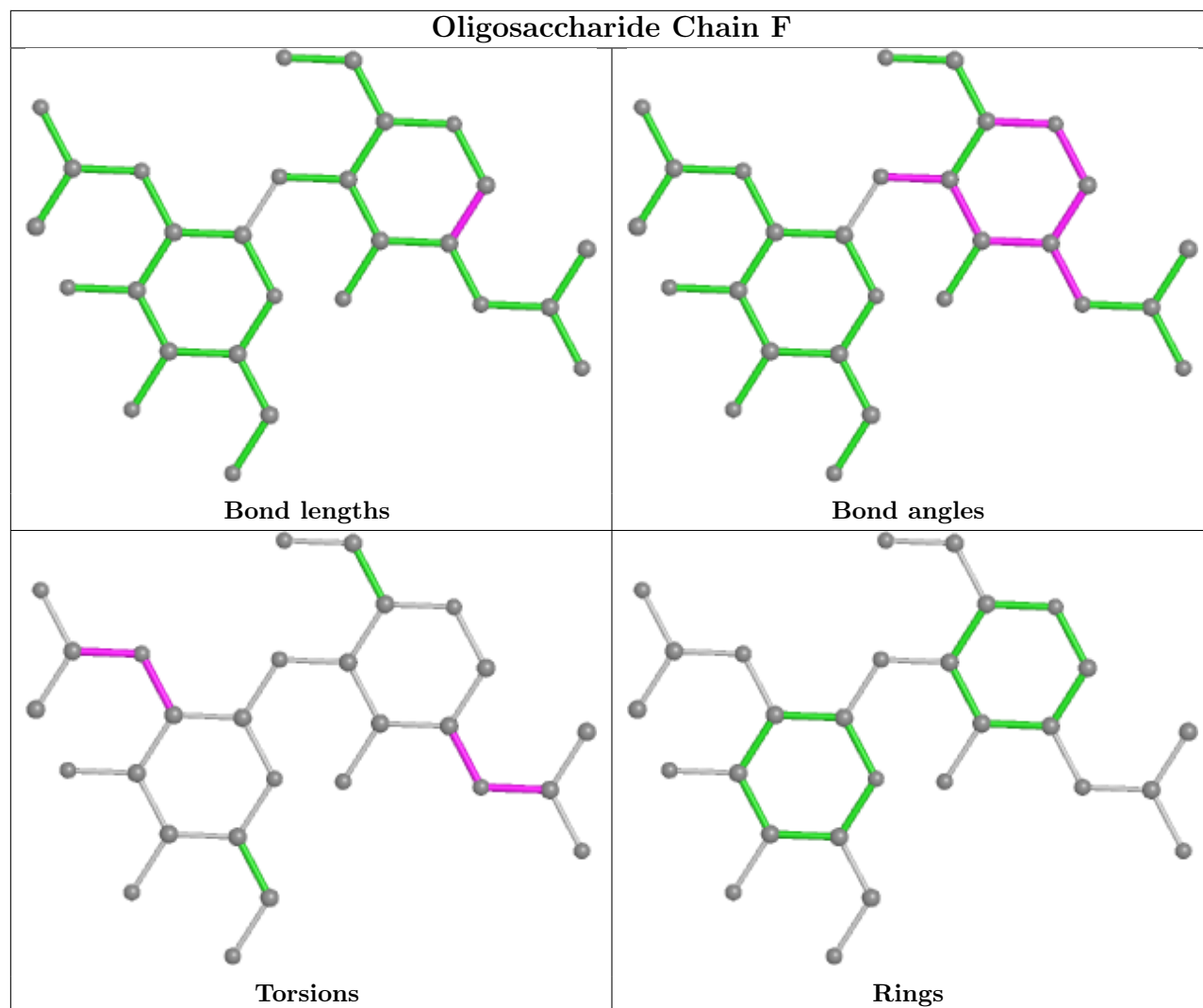
12 monomers are involved in 21 short contacts:

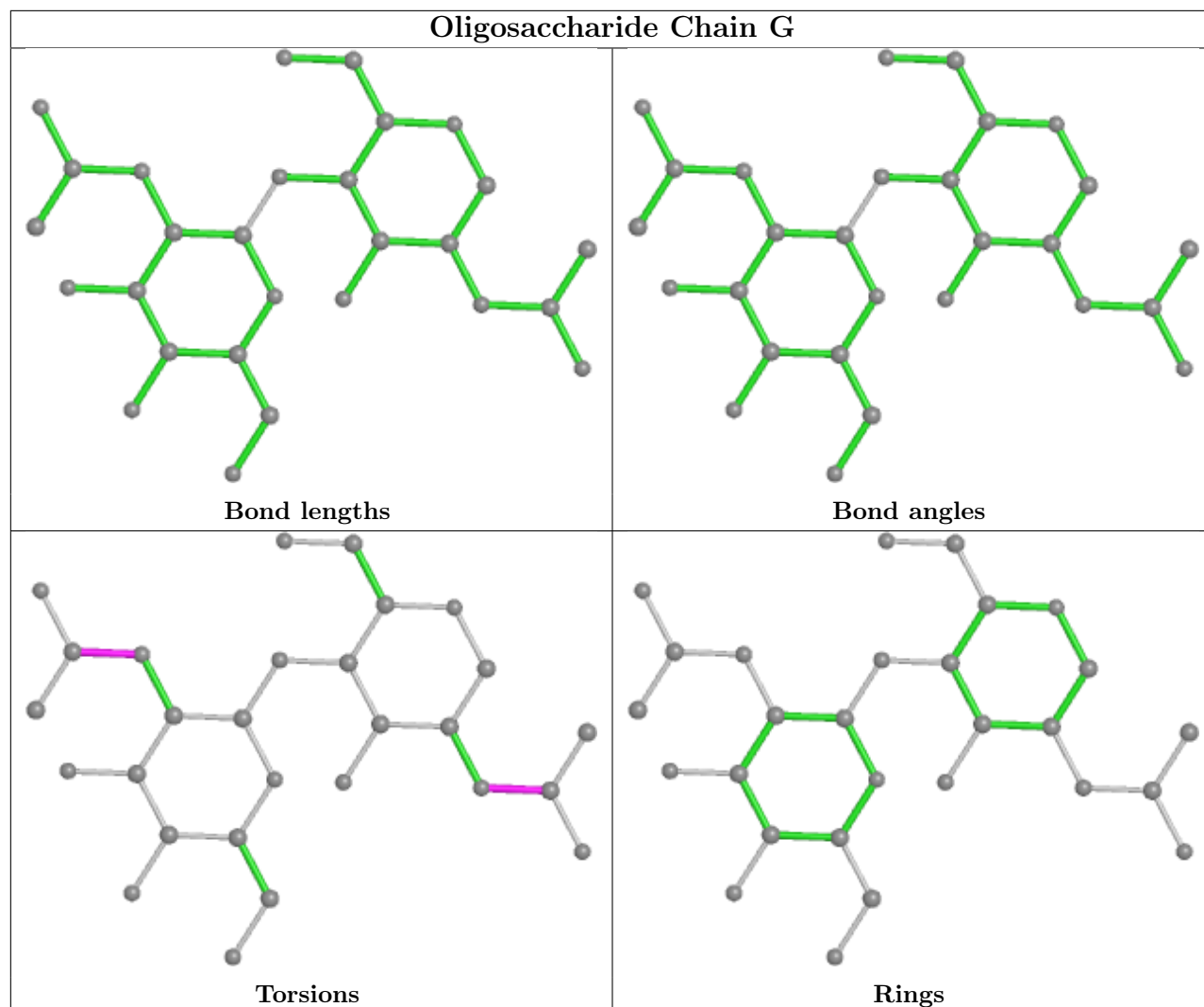
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0
3	T	2	NAG	1	0
3	L	1	NAG	2	0
3	L	2	NAG	2	0
3	F	1	NAG	3	0
3	G	2	NAG	3	0
3	E	1	NAG	2	0
3	T	1	NAG	1	0
3	E	2	NAG	1	0
3	J	1	NAG	1	0
3	Q	1	NAG	3	0
3	S	1	NAG	4	0

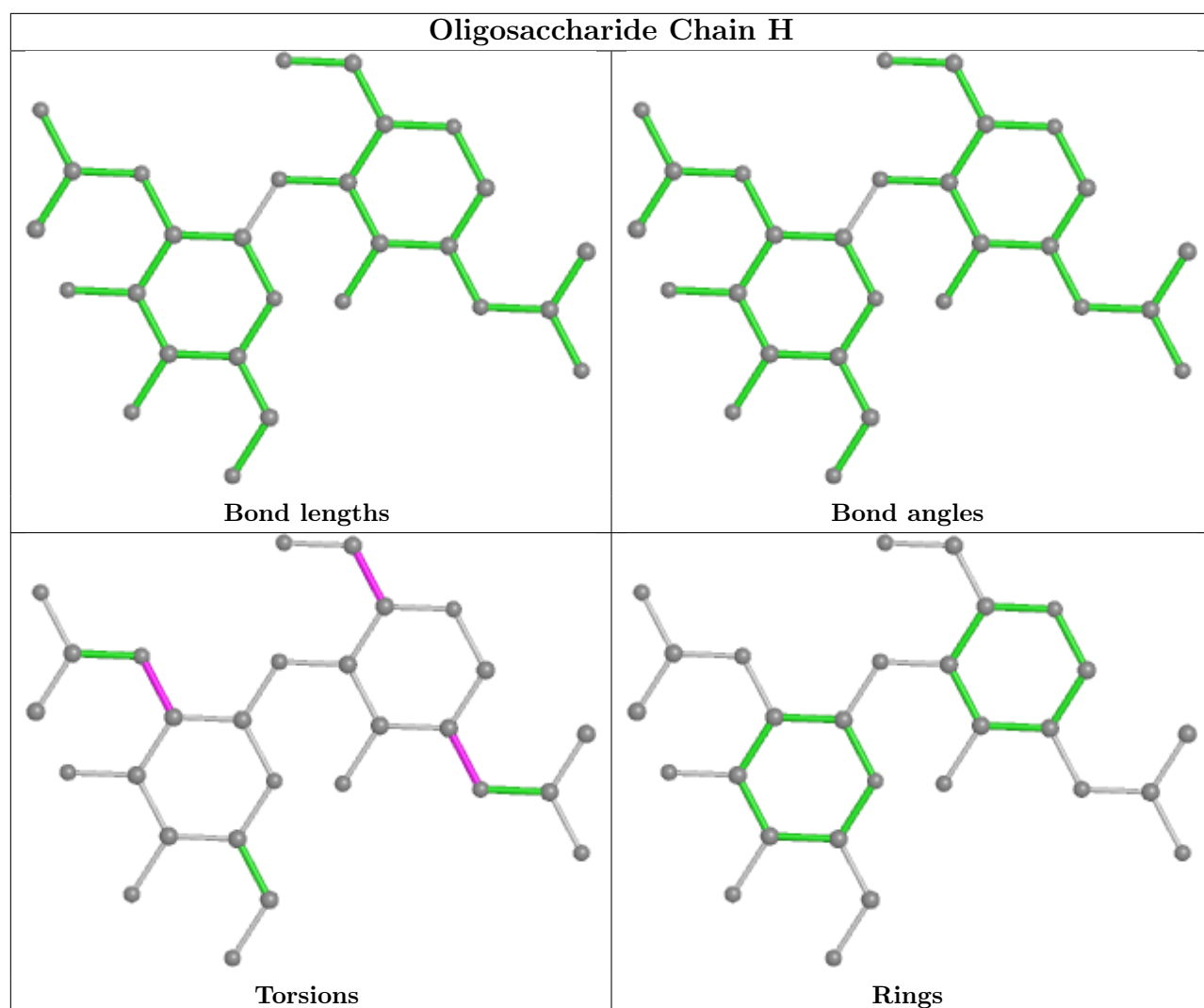
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

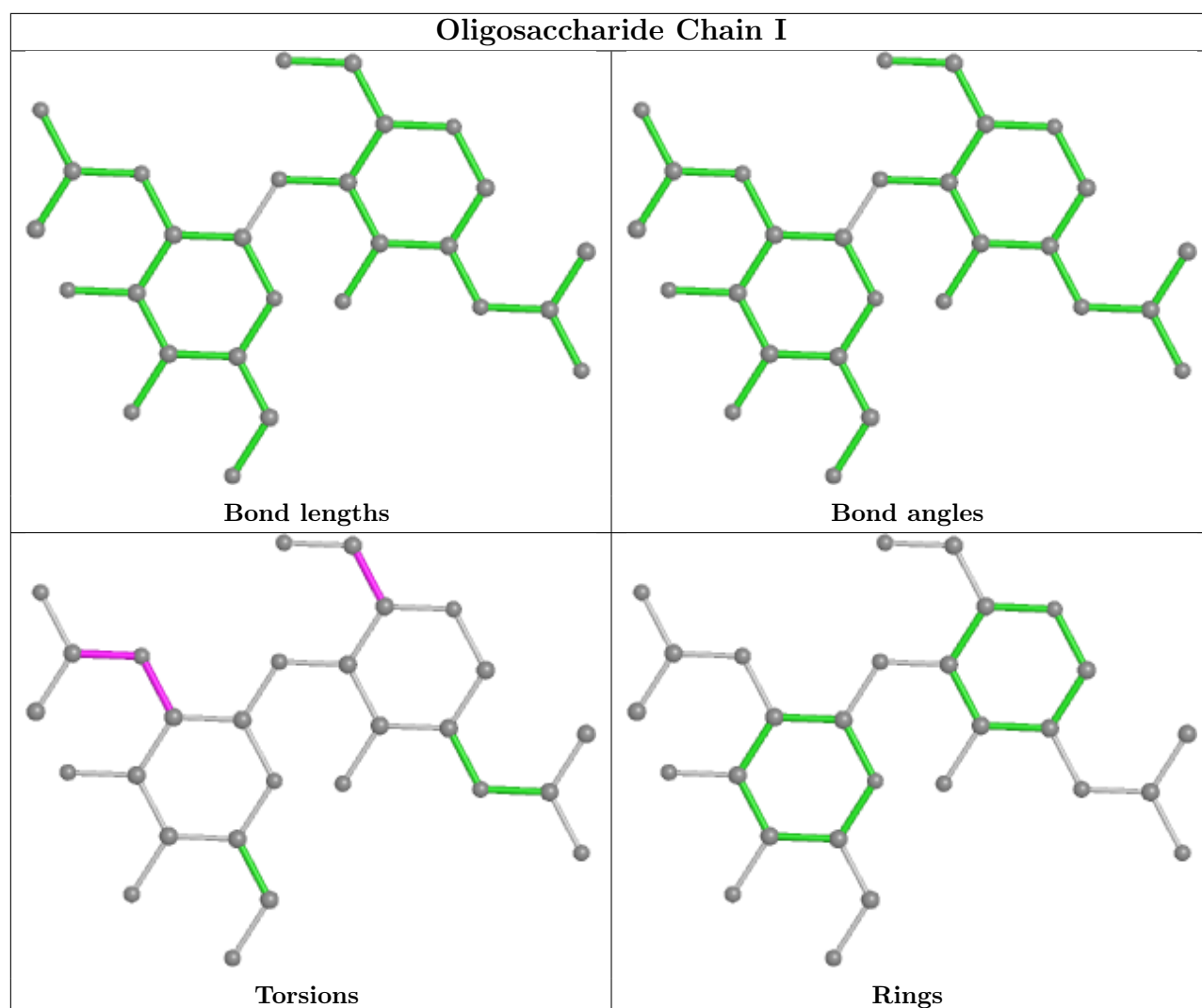


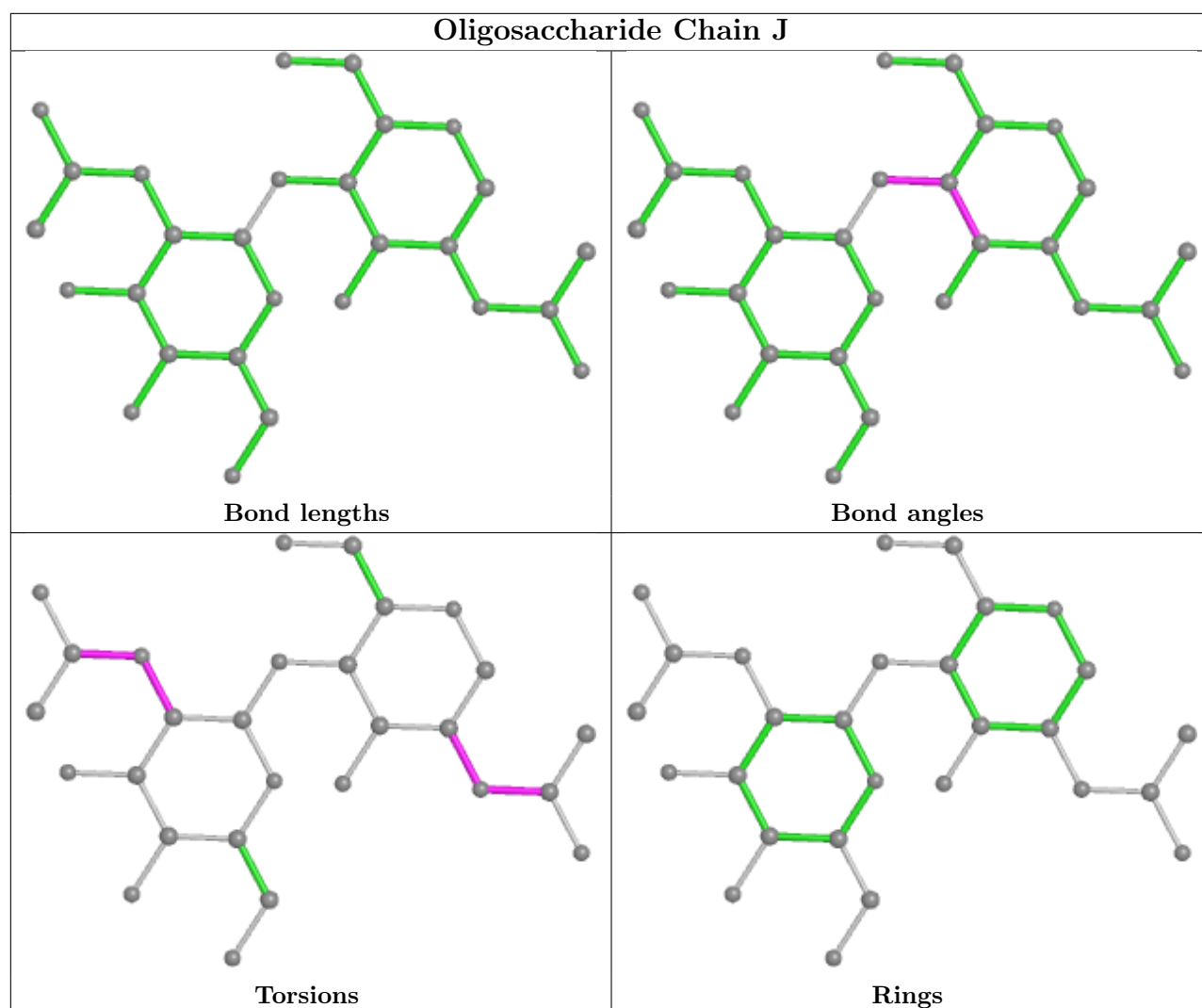


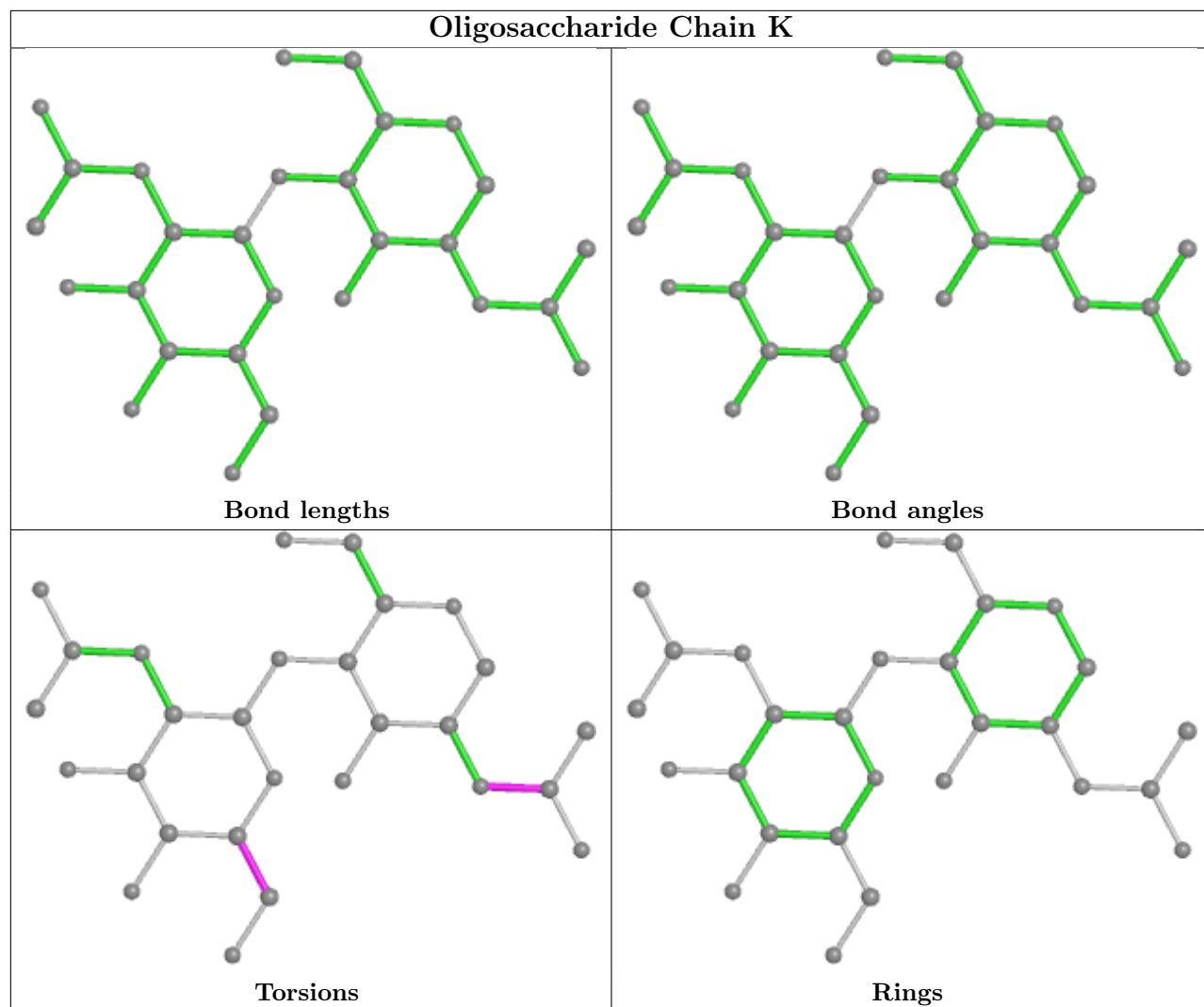


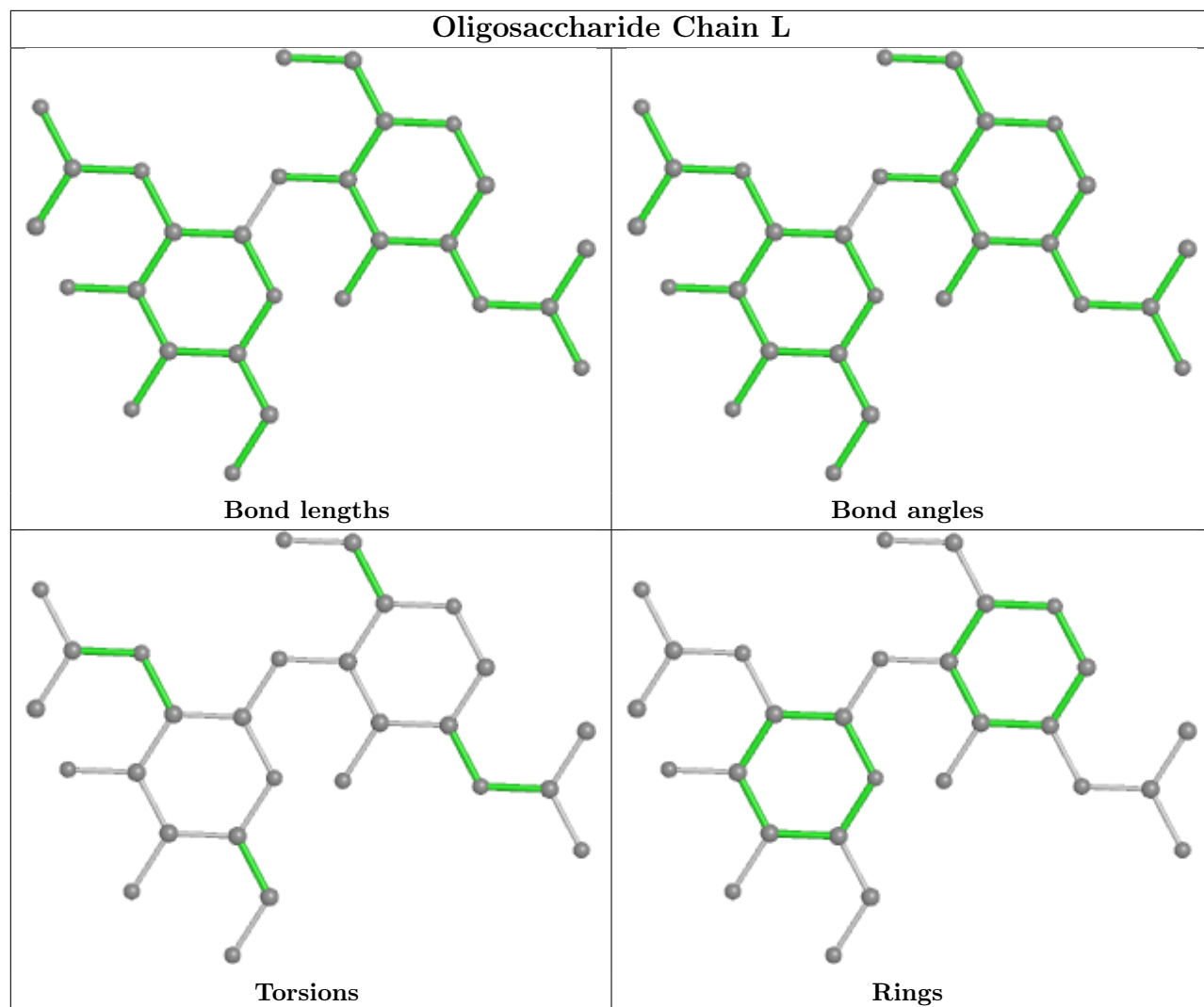


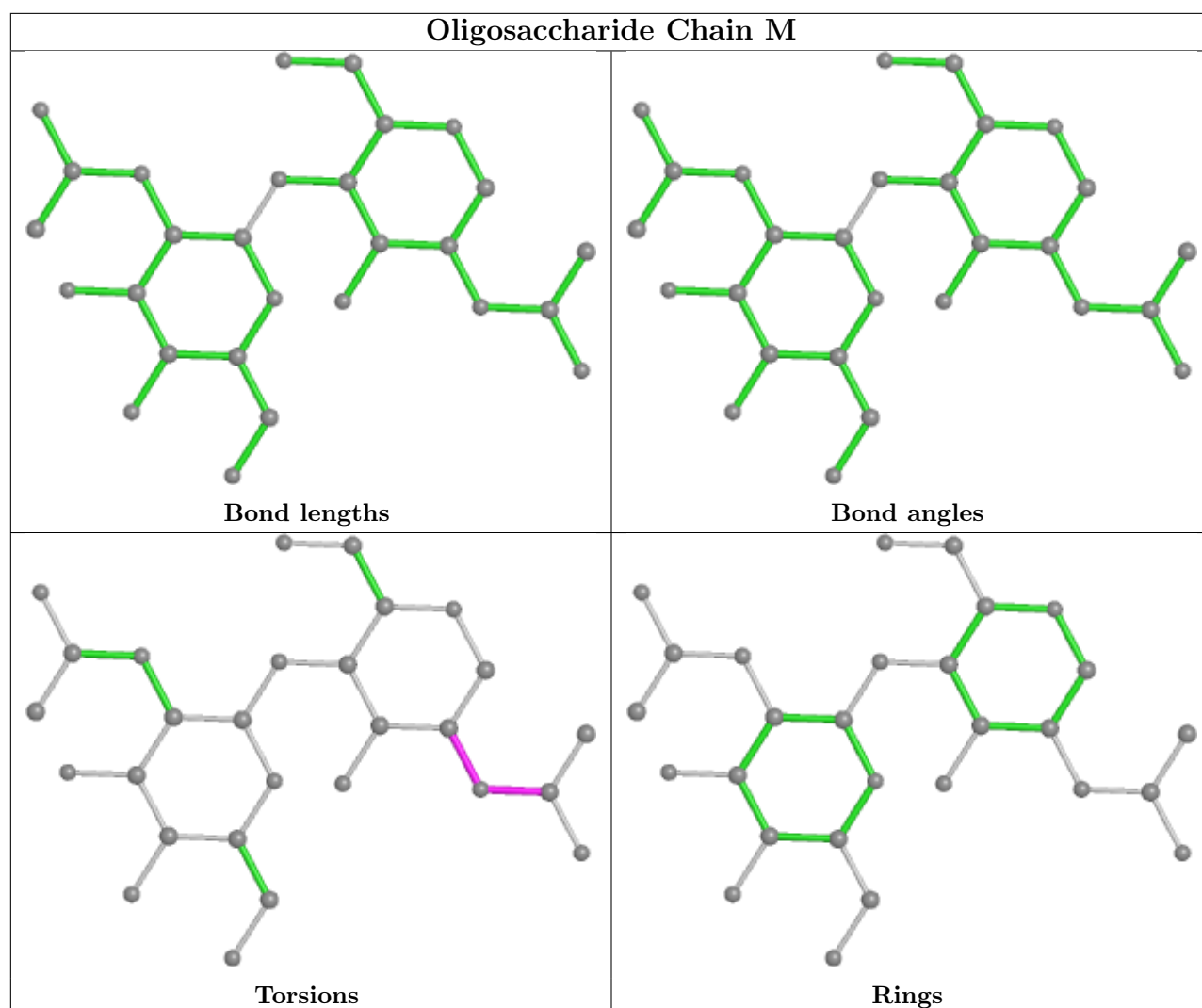




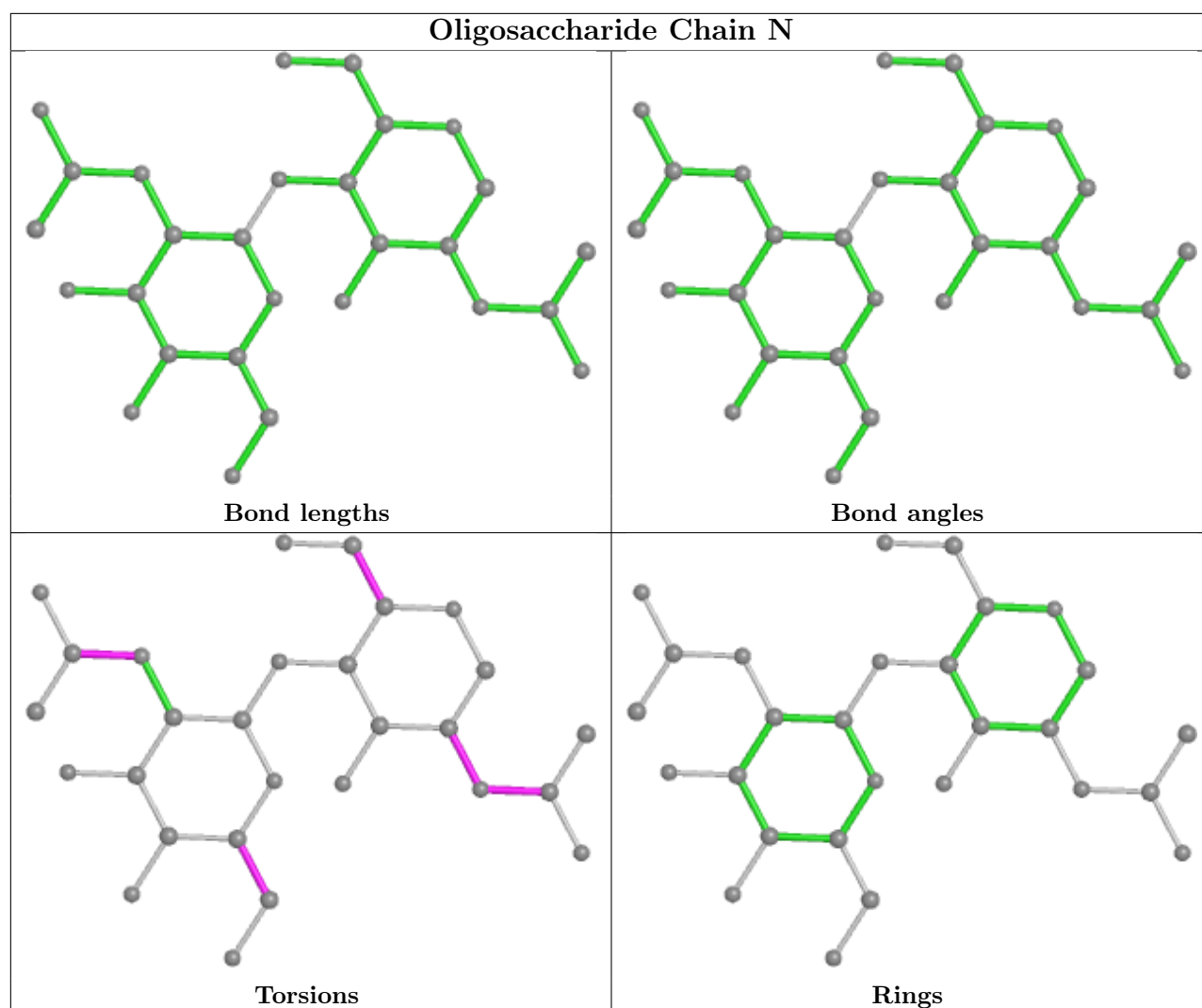


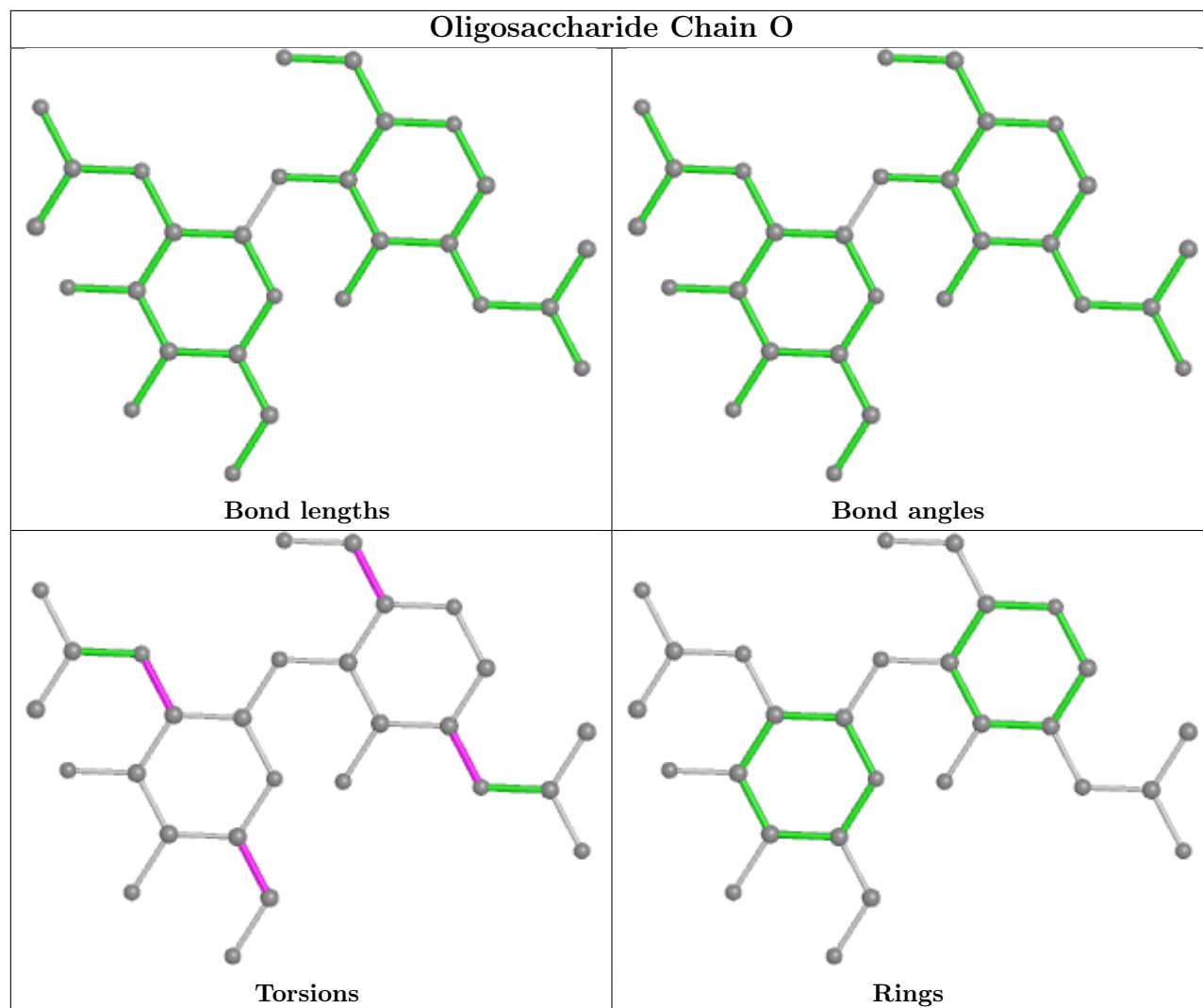


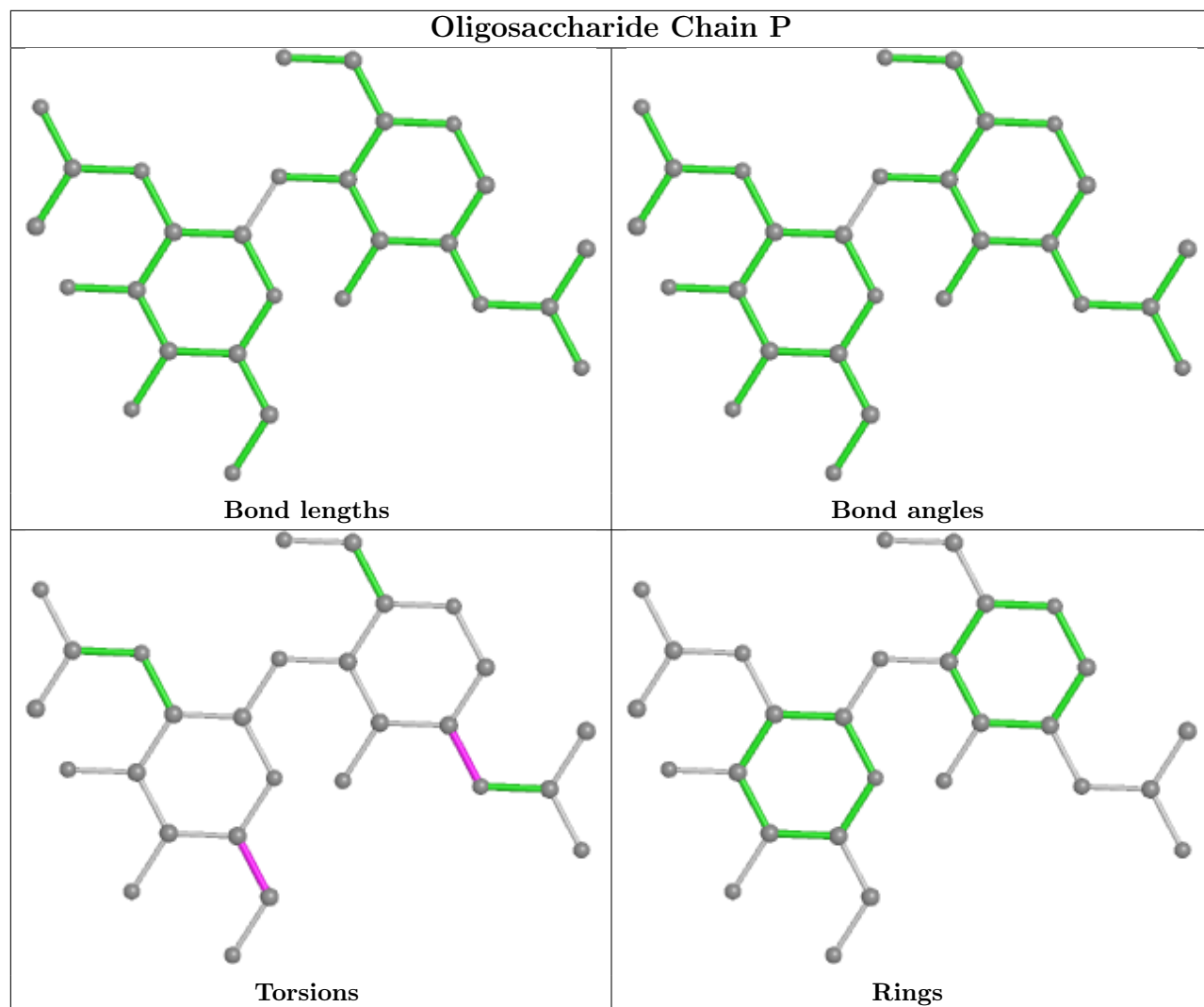


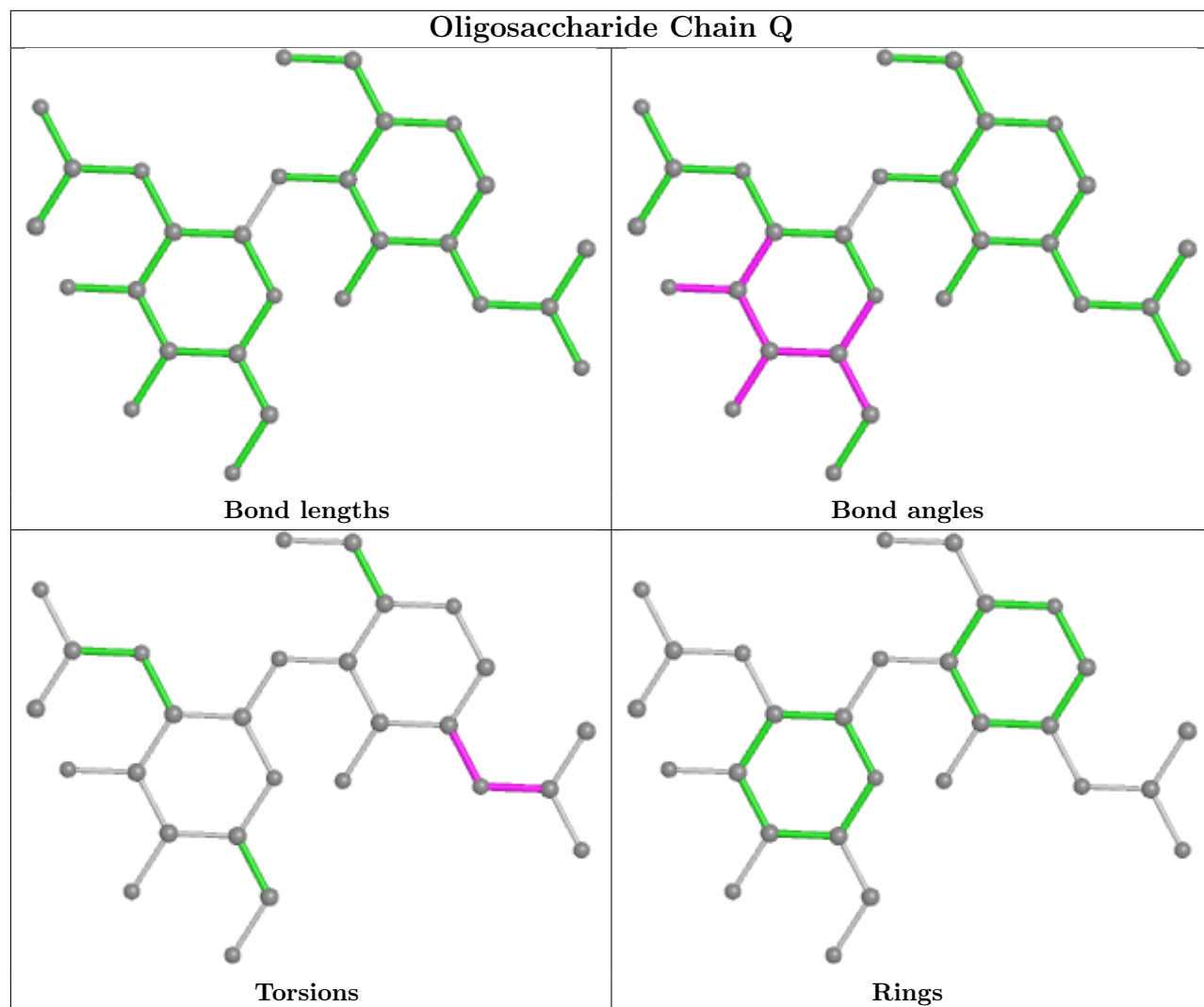


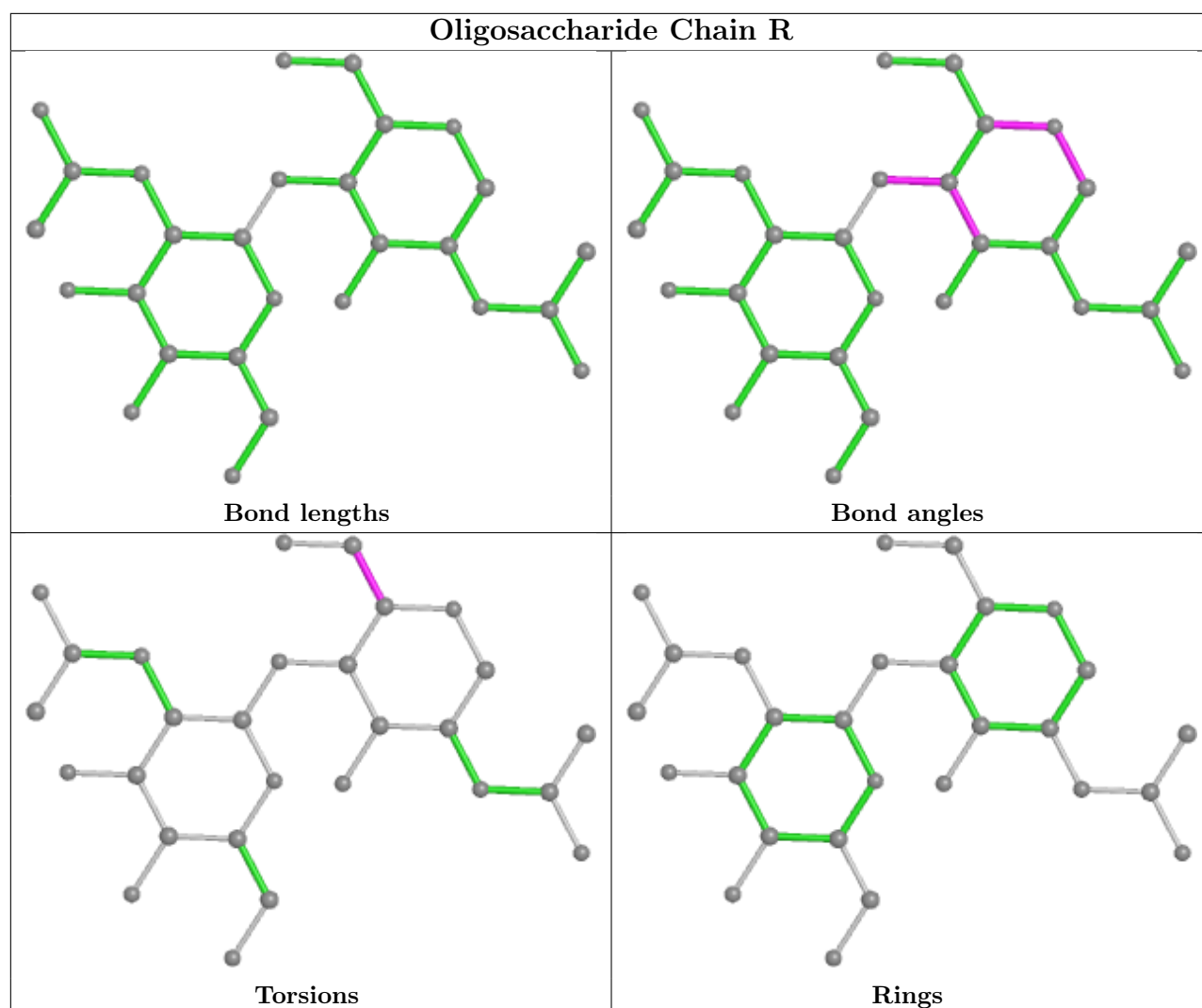


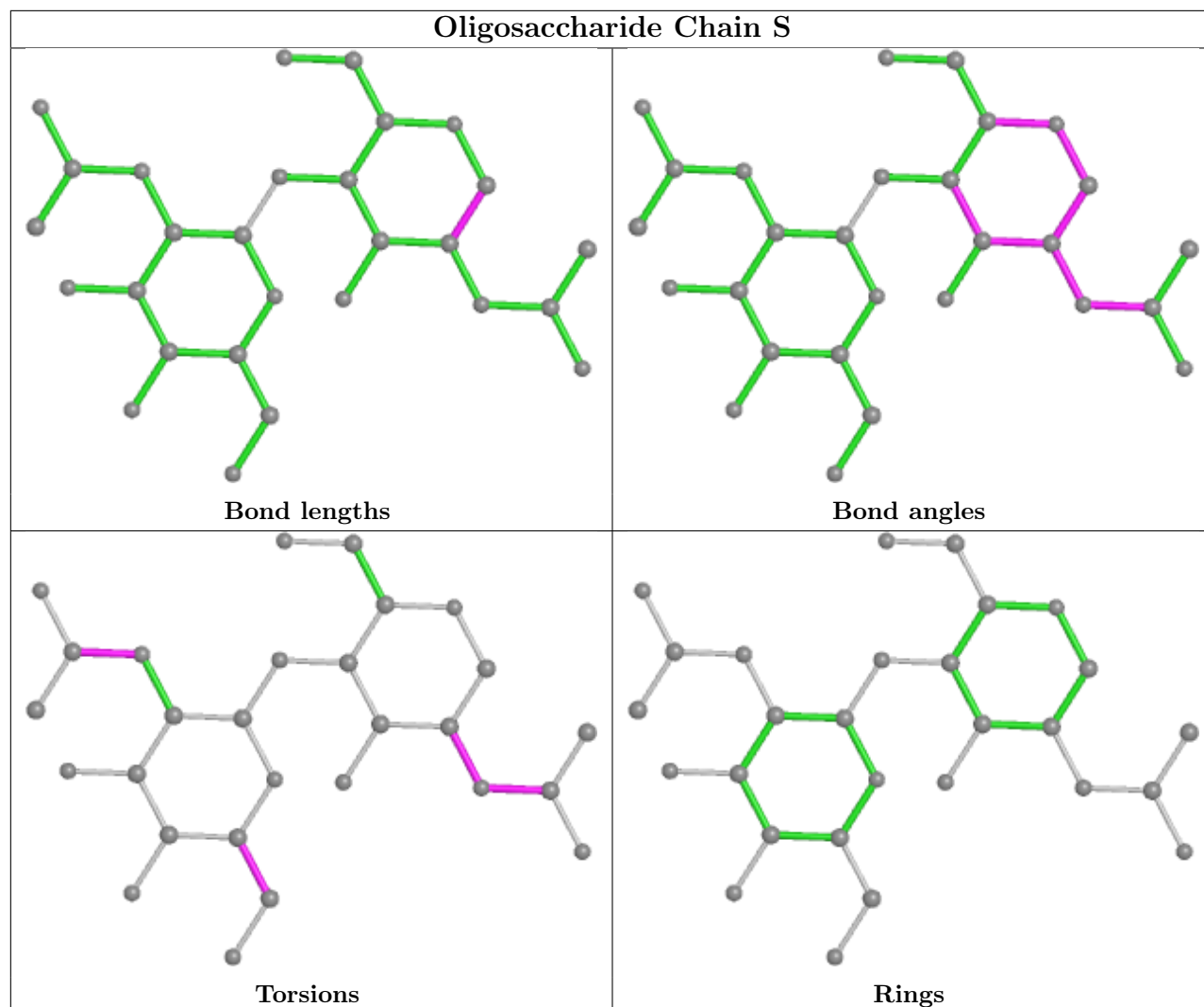


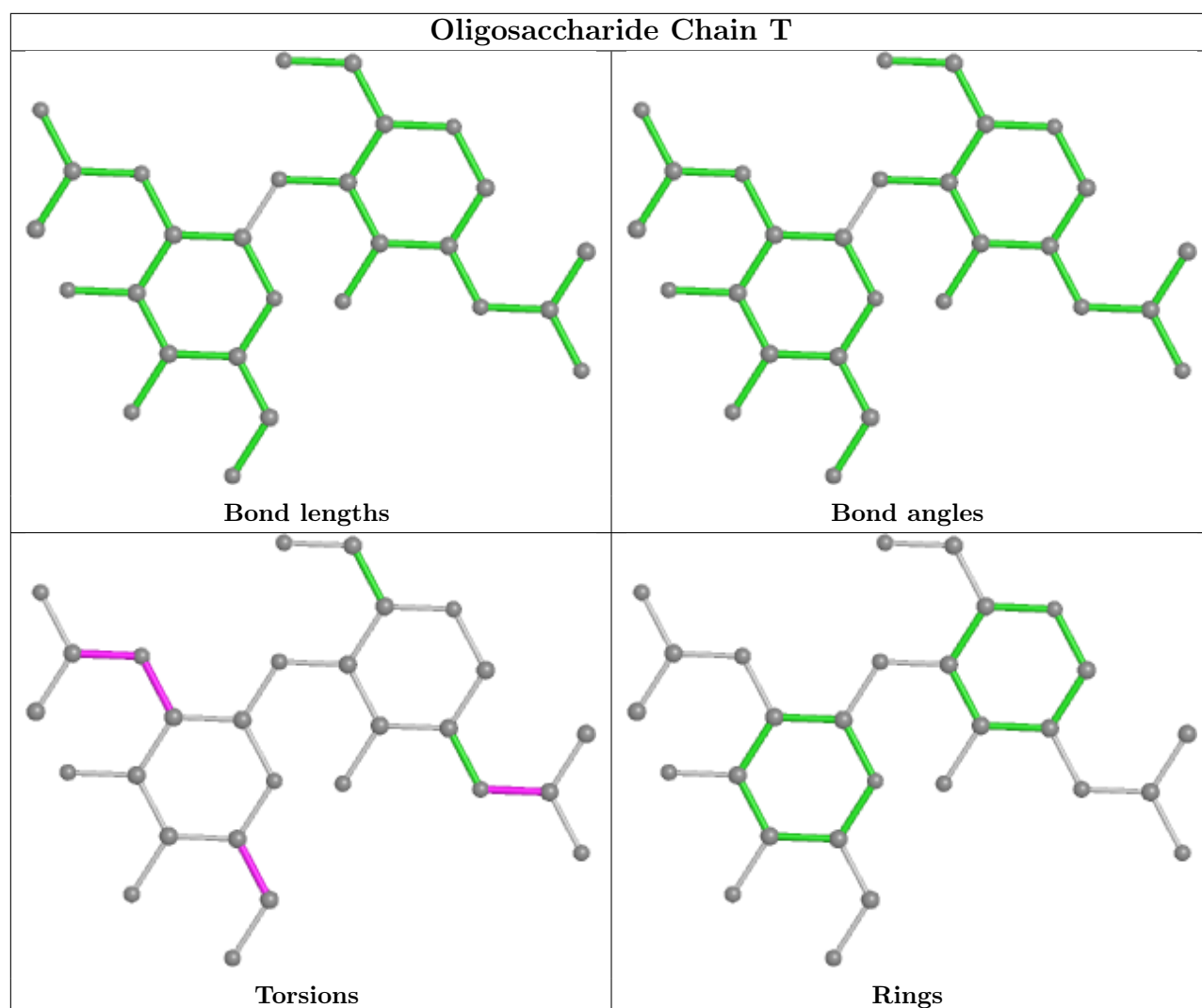


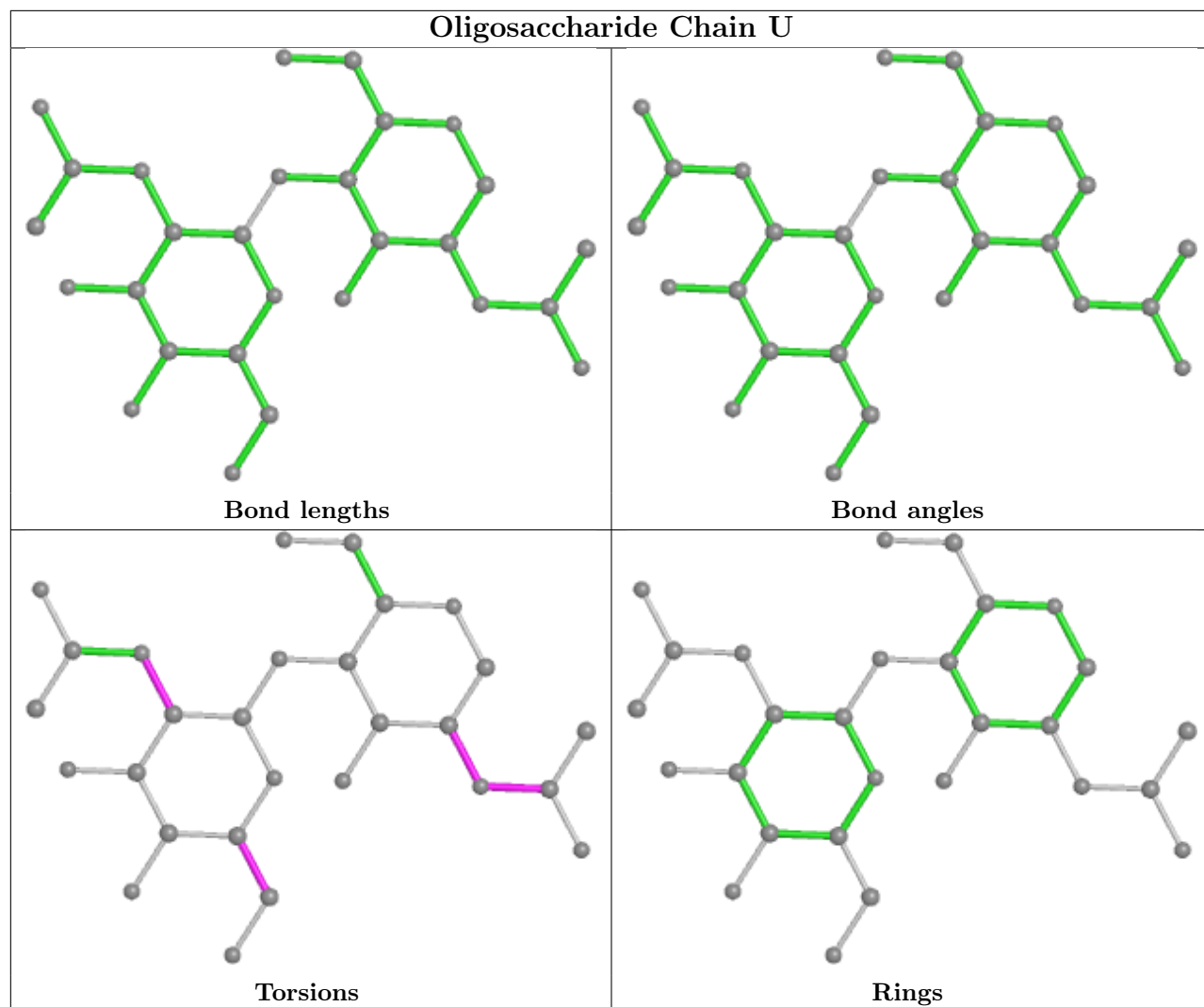




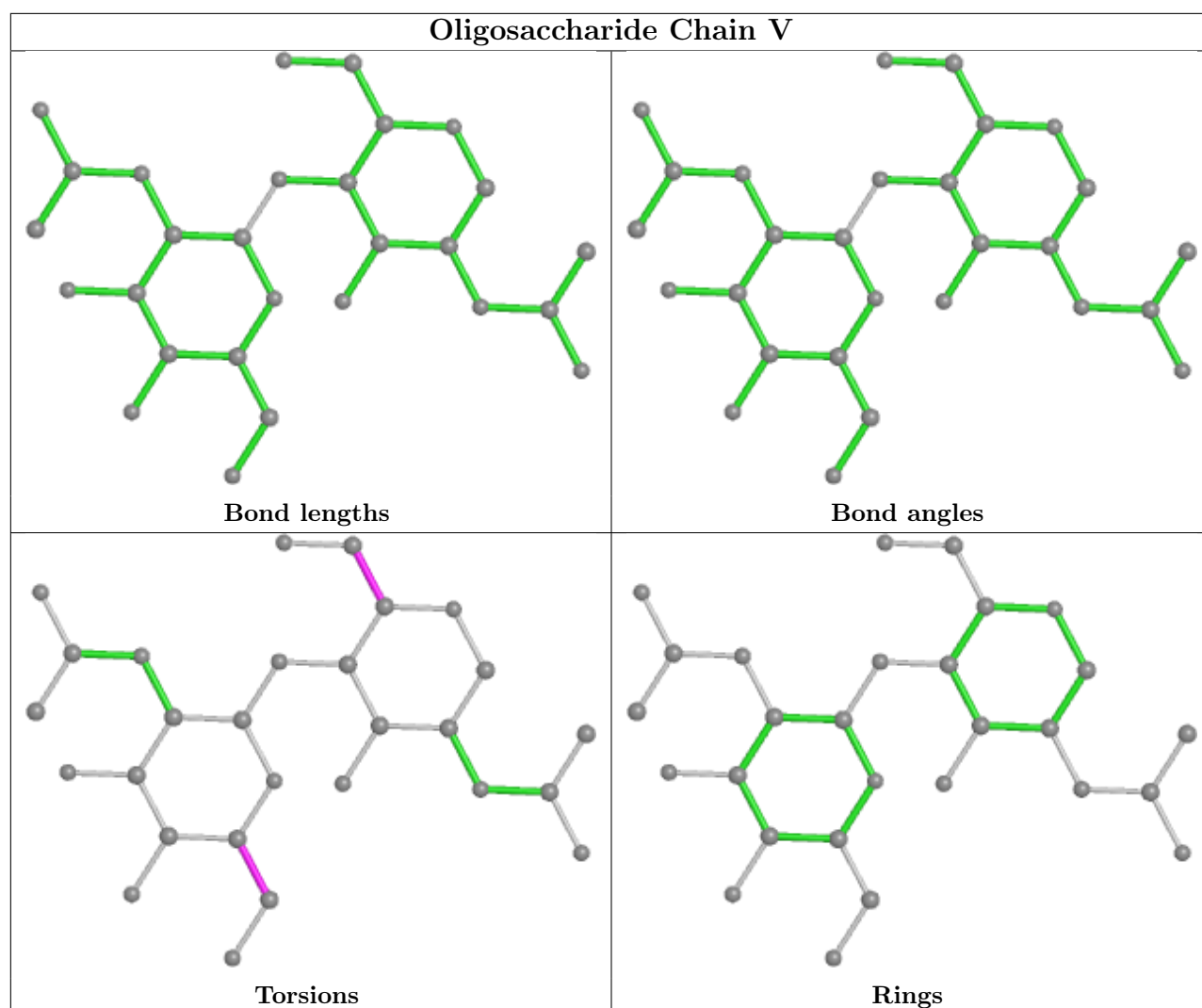












## 5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	C	1309	2	14,14,15	0.40	0	17,19,21	0.81	0
4	NAG	D	1303	2	14,14,15	0.27	0	17,19,21	0.69	0
4	NAG	B	1304	2	14,14,15	0.27	0	17,19,21	0.73	0
4	NAG	D	1302	2	14,14,15	0.27	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	1305	2	14,14,15	0.29	0	17,19,21	0.95	1 (5%)
4	NAG	D	1304	2	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	D	1310	2	14,14,15	0.40	0	17,19,21	0.81	0
4	NAG	D	1306	2	14,14,15	0.31	0	17,19,21	0.75	0
4	NAG	B	1311	2	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	C	1305	2	14,14,15	0.27	0	17,19,21	0.70	0
4	NAG	D	1309	2	14,14,15	0.40	0	17,19,21	0.82	0
4	NAG	B	1312	2	14,14,15	0.27	0	17,19,21	0.78	0
4	NAG	D	1308	2	14,14,15	0.41	0	17,19,21	0.81	0
4	NAG	C	1304	2	14,14,15	0.40	0	17,19,21	0.82	0
4	NAG	D	1307	2	14,14,15	0.28	0	17,19,21	0.75	0
4	NAG	D	1311	2	14,14,15	0.41	0	17,19,21	0.82	0
4	NAG	B	1310	2	14,14,15	0.28	0	17,19,21	0.77	0
4	NAG	B	1307	2	14,14,15	0.27	0	17,19,21	0.68	0
4	NAG	C	1311	2	14,14,15	0.27	0	17,19,21	0.65	0
4	NAG	B	1308	2	14,14,15	0.29	0	17,19,21	0.70	0
4	NAG	B	1306	2	14,14,15	0.41	0	17,19,21	0.81	0
4	NAG	B	1305	2	14,14,15	0.26	0	17,19,21	0.69	0
4	NAG	B	1309	2	14,14,15	0.40	0	17,19,21	0.82	0
4	NAG	C	1303	2	14,14,15	0.41	0	17,19,21	0.81	0
4	NAG	D	1313	2	14,14,15	0.40	0	17,19,21	0.81	0
4	NAG	C	1307	2	14,14,15	0.27	0	17,19,21	0.73	0
4	NAG	C	1308	2	14,14,15	0.39	0	17,19,21	0.82	0
4	NAG	C	1301	2	14,14,15	0.26	0	17,19,21	0.66	0
4	NAG	C	1302	2	14,14,15	0.28	0	17,19,21	0.63	0
4	NAG	B	1301	2	14,14,15	0.40	0	17,19,21	0.81	0
4	NAG	D	1312	2	14,14,15	0.27	0	17,19,21	0.81	0
4	NAG	B	1303	2	14,14,15	0.26	0	17,19,21	0.69	0
4	NAG	B	1302	2	14,14,15	0.40	0	17,19,21	0.82	0
4	NAG	C	1310	2	14,14,15	0.28	0	17,19,21	0.76	0
4	NAG	C	1306	2	14,14,15	0.39	0	17,19,21	0.81	0
4	NAG	D	1301	2	14,14,15	0.28	0	17,19,21	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1309	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1303	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1302	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1305	2	-	4/6/23/26	0/1/1/1
4	NAG	D	1304	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1310	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1306	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1311	2	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1309	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	2	-	3/6/23/26	0/1/1/1
4	NAG	D	1308	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1307	2	-	3/6/23/26	0/1/1/1
4	NAG	D	1311	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1310	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1308	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	2	-	5/6/23/26	0/1/1/1
4	NAG	B	1309	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1313	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	2	-	5/6/23/26	0/1/1/1
4	NAG	B	1301	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1312	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1303	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	2	-	0/6/23/26	0/1/1/1
4	NAG	D	1301	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1305	NAG	C1-O5-C5	2.81	116.00	112.19

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1307	NAG	C1-C2-N2-C7
4	C	1311	NAG	C3-C2-N2-C7
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	B	1310	NAG	C8-C7-N2-C2
4	B	1310	NAG	O7-C7-N2-C2
4	D	1305	NAG	C8-C7-N2-C2
4	D	1305	NAG	O7-C7-N2-C2
4	D	1312	NAG	C8-C7-N2-C2
4	D	1312	NAG	O7-C7-N2-C2
4	D	1305	NAG	O5-C5-C6-O6
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1312	NAG	C8-C7-N2-C2
4	D	1302	NAG	C8-C7-N2-C2
4	D	1303	NAG	C8-C7-N2-C2
4	D	1305	NAG	C4-C5-C6-O6
4	C	1301	NAG	C8-C7-N2-C2
4	C	1302	NAG	C8-C7-N2-C2
4	C	1311	NAG	C8-C7-N2-C2
4	B	1312	NAG	O7-C7-N2-C2
4	D	1302	NAG	O7-C7-N2-C2
4	D	1303	NAG	O7-C7-N2-C2
4	C	1311	NAG	O7-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	C	1302	NAG	O7-C7-N2-C2
4	B	1311	NAG	C8-C7-N2-C2
4	B	1306	NAG	O5-C5-C6-O6
4	B	1312	NAG	C1-C2-N2-C7
4	C	1302	NAG	C1-C2-N2-C7
4	B	1305	NAG	C1-C2-N2-C7
4	B	1305	NAG	O5-C5-C6-O6
4	B	1311	NAG	O7-C7-N2-C2
4	D	1307	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	B	1311	NAG	O5-C5-C6-O6
4	D	1306	NAG	O5-C5-C6-O6
4	D	1307	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1305	NAG	C1-C2-N2-C7
4	C	1302	NAG	C3-C2-N2-C7
4	D	1306	NAG	C8-C7-N2-C2
4	D	1306	NAG	O7-C7-N2-C2
4	D	1312	NAG	C1-C2-N2-C7
4	C	1307	NAG	C3-C2-N2-C7
4	D	1312	NAG	C3-C2-N2-C7
4	B	1306	NAG	C4-C5-C6-O6
4	C	1305	NAG	C3-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	D	1307	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1309	NAG	5	0
4	B	1304	NAG	1	0
4	B	1311	NAG	1	0
4	D	1309	NAG	1	0
4	D	1311	NAG	2	0
4	B	1310	NAG	4	0
4	B	1307	NAG	1	0
4	C	1311	NAG	5	0
4	B	1306	NAG	1	0
4	D	1313	NAG	1	0
4	C	1307	NAG	2	0
4	C	1302	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.

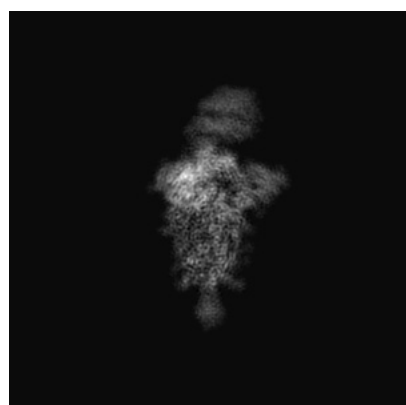
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30661. These allow visual inspection of the internal detail of the map and identification of artifacts.

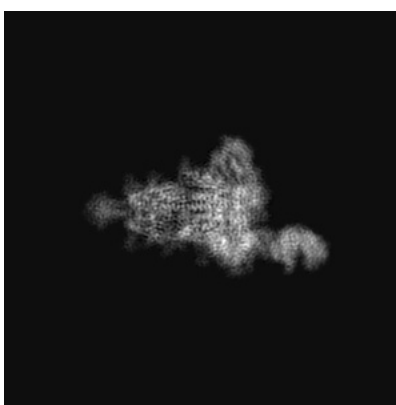
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

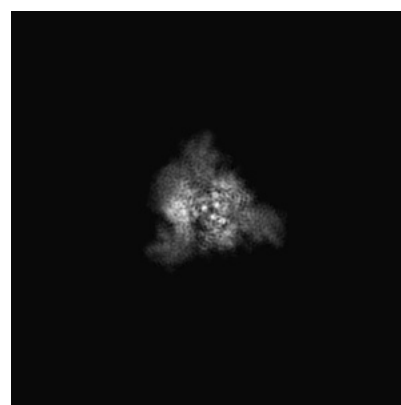
#### 6.1.1 Primary map



X



Y

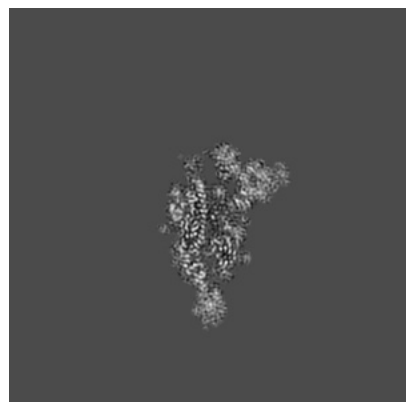


Z

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

### 6.2 Central slices [i](#)

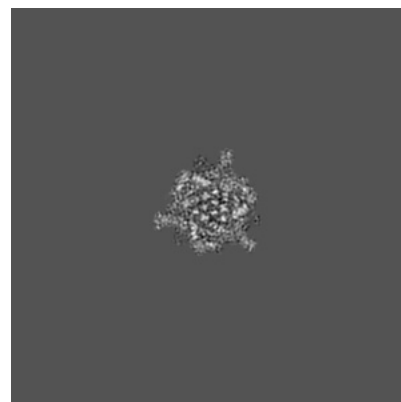
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

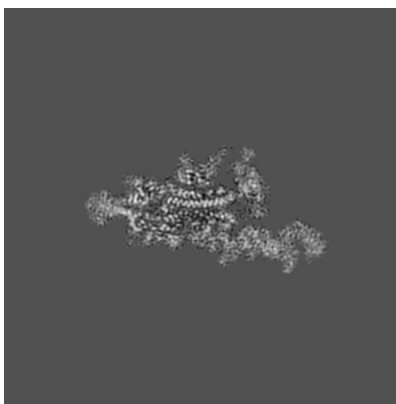
The images above show central slices of the map in three orthogonal directions.

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

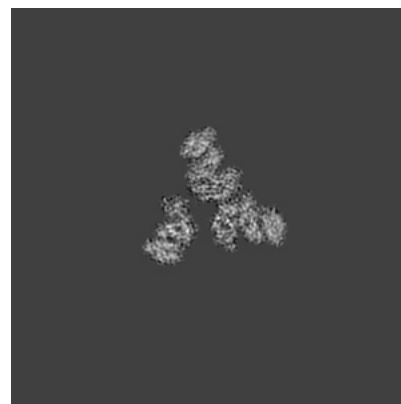
### 6.3.1 Primary map



X Index: 204



Y Index: 205

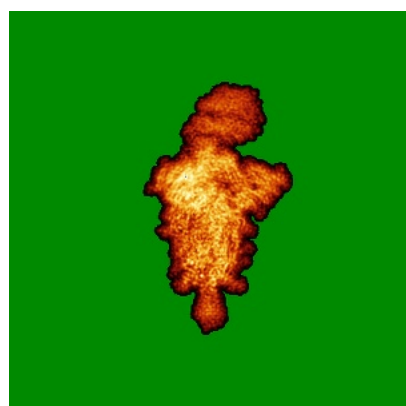


Z Index: 234

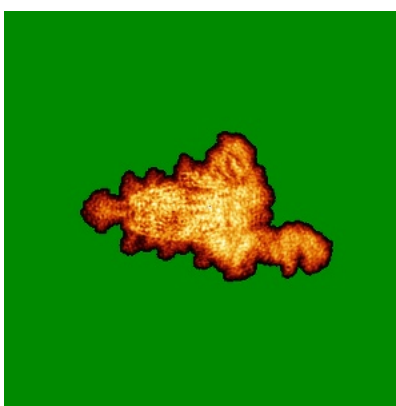
The images above show the largest variance slices of the map in three orthogonal directions.

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

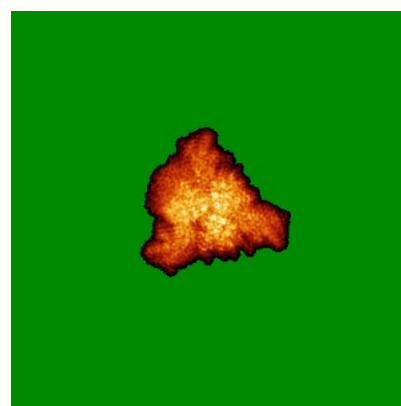
### 6.4.1 Primary map



X



Y

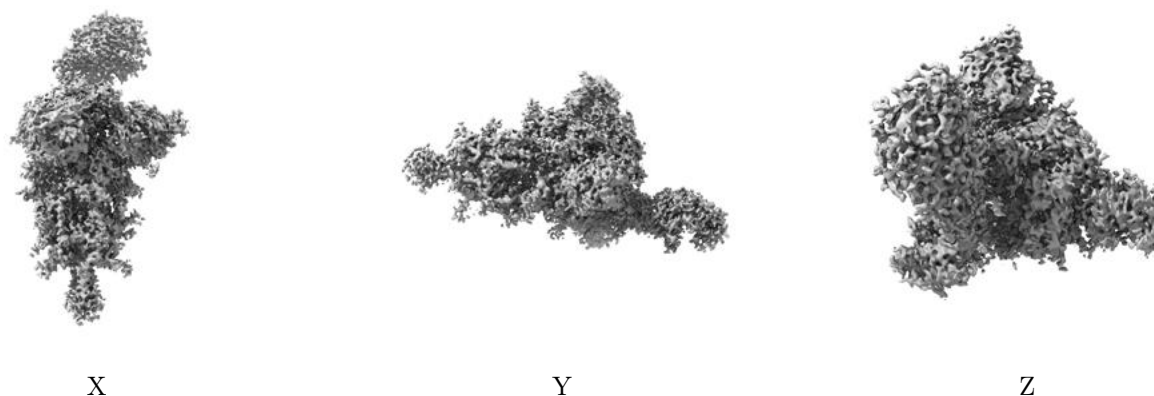


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.767. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

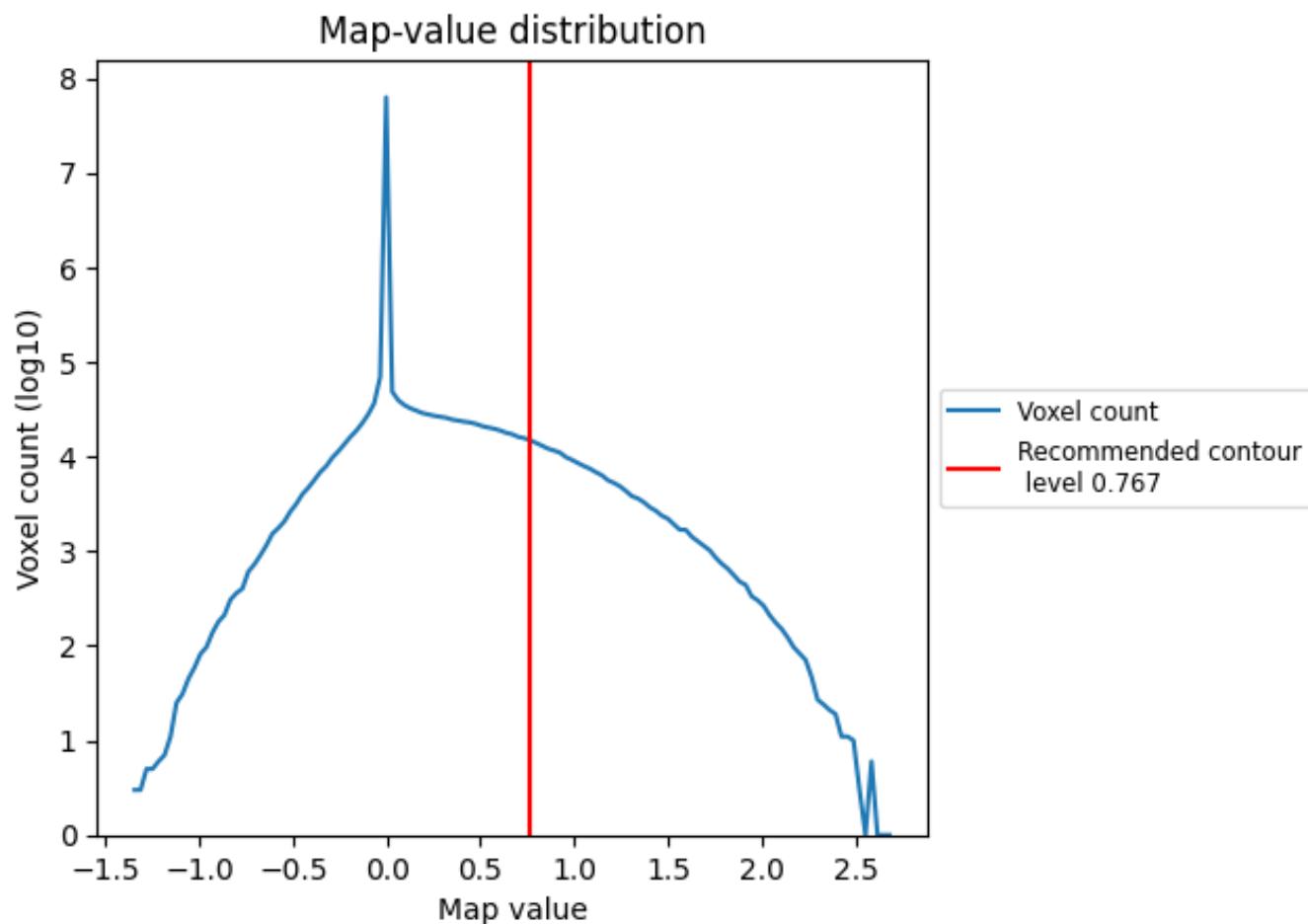
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

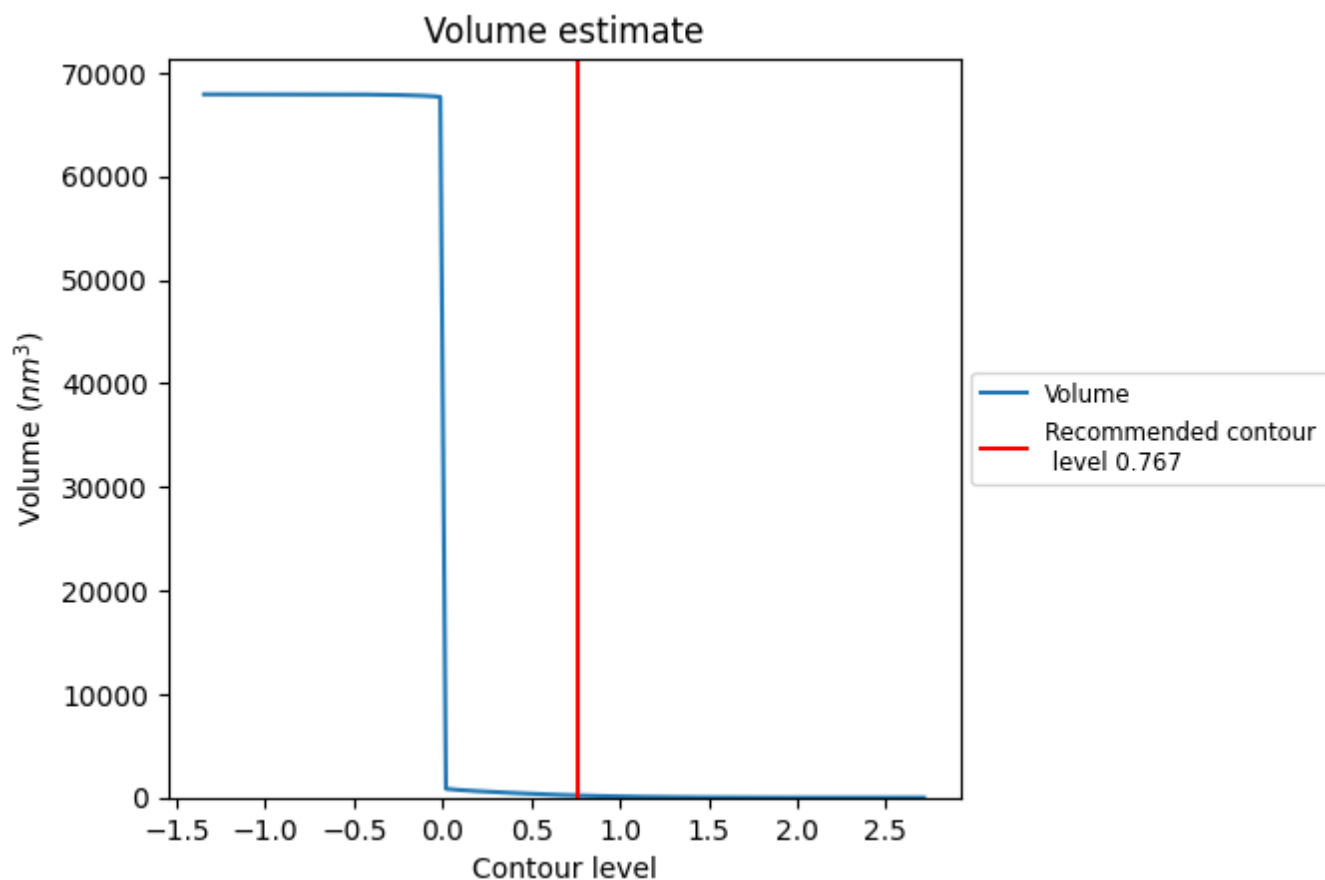
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

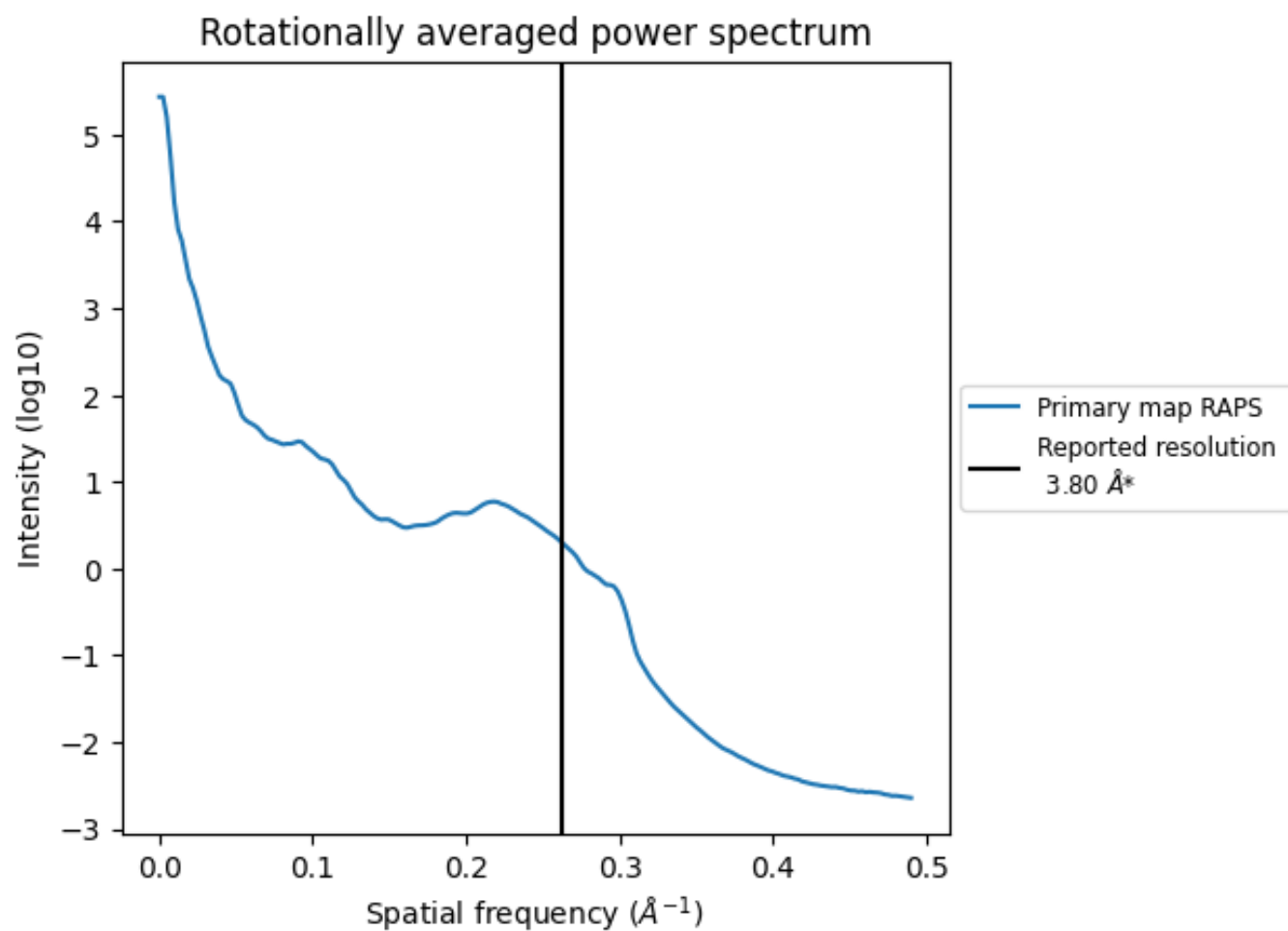
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201  $\text{nm}^3$ ; this corresponds to an approximate mass of 181 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>

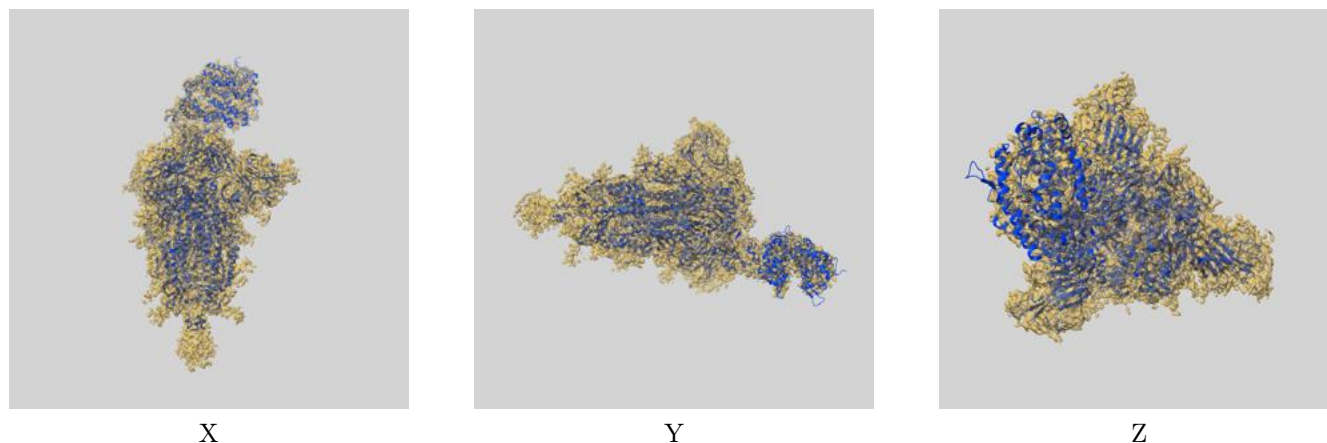
## 8 Fourier-Shell correlation ⓘ

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

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

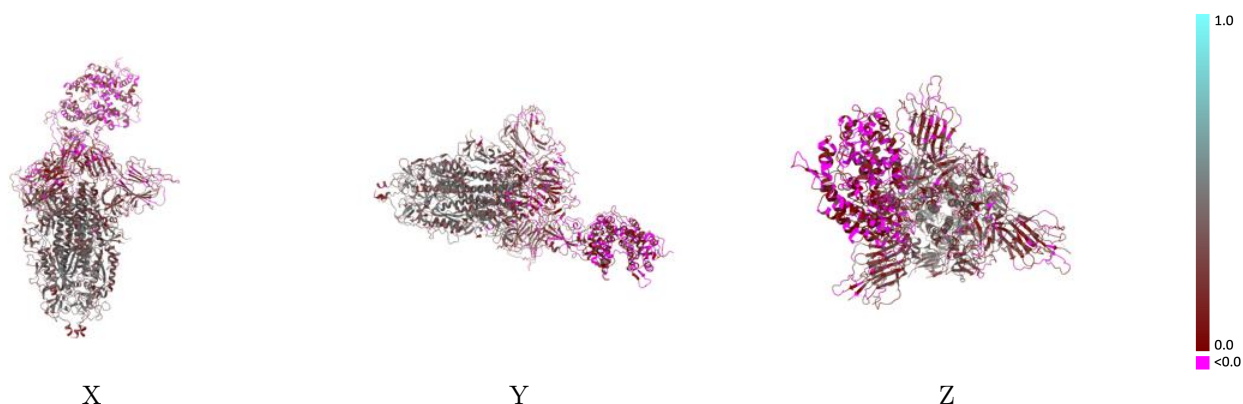
This section contains information regarding the fit between EMDB map EMD-30661 and PDB model 7DF4. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



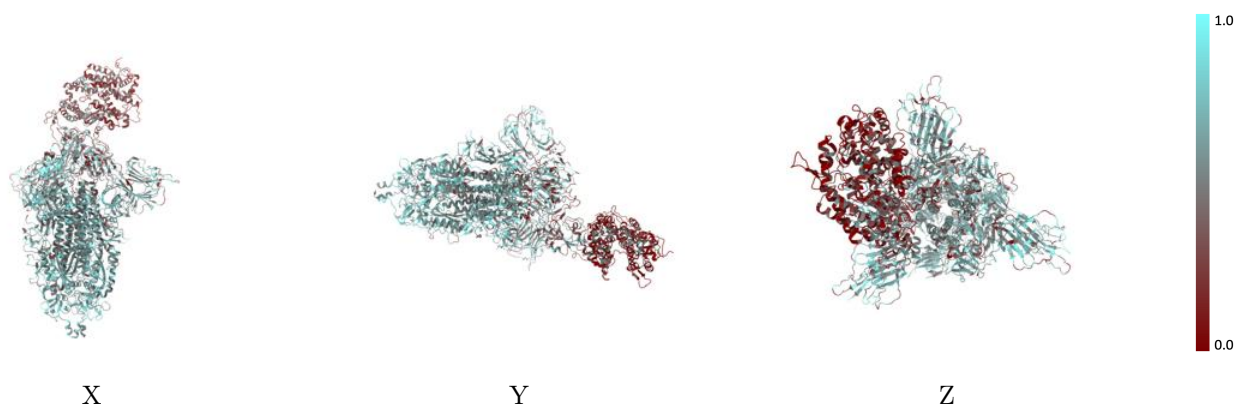
The images above show the 3D surface view of the map at the recommended contour level 0.767 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



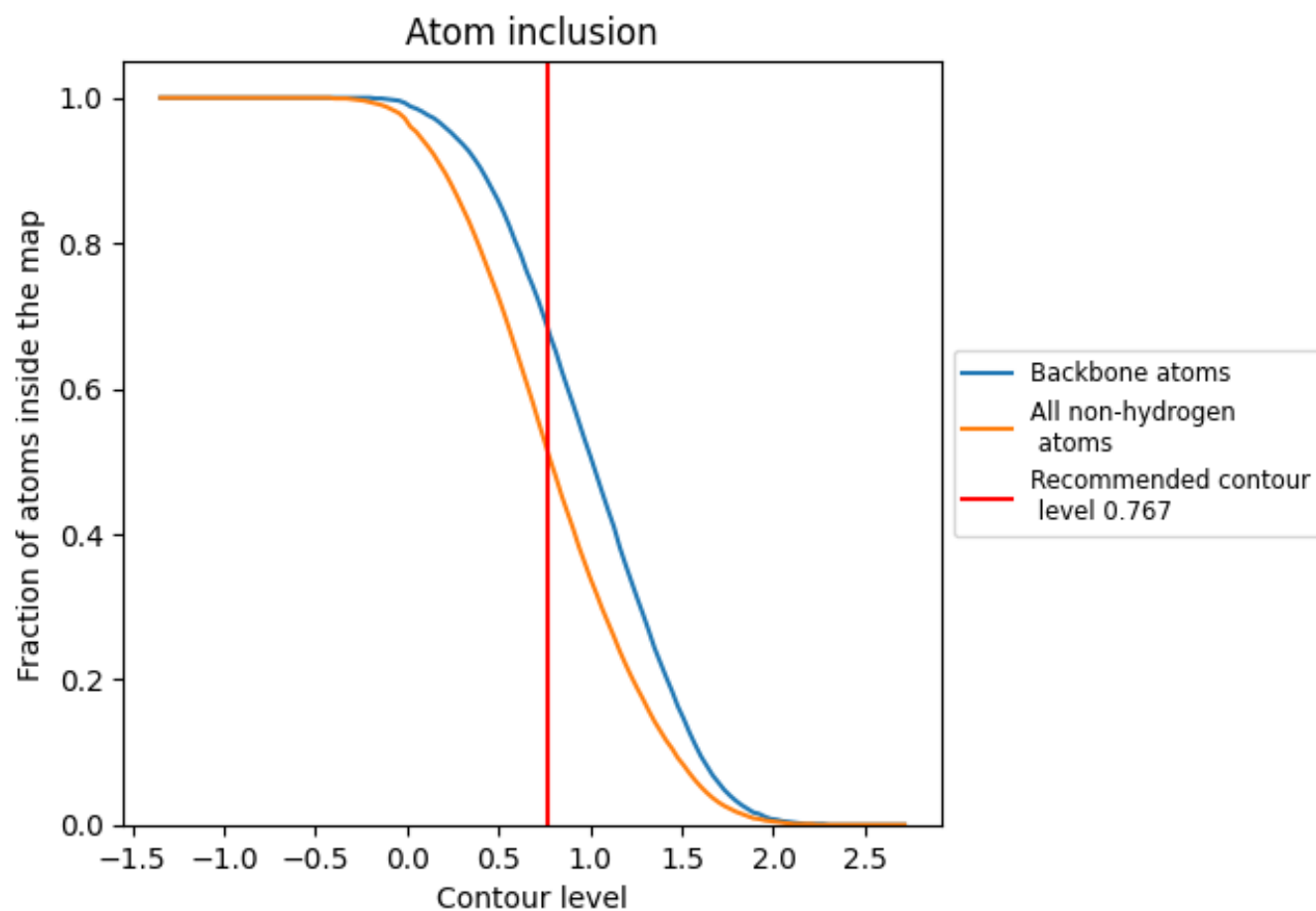
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.767).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 51% 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 (0.767) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5140	 0.2390
A	 0.2090	 0.0470
B	 0.5630	 0.2600
C	 0.5850	 0.2830
D	 0.5660	 0.2790
E	 0.6790	 0.2980
F	 0.7140	 0.2460
G	 0.4640	 0.3550
H	 0.5000	 0.1930
I	 0.7140	 0.4080
J	 0.3210	 0.2620
K	 0.6070	 0.2830
L	 0.6430	 0.3180
M	 0.6070	 0.3100
N	 0.2140	 0.1780
O	 0.7860	 0.3460
P	 0.5710	 0.3990
Q	 0.3570	 0.2170
R	 0.7500	 0.3950
S	 0.5710	 0.2830
T	 0.3570	 0.1940
U	 0.6070	 0.3160
V	 0.5360	 0.3040

