



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:00 PM UTC

PDB ID : 9D8L / pdb\_00009d8l  
EMDB ID : EMD-46641  
Title : KP.2 SARS-COV-2 Spike 2-up conformation  
Authors : Windsor, I.W.; Wu, H.  
Deposited on : 2024-08-19  
Resolution : 3.30 Å (reported)

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

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

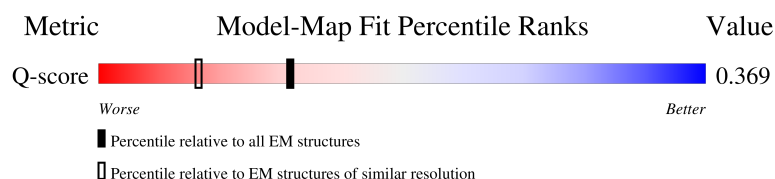
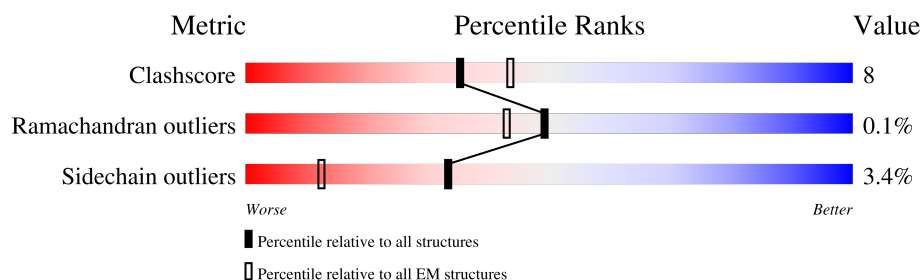
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



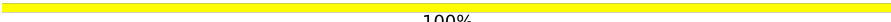
















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 ( 2.80 - 3.80 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1305	 6% 68% 17% • 14%
1	B	1305	 12% 67% 17% • 15%
1	C	1305	 • 65% 19% • 15%
2	D	2	 50% 50%

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

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27659 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	1127	Total	C	N	O	S	23	0
			9034	5782	1495	1716	41		
1	B	1106	Total	C	N	O	S	23	0
			8875	5680	1469	1687	39		
1	C	1105	Total	C	N	O	S	23	0
			8866	5675	1467	1685	39		

There are 369 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0DTC2
A	2	PHE	-	expression tag	UNP P0DTC2
A	3	VAL	-	expression tag	UNP P0DTC2
A	4	PHE	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	VAL	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	LEU	-	expression tag	UNP P0DTC2
A	9	PRO	-	expression tag	UNP P0DTC2
A	10	LEU	-	expression tag	UNP P0DTC2
A	11	VAL	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	SER	-	expression tag	UNP P0DTC2
A	14	GLN	-	expression tag	UNP P0DTC2
A	15	CYS	-	expression tag	UNP P0DTC2
A	16	VAL	-	expression tag	UNP P0DTC2
A	17	MET	-	expression tag	UNP P0DTC2
A	18	PRO	-	expression tag	UNP P0DTC2
A	19	LEU	-	expression tag	UNP P0DTC2
A	20	PHE	-	expression tag	UNP P0DTC2
A	21	ASN	-	expression tag	UNP P0DTC2
A	22	LEU	-	expression tag	UNP P0DTC2
A	23	ILE	-	expression tag	UNP P0DTC2
A	24	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	THR	-	expression tag	UNP P0DTC2
A	26	THR	-	expression tag	UNP P0DTC2
A	27	GLN	-	expression tag	UNP P0DTC2
A	28	SER	-	expression tag	UNP P0DTC2
A	51	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	126	PHE	VAL	conflict	UNP P0DTC2
A	141	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	155	SER	PHE	conflict	UNP P0DTC2
A	156	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	209	ILE	LEU	conflict	UNP P0DTC2
A	210	GLY	VAL	conflict	UNP P0DTC2
A	213	PHE	LEU	conflict	UNP P0DTC2
A	242	ASN	HIS	conflict	UNP P0DTC2
A	261	ASP	ALA	conflict	UNP P0DTC2
A	329	VAL	ILE	conflict	UNP P0DTC2
A	336	HIS	GLY	conflict	UNP P0DTC2
A	343	THR	ARG	conflict	UNP P0DTC2
A	353	THR	LYS	conflict	UNP P0DTC2
A	368	PHE	SER	conflict	UNP P0DTC2
A	370	PRO	SER	conflict	UNP P0DTC2
A	372	PHE	SER	conflict	UNP P0DTC2
A	373	ALA	THR	conflict	UNP P0DTC2
A	400	LYS	ARG	conflict	UNP P0DTC2
A	402	ASN	ASP	conflict	UNP P0DTC2
A	405	SER	ARG	conflict	UNP P0DTC2
A	414	ASN	LYS	conflict	UNP P0DTC2
A	437	LYS	ASN	conflict	UNP P0DTC2
A	442	HIS	VAL	conflict	UNP P0DTC2
A	443	SER	GLY	conflict	UNP P0DTC2
A	447	ASP	ASN	conflict	UNP P0DTC2
A	449	TRP	LEU	conflict	UNP P0DTC2
A	452	SER	LEU	conflict	UNP P0DTC2
A	453	LEU	PHE	conflict	UNP P0DTC2
A	457	LYS	ASN	conflict	UNP P0DTC2
A	474	ASN	SER	conflict	UNP P0DTC2
A	475	LYS	THR	conflict	UNP P0DTC2
A	478	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	480	LYS	GLU	conflict	UNP P0DTC2
A	482	PRO	PHE	conflict	UNP P0DTC2
A	494	ARG	GLN	conflict	UNP P0DTC2
A	497	TYR	ASN	conflict	UNP P0DTC2
A	501	HIS	TYR	conflict	UNP P0DTC2
A	550	LYS	GLU	conflict	UNP P0DTC2
A	566	VAL	ALA	conflict	UNP P0DTC2
A	610	GLY	ASP	conflict	UNP P0DTC2
A	617	SER	PRO	conflict	UNP P0DTC2
A	651	TYR	HIS	conflict	UNP P0DTC2
A	675	LYS	ASN	conflict	UNP P0DTC2
A	677	ARG	PRO	conflict	UNP P0DTC2
A	760	LYS	ASN	conflict	UNP P0DTC2
A	792	TYR	ASP	conflict	UNP P0DTC2
A	935	PHE	SER	conflict	UNP P0DTC2
A	950	HIS	GLN	conflict	UNP P0DTC2
A	965	LYS	ASN	conflict	UNP P0DTC2
A	982	PRO	LYS	conflict	UNP P0DTC2
A	983	PRO	VAL	conflict	UNP P0DTC2
A	1100	LEU	VAL	conflict	UNP P0DTC2
A	1139	LEU	PRO	conflict	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	GLY	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	TRP	-	expression tag	UNP P0DTC2
A	1281	SER	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	PRO	-	expression tag	UNP P0DTC2
A	1284	GLN	-	expression tag	UNP P0DTC2
A	1285	PHE	-	expression tag	UNP P0DTC2
A	1286	GLU	-	expression tag	UNP P0DTC2
A	1287	LYS	-	expression tag	UNP P0DTC2
A	1288	GLY	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1291	GLY	-	expression tag	UNP P0DTC2
A	1292	SER	-	expression tag	UNP P0DTC2
A	1293	GLY	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	GLY	-	expression tag	UNP P0DTC2
A	1296	GLY	-	expression tag	UNP P0DTC2
A	1297	SER	-	expression tag	UNP P0DTC2
A	1298	TRP	-	expression tag	UNP P0DTC2
A	1299	SER	-	expression tag	UNP P0DTC2
A	1300	HIS	-	expression tag	UNP P0DTC2
A	1301	PRO	-	expression tag	UNP P0DTC2
A	1302	GLN	-	expression tag	UNP P0DTC2
A	1303	PHE	-	expression tag	UNP P0DTC2
A	1304	GLU	-	expression tag	UNP P0DTC2
A	1305	LYS	-	expression tag	UNP P0DTC2
B	1	MET	-	initiating methionine	UNP P0DTC2
B	2	PHE	-	expression tag	UNP P0DTC2
B	3	VAL	-	expression tag	UNP P0DTC2
B	4	PHE	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	VAL	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	LEU	-	expression tag	UNP P0DTC2
B	9	PRO	-	expression tag	UNP P0DTC2
B	10	LEU	-	expression tag	UNP P0DTC2
B	11	VAL	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	SER	-	expression tag	UNP P0DTC2
B	14	GLN	-	expression tag	UNP P0DTC2
B	15	CYS	-	expression tag	UNP P0DTC2
B	16	VAL	-	expression tag	UNP P0DTC2
B	17	MET	-	expression tag	UNP P0DTC2
B	18	PRO	-	expression tag	UNP P0DTC2
B	19	LEU	-	expression tag	UNP P0DTC2
B	20	PHE	-	expression tag	UNP P0DTC2
B	21	ASN	-	expression tag	UNP P0DTC2
B	22	LEU	-	expression tag	UNP P0DTC2
B	23	ILE	-	expression tag	UNP P0DTC2
B	24	THR	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	THR	-	expression tag	UNP P0DTC2
B	27	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	28	SER	-	expression tag	UNP P0DTC2
B	51	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	126	PHE	VAL	conflict	UNP P0DTC2
B	141	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	155	SER	PHE	conflict	UNP P0DTC2
B	156	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	ILE	LEU	conflict	UNP P0DTC2
B	210	GLY	VAL	conflict	UNP P0DTC2
B	213	PHE	LEU	conflict	UNP P0DTC2
B	242	ASN	HIS	conflict	UNP P0DTC2
B	261	ASP	ALA	conflict	UNP P0DTC2
B	329	VAL	ILE	conflict	UNP P0DTC2
B	336	HIS	GLY	conflict	UNP P0DTC2
B	343	THR	ARG	conflict	UNP P0DTC2
B	353	THR	LYS	conflict	UNP P0DTC2
B	368	PHE	SER	conflict	UNP P0DTC2
B	370	PRO	SER	conflict	UNP P0DTC2
B	372	PHE	SER	conflict	UNP P0DTC2
B	373	ALA	THR	conflict	UNP P0DTC2
B	400	LYS	ARG	conflict	UNP P0DTC2
B	402	ASN	ASP	conflict	UNP P0DTC2
B	405	SER	ARG	conflict	UNP P0DTC2
B	414	ASN	LYS	conflict	UNP P0DTC2
B	437	LYS	ASN	conflict	UNP P0DTC2
B	442	HIS	VAL	conflict	UNP P0DTC2
B	443	SER	GLY	conflict	UNP P0DTC2
B	447	ASP	ASN	conflict	UNP P0DTC2
B	449	TRP	LEU	conflict	UNP P0DTC2
B	452	SER	LEU	conflict	UNP P0DTC2
B	453	LEU	PHE	conflict	UNP P0DTC2
B	457	LYS	ASN	conflict	UNP P0DTC2
B	474	ASN	SER	conflict	UNP P0DTC2
B	475	LYS	THR	conflict	UNP P0DTC2
B	478	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	480	LYS	GLU	conflict	UNP P0DTC2
B	482	PRO	PHE	conflict	UNP P0DTC2
B	494	ARG	GLN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	497	TYR	ASN	conflict	UNP P0DTC2
B	501	HIS	TYR	conflict	UNP P0DTC2
B	550	LYS	GLU	conflict	UNP P0DTC2
B	566	VAL	ALA	conflict	UNP P0DTC2
B	610	GLY	ASP	conflict	UNP P0DTC2
B	617	SER	PRO	conflict	UNP P0DTC2
B	651	TYR	HIS	conflict	UNP P0DTC2
B	675	LYS	ASN	conflict	UNP P0DTC2
B	677	ARG	PRO	conflict	UNP P0DTC2
B	760	LYS	ASN	conflict	UNP P0DTC2
B	792	TYR	ASP	conflict	UNP P0DTC2
B	935	PHE	SER	conflict	UNP P0DTC2
B	950	HIS	GLN	conflict	UNP P0DTC2
B	965	LYS	ASN	conflict	UNP P0DTC2
B	982	PRO	LYS	conflict	UNP P0DTC2
B	983	PRO	VAL	conflict	UNP P0DTC2
B	1100	LEU	VAL	conflict	UNP P0DTC2
B	1139	LEU	PRO	conflict	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	GLY	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	SER	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	GLY	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	TRP	-	expression tag	UNP P0DTC2
B	1281	SER	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	PRO	-	expression tag	UNP P0DTC2
B	1284	GLN	-	expression tag	UNP P0DTC2
B	1285	PHE	-	expression tag	UNP P0DTC2
B	1286	GLU	-	expression tag	UNP P0DTC2
B	1287	LYS	-	expression tag	UNP P0DTC2
B	1288	GLY	-	expression tag	UNP P0DTC2
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	GLY	-	expression tag	UNP P0DTC2
B	1291	GLY	-	expression tag	UNP P0DTC2
B	1292	SER	-	expression tag	UNP P0DTC2
B	1293	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1294	GLY	-	expression tag	UNP P0DTC2
B	1295	GLY	-	expression tag	UNP P0DTC2
B	1296	GLY	-	expression tag	UNP P0DTC2
B	1297	SER	-	expression tag	UNP P0DTC2
B	1298	TRP	-	expression tag	UNP P0DTC2
B	1299	SER	-	expression tag	UNP P0DTC2
B	1300	HIS	-	expression tag	UNP P0DTC2
B	1301	PRO	-	expression tag	UNP P0DTC2
B	1302	GLN	-	expression tag	UNP P0DTC2
B	1303	PHE	-	expression tag	UNP P0DTC2
B	1304	GLU	-	expression tag	UNP P0DTC2
B	1305	LYS	-	expression tag	UNP P0DTC2
C	1	MET	-	initiating methionine	UNP P0DTC2
C	2	PHE	-	expression tag	UNP P0DTC2
C	3	VAL	-	expression tag	UNP P0DTC2
C	4	PHE	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	VAL	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	LEU	-	expression tag	UNP P0DTC2
C	9	PRO	-	expression tag	UNP P0DTC2
C	10	LEU	-	expression tag	UNP P0DTC2
C	11	VAL	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	SER	-	expression tag	UNP P0DTC2
C	14	GLN	-	expression tag	UNP P0DTC2
C	15	CYS	-	expression tag	UNP P0DTC2
C	16	VAL	-	expression tag	UNP P0DTC2
C	17	MET	-	expression tag	UNP P0DTC2
C	18	PRO	-	expression tag	UNP P0DTC2
C	19	LEU	-	expression tag	UNP P0DTC2
C	20	PHE	-	expression tag	UNP P0DTC2
C	21	ASN	-	expression tag	UNP P0DTC2
C	22	LEU	-	expression tag	UNP P0DTC2
C	23	ILE	-	expression tag	UNP P0DTC2
C	24	THR	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	THR	-	expression tag	UNP P0DTC2
C	27	GLN	-	expression tag	UNP P0DTC2
C	28	SER	-	expression tag	UNP P0DTC2
C	51	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP P0DTC2
C	126	PHE	VAL	conflict	UNP P0DTC2
C	141	ASP	GLY	conflict	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	155	SER	PHE	conflict	UNP P0DTC2
C	156	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	209	ILE	LEU	conflict	UNP P0DTC2
C	210	GLY	VAL	conflict	UNP P0DTC2
C	213	PHE	LEU	conflict	UNP P0DTC2
C	242	ASN	HIS	conflict	UNP P0DTC2
C	261	ASP	ALA	conflict	UNP P0DTC2
C	329	VAL	ILE	conflict	UNP P0DTC2
C	336	HIS	GLY	conflict	UNP P0DTC2
C	343	THR	ARG	conflict	UNP P0DTC2
C	353	THR	LYS	conflict	UNP P0DTC2
C	368	PHE	SER	conflict	UNP P0DTC2
C	370	PRO	SER	conflict	UNP P0DTC2
C	372	PHE	SER	conflict	UNP P0DTC2
C	373	ALA	THR	conflict	UNP P0DTC2
C	400	LYS	ARG	conflict	UNP P0DTC2
C	402	ASN	ASP	conflict	UNP P0DTC2
C	405	SER	ARG	conflict	UNP P0DTC2
C	414	ASN	LYS	conflict	UNP P0DTC2
C	437	LYS	ASN	conflict	UNP P0DTC2
C	442	HIS	VAL	conflict	UNP P0DTC2
C	443	SER	GLY	conflict	UNP P0DTC2
C	447	ASP	ASN	conflict	UNP P0DTC2
C	449	TRP	LEU	conflict	UNP P0DTC2
C	452	SER	LEU	conflict	UNP P0DTC2
C	453	LEU	PHE	conflict	UNP P0DTC2
C	457	LYS	ASN	conflict	UNP P0DTC2
C	474	ASN	SER	conflict	UNP P0DTC2
C	475	LYS	THR	conflict	UNP P0DTC2
C	478	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	480	LYS	GLU	conflict	UNP P0DTC2
C	482	PRO	PHE	conflict	UNP P0DTC2
C	494	ARG	GLN	conflict	UNP P0DTC2
C	497	TYR	ASN	conflict	UNP P0DTC2
C	501	HIS	TYR	conflict	UNP P0DTC2
C	550	LYS	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	566	VAL	ALA	conflict	UNP P0DTC2
C	610	GLY	ASP	conflict	UNP P0DTC2
C	617	SER	PRO	conflict	UNP P0DTC2
C	651	TYR	HIS	conflict	UNP P0DTC2
C	675	LYS	ASN	conflict	UNP P0DTC2
C	677	ARG	PRO	conflict	UNP P0DTC2
C	760	LYS	ASN	conflict	UNP P0DTC2
C	792	TYR	ASP	conflict	UNP P0DTC2
C	935	PHE	SER	conflict	UNP P0DTC2
C	950	HIS	GLN	conflict	UNP P0DTC2
C	965	LYS	ASN	conflict	UNP P0DTC2
C	982	PRO	LYS	conflict	UNP P0DTC2
C	983	PRO	VAL	conflict	UNP P0DTC2
C	1100	LEU	VAL	conflict	UNP P0DTC2
C	1139	LEU	PRO	conflict	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	SER	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	GLY	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	TRP	-	expression tag	UNP P0DTC2
C	1281	SER	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	PRO	-	expression tag	UNP P0DTC2
C	1284	GLN	-	expression tag	UNP P0DTC2
C	1285	PHE	-	expression tag	UNP P0DTC2
C	1286	GLU	-	expression tag	UNP P0DTC2
C	1287	LYS	-	expression tag	UNP P0DTC2
C	1288	GLY	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2
C	1290	GLY	-	expression tag	UNP P0DTC2
C	1291	GLY	-	expression tag	UNP P0DTC2
C	1292	SER	-	expression tag	UNP P0DTC2
C	1293	GLY	-	expression tag	UNP P0DTC2
C	1294	GLY	-	expression tag	UNP P0DTC2
C	1295	GLY	-	expression tag	UNP P0DTC2
C	1296	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1297	SER	-	expression tag	UNP P0DTC2
C	1298	TRP	-	expression tag	UNP P0DTC2
C	1299	SER	-	expression tag	UNP P0DTC2
C	1300	HIS	-	expression tag	UNP P0DTC2
C	1301	PRO	-	expression tag	UNP P0DTC2
C	1302	GLN	-	expression tag	UNP P0DTC2
C	1303	PHE	-	expression tag	UNP P0DTC2
C	1304	GLU	-	expression tag	UNP P0DTC2
C	1305	LYS	-	expression tag	UNP P0DTC2

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



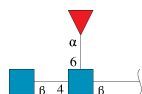
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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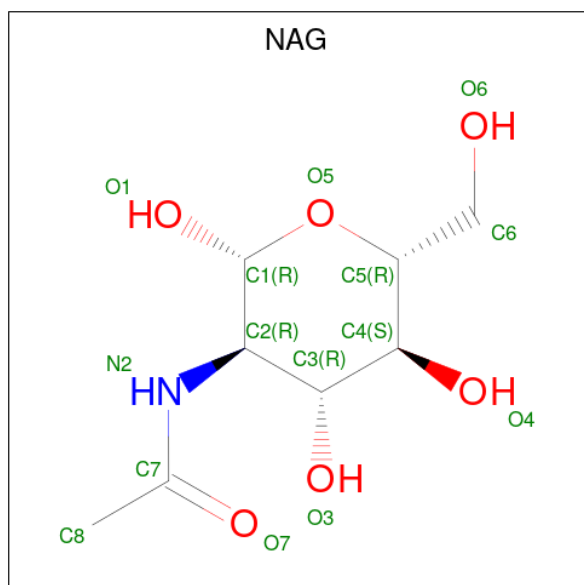
Mol	Chain	Residues	Atoms				AltConf	Trace
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	3	Total	C	N	O	0	0
			38	22	2	14		
3	K	3	Total	C	N	O	0	0
			38	22	2	14		
3	T	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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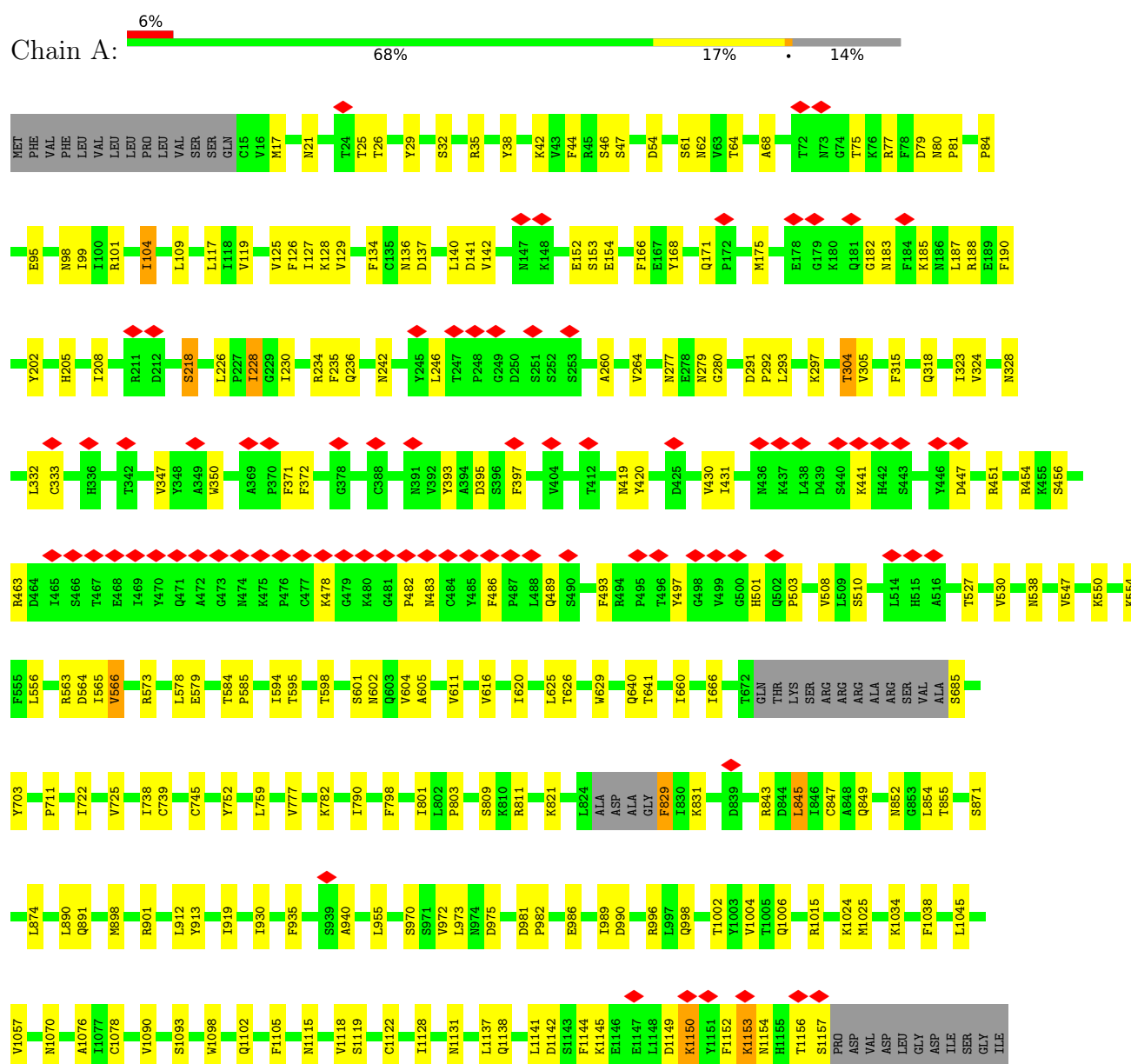
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	



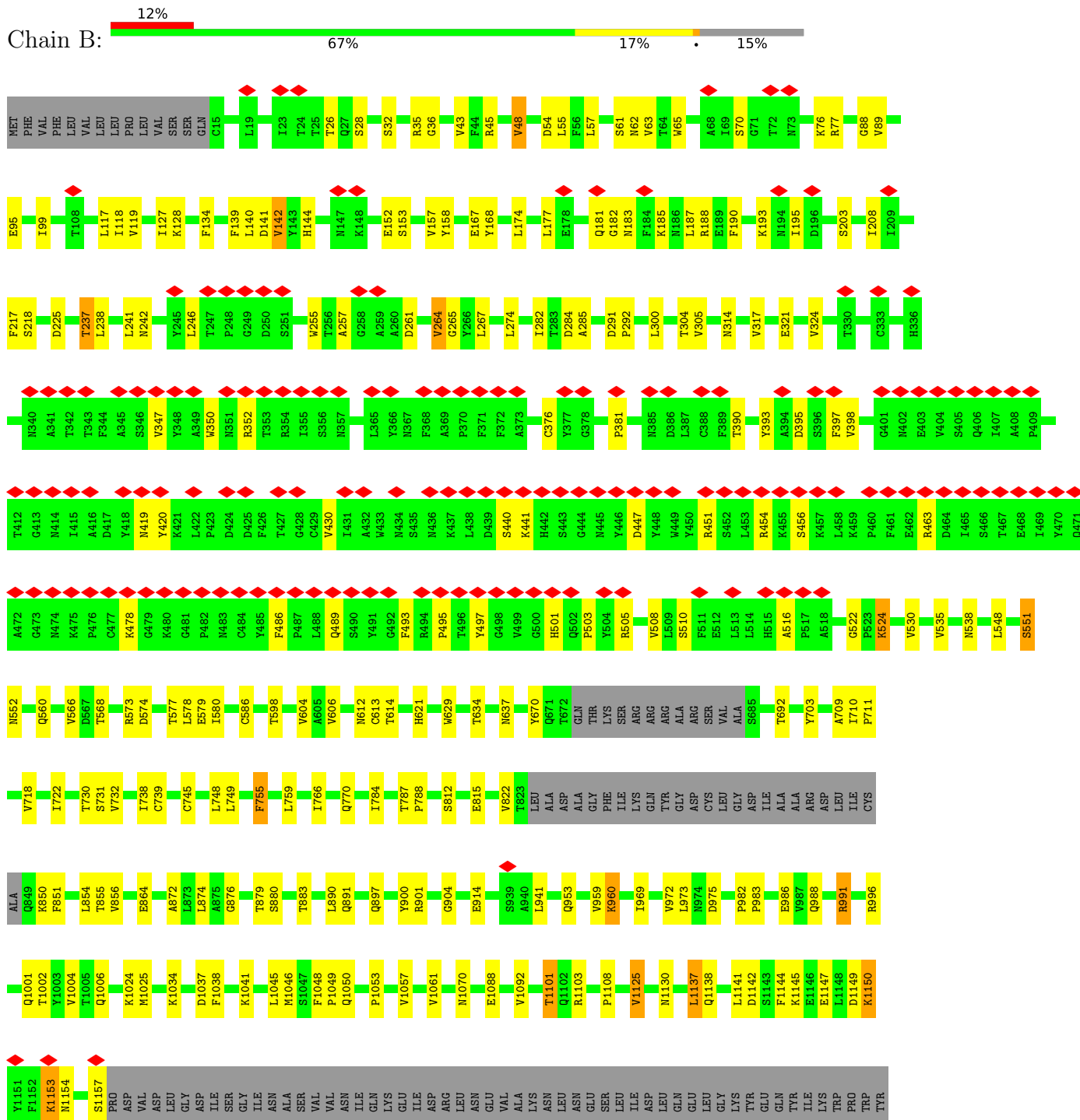
### 3 Residue-property plots

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

#### • Molecule 1: Spike glycoprotein

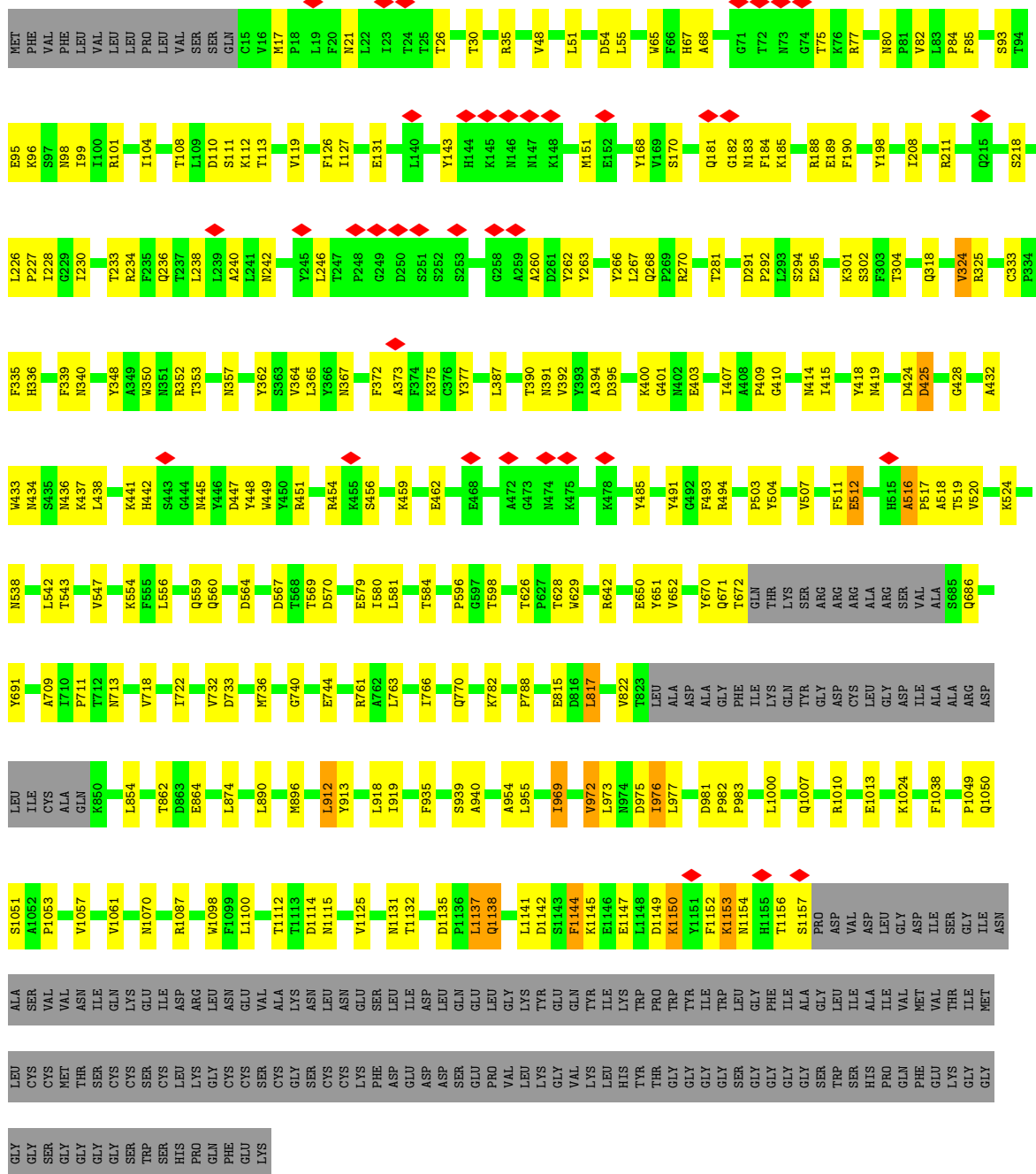


- Molecule 1: Spike glycoprotein



[illegible]

- Molecule 1: Spike glycoprotein



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

Chain D:  50% 50%

MAG1  
MAG2

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

Chain E:  100%

MAG1  
MAG2

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

Chain F:  100%

MAG1  
MAG2

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

Chain G:  100%

MAG1  
MAG2

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

Chain I:  50% 50%

MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

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

Chain L:  50% 50%

MAG1  
MAG2

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

Chain M:  50% 50%



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

Chain N:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain Q:  50% 50%



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

Chain R:  50% 50%



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

Chain S:  100%



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

Chain U:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 67% 33%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  67% 33%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54272	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 ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.540	Depositor
Minimum map value	-0.304	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	263.88, 263.88, 263.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73300004, 0.73300004, 0.73300004	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: FUC, 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	0.14	0/9253	0.28	1/12583 (0.0%)
1	B	0.14	0/9092	0.28	0/12366
1	C	0.14	0/9083	0.29	0/12354
All	All	0.14	0/27428	0.28	1/37303 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	VAL	N-CA-C	-5.05	107.41	111.91

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	9034	0	8798	157	0
1	B	8875	0	8639	141	0
1	C	8866	0	8630	162	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	1	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	0
2	R	28	0	25	2	0
2	S	28	0	25	0	0
2	U	28	0	25	1	0
3	H	38	0	34	0	0
3	K	38	0	34	2	0
3	T	38	0	34	0	0
4	A	112	0	104	4	0
4	B	112	0	104	3	0
4	C	126	0	117	0	0
All	All	27659	0	26869	433	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 8.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ASN:OD1	4:B:1407:NAG:N2	2.17	0.77
1:C:409:PRO:HB3	1:C:424:ASP:HA	1.67	0.76
1:A:182:GLY:H	1:A:185:LYS:HE3	1.51	0.76
1:A:1070:ASN:HD22	1:B:891:GLN:HE22	1.37	0.73
1:B:182:GLY:H	1:B:185:LYS:HE3	1.52	0.73
1:C:188:ARG:HB3	1:C:190:PHE:HE2	1.54	0.73
1:C:744:GLU:OE2	1:C:744:GLU:N	2.16	0.72
1:A:564:ASP:OD1	1:A:565:ILE:N	2.23	0.71
1:B:1130:ASN:OD1	3:K:1:NAG:N2	2.24	0.70
1:B:972:VAL:HG12	1:B:975:ASP:H	1.57	0.70
1:B:393:TYR:HB2	1:B:510:SER:HB2	1.74	0.69
1:A:68:ALA:HB3	1:A:260:ALA:HB3	1.74	0.69
1:A:242:ASN:HB2	1:A:246:LEU:HD11	1.75	0.69
1:A:393:TYR:HB2	1:A:510:SER:HB2	1.75	0.69
1:C:1049:PRO:O	1:C:1050:GLN:NE2	2.25	0.69
1:A:573:ARG:HD3	1:A:578:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HB	1:A:168:TYR:HB3	1.76	0.67
1:C:390:THR:OG1	1:C:512:GLU:OE1	2.12	0.67
1:B:242:ASN:HB2	1:B:246:LEU:HD11	1.77	0.66
1:C:516:ALA:HB1	1:C:560:GLN:HB2	1.77	0.66
1:A:898:MET:HE1	1:A:1045:LEU:HD13	1.76	0.66
1:C:242:ASN:HB2	1:C:246:LEU:HD11	1.77	0.65
1:C:373:ALA:HB3	1:C:432:ALA:HB3	1.77	0.65
1:C:407:ILE:O	1:C:407:ILE:HG13	1.96	0.65
1:A:84:PRO:HA	1:A:234:ARG:HD3	1.79	0.64
3:K:1:NAG:H4	3:K:3:FUC:H5	1.78	0.64
1:B:35:ARG:NH2	1:B:218:SER:OG	2.30	0.64
1:C:442:HIS:O	1:C:494:ARG:NH1	2.31	0.64
1:C:722:ILE:HG13	1:C:1057:VAL:HG22	1.80	0.64
1:B:185:LYS:HE2	1:B:208:ILE:H	1.63	0.64
1:B:904:GLY:O	1:B:1034:LYS:NZ	2.30	0.64
1:A:188:ARG:HG2	1:A:190:PHE:HE1	1.63	0.63
1:C:918:LEU:HD11	2:R:1:NAG:H3	1.80	0.63
1:B:314:ASN:ND2	1:C:733:ASP:OD2	2.32	0.63
1:B:1024:LYS:NZ	1:B:1038:PHE:O	2.27	0.63
1:C:864:GLU:OE1	1:C:864:GLU:N	2.32	0.63
1:C:912:LEU:HD12	1:C:919:ILE:HD12	1.81	0.63
1:C:969:ILE:HG12	1:C:976:ILE:HD11	1.81	0.62
1:B:193:LYS:HE2	1:B:195:ILE:HD11	1.82	0.62
1:C:182:GLY:H	1:C:185:LYS:HE3	1.63	0.62
1:B:321:GLU:H	1:B:535:VAL:HG12	1.64	0.62
1:C:372:PHE:HB3	1:C:433:TRP:HA	1.82	0.62
1:C:542:LEU:HD21	1:C:569:THR:HG21	1.82	0.62
1:C:425:ASP:OD1	1:C:425:ASP:N	2.33	0.62
1:B:28:SER:HB2	1:B:65:TRP:HB3	1.82	0.62
1:A:127:ILE:HG21	1:A:226:LEU:HD21	1.82	0.61
1:B:1049:PRO:O	1:B:1050:GLN:NE2	2.25	0.61
1:B:317:VAL:HG23	1:B:586:CYS:HB3	1.82	0.61
1:A:972:VAL:HG12	1:A:975:ASP:H	1.66	0.61
1:B:759:LEU:HG	1:B:1004:VAL:HG21	1.83	0.61
1:B:612:ASN:HB2	4:B:1403:NAG:N2	2.16	0.60
1:A:318:GLN:NE2	1:A:626:THR:OG1	2.29	0.60
1:A:1015:ARG:NH2	1:C:1013:GLU:OE2	2.34	0.60
1:B:612:ASN:OD1	1:B:614:THR:N	2.33	0.60
1:C:766:ILE:HG23	1:C:770:GLN:HE21	1.67	0.60
1:A:77:ARG:NE	1:A:79:ASP:OD2	2.33	0.60
1:A:821:LYS:HE3	1:A:935:PHE:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ARG:NH2	1:C:218:SER:OG	2.35	0.60
1:C:68:ALA:HB3	1:C:260:ALA:HB3	1.84	0.60
1:C:324:VAL:HG12	1:C:538:ASN:HB3	1.83	0.60
1:B:419:ASN:ND2	1:B:451:ARG:O	2.36	0.59
1:B:738:ILE:O	1:B:996:ARG:NH1	2.36	0.59
1:C:419:ASN:ND2	1:C:451:ARG:O	2.28	0.59
1:C:441:LYS:N	1:C:445:ASN:OD1	2.33	0.59
1:B:522:GLY:O	1:B:524:LYS:NZ	2.32	0.59
1:B:1088:GLU:HA	1:B:1103:ARG:HH21	1.68	0.59
1:C:713:ASN:OD1	2:R:1:NAG:N2	2.36	0.59
1:A:35:ARG:NH2	1:A:218:SER:OG	2.36	0.58
1:A:1024:LYS:NZ	1:A:1038:PHE:O	2.29	0.58
1:C:434:ASN:ND2	1:C:436:ASN:OD1	2.36	0.58
1:C:127:ILE:HB	1:C:168:TYR:HB3	1.84	0.58
1:C:1098:TRP:HB2	1:C:1131:ASN:ND2	2.18	0.58
1:A:1102:GLN:HE21	1:A:1105:PHE:HB3	1.69	0.58
1:C:352:ARG:H	2:U:1:NAG:H82	1.69	0.58
1:C:1007:GLN:OE1	1:C:1010:ARG:NH1	2.37	0.58
1:C:556:LEU:N	1:C:559:GLN:OE1	2.35	0.57
1:A:486:PHE:O	1:A:489:GLN:NE2	2.37	0.57
1:C:1112:THR:HG22	1:C:1114:ASP:H	1.68	0.57
1:A:419:ASN:ND2	1:A:451:ARG:O	2.37	0.57
1:A:759:LEU:HG	1:A:1004:VAL:HG21	1.87	0.57
1:A:843:ARG:NH2	1:C:570:ASP:OD1	2.37	0.57
1:C:732:VAL:HG22	1:C:763:LEU:HD12	1.87	0.57
1:A:26:THR:OG1	1:A:77:ARG:NH2	2.38	0.57
1:A:1098:TRP:HB2	1:A:1131:ASN:ND2	2.19	0.56
1:A:782:LYS:H	1:A:782:LYS:HZ3	1.52	0.56
1:C:104:ILE:HG23	1:C:238:LEU:HD21	1.87	0.56
1:B:1037:ASP:OD2	1:B:1041:LYS:NZ	2.31	0.56
1:C:650:GLU:OE1	1:C:651:TYR:N	2.38	0.56
1:A:119:VAL:HG22	1:A:140:LEU:HD11	1.87	0.56
1:A:891:GLN:HE22	1:C:1070:ASN:HD22	1.54	0.56
1:C:336:HIS:O	1:C:340:ASN:N	2.33	0.56
1:C:1098:TRP:HB2	1:C:1131:ASN:HD22	1.70	0.56
1:A:594:ILE:HG23	1:A:660:ILE:HG21	1.88	0.55
1:B:486:PHE:O	1:B:489:GLN:NE2	2.39	0.55
1:A:556:LEU:O	1:A:573:ARG:NH2	2.39	0.55
1:B:127:ILE:O	1:B:168:TYR:N	2.39	0.55
1:C:98:ASN:O	1:C:101:ARG:NE	2.38	0.55
1:B:291:ASP:OD1	1:B:291:ASP:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:THR:HA	1:B:598:THR:HG21	1.87	0.55
1:C:119:VAL:HB	1:C:126:PHE:HB2	1.87	0.55
1:A:42:LYS:HE2	1:C:517:PRO:HG3	1.89	0.55
1:C:433:TRP:HZ3	1:C:507:VAL:HG12	1.70	0.55
1:B:324:VAL:HG22	1:B:538:ASN:HB3	1.88	0.55
1:C:822:VAL:HB	1:C:1053:PRO:HG2	1.89	0.54
1:A:128:LYS:NZ	1:A:154:GLU:OE1	2.34	0.54
1:A:347:VAL:HG22	1:A:419:ASN:HB3	1.89	0.54
1:B:953:GLN:HE22	1:C:761:ARG:NH1	2.05	0.54
1:C:579:GLU:OE2	1:C:580:ILE:N	2.41	0.54
1:B:732:VAL:HG22	1:B:854:LEU:HD23	1.90	0.54
1:C:414:ASN:O	1:C:418:TYR:HB2	2.08	0.54
1:B:32:SER:N	1:B:61:SER:O	2.38	0.54
1:A:998:GLN:HB3	1:B:755:PHE:HZ	1.73	0.54
1:C:226:LEU:HG	1:C:228:ILE:HG12	1.90	0.53
1:B:63:VAL:HG22	1:B:265:GLY:HA2	1.90	0.53
1:B:1125:VAL:HG13	1:C:913:TYR:HB3	1.90	0.53
1:A:563:ARG:HD2	1:B:43:VAL:HG11	1.91	0.53
1:B:551:SER:OG	1:B:552:ASN:N	2.40	0.53
1:A:441:LYS:NZ	1:A:447:ASP:OD2	2.38	0.53
1:A:566:VAL:HG21	1:B:959:VAL:HG13	1.91	0.53
1:C:415:ILE:HD12	1:C:419:ASN:HB2	1.91	0.53
1:B:183:ASN:H	1:B:208:ILE:HG13	1.72	0.53
1:B:347:VAL:HG22	1:B:419:ASN:HB3	1.90	0.53
1:A:291:ASP:OD1	1:A:291:ASP:N	2.40	0.53
1:C:493:PHE:CG	1:C:503:PRO:HG3	2.44	0.53
1:C:722:ILE:HD13	1:C:940:ALA:HB1	1.90	0.53
1:C:454:ARG:NH1	1:C:456:SER:O	2.40	0.52
1:C:295:GLU:OE1	1:C:629:TRP:NE1	2.41	0.52
1:A:722:ILE:HD12	1:A:940:ALA:HB1	1.92	0.52
1:A:973:LEU:HD22	1:A:989:ILE:HD13	1.91	0.52
1:B:441:LYS:NZ	1:B:447:ASP:OD2	2.41	0.52
1:A:564:ASP:OD1	1:A:565:ILE:HG22	2.10	0.52
1:A:890:LEU:HD13	1:C:711:PRO:HD3	1.92	0.52
1:A:752:TYR:OH	1:A:990:ASP:OD1	2.18	0.52
1:A:982:PRO:O	1:A:986:GLU:HG2	2.09	0.52
1:C:671:GLN:NE2	1:C:672:THR:O	2.43	0.52
1:A:482:PRO:O	1:A:483:ASN:ND2	2.43	0.51
1:C:291:ASP:N	1:C:291:ASP:OD1	2.43	0.51
1:A:843:ARG:NH1	1:C:564:ASP:OD2	2.43	0.51
1:A:350:TRP:O	1:A:463:ARG:NH1	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:THR:HG22	1:A:604:VAL:HG12	1.92	0.51
1:A:315:PHE:HZ	1:A:611:VAL:HG11	1.76	0.51
1:A:803:PRO:HG3	1:A:871:SER:HB2	1.93	0.51
1:B:188:ARG:HB3	1:B:190:PHE:CE1	2.46	0.51
1:C:84:PRO:O	1:C:266:TYR:OH	2.19	0.51
1:C:168:TYR:CE1	1:C:170:SER:HB2	2.45	0.51
1:A:849:GLN:HE22	1:A:955:LEU:HB3	1.75	0.51
1:B:274:LEU:HD22	1:B:282:ILE:HD13	1.92	0.51
1:C:348:TYR:HE2	1:C:449:TRP:HB2	1.75	0.51
1:A:166:PHE:HE1	1:A:168:TYR:HB2	1.74	0.51
1:C:718:VAL:HG22	1:C:1061:VAL:HG22	1.93	0.51
1:B:139:PHE:CE2	1:B:241:LEU:HB2	2.46	0.50
1:B:141:ASP:O	1:B:153:SER:N	2.42	0.50
1:C:448:TYR:HB2	1:C:491:TYR:CD2	2.46	0.50
1:C:390:THR:OG1	1:C:391:ASN:OD1	2.29	0.50
1:A:1119:SER:OG	1:B:914:GLU:OE2	2.28	0.50
1:B:1101:THR:HG22	1:B:1108:PRO:HA	1.93	0.50
1:C:35:ARG:NE	1:C:189:GLU:OE1	2.41	0.50
1:C:709:ALA:HA	1:C:1070:ASN:HA	1.93	0.50
1:A:901:ARG:HD2	1:A:1045:LEU:O	2.11	0.50
1:C:391:ASN:OD1	1:C:391:ASN:N	2.44	0.50
1:B:722:ILE:HG12	1:B:1057:VAL:HG22	1.94	0.50
1:B:982:PRO:O	1:B:986:GLU:HG2	2.12	0.50
1:C:101:ARG:HG3	1:C:240:ALA:HB2	1.93	0.50
1:C:972:VAL:HG13	1:C:975:ASP:HB3	1.93	0.50
1:A:80:ASN:OD1	1:A:80:ASN:N	2.44	0.50
1:A:117:LEU:HD21	1:A:119:VAL:HG23	1.94	0.49
1:B:142:VAL:HB	1:B:152:GLU:HG3	1.94	0.49
1:B:241:LEU:HD23	1:B:257:ALA:HB2	1.94	0.49
1:B:292:PRO:HB2	1:B:604:VAL:HG21	1.94	0.49
1:A:912:LEU:HD12	1:A:919:ILE:HD13	1.94	0.49
1:B:347:VAL:HA	1:B:397:PHE:HB2	1.94	0.49
1:C:181:GLN:HB2	1:C:185:LYS:HD2	1.95	0.49
1:C:392:VAL:HG23	1:C:520:VAL:HG21	1.95	0.49
1:C:80:ASN:N	1:C:80:ASN:OD1	2.45	0.49
1:B:89:VAL:HG13	1:B:264:VAL:HG23	1.93	0.49
1:C:143:TYR:CZ	1:C:151:MET:HE1	2.48	0.49
1:C:390:THR:HA	1:C:518:ALA:HA	1.94	0.49
1:B:1002:THR:O	1:B:1006:GLN:HG2	2.13	0.49
1:B:117:LEU:HD21	1:B:134:PHE:HE1	1.79	0.48
1:A:95:GLU:OE1	1:A:99:ILE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:MET:SD	1:A:205:HIS:NE2	2.85	0.48
1:B:703:TYR:HD2	1:C:788:PRO:HG3	1.78	0.48
1:B:710:ILE:HD12	1:B:1092:VAL:HG11	1.95	0.48
1:A:722:ILE:HG12	1:A:1057:VAL:HG22	1.95	0.48
1:B:63:VAL:HG13	1:B:264:VAL:C	2.39	0.48
1:A:1115:ASN:OD1	1:A:1115:ASN:N	2.46	0.48
1:C:333:CYS:HB2	1:C:335:PHE:CE1	2.48	0.48
1:A:554:LYS:NZ	2:M:1:NAG:H5	2.28	0.48
1:A:1153[A]:LYS:HB3	1:A:1153[A]:LYS:HE3	1.62	0.48
1:C:437:LYS:HG3	1:C:438:LEU:HD22	1.95	0.48
1:C:815:GLU:HG2	1:C:1051:SER:H	1.78	0.48
1:A:109:LEU:HA	1:A:134:PHE:HE2	1.78	0.48
1:A:279:ASN:OD1	1:C:554:LYS:HE2	2.14	0.48
1:A:566:VAL:HG23	1:B:960:LYS:HG2	1.95	0.48
1:C:95:GLU:OE1	1:C:99:ILE:N	2.47	0.48
1:B:26:THR:OG1	1:B:77:ARG:NH2	2.46	0.48
1:B:969:ILE:HD11	1:B:988:GLN:HE21	1.78	0.48
1:C:1153[A]:LYS:HB3	1:C:1153[A]:LYS:HE3	1.59	0.48
1:A:166:PHE:CE1	1:A:168:TYR:HB2	2.48	0.48
1:A:420:TYR:HE2	1:A:508:VAL:HG21	1.80	0.47
1:A:1150[A]:LYS:HE3	1:A:1150[A]:LYS:HB3	1.72	0.47
1:C:111:SER:HA	1:C:131:GLU:HB3	1.96	0.47
1:C:362:TYR:HD2	1:C:365:LEU:HD11	1.78	0.47
1:A:1102:GLN:NE2	1:A:1105:PHE:HB3	2.28	0.47
1:B:70:SER:HB3	1:B:76:LYS:HG2	1.95	0.47
1:C:672:THR:HA	1:C:686:GLN:HA	1.96	0.47
1:C:1131:ASN:OD1	1:C:1132:THR:N	2.47	0.47
1:A:136:ASN:OD1	1:A:137:ASP:N	2.47	0.47
1:C:400:LYS:HB3	1:C:403:GLU:HB2	1.95	0.47
1:C:1135[A]:ASP:HB3	1:C:1138[A]:GLN:HB2	1.95	0.47
1:A:17:MET:SD	1:A:17:MET:N	2.88	0.47
1:B:552:ASN:N	1:B:552:ASN:OD1	2.46	0.47
1:B:812:SER:OG	1:B:815:GLU:OE1	2.30	0.47
1:C:302:SER:OG	1:C:304:THR:O	2.33	0.47
1:A:304:THR:HA	1:A:598:THR:HG21	1.96	0.47
1:B:284:ASP:OD1	1:B:285:ALA:N	2.46	0.47
1:B:350:TRP:O	1:B:463:ARG:NH1	2.38	0.47
1:A:566:VAL:HG22	1:A:566:VAL:O	2.14	0.47
1:B:988:GLN:OE1	1:B:991:ARG:NH2	2.41	0.47
1:A:38:TYR:OH	1:A:54:ASP:OD2	2.29	0.47
1:A:419:ASN:OD1	1:A:451:ARG:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LEU:HD12	1:B:187:LEU:H	1.80	0.47
1:B:237:THR:OG1	1:B:238:LEU:N	2.47	0.47
1:A:68:ALA:O	1:A:260:ALA:N	2.48	0.47
1:A:126:PHE:HE2	4:A:1406:NAG:HN2	1.62	0.47
1:B:430:VAL:HG12	1:B:508:VAL:HG22	1.97	0.47
1:B:897:GLN:O	1:B:900:TYR:HB2	2.15	0.47
1:C:93:SER:HA	1:C:262:TYR:HA	1.96	0.47
1:B:300:LEU:HD12	1:B:305:VAL:HG12	1.97	0.46
1:B:577:THR:HG23	1:B:579:GLU:HB2	1.96	0.46
1:B:497:TYR:HB3	1:B:501:HIS:HB3	1.96	0.46
1:A:25:THR:HG21	1:A:81:PRO:HG2	1.97	0.46
1:A:852:ASN:O	1:A:854:LEU:HG	2.14	0.46
1:B:95:GLU:OE1	1:B:99:ILE:N	2.48	0.46
1:B:983:PRO:HG3	1:C:410:GLY:HA3	1.96	0.46
1:C:82:VAL:HB	1:C:234:ARG:HD2	1.96	0.46
1:A:739:CYS:HB3	1:A:745:CYS:HB3	1.66	0.46
1:B:390:THR:HG21	1:B:516:ALA:HB3	1.96	0.46
1:C:441:LYS:NZ	1:C:447:ASP:OD2	2.47	0.46
1:C:350:TRP:NE1	1:C:395:ASP:OD2	2.46	0.46
1:A:821:LYS:HB2	1:A:821:LYS:HE2	1.72	0.46
1:B:1025:MET:HE2	1:B:1025:MET:HB2	1.83	0.46
1:A:1153[B]:LYS:HA	1:A:1153[B]:LYS:HD3	1.70	0.46
1:B:63:VAL:HG13	1:B:264:VAL:O	2.15	0.46
1:A:185:LYS:HA	1:A:208:ILE:HG12	1.97	0.46
1:B:901:ARG:HD2	1:B:1045:LEU:O	2.16	0.46
1:A:497:TYR:HB3	1:A:501:HIS:HB3	1.97	0.45
1:A:616:VAL:O	1:A:620:ILE:HG12	2.16	0.45
1:B:730:THR:HG22	1:B:856:VAL:HG22	1.97	0.45
1:B:784:ILE:HG23	1:B:872:ALA:HB2	1.98	0.45
1:A:125:VAL:HB	1:A:171:GLN:HB2	1.98	0.45
1:B:65:TRP:HE1	1:B:261:ASP:HB3	1.81	0.45
1:B:766:ILE:O	1:B:770:GLN:HG2	2.16	0.45
1:C:401:GLY:HA2	1:C:504:TYR:CD1	2.51	0.45
1:C:547:VAL:HG12	1:C:584:THR:HB	1.99	0.45
1:A:703:TYR:HB2	1:B:879:THR:HB	1.98	0.45
1:B:876:GLY:O	1:B:880:SER:OG	2.29	0.45
1:A:190:PHE:HA	1:A:202:TYR:O	2.17	0.45
1:B:1153[B]:LYS:HA	1:B:1153[B]:LYS:HD3	1.69	0.45
1:C:339:PHE:HE2	1:C:507:VAL:HG21	1.80	0.45
1:A:854:LEU:HD13	1:A:955:LEU:HD22	1.98	0.45
1:A:843:ARG:HD2	1:A:847:CYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:VAL:HG23	1:B:568:THR:HG23	1.99	0.45
1:C:108:THR:OG1	1:C:110:ASP:OD1	2.28	0.45
1:C:198:TYR:CE1	1:C:227:PRO:HB3	2.52	0.45
1:A:47:SER:N	1:A:277:ASN:O	2.37	0.45
1:A:640:GLN:NE2	1:A:641:THR:O	2.50	0.45
1:B:88:GLY:HA3	1:B:267:LEU:HB2	1.99	0.45
1:C:17:MET:SD	1:C:17:MET:N	2.90	0.45
1:B:157:VAL:HB	1:B:158:TYR:HD1	1.82	0.45
1:B:350:TRP:CD1	1:B:350:TRP:H	2.34	0.45
1:B:709:ALA:HA	1:B:1070:ASN:HA	1.99	0.45
1:C:228:ILE:HG22	1:C:230:ILE:HG23	1.99	0.45
1:C:1153[B]:LYS:HA	1:C:1153[B]:LYS:HD3	1.69	0.45
1:A:703:TYR:HD2	1:B:788:PRO:HG2	1.82	0.44
1:A:1078:CYS:HB2	1:A:1122:CYS:HB3	1.66	0.44
1:A:1152[B]:PHE:O	1:A:1156[B]:THR:OG1	2.27	0.44
1:B:181:GLN:HB2	1:B:185:LYS:HD2	1.98	0.44
1:B:718:VAL:HG22	1:B:1061:VAL:HG22	1.99	0.44
1:B:634:THR:H	1:B:637:ASN:HB2	1.82	0.44
1:A:21:ASN:HD22	1:A:75:THR:HG22	1.81	0.44
1:A:454:ARG:NH1	1:A:456:SER:O	2.45	0.44
1:A:913:TYR:HB3	1:C:1125:VAL:HG13	1.98	0.44
1:B:45:ARG:HD2	1:B:48:VAL:HG11	1.99	0.44
1:B:478:LYS:HB2	1:B:478:LYS:HE2	1.77	0.44
1:C:1150[A]:LYS:HE3	1:C:1150[A]:LYS:HB3	1.73	0.44
1:A:25:THR:HG23	1:A:79:ASP:HB3	2.00	0.44
1:B:217:PHE:CD2	1:B:284:ASP:HA	2.53	0.44
1:B:395:ASP:OD2	1:B:420:TYR:OH	2.27	0.44
1:B:493:PHE:CD2	1:B:503:PRO:HB3	2.52	0.44
1:C:353:THR:HG23	1:C:394:ALA:HB3	2.00	0.44
1:A:80:ASN:HB2	1:A:236:GLN:NE2	2.32	0.44
1:A:711:PRO:HD3	1:B:890:LEU:HD13	2.00	0.44
1:A:930:ILE:HD12	1:A:930:ILE:HA	1.82	0.44
1:A:228:ILE:HB	1:A:230:ILE:HG23	2.00	0.44
1:C:336:HIS:HA	1:C:339:PHE:HB2	2.00	0.44
1:A:641:THR:HG23	1:A:666:ILE:HG13	2.00	0.44
1:C:981:ASP:OD1	1:C:981:ASP:N	2.50	0.44
1:A:104:ILE:HD11	1:A:134:PHE:CE2	2.52	0.44
1:C:112:LYS:HG3	1:C:113:THR:HG23	1.99	0.44
1:C:1024:LYS:NZ	1:C:1038:PHE:O	2.39	0.44
1:B:560:GLN:HA	1:B:560:GLN:OE1	2.17	0.44
1:A:323:ILE:HA	1:A:527:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ASN:OD1	1:B:451:ARG:N	2.43	0.43
1:B:1150[A]:LYS:HB3	1:B:1150[A]:LYS:HE3	1.72	0.43
1:A:324:VAL:HG22	1:A:538:ASN:HB3	2.00	0.43
1:B:119:VAL:HG13	1:B:140:LEU:HD11	2.00	0.43
1:B:880:SER:O	1:B:883:THR:OG1	2.31	0.43
1:A:44:PHE:HE1	1:A:280:GLY:HA2	1.82	0.43
1:B:739:CYS:HB3	1:B:745:CYS:HB3	1.67	0.43
1:C:85:PHE:N	1:C:233:THR:O	2.50	0.43
1:C:736:MET:HA	1:C:740:GLY:HA2	2.00	0.43
1:A:1002:THR:O	1:A:1006:GLN:HG2	2.18	0.43
1:B:573:ARG:NH1	1:B:578:LEU:O	2.51	0.43
1:B:711:PRO:HD3	1:C:890:LEU:HD13	2.01	0.43
1:C:65:TRP:CD1	1:C:263:TYR:HE1	2.36	0.43
1:C:292:PRO:HG3	1:C:629:TRP:CE3	2.54	0.43
1:C:982:PRO:N	1:C:983:PRO:HD2	2.33	0.43
1:A:62:ASN:HB3	4:A:1405:NAG:N2	2.33	0.43
1:A:1093:SER:HB3	1:A:1098:TRP:CD2	2.54	0.43
1:B:822:VAL:HB	1:B:1053:PRO:HG2	1.99	0.43
1:C:67:HIS:HB2	1:C:77:ARG:CZ	2.48	0.43
1:C:516:ALA:HB3	1:C:517:PRO:HD3	2.01	0.43
1:B:255:TRP:H	1:B:255:TRP:CD1	2.36	0.43
1:B:292:PRO:HG3	1:B:629:TRP:CE3	2.53	0.43
1:B:440:SER:HB3	1:B:495:PRO:HD3	2.00	0.43
1:C:51:LEU:HB3	1:C:301:LYS:HZ1	1.84	0.43
1:C:596:PRO:HB3	1:C:670:TYR:HB2	1.99	0.43
1:B:629:TRP:O	1:B:629:TRP:HE3	2.02	0.43
1:B:738:ILE:HG22	1:B:739:CYS:SG	2.59	0.43
1:A:347:VAL:HA	1:A:397:PHE:HB2	2.01	0.43
1:A:831:LYS:HA	1:C:642:ARG:HH21	1.84	0.43
1:C:763:LEU:HD23	1:C:766:ILE:HD12	2.00	0.43
1:A:142:VAL:HB	1:A:152:GLU:HG3	2.01	0.43
1:A:430:VAL:HG12	1:A:508:VAL:HG22	1.99	0.43
1:A:725:VAL:HG21	1:A:777:VAL:HG11	2.00	0.43
1:B:398:VAL:HG22	1:B:505:ARG:HG2	2.01	0.43
1:B:1145[B]:LYS:HA	1:B:1145[B]:LYS:HD3	1.77	0.43
1:C:55:LEU:HB3	1:C:267:LEU:HD23	2.00	0.43
4:A:1404:NAG:H83	1:C:459:LYS:HD3	2.01	0.42
1:A:1025:MET:HE2	1:A:1025:MET:HB2	1.92	0.42
1:B:731:SER:HB3	1:B:855:THR:HG23	2.01	0.42
1:C:183:ASN:O	1:C:208:ILE:HD13	2.19	0.42
1:C:375:LYS:HB3	1:C:375:LYS:HE3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:954:ALA:HB2	1:C:1010:ARG:HH22	1.84	0.42
1:A:395:ASP:OD2	1:A:420:TYR:OH	2.31	0.42
1:A:738:ILE:O	1:A:996:ARG:NH1	2.48	0.42
1:C:1152[B]:PHE:O	1:C:1156[B]:THR:OG1	2.34	0.42
1:A:32:SER:N	1:A:61:SER:O	2.51	0.42
1:A:129:VAL:HG21	1:A:228:ILE:HG21	2.01	0.42
1:A:478:LYS:HB2	1:A:478:LYS:HE2	1.76	0.42
1:B:941:LEU:HD12	1:B:941:LEU:HA	1.86	0.42
1:C:26:THR:HG1	1:C:77:ARG:HH22	1.65	0.42
1:C:226:LEU:HD12	1:C:227:PRO:HD2	2.02	0.42
1:C:763:LEU:HD23	1:C:763:LEU:HA	1.82	0.42
1:A:183:ASN:H	1:A:208:ILE:HG13	1.84	0.42
1:C:1087:ARG:NH1	1:C:1114:ASP:O	2.53	0.42
1:C:524:LYS:HB2	1:C:524:LYS:HE2	1.72	0.42
1:C:80:ASN:HB2	1:C:236:GLN:HE21	1.85	0.42
1:A:104:ILE:HG23	1:A:236:GLN:HB3	2.02	0.42
1:B:376:CYS:HB2	1:B:381:PRO:HG3	2.02	0.42
1:B:606:VAL:HG11	1:B:629:TRP:CZ3	2.55	0.42
1:C:183:ASN:ND2	1:C:211:ARG:O	2.53	0.42
1:C:304:THR:HA	1:C:598:THR:HG21	2.02	0.42
1:A:790:ILE:HD12	2:Q:1:NAG:H82	2.01	0.42
1:B:850:LYS:HA	1:B:854:LEU:O	2.20	0.42
1:C:291:ASP:OD1	1:C:294:SER:OG	2.30	0.42
1:C:364:VAL:HA	1:C:367:ASN:ND2	2.35	0.42
1:C:377:TYR:HE2	1:C:409:PRO:HD3	1.85	0.42
1:A:849:GLN:NE2	1:A:955:LEU:HB3	2.34	0.41
1:B:36:GLY:HA3	1:B:57:LEU:HD23	2.02	0.41
1:B:352:ARG:H	4:B:1408:NAG:H82	1.84	0.41
1:C:348:TYR:CE2	1:C:449:TRP:HB2	2.54	0.41
1:C:977:LEU:HD23	1:C:977:LEU:HA	1.84	0.41
1:A:80:ASN:N	1:A:81:PRO:HD3	2.36	0.41
1:A:685:SER:O	1:A:685:SER:OG	2.32	0.41
1:B:612:ASN:OD1	1:B:613:CYS:N	2.53	0.41
1:A:547:VAL:HG12	1:A:584:THR:HB	2.01	0.41
1:C:318:GLN:NE2	1:C:626:THR:OG1	2.44	0.41
1:C:375:LYS:HD2	1:C:377:TYR:HE1	1.86	0.41
1:A:332:LEU:HD12	1:A:333:CYS:O	2.20	0.41
1:A:550:LYS:NZ	1:A:579:GLU:OE2	2.46	0.41
1:B:118:ILE:HG13	1:B:127:ILE:HG12	2.01	0.41
1:B:1046:MET:HE2	1:B:1048:PHE:CE1	2.56	0.41
1:A:1034:LYS:HE2	1:A:1034:LYS:HB2	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ASP:OD2	1:B:577:THR:HG22	2.21	0.41
1:C:183:ASN:C	1:C:185:LYS:H	2.29	0.41
1:C:1100:LEU:HD23	1:C:1115:ASN:ND2	2.36	0.41
1:A:166:PHE:C	1:A:166:PHE:CD1	2.98	0.41
1:A:372:PHE:O	1:C:485:TYR:OH	2.33	0.41
1:A:955:LEU:HA	1:A:955:LEU:HD23	1.82	0.41
1:B:174:LEU:HB2	1:B:177:LEU:HD11	2.03	0.41
1:C:324:VAL:O	1:C:325:ARG:HD2	2.21	0.41
1:A:98:ASN:HB2	1:A:101:ARG:NH2	2.35	0.41
1:A:845:LEU:O	1:A:849:GLN:HG3	2.19	0.41
1:C:854:LEU:HD13	1:C:955:LEU:HD22	2.03	0.41
1:C:896:MET:HE2	1:C:896:MET:HB3	1.73	0.41
1:A:585:PRO:HG2	1:B:851:PHE:CG	2.56	0.41
1:A:601:SER:OG	1:A:602:ASN:N	2.53	0.41
1:C:428:GLY:HA2	1:C:511:PHE:CE1	2.55	0.41
1:A:29:TYR:CD2	4:A:1405:NAG:H61	2.55	0.41
1:A:493:PHE:CD2	1:A:503:PRO:HB3	2.56	0.41
1:B:1137[A]:LEU:HD21	1:C:1137[A]:LEU:HG	2.03	0.41
1:C:96:LYS:HB3	1:C:184:PHE:CD1	2.56	0.41
1:C:1145[B]:LYS:HD3	1:C:1145[B]:LYS:HA	1.79	0.41
1:A:1145[B]:LYS:HD3	1:A:1145[B]:LYS:HA	1.81	0.41
1:B:1145[B]:LYS:HE3	1:C:1144[B]:PHE:CE2	2.55	0.41
1:C:21:ASN:HD22	1:C:75:THR:HG22	1.85	0.41
1:C:652:VAL:HG22	1:C:691:TYR:HB3	2.03	0.41
1:A:185:LYS:HE2	1:A:208:ILE:H	1.85	0.40
1:A:738:ILE:HA	1:A:996:ARG:HD3	2.02	0.40
1:A:809:SER:OG	1:A:811:ARG:NH1	2.54	0.40
1:A:1076:ALA:HB3	1:A:1128:ILE:HD12	2.02	0.40
1:B:183:ASN:C	1:B:185:LYS:H	2.29	0.40
1:B:670:TYR:HD1	1:B:670:TYR:HA	1.79	0.40
1:C:357:ASN:H	1:C:519:THR:HG23	1.87	0.40
1:A:166:PHE:C	1:A:166:PHE:HD1	2.29	0.40
1:A:293:LEU:HG	1:A:297:LYS:HE3	2.03	0.40
1:A:371:PHE:CG	1:A:431:ILE:HD11	2.56	0.40
1:C:766:ILE:HG23	1:C:770:GLN:NE2	2.35	0.40
1:A:141:ASP:O	1:A:153:SER:N	2.49	0.40
1:A:798:PHE:HD1	1:A:801:ILE:HD11	1.86	0.40
1:A:829:PHE:HD1	1:A:829:PHE:HA	1.70	0.40
1:A:845:LEU:HD13	1:A:845:LEU:HA	1.96	0.40
1:C:817:LEU:HB3	1:C:935:PHE:CZ	2.57	0.40
1:A:292:PRO:HG3	1:A:629:TRP:CE3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ILE:HB	1:A:605:ALA:HB3	2.04	0.40
1:B:128:LYS:HB3	1:B:167:GLU:HG2	2.02	0.40
1:B:864:GLU:H	1:B:864:GLU:HG3	1.67	0.40
1:C:459:LYS:HG2	1:C:462:GLU:OE1	2.22	0.40
1:B:54:ASP:OD1	1:B:55:LEU:N	2.55	0.40
1:B:454:ARG:NH1	1:B:456:SER:O	2.47	0.40
1:C:268:GLN:OE1	1:C:270:ARG:NE	2.55	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	1143/1305 (88%)	1089 (95%)	53 (5%)	1 (0%)	48 75
1	B	1122/1305 (86%)	1069 (95%)	52 (5%)	1 (0%)	48 75
1	C	1121/1305 (86%)	1076 (96%)	43 (4%)	2 (0%)	43 71
All	All	3386/3915 (86%)	3234 (96%)	148 (4%)	4 (0%)	49 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	VAL
1	B	530	VAL
1	C	516	ALA
1	C	939	SER

### 5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1008/1130 (89%)	968 (96%)	40 (4%)	28	56
1	B	992/1130 (88%)	946 (95%)	46 (5%)	24	53
1	C	991/1130 (88%)	947 (96%)	44 (4%)	25	54
All	All	2991/3390 (88%)	2861 (96%)	130 (4%)	33	54

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	64	THR
1	A	104	ILE
1	A	187	LEU
1	A	218	SER
1	A	228	ILE
1	A	235	PHE
1	A	264	VAL
1	A	304	THR
1	A	305	VAL
1	A	328	ASN
1	A	625	LEU
1	A	829	PHE
1	A	845	LEU
1	A	855	THR
1	A	874	LEU
1	A	970	SER
1	A	981	ASP
1	A	1090	VAL
1	A	1118	VAL
1	A	1137[A]	LEU
1	A	1137[B]	LEU
1	A	1138[A]	GLN
1	A	1138[B]	GLN
1	A	1141[A]	LEU
1	A	1141[B]	LEU
1	A	1142[A]	ASP
1	A	1142[B]	ASP
1	A	1144[A]	PHE
1	A	1144[B]	PHE

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Mol	Chain	Res	Type
1	A	1149[A]	ASP
1	A	1149[B]	ASP
1	A	1150[A]	LYS
1	A	1150[B]	LYS
1	A	1153[A]	LYS
1	A	1153[B]	LYS
1	A	1154[A]	ASN
1	A	1154[B]	ASN
1	A	1157[A]	SER
1	A	1157[B]	SER
1	B	48	VAL
1	B	142	VAL
1	B	144	HIS
1	B	203	SER
1	B	225	ASP
1	B	237	THR
1	B	264	VAL
1	B	524	LYS
1	B	548	LEU
1	B	551	SER
1	B	580	ILE
1	B	621	HIS
1	B	692	THR
1	B	748	LEU
1	B	749	LEU
1	B	755	PHE
1	B	787	THR
1	B	874	LEU
1	B	960	LYS
1	B	973	LEU
1	B	991	ARG
1	B	1001	GLN
1	B	1101	THR
1	B	1125	VAL
1	B	1137[A]	LEU
1	B	1137[B]	LEU
1	B	1138[A]	GLN
1	B	1138[B]	GLN
1	B	1141[A]	LEU
1	B	1141[B]	LEU
1	B	1142[A]	ASP
1	B	1142[B]	ASP

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Mol	Chain	Res	Type
1	B	1144[A]	PHE
1	B	1144[B]	PHE
1	B	1147[A]	GLU
1	B	1147[B]	GLU
1	B	1149[A]	ASP
1	B	1149[B]	ASP
1	B	1150[A]	LYS
1	B	1150[B]	LYS
1	B	1153[A]	LYS
1	B	1153[B]	LYS
1	B	1154[A]	ASN
1	B	1154[B]	ASN
1	B	1157[A]	SER
1	B	1157[B]	SER
1	C	30	THR
1	C	48	VAL
1	C	54	ASP
1	C	281	THR
1	C	324	VAL
1	C	387	LEU
1	C	425	ASP
1	C	512	GLU
1	C	543	THR
1	C	567	ASP
1	C	581	LEU
1	C	628	THR
1	C	782	LYS
1	C	817	LEU
1	C	862	THR
1	C	874	LEU
1	C	912	LEU
1	C	969	ILE
1	C	972	VAL
1	C	973	LEU
1	C	976	ILE
1	C	1000	LEU
1	C	1137[A]	LEU
1	C	1137[B]	LEU
1	C	1138[A]	GLN
1	C	1138[B]	GLN
1	C	1141[A]	LEU
1	C	1141[B]	LEU

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Mol	Chain	Res	Type
1	C	1142[A]	ASP
1	C	1142[B]	ASP
1	C	1144[A]	PHE
1	C	1144[B]	PHE
1	C	1147[A]	GLU
1	C	1147[B]	GLU
1	C	1149[A]	ASP
1	C	1149[B]	ASP
1	C	1150[A]	LYS
1	C	1150[B]	LYS
1	C	1153[A]	LYS
1	C	1153[B]	LYS
1	C	1154[A]	ASN
1	C	1154[B]	ASN
1	C	1157[A]	SER
1	C	1157[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	186	ASN
1	A	331	ASN
1	A	414	ASN
1	A	489	GLN
1	A	560	GLN
1	A	603	GLN
1	A	751	GLN
1	A	783	GLN
1	A	849	GLN
1	A	897	GLN
1	A	903	ASN
1	A	1007	GLN
1	A	1131	ASN
1	B	489	GLN
1	B	783	GLN
1	B	800	GLN
1	B	951	ASN
1	B	1007	GLN
1	B	1102	GLN
1	B	1131	ASN
1	C	31	ASN

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Mol	Chain	Res	Type
1	C	98	ASN
1	C	124	ASN
1	C	133	GLN
1	C	205	HIS
1	C	331	ASN
1	C	483	ASN
1	C	489	GLN
1	C	532	ASN
1	C	540	ASN
1	C	671	GLN
1	C	686	GLN
1	C	758	GLN
1	C	945	GLN
1	C	951	ASN
1	C	1006	GLN
1	C	1102	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 ⓘ

39 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	D	1	1,2	14,14,15	0.74	0	17,19,21	1.90	6 (35%)
2	NAG	D	2	2	14,14,15	0.77	0	17,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	E	1	1,2	14,14,15	0.77	0	17,19,21	2.28	5 (29%)
2	NAG	E	2	2	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.78	0	17,19,21	0.87	0
2	NAG	F	2	2	14,14,15	0.72	0	17,19,21	0.79	0
2	NAG	G	1	1,2	14,14,15	0.74	0	17,19,21	0.84	0
2	NAG	G	2	2	14,14,15	0.70	0	17,19,21	0.76	0
3	NAG	H	1	1,3	14,14,15	0.66	0	17,19,21	1.14	1 (5%)
3	NAG	H	2	3	14,14,15	0.77	0	17,19,21	0.76	0
3	FUC	H	3	3	10,10,11	0.80	0	14,14,16	0.89	0
2	NAG	I	1	1,2	14,14,15	0.69	0	17,19,21	0.99	1 (5%)
2	NAG	I	2	2	14,14,15	0.72	0	17,19,21	0.84	0
2	NAG	J	1	1,2	14,14,15	0.75	0	17,19,21	0.85	0
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.79	0
3	NAG	K	1	1,3	14,14,15	0.98	1 (7%)	17,19,21	1.98	6 (35%)
3	NAG	K	2	3	14,14,15	0.64	0	17,19,21	0.93	1 (5%)
3	FUC	K	3	3	10,10,11	0.73	0	14,14,16	1.02	0
2	NAG	L	1	1,2	14,14,15	0.72	0	17,19,21	0.84	1 (5%)
2	NAG	L	2	2	14,14,15	0.72	0	17,19,21	0.81	0
2	NAG	M	1	1,2	14,14,15	0.76	0	17,19,21	1.06	2 (11%)
2	NAG	M	2	2	14,14,15	0.71	0	17,19,21	0.77	0
2	NAG	N	1	1,2	14,14,15	0.82	0	17,19,21	1.29	2 (11%)
2	NAG	N	2	2	14,14,15	0.78	0	17,19,21	0.88	0
2	NAG	O	1	1,2	14,14,15	0.79	0	17,19,21	1.05	1 (5%)
2	NAG	O	2	2	14,14,15	0.73	0	17,19,21	0.84	0
2	NAG	P	1	1,2	14,14,15	0.74	0	17,19,21	0.84	0
2	NAG	P	2	2	14,14,15	0.74	0	17,19,21	0.87	0
2	NAG	Q	1	1,2	14,14,15	0.68	0	17,19,21	1.25	2 (11%)
2	NAG	Q	2	2	14,14,15	0.73	0	17,19,21	0.85	0
2	NAG	R	1	1,2	14,14,15	0.74	0	17,19,21	1.18	2 (11%)
2	NAG	R	2	2	14,14,15	0.67	0	17,19,21	0.93	1 (5%)
2	NAG	S	1	1,2	14,14,15	0.68	0	17,19,21	1.37	3 (17%)
2	NAG	S	2	2	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
3	NAG	T	1	1,3	14,14,15	0.82	0	17,19,21	1.21	1 (5%)
3	NAG	T	2	3	14,14,15	0.71	0	17,19,21	0.81	0
3	FUC	T	3	3	10,10,11	0.78	0	14,14,16	0.88	0
2	NAG	U	1	1,2	14,14,15	0.69	0	17,19,21	0.84	0
2	NAG	U	2	2	14,14,15	0.71	0	17,19,21	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	NAG	C1-C2	3.10	1.56	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O5-C1-C2	-5.38	102.96	111.29
3	K	1	NAG	C1-O5-C5	4.59	118.33	112.19
2	E	1	NAG	C2-N2-C7	4.31	128.67	122.90
2	E	1	NAG	C4-C3-C2	-3.93	105.25	111.02
2	S	1	NAG	C1-O5-C5	-3.76	107.15	112.19
2	D	1	NAG	O5-C1-C2	-3.55	105.81	111.29
3	T	1	NAG	C1-O5-C5	3.45	116.81	112.19
2	Q	1	NAG	C2-N2-C7	3.42	127.48	122.90
2	D	1	NAG	C4-C3-C2	3.34	115.92	111.02
2	D	1	NAG	C1-O5-C5	-3.16	107.96	112.19
2	I	1	NAG	O5-C1-C2	-3.15	106.41	111.29
2	O	1	NAG	O5-C1-C2	-3.15	106.41	111.29
2	D	1	NAG	C3-C4-C5	2.96	115.60	110.23
3	K	1	NAG	C4-C3-C2	-2.93	106.73	111.02
2	N	1	NAG	C2-N2-C7	2.92	126.82	122.90
3	H	1	NAG	C2-N2-C7	2.90	126.78	122.90
3	K	1	NAG	C1-C2-N2	2.86	114.94	110.43
2	E	1	NAG	C1-C2-N2	2.84	114.92	110.43
2	M	1	NAG	O5-C1-C2	-2.80	106.96	111.29
3	K	1	NAG	C3-C4-C5	-2.79	105.17	110.23
2	N	1	NAG	O5-C5-C4	-2.69	104.29	110.83
2	E	2	NAG	C1-O5-C5	2.67	115.77	112.19
3	K	1	NAG	O4-C4-C5	2.51	115.50	109.32
3	K	1	NAG	O5-C1-C2	-2.44	107.52	111.29
2	R	1	NAG	C1-O5-C5	2.42	115.43	112.19
2	D	1	NAG	C1-C2-N2	2.39	114.20	110.43
2	M	1	NAG	O4-C4-C3	-2.35	104.83	110.38
3	K	2	NAG	O5-C1-C2	-2.35	107.66	111.29
2	S	2	NAG	C1-O5-C5	2.32	115.29	112.19
2	L	1	NAG	O5-C1-C2	-2.27	107.78	111.29
2	S	1	NAG	O5-C1-C2	-2.17	107.93	111.29
2	R	1	NAG	O5-C1-C2	-2.15	107.96	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	1	NAG	O4-C4-C3	-2.13	105.36	110.38
2	R	2	NAG	O5-C1-C2	-2.11	108.03	111.29
2	Q	1	NAG	O5-C1-C2	-2.11	108.03	111.29
2	E	1	NAG	O3-C3-C4	2.10	115.32	110.38
2	D	1	NAG	O4-C4-C3	-2.08	105.46	110.38

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	P	2	NAG	C8-C7-N2-C2
2	P	2	NAG	O7-C7-N2-C2
2	U	2	NAG	C8-C7-N2-C2
2	U	2	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	N	1	NAG	C1-C2-N2-C7
2	Q	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	Q	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C1-C2-N2-C7
3	K	2	NAG	C1-C2-N2-C7
2	N	1	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 7 short contacts:

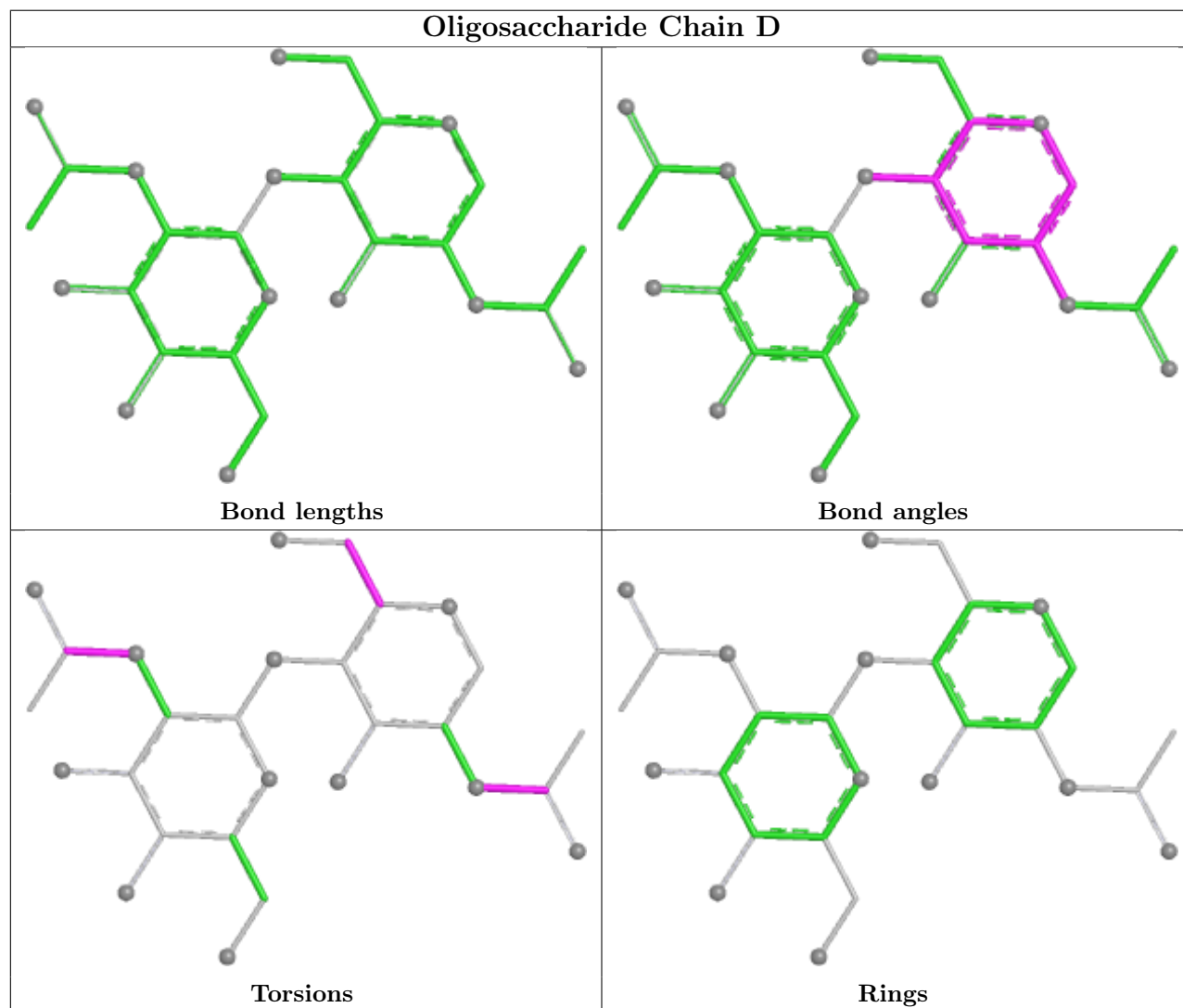
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	3	FUC	1	0
2	M	1	NAG	1	0

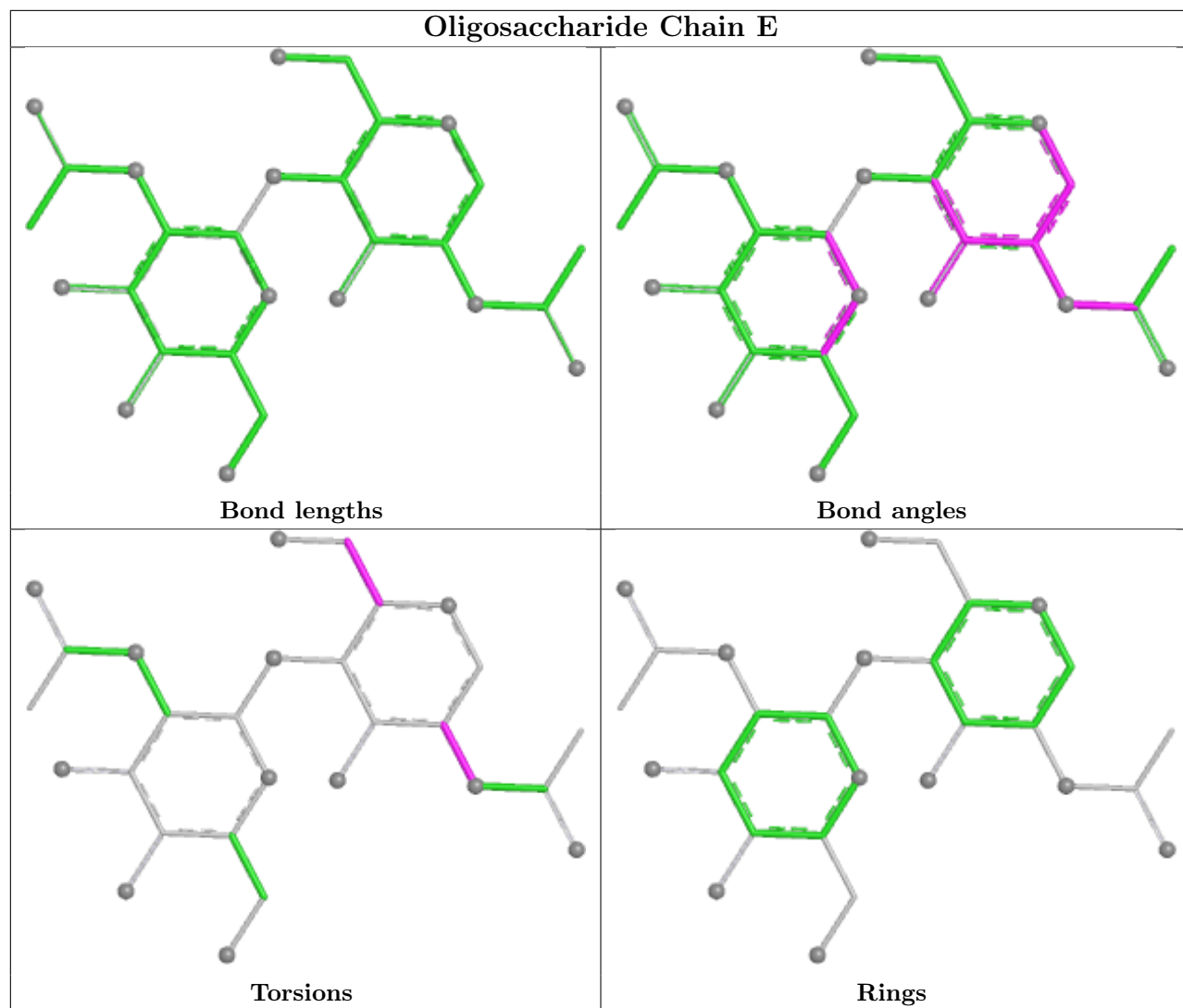
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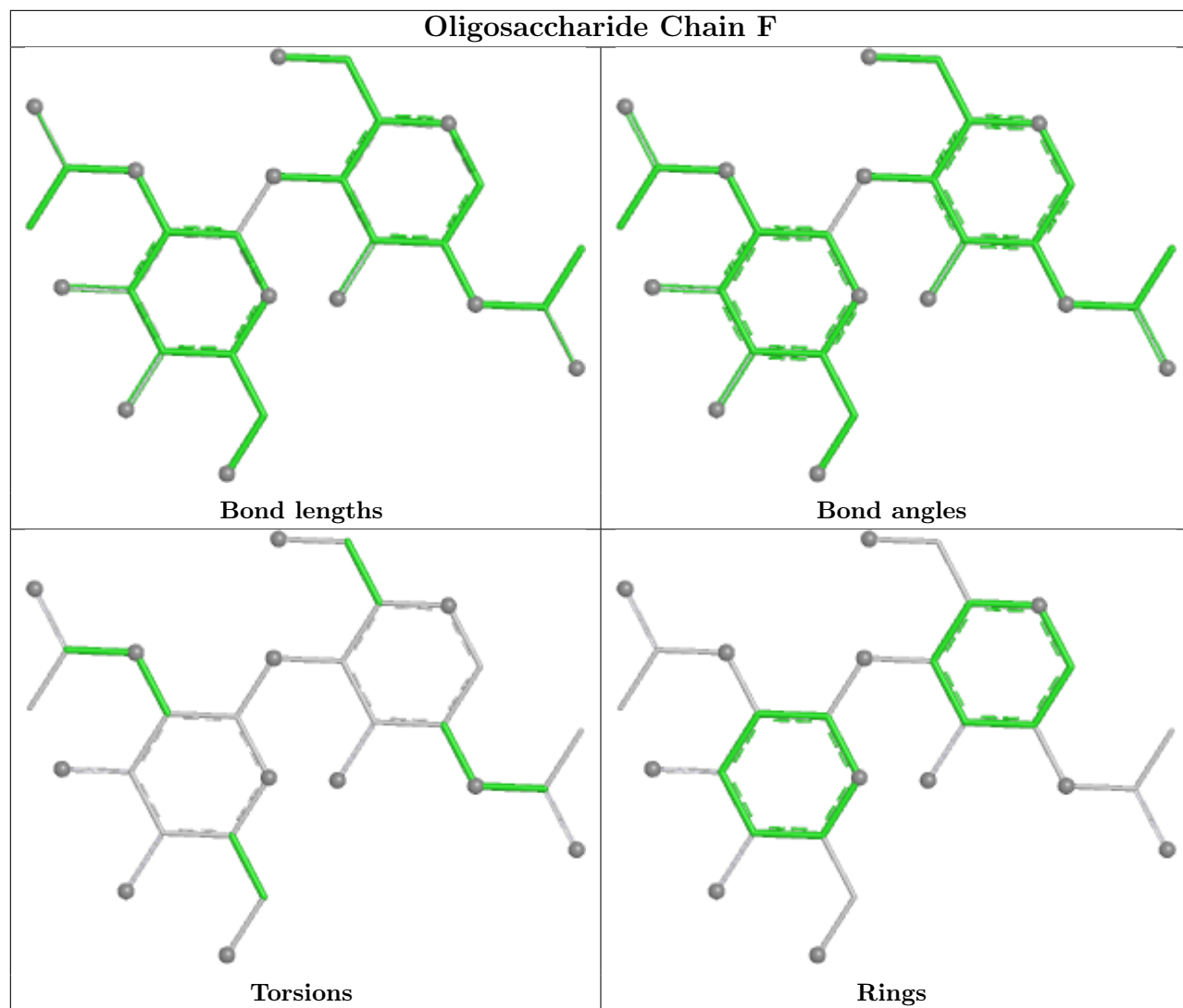
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	1	NAG	2	0
3	K	1	NAG	2	0
2	Q	1	NAG	1	0
2	U	1	NAG	1	0

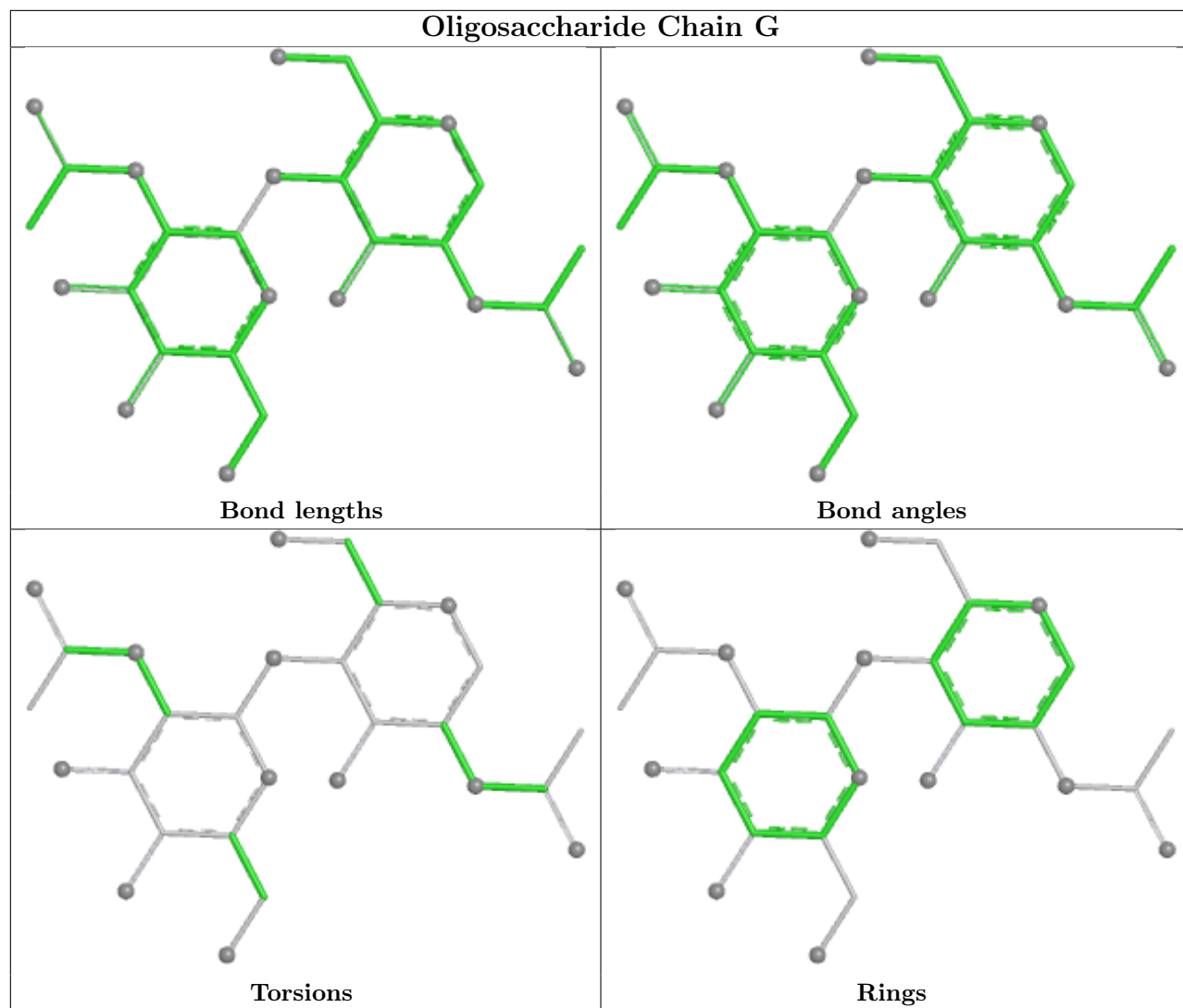
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

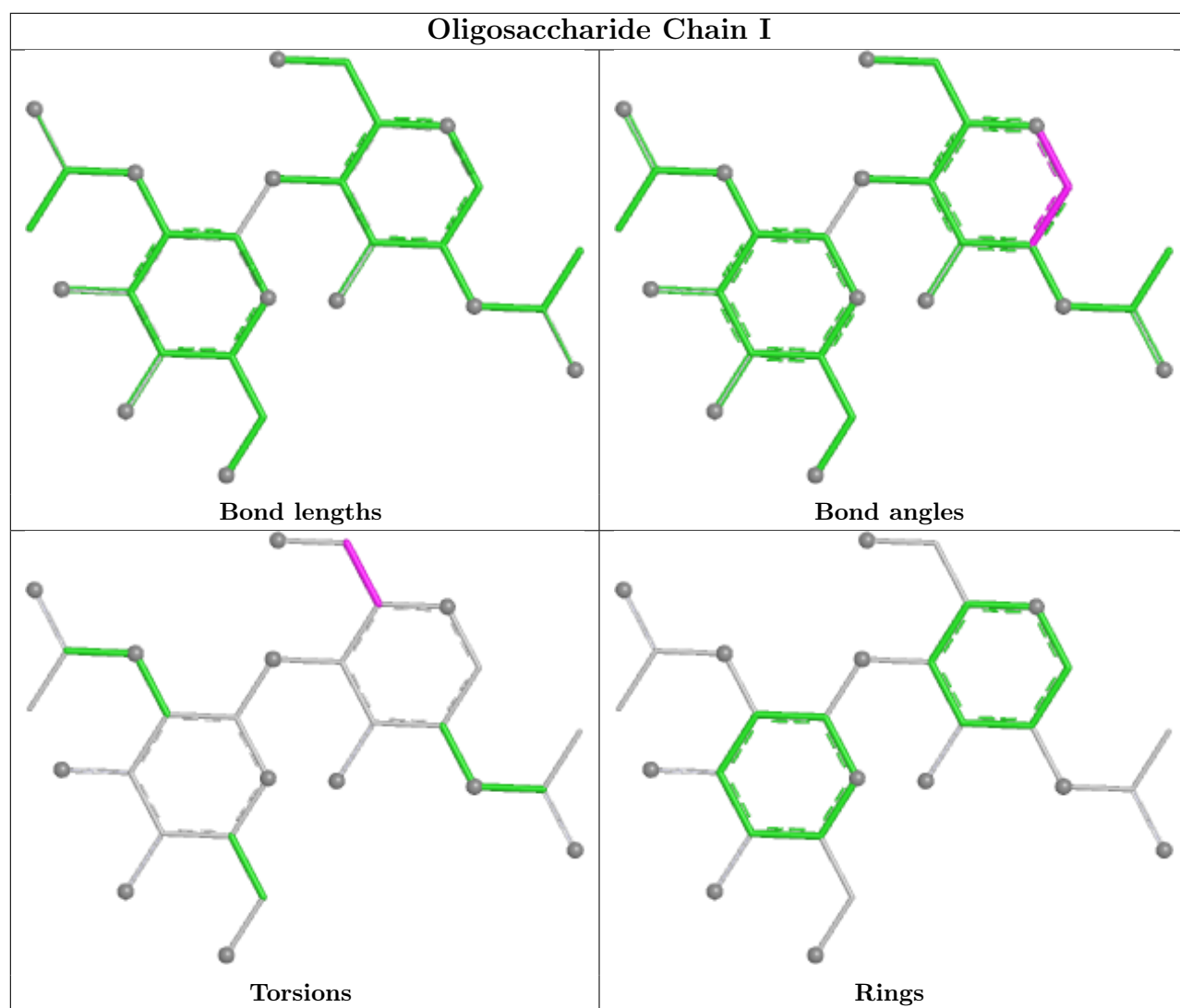


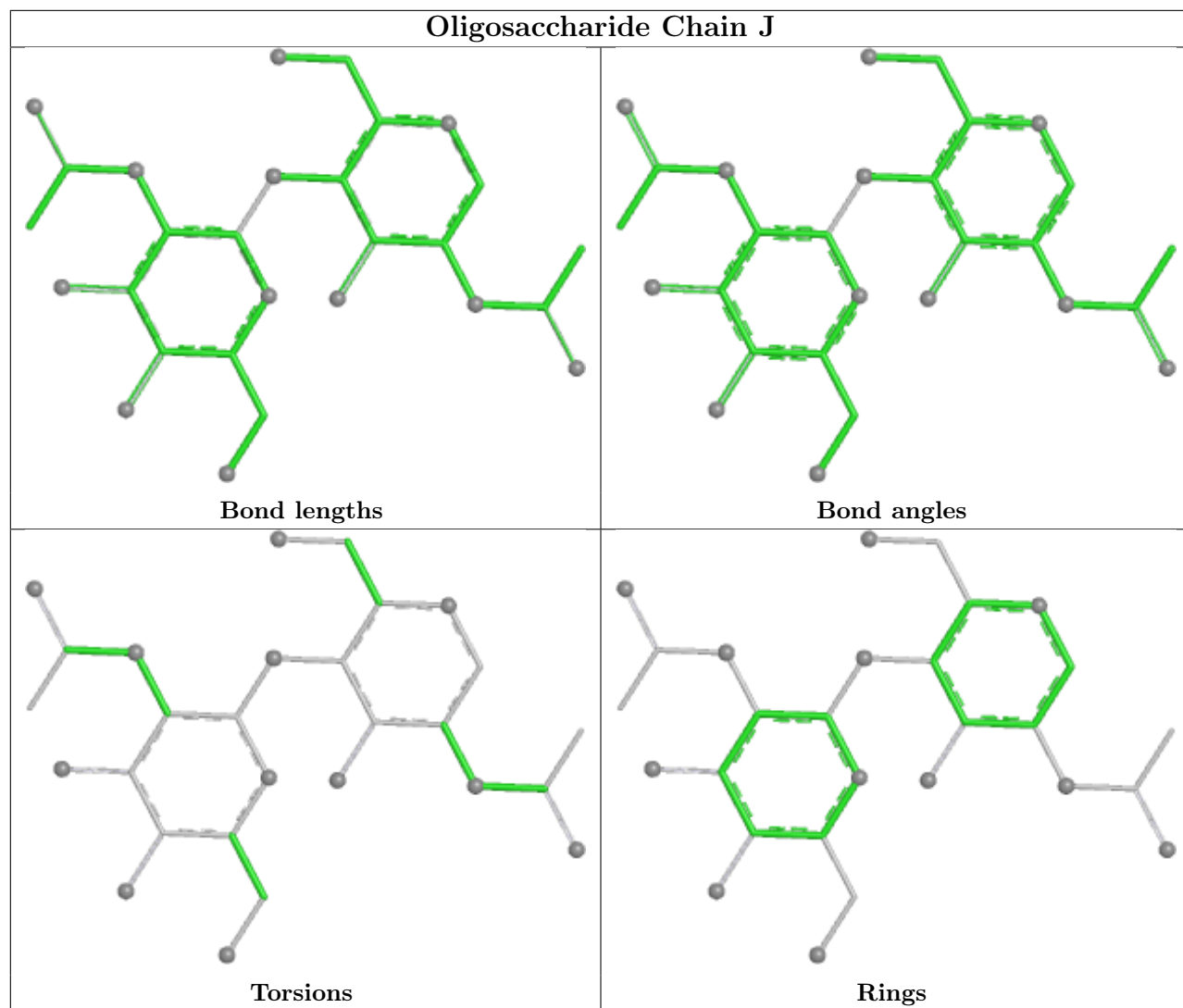


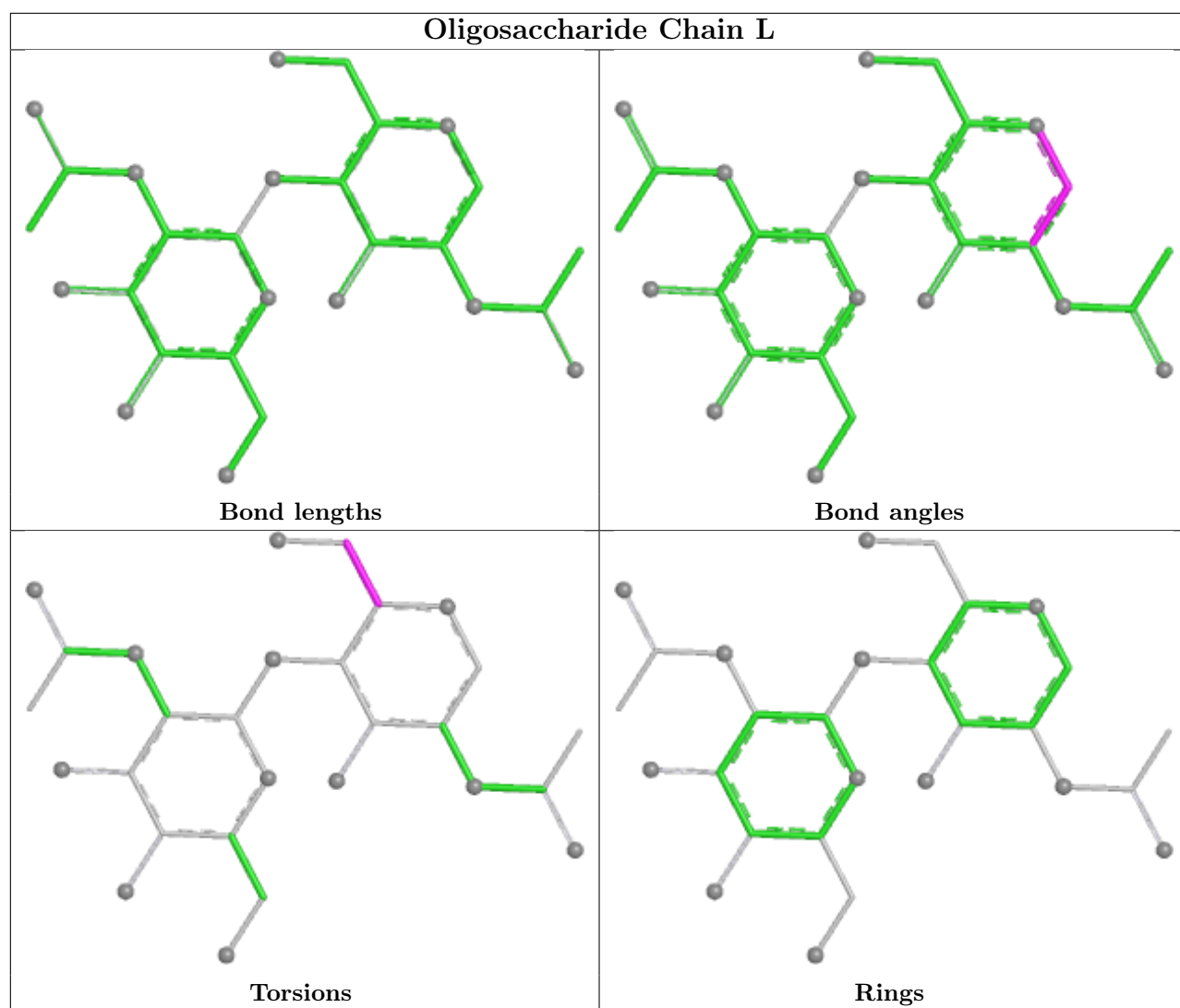


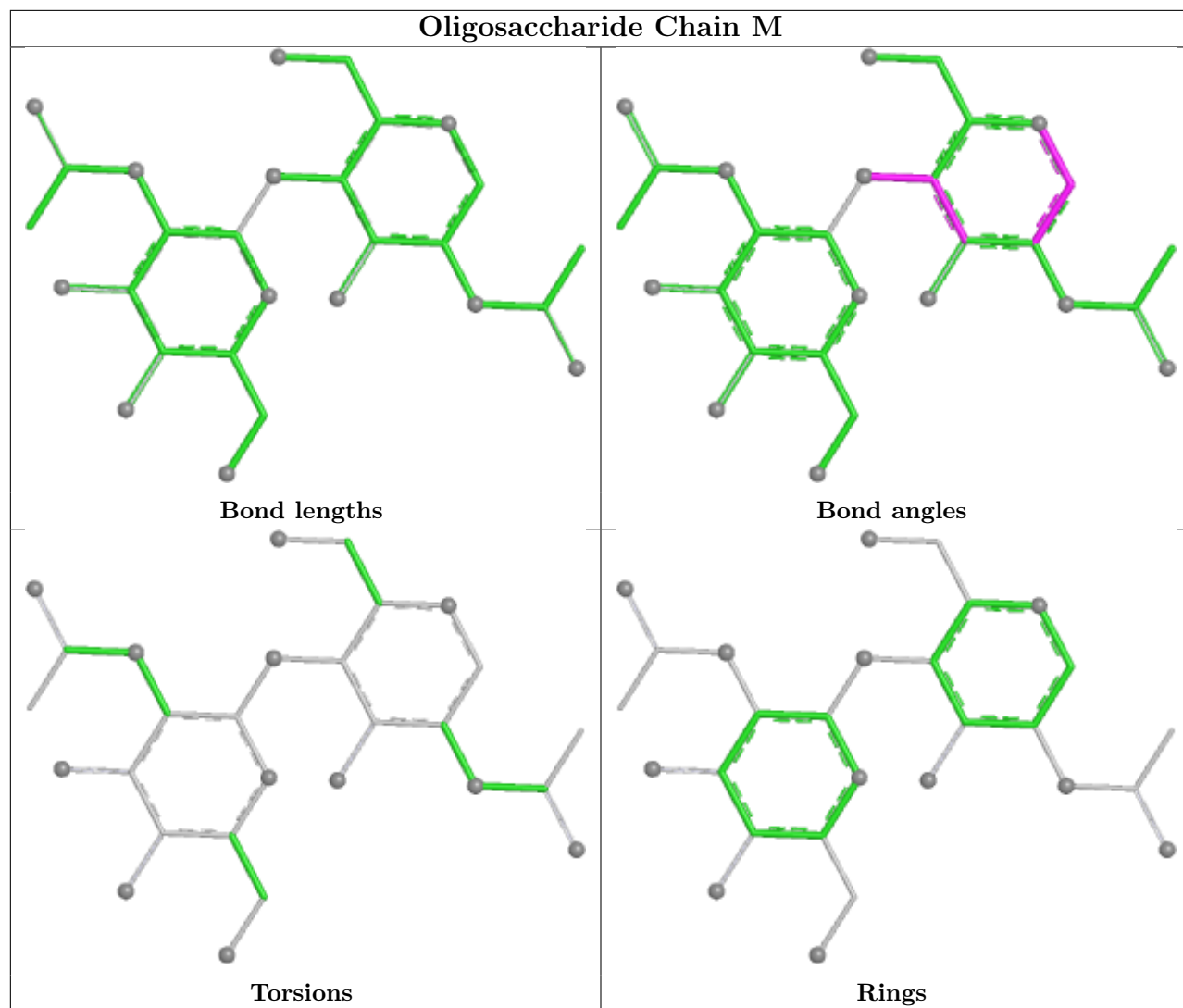


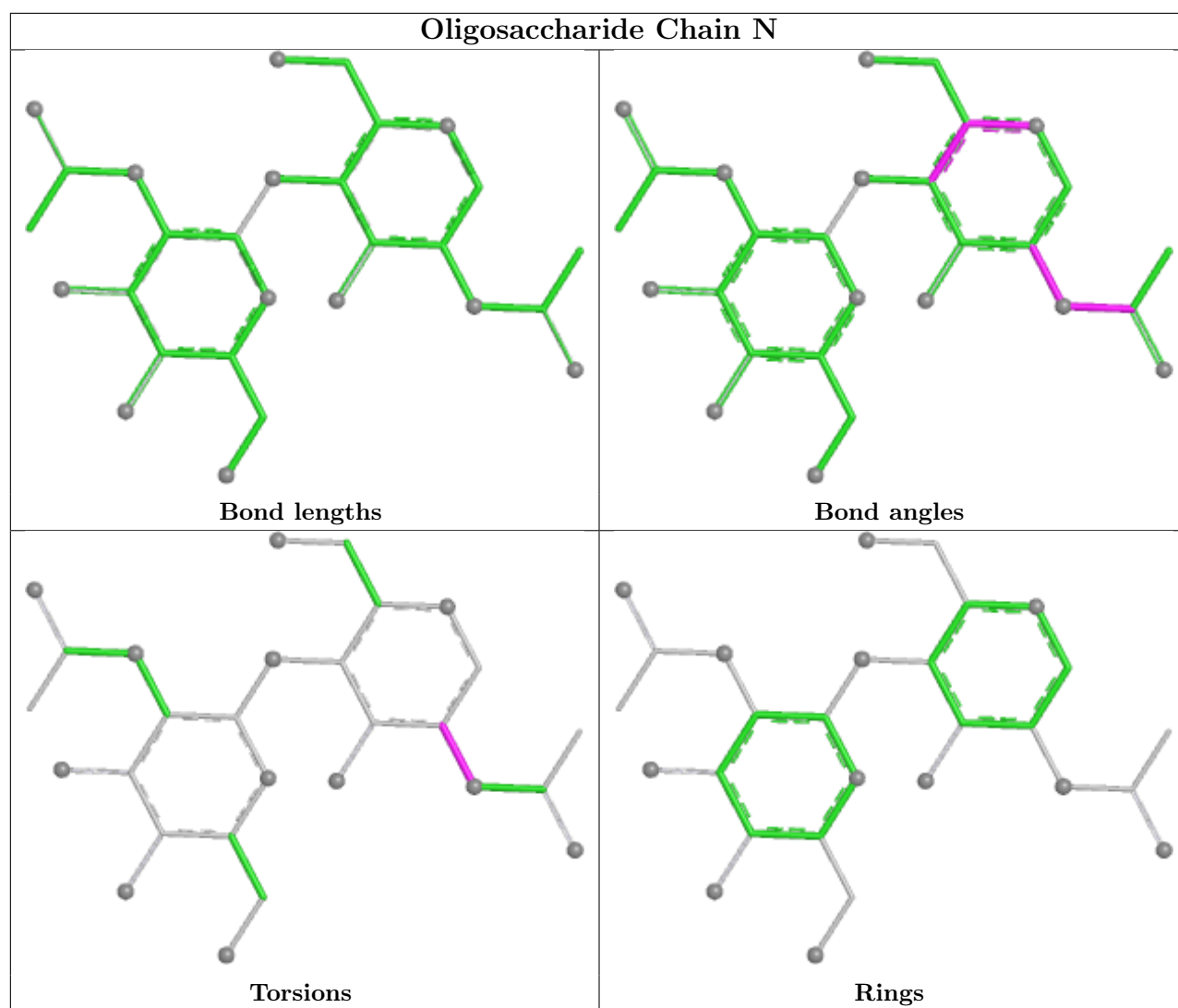


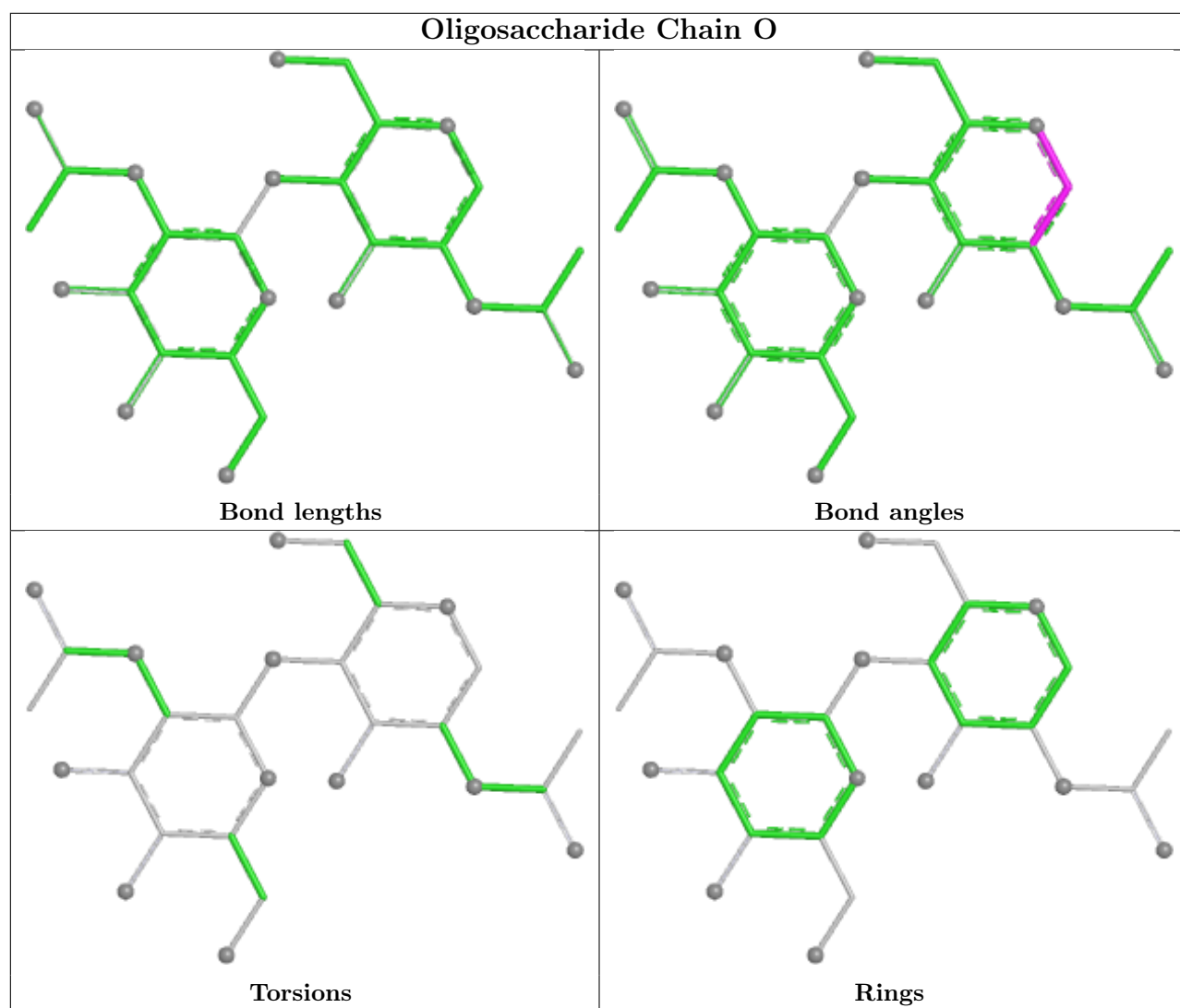


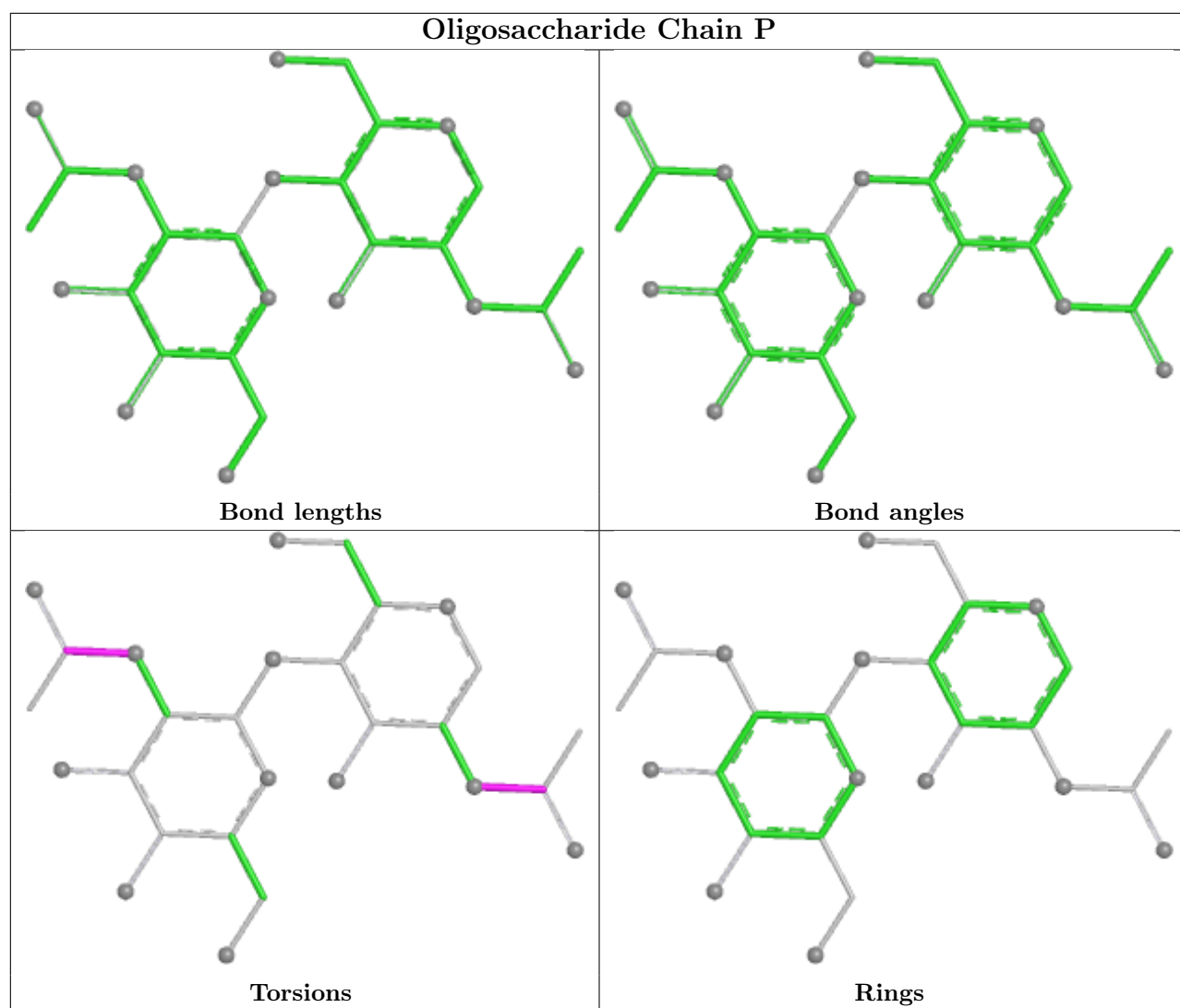




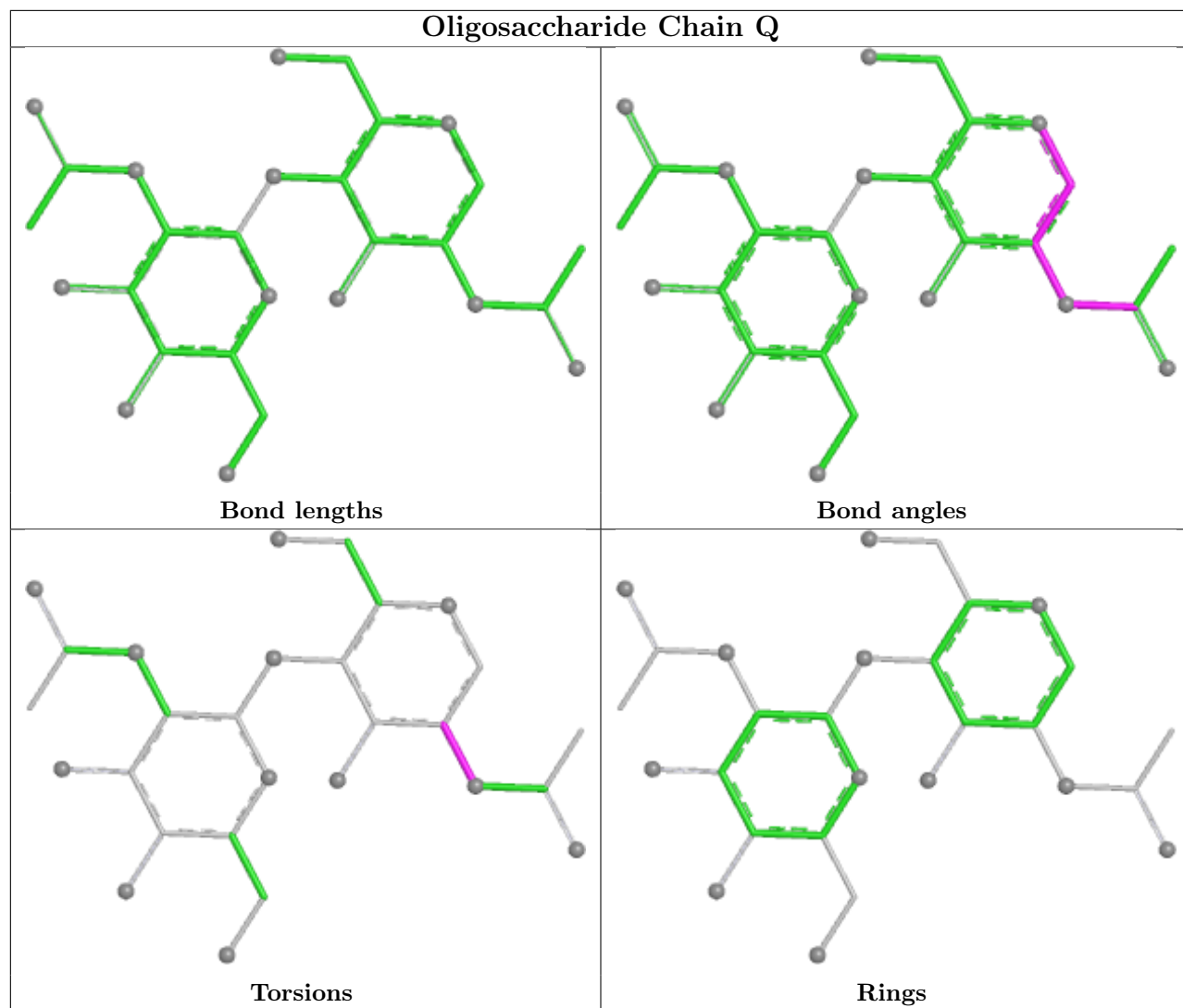


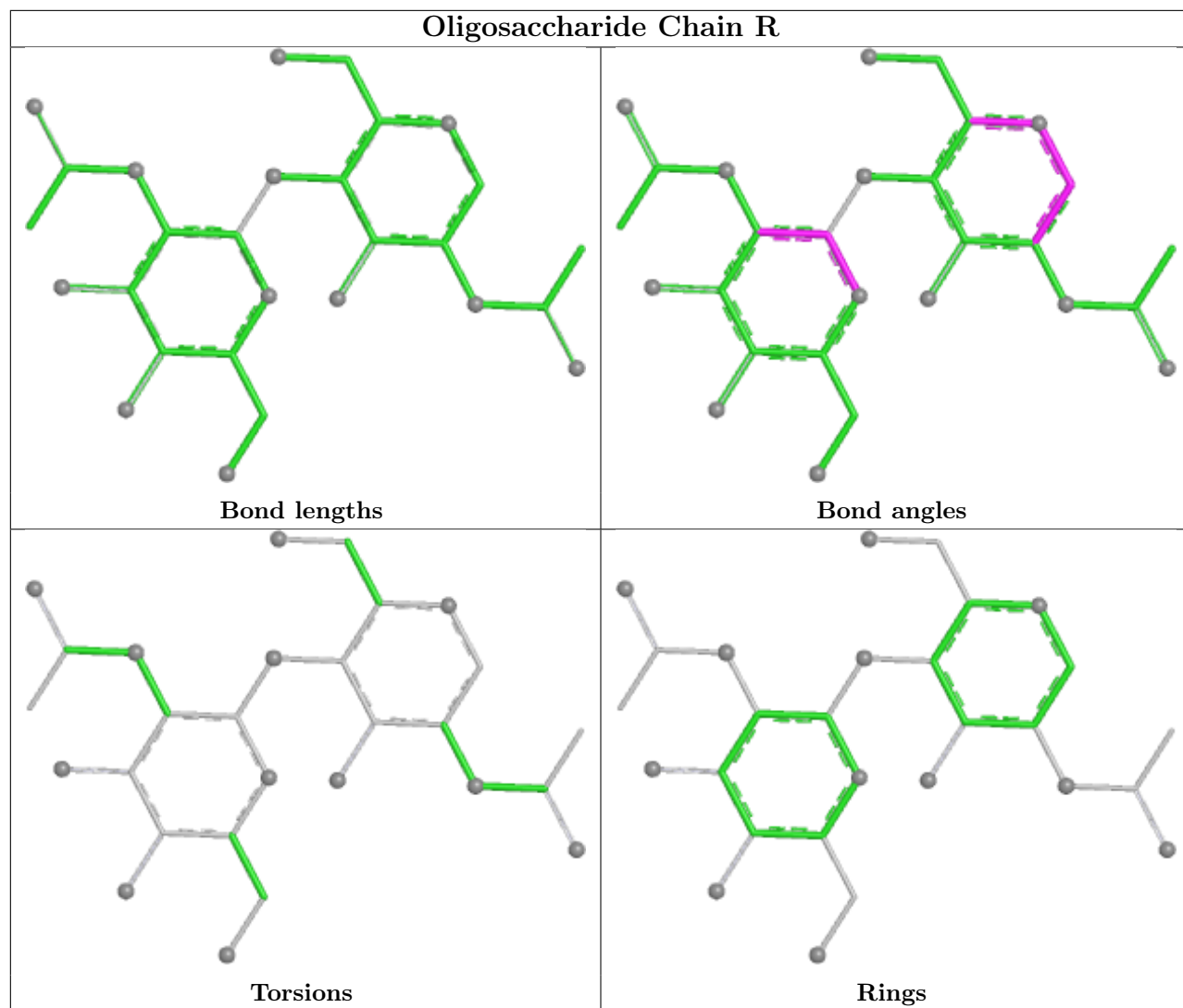


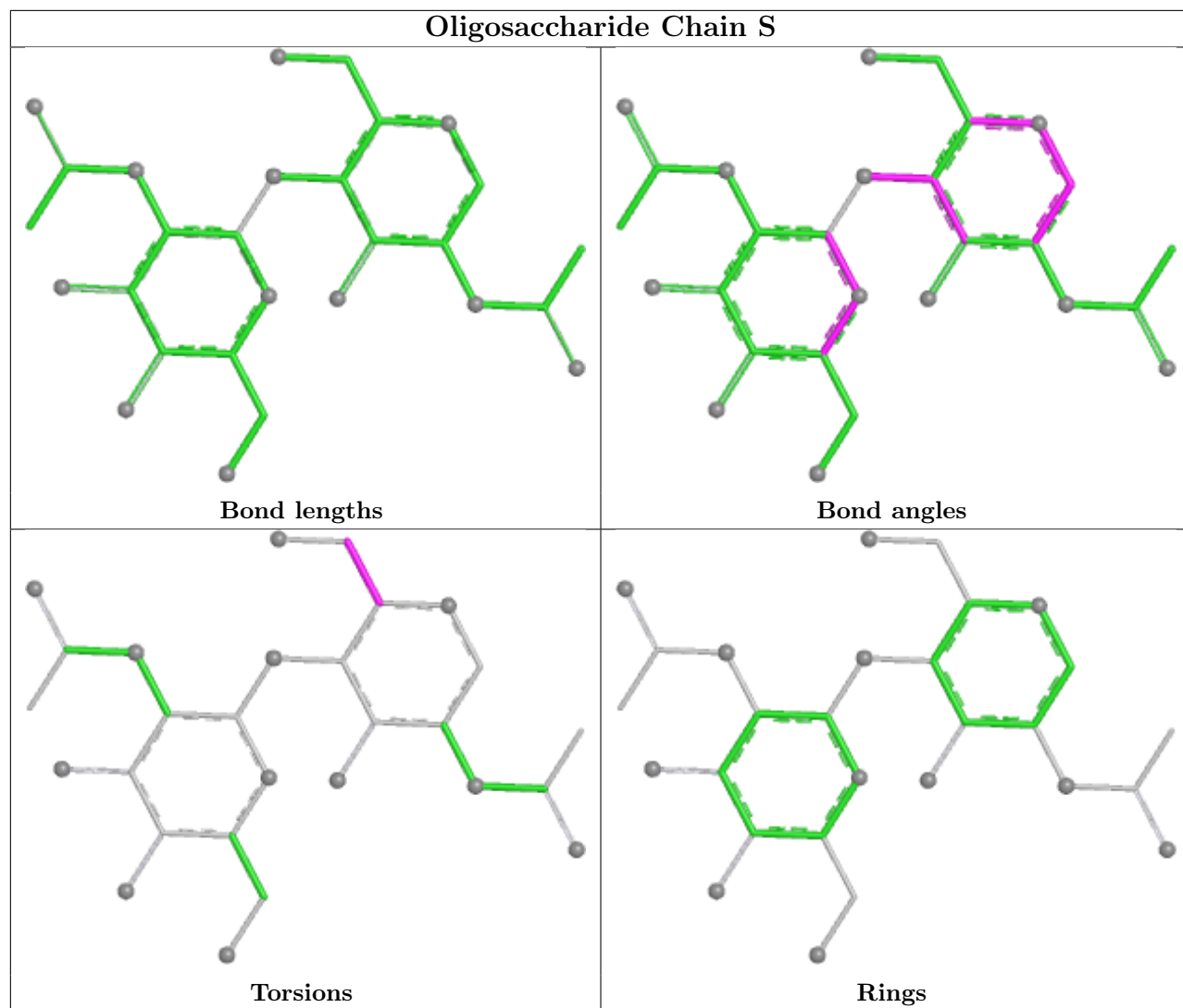


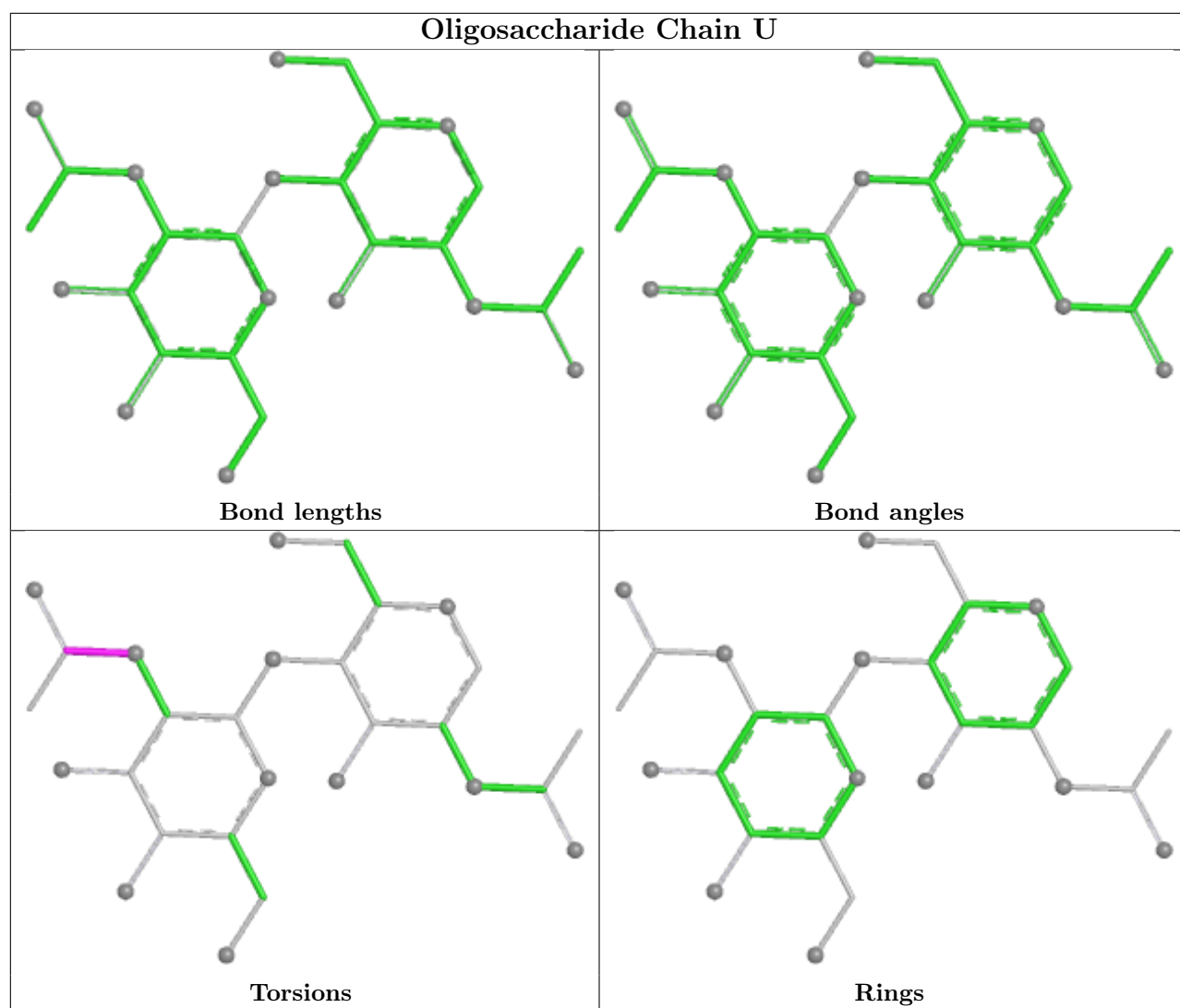


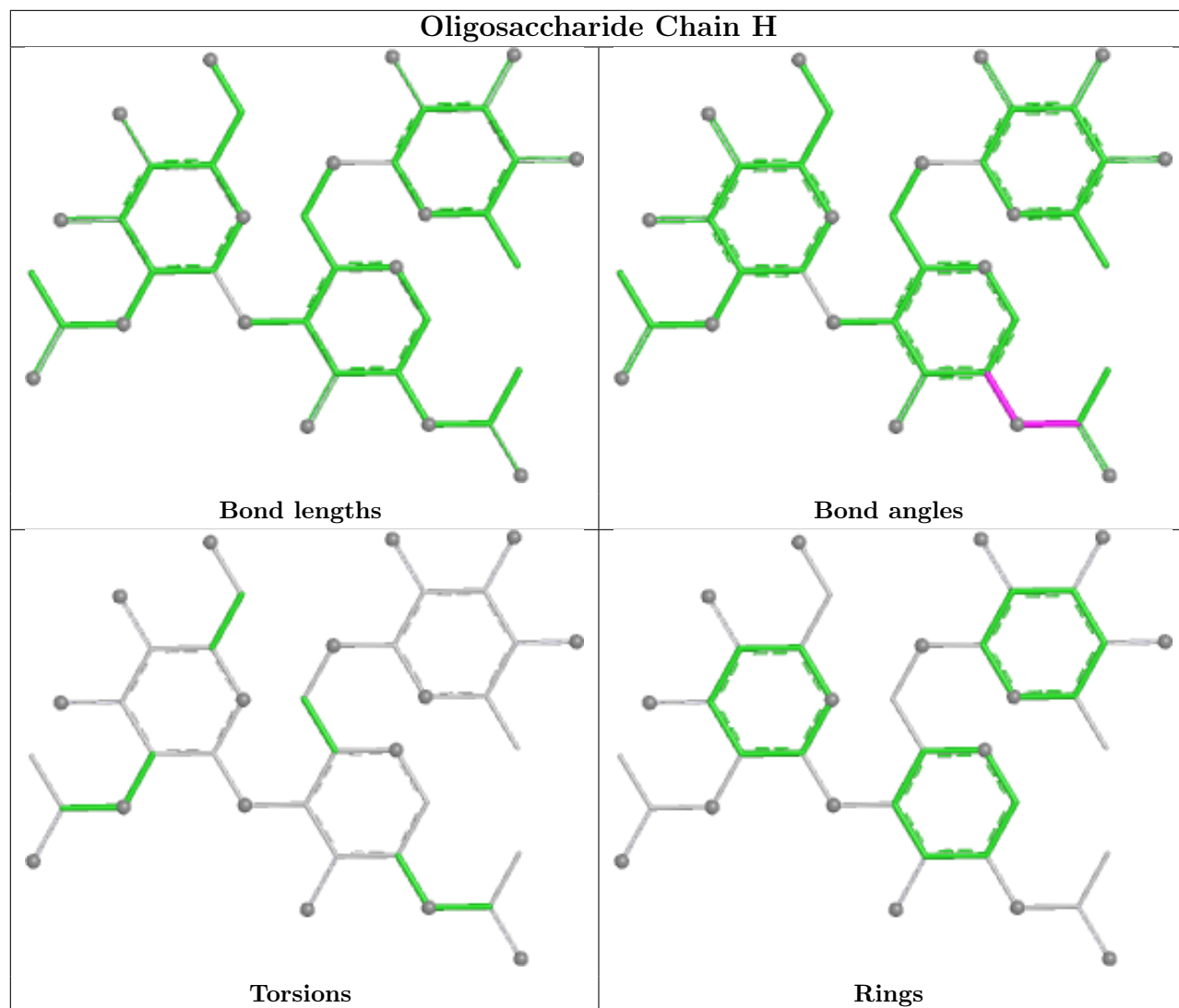


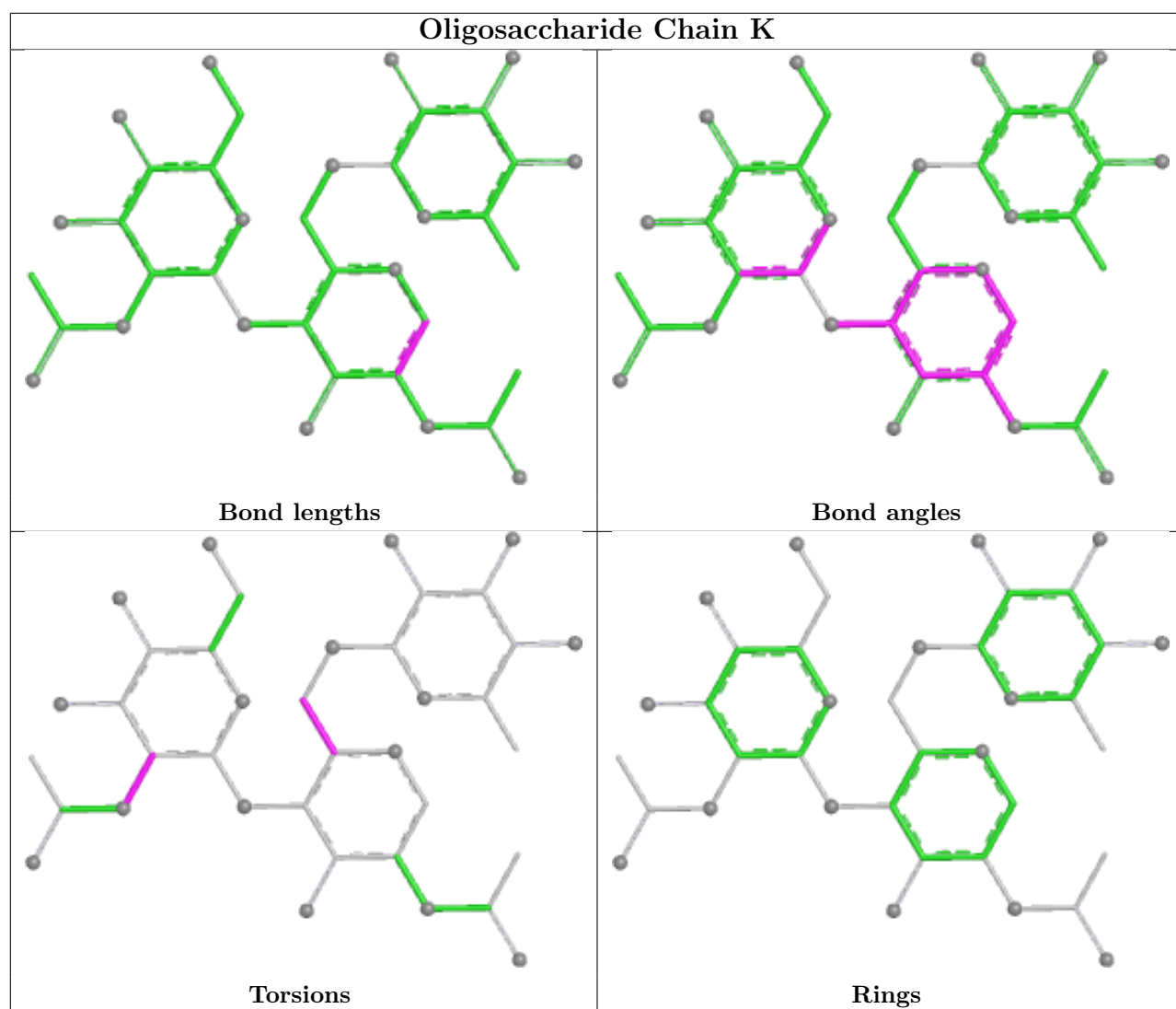


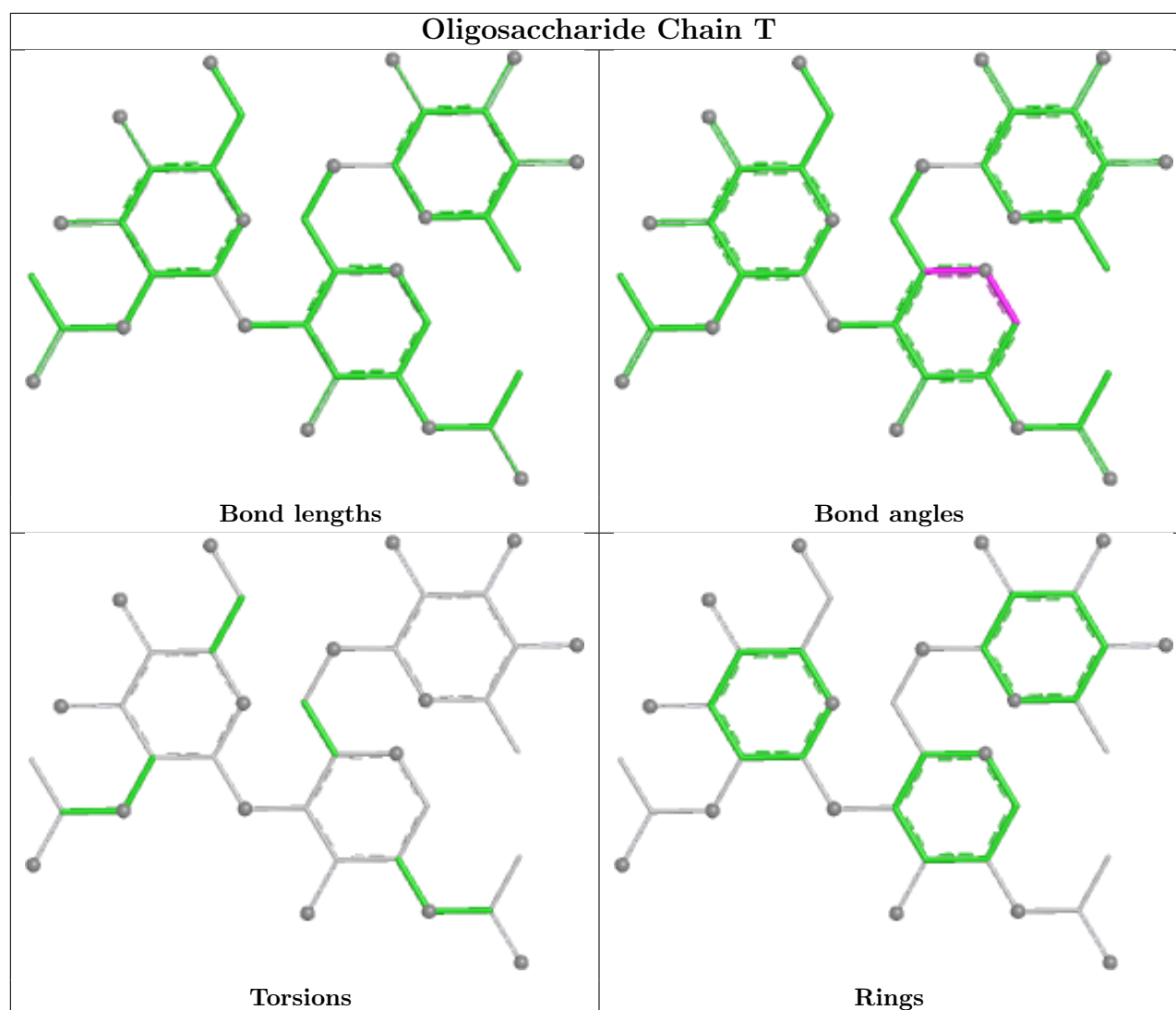












## 5.6 Ligand geometry [i](#)

25 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	B	1408	1	14,14,15	0.70	0	17,19,21	0.76	0
4	NAG	B	1406	1	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
4	NAG	C	1402	1	14,14,15	0.73	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1403	1	14,14,15	0.88	1 (7%)	17,19,21	1.63	2 (11%)
4	NAG	A	1403	1	14,14,15	0.77	0	17,19,21	1.19	1 (5%)
4	NAG	C	1406	1	14,14,15	0.70	0	17,19,21	1.18	1 (5%)
4	NAG	C	1409	1	14,14,15	0.71	0	17,19,21	1.23	2 (11%)
4	NAG	A	1404	1	14,14,15	0.70	0	17,19,21	0.79	0
4	NAG	B	1402	1	14,14,15	0.67	0	17,19,21	1.08	2 (11%)
4	NAG	A	1405	1	14,14,15	0.93	1 (7%)	17,19,21	1.37	2 (11%)
4	NAG	A	1402	1	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	B	1405	1	14,14,15	0.79	0	17,19,21	2.35	3 (17%)
4	NAG	B	1407	1	14,14,15	0.71	0	17,19,21	1.86	4 (23%)
4	NAG	C	1403	1	14,14,15	0.66	0	17,19,21	0.90	1 (5%)
4	NAG	B	1404	1	14,14,15	0.69	0	17,19,21	0.80	0
4	NAG	A	1407	1	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
4	NAG	B	1401	1	14,14,15	0.72	0	17,19,21	0.78	0
4	NAG	A	1401	1	14,14,15	0.74	0	17,19,21	0.84	1 (5%)
4	NAG	A	1408	1	14,14,15	0.71	0	17,19,21	0.79	0
4	NAG	C	1405	1	14,14,15	0.75	0	17,19,21	1.15	2 (11%)
4	NAG	C	1407	1	14,14,15	0.72	0	17,19,21	0.85	1 (5%)
4	NAG	A	1406	1	14,14,15	0.79	0	17,19,21	2.34	2 (11%)
4	NAG	C	1408	1	14,14,15	0.71	0	17,19,21	2.49	3 (17%)
4	NAG	C	1404	1	14,14,15	0.73	0	17,19,21	0.80	0
4	NAG	C	1401	1	14,14,15	0.72	0	17,19,21	0.89	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	B	1408	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1405	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1401	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)
4	A	1405	NAG	C1-C2	2.71	1.56	1.52
4	B	1403	NAG	C1-C2	2.36	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1406	NAG	C2-N2-C7	8.35	134.09	122.90
4	B	1405	NAG	C2-N2-C7	8.32	134.06	122.90
4	C	1408	NAG	C1-O5-C5	8.16	123.13	112.19
4	B	1407	NAG	C2-N2-C7	4.74	129.25	122.90
4	C	1408	NAG	O5-C1-C2	4.51	118.27	111.29
4	B	1403	NAG	C1-O5-C5	4.51	118.23	112.19
4	B	1407	NAG	C1-O5-C5	-4.09	106.70	112.19
4	C	1409	NAG	C1-O5-C5	-3.53	107.46	112.19
4	C	1406	NAG	C2-N2-C7	3.30	127.32	122.90
4	B	1406	NAG	C2-N2-C7	3.28	127.29	122.90
4	A	1407	NAG	C2-N2-C7	3.19	127.17	122.90
4	A	1405	NAG	C1-O5-C5	3.12	116.37	112.19
4	A	1403	NAG	C2-N2-C7	3.04	126.97	122.90
4	B	1403	NAG	C2-N2-C7	2.94	126.84	122.90
4	C	1403	NAG	O5-C1-C2	-2.68	107.15	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1405	NAG	C2-N2-C7	2.63	126.42	122.90
4	A	1406	NAG	C8-C7-N2	2.60	120.43	116.12
4	B	1405	NAG	C8-C7-N2	2.55	120.35	116.12
4	C	1405	NAG	C1-O5-C5	2.42	115.43	112.19
4	B	1402	NAG	C1-O5-C5	2.35	115.34	112.19
4	B	1402	NAG	O5-C1-C2	-2.33	107.68	111.29
4	C	1408	NAG	C3-C4-C5	-2.30	106.06	110.23
4	C	1407	NAG	O5-C1-C2	-2.26	107.80	111.29
4	A	1405	NAG	C2-N2-C7	2.25	125.92	122.90
4	B	1405	NAG	C1-C2-N2	2.12	113.78	110.43
4	B	1407	NAG	C1-C2-N2	2.12	113.78	110.43
4	B	1407	NAG	O4-C4-C3	-2.05	105.54	110.38
4	A	1401	NAG	O5-C1-C2	-2.02	108.16	111.29
4	C	1409	NAG	O4-C4-C3	-2.02	105.62	110.38

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1409	NAG	C4-C5-C6-O6
4	C	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C8-C7-N2-C2
4	A	1406	NAG	O7-C7-N2-C2
4	B	1405	NAG	C8-C7-N2-C2
4	B	1405	NAG	O7-C7-N2-C2
4	B	1407	NAG	C8-C7-N2-C2
4	B	1407	NAG	O7-C7-N2-C2
4	C	1401	NAG	C8-C7-N2-C2
4	C	1401	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	A	1405	NAG	O5-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	B	1407	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	A	1407	NAG	C1-C2-N2-C7
4	B	1403	NAG	C1-C2-N2-C7
4	B	1406	NAG	C1-C2-N2-C7
4	C	1406	NAG	C1-C2-N2-C7
4	A	1403	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	B	1403	NAG	C3-C2-N2-C7
4	A	1403	NAG	C1-C2-N2-C7
4	A	1406	NAG	C1-C2-N2-C7
4	B	1405	NAG	C1-C2-N2-C7
4	C	1407	NAG	C1-C2-N2-C7
4	A	1406	NAG	C3-C2-N2-C7
4	A	1407	NAG	C3-C2-N2-C7
4	B	1405	NAG	C3-C2-N2-C7
4	B	1406	NAG	C3-C2-N2-C7
4	C	1406	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1408	NAG	1	0
4	B	1403	NAG	1	0
4	A	1404	NAG	1	0
4	A	1405	NAG	2	0
4	B	1407	NAG	1	0
4	A	1406	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.

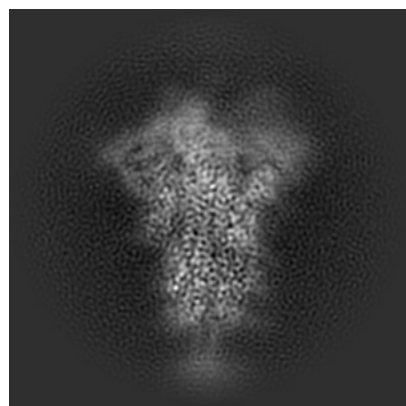
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46641. These allow visual inspection of the internal detail of the map and identification of artifacts.

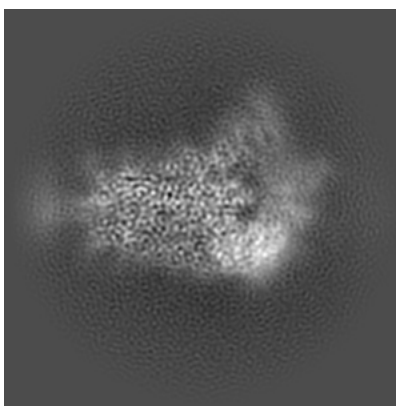
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

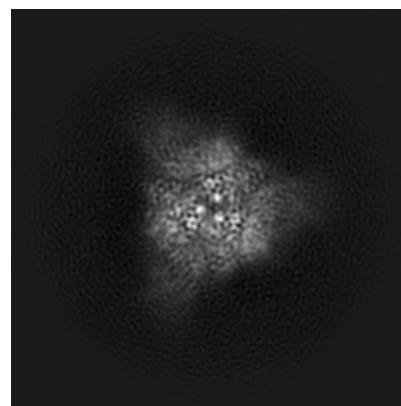
#### 6.1.1 Primary map



X

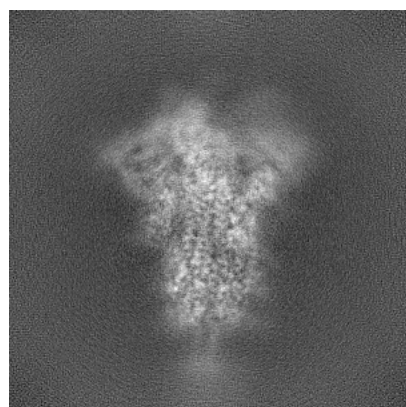


Y

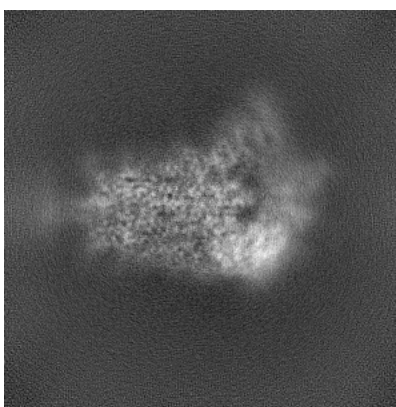


Z

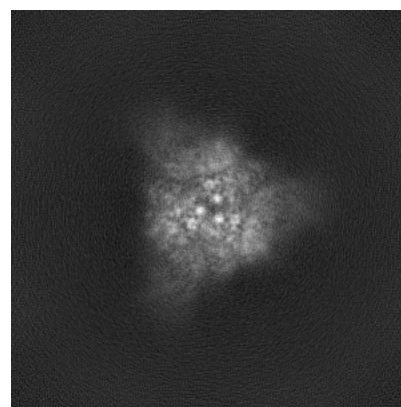
#### 6.1.2 Raw map



X



Y

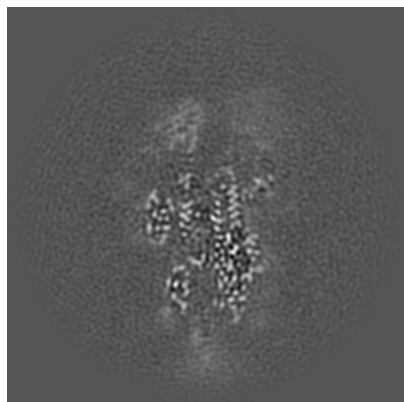


Z

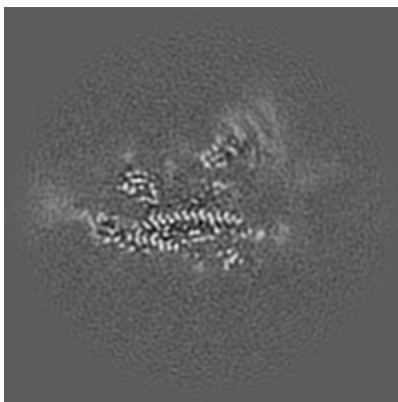
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

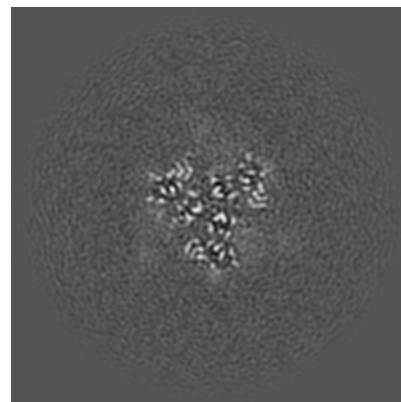
### 6.2.1 Primary map



X Index: 180

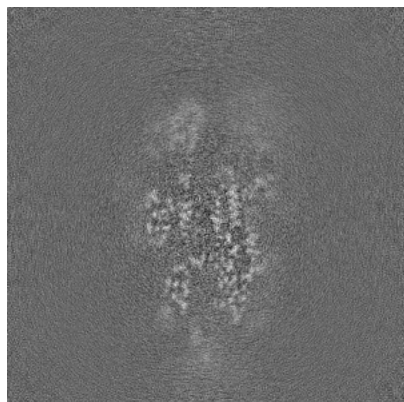


Y Index: 180

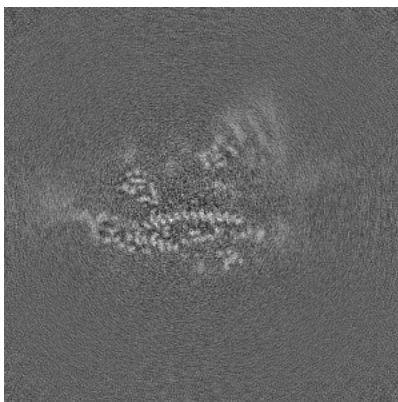


Z Index: 180

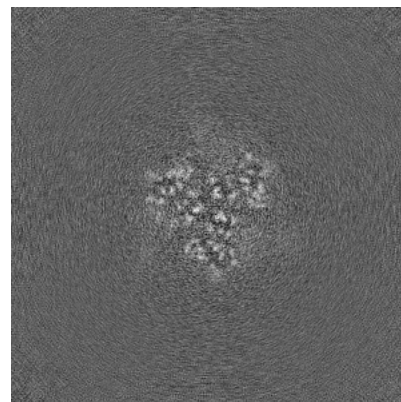
### 6.2.2 Raw map



X Index: 180



Y Index: 180



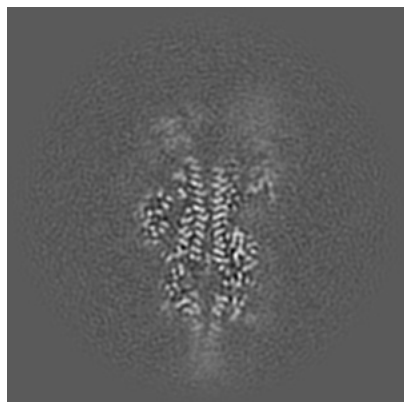
Z Index: 180

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

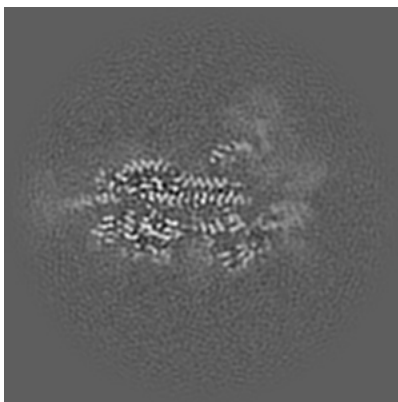


## 6.3 Largest variance slices [i](#)

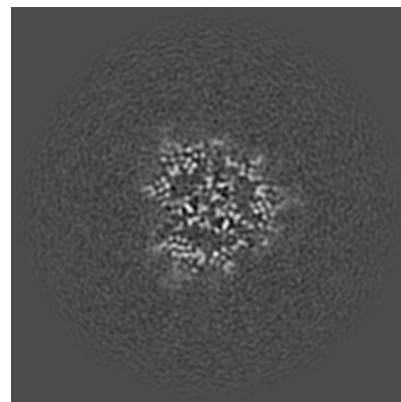
### 6.3.1 Primary map



X Index: 185

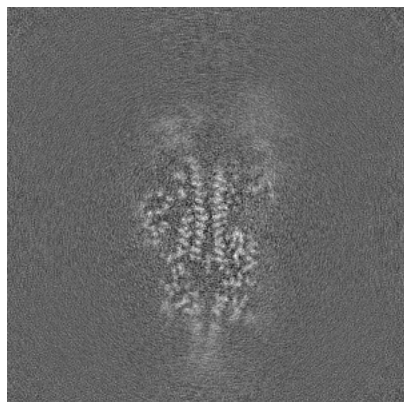


Y Index: 170

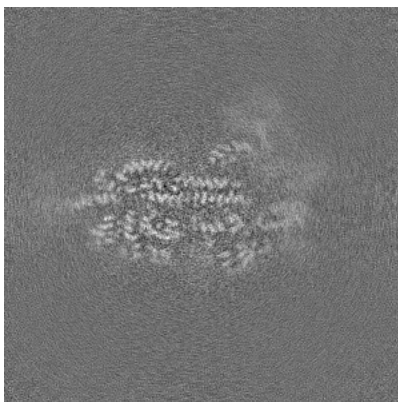


Z Index: 191

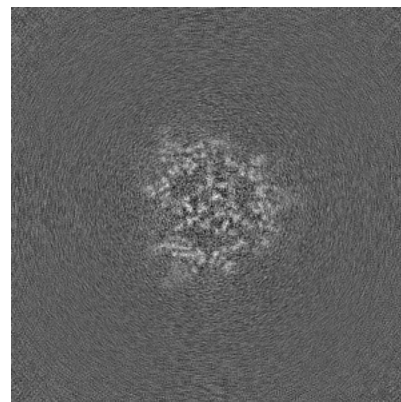
### 6.3.2 Raw map



X Index: 185



Y Index: 170

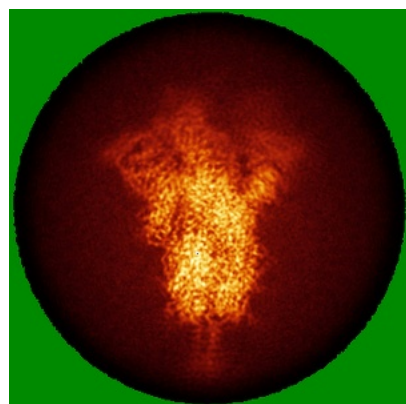


Z Index: 191

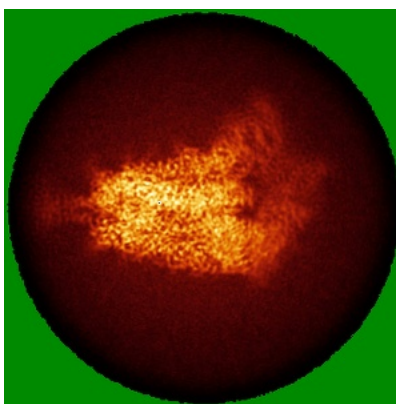
The images above show the largest variance slices of the map in three orthogonal directions.

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

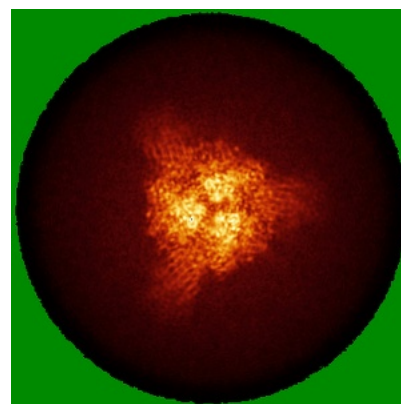
### 6.4.1 Primary map



X

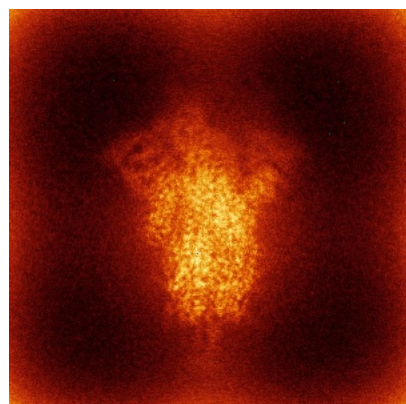


Y

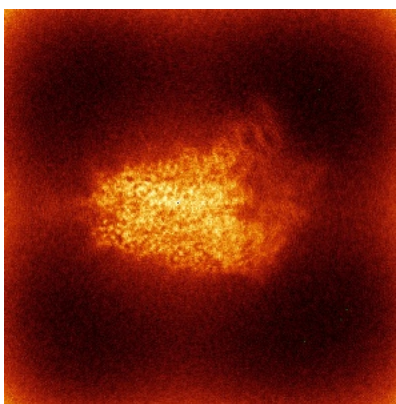


Z

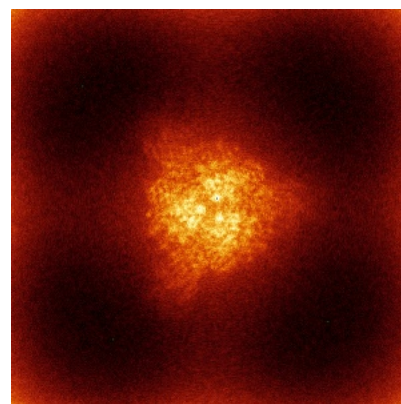
### 6.4.2 Raw map



X



Y

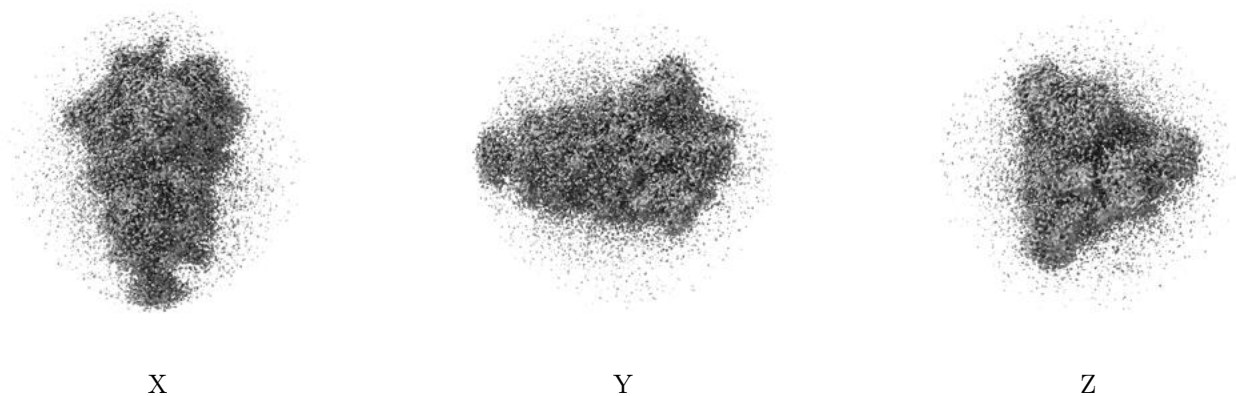


Z

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.

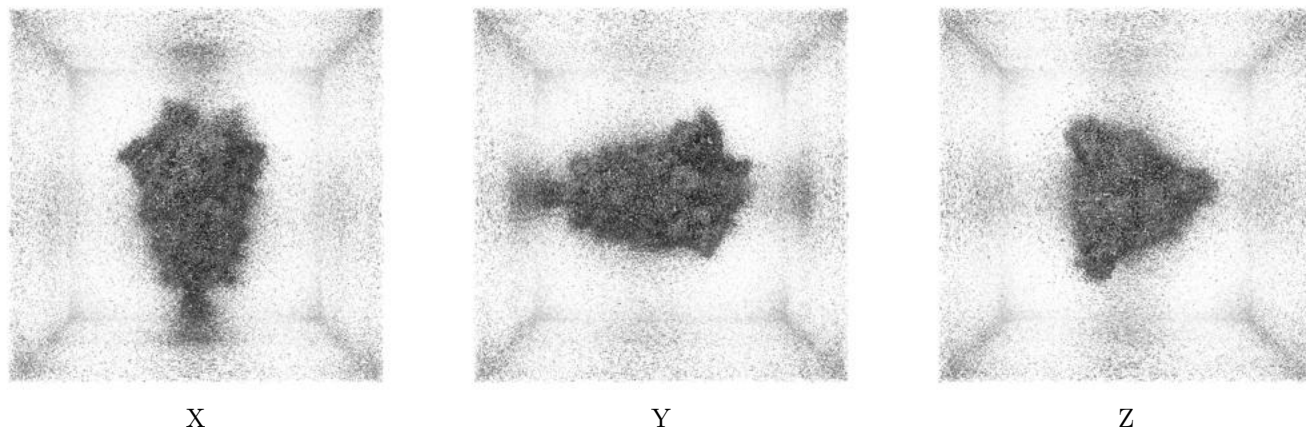
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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](#)

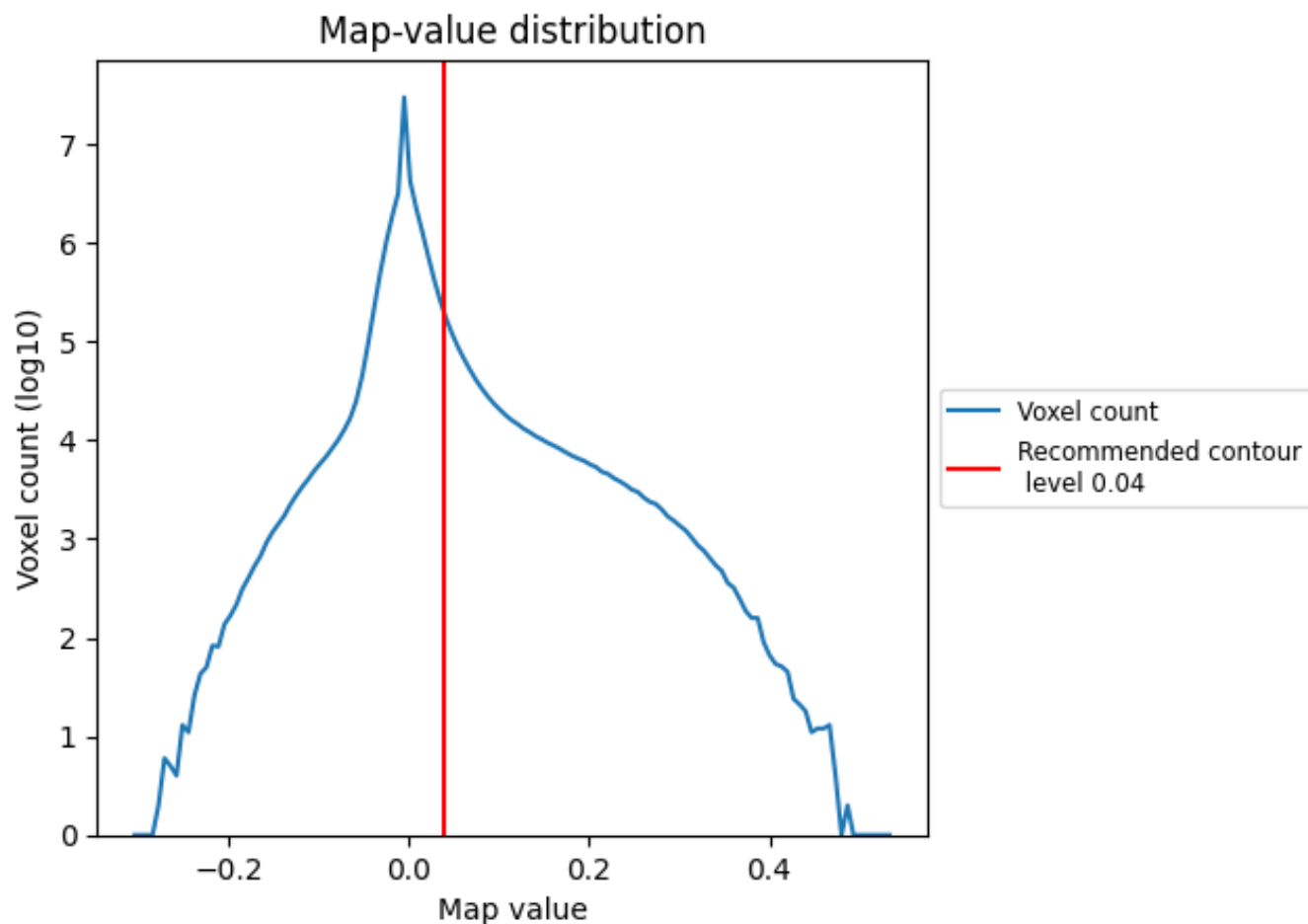
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

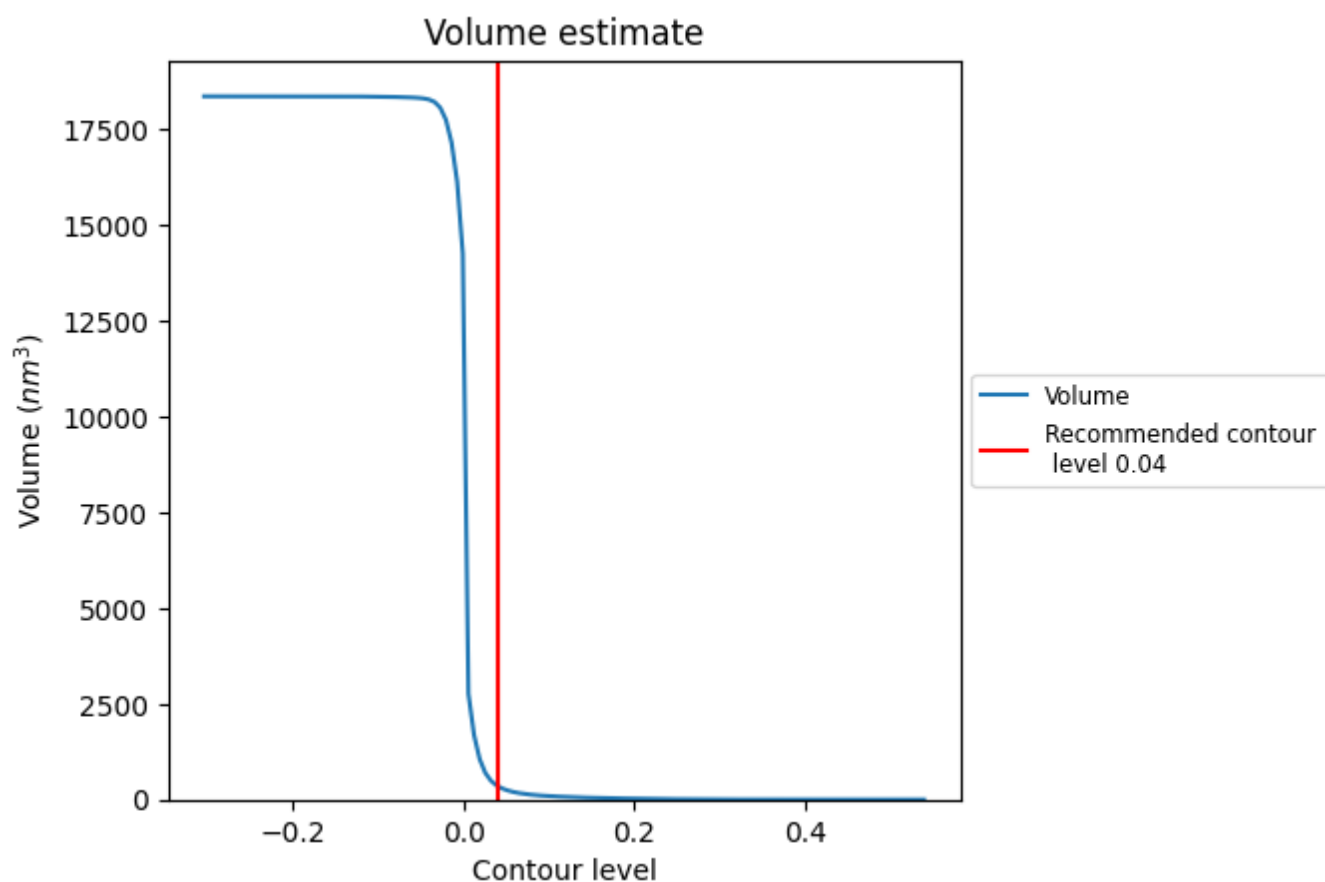
This section contains the results of statistical analysis of the map.

### 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.

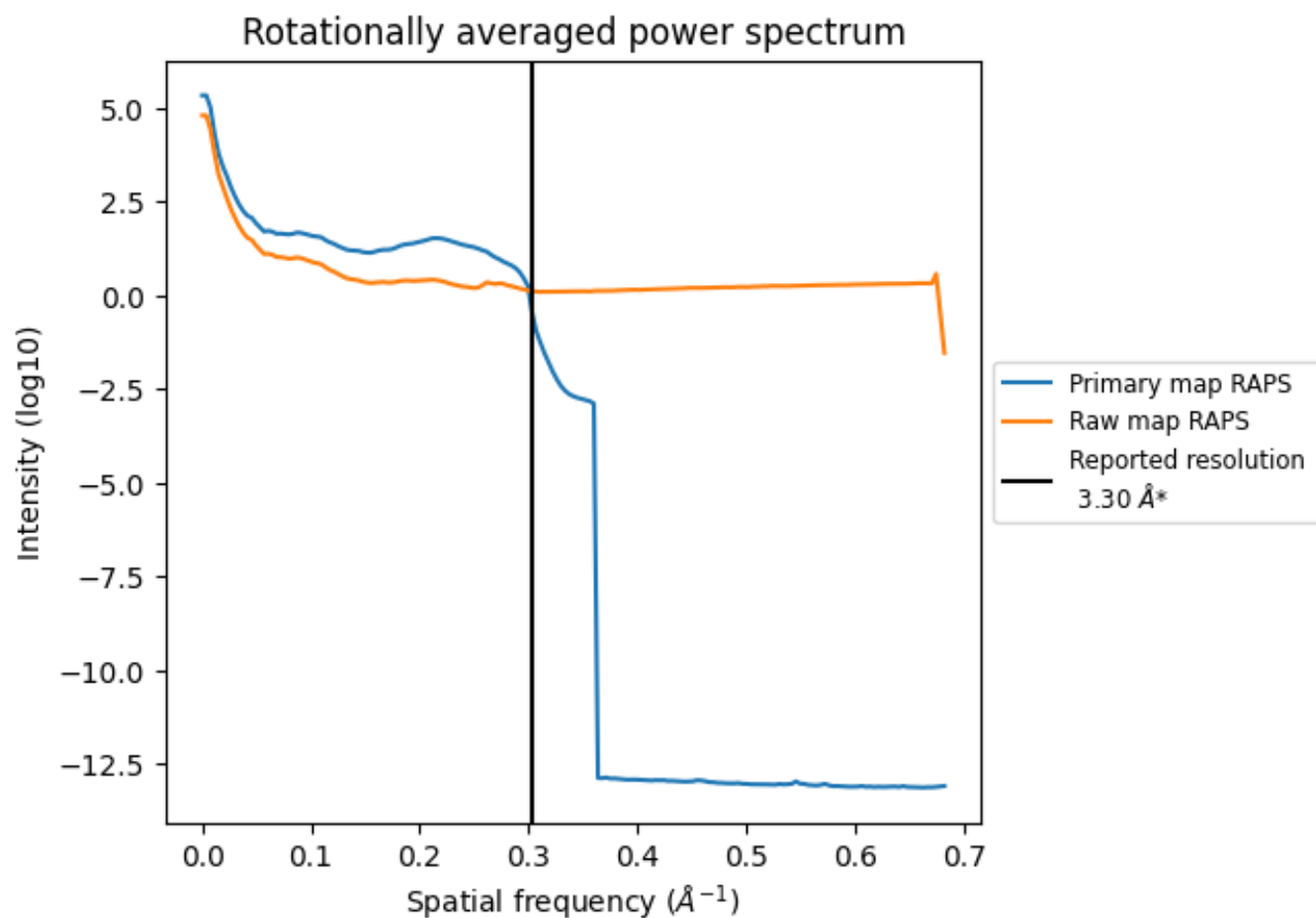
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 353 nm<sup>3</sup>; this corresponds to an approximate mass of 319 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

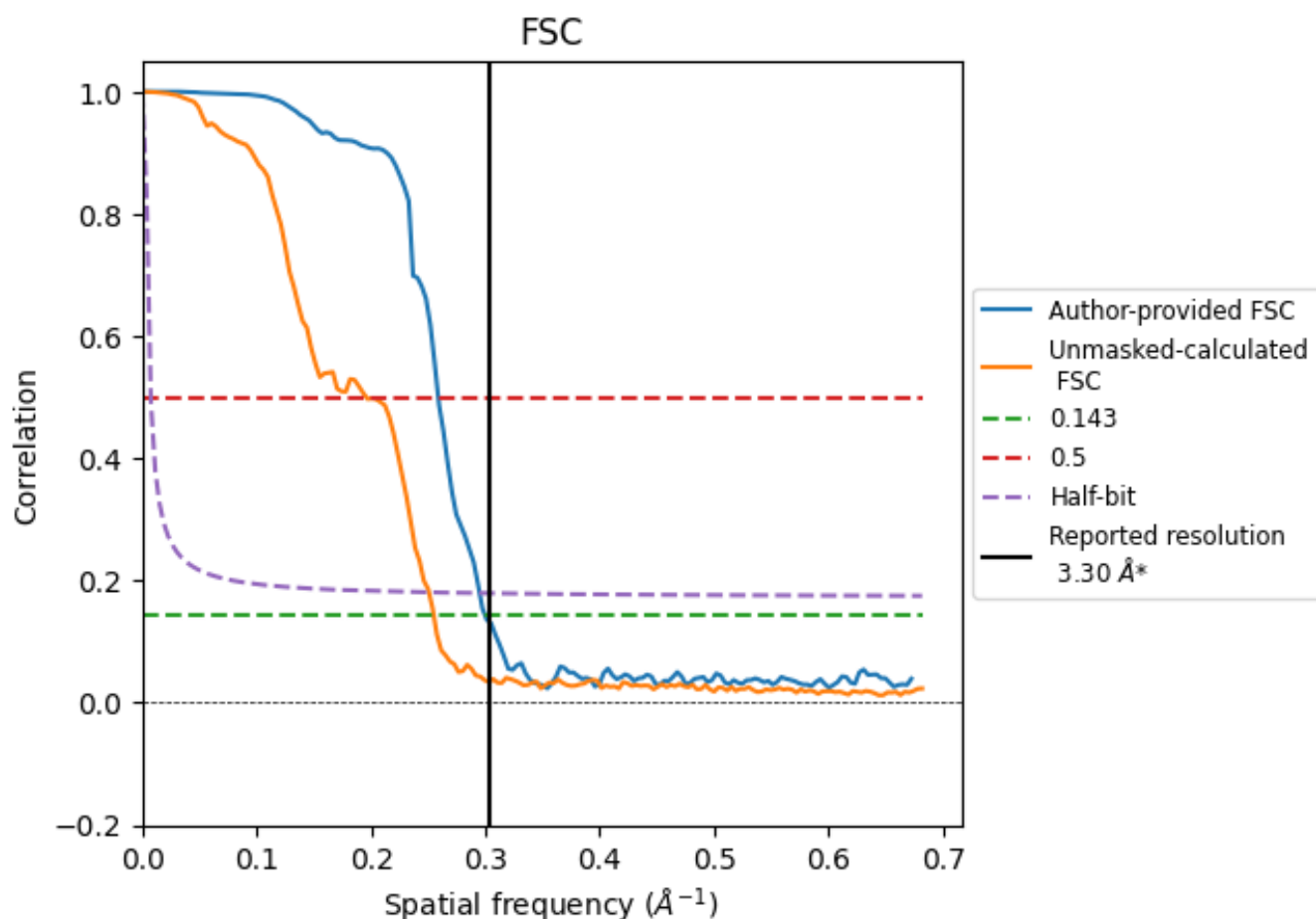


\*Reported resolution corresponds to spatial frequency of 0.303  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [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 0.303  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

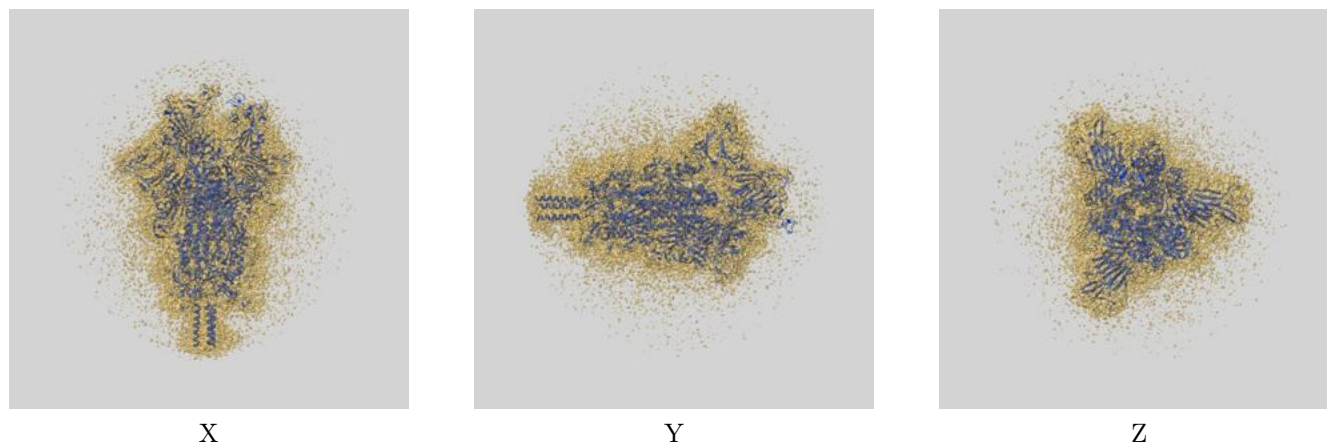
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.34	3.86	3.39
Unmasked-calculated*	3.92	5.10	3.99

\*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 3.92 differs from the reported value 3.3 by more than 10 %

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

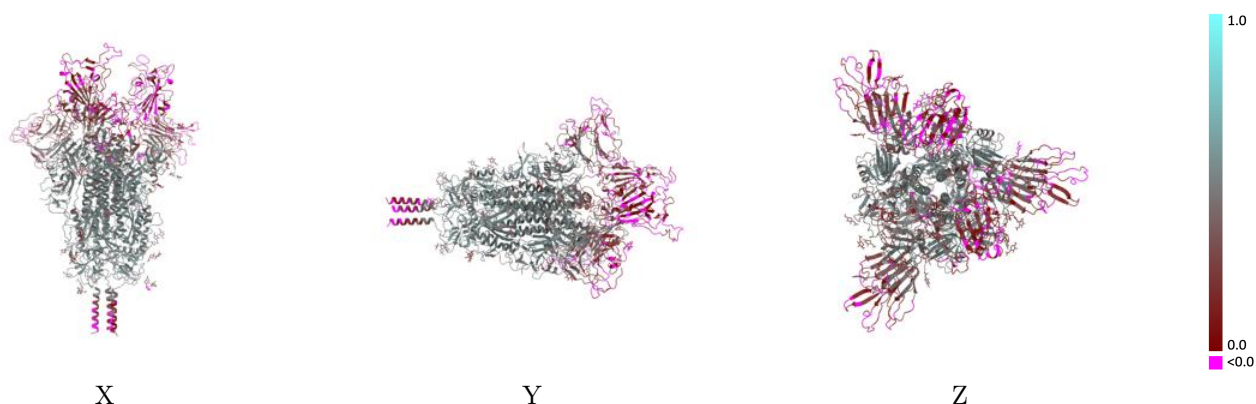
This section contains information regarding the fit between EMDB map EMD-46641 and PDB model 9D8L. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



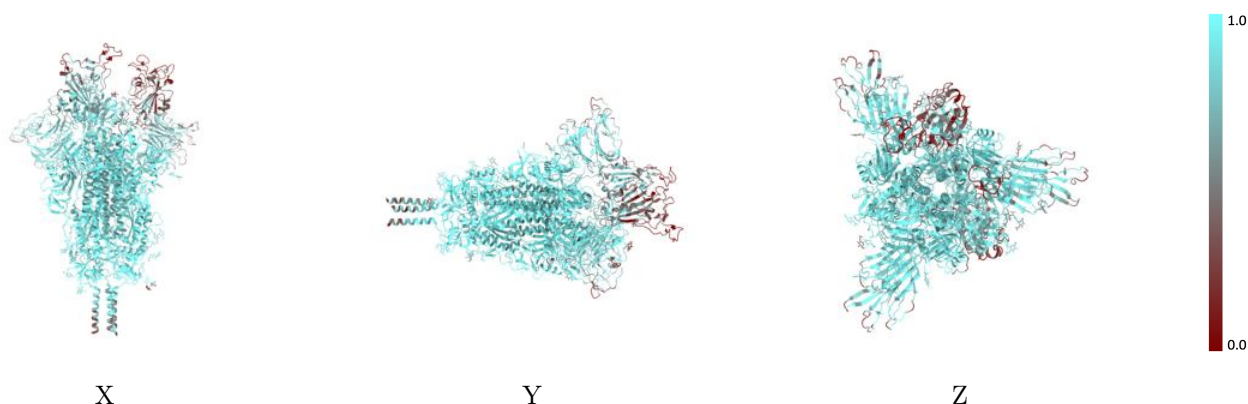
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



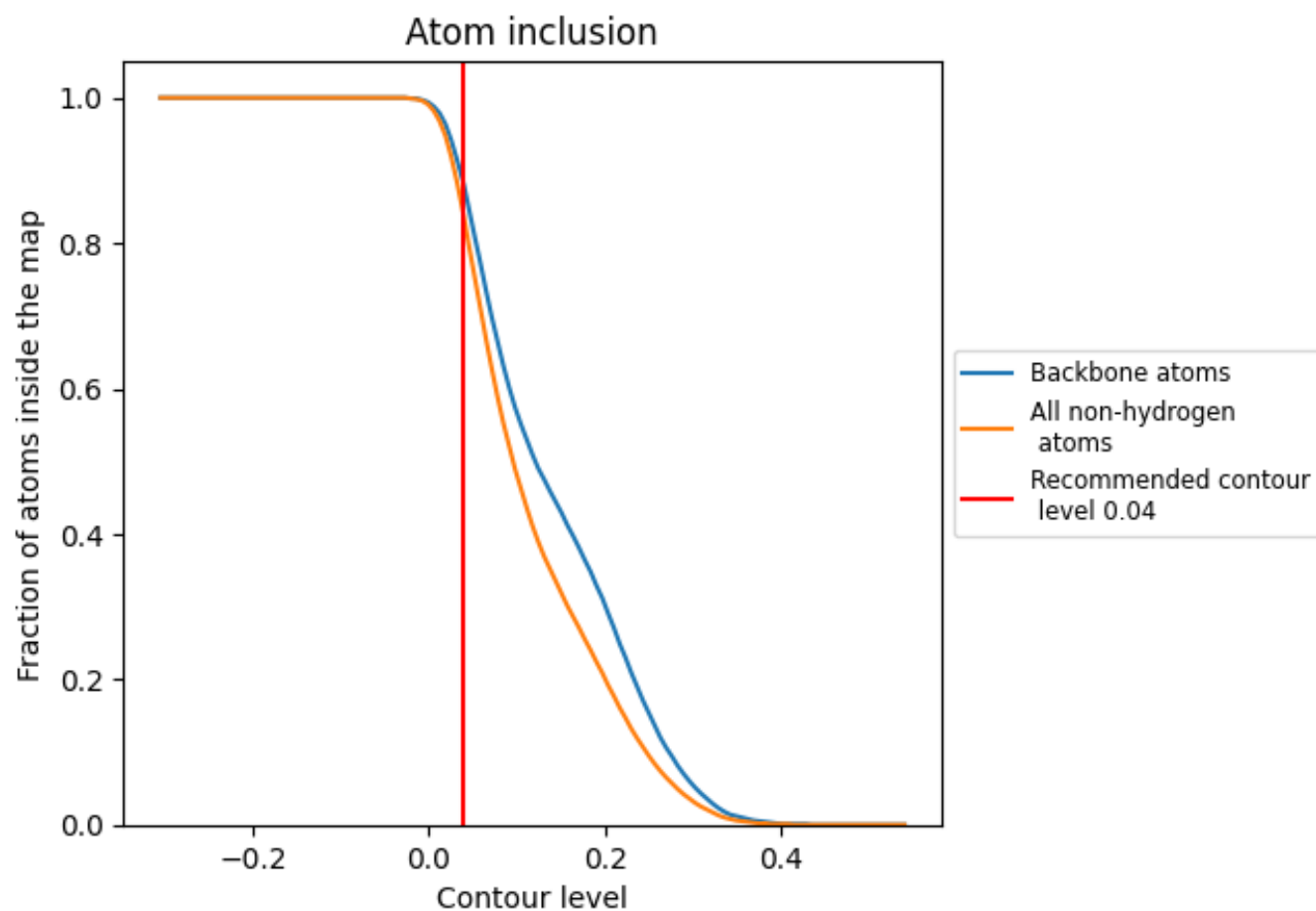
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

## 9.4 Atom inclusion [i](#)















































At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.3690
A	 0.8390	 0.3700
B	 0.7890	 0.3440
C	 0.8840	 0.3950
D	 0.6430	 0.2110
E	 0.6790	 0.2430
F	 0.8930	 0.3980
G	 0.9290	 0.4140
H	 0.8680	 0.3770
I	 0.8570	 0.2700
J	 0.8210	 0.1900
K	 0.5790	 0.2020
L	 0.6070	 0.2070
M	 0.6790	 0.2550
N	 0.8570	 0.2870
O	 0.9640	 0.4390
P	 0.8930	 0.4080
Q	 0.7500	 0.2790
R	 0.9290	 0.4890
S	 0.8210	 0.3350
T	 0.8680	 0.3610
U	 0.7140	 0.2550

