



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:33 PM UTC

PDB ID : 8WLY / pdb_00008wly
EMDB ID : EMD-37635
Title : Cryo-EM structure of bat WIV1 spike glycoprotein
Authors : Wang, X.; Qiao, S.
Deposited on : 2023-10-01
Resolution : 3.96 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

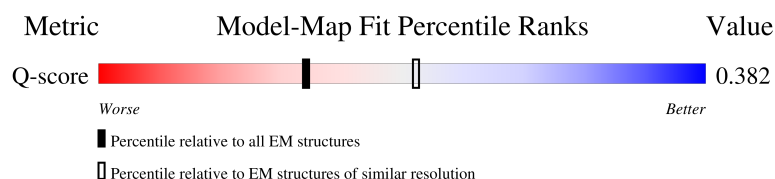
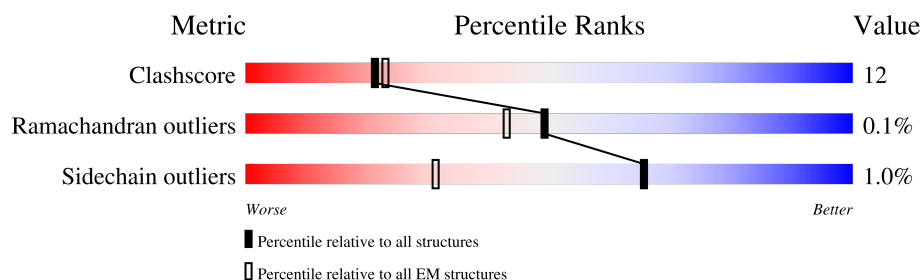
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.96 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	7646 (3.46 - 4.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1271	
1	B	1271	
1	C	1271	
2	D	2	

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22598 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	870	Total	C	N	O	S	0	0
			6757	4303	1128	1293	33		
1	B	1067	Total	C	N	O	S	0	0
			8325	5312	1386	1586	41		
1	C	871	Total	C	N	O	S	0	0
			6769	4312	1129	1295	33		

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	969	PRO	LYS	conflict	UNP U5WI05
A	970	PRO	VAL	conflict	UNP U5WI05
A	1192	GLY	-	linker	UNP U5WI05
A	1193	SER	-	linker	UNP U5WI05
A	1220	LEU	-	expression tag	UNP A0A346FJN8
A	1221	GLY	-	expression tag	UNP A0A346FJN8
A	1222	ARG	-	expression tag	UNP A0A346FJN8
A	1223	SER	-	expression tag	UNP A0A346FJN8
A	1224	LEU	-	expression tag	UNP A0A346FJN8
A	1225	GLU	-	expression tag	UNP A0A346FJN8
A	1226	VAL	-	expression tag	UNP A0A346FJN8
A	1227	LEU	-	expression tag	UNP A0A346FJN8
A	1228	PHE	-	expression tag	UNP A0A346FJN8
A	1229	GLN	-	expression tag	UNP A0A346FJN8
A	1230	GLY	-	expression tag	UNP A0A346FJN8
A	1231	PRO	-	expression tag	UNP A0A346FJN8
A	1232	GLY	-	expression tag	UNP A0A346FJN8
A	1233	HIS	-	expression tag	UNP A0A346FJN8
A	1234	HIS	-	expression tag	UNP A0A346FJN8
A	1235	HIS	-	expression tag	UNP A0A346FJN8
A	1236	HIS	-	expression tag	UNP A0A346FJN8
A	1237	HIS	-	expression tag	UNP A0A346FJN8
A	1238	HIS	-	expression tag	UNP A0A346FJN8
A	1239	HIS	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	HIS	-	expression tag	UNP A0A346FJN8
A	1241	SER	-	expression tag	UNP A0A346FJN8
A	1242	ALA	-	expression tag	UNP A0A346FJN8
A	1243	TRP	-	expression tag	UNP A0A346FJN8
A	1244	SER	-	expression tag	UNP A0A346FJN8
A	1245	HIS	-	expression tag	UNP A0A346FJN8
A	1246	PRO	-	expression tag	UNP A0A346FJN8
A	1247	GLN	-	expression tag	UNP A0A346FJN8
A	1248	PHE	-	expression tag	UNP A0A346FJN8
A	1249	GLU	-	expression tag	UNP A0A346FJN8
A	1250	LYS	-	expression tag	UNP A0A346FJN8
A	1251	GLY	-	expression tag	UNP A0A346FJN8
A	1252	GLY	-	expression tag	UNP A0A346FJN8
A	1253	GLY	-	expression tag	UNP A0A346FJN8
A	1254	SER	-	expression tag	UNP A0A346FJN8
A	1255	GLY	-	expression tag	UNP A0A346FJN8
A	1256	GLY	-	expression tag	UNP A0A346FJN8
A	1257	GLY	-	expression tag	UNP A0A346FJN8
A	1258	GLY	-	expression tag	UNP A0A346FJN8
A	1259	SER	-	expression tag	UNP A0A346FJN8
A	1260	GLY	-	expression tag	UNP A0A346FJN8
A	1261	GLY	-	expression tag	UNP A0A346FJN8
A	1262	SER	-	expression tag	UNP A0A346FJN8
A	1263	ALA	-	expression tag	UNP A0A346FJN8
A	1264	TRP	-	expression tag	UNP A0A346FJN8
A	1265	SER	-	expression tag	UNP A0A346FJN8
A	1266	HIS	-	expression tag	UNP A0A346FJN8
A	1267	PRO	-	expression tag	UNP A0A346FJN8
A	1268	GLN	-	expression tag	UNP A0A346FJN8
A	1269	PHE	-	expression tag	UNP A0A346FJN8
A	1270	GLU	-	expression tag	UNP A0A346FJN8
A	1271	LYS	-	expression tag	UNP A0A346FJN8
B	969	PRO	LYS	conflict	UNP U5WI05
B	970	PRO	VAL	conflict	UNP U5WI05
B	1192	GLY	-	linker	UNP U5WI05
B	1193	SER	-	linker	UNP U5WI05
B	1220	LEU	-	expression tag	UNP A0A346FJN8
B	1221	GLY	-	expression tag	UNP A0A346FJN8
B	1222	ARG	-	expression tag	UNP A0A346FJN8
B	1223	SER	-	expression tag	UNP A0A346FJN8
B	1224	LEU	-	expression tag	UNP A0A346FJN8
B	1225	GLU	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1226	VAL	-	expression tag	UNP A0A346FJN8
B	1227	LEU	-	expression tag	UNP A0A346FJN8
B	1228	PHE	-	expression tag	UNP A0A346FJN8
B	1229	GLN	-	expression tag	UNP A0A346FJN8
B	1230	GLY	-	expression tag	UNP A0A346FJN8
B	1231	PRO	-	expression tag	UNP A0A346FJN8
B	1232	GLY	-	expression tag	UNP A0A346FJN8
B	1233	HIS	-	expression tag	UNP A0A346FJN8
B	1234	HIS	-	expression tag	UNP A0A346FJN8
B	1235	HIS	-	expression tag	UNP A0A346FJN8
B	1236	HIS	-	expression tag	UNP A0A346FJN8
B	1237	HIS	-	expression tag	UNP A0A346FJN8
B	1238	HIS	-	expression tag	UNP A0A346FJN8
B	1239	HIS	-	expression tag	UNP A0A346FJN8
B	1240	HIS	-	expression tag	UNP A0A346FJN8
B	1241	SER	-	expression tag	UNP A0A346FJN8
B	1242	ALA	-	expression tag	UNP A0A346FJN8
B	1243	TRP	-	expression tag	UNP A0A346FJN8
B	1244	SER	-	expression tag	UNP A0A346FJN8
B	1245	HIS	-	expression tag	UNP A0A346FJN8
B	1246	PRO	-	expression tag	UNP A0A346FJN8
B	1247	GLN	-	expression tag	UNP A0A346FJN8
B	1248	PHE	-	expression tag	UNP A0A346FJN8
B	1249	GLU	-	expression tag	UNP A0A346FJN8
B	1250	LYS	-	expression tag	UNP A0A346FJN8
B	1251	GLY	-	expression tag	UNP A0A346FJN8
B	1252	GLY	-	expression tag	UNP A0A346FJN8
B	1253	GLY	-	expression tag	UNP A0A346FJN8
B	1254	SER	-	expression tag	UNP A0A346FJN8
B	1255	GLY	-	expression tag	UNP A0A346FJN8
B	1256	GLY	-	expression tag	UNP A0A346FJN8
B	1257	GLY	-	expression tag	UNP A0A346FJN8
B	1258	GLY	-	expression tag	UNP A0A346FJN8
B	1259	SER	-	expression tag	UNP A0A346FJN8
B	1260	GLY	-	expression tag	UNP A0A346FJN8
B	1261	GLY	-	expression tag	UNP A0A346FJN8
B	1262	SER	-	expression tag	UNP A0A346FJN8
B	1263	ALA	-	expression tag	UNP A0A346FJN8
B	1264	TRP	-	expression tag	UNP A0A346FJN8
B	1265	SER	-	expression tag	UNP A0A346FJN8
B	1266	HIS	-	expression tag	UNP A0A346FJN8
B	1267	PRO	-	expression tag	UNP A0A346FJN8

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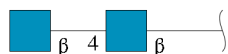
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B	1269	PHE	-	expression tag	UNP A0A346FJN8
B	1270	GLU	-	expression tag	UNP A0A346FJN8
B	1271	LYS	-	expression tag	UNP A0A346FJN8
C	969	PRO	LYS	conflict	UNP U5WI05
C	970	PRO	VAL	conflict	UNP U5WI05
C	1192	GLY	-	linker	UNP U5WI05
C	1193	SER	-	linker	UNP U5WI05
C	1220	LEU	-	expression tag	UNP A0A346FJN8
C	1221	GLY	-	expression tag	UNP A0A346FJN8
C	1222	ARG	-	expression tag	UNP A0A346FJN8
C	1223	SER	-	expression tag	UNP A0A346FJN8
C	1224	LEU	-	expression tag	UNP A0A346FJN8
C	1225	GLU	-	expression tag	UNP A0A346FJN8
C	1226	VAL	-	expression tag	UNP A0A346FJN8
C	1227	LEU	-	expression tag	UNP A0A346FJN8
C	1228	PHE	-	expression tag	UNP A0A346FJN8
C	1229	GLN	-	expression tag	UNP A0A346FJN8
C	1230	GLY	-	expression tag	UNP A0A346FJN8
C	1231	PRO	-	expression tag	UNP A0A346FJN8
C	1232	GLY	-	expression tag	UNP A0A346FJN8
C	1233	HIS	-	expression tag	UNP A0A346FJN8
C	1234	HIS	-	expression tag	UNP A0A346FJN8
C	1235	HIS	-	expression tag	UNP A0A346FJN8
C	1236	HIS	-	expression tag	UNP A0A346FJN8
C	1237	HIS	-	expression tag	UNP A0A346FJN8
C	1238	HIS	-	expression tag	UNP A0A346FJN8
C	1239	HIS	-	expression tag	UNP A0A346FJN8
C	1240	HIS	-	expression tag	UNP A0A346FJN8
C	1241	SER	-	expression tag	UNP A0A346FJN8
C	1242	ALA	-	expression tag	UNP A0A346FJN8
C	1243	TRP	-	expression tag	UNP A0A346FJN8
C	1244	SER	-	expression tag	UNP A0A346FJN8
C	1245	HIS	-	expression tag	UNP A0A346FJN8
C	1246	PRO	-	expression tag	UNP A0A346FJN8
C	1247	GLN	-	expression tag	UNP A0A346FJN8
C	1248	PHE	-	expression tag	UNP A0A346FJN8
C	1249	GLU	-	expression tag	UNP A0A346FJN8
C	1250	LYS	-	expression tag	UNP A0A346FJN8
C	1251	GLY	-	expression tag	UNP A0A346FJN8
C	1252	GLY	-	expression tag	UNP A0A346FJN8
C	1253	GLY	-	expression tag	UNP A0A346FJN8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1254	SER	-	expression tag	UNP A0A346FJN8
C	1255	GLY	-	expression tag	UNP A0A346FJN8
C	1256	GLY	-	expression tag	UNP A0A346FJN8
C	1257	GLY	-	expression tag	UNP A0A346FJN8
C	1258	GLY	-	expression tag	UNP A0A346FJN8
C	1259	SER	-	expression tag	UNP A0A346FJN8
C	1260	GLY	-	expression tag	UNP A0A346FJN8
C	1261	GLY	-	expression tag	UNP A0A346FJN8
C	1262	SER	-	expression tag	UNP A0A346FJN8
C	1263	ALA	-	expression tag	UNP A0A346FJN8
C	1264	TRP	-	expression tag	UNP A0A346FJN8
C	1265	SER	-	expression tag	UNP A0A346FJN8
C	1266	HIS	-	expression tag	UNP A0A346FJN8
C	1267	PRO	-	expression tag	UNP A0A346FJN8
C	1268	GLN	-	expression tag	UNP A0A346FJN8
C	1269	PHE	-	expression tag	UNP A0A346FJN8
C	1270	GLU	-	expression tag	UNP A0A346FJN8
C	1271	LYS	-	expression tag	UNP A0A346FJN8

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



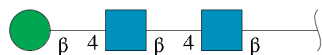
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
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	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		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

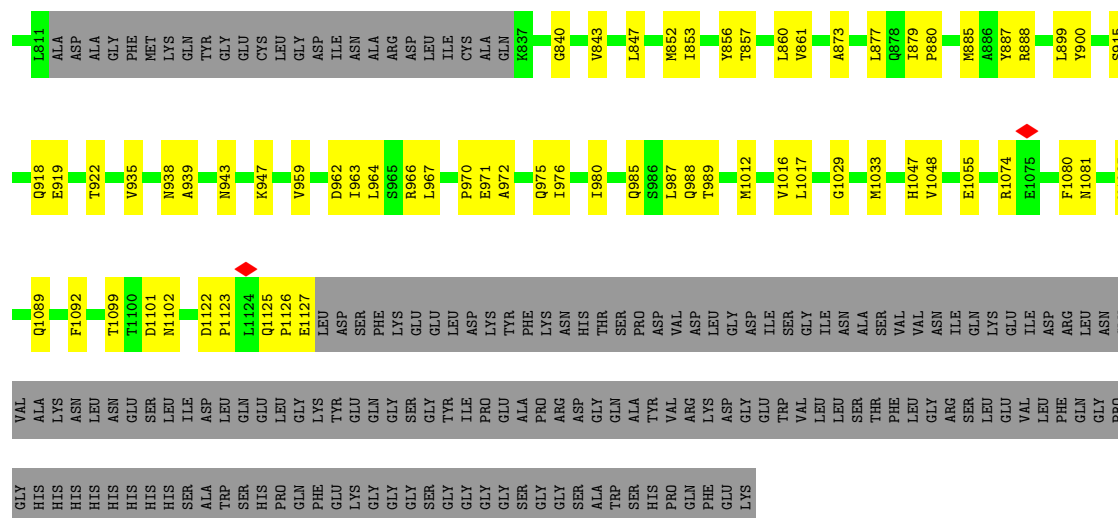


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4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

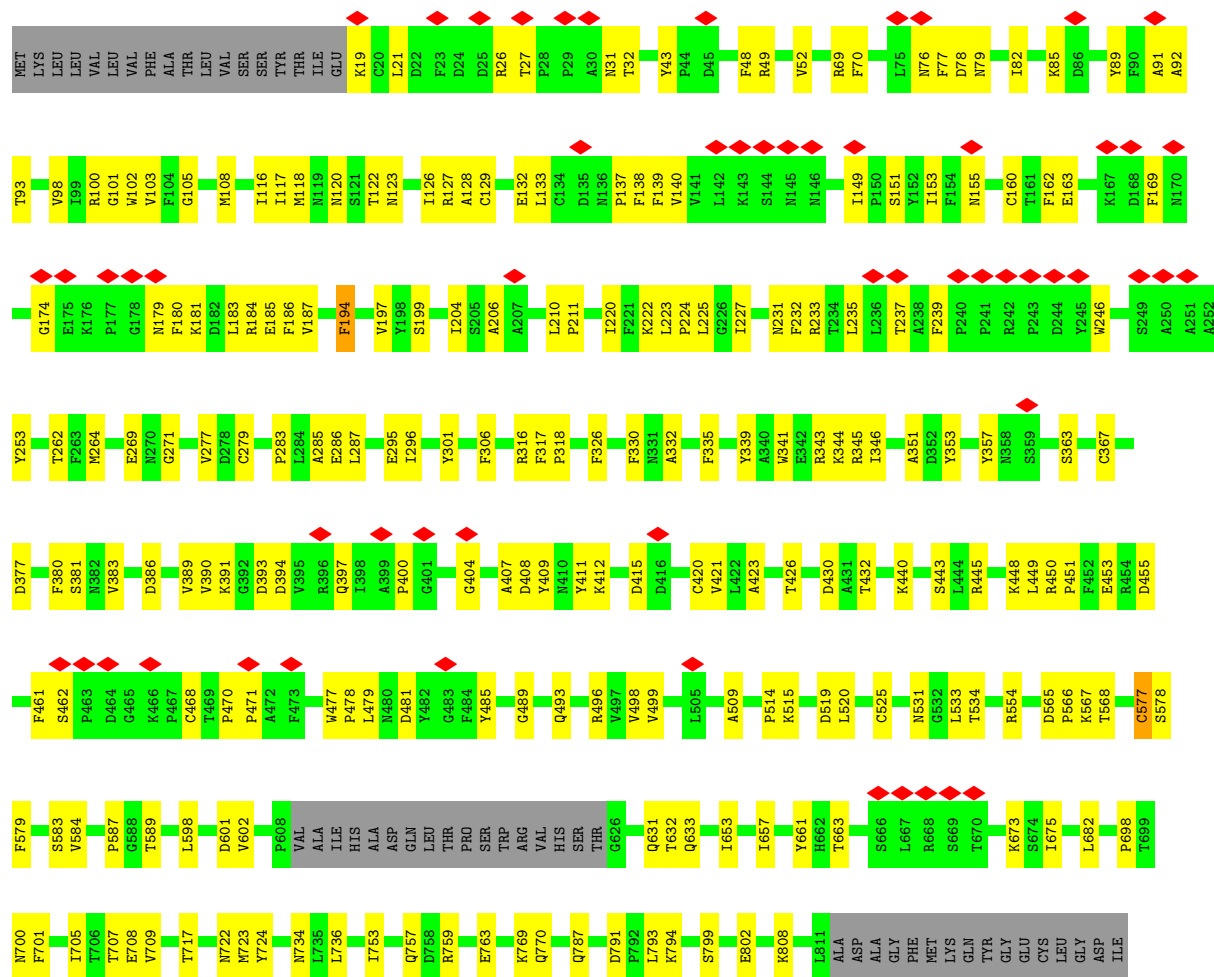
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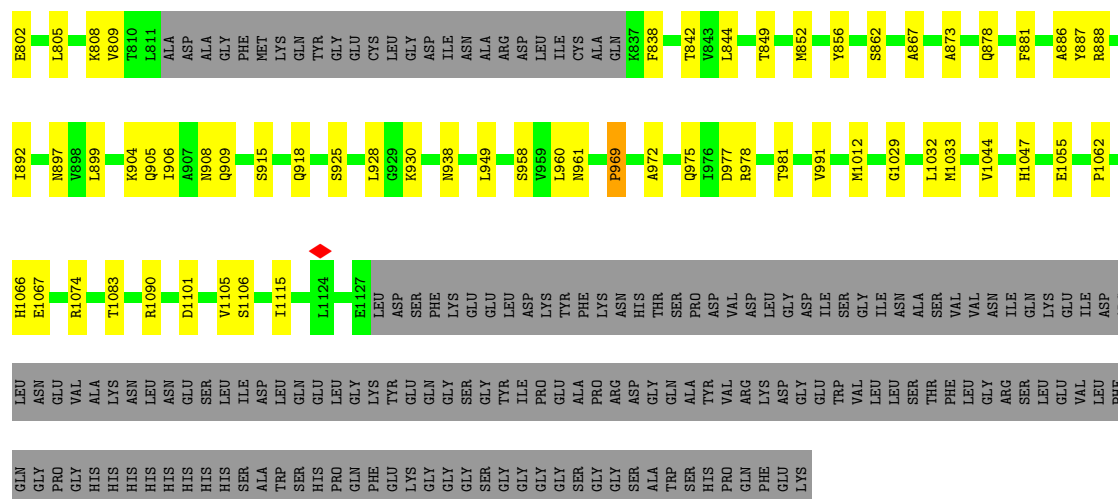
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

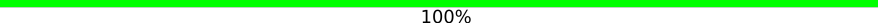


• Molecule 1: Spike glycoprotein, Fibrin





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

Chain D:  100%



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

Chain E:  50%

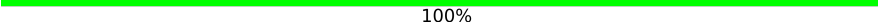


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50%



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

Chain G:  100%



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

Chain H:  50%



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

Chain I:  50% 50%

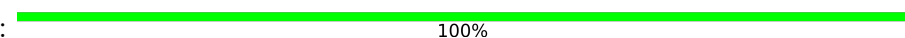


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100% 50% 50%



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

Chain M:  100%



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

Chain N:  50% 50%

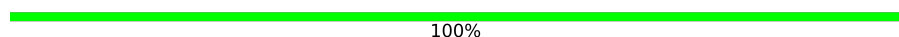


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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 R:  50% 50%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

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

Chain K:  100%

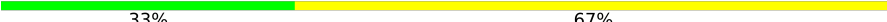
MAG1
MAG2
BMA3

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

Chain L:  100%

MAG1
MAG2
BMA3

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

Chain Q:  33% 67%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59319	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0106	Depositor
Map size ($\text{\AA}$)	300.776, 300.776, 300.776	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.21	0/6907	0.45	0/9391
1	B	0.21	0/8527	0.50	5/11611 (0.0%)
1	C	0.26	0/6921	0.58	8/9412 (0.1%)
All	All	0.23	0/22355	0.51	13/30414 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	734	ASN	N-CA-C	-9.56	100.94	111.36
1	B	578	SER	N-CA-C	8.99	123.79	111.39
1	C	119	ASN	N-CA-C	-8.74	96.21	108.54
1	C	740	GLY	N-CA-C	8.54	121.35	111.36
1	B	724	TYR	N-CA-C	-8.25	101.06	112.12
1	B	577	CYS	N-CA-C	7.92	123.22	107.62
1	C	734	ASN	N-CA-C	-7.89	102.62	111.14
1	C	725	ILE	N-CA-C	6.84	116.96	110.53
1	C	240	PRO	CA-C-N	-6.00	113.50	119.56
1	C	240	PRO	C-N-CA	-6.00	113.50	119.56
1	C	120	ASN	N-CA-C	5.92	117.74	111.28
1	C	969	PRO	N-CA-C	5.66	117.60	110.70
1	B	954	GLY	N-CA-C	-5.12	108.26	115.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6757	0	6607	189	0
1	B	8325	0	8085	205	0
1	C	6769	0	6611	160	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	O	28	0	25	1	0
2	P	28	0	25	0	0
2	R	28	0	25	1	0
2	S	28	0	25	0	0
3	K	39	0	34	0	0
3	L	39	0	34	0	0
3	Q	39	0	34	1	0
4	A	56	0	52	1	0
4	B	84	0	78	0	0
4	C	126	0	117	2	0
All	All	22598	0	21977	527	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (527) 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:A:128:ALA:HB3	1:A:162:PHE:HB3	1.52	0.90
1:A:315:VAL:HG23	1:A:529:ASN:HB3	1.55	0.86
1:A:69:ARG:HH22	1:A:210:LEU:HB2	1.46	0.80
1:A:1099:THR:HG22	1:A:1101:ASP:H	1.47	0.80
1:A:852:MET:HG2	1:C:682:LEU:HD21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ILE:HD11	1:C:231:ASN:HB2	1.67	0.76
1:C:598:LEU:HD11	1:C:653:ILE:HG23	1.67	0.76
1:A:104:PHE:HB2	1:A:115:VAL:HG22	1.69	0.75
1:B:663:THR:HA	1:B:673:LYS:HA	1.68	0.75
1:C:27:THR:HB	1:C:76:ASN:HB3	1.69	0.75
1:C:599:TYR:O	1:C:635:GLY:HA3	1.87	0.74
1:A:629:VAL:HG13	1:A:638:ILE:HG13	1.70	0.74
1:A:36:SER:HB3	1:A:65:SER:H	1.53	0.74
1:B:377:ASP:HA	1:B:515:LYS:HD2	1.70	0.74
1:C:39:ARG:HH22	1:C:202:GLN:HE22	1.37	0.73
1:C:522:LYS:HD3	1:C:541:PRO:HD3	1.71	0.72
1:A:104:PHE:HB3	1:A:229:ILE:HG21	1.71	0.72
1:B:129:CYS:SG	1:B:160:CYS:N	2.63	0.71
1:B:128:ALA:HB3	1:B:162:PHE:HB3	1.73	0.71
1:B:264:MET:HB3	1:B:277:VAL:HG22	1.72	0.71
1:A:959:VAL:HG12	1:A:962:ASP:H	1.55	0.70
1:B:448:LYS:HB3	1:B:448:LYS:HZ2	1.55	0.70
1:B:79:ASN:O	1:B:233:ARG:NH2	2.26	0.68
1:B:404:GLY:O	1:B:408:ASP:N	2.25	0.68
1:B:326:PHE:HB3	1:B:330:PHE:CE2	2.29	0.67
1:C:115:VAL:HG21	1:C:225:LEU:HD13	1.75	0.67
1:A:656:GLY:HA3	1:B:852:MET:HE1	1.76	0.67
1:A:69:ARG:NH2	1:A:210:LEU:HB2	2.10	0.67
1:B:391:LYS:HE3	1:B:393:ASP:HB2	1.77	0.66
1:C:774:THR:HG23	1:C:789:LEU:HD22	1.77	0.66
1:A:118:MET:HE1	1:A:125:VAL:HB	1.77	0.65
1:B:194:PHE:CE2	1:B:222:LYS:HG2	2.31	0.65
1:B:117:ILE:HG23	1:B:126:ILE:HG12	1.79	0.65
1:A:189:ARG:NH2	1:A:190:ASN:O	2.29	0.65
1:C:32:THR:HG23	1:C:69:ARG:HB3	1.78	0.65
1:B:98:VAL:HG13	1:B:237:THR:HG22	1.79	0.65
1:A:77:PHE:HE1	1:A:79:ASN:HB2	1.62	0.64
1:B:326:PHE:HB3	1:B:330:PHE:HE2	1.62	0.64
1:B:705:ILE:HD12	1:B:1048:VAL:HG22	1.79	0.64
1:C:746:LEU:HD22	1:C:991:VAL:HG21	1.79	0.64
1:A:1029:GLY:HA2	1:B:873:ALA:HB1	1.80	0.64
1:A:561:ASP:O	1:A:574:ILE:N	2.28	0.63
1:C:298:LYS:HG2	1:C:651:ILE:HD11	1.80	0.63
1:B:122:THR:O	1:B:169:PHE:N	2.32	0.63
1:C:195:LEU:HD12	1:C:225:LEU:HD12	1.80	0.63
1:A:682:LEU:HD11	1:B:852:MET:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HB	1:B:233:ARG:HG2	1.80	0.63
1:C:975:GLN:OE1	1:C:978:ARG:NH2	2.32	0.62
1:B:972:ALA:O	1:B:976:ILE:HG13	2.00	0.62
1:C:314:VAL:HB	1:C:316:ARG:HH12	1.64	0.62
1:C:794:LYS:NZ	1:C:798:ARG:O	2.32	0.62
1:A:122:THR:HB	1:A:168:ASP:HB3	1.82	0.62
1:A:533:LEU:HD11	1:A:560:THR:HG21	1.81	0.62
1:C:62:PRO:HG2	1:C:259:LYS:HD3	1.81	0.62
1:C:709:VAL:HG22	1:C:1044:VAL:HG22	1.81	0.62
1:A:585:ILE:HG23	1:A:651:ILE:HG21	1.80	0.61
1:A:879:ILE:HG13	1:C:695:ILE:HD13	1.82	0.61
1:B:430:ASP:OD1	1:B:496:ARG:NH2	2.34	0.61
1:C:307:ARG:HH11	1:C:579:PHE:HB3	1.64	0.61
1:C:24:ASP:H	1:C:246:TRP:HZ3	1.45	0.61
1:B:103:VAL:HG23	1:B:235:LEU:HD11	1.81	0.61
1:B:1074:ARG:HG2	1:B:1075:GLU:HG2	1.83	0.61
1:C:29:PRO:HG3	1:C:78:ASP:HB3	1.81	0.61
1:B:440:LYS:HG2	1:B:481:ASP:HB3	1.83	0.60
1:A:717:THR:HG22	1:A:843:VAL:HG22	1.82	0.60
1:B:76:ASN:ND2	1:B:78:ASP:OD2	2.34	0.60
1:B:363:SER:N	1:B:423:ALA:O	2.34	0.60
1:B:969:PRO:HG2	1:B:970:PRO:HD3	1.83	0.60
1:C:1105:VAL:HG23	1:C:1106:SER:H	1.67	0.60
1:B:421:VAL:HG22	1:B:499:VAL:HG22	1.82	0.59
1:B:860:LEU:HD13	1:B:1012:MET:HE2	1.84	0.59
1:B:21:LEU:HB2	1:B:138:PHE:HZ	1.68	0.59
1:A:915:SER:O	1:A:919:GLU:HG2	2.03	0.58
1:B:477:TRP:HE3	1:B:478:PRO:HD2	1.68	0.58
1:B:204:ILE:HG21	1:B:211:PRO:HG3	1.85	0.58
1:A:115:VAL:HG11	1:A:225:LEU:HD13	1.85	0.58
1:C:641:GLU:OE2	1:C:641:GLU:N	2.35	0.58
1:A:101:GLY:HA3	1:A:117:ILE:O	2.04	0.58
1:C:87:GLY:HA2	1:C:188:PHE:O	2.03	0.58
1:C:265:LEU:HD23	1:C:273:ILE:HD13	1.85	0.58
1:A:34:PHE:HD1	1:A:69:ARG:HG3	1.69	0.57
1:A:307:ARG:HE	1:A:308:VAL:H	1.49	0.57
1:B:225:LEU:HB3	1:B:227:ILE:HG12	1.86	0.57
1:A:236:LEU:HD11	1:A:253:TYR:CE1	2.39	0.57
1:C:202:GLN:OE1	1:C:215:ASN:ND2	2.37	0.57
1:A:972:ALA:O	1:A:976:ILE:HG12	2.03	0.57
1:C:316:ARG:NH1	1:C:519:ASP:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:HIS:CE1	1:C:260:PRO:HB3	2.39	0.57
1:A:100:ARG:HH21	1:A:141:VAL:HG21	1.70	0.57
1:B:914:ILE:O	1:B:917:ILE:HG22	2.03	0.57
1:A:34:PHE:HB2	1:A:69:ARG:NE	2.20	0.57
1:A:97:ASN:ND2	1:A:172:ASP:O	2.35	0.57
1:A:196:HIS:HB3	1:A:198:TYR:HE1	1.70	0.57
1:A:287:LEU:HD12	1:A:584:VAL:HB	1.86	0.56
1:A:726:CYS:SG	1:A:733:ALA:N	2.78	0.56
2:F:2:NAG:H3	2:F:2:NAG:H83	1.85	0.56
1:A:36:SER:HB2	1:A:67:VAL:HG21	1.86	0.56
1:A:55:LEU:HD12	1:A:264:MET:HG2	1.87	0.56
1:A:57:GLN:HG2	1:A:262:THR:HG22	1.86	0.56
1:A:985:GLN:O	1:A:989:THR:HG23	2.05	0.56
1:B:101:GLY:HA3	1:B:117:ILE:O	2.05	0.56
1:B:194:PHE:HE2	1:B:222:LYS:HG2	1.70	0.56
1:A:853:ILE:O	1:A:857:THR:HG23	2.04	0.56
1:B:103:VAL:HG22	1:B:116:ILE:HG12	1.88	0.56
1:A:880:PRO:HA	1:C:690:TYR:HE1	1.69	0.56
1:A:295:GLU:HA	1:A:589:THR:HG21	1.87	0.56
1:C:888:ARG:O	1:C:892:ILE:HD12	2.05	0.56
1:B:132:GLU:OE2	1:B:155:ASN:ND2	2.33	0.56
1:C:304:SER:OG	1:C:305:ASN:N	2.34	0.56
1:C:1074:ARG:NH2	1:C:1101:ASP:O	2.35	0.56
1:A:129:CYS:SG	1:A:160:CYS:N	2.78	0.56
1:A:198:TYR:CE2	1:A:219:PRO:HB3	2.41	0.56
1:B:341:TRP:CZ3	1:B:343:ARG:HB2	2.40	0.56
1:A:746:LEU:HD21	1:A:988:GLN:HG2	1.88	0.55
1:B:140:VAL:HB	1:B:149:ILE:HB	1.87	0.55
1:A:138:PHE:CE2	1:A:140:VAL:HG22	2.41	0.55
1:B:199:SER:HB3	1:B:220:ILE:HG21	1.88	0.55
1:B:793:LEU:HB2	1:B:794:LYS:HZ2	1.72	0.55
1:B:793:LEU:HB2	1:B:794:LYS:NZ	2.21	0.55
1:A:287:LEU:HD11	1:A:301:TYR:HD2	1.71	0.55
1:A:791:ASP:HB2	1:A:794:LYS:HD2	1.88	0.55
1:B:477:TRP:CE3	1:B:478:PRO:HD2	2.42	0.55
1:A:530:PHE:HE1	1:A:572:LEU:HD12	1.71	0.55
1:A:705:ILE:HA	1:A:1047:HIS:O	2.07	0.55
1:B:27:THR:O	1:B:76:ASN:ND2	2.39	0.55
1:B:1059:THR:HB	1:B:1080:PHE:HB3	1.88	0.55
1:B:1104:PHE:HE2	1:C:897:ASN:HD21	1.55	0.55
1:B:1036:PRO:O	1:B:1037:GLN:NE2	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:SER:OG	1:C:842:THR:OG1	2.22	0.55
1:A:113:GLN:HB2	1:A:227:ILE:HG21	1.88	0.55
1:A:98:VAL:HA	1:A:237:THR:HG22	1.89	0.55
1:B:180:PHE:HB2	1:B:206:ALA:HB3	1.88	0.54
1:B:791:ASP:HB2	1:B:794:LYS:HG2	1.88	0.54
1:B:915:SER:O	1:B:919:GLU:HG3	2.07	0.54
1:B:137:PRO:HB3	1:B:153:ILE:HG23	1.90	0.54
1:B:400:PRO:HB3	1:B:415:ASP:HA	1.90	0.54
1:A:262:THR:OG1	1:A:279:CYS:SG	2.65	0.54
1:C:299:GLY:HA2	1:C:651:ILE:HD12	1.88	0.54
1:B:91:ALA:HB1	1:B:183:LEU:HD11	1.89	0.54
1:A:1122:ASP:OD2	1:A:1125:GLN:NE2	2.41	0.54
1:B:117:ILE:HG12	1:B:126:ILE:HG23	1.90	0.54
1:B:318:PRO:HA	1:B:567:LYS:HZ3	1.72	0.53
1:B:381:SER:HB3	1:B:509:ALA:HA	1.91	0.53
1:A:1081:ASN:ND2	2:E:1:NAG:O7	2.42	0.53
1:C:126:ILE:HG12	1:C:164:TYR:HD2	1.73	0.53
1:C:802:GLU:HA	1:C:805:LEU:HD12	1.89	0.53
1:B:102:TRP:HD1	1:B:232:PHE:HE1	1.57	0.53
1:A:552:PHE:O	1:B:48:PHE:N	2.25	0.53
1:A:731:GLU:OE2	1:A:964:LEU:HD22	2.09	0.53
1:B:707:THR:HG22	1:B:917:ILE:HD11	1.91	0.53
1:C:805:LEU:O	1:C:809:VAL:HG12	2.09	0.53
1:B:583:SER:OG	1:B:598:LEU:HB3	2.09	0.52
1:C:59:HIS:HB2	1:C:189:ARG:NH1	2.24	0.52
1:C:714:MET:HB2	1:C:938:ASN:HD21	1.74	0.52
1:C:733:ALA:HA	1:C:736:LEU:HB3	1.89	0.52
1:A:522:LYS:NZ	1:A:541:PRO:HG3	2.24	0.52
1:A:663:THR:HA	1:A:673:LYS:HA	1.91	0.52
1:C:200:GLY:HA3	1:C:217:LEU:HD22	1.91	0.52
1:A:553:GLY:N	1:A:562:SER:O	2.42	0.52
1:A:691:SER:HB3	1:A:694:THR:HG22	1.91	0.52
1:C:287:LEU:HD13	1:C:584:VAL:HB	1.90	0.52
1:A:104:PHE:HB3	1:A:229:ILE:HD13	1.91	0.52
1:A:121:SER:HA	1:A:171:LEU:HB3	1.91	0.52
1:A:1016:VAL:HG12	1:A:1017:LEU:HD23	1.92	0.52
1:B:89:TYR:HE1	1:B:185:GLU:HB3	1.75	0.52
1:B:717:THR:HG22	1:B:843:VAL:HG22	1.92	0.52
1:C:269:GLU:OE1	2:O:1:NAG:N2	2.40	0.52
1:C:307:ARG:NH1	1:C:578:SER:O	2.43	0.52
1:C:767:GLN:HG3	1:C:1012:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:ARG:HD3	1:A:1033:MET:HG2	1.91	0.52
1:C:39:ARG:NH1	1:C:185:GLU:OE2	2.43	0.52
1:C:317:PHE:HE2	1:C:516:LEU:HA	1.74	0.52
1:C:888:ARG:HD3	1:C:1032:LEU:O	2.09	0.52
1:A:663:THR:HB	1:A:673:LYS:HG2	1.91	0.51
1:C:305:ASN:HA	1:C:581:GLY:HA2	1.92	0.51
1:B:633:GLN:H	1:B:633:GLN:CD	2.19	0.51
1:B:948:GLN:HG2	1:B:986:SER:OG	2.10	0.51
1:A:1125:GLN:HG3	1:A:1126:PRO:HD3	1.92	0.51
1:B:426:THR:HG21	1:B:496:ARG:HG3	1.92	0.51
1:B:102:TRP:HD1	1:B:232:PHE:CE1	2.28	0.51
1:A:54:HIS:CE1	1:A:56:VAL:HB	2.45	0.51
1:A:318:PRO:HD3	1:A:531:ASN:HA	1.92	0.51
1:B:1029:GLY:HA2	1:C:873:ALA:HB1	1.92	0.51
1:C:808:LYS:HZ1	1:C:925:SER:H	1.58	0.51
1:A:200:GLY:HA3	1:A:217:LEU:HD22	1.92	0.51
1:B:390:VAL:HB	1:B:394:ASP:HB2	1.92	0.51
1:B:1031:HIS:HA	1:B:1049:THR:HG22	1.92	0.51
1:B:103:VAL:HG12	1:B:108:MET:HE2	1.93	0.51
1:A:268:ASP:OD1	1:A:272:THR:N	2.41	0.51
1:B:977:ASP:HA	1:B:980:ILE:HG22	1.92	0.51
1:A:264:MET:SD	1:A:289:CYS:HA	2.51	0.51
1:B:326:PHE:CE1	1:B:346:ILE:HG21	2.46	0.51
1:B:682:LEU:HD21	1:C:852:MET:HG2	1.92	0.51
1:A:1089:GLN:HE21	1:A:1092:PHE:HB3	1.76	0.51
1:B:339:TYR:HE1	1:B:440:LYS:HB2	1.76	0.51
1:B:1090:ARG:NH2	1:C:887:TYR:HB2	2.26	0.51
1:C:718:SER:HB3	1:C:844:LEU:HD11	1.93	0.51
1:C:516:LEU:HG	1:C:517:SER:H	1.76	0.50
1:C:588:GLY:O	1:C:591:THR:N	2.43	0.50
1:A:179:ASN:HB3	1:A:181:LYS:HG2	1.94	0.50
1:C:69:ARG:NH2	1:C:208:SER:O	2.28	0.50
1:B:82:ILE:HD12	1:B:232:PHE:CE2	2.47	0.50
1:C:653:ILE:HD11	1:C:659:ALA:HB2	1.92	0.50
1:A:189:ARG:HH21	1:A:191:LYS:HG3	1.75	0.50
1:C:162:PHE:HE2	1:C:224:PRO:HD2	1.77	0.50
1:C:668:ARG:CD	1:C:669:SER:H	2.25	0.50
1:A:719:VAL:HG11	1:A:987:LEU:HD11	1.93	0.50
1:C:809:VAL:HB	1:C:928:LEU:HD23	1.94	0.50
1:A:918:GLN:O	1:A:922:THR:OG1	2.21	0.50
1:A:34:PHE:H	1:A:69:ARG:HD3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ALA:O	1:B:514:PRO:HD3	2.11	0.50
1:C:314:VAL:HG23	1:C:528:PHE:HA	1.94	0.50
1:A:104:PHE:HB2	1:A:115:VAL:CG2	2.40	0.50
1:A:118:MET:HB3	1:A:139:PHE:HZ	1.77	0.50
1:B:346:ILE:HB	1:B:383:VAL:HG13	1.94	0.50
1:B:682:LEU:HB3	1:C:856:TYR:CZ	2.47	0.50
1:B:968:ASP:OD1	1:B:969:PRO:HD2	2.12	0.50
1:B:1073:PRO:HD3	1:B:1078:PHE:CE2	2.47	0.50
1:A:59:HIS:O	1:A:258:LEU:HD12	2.12	0.49
1:C:246:TRP:CD1	1:C:246:TRP:N	2.80	0.49
1:C:599:TYR:HB3	1:C:602:VAL:HG22	1.93	0.49
1:B:210:LEU:HD12	1:B:211:PRO:HD2	1.94	0.49
1:B:885:MET:HG3	1:B:899:LEU:HD11	1.94	0.49
1:A:27:THR:N	1:A:76:ASN:OD1	2.45	0.49
1:B:326:PHE:HE1	1:B:346:ILE:HG21	1.77	0.49
1:B:332:ALA:HB3	1:B:335:PHE:CE1	2.47	0.49
1:C:239:PHE:N	1:C:247:GLY:O	2.44	0.49
1:C:791:ASP:HB2	1:C:794:LYS:HG2	1.94	0.49
1:A:99:ILE:CD1	1:A:253:TYR:HB3	2.43	0.49
1:A:115:VAL:HG12	1:A:128:ALA:HB2	1.94	0.49
1:B:269:GLU:HB3	2:N:1:NAG:H82	1.94	0.49
1:B:301:TYR:O	1:B:584:VAL:N	2.35	0.49
1:B:397:GLN:HE21	1:B:407:ALA:HB2	1.77	0.49
1:C:563:VAL:HB	1:C:574:ILE:HD11	1.94	0.49
1:B:264:MET:HE2	1:B:264:MET:HA	1.95	0.49
1:C:287:LEU:HD11	1:C:301:TYR:HB3	1.95	0.49
1:A:115:VAL:HA	1:A:128:ALA:HA	1.94	0.49
1:A:129:CYS:HA	1:A:160:CYS:HA	1.94	0.49
1:A:1080:PHE:HB2	1:A:1085:TRP:CZ3	2.48	0.49
1:B:579:PHE:HB2	1:C:838:PHE:CZ	2.48	0.49
1:B:389:VAL:HG22	1:B:496:ARG:HG2	1.95	0.49
1:C:181:LYS:HA	1:C:205:SER:HB3	1.94	0.49
1:C:886:ALA:HB2	1:C:899:LEU:HD22	1.95	0.49
1:C:284:LEU:HB2	1:C:595:VAL:HG11	1.94	0.49
1:A:287:LEU:HD11	1:A:301:TYR:CD2	2.46	0.48
1:B:409:TYR:CD2	1:B:445:ARG:HB3	2.48	0.48
1:B:1087:ILE:HG21	1:B:1102:ASN:HB3	1.94	0.48
1:C:51:ASN:CA	1:C:267:TYR:O	2.61	0.48
1:C:51:ASN:N	1:C:267:TYR:O	2.46	0.48
1:C:312:LYS:HD3	1:C:521:ILE:HG13	1.96	0.48
1:A:202:GLN:OE1	1:A:215:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:MET:HE1	1:C:656:GLY:HA3	1.96	0.48
1:B:100:ARG:HB2	1:B:139:PHE:HE2	1.78	0.48
1:B:102:TRP:CD1	1:B:232:PHE:HE1	2.31	0.48
1:C:129:CYS:HB3	1:C:131:PHE:CE2	2.48	0.48
1:A:308:VAL:HB	1:A:577:CYS:SG	2.54	0.48
1:A:628:ASN:ND2	1:A:641:GLU:HG3	2.27	0.48
1:B:736:LEU:HG	1:B:980:ILE:HD11	1.96	0.48
1:B:960:LEU:HD23	1:B:960:LEU:H	1.78	0.48
1:C:142:LEU:HD21	1:C:149:ILE:CD1	2.44	0.48
1:C:156:ASN:OD1	1:C:156:ASN:N	2.46	0.48
1:C:709:VAL:O	1:C:930:LYS:NZ	2.30	0.48
1:A:185:GLU:O	1:A:199:SER:HA	2.13	0.48
1:C:977:ASP:OD1	1:C:978:ARG:N	2.47	0.48
1:B:26:ARG:HD2	1:B:77:PHE:HD2	1.78	0.48
1:C:522:LYS:HB2	1:C:522:LYS:HE2	1.53	0.48
1:C:881:PHE:CE1	1:C:1033:MET:HE1	2.49	0.48
1:A:95:LYS:NZ	1:A:250:ALA:O	2.40	0.47
1:B:187:VAL:O	1:B:197:VAL:HA	2.14	0.47
1:A:559:PHE:HZ	1:B:946:VAL:HG11	1.79	0.47
1:B:890:ASN:HD22	1:B:890:ASN:HA	1.51	0.47
1:B:698:PRO:HA	1:B:1055:GLU:HA	1.95	0.47
1:A:100:ARG:HH22	1:A:173:LEU:HB3	1.80	0.47
1:C:561:ASP:O	1:C:574:ILE:N	2.36	0.47
1:C:698:PRO:HA	1:C:1055:GLU:HA	1.96	0.47
1:A:522:LYS:HD3	1:A:541:PRO:HD3	1.97	0.47
1:A:21:LEU:HD23	1:A:21:LEU:H	1.80	0.47
1:A:970:PRO:HB2	1:A:971:GLU:OE2	2.15	0.47
1:B:317:PHE:O	1:B:567:LYS:HD3	2.14	0.47
1:B:450:ARG:HB2	1:B:453:GLU:HG3	1.97	0.47
1:A:108:MET:SD	1:A:133:LEU:HG	2.55	0.47
1:C:51:ASN:HA	1:C:267:TYR:O	2.15	0.47
1:C:70:PHE:HB2	1:C:253:TYR:CZ	2.50	0.47
1:C:1066:HIS:CD2	1:C:1067:GLU:HB2	2.50	0.47
1:A:72:THR:O	1:A:72:THR:HG23	2.14	0.47
1:B:661:TYR:HD1	1:B:675:ILE:HG12	1.80	0.47
1:C:627:ASN:OD1	1:C:627:ASN:N	2.48	0.47
1:C:958:SER:O	1:C:958:SER:OG	2.32	0.47
1:B:27:THR:HB	1:B:76:ASN:HA	1.97	0.47
1:A:847:LEU:HD12	1:C:654:GLY:HA2	1.97	0.47
1:B:330:PHE:CD1	1:B:498:VAL:HG21	2.50	0.47
1:B:332:ALA:HB3	1:B:335:PHE:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:NH1	1:A:565:ASP:OD1	2.49	0.46
1:B:554:ARG:HG3	1:C:47:ILE:HG21	1.97	0.46
1:C:668:ARG:HD3	1:C:669:SER:H	1.80	0.46
1:C:905:GLN:O	1:C:909:GLN:HG3	2.16	0.46
1:A:316:ARG:HG2	1:A:566:PRO:HG2	1.97	0.46
1:B:105:GLY:O	1:B:231:ASN:HB3	2.16	0.46
1:B:587:PRO:HG3	1:B:661:TYR:CD1	2.49	0.46
1:B:957:SER:O	1:B:963:ILE:HD11	2.15	0.46
1:A:307:ARG:HD2	1:A:307:ARG:HA	1.72	0.46
1:A:963:ILE:HD13	1:A:975:GLN:HB3	1.97	0.46
1:C:892:ILE:HD12	1:C:892:ILE:H	1.80	0.46
1:A:774:THR:HG21	1:A:790:PRO:HG2	1.97	0.46
1:A:880:PRO:HA	1:C:690:TYR:CE1	2.49	0.46
1:A:1099:THR:HG23	1:A:1123:PRO:HD3	1.97	0.46
1:B:601:ASP:OD1	1:C:842:THR:HG21	2.15	0.46
1:A:705:ILE:HG12	1:A:1048:VAL:HG22	1.97	0.46
1:B:174:GLY:HA2	1:B:239:PHE:HE2	1.81	0.46
1:B:808:LYS:HA	1:B:808:LYS:HD3	1.68	0.46
1:C:653:ILE:HB	1:C:657:ILE:HG13	1.96	0.46
1:A:183:LEU:HB2	1:A:202:GLN:HB2	1.98	0.46
1:B:127:ARG:HD2	1:B:160:CYS:SG	2.55	0.46
1:B:455:ASP:OD1	1:B:455:ASP:N	2.49	0.46
1:B:1021:LYS:O	1:B:1022:ARG:C	2.59	0.46
1:B:287:LEU:HD22	1:B:296:ILE:HG13	1.98	0.46
1:A:204:ILE:HG23	1:A:211:PRO:HG2	1.98	0.45
1:A:296:ILE:HD13	1:A:296:ILE:HA	1.83	0.45
1:A:587:PRO:HG3	1:A:661:TYR:CD1	2.51	0.45
1:B:1033:MET:HE2	1:B:1035:PHE:CZ	2.51	0.45
1:C:969:PRO:HA	1:C:972:ALA:HB3	1.96	0.45
1:C:142:LEU:HD21	1:C:149:ILE:HG12	1.99	0.45
1:C:238:ALA:C	1:C:240:PRO:HD3	2.42	0.45
1:A:118:MET:SD	1:A:118:MET:N	2.89	0.45
1:B:386:ASP:OD2	1:B:411:TYR:OH	2.33	0.45
1:A:857:THR:O	1:A:861:VAL:HG23	2.17	0.45
1:C:1083:THR:HG21	2:R:1:NAG:H3	1.99	0.45
1:A:887:TYR:HB2	1:C:1090:ARG:NH2	2.31	0.45
1:B:120:ASN:HB3	1:B:123:ASN:O	2.16	0.45
1:B:140:VAL:HG23	1:B:151:SER:HB3	1.98	0.45
1:B:92:ALA:O	1:B:183:LEU:HA	2.17	0.45
2:I:1:NAG:H61	2:I:2:NAG:HN2	1.82	0.45
1:A:529:ASN:ND2	1:A:534:THR:OG1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:LEU:H	1:A:793:LEU:HD23	1.81	0.45
1:B:448:LYS:HB3	1:B:448:LYS:NZ	2.23	0.45
1:B:977:ASP:O	1:B:980:ILE:HG22	2.16	0.45
1:B:1080:PHE:HB2	1:B:1085:TRP:CZ3	2.51	0.45
1:C:73:PHE:HA	1:C:250:ALA:HA	1.99	0.45
1:B:140:VAL:HG12	1:B:149:ILE:HD12	1.99	0.45
1:B:462:SER:HB2	1:B:468:CYS:SG	2.57	0.45
1:B:525:CYS:HB2	1:B:577:CYS:HB3	1.84	0.45
1:A:143:LYS:HD3	1:A:239:PHE:HB3	1.99	0.45
1:A:287:LEU:O	1:A:291:VAL:HG23	2.17	0.45
1:A:885:MET:HB3	1:A:899:LEU:HD11	1.99	0.45
1:B:533:LEU:HD12	1:B:533:LEU:HA	1.77	0.45
1:C:562:SER:HA	1:C:572:LEU:O	2.17	0.45
1:C:1012:MET:HE2	1:C:1012:MET:HB2	1.93	0.45
1:A:142:LEU:HA	1:A:240:PRO:HD2	1.98	0.44
1:A:222:LYS:HB2	1:A:222:LYS:HE3	1.81	0.44
1:A:264:MET:HE2	1:A:264:MET:HB3	1.60	0.44
1:A:317:PHE:CD2	1:A:318:PRO:HD2	2.52	0.44
1:A:852:MET:CG	1:C:682:LEU:HD21	2.42	0.44
1:B:579:PHE:HB2	1:C:838:PHE:CE1	2.52	0.44
1:C:121:SER:HB3	4:C:1309:NAG:H82	1.99	0.44
1:B:461:PHE:N	1:B:478:PRO:HD3	2.33	0.44
1:A:42:TYR:HB2	1:A:198:TYR:CD2	2.53	0.44
1:A:962:ASP:OD1	1:A:966:ARG:HD2	2.18	0.44
1:B:849:THR:HG23	1:B:852:MET:HE3	1.99	0.44
1:C:977:ASP:O	1:C:981:THR:HG23	2.18	0.44
1:B:93:THR:HB	1:B:180:PHE:HB3	1.99	0.44
1:B:316:ARG:NH2	1:B:520:LEU:HB2	2.32	0.44
1:B:955:ALA:HA	1:B:975:GLN:OE1	2.18	0.44
1:A:58:ASP:CG	1:A:59:HIS:H	2.26	0.44
1:A:99:ILE:HD11	1:A:253:TYR:HB3	2.00	0.44
1:A:808:LYS:HA	1:A:808:LYS:HD3	1.79	0.44
1:B:43:TYR:OH	1:B:271:GLY:O	2.28	0.44
1:B:70:PHE:HB2	1:B:253:TYR:CZ	2.52	0.44
1:B:295:GLU:HA	1:B:589:THR:HG21	2.00	0.44
1:B:565:ASP:HB3	1:B:568:THR:O	2.18	0.44
1:C:87:GLY:CA	1:C:188:PHE:O	2.65	0.44
1:A:198:TYR:CZ	1:A:219:PRO:HB3	2.51	0.44
1:C:568:THR:HG22	1:C:569:SER:N	2.33	0.44
1:A:935:VAL:O	1:A:938:ASN:HB3	2.17	0.44
1:B:49:ARG:HB3	1:B:52:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:GLN:NE2	1:B:632:THR:O	2.51	0.44
1:B:682:LEU:HB2	1:C:771:MET:HE2	2.00	0.44
1:C:904:LYS:HE2	1:C:908:ASN:ND2	2.32	0.44
1:B:335:PHE:CE2	1:B:496:ARG:HD3	2.53	0.43
1:A:105:GLY:HA3	1:A:108:MET:HE1	2.01	0.43
1:A:312:LYS:HE3	1:A:312:LYS:HB2	1.80	0.43
1:B:262:THR:HG23	1:B:279:CYS:SG	2.58	0.43
1:B:759:ARG:NH2	1:B:763:GLU:OE1	2.51	0.43
1:C:520:LEU:O	1:C:521:ILE:HD13	2.18	0.43
1:A:522:LYS:HZ3	1:A:541:PRO:HG3	1.83	0.43
1:B:753:ILE:O	1:B:757:GLN:HG2	2.17	0.43
1:A:976:ILE:O	1:A:980:ILE:HD12	2.18	0.43
1:B:19:LYS:HA	1:B:19:LYS:HD3	1.79	0.43
1:A:70:PHE:CE2	1:A:80:PRO:HG2	2.53	0.43
1:A:791:ASP:HB3	1:A:793:LEU:HD23	2.00	0.43
1:B:21:LEU:HB2	1:B:138:PHE:CZ	2.51	0.43
1:B:179:ASN:O	1:B:181:LYS:N	2.51	0.43
1:A:115:VAL:HG12	1:A:128:ALA:CB	2.49	0.43
1:A:741:SER:HB3	1:A:744:THR:HG22	2.00	0.43
1:A:1055:GLU:H	1:A:1055:GLU:HG2	1.55	0.43
1:B:32:THR:OG1	1:B:69:ARG:HB3	2.18	0.43
1:B:184:ARG:HB3	1:B:186:PHE:HE1	1.83	0.43
1:B:479:LEU:HD13	1:B:479:LEU:HA	1.90	0.43
1:C:36:SER:HG	1:C:65:SER:C	2.20	0.43
1:A:873:ALA:HB1	1:C:1029:GLY:HA2	1.99	0.43
1:C:701:PHE:HE2	1:C:906:ILE:HG22	1.83	0.43
1:C:705:ILE:HA	1:C:1047:HIS:O	2.18	0.43
1:B:85:LYS:HB2	1:B:85:LYS:HE2	1.82	0.43
1:B:470:PRO:N	1:B:471:PRO:HD2	2.33	0.43
1:B:653:ILE:HD13	1:B:653:ILE:HA	1.79	0.43
1:B:1012:MET:O	1:B:1016:VAL:HB	2.18	0.43
1:B:1123:PRO:O	1:B:1126:PRO:HD2	2.19	0.43
1:A:857:THR:HA	1:A:860:LEU:HD12	2.01	0.43
1:A:947:LYS:HD3	1:A:947:LYS:N	2.33	0.43
1:B:127:ARG:NH2	1:B:163:GLU:OE2	2.52	0.43
1:B:885:MET:CG	1:B:899:LEU:HD11	2.48	0.43
1:B:705:ILE:HG12	1:B:913:ALA:HB1	2.01	0.43
1:B:1055:GLU:H	1:B:1055:GLU:CD	2.23	0.43
1:C:540:THR:O	1:C:573:ASP:N	2.52	0.43
1:A:58:ASP:HB3	1:A:60:PHE:CZ	2.54	0.42
1:B:316:ARG:HA	1:B:316:ARG:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:HE2	1:B:345:ARG:O	2.19	0.42
1:B:461:PHE:H	1:B:478:PRO:HD3	1.83	0.42
1:C:126:ILE:O	1:C:126:ILE:HG13	2.19	0.42
1:A:42:TYR:HB2	1:A:198:TYR:HD2	1.83	0.42
1:B:339:TYR:CE1	1:B:440:LYS:HB2	2.54	0.42
1:B:489:GLY:O	1:B:493:GLN:N	2.50	0.42
1:B:799:SER:HB2	1:B:802:GLU:HG3	2.02	0.42
1:B:963:ILE:O	1:B:967:LEU:HB2	2.18	0.42
1:B:133:LEU:HD21	1:B:233:ARG:NH1	2.35	0.42
1:C:106:SER:HB3	1:C:107:THR:H	1.57	0.42
1:B:432:THR:O	1:B:485:TYR:HA	2.20	0.42
1:B:709:VAL:HG22	1:B:1044:VAL:HG22	2.00	0.42
1:C:654:GLY:O	1:C:657:ILE:HG12	2.19	0.42
1:A:37:SER:OG	1:A:38:HIS:N	2.51	0.42
1:A:61:LEU:HD22	1:A:89:TYR:CD2	2.55	0.42
1:A:939:ALA:O	1:A:943:ASN:N	2.49	0.42
1:A:971:GLU:CD	1:A:971:GLU:H	2.28	0.42
1:B:534:THR:HG23	1:C:961:ASN:HB3	2.01	0.42
1:C:26:ARG:HD2	1:C:77:PHE:HD1	1.83	0.42
1:C:187:VAL:CG2	1:C:217:LEU:HD12	2.50	0.42
1:C:797:LYS:HD2	1:C:797:LYS:HA	1.93	0.42
1:C:849:THR:HG23	1:C:852:MET:HB2	2.01	0.42
1:A:140:VAL:HB	1:A:149:ILE:HB	2.01	0.42
1:B:353:TYR:CE1	1:B:357:TYR:HB2	2.54	0.42
1:B:857:THR:HG21	1:B:1037:GLN:HA	2.02	0.42
3:Q:1:NAG:H61	3:Q:2:NAG:N2	2.35	0.42
1:C:50:SER:O	1:C:52:VAL:HG13	2.20	0.42
1:C:59:HIS:ND1	1:C:86:ASP:OD1	2.51	0.42
1:C:287:LEU:HD11	1:C:301:TYR:CB	2.50	0.42
1:C:915:SER:O	1:C:918:GLN:HG2	2.19	0.42
1:A:41:VAL:HG21	1:A:214:PHE:HE1	1.84	0.42
1:A:900:TYR:CE1	1:C:1062:PRO:HB3	2.55	0.42
1:C:84:PHE:CD2	1:C:88:ILE:HG23	2.55	0.42
1:C:521:ILE:HB	1:C:526:VAL:HG11	2.01	0.42
1:A:856:TYR:CE2	1:C:682:LEU:HD22	2.55	0.42
1:A:1074:ARG:HG2	1:A:1102:ASN:O	2.20	0.42
1:B:960:LEU:HA	1:B:963:ILE:HD12	2.01	0.42
1:A:132:GLU:CD	1:A:155:ASN:HD22	2.28	0.41
1:B:223:LEU:HA	1:B:224:PRO:HD3	1.85	0.41
1:B:283:PRO:HA	1:B:286:GLU:CD	2.44	0.41
1:B:888:ARG:HD3	1:B:1032:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:GLN:HE21	1:B:940:GLN:HB3	1.64	0.41
1:C:43:TYR:CE1	1:C:216:ALA:HB1	2.55	0.41
1:A:73:PHE:HA	1:A:249:SER:O	2.20	0.41
1:B:306:PHE:HD2	1:B:602:VAL:HG21	1.85	0.41
1:B:956:ILE:HG12	1:B:975:GLN:HG3	2.02	0.41
1:C:162:PHE:CE2	1:C:224:PRO:HD2	2.54	0.41
1:A:141:VAL:O	1:A:239:PHE:HA	2.21	0.41
1:A:720:ASP:OD2	1:A:722:ASN:N	2.53	0.41
1:B:412:LYS:O	1:B:451:PRO:HA	2.19	0.41
1:B:653:ILE:HB	1:B:657:ILE:O	2.20	0.41
1:B:961:ASN:HA	1:B:964:LEU:HG	2.03	0.41
1:B:443:SER:OG	1:B:478:PRO:O	2.36	0.41
1:A:131:PHE:HA	1:A:158:PHE:HD2	1.86	0.41
1:A:516:LEU:HD12	1:A:516:LEU:HA	1.89	0.41
1:C:528:PHE:HB2	1:C:530:PHE:CE1	2.56	0.41
1:A:39:ARG:O	1:A:61:LEU:HD23	2.20	0.41
1:A:43:TYR:O	1:A:198:TYR:HE2	2.03	0.41
1:A:603:ASN:HD22	4:A:1302:NAG:C7	2.34	0.41
1:A:694:THR:O	1:B:880:PRO:HD3	2.21	0.41
1:A:1012:MET:HE2	1:A:1012:MET:HB2	1.99	0.41
1:B:194:PHE:CD2	1:B:222:LYS:HG2	2.54	0.41
1:A:181:LYS:HE3	1:A:203:PRO:O	2.21	0.41
1:B:531:ASN:OD1	1:B:566:PRO:HG3	2.20	0.41
1:B:566:PRO:C	1:B:567:LYS:HD2	2.46	0.41
1:C:117:ILE:HG23	1:C:126:ILE:HG22	2.02	0.41
1:A:59:HIS:HE1	1:A:258:LEU:O	2.03	0.41
1:A:877:LEU:HD11	1:C:698:PRO:HG3	2.03	0.41
1:A:1125:GLN:H	1:A:1125:GLN:HG2	1.71	0.41
1:B:519:ASP:OD2	1:B:519:ASP:N	2.53	0.41
1:B:700:ASN:OD1	1:B:701:PHE:N	2.49	0.41
1:C:60:PHE:C	1:C:258:LEU:HD22	2.46	0.41
1:C:554:ARG:HD3	1:C:558:ASP:OD1	2.19	0.41
1:C:775:PRO:HD3	1:C:862:SER:HB2	2.02	0.41
1:C:867:ALA:HA	1:C:878:GLN:HA	2.02	0.41
1:C:1115:ILE:HD12	1:C:1115:ILE:HA	1.87	0.41
1:A:967:LEU:HD23	1:A:967:LEU:HA	1.85	0.41
1:B:708:GLU:OE2	1:B:1011:LYS:HE2	2.21	0.41
1:A:139:PHE:O	1:A:237:THR:HA	2.20	0.40
1:A:139:PHE:N	1:A:236:LEU:O	2.49	0.40
1:A:214:PHE:HZ	1:A:273:ILE:HG22	1.86	0.40
1:A:788:ILE:H	1:A:788:ILE:HG12	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:PHE:HD2	1:C:75:LEU:HG	1.86	0.40
1:C:307:ARG:HA	1:C:307:ARG:HD2	1.91	0.40
1:C:670:THR:HG22	1:C:670:THR:O	2.21	0.40
1:A:976:ILE:HG22	1:A:980:ILE:HD11	2.02	0.40
1:A:1126:PRO:HB2	1:A:1127:GLU:OE1	2.21	0.40
1:B:449:LEU:HD23	1:B:449:LEU:HA	1.87	0.40
1:C:125:VAL:HG21	4:C:1309:NAG:H62	2.04	0.40
1:C:190:ASN:HA	1:C:195:LEU:HD23	2.02	0.40
1:C:275:ASP:OD1	1:C:276:ALA:N	2.54	0.40
1:C:949:LEU:HD23	1:C:949:LEU:HA	1.87	0.40
1:A:118:MET:HB3	1:A:139:PHE:CZ	2.54	0.40
1:A:264:MET:HE1	1:A:292:LYS:HA	2.02	0.40
1:A:293:SER:C	1:A:295:GLU:H	2.30	0.40
1:A:719:VAL:HA	1:A:840:GLY:O	2.21	0.40
1:A:976:ILE:HG22	1:A:980:ILE:CD1	2.51	0.40
1:B:367:CYS:HA	1:B:420:CYS:HA	2.04	0.40
1:B:567:LYS:HD2	1:B:567:LYS:N	2.36	0.40
1:B:769:LYS:HG3	1:B:770:GLN:HG2	2.04	0.40
1:B:968:ASP:C	1:B:970:PRO:HD2	2.46	0.40
1:C:539:LEU:HD23	1:C:539:LEU:HA	1.97	0.40
1:A:62:PRO:CD	1:A:259:LYS:HG3	2.51	0.40
1:A:108:MET:HE1	1:A:114:SER:OG	2.21	0.40
1:A:182:ASP:OD1	1:A:201:TYR:OH	2.39	0.40
1:A:989:THR:HG22	1:B:988:GLN:NE2	2.37	0.40
1:C:100:ARG:HG2	1:C:237:THR:HG23	2.03	0.40
1:B:279:CYS:HA	1:B:285:ALA:HB1	2.03	0.40
1:B:787:GLN:H	1:B:787:GLN:HG2	1.72	0.40
1:B:1011:LYS:HE3	1:B:1025:PHE:O	2.21	0.40
1:C:59:HIS:HA	1:C:260:PRO:HA	2.03	0.40
1:C:307:ARG:NH1	1:C:579:PHE:HB3	2.34	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	860/1271 (68%)	807 (94%)	52 (6%)	1 (0%)	48	81
1	B	1061/1271 (84%)	1022 (96%)	37 (4%)	2 (0%)	43	75
1	C	863/1271 (68%)	826 (96%)	37 (4%)	0	100	100
All	All	2784/3813 (73%)	2655 (95%)	126 (4%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	604	CYS
1	B	246	TRP
1	B	722	ASN

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	759/1100 (69%)	756 (100%)	3 (0%)	84	84
1	B	931/1100 (85%)	918 (99%)	13 (1%)	59	71
1	C	760/1100 (69%)	751 (99%)	9 (1%)	63	73
All	All	2450/3300 (74%)	2425 (99%)	25 (1%)	65	76

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	607	VAL
1	A	680	MET
1	A	756	GLU
1	B	31	ASN
1	B	118	MET
1	B	194	PHE
1	B	380	PHE

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Mol	Chain	Res	Type
1	B	723	MET
1	B	839	ASN
1	B	890	ASN
1	B	935	VAL
1	B	940	GLN
1	B	948	GLN
1	B	994	GLN
1	B	1026	CYS
1	B	1067	GLU
1	C	106	SER
1	C	108	MET
1	C	125	VAL
1	C	232	PHE
1	C	294	PHE
1	C	540	THR
1	C	731	GLU
1	C	756	GLU
1	C	960	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	527	ASN
1	A	734	ASN
1	A	878	GLN
1	A	975	GLN
1	A	988	GLN
1	A	993	GLN
1	A	994	GLN
1	B	59	HIS
1	B	397	GLN
1	B	642	HIS
1	B	760	ASN
1	B	770	GLN
1	B	787	GLN
1	B	839	ASN
1	B	884	GLN
1	B	890	ASN
1	B	896	GLN
1	B	932	GLN
1	B	938	ASN

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Mol	Chain	Res	Type
1	B	940	GLN
1	B	993	GLN
1	B	994	GLN
1	C	196	HIS
1	C	231	ASN
1	C	722	ASN
1	C	745	GLN
1	C	747	ASN
1	C	897	ASN
1	C	908	ASN
1	C	988	GLN
1	C	1066	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

35 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	E	1	2,1	14,14,15	0.48	0	17,19,21	0.58	0
2	NAG	E	2	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	F	1	2,1	14,14,15	0.18	0	17,19,21	0.49	0
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	1	2,1	14,14,15	0.38	0	17,19,21	0.52	0
2	NAG	G	2	2	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	H	1	2,1	14,14,15	0.60	0	17,19,21	0.82	1 (5%)
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	I	1	2,1	14,14,15	0.76	1 (7%)	17,19,21	0.84	1 (5%)
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.55	0
2	NAG	J	1	2,1	14,14,15	0.22	0	17,19,21	0.71	0
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	0.62	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.26	0	17,19,21	0.53	0
3	BMA	K	3	3	11,11,12	0.62	0	15,15,17	0.69	0
3	NAG	L	1	1,3	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	L	2	3	14,14,15	0.20	0	17,19,21	0.51	0
3	BMA	L	3	3	11,11,12	0.64	0	15,15,17	0.68	0
2	NAG	M	1	2,1	14,14,15	0.32	0	17,19,21	0.60	0
2	NAG	M	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	N	1	2,1	14,14,15	0.25	0	17,19,21	0.46	0
2	NAG	N	2	2	14,14,15	0.18	0	17,19,21	0.49	0
2	NAG	O	1	2,1	14,14,15	0.45	0	17,19,21	0.46	0
2	NAG	O	2	2	14,14,15	0.29	0	17,19,21	0.48	0
2	NAG	P	1	2,1	14,14,15	0.34	0	17,19,21	0.46	0
2	NAG	P	2	2	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	Q	1	1,3	14,14,15	0.26	0	17,19,21	0.61	0
3	NAG	Q	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	Q	3	3	11,11,12	0.61	0	15,15,17	0.63	0
2	NAG	R	1	2,1	14,14,15	0.27	0	17,19,21	0.50	0
2	NAG	R	2	2	14,14,15	0.33	0	17,19,21	0.46	0
2	NAG	S	1	2,1	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	S	2	2	14,14,15	0.20	0	17,19,21	0.43	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	2	2	-	6/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
2	NAG	R	1	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	-2.50	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C2-N2-C7	4.50	128.93	122.90
2	H	1	NAG	C1-O5-C5	2.41	115.41	112.19
2	I	1	NAG	C3-C4-C5	2.20	114.22	110.23
2	J	2	NAG	C1-O5-C5	2.13	115.04	112.19
2	F	2	NAG	C1-C2-N2	2.04	113.65	110.43

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	M	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6

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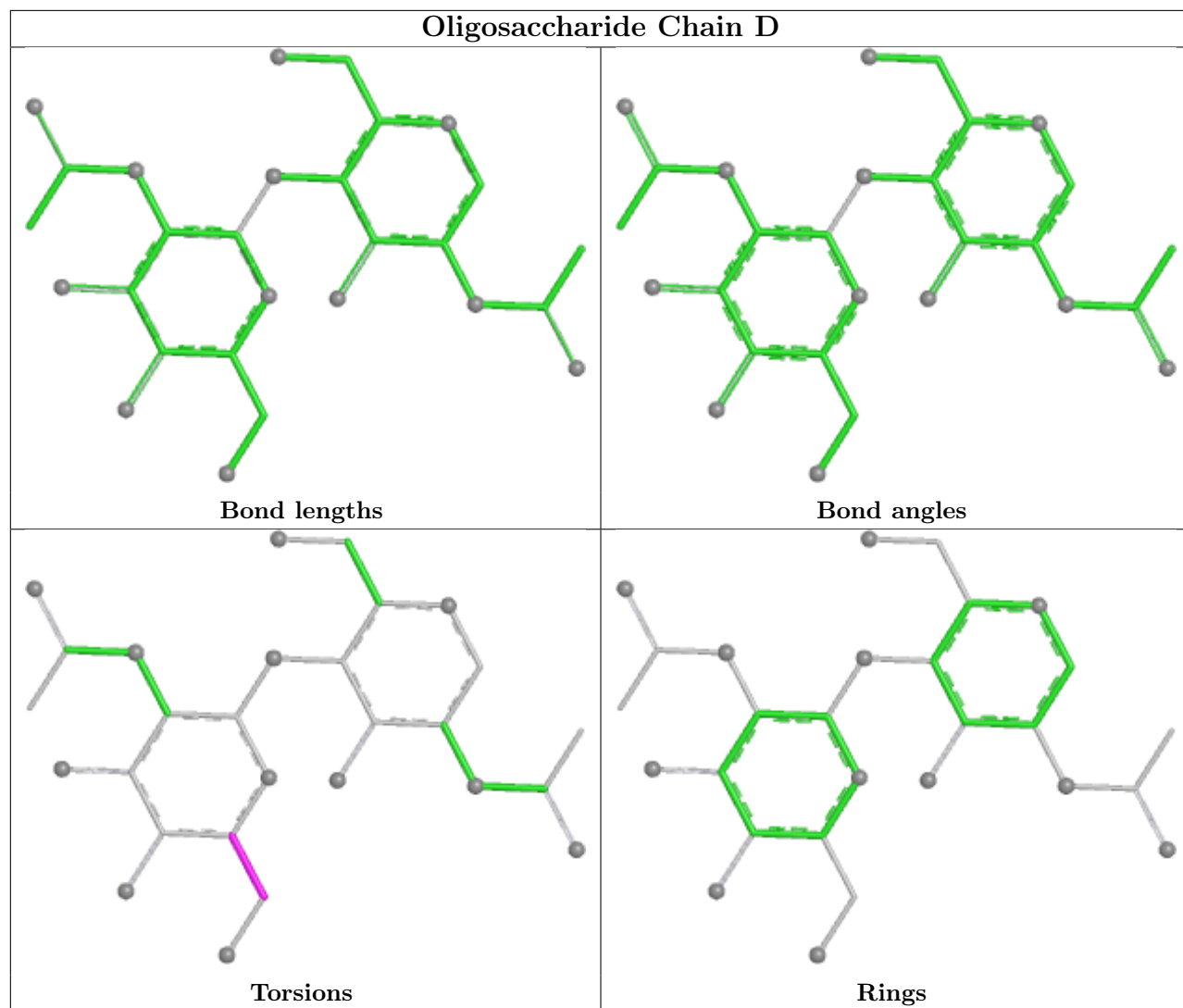
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7

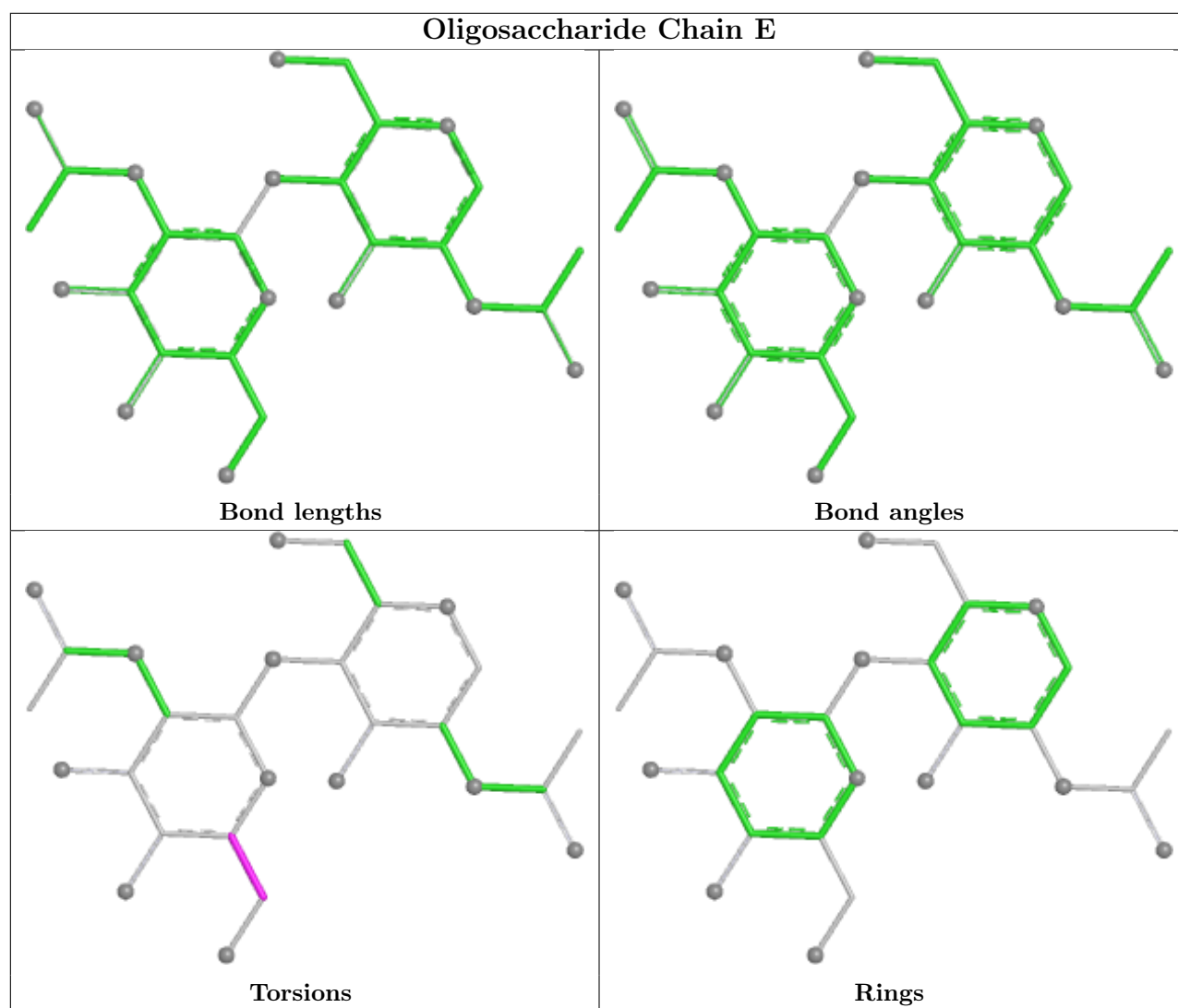
There are no ring outliers.

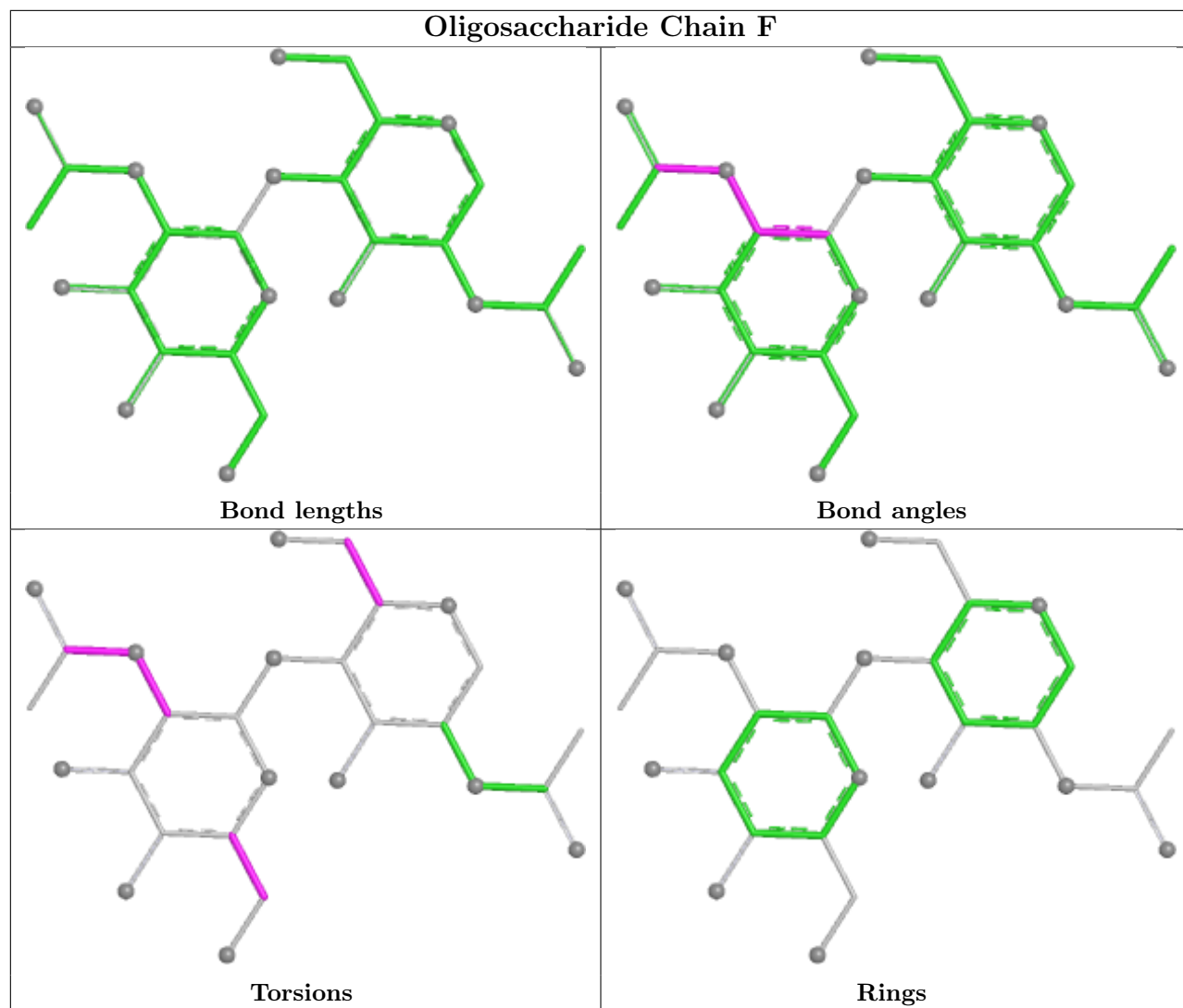
9 monomers are involved in 7 short contacts:

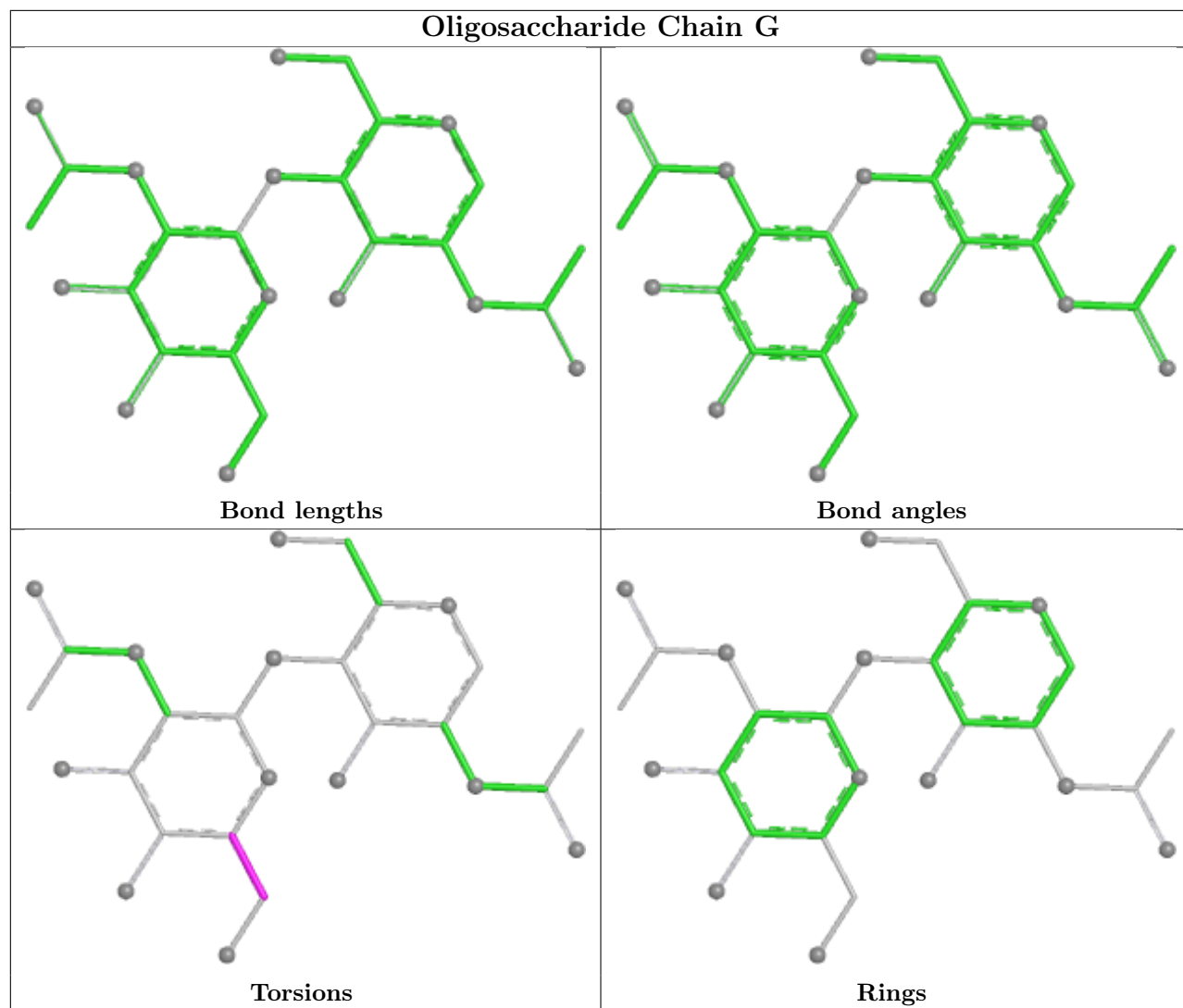
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	1	0
3	Q	2	NAG	1	0
2	I	2	NAG	1	0
2	N	1	NAG	1	0
2	F	2	NAG	1	0
2	E	1	NAG	1	0
2	R	1	NAG	1	0
2	O	1	NAG	1	0
3	Q	1	NAG	1	0

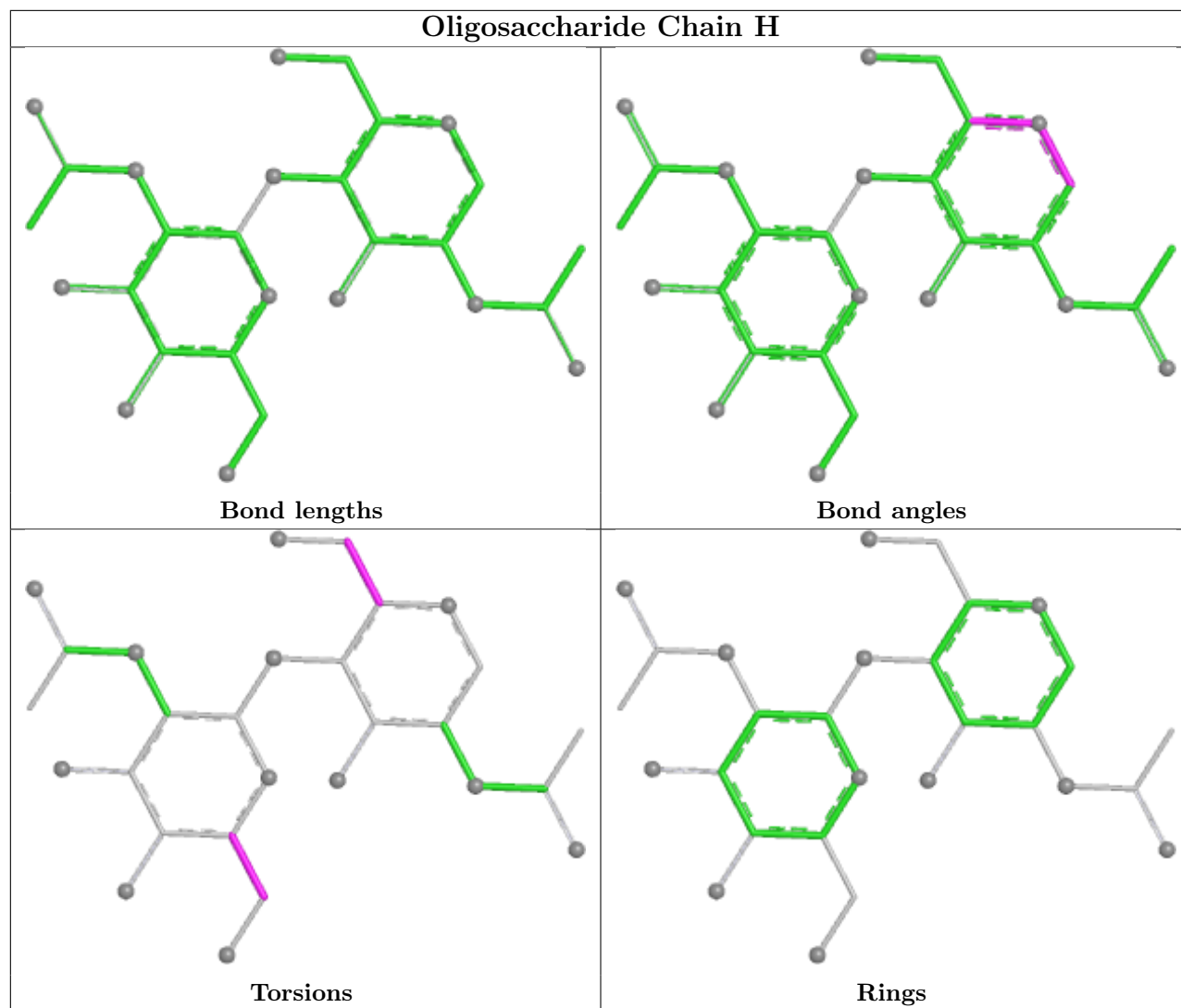
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

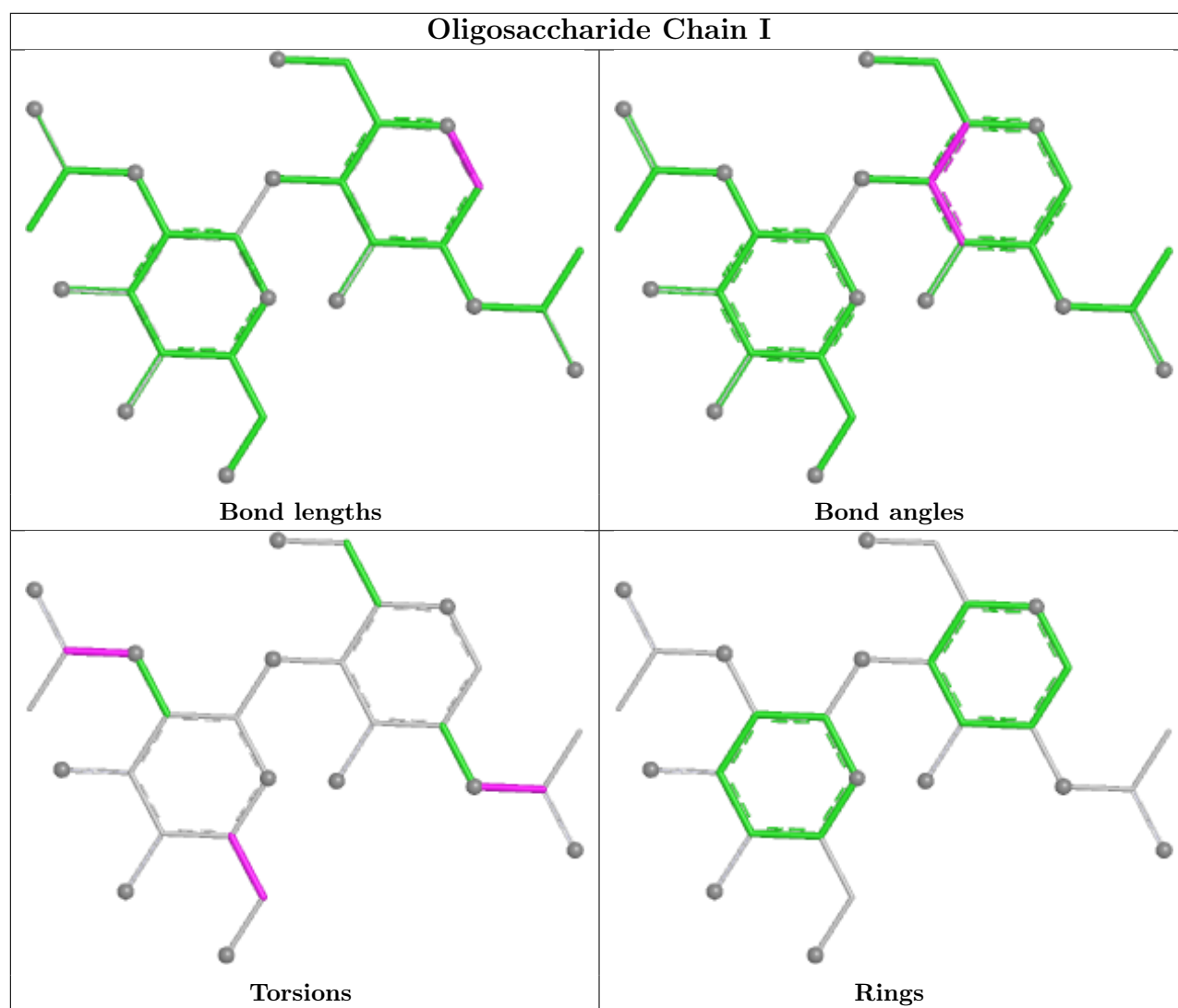


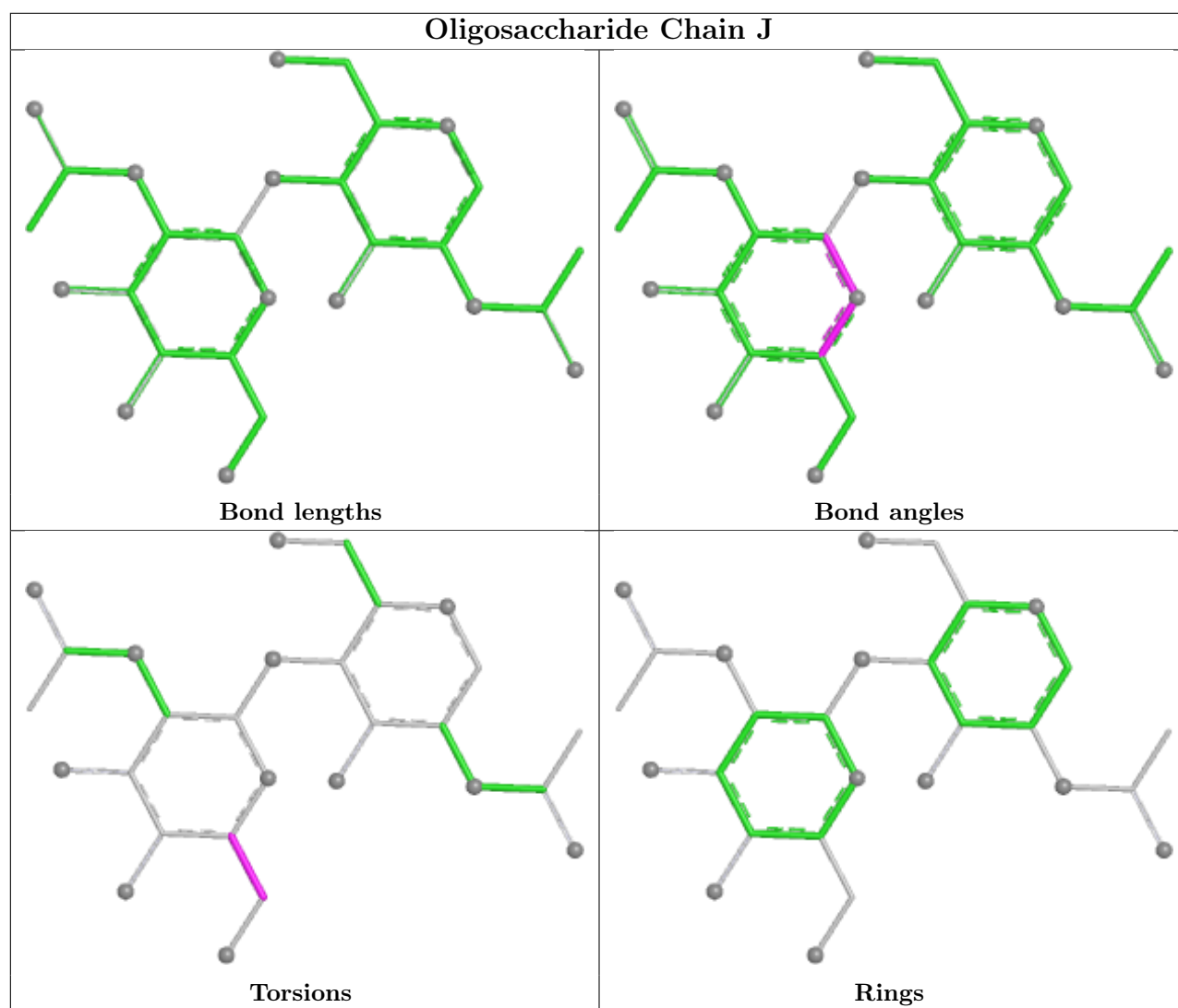


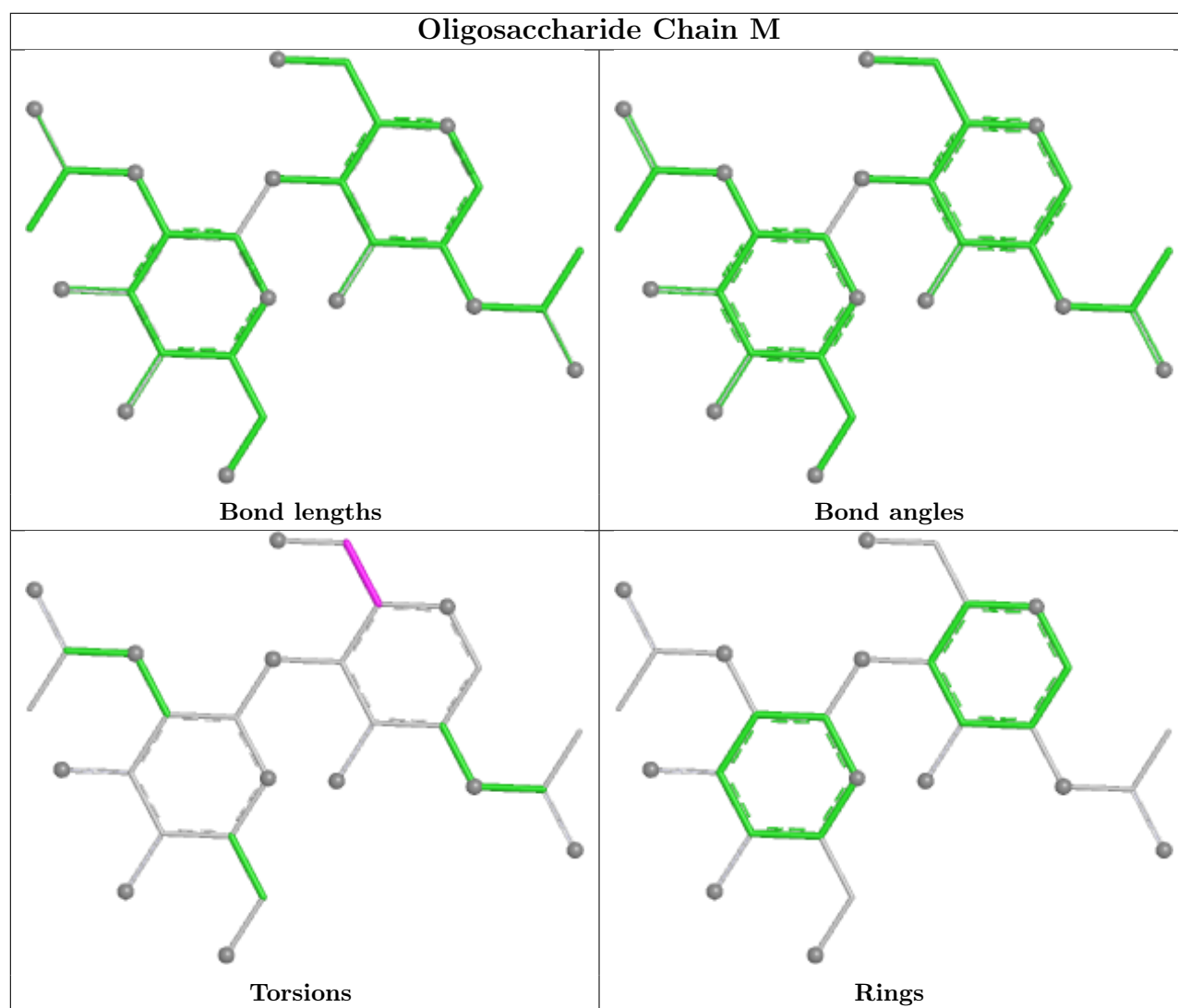


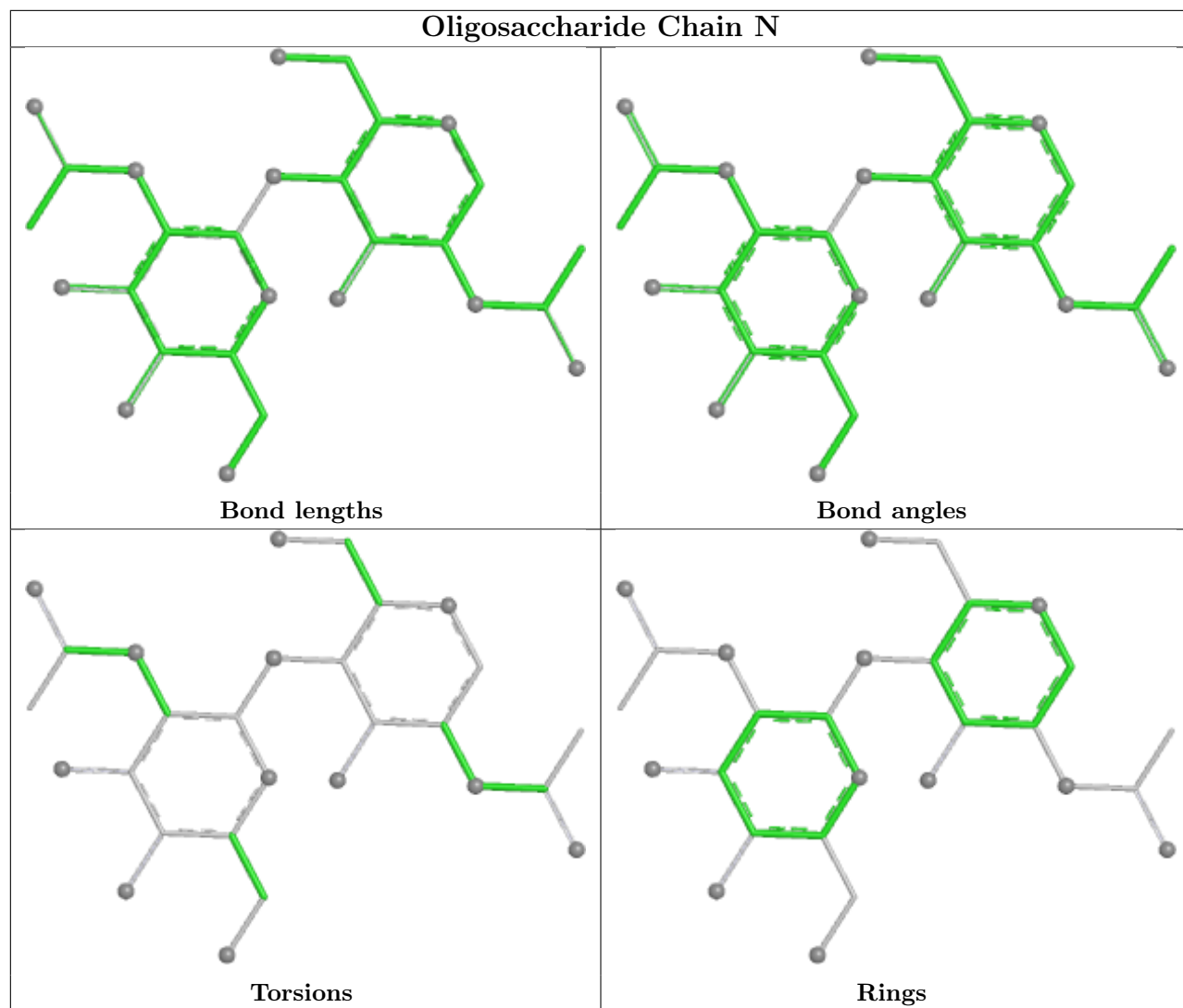


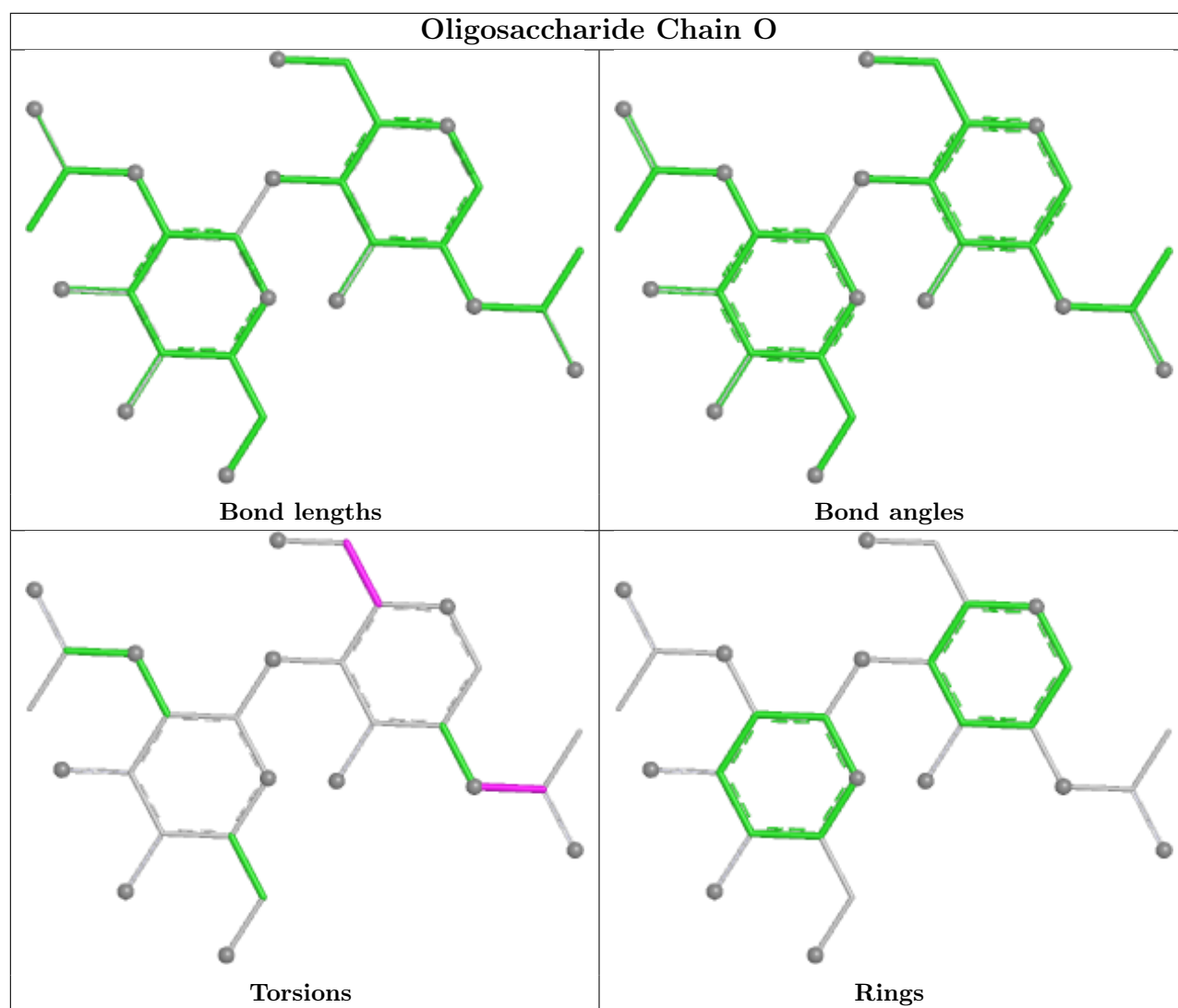


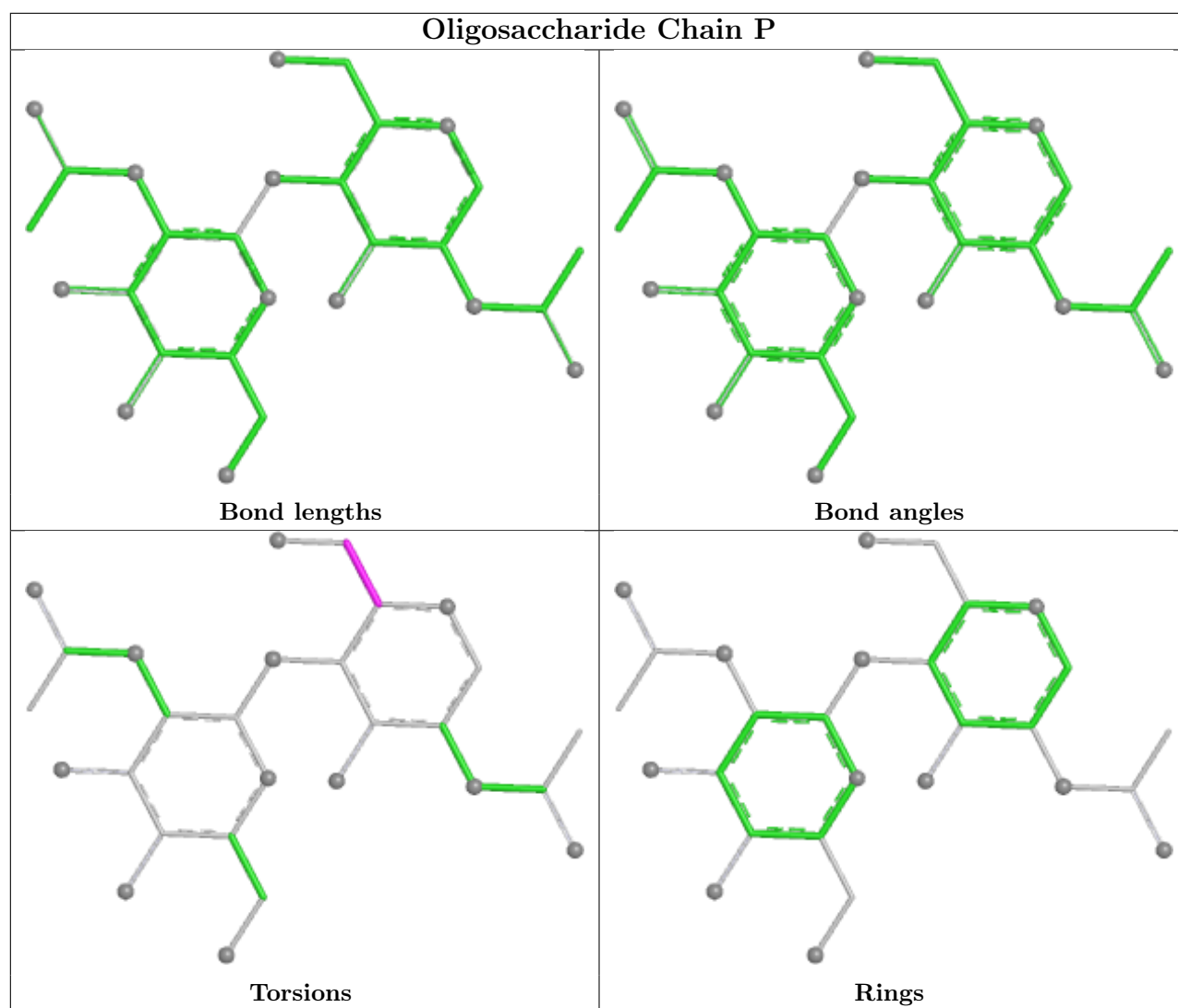


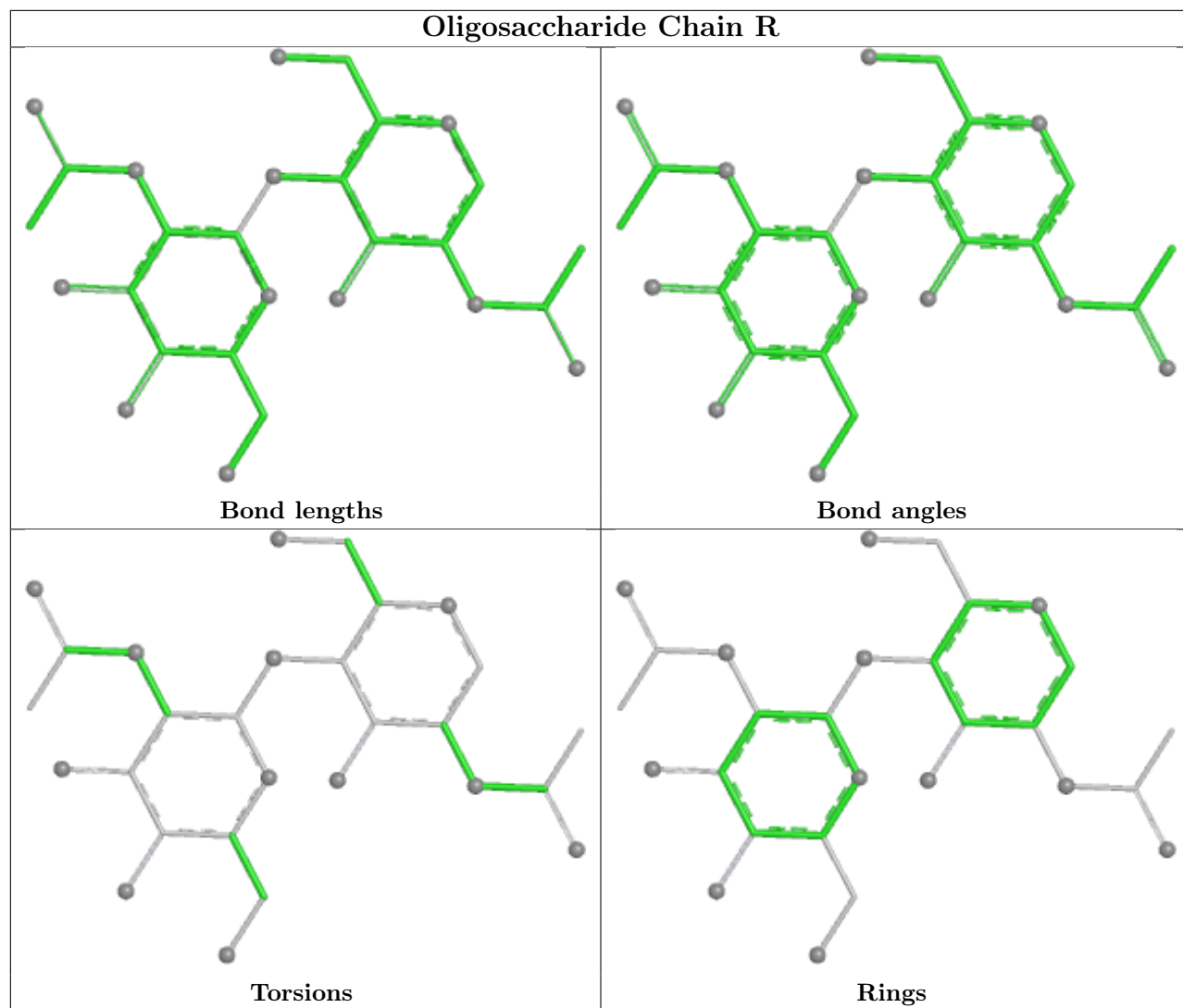


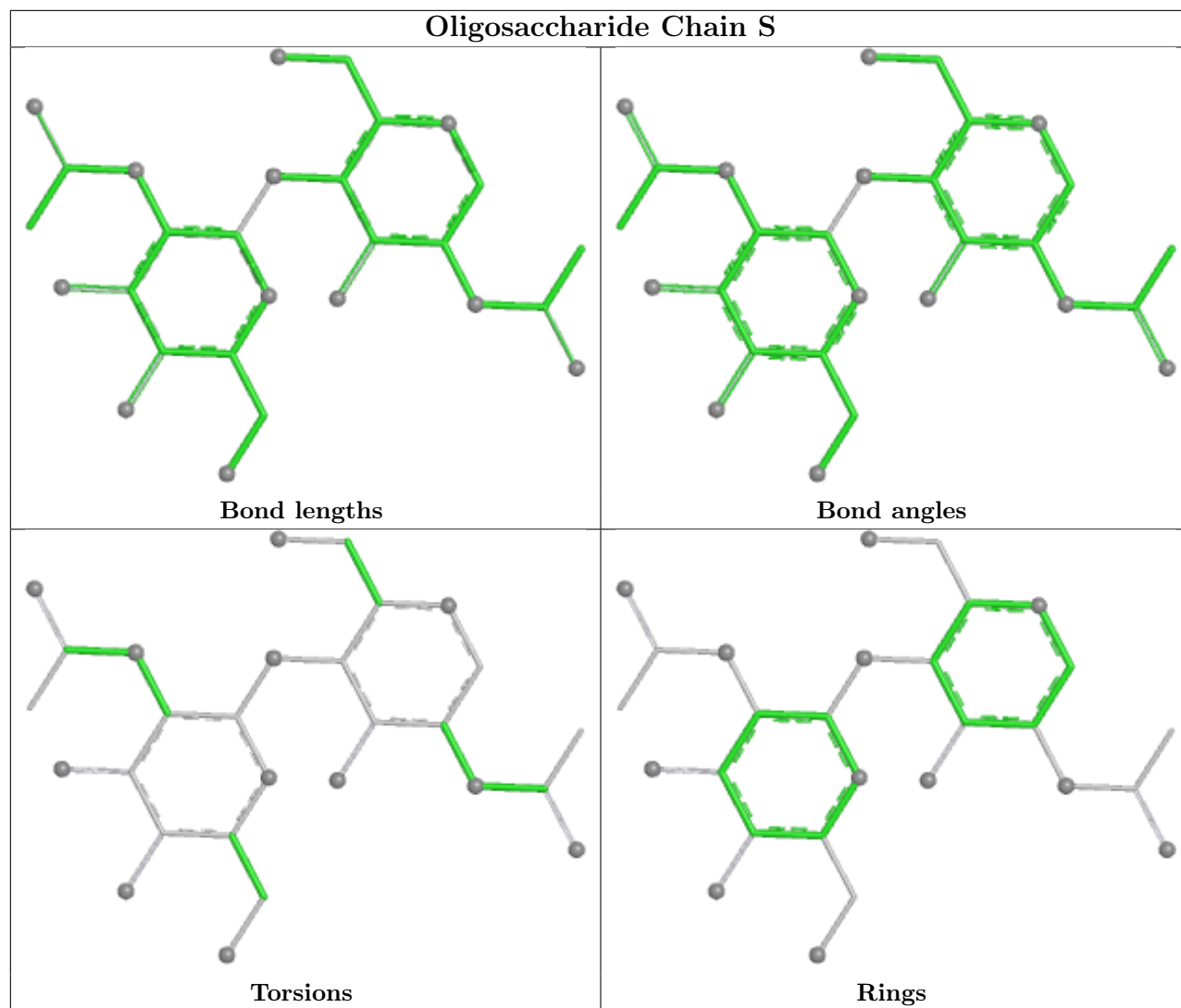


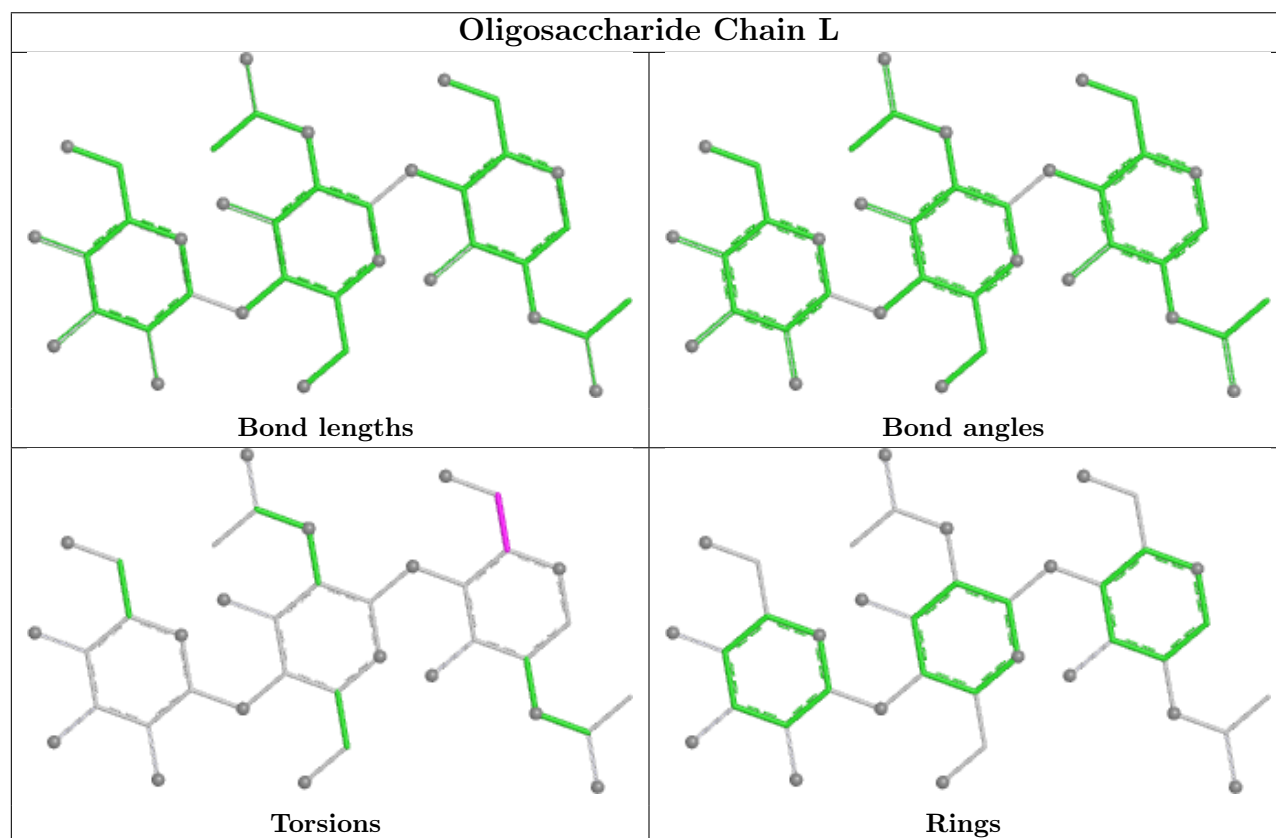
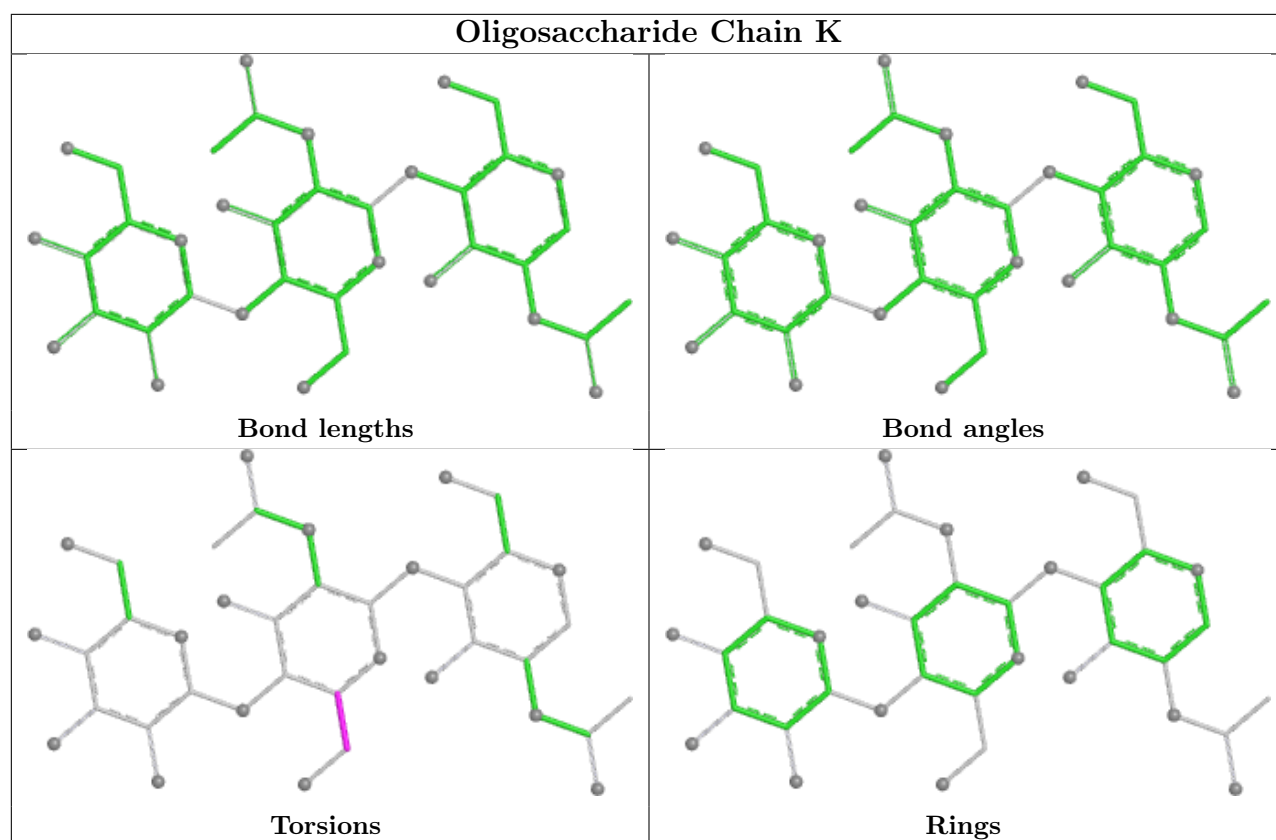


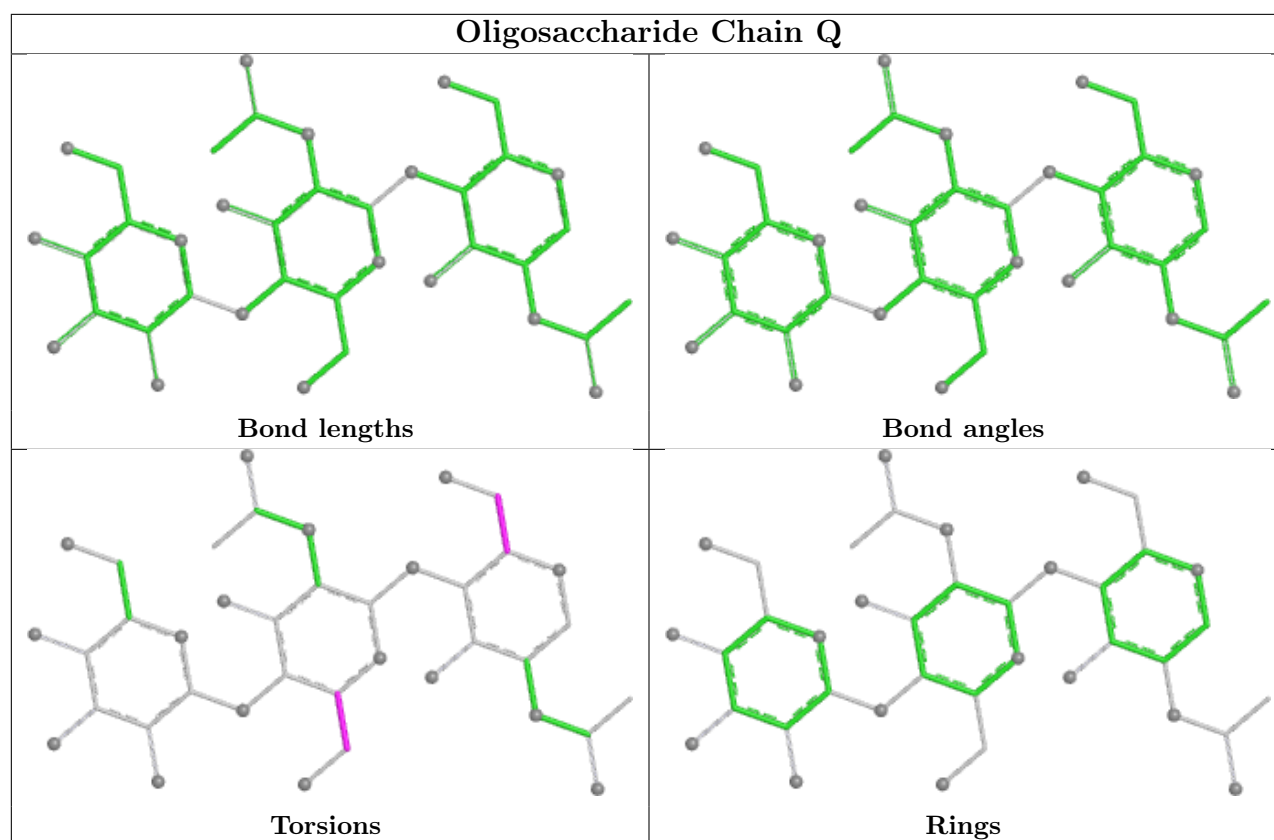












5.6 Ligand geometry [i](#)

19 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	1302	1	14,14,15	0.17	0	17,19,21	0.49	0
4	NAG	A	1304	1	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.42	0
4	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	C	1302	1	14,14,15	0.33	0	17,19,21	0.35	0
4	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1305	1	14,14,15	0.16	0	17,19,21	0.45	0
4	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1307	1	14,14,15	0.29	0	17,19,21	0.36	0
4	NAG	C	1303	1	14,14,15	0.17	0	17,19,21	0.37	0
4	NAG	C	1308	1	14,14,15	0.35	0	17,19,21	0.45	0
4	NAG	B	1305	1	14,14,15	0.19	0	17,19,21	0.57	0
4	NAG	B	1304	1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	A	1301	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	B	1303	1	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	C	1309	1	14,14,15	0.17	0	17,19,21	0.43	0
4	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.59	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	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1301	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	C	1308	NAG	C8-C7-N2-C2
4	C	1308	NAG	O7-C7-N2-C2
4	C	1302	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	C	1304	NAG	C1-C2-N2-C7
4	A	1303	NAG	O5-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	C	1304	NAG	C3-C2-N2-C7
4	B	1304	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	C	1302	NAG	C3-C2-N2-C7
4	C	1309	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	NAG	1	0
4	C	1309	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

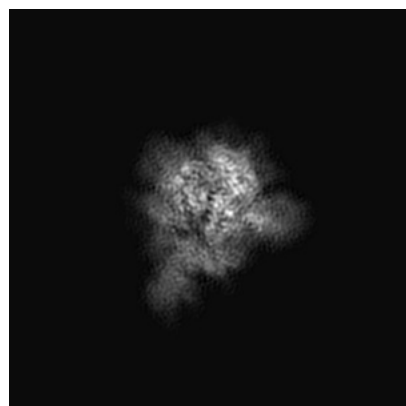
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37635. These allow visual inspection of the internal detail of the map and identification of artifacts.

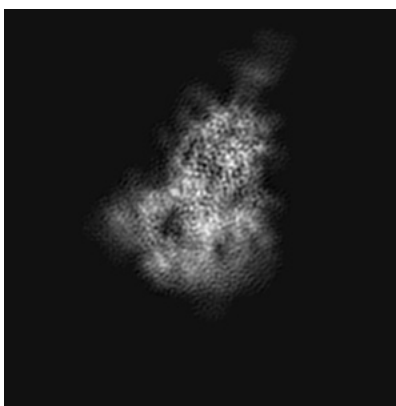
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

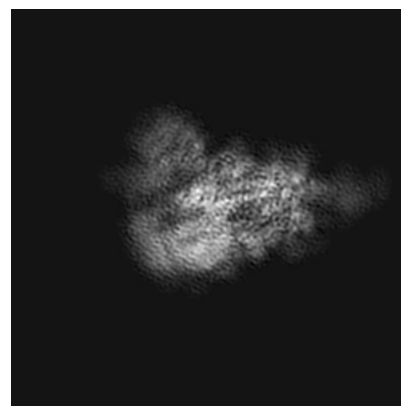
6.1.1 Primary map



X

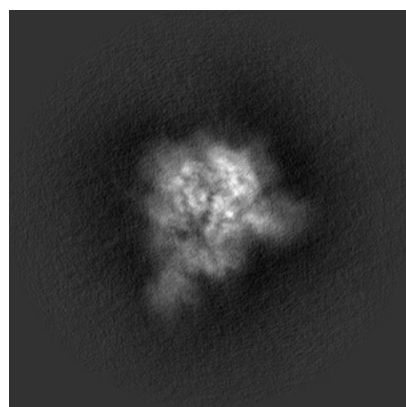


Y

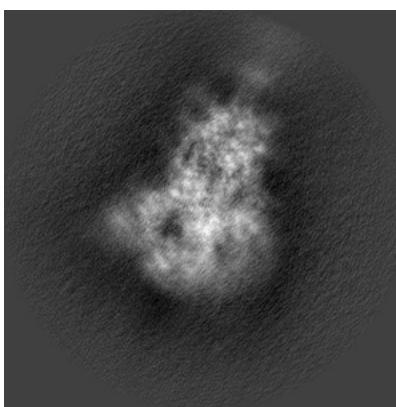


Z

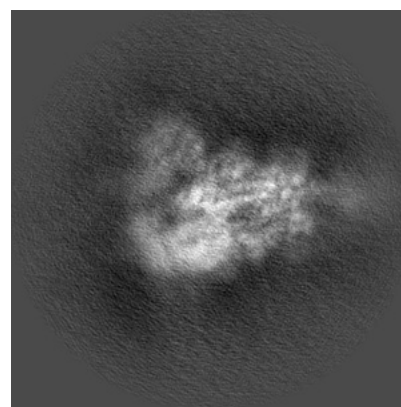
6.1.2 Raw map



X



Y

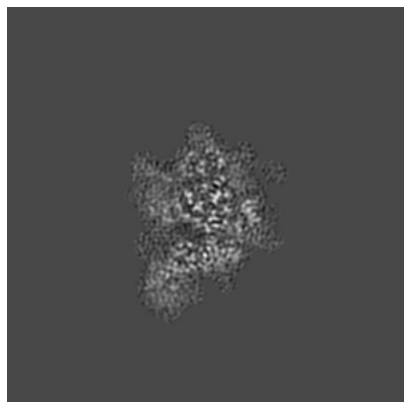


Z

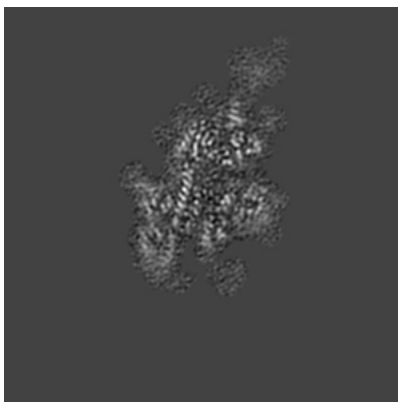
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

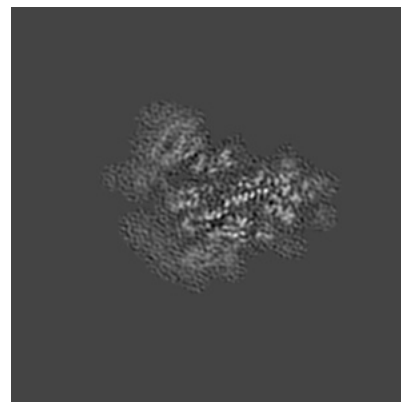
6.2.1 Primary map



X Index: 140

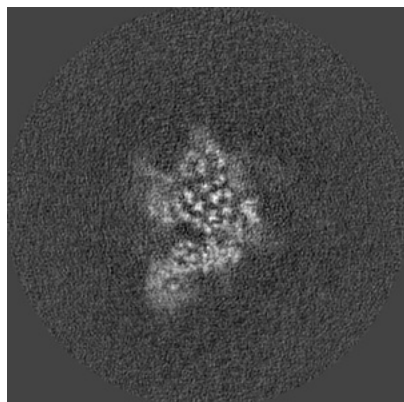


Y Index: 140

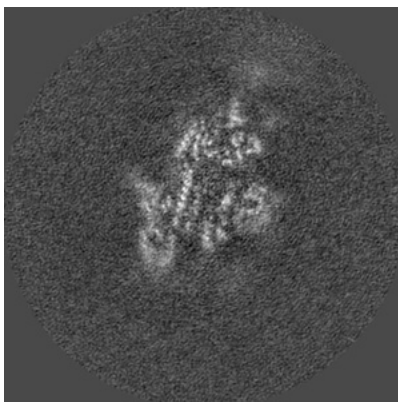


Z Index: 140

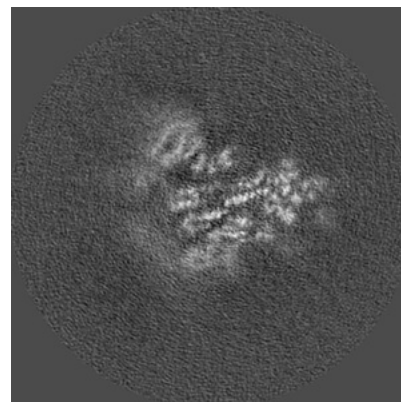
6.2.2 Raw map



X Index: 140



Y Index: 140

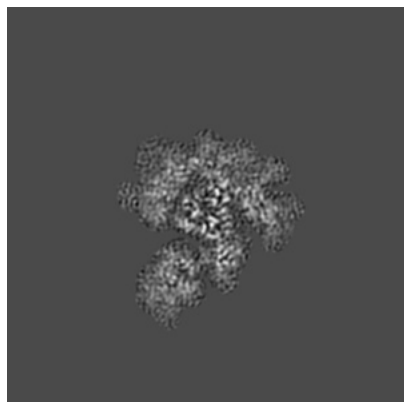


Z Index: 140

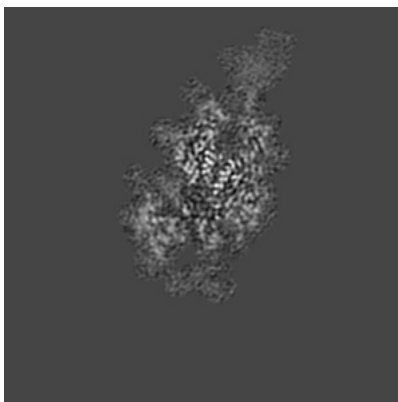
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

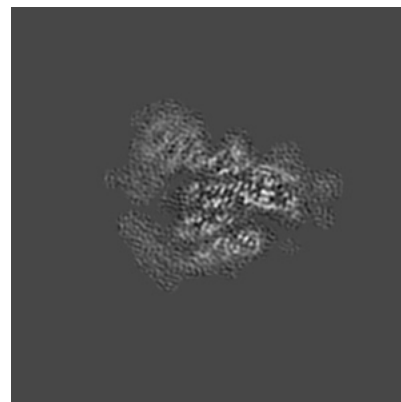
6.3.1 Primary map



X Index: 131

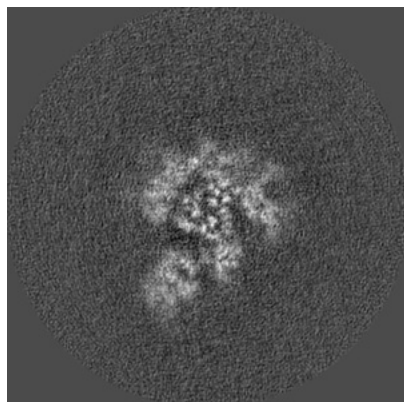


Y Index: 148

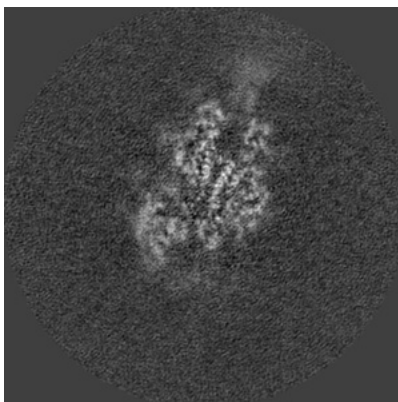


Z Index: 134

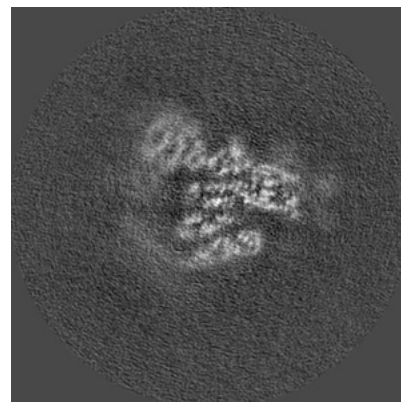
6.3.2 Raw map



X Index: 131



Y Index: 147

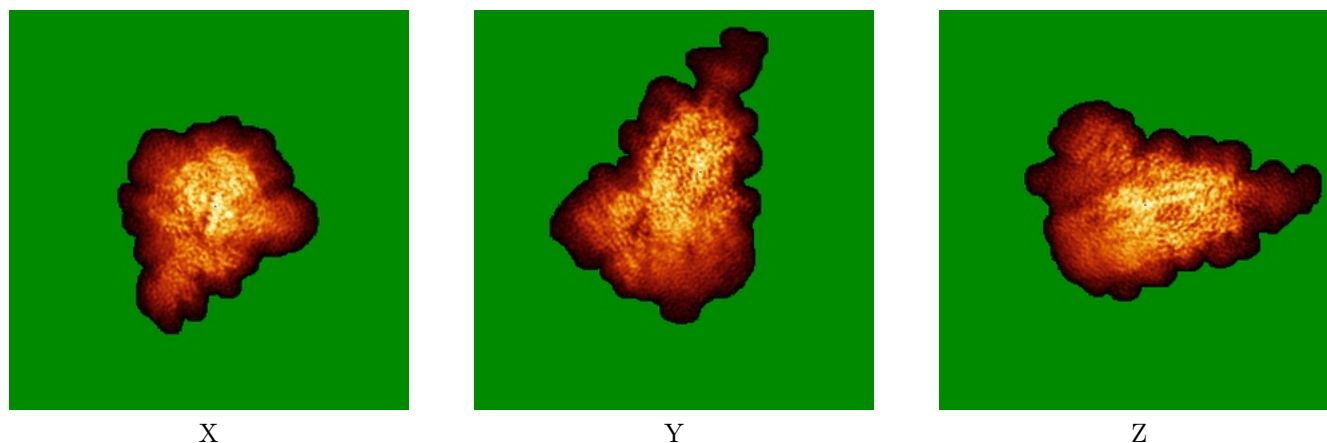


Z Index: 134

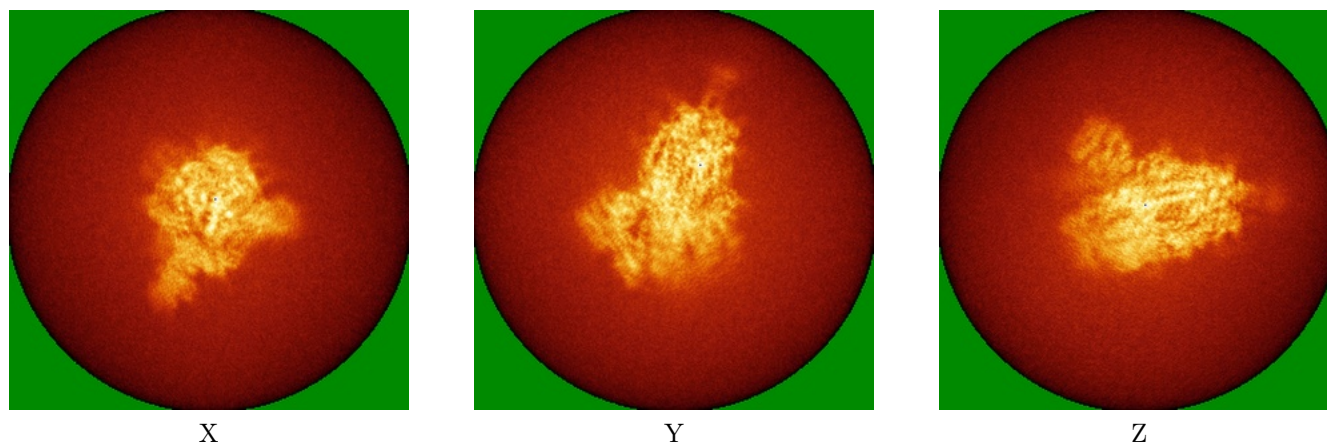
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

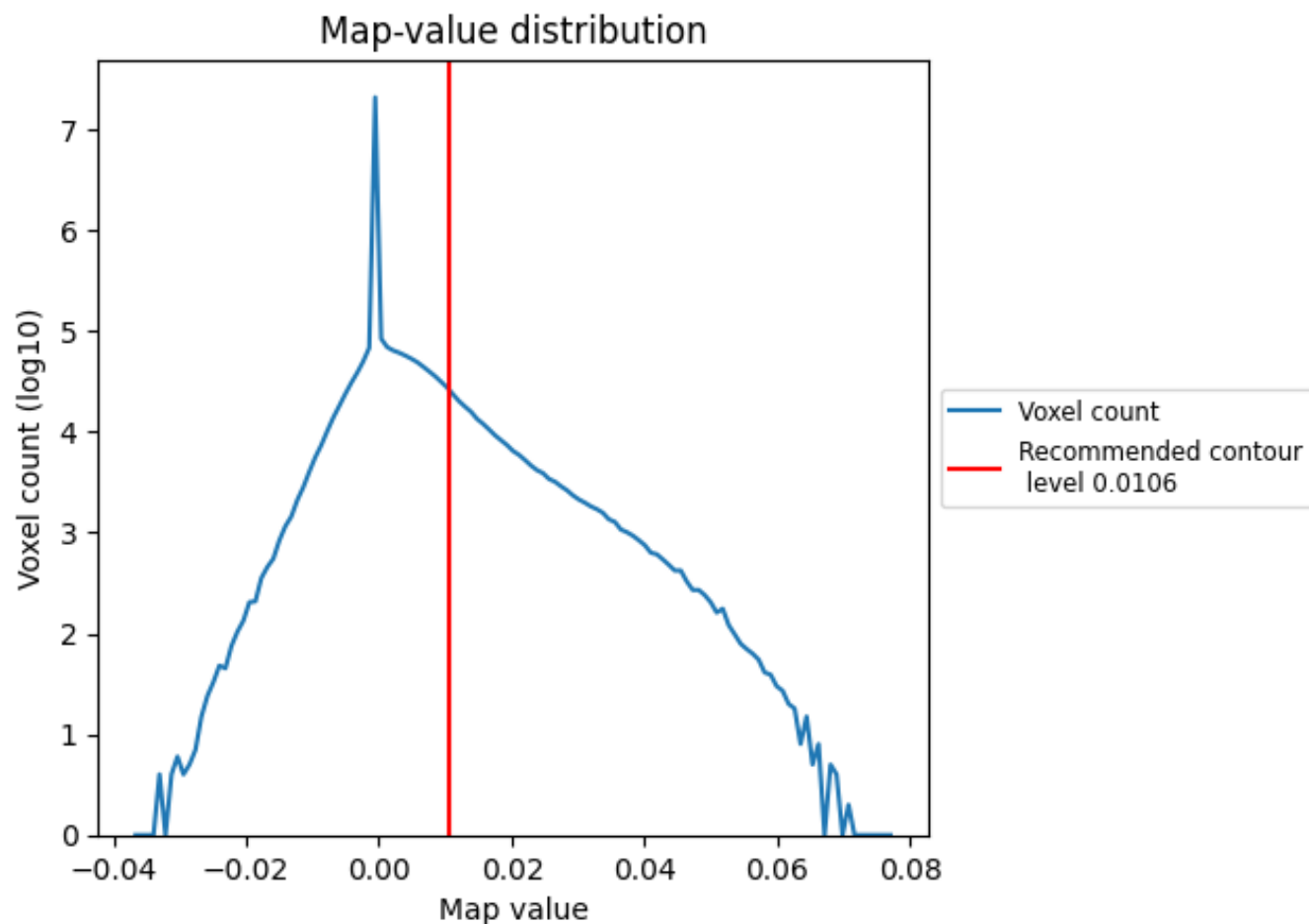
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

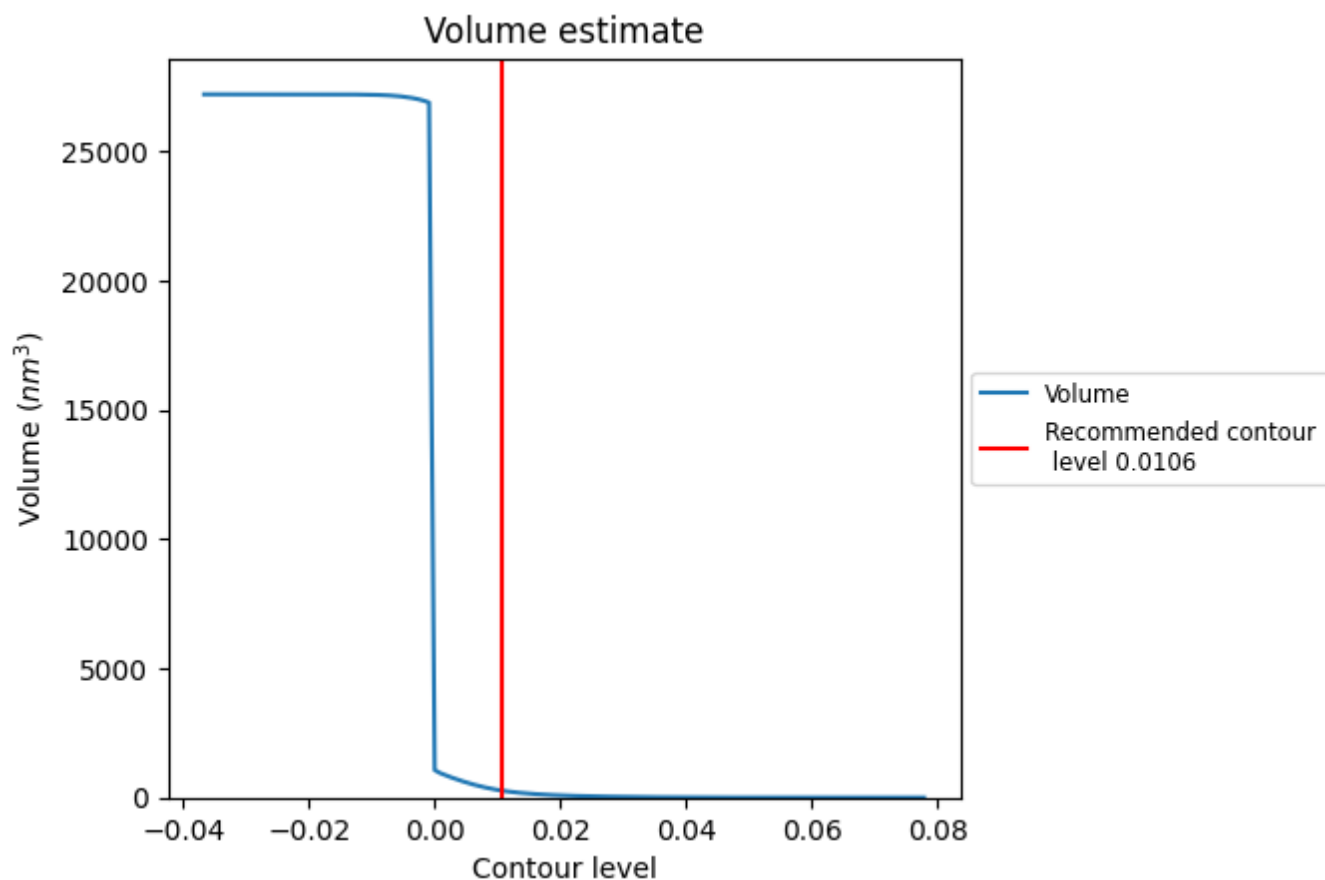
This section contains the results of statistical analysis of the map.

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.

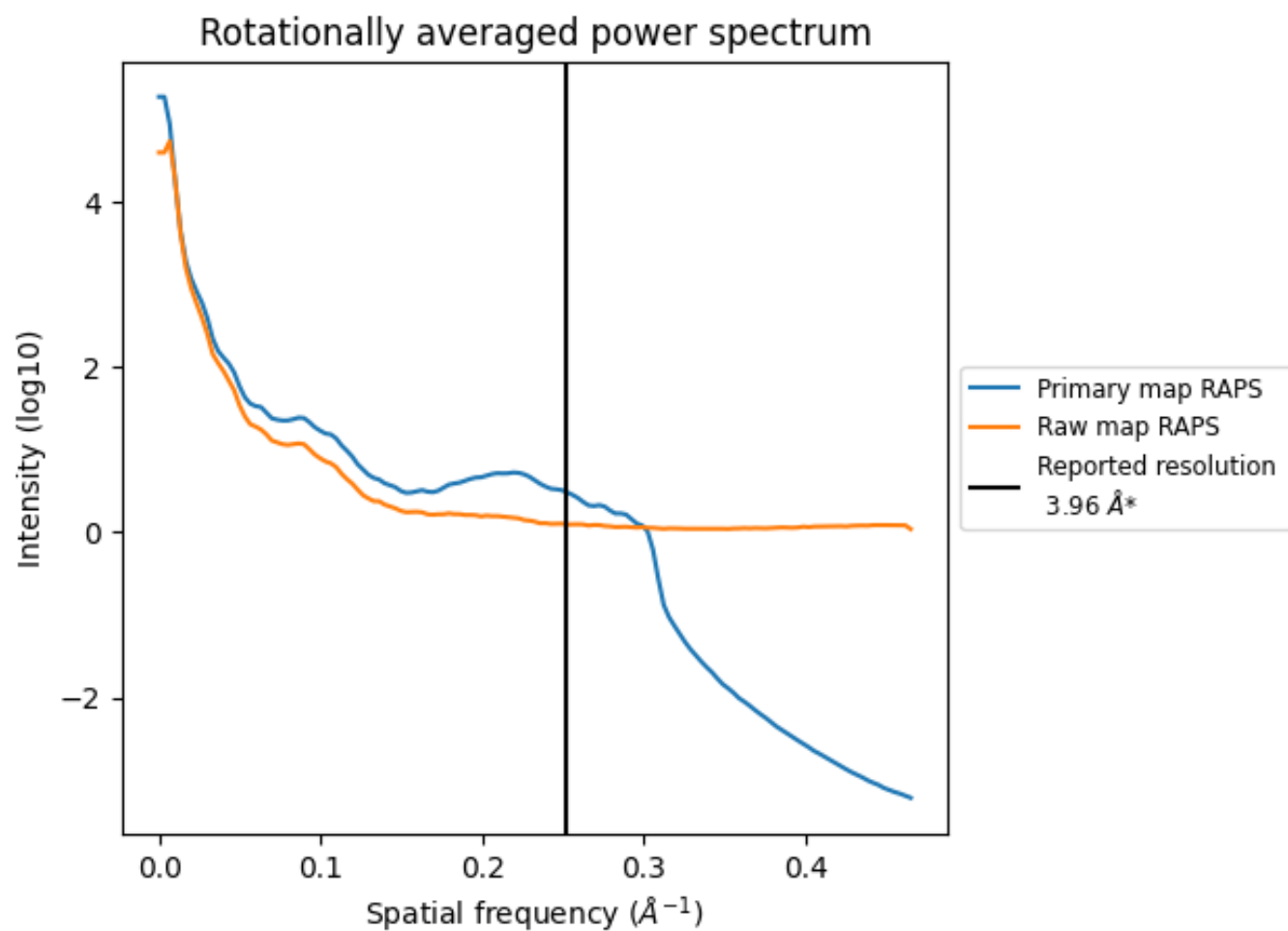
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 275 nm³; this corresponds to an approximate mass of 248 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 ⓘ

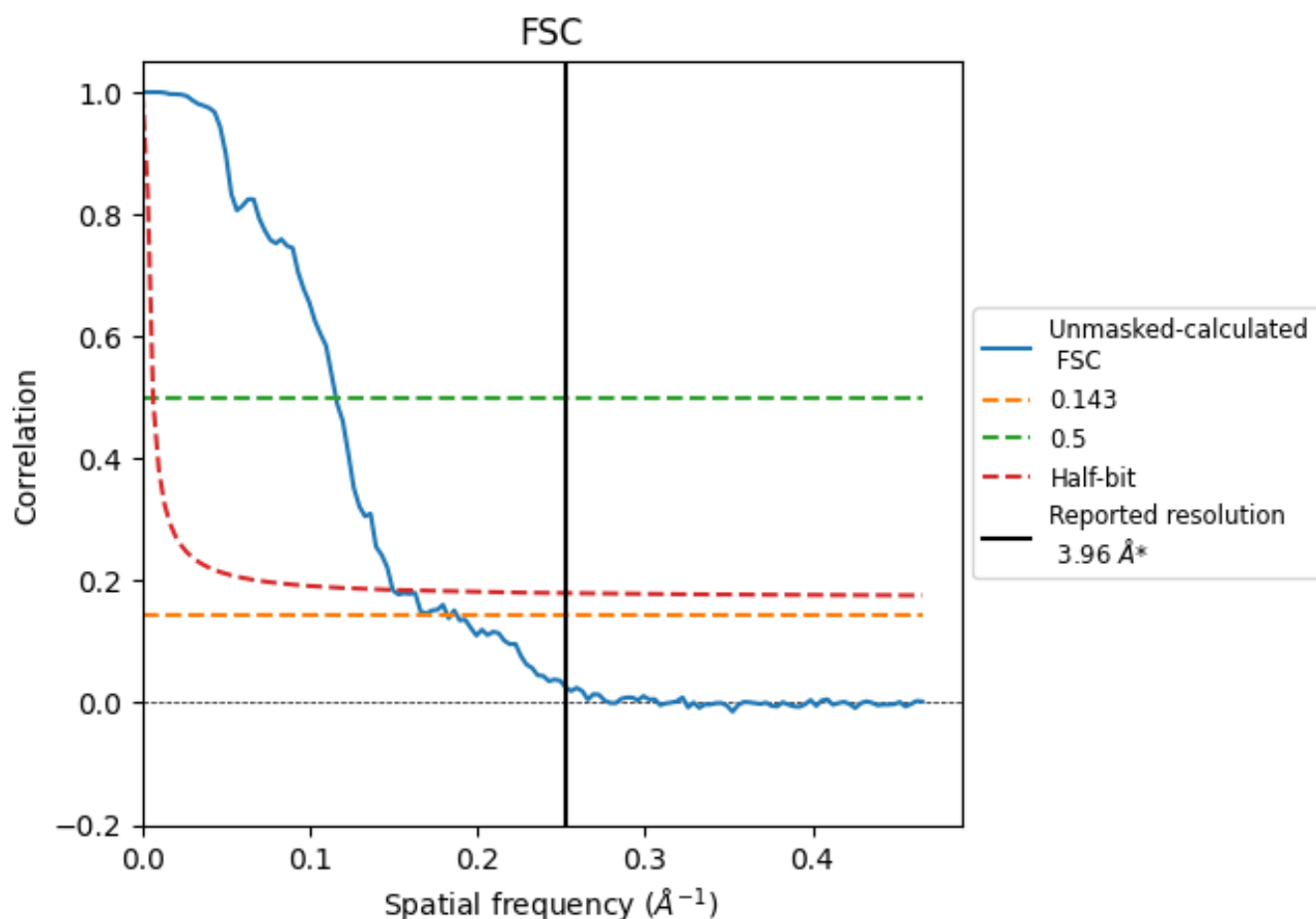


*Reported resolution corresponds to spatial frequency of 0.253 $\text{\AA}^{-1}$

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 0.253 Å⁻¹

8.2 Resolution estimates [i](#)

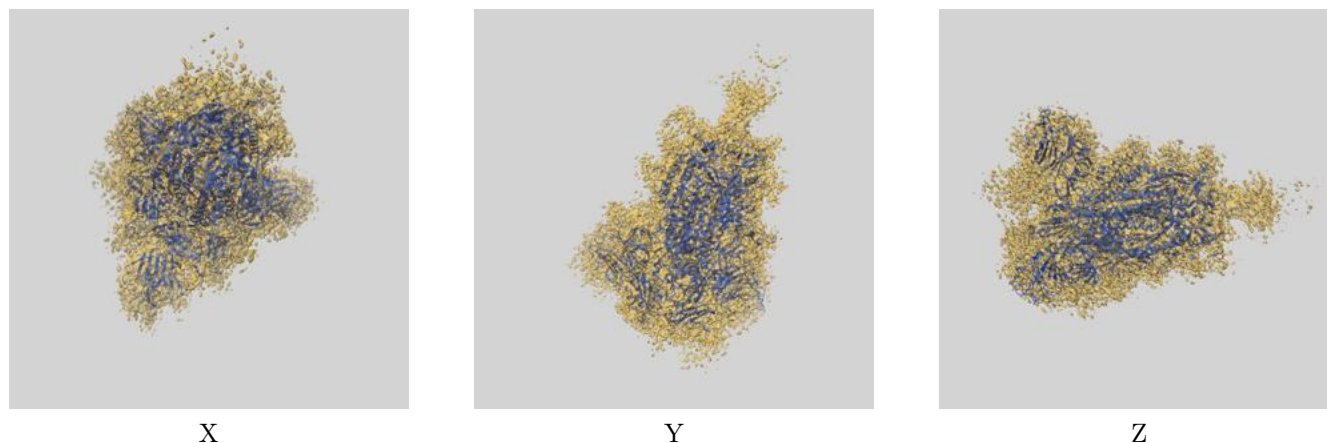
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.49	8.65	6.68

*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 5.49 differs from the reported value 3.96 by more than 10 %

9 Map-model fit [i](#)

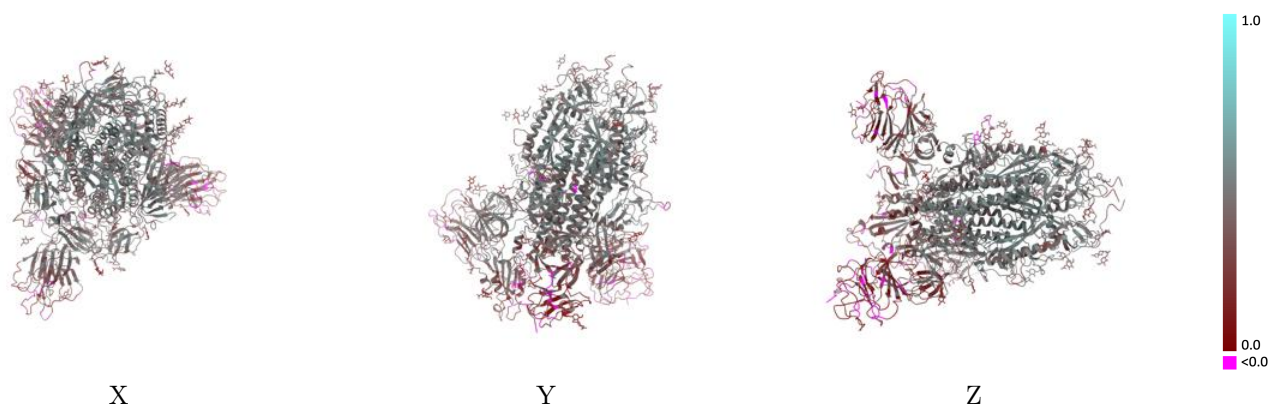
This section contains information regarding the fit between EMDB map EMD-37635 and PDB model 8WLY. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



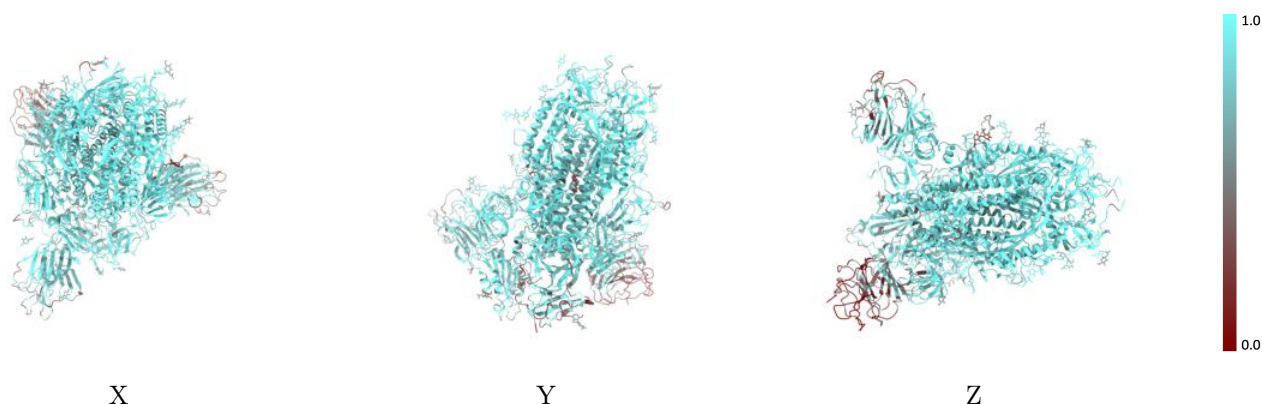
The images above show the 3D surface view of the map at the recommended contour level 0.0106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



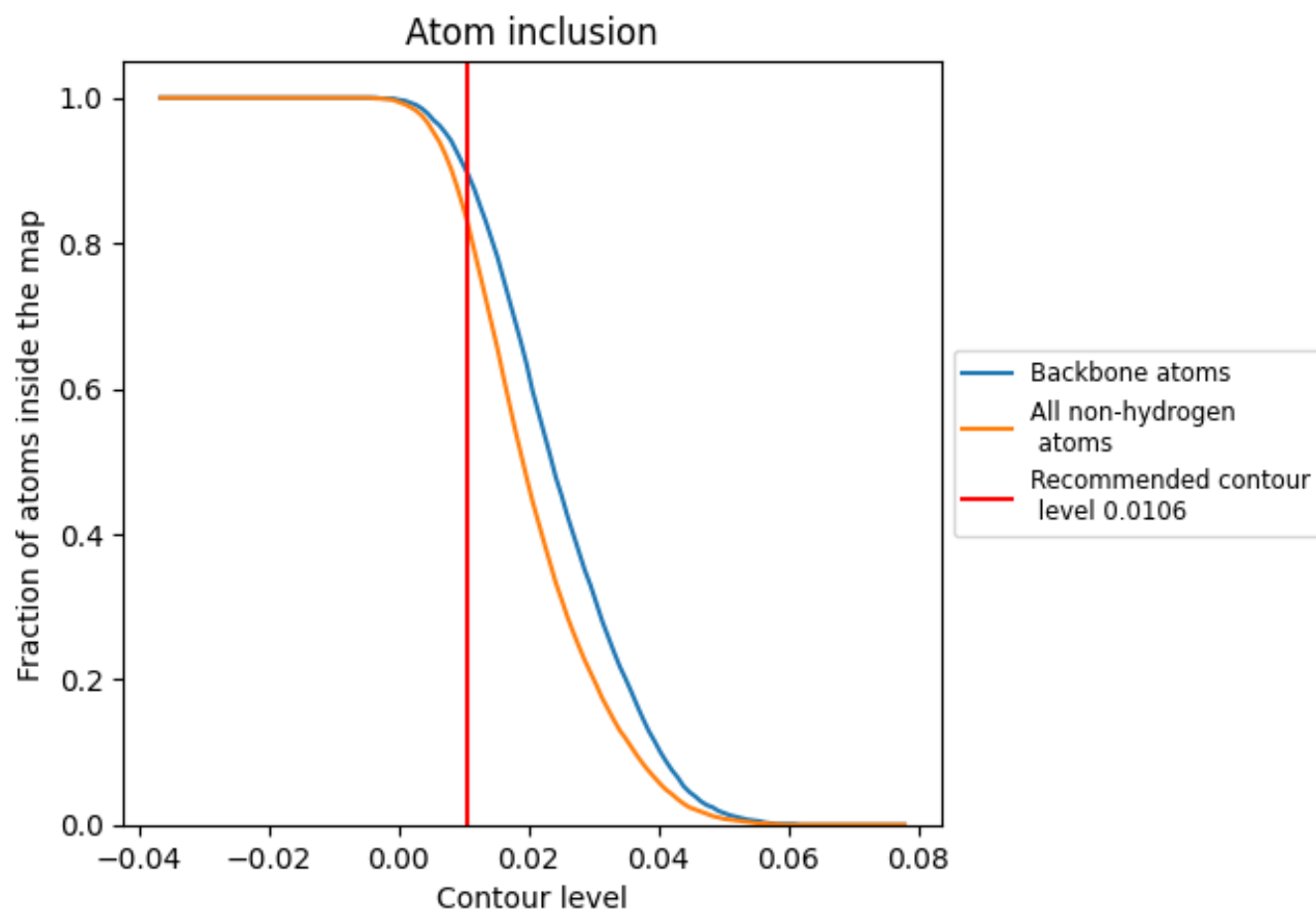
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0106).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.0106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8300	 0.3820
A	 0.7620	 0.3630
B	 0.8500	 0.3800
C	 0.8790	 0.4110
D	 0.8210	 0.3450
E	 0.7140	 0.3060
F	 0.7500	 0.3220
G	 0.9640	 0.4560
H	 0.5360	 0.1370
I	 0.4290	 0.1150
J	 0.1070	 0.0600
K	 0.7690	 0.3230
L	 0.8210	 0.3130
M	 0.8570	 0.3740
N	 0.7860	 0.2790
O	 0.7140	 0.1650
P	 0.8210	 0.3910
Q	 0.8720	 0.3620
R	 0.7860	 0.2440
S	 0.7500	 0.3330

