



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:40 PM UTC

PDB ID : 7USA / pdb_00007usa
EMDB ID : EMD-26730
Title : Structure of the human coronavirus CCoV-HuPn-2018 spike glycoprotein with domain 0 in the swung out conformation
Authors : Tortorici, M.A.; Veessler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2022-04-23
Resolution : 2.80 Å(reported)

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

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

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:

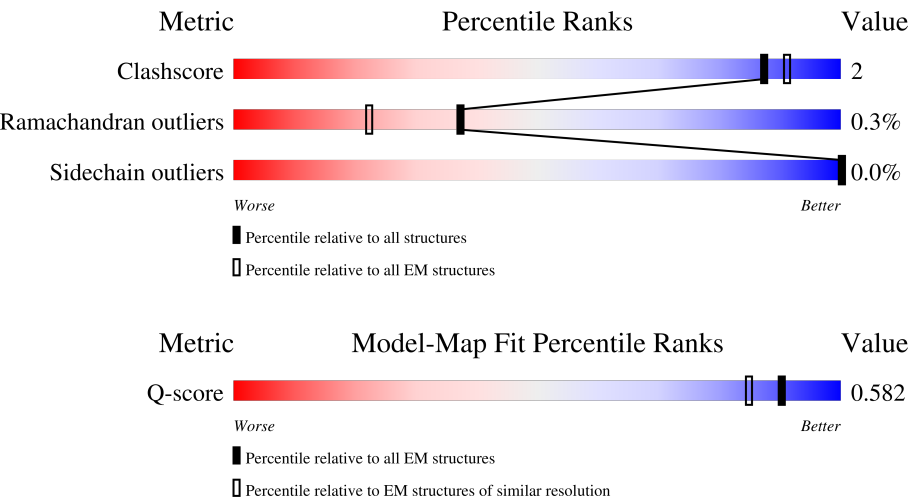
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	1469	8% 68% 28%
1	B	1469	8% 68% 28%
1	C	1469	9% 68% 28%
2	D	2	50% 100%

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

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Mol	Chain	Length	Quality of chain
3	d	3	33% 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1508	X	-	-	-
4	NAG	B	1508	X	-	-	-
4	NAG	C	1508	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24307 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	1061	Total	C	N	O	S	0	0
			7694	4926	1297	1429	42		
1	B	1058	Total	C	N	O	S	0	0
			7678	4903	1296	1437	42		
1	C	1062	Total	C	N	O	S	0	0
			7693	4916	1296	1439	42		

There are 297 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP A0A8E6CMP0
A	-14	GLY	-	expression tag	UNP A0A8E6CMP0
A	-13	ILE	-	expression tag	UNP A0A8E6CMP0
A	-12	LEU	-	expression tag	UNP A0A8E6CMP0
A	-11	PRO	-	expression tag	UNP A0A8E6CMP0
A	-10	SER	-	expression tag	UNP A0A8E6CMP0
A	-9	PRO	-	expression tag	UNP A0A8E6CMP0
A	-8	GLY	-	expression tag	UNP A0A8E6CMP0
A	-7	MET	-	expression tag	UNP A0A8E6CMP0
A	-6	PRO	-	expression tag	UNP A0A8E6CMP0
A	-5	ALA	-	expression tag	UNP A0A8E6CMP0
A	-4	LEU	-	expression tag	UNP A0A8E6CMP0
A	-3	LEU	-	expression tag	UNP A0A8E6CMP0
A	-2	SER	-	expression tag	UNP A0A8E6CMP0
A	-1	LEU	-	expression tag	UNP A0A8E6CMP0
A	0	VAL	-	expression tag	UNP A0A8E6CMP0
A	1	SER	-	expression tag	UNP A0A8E6CMP0
A	2	LEU	-	expression tag	UNP A0A8E6CMP0
A	3	LEU	-	expression tag	UNP A0A8E6CMP0
A	4	SER	-	expression tag	UNP A0A8E6CMP0
A	5	VAL	-	expression tag	UNP A0A8E6CMP0
A	6	LEU	-	expression tag	UNP A0A8E6CMP0
A	7	LEU	-	expression tag	UNP A0A8E6CMP0
A	8	MET	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP A0A8E6CMP0
A	10	CYS	-	expression tag	UNP A0A8E6CMP0
A	11	VAL	-	expression tag	UNP A0A8E6CMP0
A	12	ALA	-	expression tag	UNP A0A8E6CMP0
A	13	GLU	-	expression tag	UNP A0A8E6CMP0
A	14	THR	-	expression tag	UNP A0A8E6CMP0
A	15	GLY	-	expression tag	UNP A0A8E6CMP0
A	16	THR	-	expression tag	UNP A0A8E6CMP0
A	1140	PRO	GLU	conflict	UNP A0A8E6CMP0
A	1141	PRO	LEU	conflict	UNP A0A8E6CMP0
A	1388	SER	TRP	conflict	UNP A0A8E6CMP0
A	1389	GLY	PRO	conflict	UNP A0A8E6CMP0
A	1390	GLY	TRP	conflict	UNP A0A8E6CMP0
A	1392	ILE	VAL	conflict	UNP A0A8E6CMP0
A	1393	PRO	-	expression tag	UNP A0A8E6CMP0
A	1394	GLU	-	expression tag	UNP A0A8E6CMP0
A	1395	ALA	-	expression tag	UNP A0A8E6CMP0
A	1396	PRO	-	expression tag	UNP A0A8E6CMP0
A	1397	ARG	-	expression tag	UNP A0A8E6CMP0
A	1398	ASP	-	expression tag	UNP A0A8E6CMP0
A	1399	GLY	-	expression tag	UNP A0A8E6CMP0
A	1400	GLN	-	expression tag	UNP A0A8E6CMP0
A	1401	ALA	-	expression tag	UNP A0A8E6CMP0
A	1402	TYR	-	expression tag	UNP A0A8E6CMP0
A	1403	VAL	-	expression tag	UNP A0A8E6CMP0
A	1404	ARG	-	expression tag	UNP A0A8E6CMP0
A	1405	LYS	-	expression tag	UNP A0A8E6CMP0
A	1406	ASP	-	expression tag	UNP A0A8E6CMP0
A	1407	GLY	-	expression tag	UNP A0A8E6CMP0
A	1408	GLU	-	expression tag	UNP A0A8E6CMP0
A	1409	TRP	-	expression tag	UNP A0A8E6CMP0
A	1410	VAL	-	expression tag	UNP A0A8E6CMP0
A	1411	LEU	-	expression tag	UNP A0A8E6CMP0
A	1412	LEU	-	expression tag	UNP A0A8E6CMP0
A	1413	SER	-	expression tag	UNP A0A8E6CMP0
A	1414	THR	-	expression tag	UNP A0A8E6CMP0
A	1415	PHE	-	expression tag	UNP A0A8E6CMP0
A	1416	LEU	-	expression tag	UNP A0A8E6CMP0
A	1417	VAL	-	expression tag	UNP A0A8E6CMP0
A	1418	PRO	-	expression tag	UNP A0A8E6CMP0
A	1419	ARG	-	expression tag	UNP A0A8E6CMP0
A	1420	GLY	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1421	SER	-	expression tag	UNP A0A8E6CMP0
A	1422	GLY	-	expression tag	UNP A0A8E6CMP0
A	1423	GLY	-	expression tag	UNP A0A8E6CMP0
A	1424	SER	-	expression tag	UNP A0A8E6CMP0
A	1425	GLY	-	expression tag	UNP A0A8E6CMP0
A	1426	GLY	-	expression tag	UNP A0A8E6CMP0
A	1427	SER	-	expression tag	UNP A0A8E6CMP0
A	1428	GLY	-	expression tag	UNP A0A8E6CMP0
A	1429	LEU	-	expression tag	UNP A0A8E6CMP0
A	1430	ASN	-	expression tag	UNP A0A8E6CMP0
A	1431	ASP	-	expression tag	UNP A0A8E6CMP0
A	1432	ILE	-	expression tag	UNP A0A8E6CMP0
A	1433	PHE	-	expression tag	UNP A0A8E6CMP0
A	1434	GLU	-	expression tag	UNP A0A8E6CMP0
A	1435	ALA	-	expression tag	UNP A0A8E6CMP0
A	1436	GLN	-	expression tag	UNP A0A8E6CMP0
A	1437	LYS	-	expression tag	UNP A0A8E6CMP0
A	1438	ILE	-	expression tag	UNP A0A8E6CMP0
A	1439	GLU	-	expression tag	UNP A0A8E6CMP0
A	1440	TRP	-	expression tag	UNP A0A8E6CMP0
A	1441	HIS	-	expression tag	UNP A0A8E6CMP0
A	1442	GLU	-	expression tag	UNP A0A8E6CMP0
A	1443	GLY	-	expression tag	UNP A0A8E6CMP0
A	1444	GLY	-	expression tag	UNP A0A8E6CMP0
A	1445	SER	-	expression tag	UNP A0A8E6CMP0
A	1446	HIS	-	expression tag	UNP A0A8E6CMP0
A	1447	HIS	-	expression tag	UNP A0A8E6CMP0
A	1448	HIS	-	expression tag	UNP A0A8E6CMP0
A	1449	HIS	-	expression tag	UNP A0A8E6CMP0
A	1450	HIS	-	expression tag	UNP A0A8E6CMP0
A	1451	HIS	-	expression tag	UNP A0A8E6CMP0
A	1452	HIS	-	expression tag	UNP A0A8E6CMP0
A	1453	HIS	-	expression tag	UNP A0A8E6CMP0
B	-15	MET	-	initiating methionine	UNP A0A8E6CMP0
B	-14	GLY	-	expression tag	UNP A0A8E6CMP0
B	-13	ILE	-	expression tag	UNP A0A8E6CMP0
B	-12	LEU	-	expression tag	UNP A0A8E6CMP0
B	-11	PRO	-	expression tag	UNP A0A8E6CMP0
B	-10	SER	-	expression tag	UNP A0A8E6CMP0
B	-9	PRO	-	expression tag	UNP A0A8E6CMP0
B	-8	GLY	-	expression tag	UNP A0A8E6CMP0
B	-7	MET	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	PRO	-	expression tag	UNP A0A8E6CMP0
B	-5	ALA	-	expression tag	UNP A0A8E6CMP0
B	-4	LEU	-	expression tag	UNP A0A8E6CMP0
B	-3	LEU	-	expression tag	UNP A0A8E6CMP0
B	-2	SER	-	expression tag	UNP A0A8E6CMP0
B	-1	LEU	-	expression tag	UNP A0A8E6CMP0
B	0	VAL	-	expression tag	UNP A0A8E6CMP0
B	1	SER	-	expression tag	UNP A0A8E6CMP0
B	2	LEU	-	expression tag	UNP A0A8E6CMP0
B	3	LEU	-	expression tag	UNP A0A8E6CMP0
B	4	SER	-	expression tag	UNP A0A8E6CMP0
B	5	VAL	-	expression tag	UNP A0A8E6CMP0
B	6	LEU	-	expression tag	UNP A0A8E6CMP0
B	7	LEU	-	expression tag	UNP A0A8E6CMP0
B	8	MET	-	expression tag	UNP A0A8E6CMP0
B	9	GLY	-	expression tag	UNP A0A8E6CMP0
B	10	CYS	-	expression tag	UNP A0A8E6CMP0
B	11	VAL	-	expression tag	UNP A0A8E6CMP0
B	12	ALA	-	expression tag	UNP A0A8E6CMP0
B	13	GLU	-	expression tag	UNP A0A8E6CMP0
B	14	THR	-	expression tag	UNP A0A8E6CMP0
B	15	GLY	-	expression tag	UNP A0A8E6CMP0
B	16	THR	-	expression tag	UNP A0A8E6CMP0
B	1140	PRO	GLU	conflict	UNP A0A8E6CMP0
B	1141	PRO	LEU	conflict	UNP A0A8E6CMP0
B	1388	SER	TRP	conflict	UNP A0A8E6CMP0
B	1389	GLY	PRO	conflict	UNP A0A8E6CMP0
B	1390	GLY	TRP	conflict	UNP A0A8E6CMP0
B	1392	ILE	VAL	conflict	UNP A0A8E6CMP0
B	1393	PRO	-	expression tag	UNP A0A8E6CMP0
B	1394	GLU	-	expression tag	UNP A0A8E6CMP0
B	1395	ALA	-	expression tag	UNP A0A8E6CMP0
B	1396	PRO	-	expression tag	UNP A0A8E6CMP0
B	1397	ARG	-	expression tag	UNP A0A8E6CMP0
B	1398	ASP	-	expression tag	UNP A0A8E6CMP0
B	1399	GLY	-	expression tag	UNP A0A8E6CMP0
B	1400	GLN	-	expression tag	UNP A0A8E6CMP0
B	1401	ALA	-	expression tag	UNP A0A8E6CMP0
B	1402	TYR	-	expression tag	UNP A0A8E6CMP0
B	1403	VAL	-	expression tag	UNP A0A8E6CMP0
B	1404	ARG	-	expression tag	UNP A0A8E6CMP0
B	1405	LYS	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1406	ASP	-	expression tag	UNP A0A8E6CMP0
B	1407	GLY	-	expression tag	UNP A0A8E6CMP0
B	1408	GLU	-	expression tag	UNP A0A8E6CMP0
B	1409	TRP	-	expression tag	UNP A0A8E6CMP0
B	1410	VAL	-	expression tag	UNP A0A8E6CMP0
B	1411	LEU	-	expression tag	UNP A0A8E6CMP0
B	1412	LEU	-	expression tag	UNP A0A8E6CMP0
B	1413	SER	-	expression tag	UNP A0A8E6CMP0
B	1414	THR	-	expression tag	UNP A0A8E6CMP0
B	1415	PHE	-	expression tag	UNP A0A8E6CMP0
B	1416	LEU	-	expression tag	UNP A0A8E6CMP0
B	1417	VAL	-	expression tag	UNP A0A8E6CMP0
B	1418	PRO	-	expression tag	UNP A0A8E6CMP0
B	1419	ARG	-	expression tag	UNP A0A8E6CMP0
B	1420	GLY	-	expression tag	UNP A0A8E6CMP0
B	1421	SER	-	expression tag	UNP A0A8E6CMP0
B	1422	GLY	-	expression tag	UNP A0A8E6CMP0
B	1423	GLY	-	expression tag	UNP A0A8E6CMP0
B	1424	SER	-	expression tag	UNP A0A8E6CMP0
B	1425	GLY	-	expression tag	UNP A0A8E6CMP0
B	1426	GLY	-	expression tag	UNP A0A8E6CMP0
B	1427	SER	-	expression tag	UNP A0A8E6CMP0
B	1428	GLY	-	expression tag	UNP A0A8E6CMP0
B	1429	LEU	-	expression tag	UNP A0A8E6CMP0
B	1430	ASN	-	expression tag	UNP A0A8E6CMP0
B	1431	ASP	-	expression tag	UNP A0A8E6CMP0
B	1432	ILE	-	expression tag	UNP A0A8E6CMP0
B	1433	PHE	-	expression tag	UNP A0A8E6CMP0
B	1434	GLU	-	expression tag	UNP A0A8E6CMP0
B	1435	ALA	-	expression tag	UNP A0A8E6CMP0
B	1436	GLN	-	expression tag	UNP A0A8E6CMP0
B	1437	LYS	-	expression tag	UNP A0A8E6CMP0
B	1438	ILE	-	expression tag	UNP A0A8E6CMP0
B	1439	GLU	-	expression tag	UNP A0A8E6CMP0
B	1440	TRP	-	expression tag	UNP A0A8E6CMP0
B	1441	HIS	-	expression tag	UNP A0A8E6CMP0
B	1442	GLU	-	expression tag	UNP A0A8E6CMP0
B	1443	GLY	-	expression tag	UNP A0A8E6CMP0
B	1444	GLY	-	expression tag	UNP A0A8E6CMP0
B	1445	SER	-	expression tag	UNP A0A8E6CMP0
B	1446	HIS	-	expression tag	UNP A0A8E6CMP0
B	1447	HIS	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1448	HIS	-	expression tag	UNP A0A8E6CMP0
B	1449	HIS	-	expression tag	UNP A0A8E6CMP0
B	1450	HIS	-	expression tag	UNP A0A8E6CMP0
B	1451	HIS	-	expression tag	UNP A0A8E6CMP0
B	1452	HIS	-	expression tag	UNP A0A8E6CMP0
B	1453	HIS	-	expression tag	UNP A0A8E6CMP0
C	-15	MET	-	initiating methionine	UNP A0A8E6CMP0
C	-14	GLY	-	expression tag	UNP A0A8E6CMP0
C	-13	ILE	-	expression tag	UNP A0A8E6CMP0
C	-12	LEU	-	expression tag	UNP A0A8E6CMP0
C	-11	PRO	-	expression tag	UNP A0A8E6CMP0
C	-10	SER	-	expression tag	UNP A0A8E6CMP0
C	-9	PRO	-	expression tag	UNP A0A8E6CMP0
C	-8	GLY	-	expression tag	UNP A0A8E6CMP0
C	-7	MET	-	expression tag	UNP A0A8E6CMP0
C	-6	PRO	-	expression tag	UNP A0A8E6CMP0
C	-5	ALA	-	expression tag	UNP A0A8E6CMP0
C	-4	LEU	-	expression tag	UNP A0A8E6CMP0
C	-3	LEU	-	expression tag	UNP A0A8E6CMP0
C	-2	SER	-	expression tag	UNP A0A8E6CMP0
C	-1	LEU	-	expression tag	UNP A0A8E6CMP0
C	0	VAL	-	expression tag	UNP A0A8E6CMP0
C	1	SER	-	expression tag	UNP A0A8E6CMP0
C	2	LEU	-	expression tag	UNP A0A8E6CMP0
C	3	LEU	-	expression tag	UNP A0A8E6CMP0
C	4	SER	-	expression tag	UNP A0A8E6CMP0
C	5	VAL	-	expression tag	UNP A0A8E6CMP0
C	6	LEU	-	expression tag	UNP A0A8E6CMP0
C	7	LEU	-	expression tag	UNP A0A8E6CMP0
C	8	MET	-	expression tag	UNP A0A8E6CMP0
C	9	GLY	-	expression tag	UNP A0A8E6CMP0
C	10	CYS	-	expression tag	UNP A0A8E6CMP0
C	11	VAL	-	expression tag	UNP A0A8E6CMP0
C	12	ALA	-	expression tag	UNP A0A8E6CMP0
C	13	GLU	-	expression tag	UNP A0A8E6CMP0
C	14	THR	-	expression tag	UNP A0A8E6CMP0
C	15	GLY	-	expression tag	UNP A0A8E6CMP0
C	16	THR	-	expression tag	UNP A0A8E6CMP0
C	1140	PRO	GLU	conflict	UNP A0A8E6CMP0
C	1141	PRO	LEU	conflict	UNP A0A8E6CMP0
C	1388	SER	TRP	conflict	UNP A0A8E6CMP0
C	1389	GLY	PRO	conflict	UNP A0A8E6CMP0

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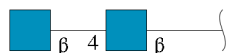
Chain	Residue	Modelled	Actual	Comment	Reference
C	1390	GLY	TRP	conflict	UNP A0A8E6CMP0
C	1392	ILE	VAL	conflict	UNP A0A8E6CMP0
C	1393	PRO	-	expression tag	UNP A0A8E6CMP0
C	1394	GLU	-	expression tag	UNP A0A8E6CMP0
C	1395	ALA	-	expression tag	UNP A0A8E6CMP0
C	1396	PRO	-	expression tag	UNP A0A8E6CMP0
C	1397	ARG	-	expression tag	UNP A0A8E6CMP0
C	1398	ASP	-	expression tag	UNP A0A8E6CMP0
C	1399	GLY	-	expression tag	UNP A0A8E6CMP0
C	1400	GLN	-	expression tag	UNP A0A8E6CMP0
C	1401	ALA	-	expression tag	UNP A0A8E6CMP0
C	1402	TYR	-	expression tag	UNP A0A8E6CMP0
C	1403	VAL	-	expression tag	UNP A0A8E6CMP0
C	1404	ARG	-	expression tag	UNP A0A8E6CMP0
C	1405	LYS	-	expression tag	UNP A0A8E6CMP0
C	1406	ASP	-	expression tag	UNP A0A8E6CMP0
C	1407	GLY	-	expression tag	UNP A0A8E6CMP0
C	1408	GLU	-	expression tag	UNP A0A8E6CMP0
C	1409	TRP	-	expression tag	UNP A0A8E6CMP0
C	1410	VAL	-	expression tag	UNP A0A8E6CMP0
C	1411	LEU	-	expression tag	UNP A0A8E6CMP0
C	1412	LEU	-	expression tag	UNP A0A8E6CMP0
C	1413	SER	-	expression tag	UNP A0A8E6CMP0
C	1414	THR	-	expression tag	UNP A0A8E6CMP0
C	1415	PHE	-	expression tag	UNP A0A8E6CMP0
C	1416	LEU	-	expression tag	UNP A0A8E6CMP0
C	1417	VAL	-	expression tag	UNP A0A8E6CMP0
C	1418	PRO	-	expression tag	UNP A0A8E6CMP0
C	1419	ARG	-	expression tag	UNP A0A8E6CMP0
C	1420	GLY	-	expression tag	UNP A0A8E6CMP0
C	1421	SER	-	expression tag	UNP A0A8E6CMP0
C	1422	GLY	-	expression tag	UNP A0A8E6CMP0
C	1423	GLY	-	expression tag	UNP A0A8E6CMP0
C	1424	SER	-	expression tag	UNP A0A8E6CMP0
C	1425	GLY	-	expression tag	UNP A0A8E6CMP0
C	1426	GLY	-	expression tag	UNP A0A8E6CMP0
C	1427	SER	-	expression tag	UNP A0A8E6CMP0
C	1428	GLY	-	expression tag	UNP A0A8E6CMP0
C	1429	LEU	-	expression tag	UNP A0A8E6CMP0
C	1430	ASN	-	expression tag	UNP A0A8E6CMP0
C	1431	ASP	-	expression tag	UNP A0A8E6CMP0
C	1432	ILE	-	expression tag	UNP A0A8E6CMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1433	PHE	-	expression tag	UNP A0A8E6CMP0
C	1434	GLU	-	expression tag	UNP A0A8E6CMP0
C	1435	ALA	-	expression tag	UNP A0A8E6CMP0
C	1436	GLN	-	expression tag	UNP A0A8E6CMP0
C	1437	LYS	-	expression tag	UNP A0A8E6CMP0
C	1438	ILE	-	expression tag	UNP A0A8E6CMP0
C	1439	GLU	-	expression tag	UNP A0A8E6CMP0
C	1440	TRP	-	expression tag	UNP A0A8E6CMP0
C	1441	HIS	-	expression tag	UNP A0A8E6CMP0
C	1442	GLU	-	expression tag	UNP A0A8E6CMP0
C	1443	GLY	-	expression tag	UNP A0A8E6CMP0
C	1444	GLY	-	expression tag	UNP A0A8E6CMP0
C	1445	SER	-	expression tag	UNP A0A8E6CMP0
C	1446	HIS	-	expression tag	UNP A0A8E6CMP0
C	1447	HIS	-	expression tag	UNP A0A8E6CMP0
C	1448	HIS	-	expression tag	UNP A0A8E6CMP0
C	1449	HIS	-	expression tag	UNP A0A8E6CMP0
C	1450	HIS	-	expression tag	UNP A0A8E6CMP0
C	1451	HIS	-	expression tag	UNP A0A8E6CMP0
C	1452	HIS	-	expression tag	UNP A0A8E6CMP0
C	1453	HIS	-	expression tag	UNP A0A8E6CMP0

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



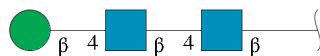
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	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		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	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.



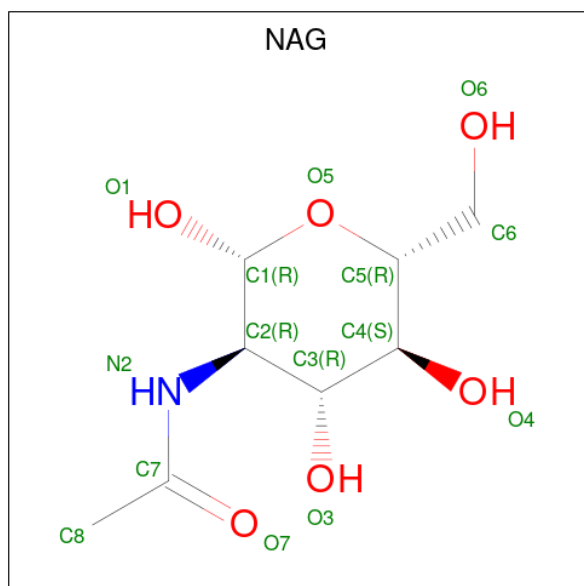
Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	b	3	Total	C	N	O	0	0
			39	22	2	15		
3	d	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: $C_8H_{15}NO_6$).



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	

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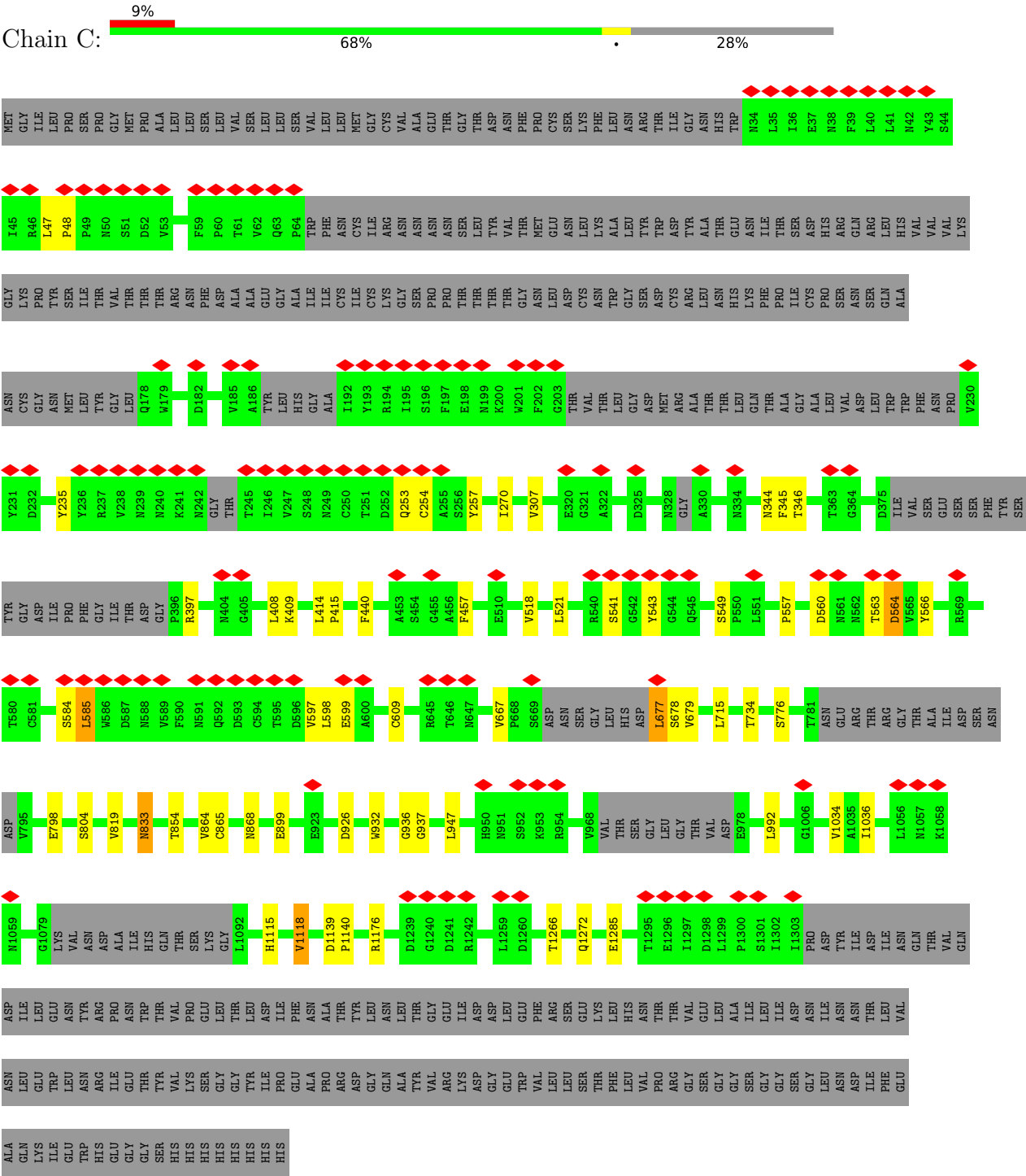
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B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

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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	

- Molecule 1: Spike glycoprotein



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



NAG1
NAG2

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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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





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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70990	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.425	Depositor
Minimum map value	-3.136	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.706	Depositor
Map size ($\text{\AA}$)	431.616, 431.616, 431.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.843, 0.843, 0.843	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	0.75	2/7849 (0.0%)	1.11	62/10741 (0.6%)
1	B	0.74	2/7835 (0.0%)	1.11	60/10723 (0.6%)
1	C	0.75	2/7850 (0.0%)	1.11	62/10745 (0.6%)
All	All	0.75	6/23534 (0.0%)	1.11	184/32209 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	865	CYS	C-O	9.51	1.34	1.23
1	B	865	CYS	C-O	9.48	1.34	1.23
1	C	865	CYS	C-O	9.47	1.34	1.23
1	A	865	CYS	C-N	-5.43	1.27	1.33
1	B	865	CYS	C-N	-5.42	1.27	1.33
1	C	865	CYS	C-N	-5.38	1.27	1.33

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	584	SER	N-CA-C	25.52	146.97	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	584	SER	N-CA-C	25.51	146.96	114.56
1	A	584	SER	N-CA-C	25.49	146.93	114.56
1	C	585	LEU	N-CA-CB	17.99	140.89	110.49
1	A	585	LEU	N-CA-CB	17.97	140.86	110.49
1	B	585	LEU	N-CA-CB	17.97	140.85	110.49
1	C	819	VAL	CA-CB-CG2	10.90	128.94	110.40
1	A	819	VAL	CA-CB-CG2	10.90	128.93	110.40
1	B	819	VAL	CA-CB-CG2	10.89	128.92	110.40
1	B	584	SER	CB-CA-C	-10.66	92.50	109.13
1	A	584	SER	CB-CA-C	-10.65	92.51	109.13
1	C	584	SER	CB-CA-C	-10.65	92.52	109.13
1	C	47	LEU	CA-C-N	10.18	127.09	119.66
1	C	47	LEU	C-N-CA	10.18	127.09	119.66
1	A	47	LEU	CA-C-N	10.15	127.07	119.66
1	A	47	LEU	C-N-CA	10.15	127.07	119.66
1	B	47	LEU	CA-C-N	10.14	127.06	119.66
1	B	47	LEU	C-N-CA	10.14	127.06	119.66
1	C	541	SER	CB-CA-C	9.47	129.57	111.48
1	A	541	SER	CB-CA-C	9.47	129.56	111.48
1	B	541	SER	CB-CA-C	9.46	129.55	111.48
1	B	1118	VAL	CG1-CB-CG2	9.22	131.09	110.80
1	C	1118	VAL	CG1-CB-CG2	9.22	131.08	110.80
1	A	1118	VAL	CG1-CB-CG2	9.21	131.07	110.80
1	B	992	LEU	CD1-CG-CD2	8.80	130.17	110.80
1	A	992	LEU	CD1-CG-CD2	8.80	130.17	110.80
1	C	992	LEU	CD1-CG-CD2	8.79	130.15	110.80
1	B	543	TYR	N-CA-C	-8.45	102.41	112.89
1	A	543	TYR	N-CA-C	-8.43	102.43	112.89
1	C	543	TYR	N-CA-C	-8.43	102.43	112.89
1	A	585	LEU	N-CA-C	-8.03	93.70	110.80
1	B	585	LEU	N-CA-C	-8.02	93.72	110.80
1	C	585	LEU	N-CA-C	-8.02	93.73	110.80
1	B	48	PRO	CA-C-N	7.66	127.30	119.56
1	B	48	PRO	C-N-CA	7.66	127.30	119.56
1	C	48	PRO	CA-C-N	7.64	127.28	119.56
1	C	48	PRO	C-N-CA	7.64	127.28	119.56
1	A	48	PRO	CA-C-N	7.64	127.28	119.56
1	A	48	PRO	C-N-CA	7.64	127.28	119.56
1	A	307	VAL	CA-C-N	7.37	127.80	119.92
1	A	307	VAL	C-N-CA	7.37	127.80	119.92
1	B	307	VAL	CA-C-N	7.36	127.79	119.92
1	B	307	VAL	C-N-CA	7.36	127.79	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	VAL	CA-C-N	7.35	127.78	119.92
1	C	307	VAL	C-N-CA	7.35	127.78	119.92
1	A	408	LEU	N-CA-C	6.91	120.19	111.69
1	C	408	LEU	N-CA-C	6.90	120.18	111.69
1	B	408	LEU	N-CA-C	6.89	120.17	111.69
1	C	926	ASP	CA-C-N	6.72	127.26	119.47
1	C	926	ASP	C-N-CA	6.72	127.26	119.47
1	A	926	ASP	CA-C-N	6.71	127.26	119.47
1	A	926	ASP	C-N-CA	6.71	127.26	119.47
1	B	926	ASP	CA-C-N	6.70	127.24	119.47
1	B	926	ASP	C-N-CA	6.70	127.24	119.47
1	B	947	LEU	CA-C-N	6.55	126.53	119.78
1	B	947	LEU	C-N-CA	6.55	126.53	119.78
1	A	947	LEU	CA-C-N	6.55	126.52	119.78
1	A	947	LEU	C-N-CA	6.55	126.52	119.78
1	C	947	LEU	CA-C-N	6.55	126.52	119.78
1	C	947	LEU	C-N-CA	6.55	126.52	119.78
1	A	864	VAL	CA-C-N	6.37	132.56	123.14
1	A	864	VAL	C-N-CA	6.37	132.56	123.14
1	B	864	VAL	CA-C-N	6.37	132.56	123.14
1	B	864	VAL	C-N-CA	6.37	132.56	123.14
1	C	864	VAL	CA-C-N	6.36	132.56	123.14
1	C	864	VAL	C-N-CA	6.36	132.56	123.14
1	A	854	THR	CA-C-N	6.09	126.06	119.78
1	A	854	THR	C-N-CA	6.09	126.06	119.78
1	C	521	LEU	CA-C-N	6.09	126.00	119.85
1	C	521	LEU	C-N-CA	6.09	126.00	119.85
1	B	854	THR	CA-C-N	6.08	126.05	119.78
1	B	854	THR	C-N-CA	6.08	126.05	119.78
1	B	521	LEU	CA-C-N	6.08	125.99	119.85
1	B	521	LEU	C-N-CA	6.08	125.99	119.85
1	C	854	THR	CA-C-N	6.06	126.02	119.78
1	C	854	THR	C-N-CA	6.06	126.02	119.78
1	A	521	LEU	CA-C-N	6.06	125.97	119.85
1	A	521	LEU	C-N-CA	6.06	125.97	119.85
1	A	1036	ILE	CA-C-N	6.00	125.96	119.78
1	A	1036	ILE	C-N-CA	6.00	125.96	119.78
1	C	1036	ILE	CA-C-N	6.00	125.96	119.78
1	C	1036	ILE	C-N-CA	6.00	125.96	119.78
1	B	1036	ILE	CA-C-N	5.99	125.95	119.78
1	B	1036	ILE	C-N-CA	5.99	125.95	119.78
1	C	549	SER	CA-C-N	5.99	126.77	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	549	SER	C-N-CA	5.99	126.77	120.12
1	A	549	SER	CA-C-N	5.99	126.77	120.12
1	A	549	SER	C-N-CA	5.99	126.77	120.12
1	B	549	SER	CA-C-N	5.97	126.74	120.12
1	B	549	SER	C-N-CA	5.97	126.74	120.12
1	A	541	SER	N-CA-C	-5.91	101.44	109.95
1	C	541	SER	N-CA-C	-5.90	101.45	109.95
1	B	541	SER	N-CA-C	-5.89	101.46	109.95
1	A	1272	GLN	CA-C-N	5.77	125.67	119.85
1	A	1272	GLN	C-N-CA	5.77	125.67	119.85
1	B	804	SER	CB-CA-C	-5.76	109.95	116.63
1	C	1272	GLN	CA-C-N	5.75	125.65	119.85
1	C	1272	GLN	C-N-CA	5.75	125.65	119.85
1	C	804	SER	CB-CA-C	-5.74	109.97	116.63
1	A	804	SER	CB-CA-C	-5.72	110.00	116.63
1	B	1272	GLN	CA-C-N	5.72	125.63	119.85
1	B	1272	GLN	C-N-CA	5.72	125.63	119.85
1	B	270	ILE	CA-C-N	5.71	125.71	119.89
1	B	270	ILE	C-N-CA	5.71	125.71	119.89
1	C	270	ILE	CA-C-N	5.70	125.71	119.89
1	C	270	ILE	C-N-CA	5.70	125.71	119.89
1	A	270	ILE	CA-C-N	5.70	125.70	119.89
1	A	270	ILE	C-N-CA	5.70	125.70	119.89
1	B	1140	PRO	N-CA-C	5.69	117.64	110.70
1	C	1140	PRO	N-CA-C	5.68	117.63	110.70
1	A	1140	PRO	N-CA-C	5.67	117.62	110.70
1	A	734	THR	CA-C-N	5.53	125.47	119.78
1	A	734	THR	C-N-CA	5.53	125.47	119.78
1	C	734	THR	CA-C-N	5.50	125.44	119.78
1	C	734	THR	C-N-CA	5.50	125.44	119.78
1	B	734	THR	CA-C-N	5.49	125.44	119.78
1	B	734	THR	C-N-CA	5.49	125.44	119.78
1	C	609	CYS	CA-C-N	5.47	126.67	119.84
1	C	609	CYS	C-N-CA	5.47	126.67	119.84
1	A	609	CYS	CA-C-N	5.46	126.66	119.84
1	A	609	CYS	C-N-CA	5.46	126.66	119.84
1	B	798	GLU	CA-C-N	5.45	125.36	119.85
1	B	798	GLU	C-N-CA	5.45	125.36	119.85
1	B	609	CYS	CA-C-N	5.44	126.64	119.84
1	B	609	CYS	C-N-CA	5.44	126.64	119.84
1	C	798	GLU	CA-C-N	5.44	125.34	119.85
1	C	798	GLU	C-N-CA	5.44	125.34	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	798	GLU	CA-C-N	5.43	125.33	119.85
1	A	798	GLU	C-N-CA	5.43	125.33	119.85
1	B	868	ASN	CA-C-N	5.41	126.60	119.84
1	B	868	ASN	C-N-CA	5.41	126.60	119.84
1	C	868	ASN	CA-C-N	5.41	126.60	119.84
1	C	868	ASN	C-N-CA	5.41	126.60	119.84
1	A	868	ASN	CA-C-N	5.40	126.59	119.84
1	A	868	ASN	C-N-CA	5.40	126.59	119.84
1	A	667	VAL	CA-C-N	5.39	124.91	119.19
1	A	667	VAL	C-N-CA	5.39	124.91	119.19
1	A	776	SER	N-CA-C	5.39	116.18	108.74
1	B	776	SER	N-CA-C	5.39	116.18	108.74
1	C	776	SER	N-CA-C	5.38	116.17	108.74
1	A	1139	ASP	CA-C-N	5.31	125.84	120.38
1	A	1139	ASP	C-N-CA	5.31	125.84	120.38
1	B	667	VAL	CA-C-N	5.30	124.92	119.56
1	B	667	VAL	C-N-CA	5.30	124.92	119.56
1	C	932	TRP	CA-C-N	5.30	124.81	119.19
1	C	932	TRP	C-N-CA	5.30	124.81	119.19
1	C	667	VAL	CA-C-N	5.30	124.91	119.56
1	C	667	VAL	C-N-CA	5.30	124.91	119.56
1	A	932	TRP	CA-C-N	5.29	124.80	119.19
1	A	932	TRP	C-N-CA	5.29	124.80	119.19
1	C	1139	ASP	CA-C-N	5.26	125.80	120.38
1	C	1139	ASP	C-N-CA	5.26	125.80	120.38
1	A	415	PRO	CA-C-N	5.25	126.28	120.45
1	A	415	PRO	C-N-CA	5.25	126.28	120.45
1	B	1139	ASP	CA-C-N	5.25	125.79	120.38
1	B	1139	ASP	C-N-CA	5.25	125.79	120.38
1	B	932	TRP	CA-C-N	5.25	124.75	119.19
1	B	932	TRP	C-N-CA	5.25	124.75	119.19
1	B	415	PRO	CA-C-N	5.25	126.28	120.45
1	B	415	PRO	C-N-CA	5.25	126.28	120.45
1	C	415	PRO	CA-C-N	5.24	126.27	120.45
1	C	415	PRO	C-N-CA	5.24	126.27	120.45
1	A	1285	GLU	N-CA-C	5.18	116.93	111.28
1	C	1285	GLU	N-CA-C	5.17	116.91	111.28
1	B	1285	GLU	N-CA-C	5.16	116.90	111.28
1	A	1266	THR	CA-C-N	5.06	124.96	119.85
1	A	1266	THR	C-N-CA	5.06	124.96	119.85
1	C	409	LYS	N-CA-CB	-5.06	102.12	111.53
1	B	409	LYS	N-CA-CB	-5.06	102.12	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1266	THR	CA-C-N	5.05	124.95	119.85
1	C	1266	THR	C-N-CA	5.05	124.95	119.85
1	B	1266	THR	CA-C-N	5.05	124.95	119.85
1	B	1266	THR	C-N-CA	5.05	124.95	119.85
1	A	409	LYS	N-CA-CB	-5.05	102.14	111.53
1	C	819	VAL	CG1-CB-CG2	-5.04	99.71	110.80
1	B	819	VAL	CG1-CB-CG2	-5.03	99.73	110.80
1	A	819	VAL	CG1-CB-CG2	-5.03	99.73	110.80
1	B	865	CYS	CA-C-O	-5.03	114.97	120.70
1	A	865	CYS	CA-C-O	-5.03	114.97	120.70
1	A	440	PHE	CA-C-N	5.02	125.02	119.90
1	A	440	PHE	C-N-CA	5.02	125.02	119.90
1	C	440	PHE	CA-C-N	5.01	125.01	119.90
1	C	440	PHE	C-N-CA	5.01	125.01	119.90
1	C	865	CYS	CA-C-O	-5.01	114.99	120.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	833	ASN	Mainchain
1	B	833	ASN	Mainchain
1	C	833	ASN	Mainchain

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	7694	0	7149	32	0
1	B	7678	0	7101	33	0
1	C	7693	0	7108	33	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
2	H	28	0	25	1	0
2	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	M	28	0	25	0	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	0	0
2	T	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	1	0
2	a	28	0	25	0	0
2	c	28	0	25	0	0
3	J	39	0	34	0	0
3	L	39	0	34	0	0
3	S	39	0	34	0	0
3	U	39	0	34	0	0
3	b	39	0	34	0	0
3	d	39	0	34	0	0
4	A	140	0	130	0	0
4	B	140	0	130	0	0
4	C	140	0	130	0	0
All	All	24307	0	22477	91	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 2.

All (91) 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:235:TYR:HE2	1:B:457:PHE:CZ	1.46	1.34
1:C:235:TYR:HE2	1:C:457:PHE:CZ	1.46	1.33
1:A:235:TYR:HE2	1:A:457:PHE:CZ	1.46	1.33
1:C:235:TYR:CE2	1:C:457:PHE:CZ	2.26	1.23
1:A:235:TYR:CE2	1:A:457:PHE:CZ	2.26	1.22
1:B:235:TYR:CE2	1:B:457:PHE:CZ	2.26	1.21
1:B:397:ARG:CD	1:B:414:LEU:HD12	1.70	1.21
1:C:397:ARG:CD	1:C:414:LEU:HD12	1.70	1.21
1:A:397:ARG:CD	1:A:414:LEU:HD12	1.70	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ARG:HD2	1:C:414:LEU:CD1	1.79	1.12
1:A:397:ARG:HD2	1:A:414:LEU:CD1	1.79	1.12
1:B:397:ARG:HD2	1:B:414:LEU:CD1	1.79	1.10
1:B:397:ARG:HD2	1:B:414:LEU:HD12	0.88	0.88
1:A:397:ARG:HD2	1:A:414:LEU:HD12	0.88	0.86
1:C:397:ARG:HD2	1:C:414:LEU:HD12	0.88	0.83
1:B:541:SER:OG	1:C:560:ASP:OD2	1.97	0.81
1:C:235:TYR:HE2	1:C:457:PHE:CE1	2.02	0.77
1:A:235:TYR:HE2	1:A:457:PHE:CE1	2.02	0.76
1:B:235:TYR:HE2	1:B:457:PHE:CE1	2.02	0.75
1:B:254:CYS:HA	1:B:257:TYR:HD1	1.57	0.70
1:A:254:CYS:HA	1:A:257:TYR:HD1	1.57	0.69
1:C:254:CYS:HA	1:C:257:TYR:HD1	1.57	0.69
1:B:518:VAL:O	1:B:678:SER:HA	1.95	0.67
1:A:518:VAL:O	1:A:678:SER:HA	1.95	0.66
1:C:518:VAL:O	1:C:678:SER:HA	1.95	0.66
1:C:253:GLN:O	1:C:257:TYR:CE1	2.49	0.66
1:A:253:GLN:O	1:A:257:TYR:CE1	2.49	0.66
1:B:253:GLN:O	1:B:257:TYR:CE1	2.49	0.66
1:B:235:TYR:CE2	1:B:457:PHE:HZ	2.10	0.63
1:C:235:TYR:HE2	1:C:457:PHE:CE2	2.12	0.63
1:C:235:TYR:CE2	1:C:457:PHE:CE2	2.86	0.63
1:C:254:CYS:HA	1:C:257:TYR:CD1	2.34	0.63
1:A:254:CYS:HA	1:A:257:TYR:CD1	2.34	0.63
1:B:254:CYS:HA	1:B:257:TYR:CD1	2.34	0.62
1:A:235:TYR:CE2	1:A:457:PHE:CE2	2.86	0.61
1:B:235:TYR:CE2	1:B:457:PHE:CE2	2.86	0.61
1:C:235:TYR:CE2	1:C:457:PHE:HZ	2.09	0.59
1:A:235:TYR:HE2	1:A:457:PHE:CE2	2.12	0.59
1:C:397:ARG:O	1:C:397:ARG:HG3	2.05	0.56
1:C:557:PRO:HB2	1:C:566:TYR:CE1	2.40	0.56
1:A:397:ARG:O	1:A:397:ARG:HG3	2.05	0.56
1:B:235:TYR:HE2	1:B:457:PHE:CE2	2.12	0.56
1:A:557:PRO:HB2	1:A:566:TYR:CE1	2.40	0.56
1:B:557:PRO:HB2	1:B:566:TYR:CE1	2.40	0.56
1:B:235:TYR:CE2	1:B:457:PHE:CE1	2.86	0.56
1:B:397:ARG:O	1:B:397:ARG:HG3	2.05	0.55
1:A:235:TYR:CE2	1:A:457:PHE:HZ	2.10	0.54
1:A:235:TYR:CE2	1:A:457:PHE:CE1	2.86	0.54
1:B:597:VAL:C	1:B:599:GLU:H	2.16	0.54
1:A:597:VAL:C	1:A:599:GLU:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:VAL:C	1:C:599:GLU:H	2.16	0.53
1:C:235:TYR:CE2	1:C:457:PHE:CE1	2.86	0.53
1:A:563:THR:O	1:A:564:ASP:C	2.52	0.52
1:B:563:THR:O	1:B:564:ASP:C	2.52	0.52
1:C:563:THR:O	1:C:564:ASP:C	2.52	0.52
1:A:715:LEU:HD11	1:C:1118:VAL:CG1	2.46	0.45
1:B:1118:VAL:CG1	1:C:715:LEU:HD11	2.46	0.45
1:A:1118:VAL:CG1	1:B:715:LEU:HD11	2.46	0.45
1:A:344:ASN:O	1:A:346:THR:N	2.48	0.45
1:C:677:LEU:HG	1:C:678:SER:N	2.31	0.45
1:A:235:TYR:CD2	1:A:457:PHE:CZ	3.00	0.44
1:A:1115:HIS:O	1:A:1118:VAL:HG22	2.18	0.44
1:C:235:TYR:CD2	1:C:457:PHE:CZ	3.00	0.44
1:C:1115:HIS:O	1:C:1118:VAL:HG22	2.18	0.44
1:A:715:LEU:HD11	1:C:1118:VAL:HG12	2.00	0.44
1:C:833:ASN:ND2	2:Z:1:NAG:O7	2.51	0.43
1:B:344:ASN:O	1:B:346:THR:N	2.48	0.43
1:C:344:ASN:O	1:C:346:THR:N	2.48	0.43
1:B:899:GLU:OE1	1:B:1176:ARG:NH1	2.52	0.43
1:A:1118:VAL:HG12	1:B:715:LEU:HD11	2.00	0.42
1:B:345:PHE:HE2	1:B:397:ARG:NH1	2.18	0.42
1:C:899:GLU:OE1	1:C:1176:ARG:NH1	2.52	0.42
1:B:833:ASN:ND2	2:Q:1:NAG:O7	2.51	0.42
1:B:1115:HIS:O	1:B:1118:VAL:HG22	2.18	0.42
1:B:1118:VAL:HG12	1:C:715:LEU:HD11	2.00	0.42
1:A:833:ASN:ND2	2:H:1:NAG:O7	2.51	0.42
1:A:899:GLU:OE1	1:A:1176:ARG:NH1	2.52	0.42
1:A:597:VAL:C	1:A:599:GLU:N	2.78	0.42
1:C:345:PHE:HE2	1:C:397:ARG:NH1	2.18	0.42
1:A:345:PHE:HE2	1:A:397:ARG:NH1	2.18	0.41
1:B:936:GLY:O	1:B:937:GLY:C	2.64	0.41
1:C:677:LEU:HD11	1:C:679:VAL:HG23	2.03	0.41
1:B:597:VAL:C	1:B:599:GLU:N	2.78	0.41
1:A:1140:PRO:HG2	1:A:1141:PRO:HD3	2.02	0.41
1:A:936:GLY:O	1:A:937:GLY:C	2.64	0.41
1:B:1140:PRO:HG2	1:B:1141:PRO:HD3	2.02	0.41
1:A:1034:VAL:O	1:A:1034:VAL:HG13	2.20	0.40
1:B:1034:VAL:HG13	1:B:1034:VAL:O	2.20	0.40
1:C:936:GLY:O	1:C:937:GLY:C	2.64	0.40
1:B:563:THR:O	1:B:565:VAL:N	2.55	0.40
1:C:1034:VAL:HG13	1:C:1034:VAL:O	2.20	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	1039/1469 (71%)	999 (96%)	37 (4%)	3 (0%)	36	66
1	B	1036/1469 (70%)	997 (96%)	36 (4%)	3 (0%)	36	66
1	C	1040/1469 (71%)	1001 (96%)	36 (4%)	3 (0%)	36	66
All	All	3115/4407 (71%)	2997 (96%)	109 (4%)	9 (0%)	37	66

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	LEU
1	B	585	LEU
1	C	585	LEU
1	A	564	ASP
1	B	564	ASP
1	C	564	ASP
1	A	598	LEU
1	B	598	LEU
1	C	598	LEU

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	763/1269 (60%)	763 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	766/1269 (60%)	766 (100%)	0	100	100
1	C	764/1269 (60%)	763 (100%)	1 (0%)	88	97
All	All	2293/3807 (60%)	2292 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	677	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	HIS
1	A	647	ASN
1	A	1107	ASN
1	A	1164	GLN
1	A	1192	GLN
1	B	647	ASN
1	B	1107	ASN
1	B	1192	GLN
1	C	428	HIS
1	C	771	ASN
1	C	1061	GLN
1	C	1107	ASN
1	C	1192	GLN
1	C	1208	ASN

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 ⓘ

60 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	1.53	2 (14%)	17,19,21	1.09	1 (5%)
2	NAG	D	2	2	14,14,15	1.48	2 (14%)	17,19,21	0.90	1 (5%)
2	NAG	E	1	1,2	14,14,15	1.56	2 (14%)	17,19,21	0.96	1 (5%)
2	NAG	E	2	2	14,14,15	1.50	2 (14%)	17,19,21	0.83	1 (5%)
2	NAG	F	1	1,2	14,14,15	1.42	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	F	2	2	14,14,15	1.42	2 (14%)	17,19,21	0.80	0
2	NAG	G	1	1,2	14,14,15	1.51	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	G	2	2	14,14,15	1.46	2 (14%)	17,19,21	0.95	1 (5%)
2	NAG	H	1	1,2	14,14,15	1.96	3 (21%)	17,19,21	0.89	0
2	NAG	H	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.77	4 (23%)
2	NAG	I	1	1,2	14,14,15	1.58	1 (7%)	17,19,21	0.92	0
2	NAG	I	2	2	14,14,15	1.49	2 (14%)	17,19,21	0.96	2 (11%)
3	NAG	J	1	1,3	14,14,15	2.29	4 (28%)	17,19,21	2.50	5 (29%)
3	NAG	J	2	3	14,14,15	0.53	0	17,19,21	1.40	2 (11%)
3	BMA	J	3	3	11,11,12	1.40	3 (27%)	15,15,17	0.67	0
2	NAG	K	1	1,2	14,14,15	1.70	2 (14%)	17,19,21	1.48	2 (11%)
2	NAG	K	2	2	14,14,15	1.51	2 (14%)	17,19,21	1.11	2 (11%)
3	NAG	L	1	1,3	14,14,15	1.69	1 (7%)	17,19,21	1.76	4 (23%)
3	NAG	L	2	3	14,14,15	0.50	0	17,19,21	1.29	1 (5%)
3	BMA	L	3	3	11,11,12	1.50	3 (27%)	15,15,17	0.61	0
2	NAG	M	1	1,2	14,14,15	1.54	2 (14%)	17,19,21	1.09	1 (5%)
2	NAG	M	2	2	14,14,15	1.47	2 (14%)	17,19,21	0.90	1 (5%)
2	NAG	N	1	1,2	14,14,15	1.56	2 (14%)	17,19,21	0.96	1 (5%)
2	NAG	N	2	2	14,14,15	1.50	2 (14%)	17,19,21	0.83	1 (5%)
2	NAG	O	1	1,2	14,14,15	1.42	1 (7%)	17,19,21	1.12	1 (5%)
2	NAG	O	2	2	14,14,15	1.42	2 (14%)	17,19,21	0.80	0
2	NAG	P	1	1,2	14,14,15	1.51	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	P	2	2	14,14,15	1.46	2 (14%)	17,19,21	0.95	1 (5%)
2	NAG	Q	1	1,2	14,14,15	1.96	3 (21%)	17,19,21	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Q	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.77	4 (23%)
2	NAG	R	1	1,2	14,14,15	1.58	1 (7%)	17,19,21	0.93	1 (5%)
2	NAG	R	2	2	14,14,15	1.49	2 (14%)	17,19,21	0.95	1 (5%)
3	NAG	S	1	1,3	14,14,15	2.29	4 (28%)	17,19,21	2.50	5 (29%)
3	NAG	S	2	3	14,14,15	0.53	0	17,19,21	1.39	2 (11%)
3	BMA	S	3	3	11,11,12	1.41	3 (27%)	15,15,17	0.68	0
2	NAG	T	1	1,2	14,14,15	1.69	2 (14%)	17,19,21	1.47	2 (11%)
2	NAG	T	2	2	14,14,15	1.51	2 (14%)	17,19,21	1.11	2 (11%)
3	NAG	U	1	1,3	14,14,15	1.69	1 (7%)	17,19,21	1.76	4 (23%)
3	NAG	U	2	3	14,14,15	0.50	0	17,19,21	1.30	1 (5%)
3	BMA	U	3	3	11,11,12	1.50	3 (27%)	15,15,17	0.61	0
2	NAG	V	1	1,2	14,14,15	1.54	2 (14%)	17,19,21	1.10	1 (5%)
2	NAG	V	2	2	14,14,15	1.47	2 (14%)	17,19,21	0.90	1 (5%)
2	NAG	W	1	1,2	14,14,15	1.56	2 (14%)	17,19,21	0.96	1 (5%)
2	NAG	W	2	2	14,14,15	1.50	2 (14%)	17,19,21	0.83	1 (5%)
2	NAG	X	1	1,2	14,14,15	1.41	2 (14%)	17,19,21	1.12	1 (5%)
2	NAG	X	2	2	14,14,15	1.42	2 (14%)	17,19,21	0.80	0
2	NAG	Y	1	1,2	14,14,15	1.52	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	Y	2	2	14,14,15	1.46	2 (14%)	17,19,21	0.95	1 (5%)
2	NAG	Z	1	1,2	14,14,15	1.96	3 (21%)	17,19,21	0.88	0
2	NAG	Z	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.77	4 (23%)
2	NAG	a	1	1,2	14,14,15	1.57	1 (7%)	17,19,21	0.92	0
2	NAG	a	2	2	14,14,15	1.48	2 (14%)	17,19,21	0.96	2 (11%)
3	NAG	b	1	1,3	14,14,15	2.28	4 (28%)	17,19,21	2.50	5 (29%)
3	NAG	b	2	3	14,14,15	0.52	0	17,19,21	1.40	2 (11%)
3	BMA	b	3	3	11,11,12	1.40	3 (27%)	15,15,17	0.67	0
2	NAG	c	1	1,2	14,14,15	1.70	2 (14%)	17,19,21	1.48	2 (11%)
2	NAG	c	2	2	14,14,15	1.50	2 (14%)	17,19,21	1.12	2 (11%)
3	NAG	d	1	1,3	14,14,15	1.69	1 (7%)	17,19,21	1.76	4 (23%)
3	NAG	d	2	3	14,14,15	0.50	0	17,19,21	1.30	1 (5%)
3	BMA	d	3	3	11,11,12	1.50	3 (27%)	15,15,17	0.62	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	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	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	-	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	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	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	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
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	BMA	S	3	3	-	2/2/19/22	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	BMA	U	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	3/6/23/26	0/1/1/1
2	NAG	a	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	BMA	b	3	3	-	2/2/19/22	0/1/1/1
2	NAG	c	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
3	NAG	d	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	d	2	3	-	3/6/23/26	0/1/1/1
3	BMA	d	3	3	-	2/2/19/22	0/1/1/1

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	C1-C2	7.00	1.61	1.52
3	S	1	NAG	C1-C2	6.99	1.61	1.52
3	b	1	NAG	C1-C2	6.98	1.61	1.52
2	H	2	NAG	C1-C2	5.74	1.60	1.52
2	Z	2	NAG	C1-C2	5.74	1.60	1.52
2	Q	2	NAG	C1-C2	5.73	1.60	1.52
2	H	1	NAG	C1-C2	5.64	1.60	1.52
2	Q	1	NAG	C1-C2	5.61	1.60	1.52
2	Z	1	NAG	C1-C2	5.61	1.60	1.52
3	U	1	NAG	C1-C2	4.74	1.58	1.52
3	L	1	NAG	C1-C2	4.73	1.58	1.52
3	d	1	NAG	C1-C2	4.72	1.58	1.52
2	I	1	NAG	C1-C2	4.71	1.58	1.52
2	R	1	NAG	C1-C2	4.66	1.58	1.52
2	a	1	NAG	C1-C2	4.66	1.58	1.52
2	K	1	NAG	C1-C2	4.65	1.58	1.52
2	c	1	NAG	C1-C2	4.63	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	1	NAG	C1-C2	4.58	1.58	1.52
2	Y	1	NAG	C1-C2	4.57	1.58	1.52
2	P	1	NAG	C1-C2	4.55	1.58	1.52
2	G	1	NAG	C1-C2	4.53	1.58	1.52
2	M	1	NAG	C1-C2	4.32	1.58	1.52
2	V	1	NAG	C1-C2	4.29	1.58	1.52
2	W	1	NAG	C1-C2	4.29	1.58	1.52
2	E	1	NAG	C1-C2	4.28	1.58	1.52
2	N	1	NAG	C1-C2	4.27	1.58	1.52
2	D	1	NAG	C1-C2	4.27	1.58	1.52
2	O	1	NAG	C1-C2	3.76	1.57	1.52
2	F	1	NAG	C1-C2	3.73	1.57	1.52
2	X	1	NAG	C1-C2	3.71	1.57	1.52
2	W	2	NAG	C1-C2	3.58	1.57	1.52
2	E	2	NAG	C1-C2	3.55	1.57	1.52
2	N	2	NAG	C1-C2	3.53	1.57	1.52
2	P	2	NAG	C1-C2	3.51	1.57	1.52
2	G	2	NAG	C1-C2	3.51	1.57	1.52
2	Y	2	NAG	C1-C2	3.50	1.57	1.52
2	T	2	NAG	C1-C2	3.47	1.57	1.52
2	K	2	NAG	C1-C2	3.47	1.57	1.52
2	c	2	NAG	C1-C2	3.44	1.57	1.52
2	D	2	NAG	C1-C2	3.43	1.57	1.52
2	M	2	NAG	C1-C2	3.41	1.57	1.52
2	a	2	NAG	C1-C2	3.40	1.57	1.52
2	I	2	NAG	C1-C2	3.39	1.57	1.52
2	V	2	NAG	C1-C2	3.39	1.57	1.52
2	R	2	NAG	C1-C2	3.38	1.57	1.52
2	T	2	NAG	O5-C5	3.25	1.49	1.43
2	F	2	NAG	C1-C2	3.25	1.56	1.52
2	K	2	NAG	O5-C5	3.24	1.49	1.43
2	c	2	NAG	O5-C5	3.24	1.49	1.43
2	O	2	NAG	C1-C2	3.23	1.56	1.52
2	X	2	NAG	C1-C2	3.23	1.56	1.52
2	O	2	NAG	O5-C5	2.90	1.49	1.43
2	F	2	NAG	O5-C5	2.90	1.49	1.43
2	X	2	NAG	O5-C5	2.89	1.49	1.43
2	P	2	NAG	O5-C5	2.87	1.49	1.43
2	E	2	NAG	O5-C5	2.87	1.49	1.43
2	G	2	NAG	O5-C5	2.86	1.49	1.43
2	N	2	NAG	O5-C5	2.85	1.49	1.43
2	W	2	NAG	O5-C5	2.84	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	2	NAG	O5-C5	2.84	1.49	1.43
2	H	2	NAG	O5-C5	2.83	1.48	1.43
2	Y	2	NAG	O5-C5	2.83	1.48	1.43
3	U	3	BMA	O5-C5	2.83	1.48	1.43
3	d	3	BMA	O5-C5	2.83	1.48	1.43
3	L	3	BMA	O5-C5	2.83	1.48	1.43
2	Z	2	NAG	O5-C5	2.82	1.48	1.43
2	D	2	NAG	O5-C5	2.82	1.48	1.43
2	M	2	NAG	O5-C5	2.80	1.48	1.43
2	V	2	NAG	O5-C5	2.80	1.48	1.43
2	I	2	NAG	O5-C5	2.72	1.48	1.43
2	R	2	NAG	O5-C5	2.70	1.48	1.43
2	a	2	NAG	O5-C5	2.68	1.48	1.43
2	Z	1	NAG	O5-C5	2.58	1.48	1.43
2	Q	1	NAG	O5-C5	2.58	1.48	1.43
2	H	1	NAG	O5-C5	2.56	1.48	1.43
3	S	1	NAG	C3-C2	2.51	1.57	1.52
3	S	3	BMA	O5-C5	2.51	1.48	1.43
3	J	1	NAG	C3-C2	2.50	1.57	1.52
3	b	3	BMA	O5-C5	2.50	1.48	1.43
3	b	1	NAG	C3-C2	2.49	1.57	1.52
3	J	3	BMA	O5-C5	2.49	1.48	1.43
2	H	2	NAG	C3-C2	2.39	1.57	1.52
2	Z	2	NAG	C3-C2	2.38	1.57	1.52
2	Q	2	NAG	C3-C2	2.36	1.57	1.52
3	d	3	BMA	C2-C3	2.24	1.55	1.52
3	L	3	BMA	C2-C3	2.24	1.55	1.52
3	U	3	BMA	C2-C3	2.23	1.55	1.52
2	V	1	NAG	O5-C5	2.21	1.47	1.43
2	D	1	NAG	O5-C5	2.20	1.47	1.43
2	M	1	NAG	O5-C5	2.20	1.47	1.43
3	S	1	NAG	O4-C4	2.19	1.48	1.43
3	J	1	NAG	O4-C4	2.18	1.48	1.43
3	b	1	NAG	O4-C4	2.18	1.48	1.43
2	W	1	NAG	O5-C5	2.16	1.47	1.43
2	E	1	NAG	O5-C5	2.15	1.47	1.43
2	K	1	NAG	C3-C2	2.15	1.57	1.52
2	Q	2	NAG	C4-C5	2.15	1.57	1.53
2	c	1	NAG	C3-C2	2.14	1.57	1.52
2	T	1	NAG	C3-C2	2.14	1.57	1.52
2	H	2	NAG	C4-C5	2.14	1.57	1.53
2	N	1	NAG	O5-C5	2.14	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	2	NAG	C4-C5	2.14	1.57	1.53
3	J	3	BMA	C2-C3	2.14	1.55	1.52
2	Q	1	NAG	O4-C4	2.12	1.48	1.43
3	S	3	BMA	C2-C3	2.11	1.55	1.52
2	Z	1	NAG	O4-C4	2.11	1.48	1.43
2	H	1	NAG	O4-C4	2.11	1.48	1.43
3	b	3	BMA	C2-C3	2.11	1.55	1.52
3	S	1	NAG	C4-C3	2.04	1.57	1.52
3	U	3	BMA	C4-C5	2.03	1.57	1.53
3	b	1	NAG	C4-C3	2.03	1.57	1.52
3	d	3	BMA	C4-C5	2.03	1.57	1.53
3	b	3	BMA	C1-C2	2.01	1.57	1.52
3	L	3	BMA	C4-C5	2.01	1.57	1.53
3	J	1	NAG	C4-C3	2.01	1.57	1.52
3	J	3	BMA	C1-C2	2.01	1.57	1.52
2	X	1	NAG	O5-C5	2.01	1.47	1.43
3	S	3	BMA	C1-C2	2.00	1.57	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1	NAG	C8-C7-N2	5.54	125.31	116.12
3	S	1	NAG	C8-C7-N2	5.54	125.31	116.12
3	b	1	NAG	C8-C7-N2	5.52	125.28	116.12
3	L	1	NAG	C2-N2-C7	5.32	130.03	122.90
3	U	1	NAG	C2-N2-C7	5.32	130.03	122.90
3	d	1	NAG	C2-N2-C7	5.32	130.03	122.90
3	J	1	NAG	O7-C7-C8	-4.86	113.40	122.05
3	b	1	NAG	O7-C7-C8	-4.85	113.41	122.05
3	S	1	NAG	O7-C7-C8	-4.84	113.43	122.05
3	b	2	NAG	O5-C1-C2	-4.50	104.33	111.29
3	J	2	NAG	O5-C1-C2	-4.49	104.34	111.29
3	S	2	NAG	O5-C1-C2	-4.48	104.36	111.29
3	b	1	NAG	O3-C3-C2	-4.37	100.33	109.40
3	J	1	NAG	O3-C3-C2	-4.36	100.34	109.40
3	S	1	NAG	O3-C3-C2	-4.36	100.34	109.40
3	d	2	NAG	O5-C1-C2	-4.16	104.85	111.29
3	U	2	NAG	O5-C1-C2	-4.16	104.85	111.29
3	L	2	NAG	O5-C1-C2	-4.16	104.85	111.29
2	H	2	NAG	C1-C2-N2	3.99	116.72	110.43
2	Z	2	NAG	C1-C2-N2	3.98	116.71	110.43
2	Q	2	NAG	C1-C2-N2	3.98	116.70	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	2	NAG	C2-N2-C7	3.94	128.17	122.90
2	Q	2	NAG	C2-N2-C7	3.93	128.17	122.90
2	H	2	NAG	C2-N2-C7	3.93	128.17	122.90
3	b	1	NAG	O4-C4-C5	-3.79	99.99	109.32
3	J	1	NAG	O4-C4-C5	-3.79	100.00	109.32
3	S	1	NAG	O4-C4-C5	-3.79	100.00	109.32
3	S	1	NAG	C1-O5-C5	3.74	117.19	112.19
3	b	1	NAG	C1-O5-C5	3.73	117.18	112.19
3	J	1	NAG	C1-O5-C5	3.73	117.18	112.19
2	c	1	NAG	C1-C2-N2	-3.70	104.60	110.43
2	K	1	NAG	C1-C2-N2	-3.69	104.62	110.43
2	T	1	NAG	C1-C2-N2	-3.68	104.63	110.43
2	K	1	NAG	C2-N2-C7	-3.39	118.35	122.90
2	c	1	NAG	C2-N2-C7	-3.38	118.36	122.90
2	T	1	NAG	C2-N2-C7	-3.38	118.38	122.90
2	c	2	NAG	C8-C7-N2	2.90	120.93	116.12
2	K	2	NAG	C8-C7-N2	2.89	120.91	116.12
2	T	2	NAG	C8-C7-N2	2.88	120.89	116.12
2	M	1	NAG	C8-C7-N2	2.72	120.62	116.12
2	V	1	NAG	C8-C7-N2	2.71	120.61	116.12
2	D	1	NAG	C8-C7-N2	2.70	120.59	116.12
3	d	1	NAG	C1-C2-N2	-2.67	106.23	110.43
2	I	2	NAG	C8-C7-N2	2.67	120.54	116.12
3	L	1	NAG	C1-C2-N2	-2.66	106.23	110.43
3	U	1	NAG	C1-C2-N2	-2.66	106.24	110.43
2	a	2	NAG	C8-C7-N2	2.66	120.53	116.12
3	L	1	NAG	C8-C7-N2	2.65	120.51	116.12
3	d	1	NAG	C8-C7-N2	2.64	120.50	116.12
3	U	1	NAG	C8-C7-N2	2.64	120.49	116.12
2	R	2	NAG	C8-C7-N2	2.63	120.48	116.12
2	P	2	NAG	C8-C7-N2	2.60	120.44	116.12
2	Y	2	NAG	C8-C7-N2	2.60	120.43	116.12
2	G	2	NAG	C8-C7-N2	2.59	120.41	116.12
2	O	1	NAG	C8-C7-N2	2.52	120.31	116.12
2	F	1	NAG	C8-C7-N2	2.52	120.30	116.12
2	X	1	NAG	C8-C7-N2	2.51	120.28	116.12
2	H	2	NAG	C4-C3-C2	-2.49	107.37	111.02
2	Q	2	NAG	C4-C3-C2	-2.49	107.37	111.02
2	Z	2	NAG	C4-C3-C2	-2.48	107.38	111.02
2	N	1	NAG	C8-C7-N2	2.47	120.22	116.12
2	E	1	NAG	C8-C7-N2	2.47	120.21	116.12
2	Y	1	NAG	C1-C2-N2	-2.46	106.56	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	1	NAG	C8-C7-N2	2.46	120.19	116.12
2	G	1	NAG	C1-C2-N2	-2.45	106.57	110.43
2	P	1	NAG	C1-C2-N2	-2.43	106.61	110.43
3	d	1	NAG	O7-C7-C8	-2.32	117.92	122.05
3	U	1	NAG	O7-C7-C8	-2.30	117.95	122.05
3	L	1	NAG	O7-C7-C8	-2.30	117.96	122.05
2	Z	2	NAG	O7-C7-C8	-2.26	118.03	122.05
2	H	2	NAG	O7-C7-C8	-2.26	118.03	122.05
2	Q	2	NAG	O7-C7-C8	-2.26	118.04	122.05
2	W	2	NAG	C8-C7-N2	2.23	119.81	116.12
2	M	2	NAG	C8-C7-N2	2.20	119.77	116.12
2	V	2	NAG	C8-C7-N2	2.20	119.77	116.12
2	D	2	NAG	C8-C7-N2	2.20	119.76	116.12
2	E	2	NAG	C8-C7-N2	2.19	119.76	116.12
2	N	2	NAG	C8-C7-N2	2.19	119.75	116.12
3	J	2	NAG	C2-N2-C7	-2.11	120.08	122.90
3	S	2	NAG	C2-N2-C7	-2.10	120.08	122.90
3	b	2	NAG	C2-N2-C7	-2.10	120.09	122.90
2	T	2	NAG	O7-C7-C8	-2.05	118.40	122.05
2	K	2	NAG	O7-C7-C8	-2.05	118.41	122.05
2	c	2	NAG	O7-C7-C8	-2.05	118.41	122.05
2	a	2	NAG	O7-C7-C8	-2.02	118.45	122.05
2	I	2	NAG	O7-C7-C8	-2.01	118.47	122.05
2	R	1	NAG	C8-C7-N2	2.01	119.45	116.12

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C1-C2-N2-C7
2	Q	2	NAG	C1-C2-N2-C7
2	Z	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	L	2	NAG	C8-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	b	2	NAG	C8-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
3	d	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	U	2	NAG	O7-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2
3	L	3	BMA	O5-C5-C6-O6
3	U	3	BMA	O5-C5-C6-O6
3	d	3	BMA	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
3	U	3	BMA	C4-C5-C6-O6
3	d	3	BMA	C4-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
3	S	3	BMA	C4-C5-C6-O6
3	b	3	BMA	C4-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6
3	b	3	BMA	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C3-C2-N2-C7
2	Q	1	NAG	C3-C2-N2-C7
2	Z	1	NAG	C3-C2-N2-C7
2	H	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C1-C2-N2-C7
2	H	1	NAG	C1-C2-N2-C7
2	P	2	NAG	C1-C2-N2-C7
2	Q	1	NAG	C1-C2-N2-C7
2	Y	2	NAG	C1-C2-N2-C7
2	Z	1	NAG	C1-C2-N2-C7
3	L	2	NAG	C1-C2-N2-C7

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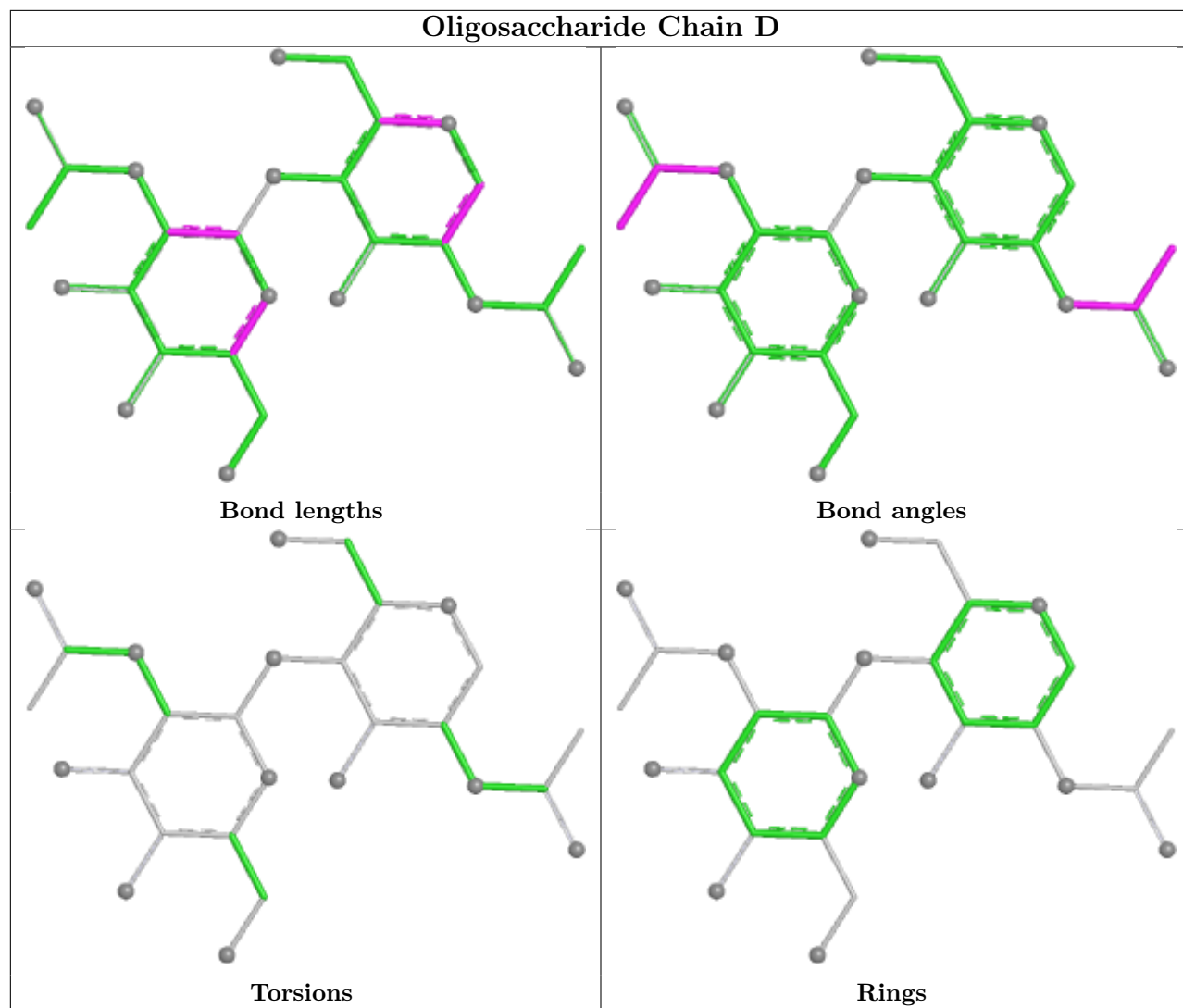
Mol	Chain	Res	Type	Atoms
3	U	2	NAG	C1-C2-N2-C7
3	d	2	NAG	C1-C2-N2-C7
3	L	1	NAG	C3-C2-N2-C7
3	U	1	NAG	C3-C2-N2-C7
3	d	1	NAG	C3-C2-N2-C7
2	G	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6

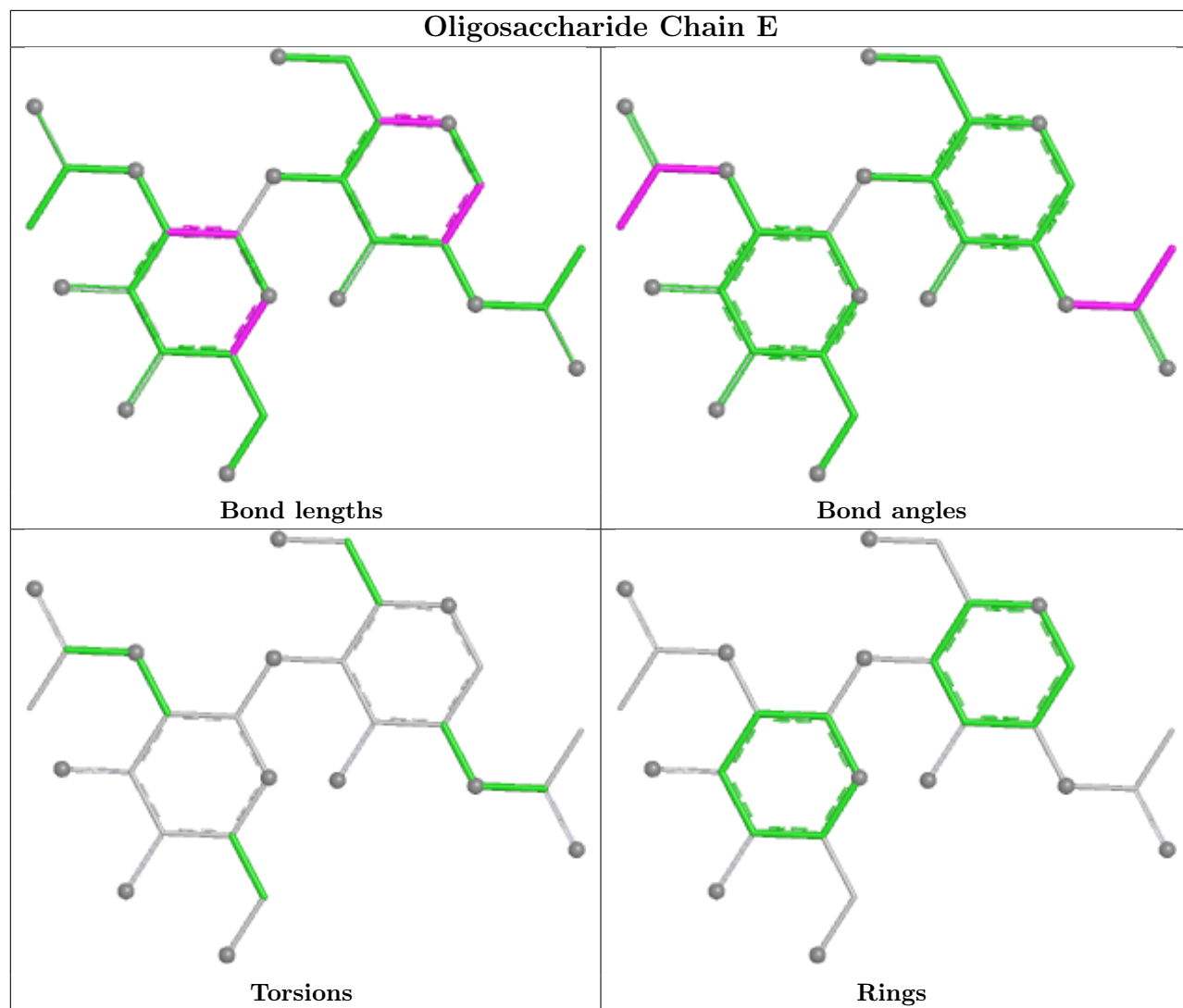
There are no ring outliers.

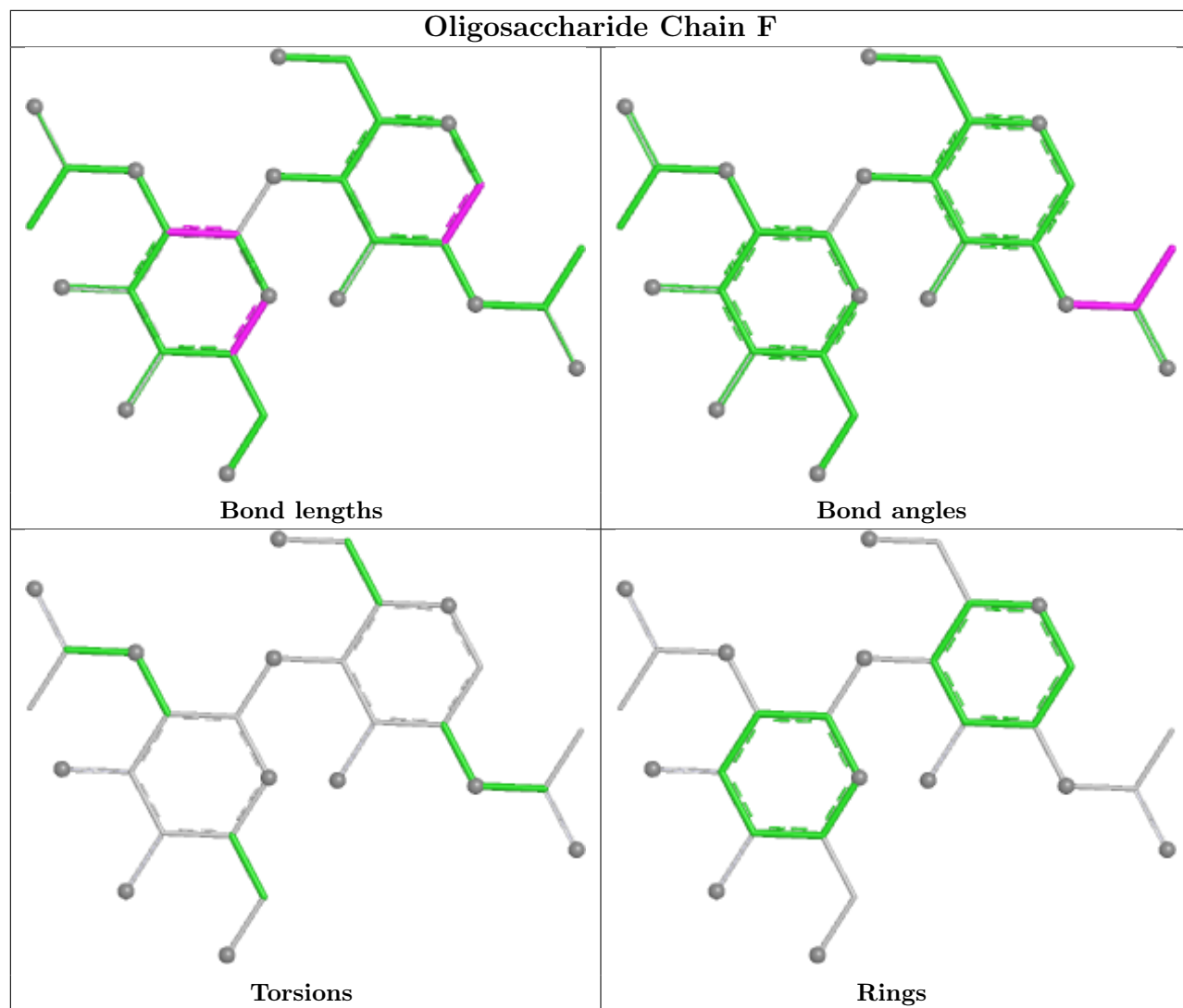
3 monomers are involved in 3 short contacts:

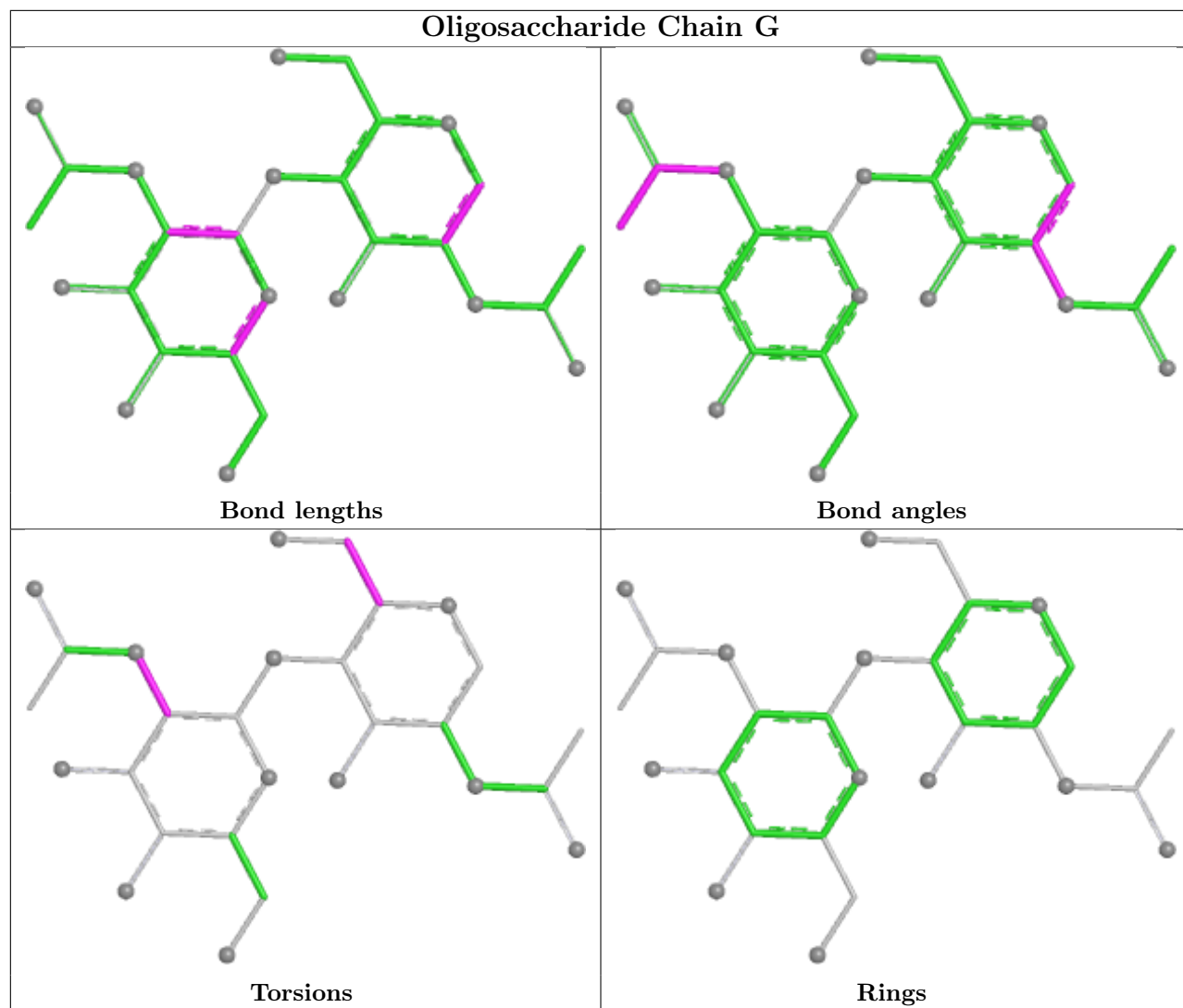
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	Z	1	NAG	1	0
2	Q	1	NAG	1	0

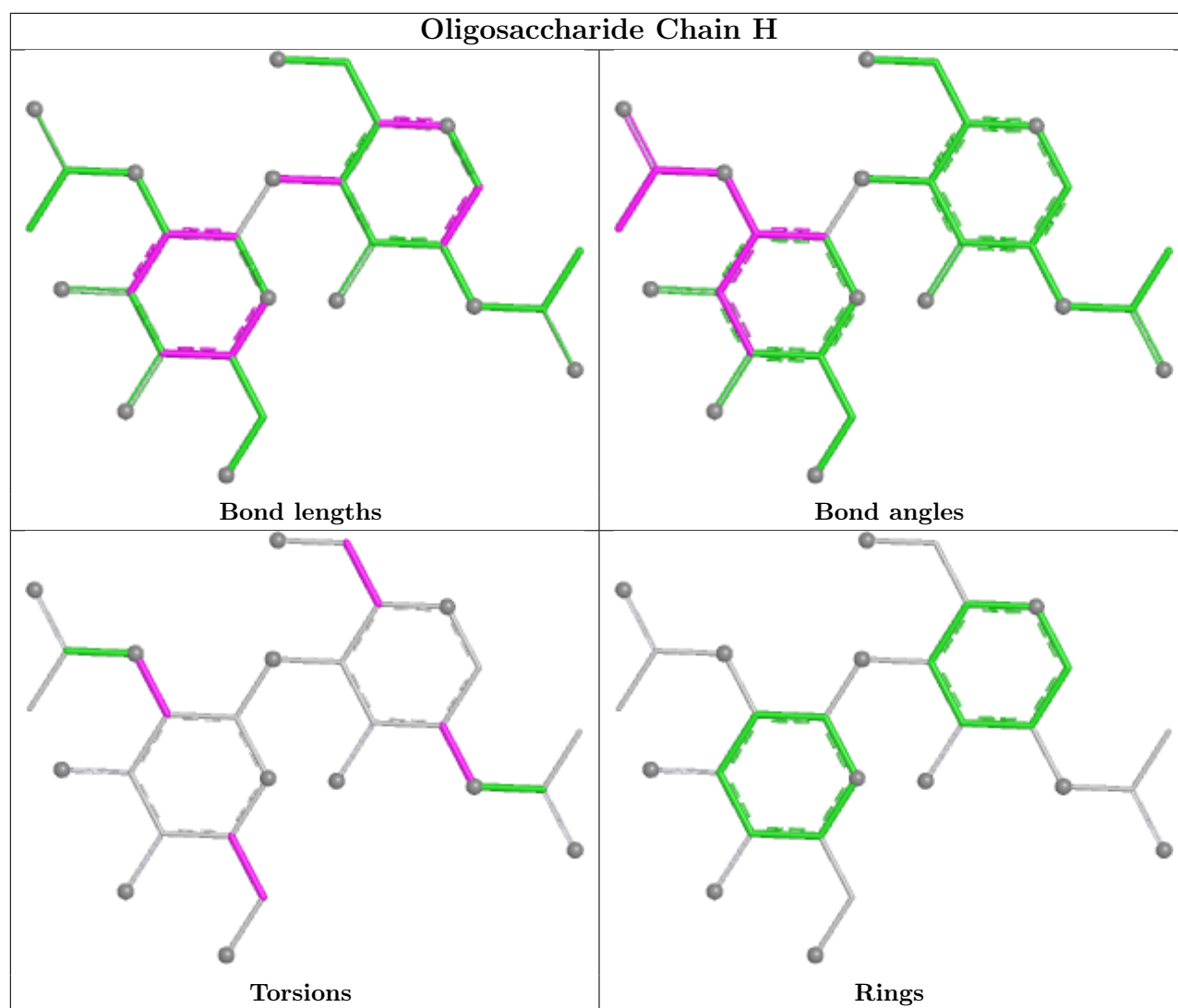
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

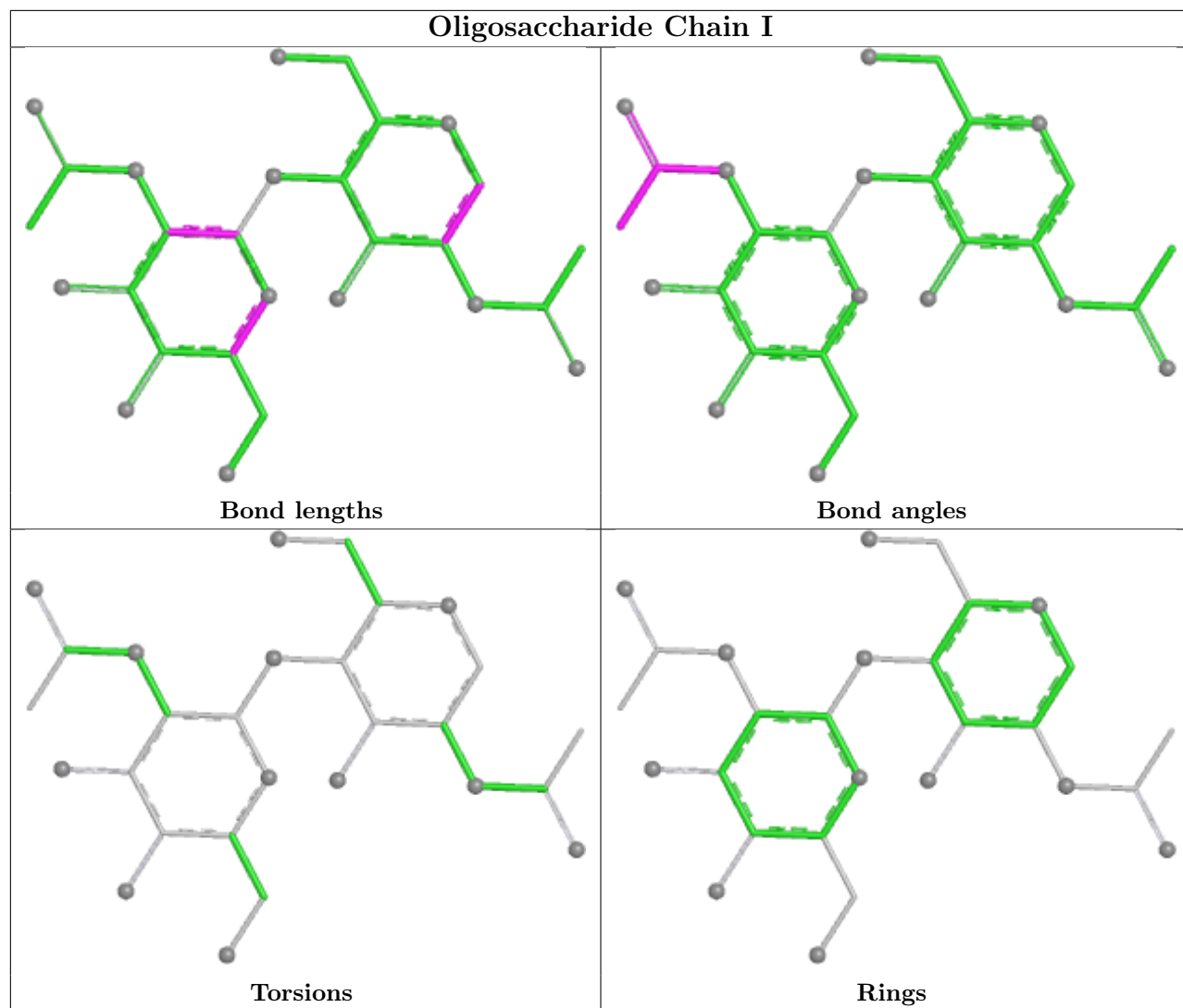


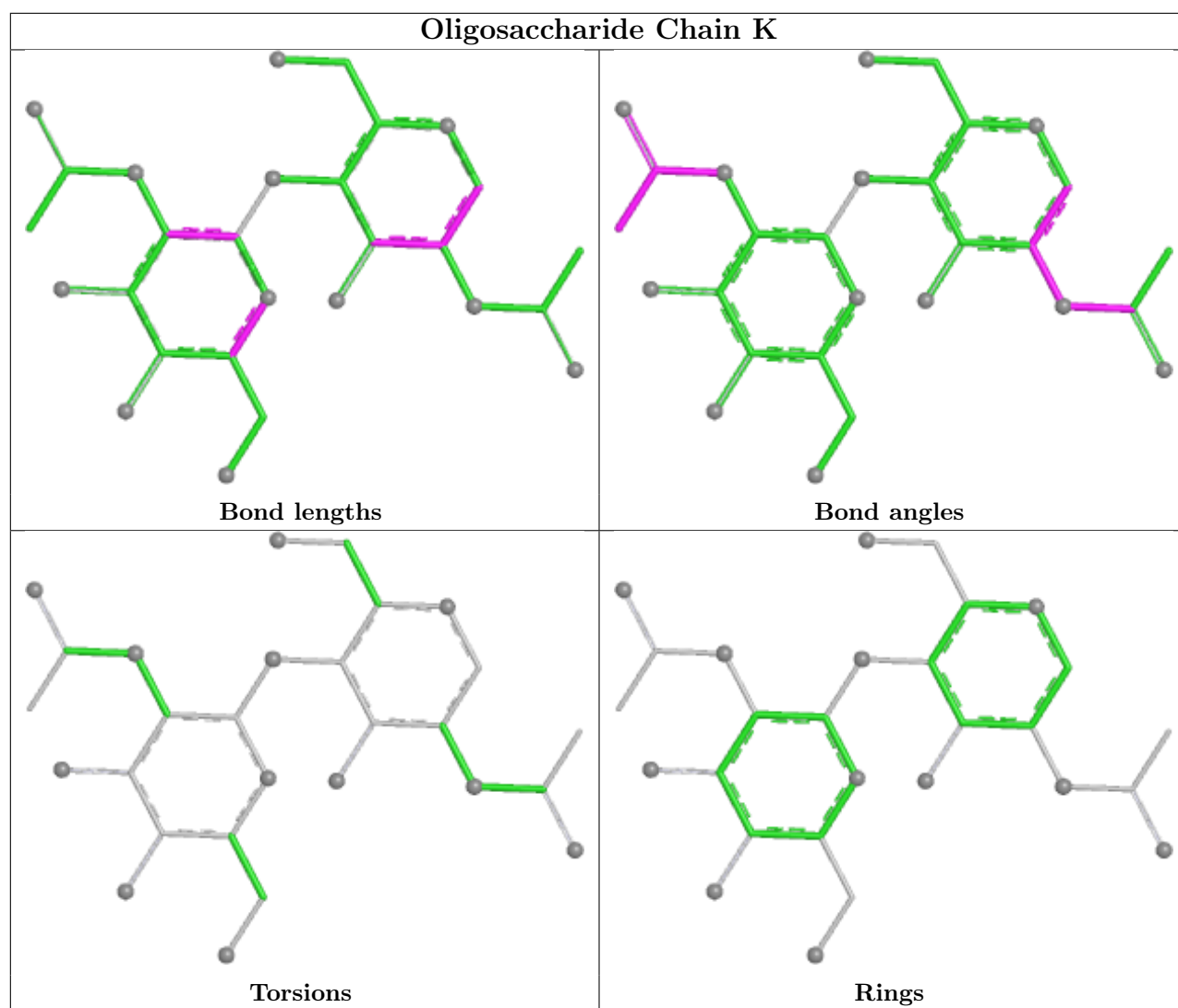


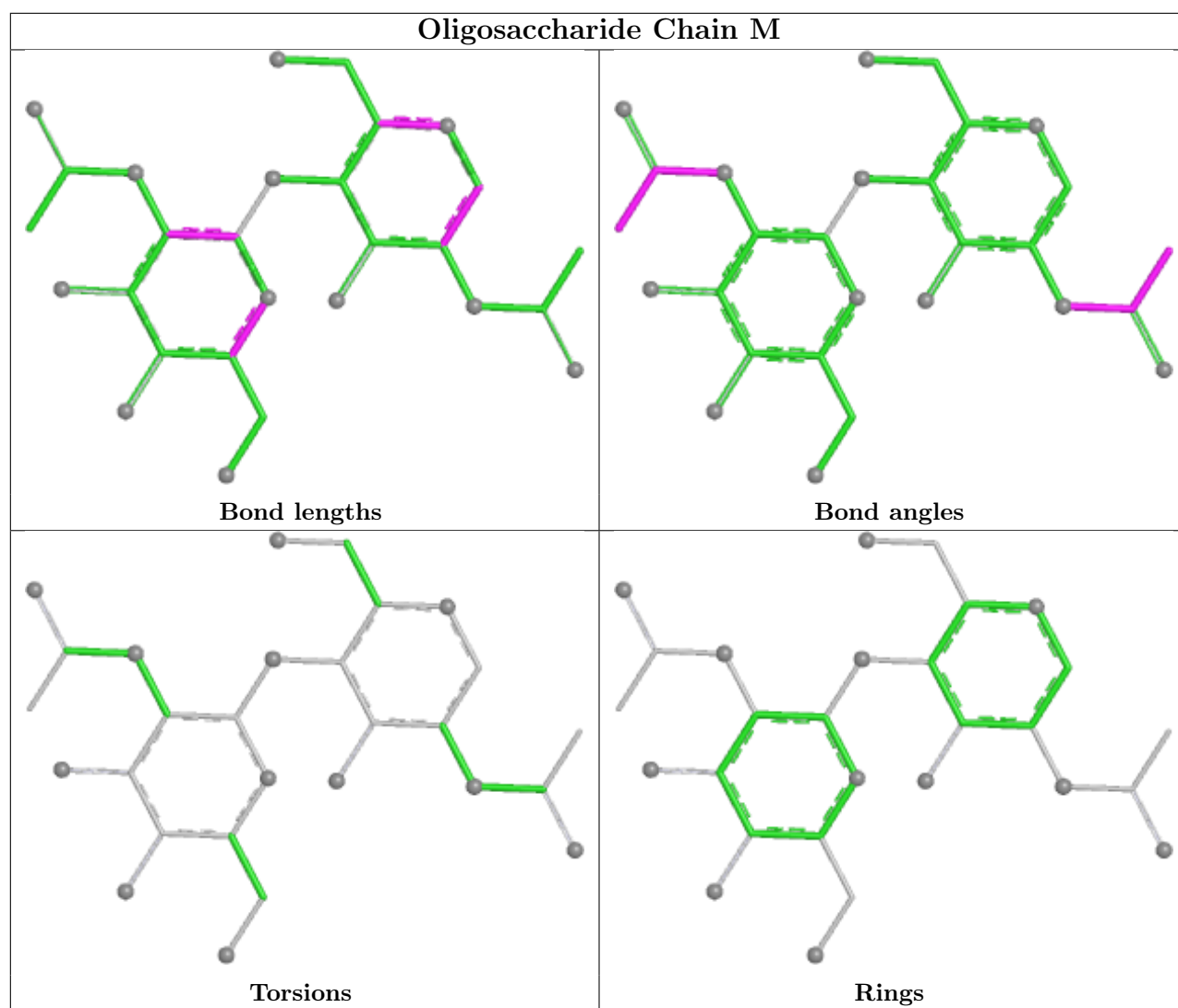


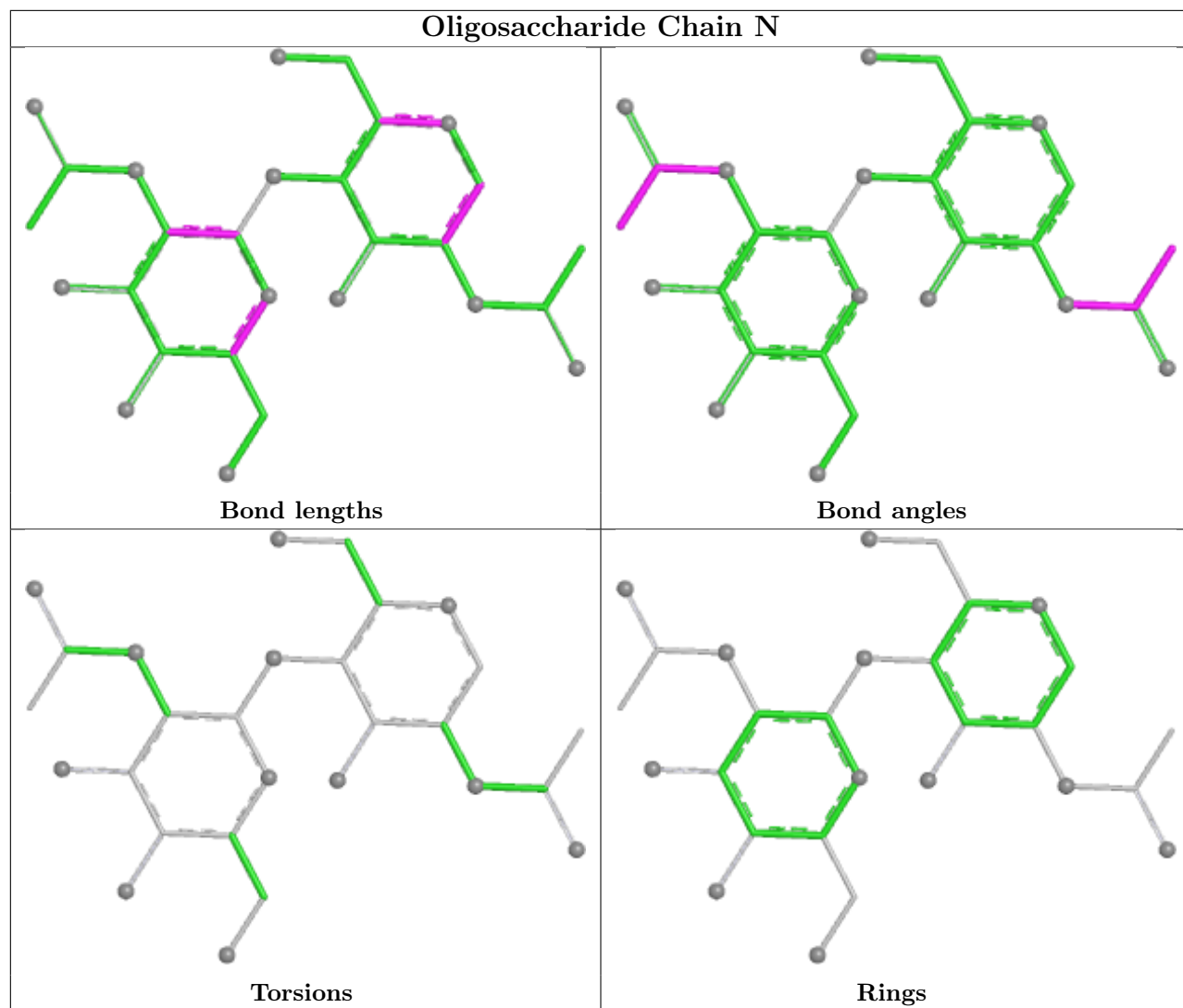


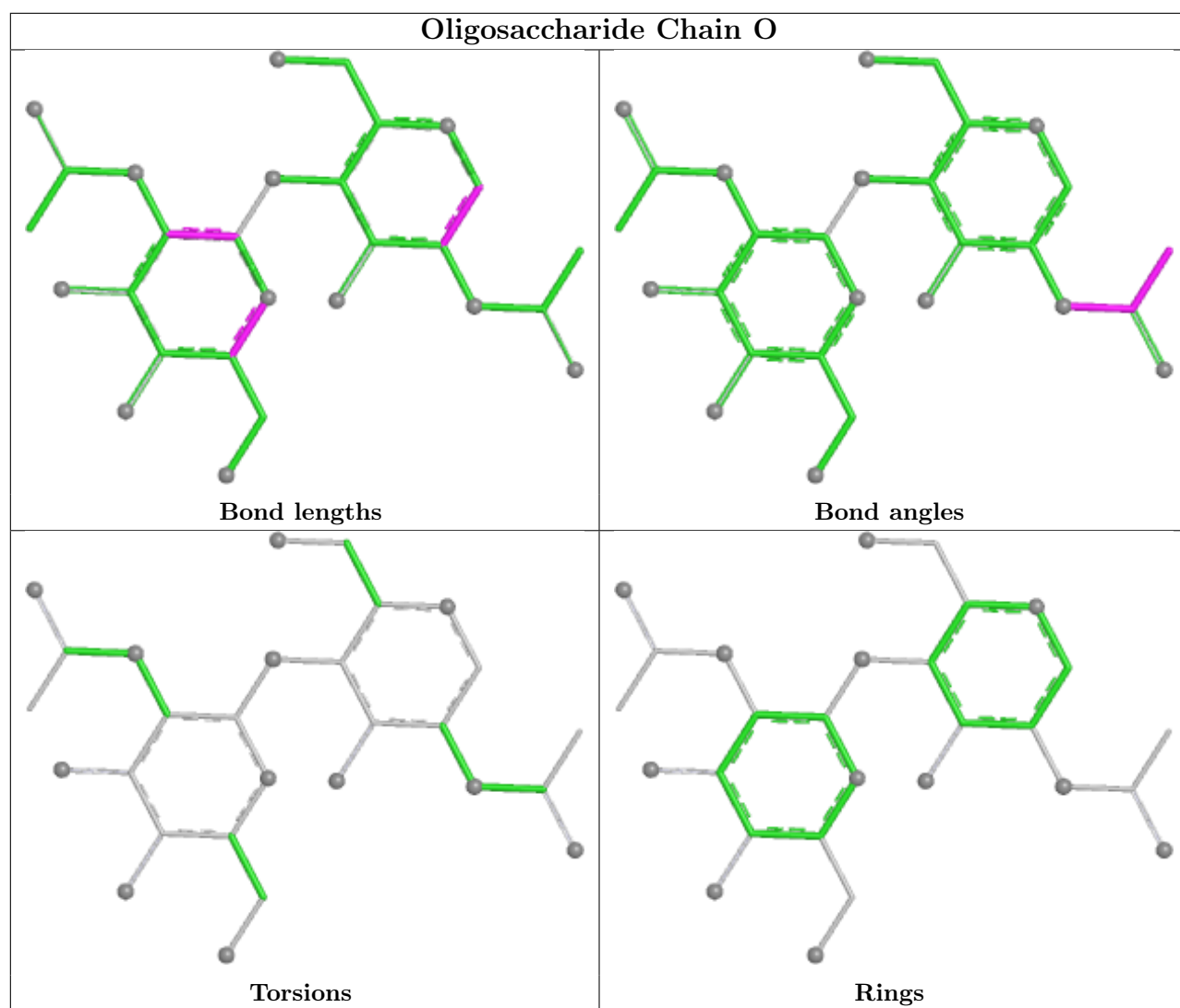


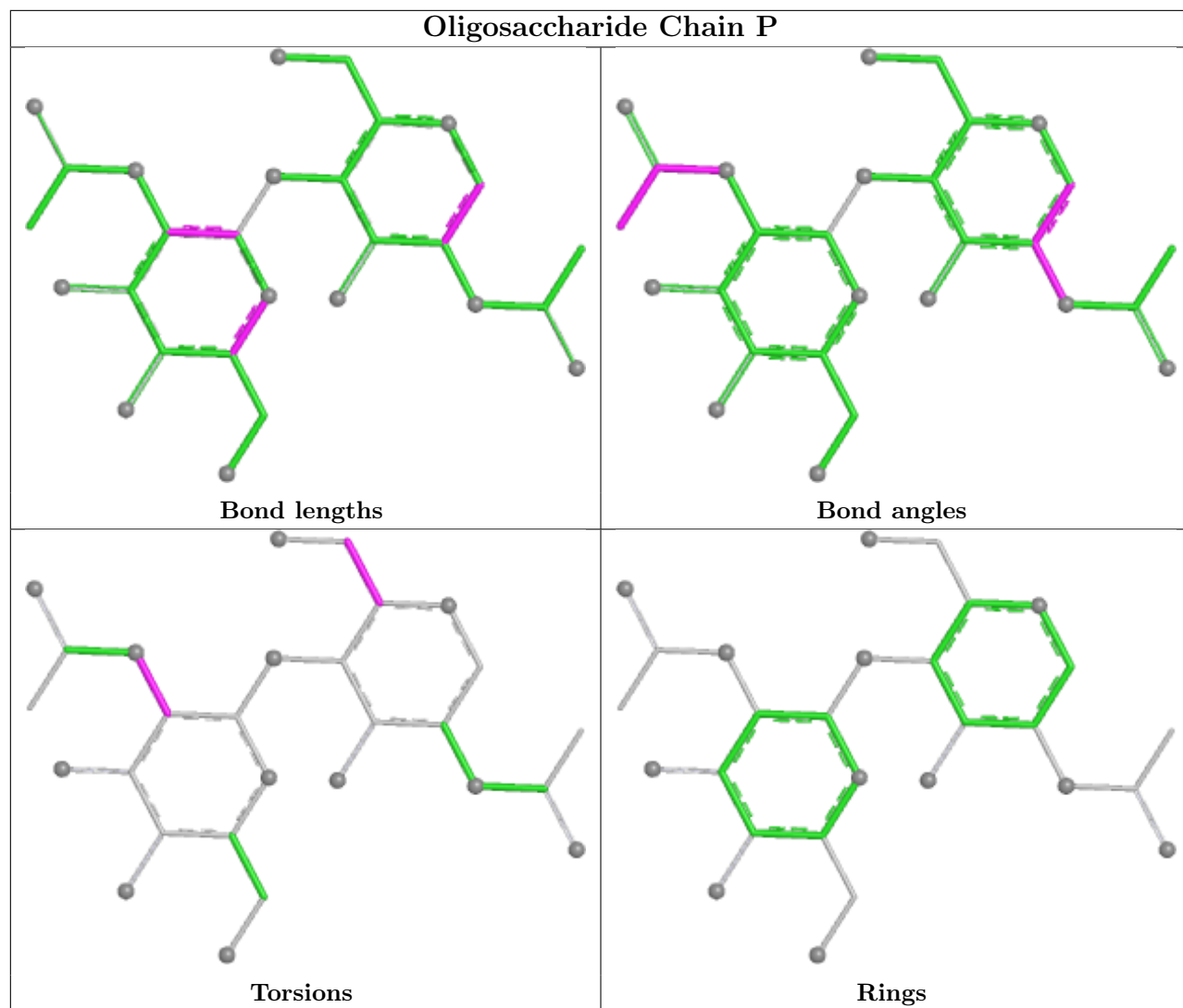


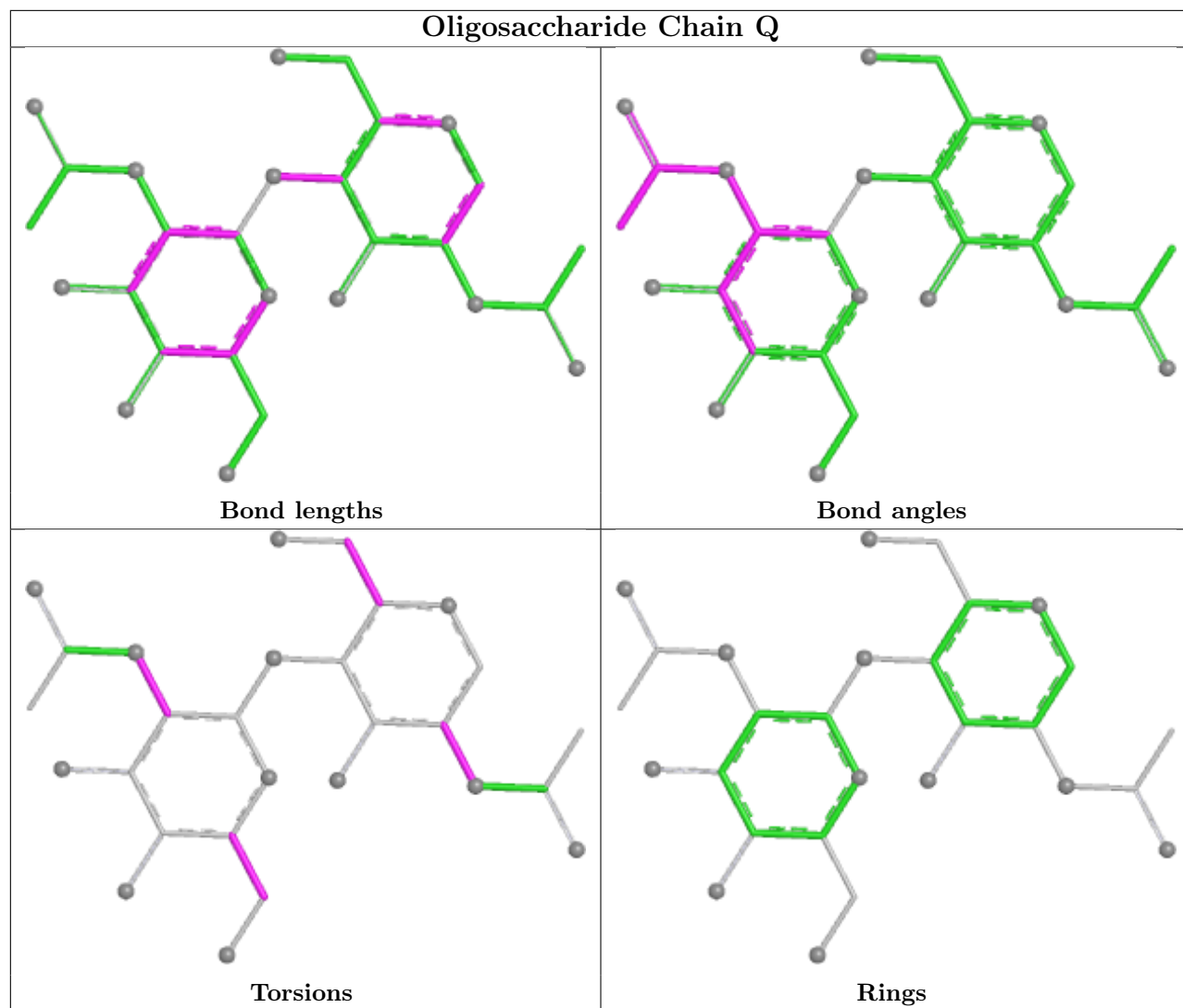


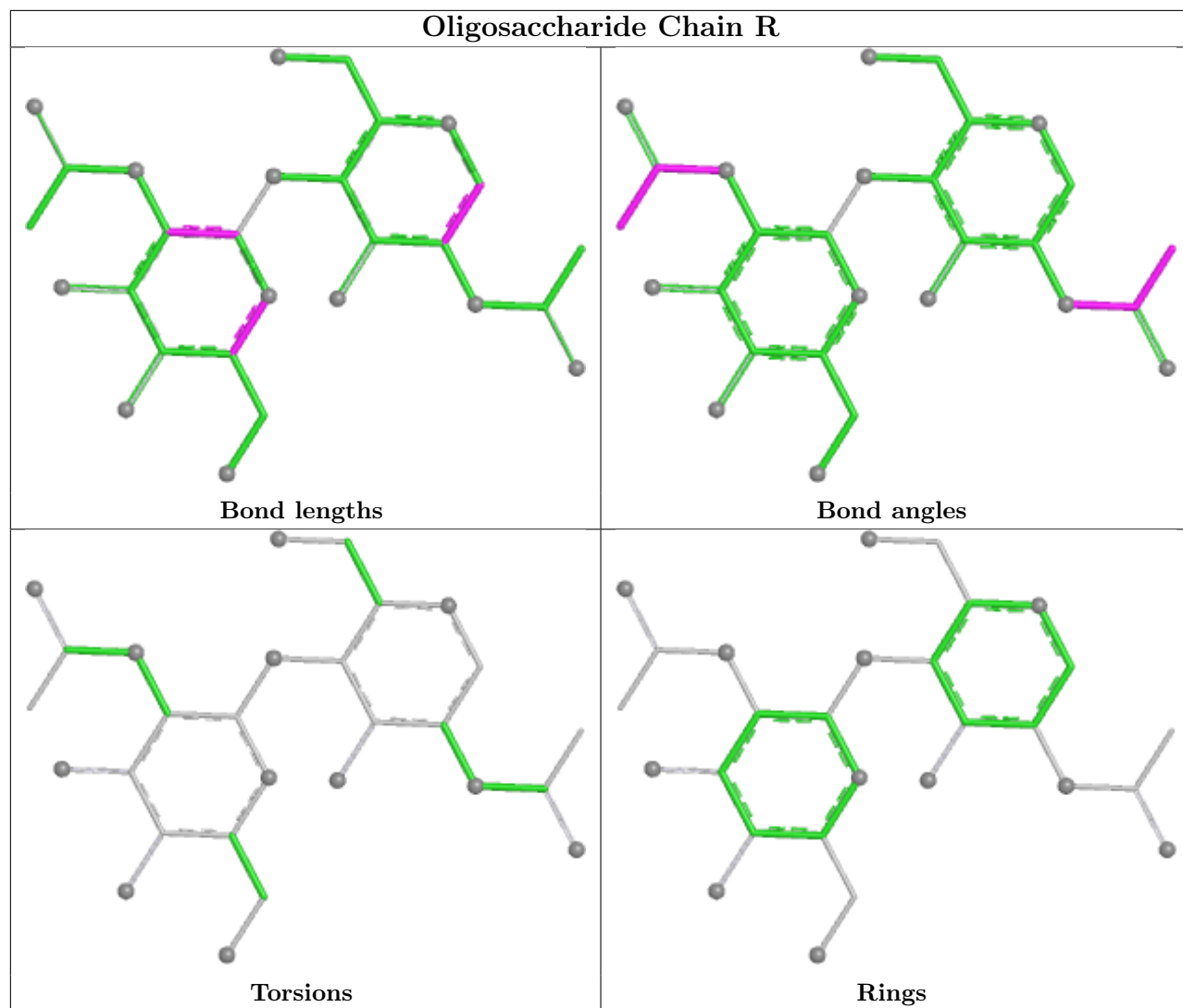


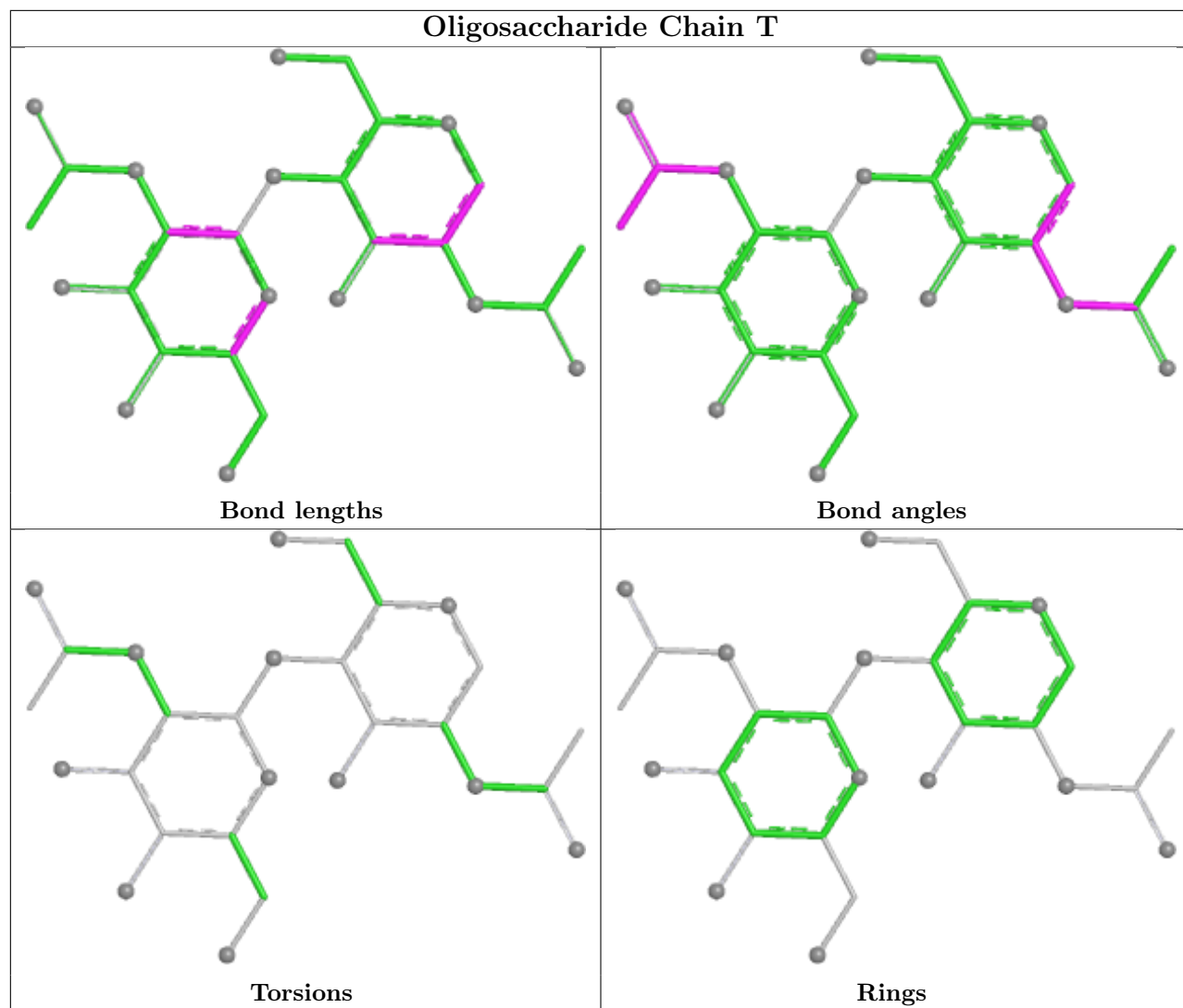


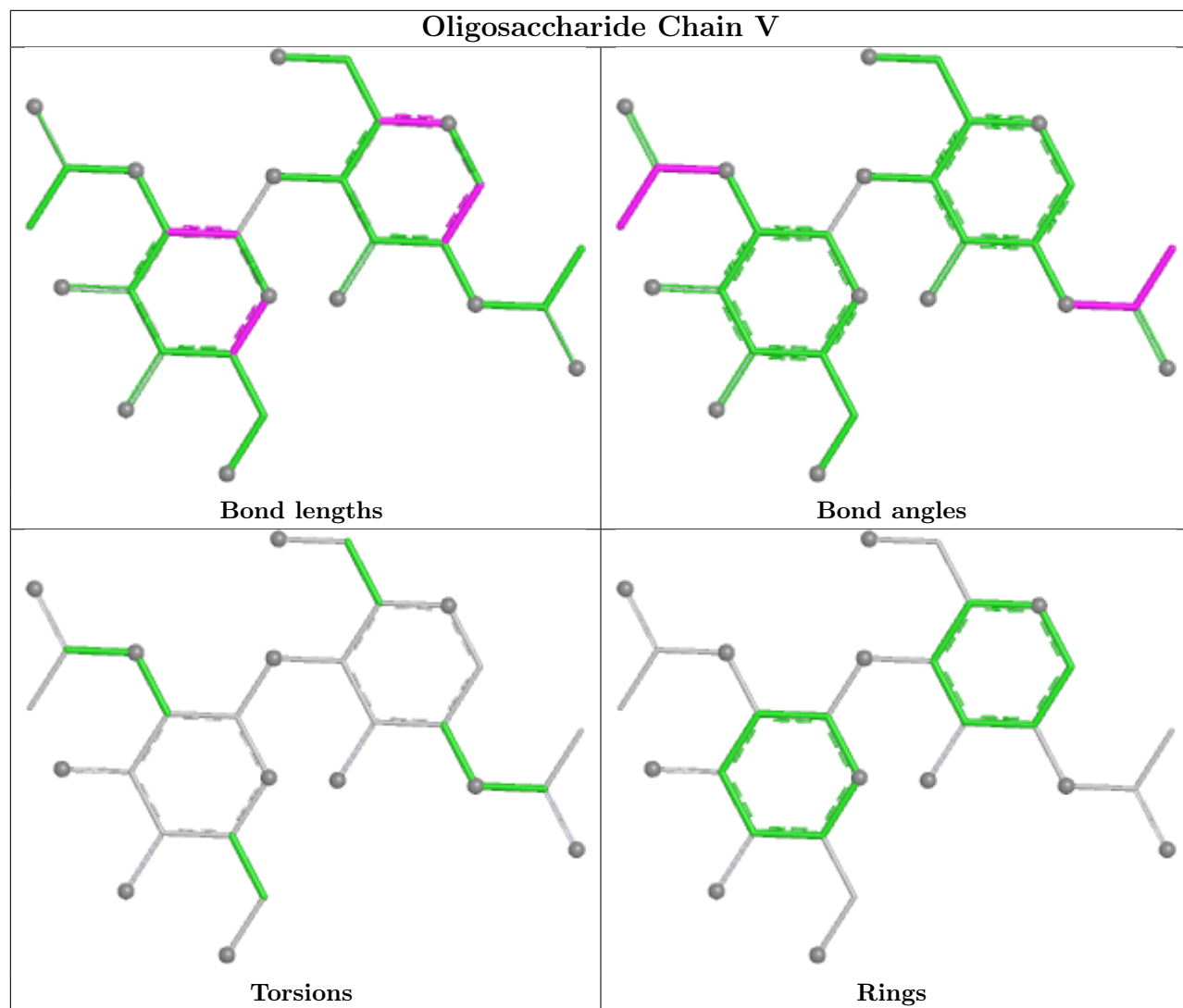


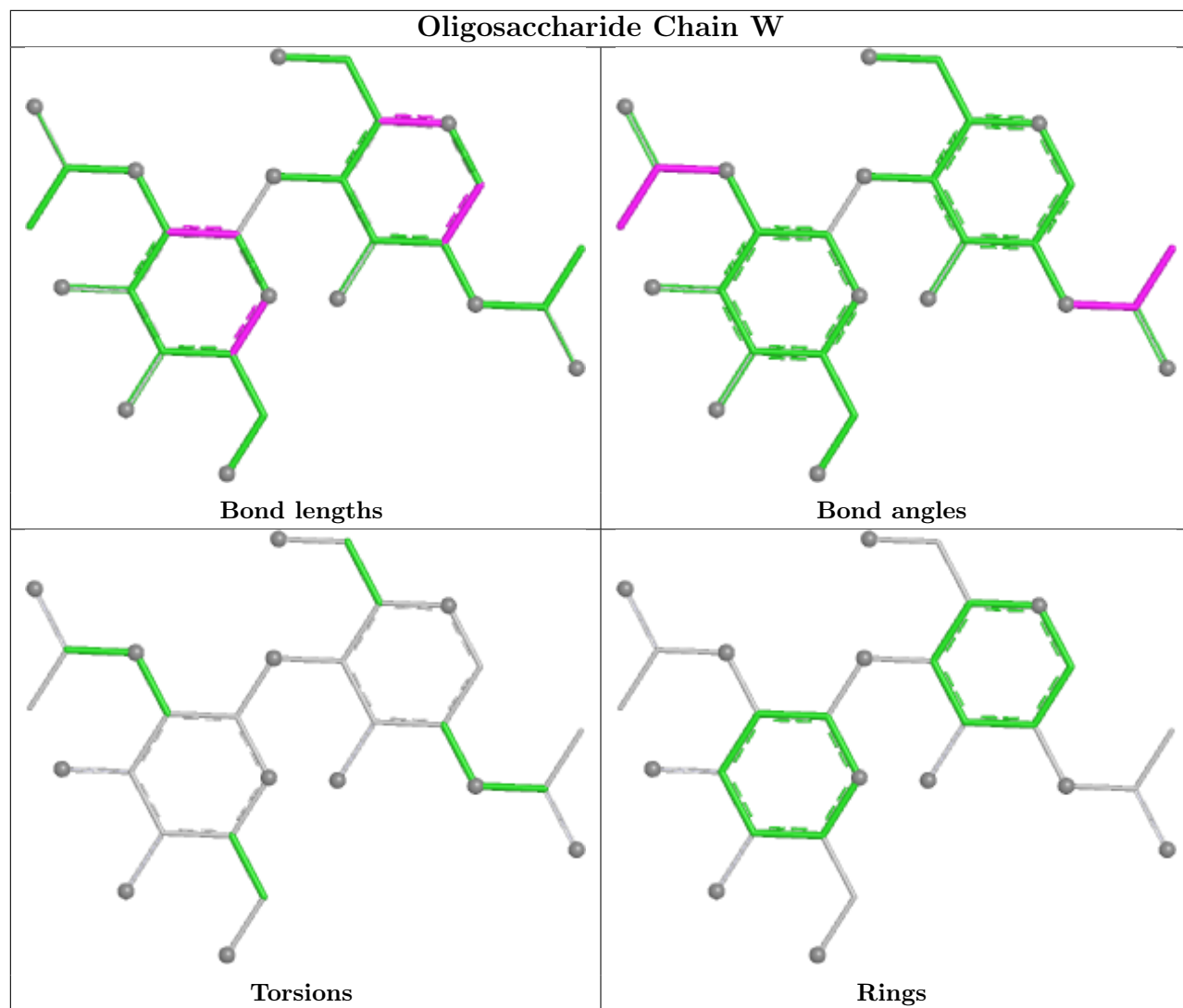


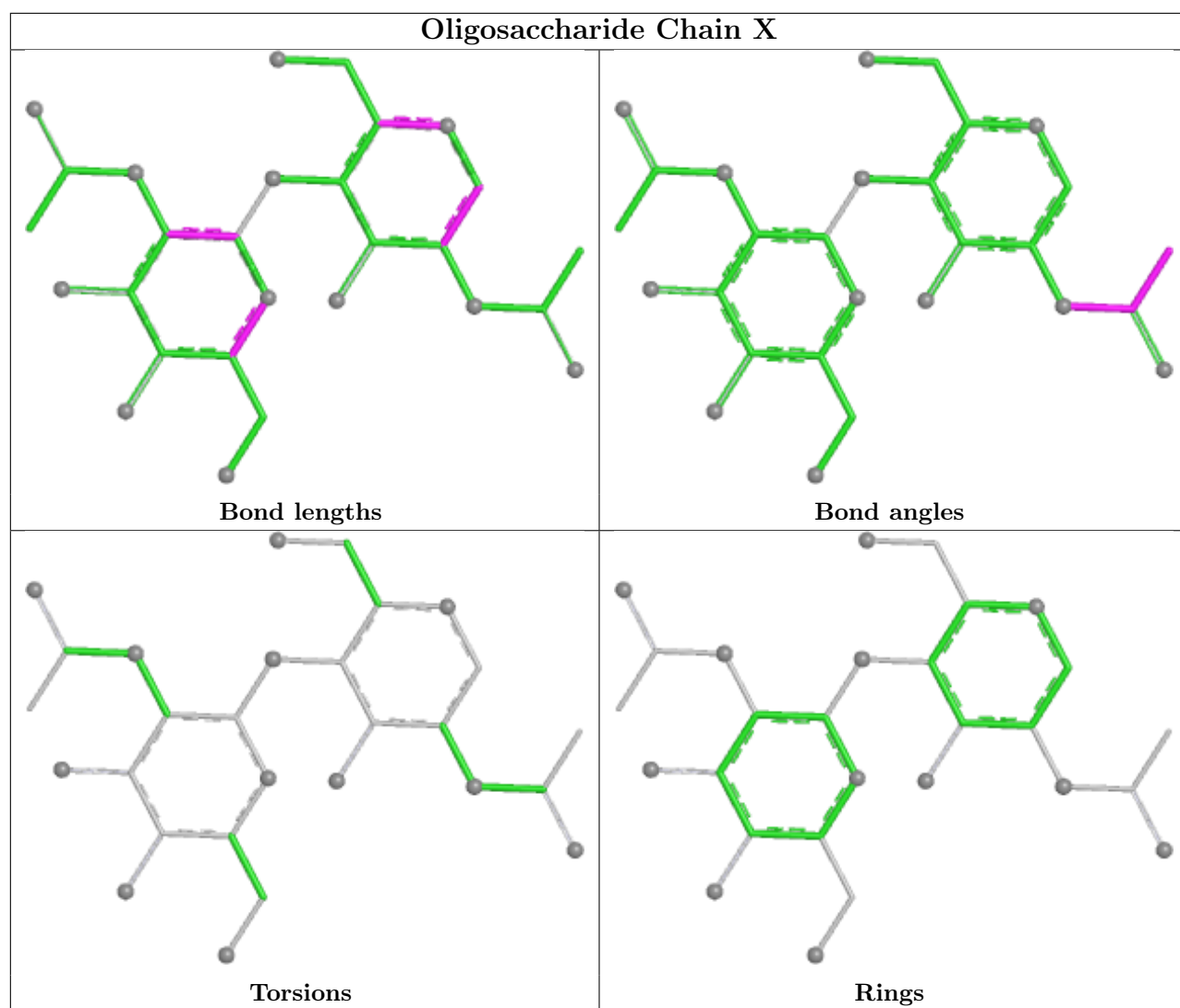


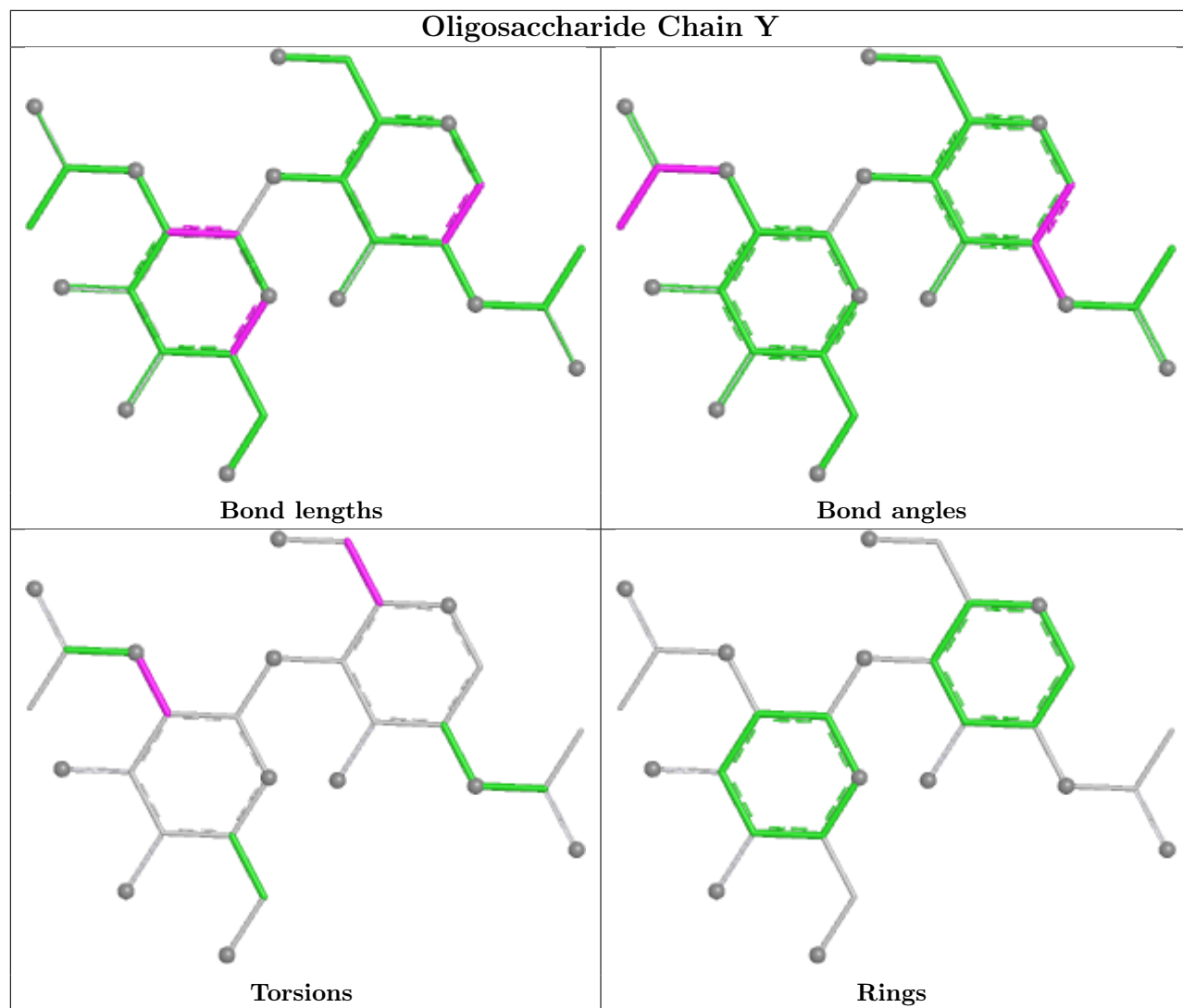


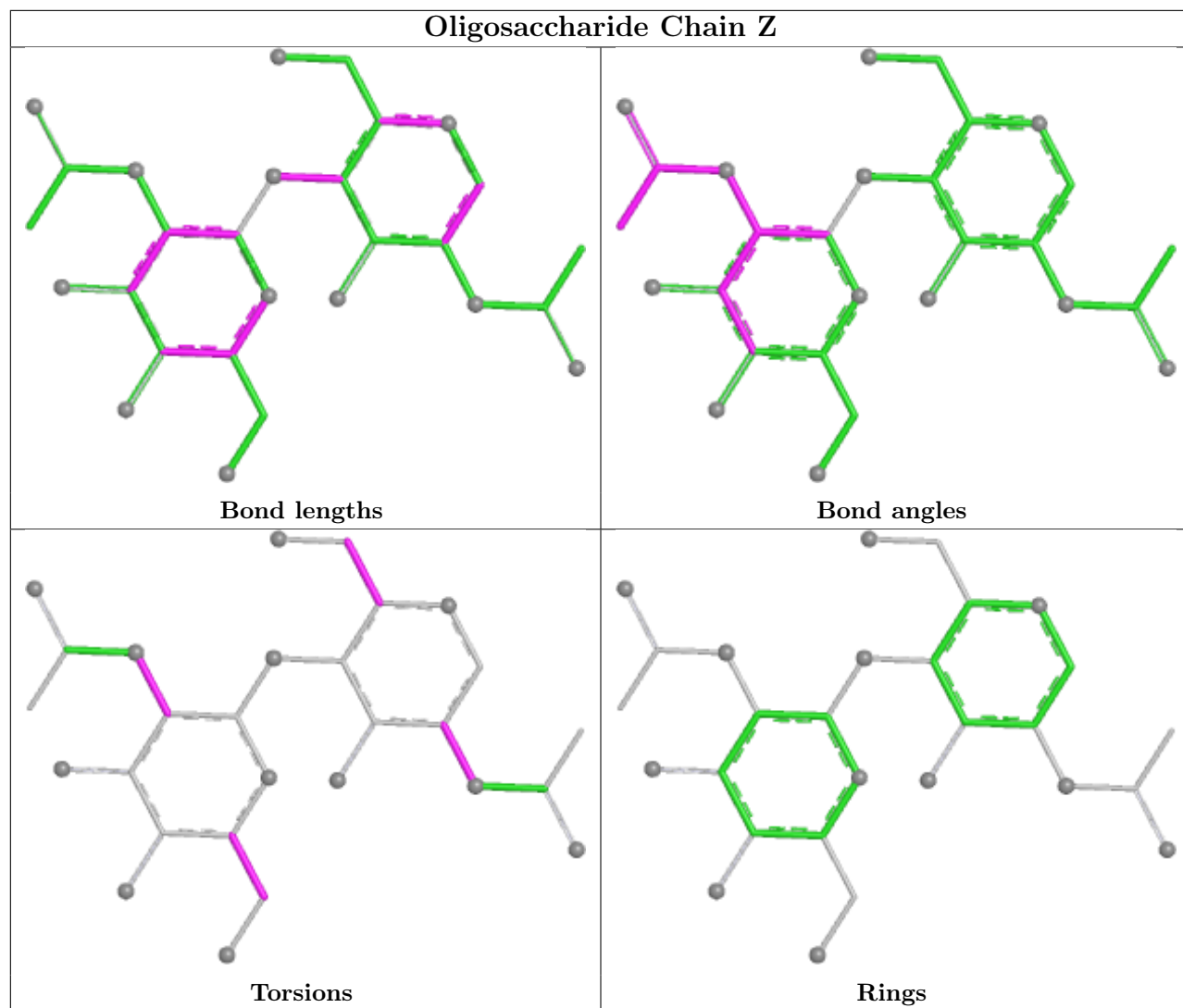


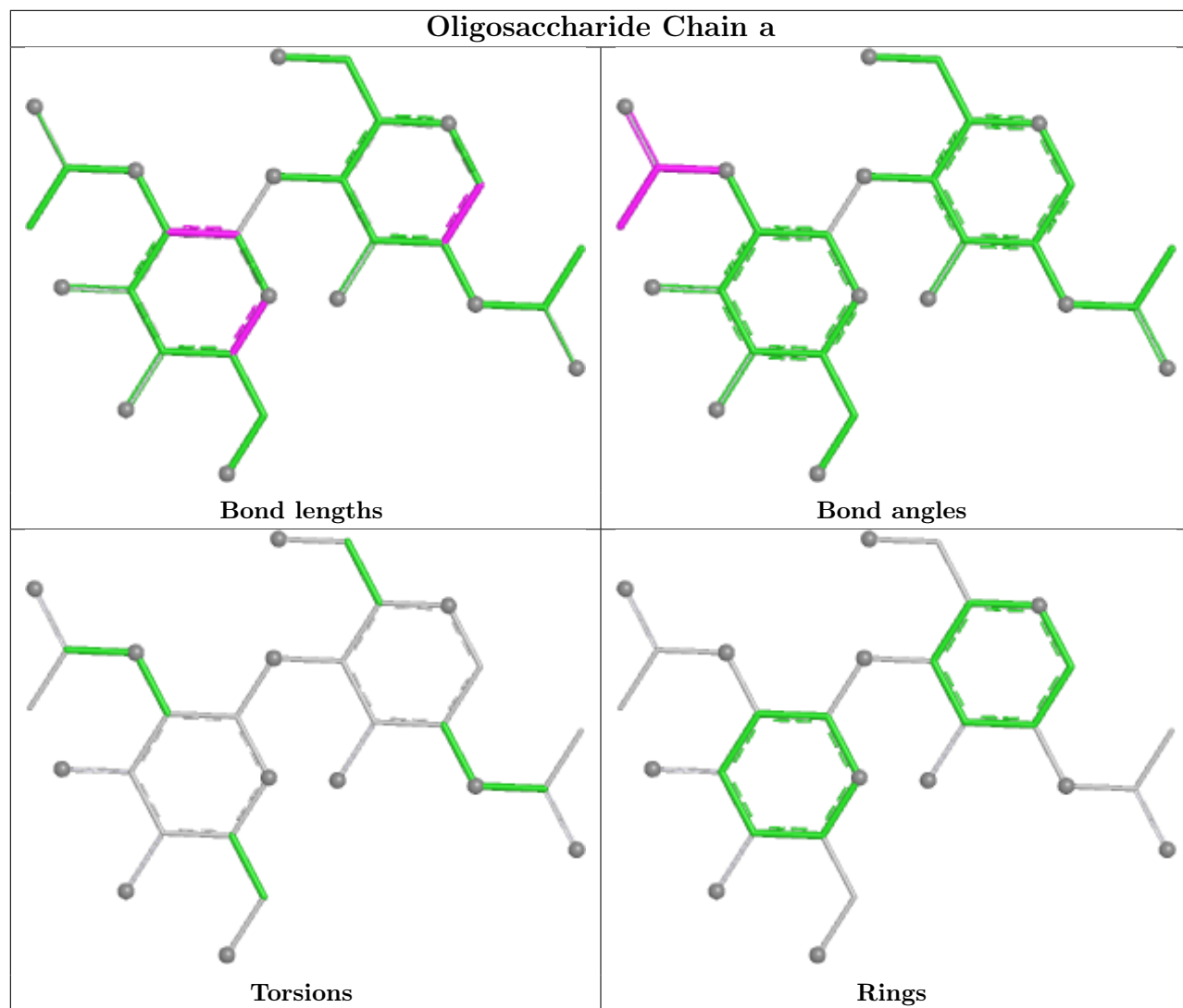


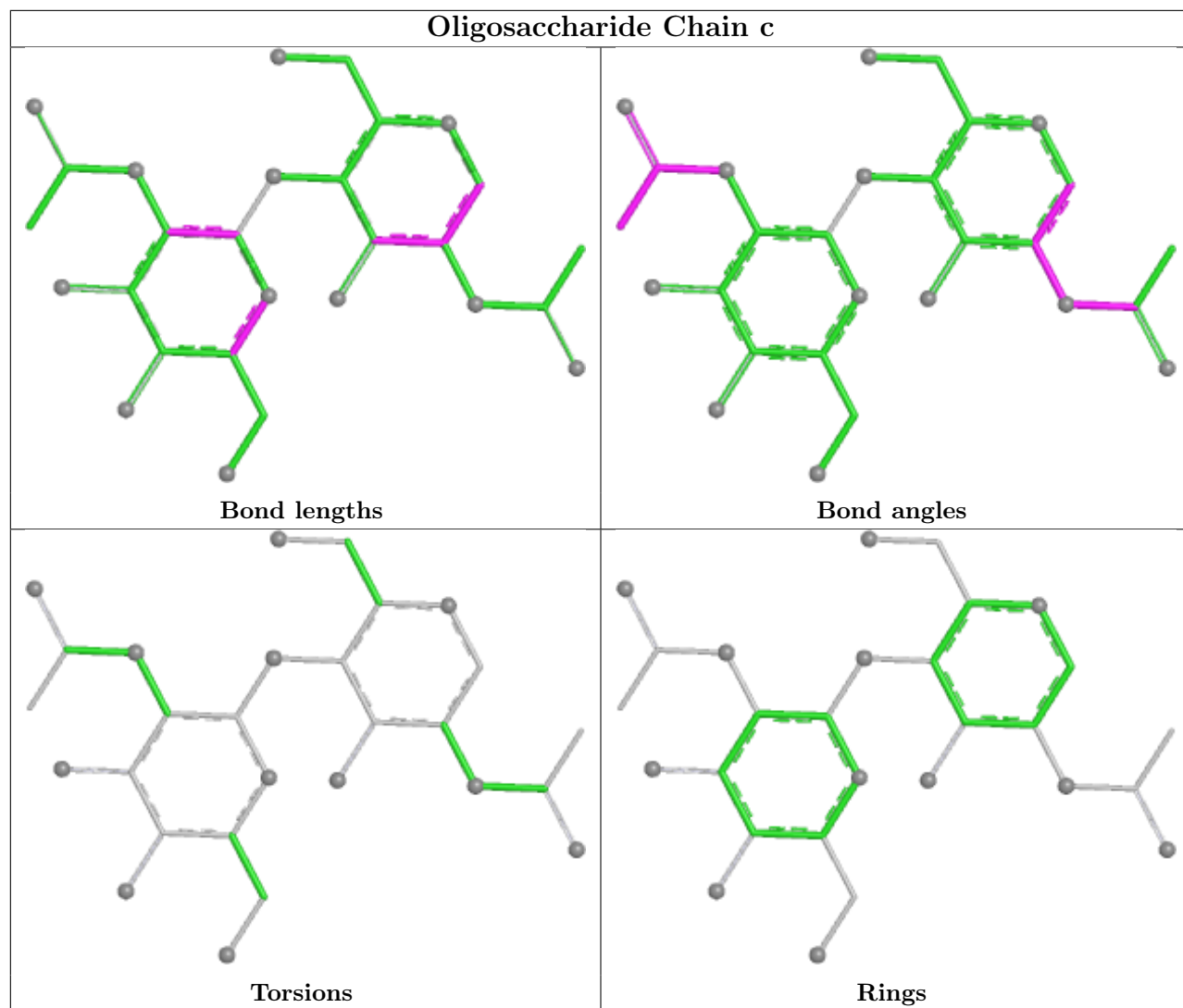


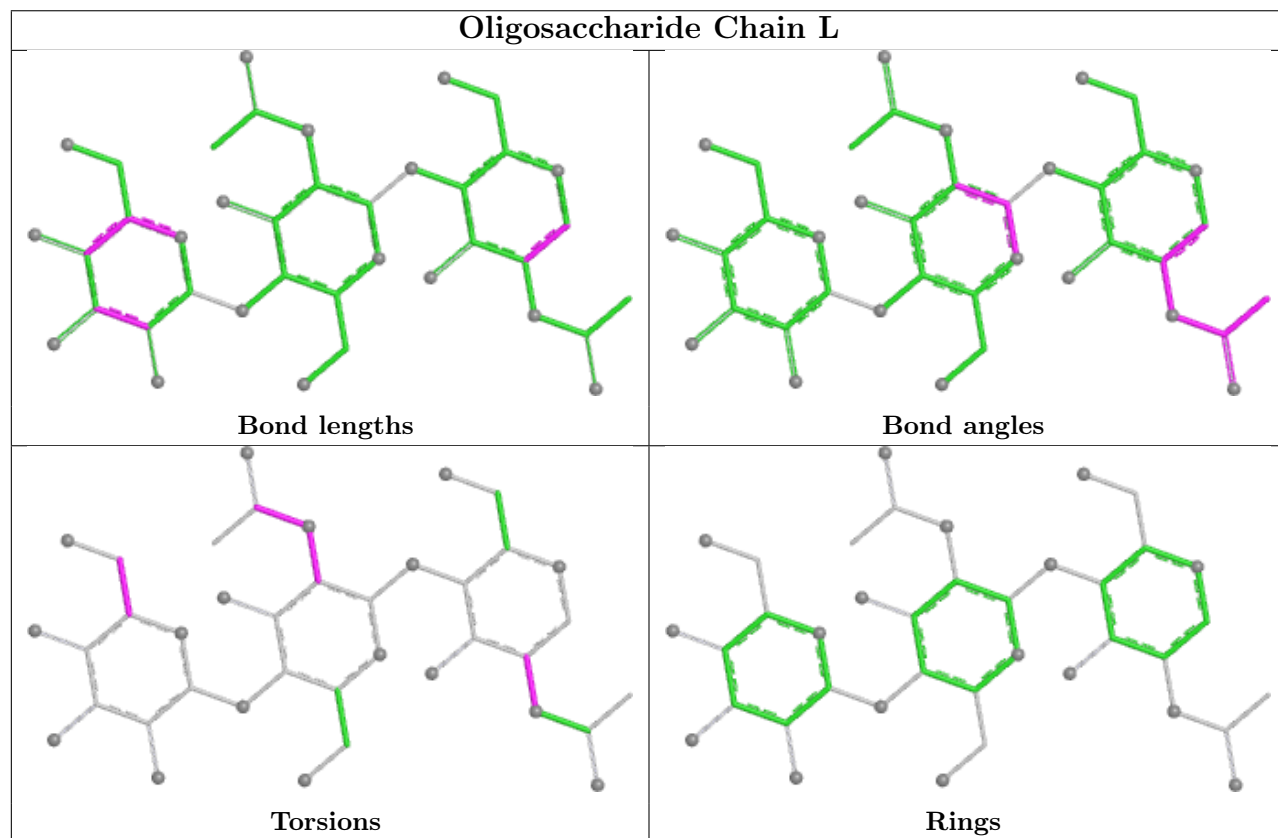
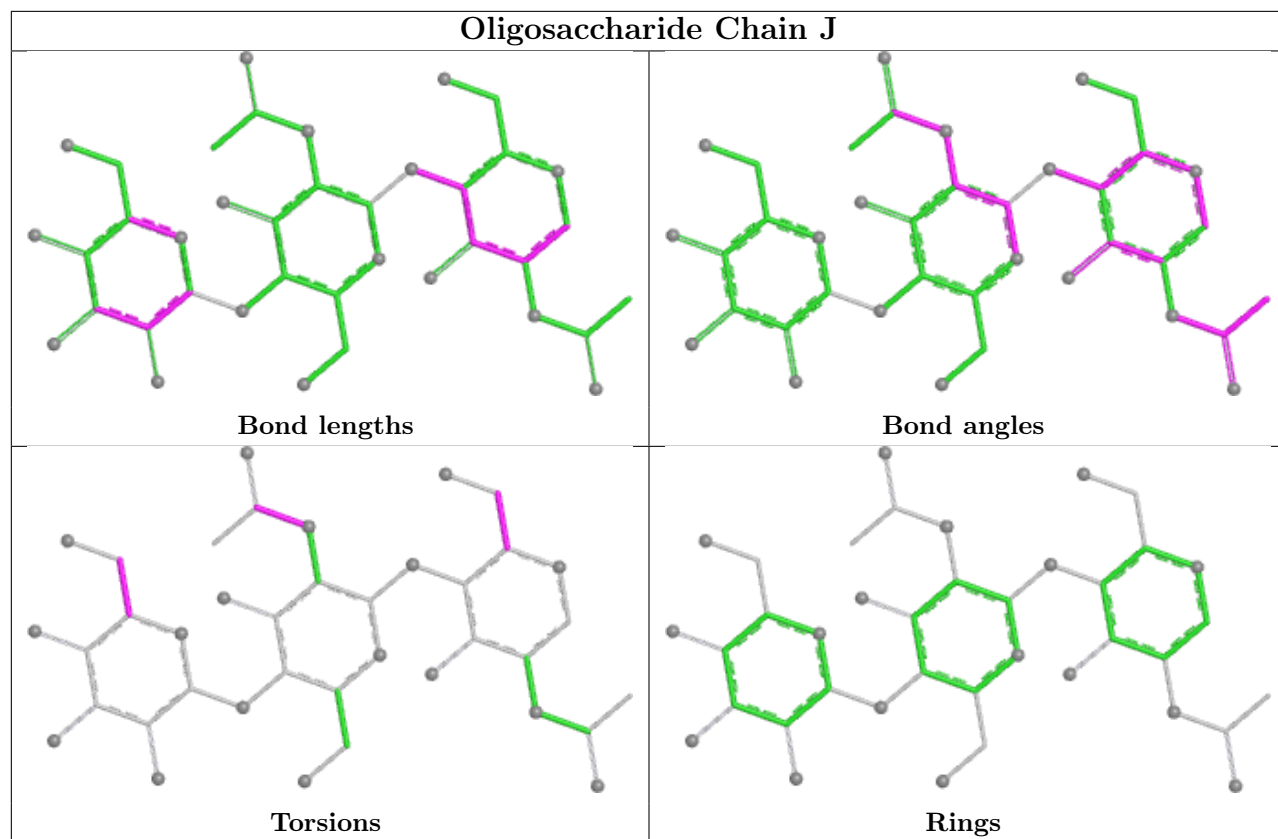


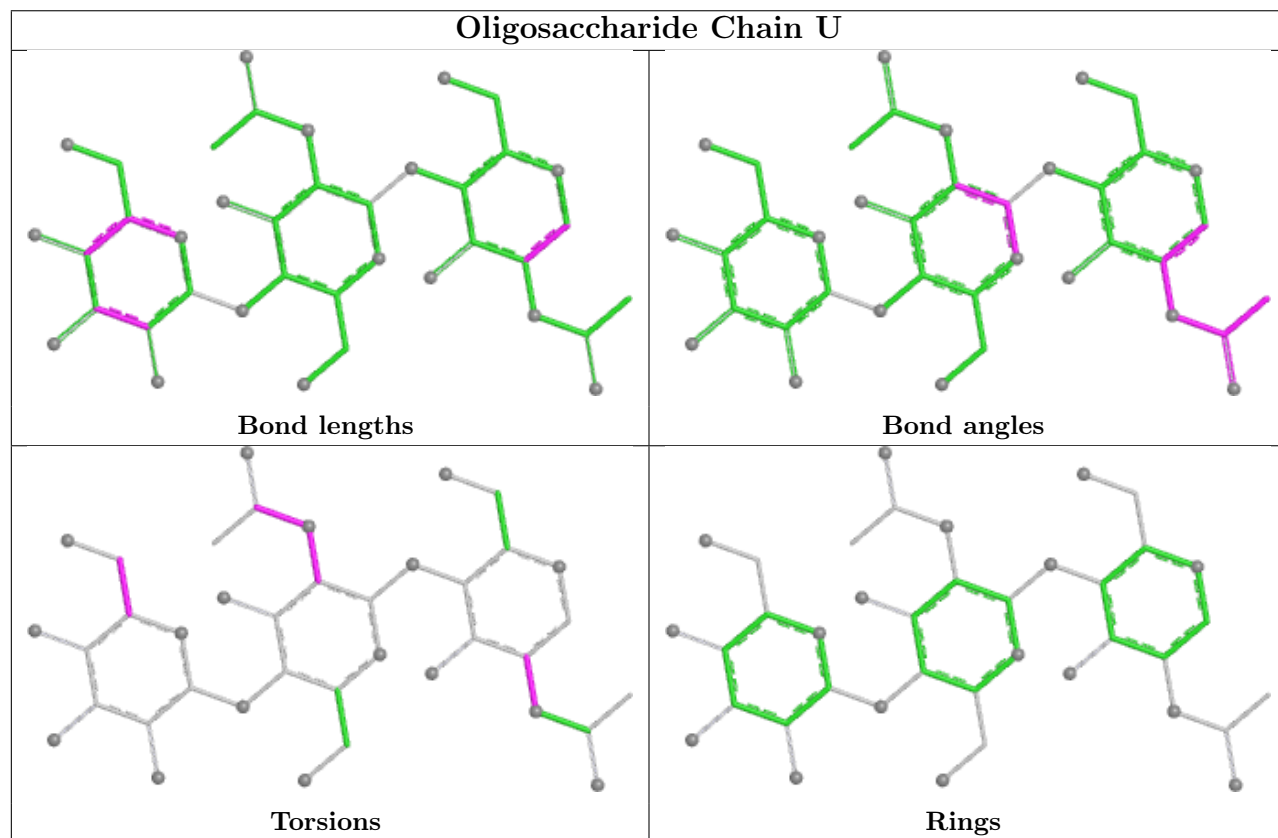
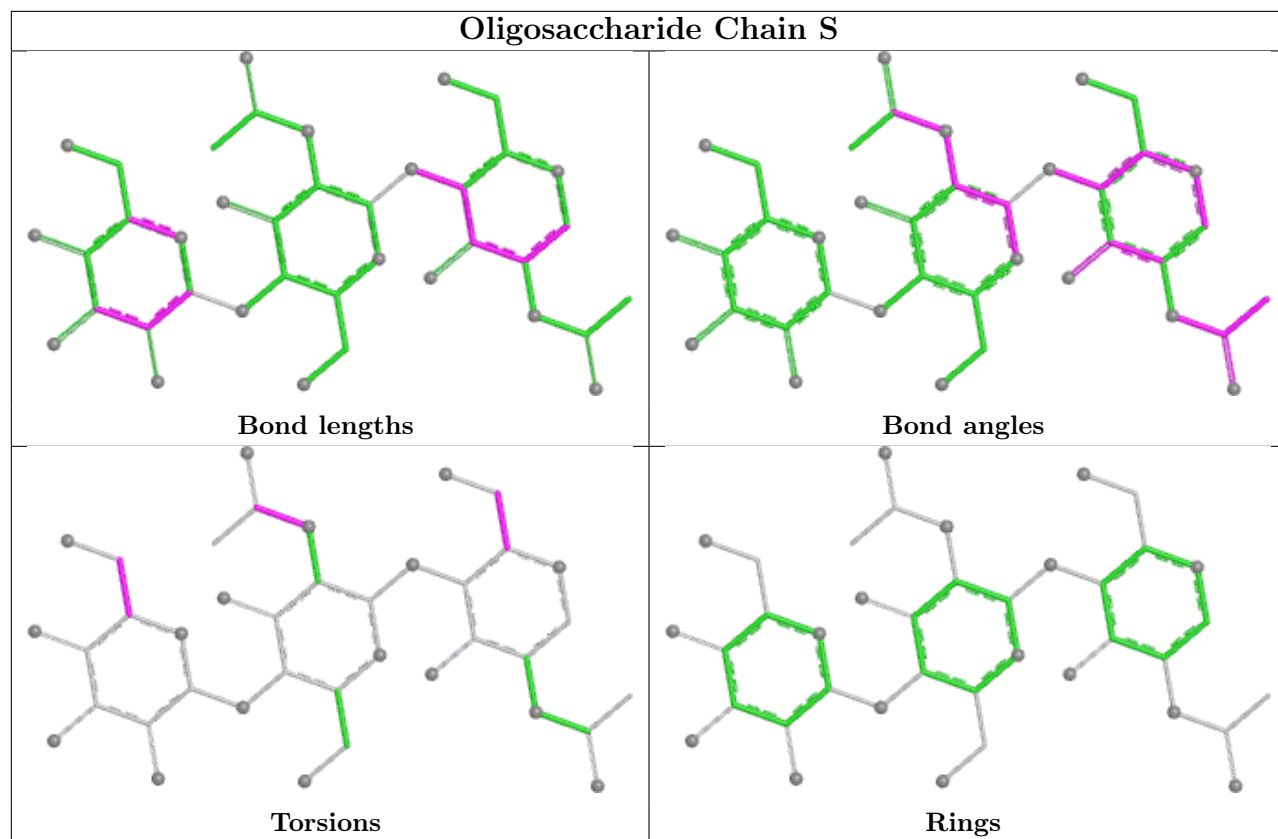


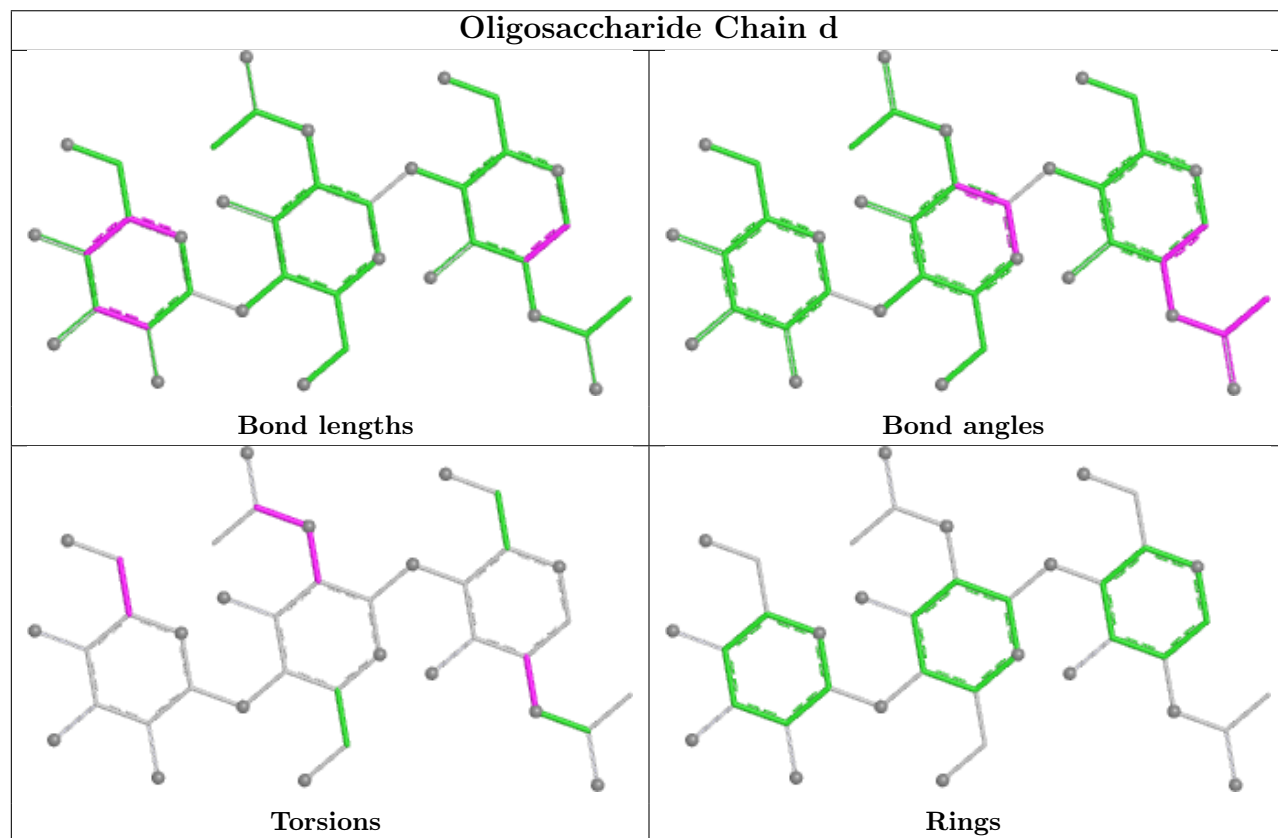
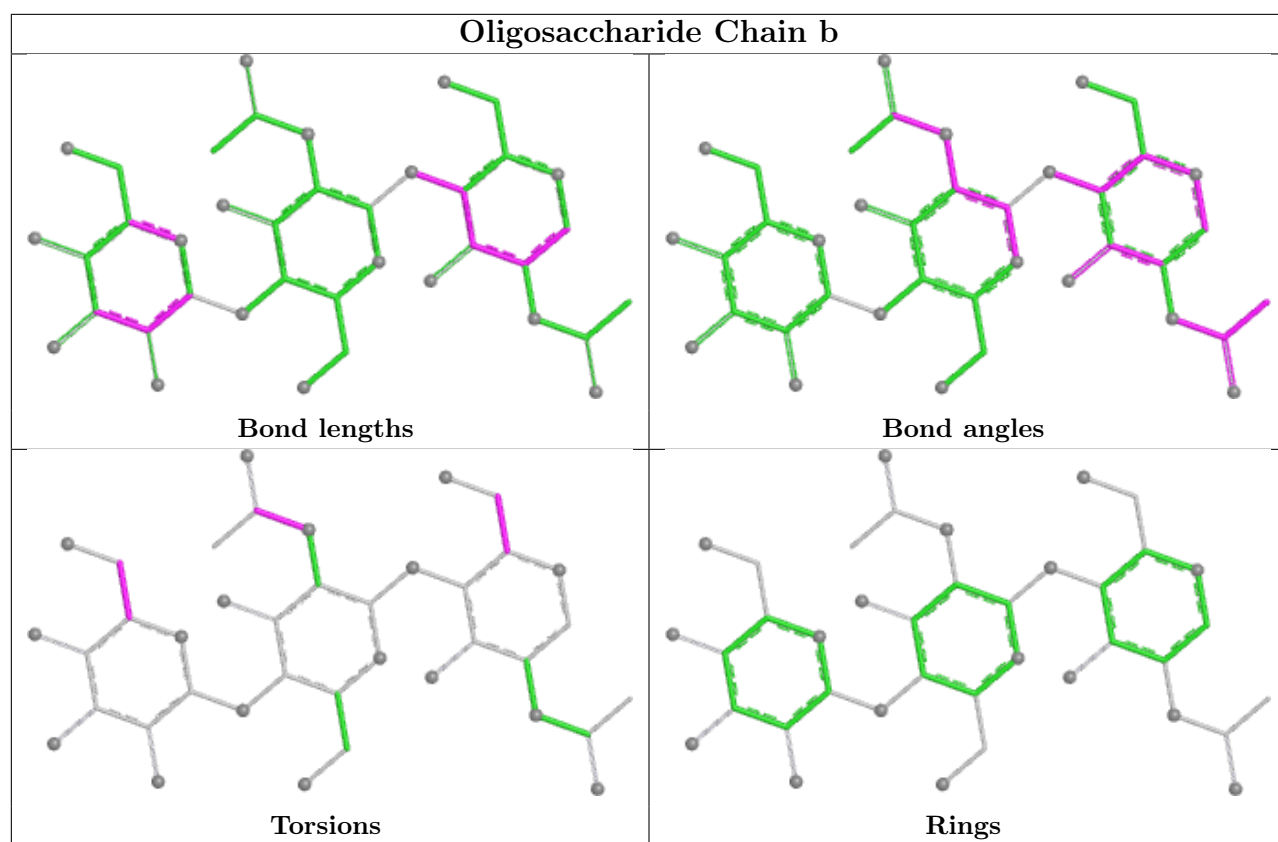












5.6 Ligand geometry

30 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	1505	1	14,14,15	1.70	2 (14%)	17,19,21	1.32	2 (11%)
4	NAG	A	1508	1	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	B	1510	1	14,14,15	0.32	0	17,19,21	0.86	1 (5%)
4	NAG	C	1507	1	14,14,15	1.68	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	C	1509	1	14,14,15	1.55	2 (14%)	17,19,21	1.43	1 (5%)
4	NAG	B	1502	1	14,14,15	0.33	0	17,19,21	0.66	0
4	NAG	C	1504	1	14,14,15	1.70	2 (14%)	17,19,21	0.97	1 (5%)
4	NAG	B	1506	1	14,14,15	1.62	2 (14%)	17,19,21	0.92	1 (5%)
4	NAG	A	1502	1	14,14,15	0.33	0	17,19,21	0.66	0
4	NAG	A	1501	1	14,14,15	1.55	2 (14%)	17,19,21	1.20	2 (11%)
4	NAG	B	1501	1	14,14,15	1.55	2 (14%)	17,19,21	1.20	2 (11%)
4	NAG	A	1510	1	14,14,15	0.33	0	17,19,21	0.85	1 (5%)
4	NAG	B	1509	1	14,14,15	1.54	2 (14%)	17,19,21	1.43	1 (5%)
4	NAG	C	1503	1	14,14,15	1.59	2 (14%)	17,19,21	1.00	1 (5%)
4	NAG	C	1506	1	14,14,15	1.63	2 (14%)	17,19,21	0.92	1 (5%)
4	NAG	C	1508	1	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	C	1502	1	14,14,15	0.34	0	17,19,21	0.65	0
4	NAG	C	1501	1	14,14,15	1.54	2 (14%)	17,19,21	1.20	2 (11%)
4	NAG	C	1510	1	14,14,15	0.33	0	17,19,21	0.86	1 (5%)
4	NAG	A	1507	1	14,14,15	1.69	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	B	1503	1	14,14,15	1.59	2 (14%)	17,19,21	1.00	1 (5%)
4	NAG	A	1503	1	14,14,15	1.59	2 (14%)	17,19,21	1.00	1 (5%)
4	NAG	B	1508	1	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	C	1505	1	14,14,15	1.70	2 (14%)	17,19,21	1.31	2 (11%)
4	NAG	A	1509	1	14,14,15	1.54	2 (14%)	17,19,21	1.43	1 (5%)
4	NAG	A	1504	1	14,14,15	1.70	2 (14%)	17,19,21	0.97	1 (5%)
4	NAG	B	1507	1	14,14,15	1.69	2 (14%)	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1505	1	14,14,15	1.70	2 (14%)	17,19,21	1.32	2 (11%)
4	NAG	B	1504	1	14,14,15	1.70	2 (14%)	17,19,21	0.96	1 (5%)
4	NAG	A	1506	1	14,14,15	1.63	2 (14%)	17,19,21	0.92	1 (5%)

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	1505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1508	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	1510	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1507	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1509	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1504	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1506	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1510	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1509	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1503	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1506	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1508	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	1502	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1501	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1510	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1507	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1503	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1503	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1508	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	1505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1509	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1504	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1507	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1505	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1504	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1506	1	-	2/6/23/26	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1504	NAG	C1-C2	5.07	1.59	1.52
4	B	1504	NAG	C1-C2	5.07	1.59	1.52
4	C	1504	NAG	C1-C2	5.06	1.59	1.52
4	B	1505	NAG	C1-C2	4.73	1.58	1.52
4	A	1505	NAG	C1-C2	4.72	1.58	1.52
4	B	1507	NAG	C1-C2	4.71	1.58	1.52
4	A	1507	NAG	C1-C2	4.71	1.58	1.52
4	C	1505	NAG	C1-C2	4.70	1.58	1.52
4	C	1507	NAG	C1-C2	4.68	1.58	1.52
4	C	1506	NAG	C1-C2	4.44	1.58	1.52
4	A	1506	NAG	C1-C2	4.43	1.58	1.52
4	A	1503	NAG	C1-C2	4.43	1.58	1.52
4	C	1503	NAG	C1-C2	4.43	1.58	1.52
4	B	1503	NAG	C1-C2	4.42	1.58	1.52
4	B	1506	NAG	C1-C2	4.41	1.58	1.52
4	C	1509	NAG	C1-C2	4.23	1.58	1.52
4	A	1509	NAG	C1-C2	4.22	1.58	1.52
4	B	1509	NAG	C1-C2	4.18	1.58	1.52
4	A	1501	NAG	C1-C2	3.82	1.57	1.52
4	B	1501	NAG	C1-C2	3.76	1.57	1.52
4	C	1501	NAG	C1-C2	3.74	1.57	1.52
4	B	1501	NAG	O5-C5	2.89	1.49	1.43
4	C	1501	NAG	O5-C5	2.88	1.49	1.43
4	A	1501	NAG	O5-C5	2.87	1.49	1.43
4	A	1505	NAG	O5-C5	2.45	1.48	1.43
4	B	1505	NAG	O5-C5	2.44	1.48	1.43
4	C	1505	NAG	O5-C5	2.43	1.48	1.43
4	B	1507	NAG	O5-C5	2.37	1.48	1.43
4	A	1507	NAG	O5-C5	2.37	1.48	1.43
4	C	1507	NAG	O5-C5	2.35	1.48	1.43
4	C	1506	NAG	O5-C5	2.31	1.47	1.43
4	A	1506	NAG	O5-C5	2.29	1.47	1.43
4	B	1506	NAG	O5-C5	2.29	1.47	1.43
4	B	1503	NAG	O5-C5	2.26	1.47	1.43
4	C	1503	NAG	O5-C5	2.26	1.47	1.43
4	A	1503	NAG	O5-C5	2.25	1.47	1.43
4	A	1504	NAG	O5-C5	2.23	1.47	1.43
4	B	1504	NAG	O5-C5	2.23	1.47	1.43
4	C	1504	NAG	O5-C5	2.21	1.47	1.43
4	A	1509	NAG	O5-C5	2.11	1.47	1.43
4	C	1509	NAG	O5-C5	2.11	1.47	1.43
4	B	1509	NAG	O5-C5	2.10	1.47	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1509	NAG	C1-C2-N2	-5.26	102.15	110.43
4	A	1509	NAG	C1-C2-N2	-5.25	102.16	110.43
4	B	1509	NAG	C1-C2-N2	-5.25	102.16	110.43
4	B	1505	NAG	C8-C7-N2	3.76	122.35	116.12
4	A	1505	NAG	C8-C7-N2	3.75	122.34	116.12
4	C	1505	NAG	C8-C7-N2	3.72	122.29	116.12
4	A	1501	NAG	C8-C7-N2	3.26	121.53	116.12
4	C	1501	NAG	C8-C7-N2	3.26	121.52	116.12
4	B	1501	NAG	C8-C7-N2	3.26	121.52	116.12
4	C	1503	NAG	C8-C7-N2	2.58	120.40	116.12
4	A	1503	NAG	C8-C7-N2	2.58	120.39	116.12
4	B	1503	NAG	C8-C7-N2	2.58	120.39	116.12
4	C	1501	NAG	O7-C7-C8	-2.54	117.54	122.05
4	B	1501	NAG	O7-C7-C8	-2.52	117.57	122.05
4	A	1501	NAG	O7-C7-C8	-2.51	117.58	122.05
4	B	1505	NAG	O7-C7-C8	-2.50	117.60	122.05
4	A	1505	NAG	O7-C7-C8	-2.48	117.63	122.05
4	C	1505	NAG	O7-C7-C8	-2.47	117.66	122.05
4	A	1504	NAG	C8-C7-N2	2.41	120.11	116.12
4	C	1504	NAG	C8-C7-N2	2.40	120.09	116.12
4	B	1504	NAG	C8-C7-N2	2.38	120.07	116.12
4	A	1506	NAG	C8-C7-N2	2.33	119.98	116.12
4	C	1506	NAG	C8-C7-N2	2.32	119.97	116.12
4	B	1506	NAG	C8-C7-N2	2.31	119.95	116.12
4	B	1510	NAG	C2-N2-C7	-2.23	119.92	122.90
4	C	1510	NAG	C2-N2-C7	-2.22	119.93	122.90
4	A	1510	NAG	C2-N2-C7	-2.21	119.94	122.90
4	A	1507	NAG	C8-C7-N2	2.07	119.55	116.12
4	B	1507	NAG	C8-C7-N2	2.06	119.54	116.12
4	C	1507	NAG	C8-C7-N2	2.06	119.54	116.12

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1508	NAG	C1
4	B	1508	NAG	C1
4	C	1508	NAG	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1509	NAG	O5-C5-C6-O6
4	B	1509	NAG	O5-C5-C6-O6
4	C	1509	NAG	O5-C5-C6-O6
4	A	1510	NAG	C8-C7-N2-C2
4	B	1510	NAG	C8-C7-N2-C2
4	C	1510	NAG	C8-C7-N2-C2
4	A	1510	NAG	O7-C7-N2-C2
4	B	1510	NAG	O7-C7-N2-C2
4	C	1510	NAG	O7-C7-N2-C2
4	A	1509	NAG	C4-C5-C6-O6
4	B	1509	NAG	C4-C5-C6-O6
4	C	1509	NAG	C4-C5-C6-O6
4	A	1506	NAG	C4-C5-C6-O6
4	B	1506	NAG	C4-C5-C6-O6
4	C	1506	NAG	C4-C5-C6-O6
4	A	1506	NAG	O5-C5-C6-O6
4	C	1506	NAG	O5-C5-C6-O6
4	B	1506	NAG	O5-C5-C6-O6
4	B	1504	NAG	C4-C5-C6-O6
4	A	1504	NAG	C4-C5-C6-O6
4	C	1504	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

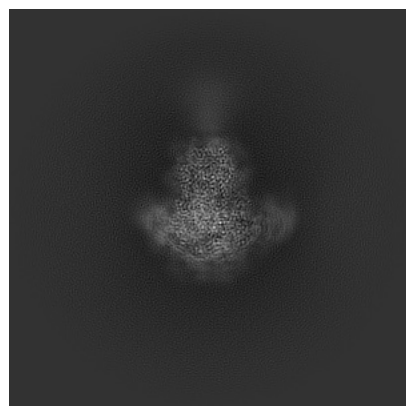
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26730. These allow visual inspection of the internal detail of the map and identification of artifacts.

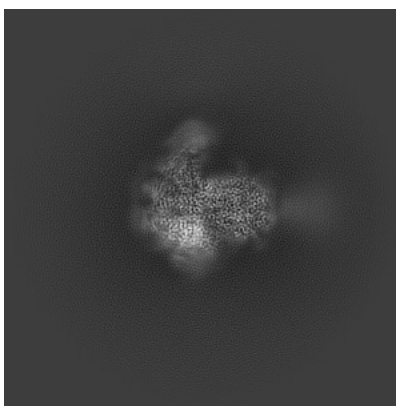
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

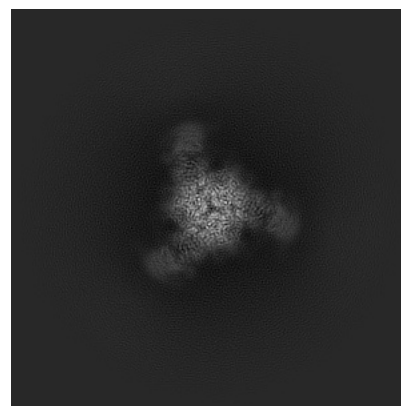
6.1.1 Primary map



X

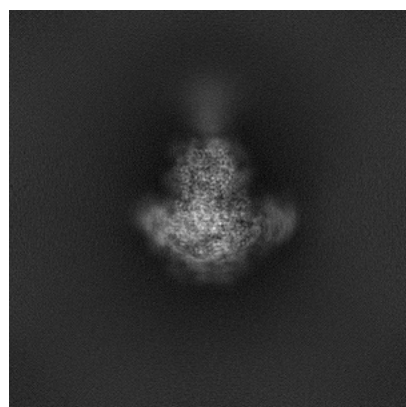


Y

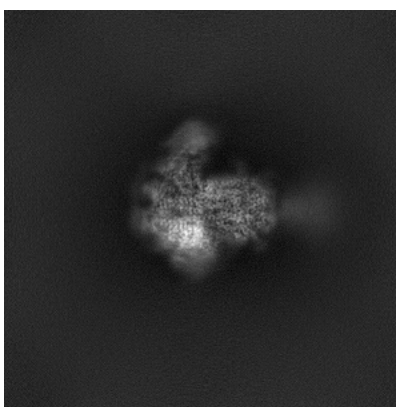


Z

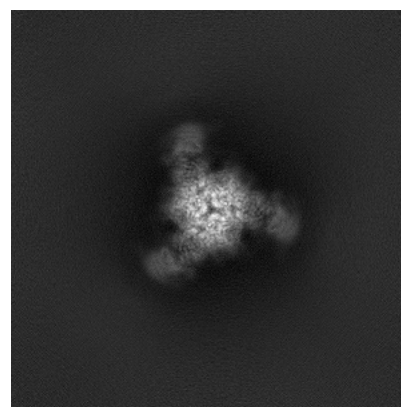
6.1.2 Raw map



X



Y

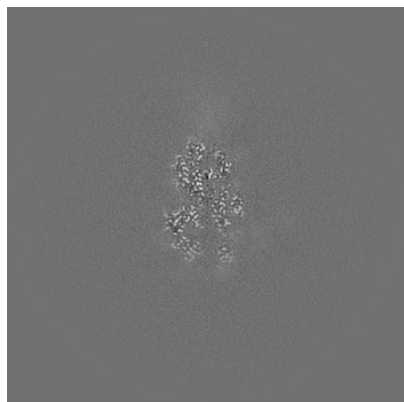


Z

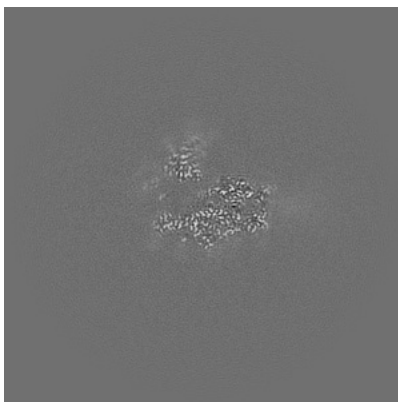
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

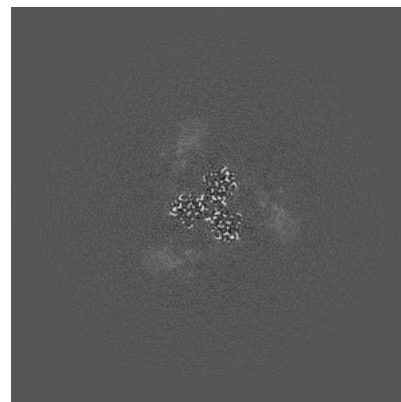
6.2.1 Primary map



X Index: 256

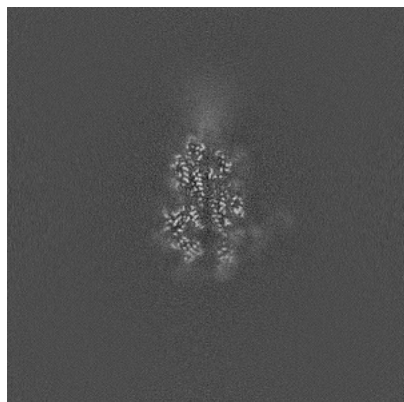


Y Index: 256

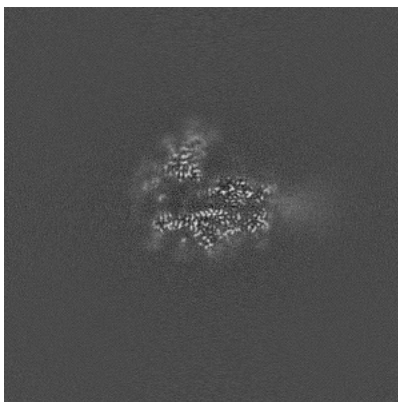


Z Index: 256

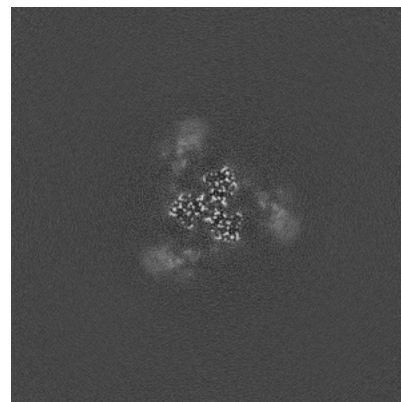
6.2.2 Raw map



X Index: 256



Y Index: 256

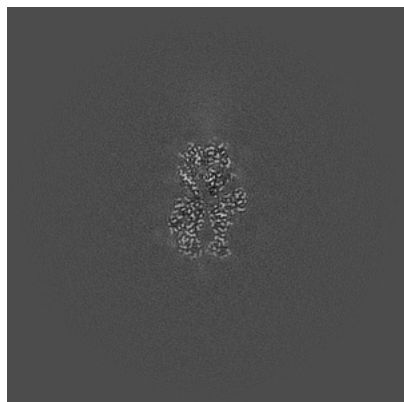


Z Index: 256

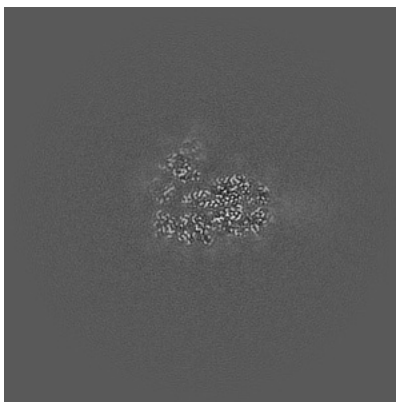
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

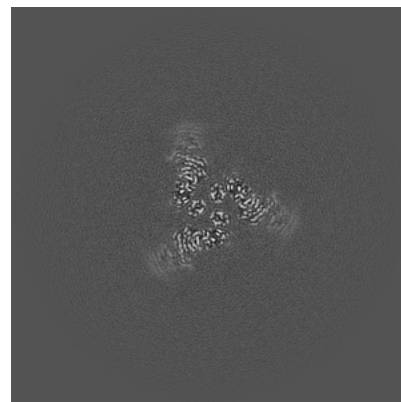
6.3.1 Primary map



X Index: 267

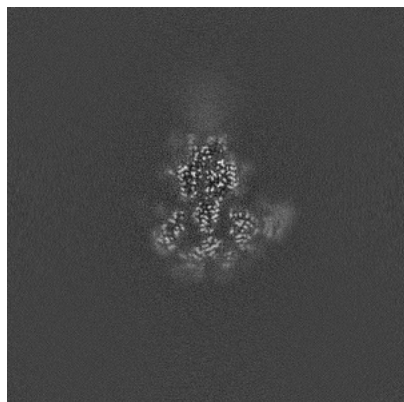


Y Index: 262

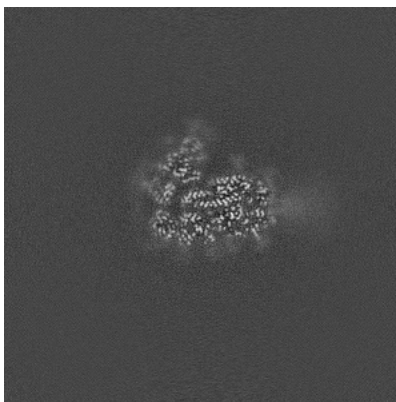


Z Index: 232

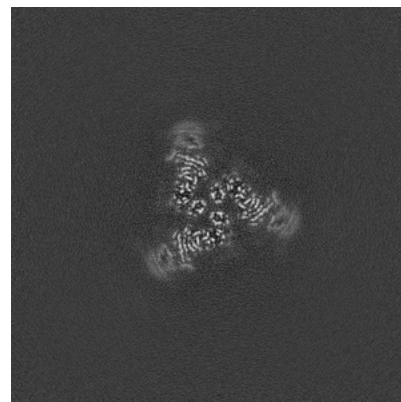
6.3.2 Raw map



X Index: 242



Y Index: 263

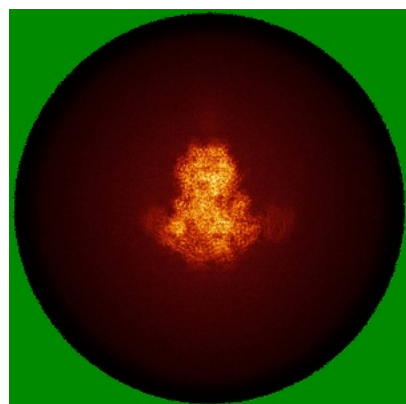


Z Index: 232

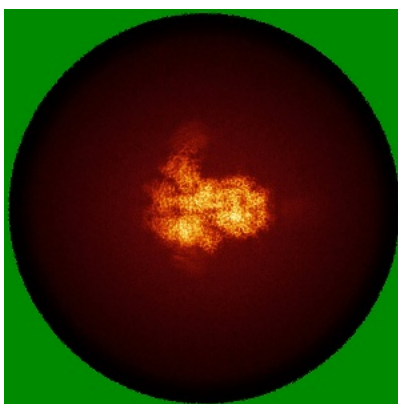
The images above show the largest variance slices of the map in three orthogonal directions.

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

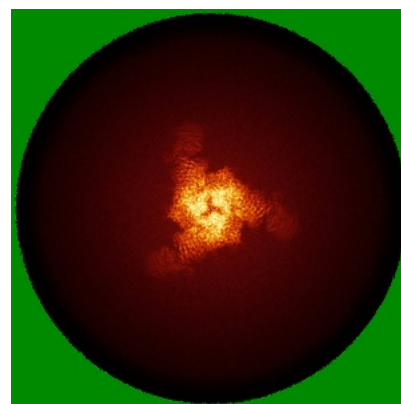
6.4.1 Primary map



X

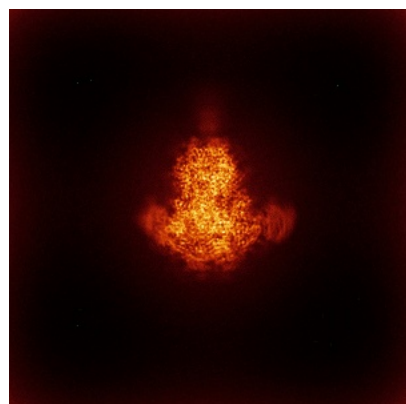


Y

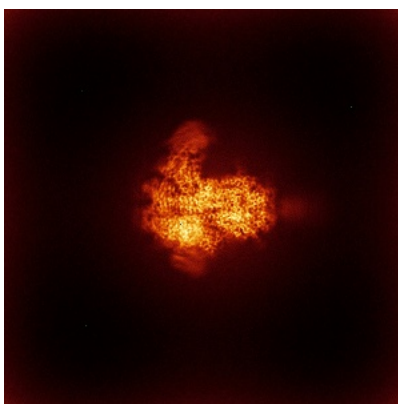


Z

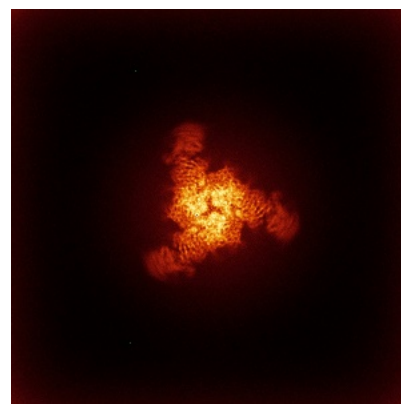
6.4.2 Raw map



X



Y

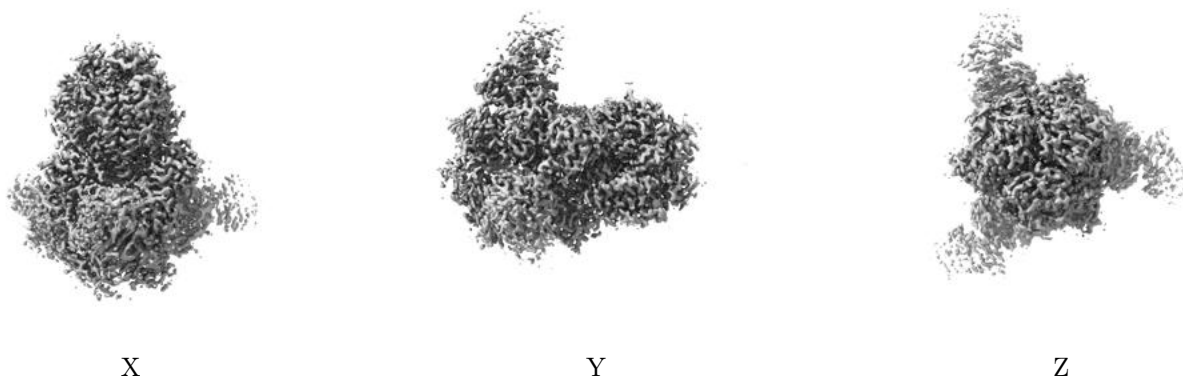


Z

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.

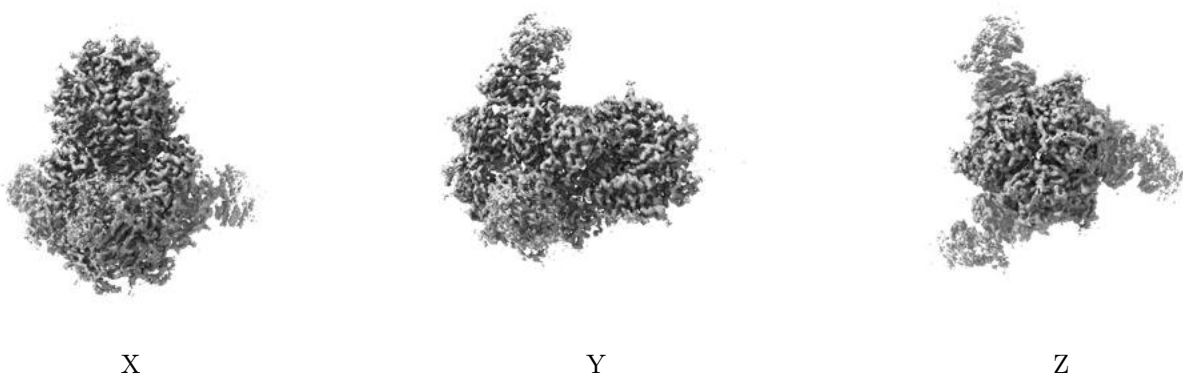
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.706. 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.

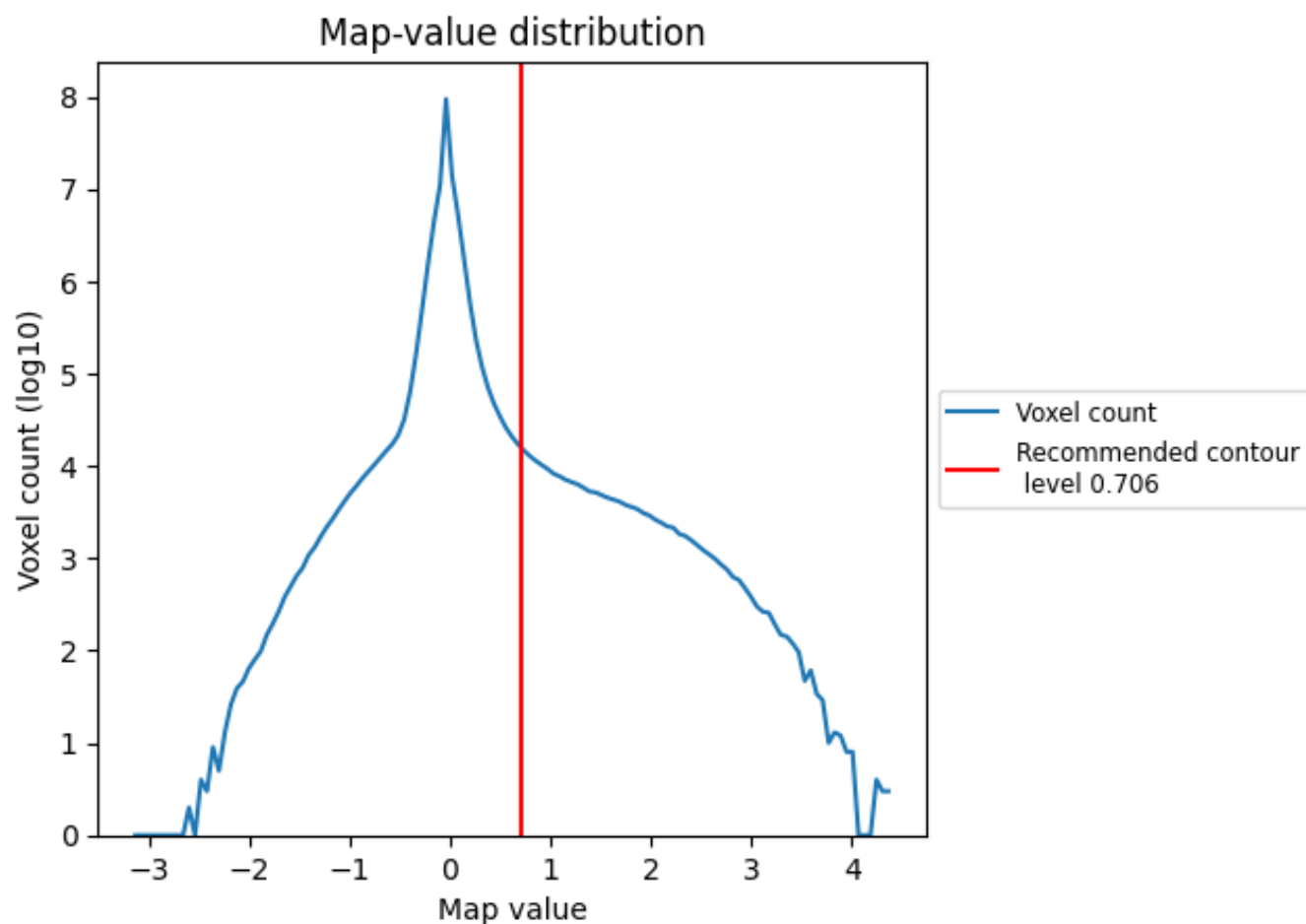
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

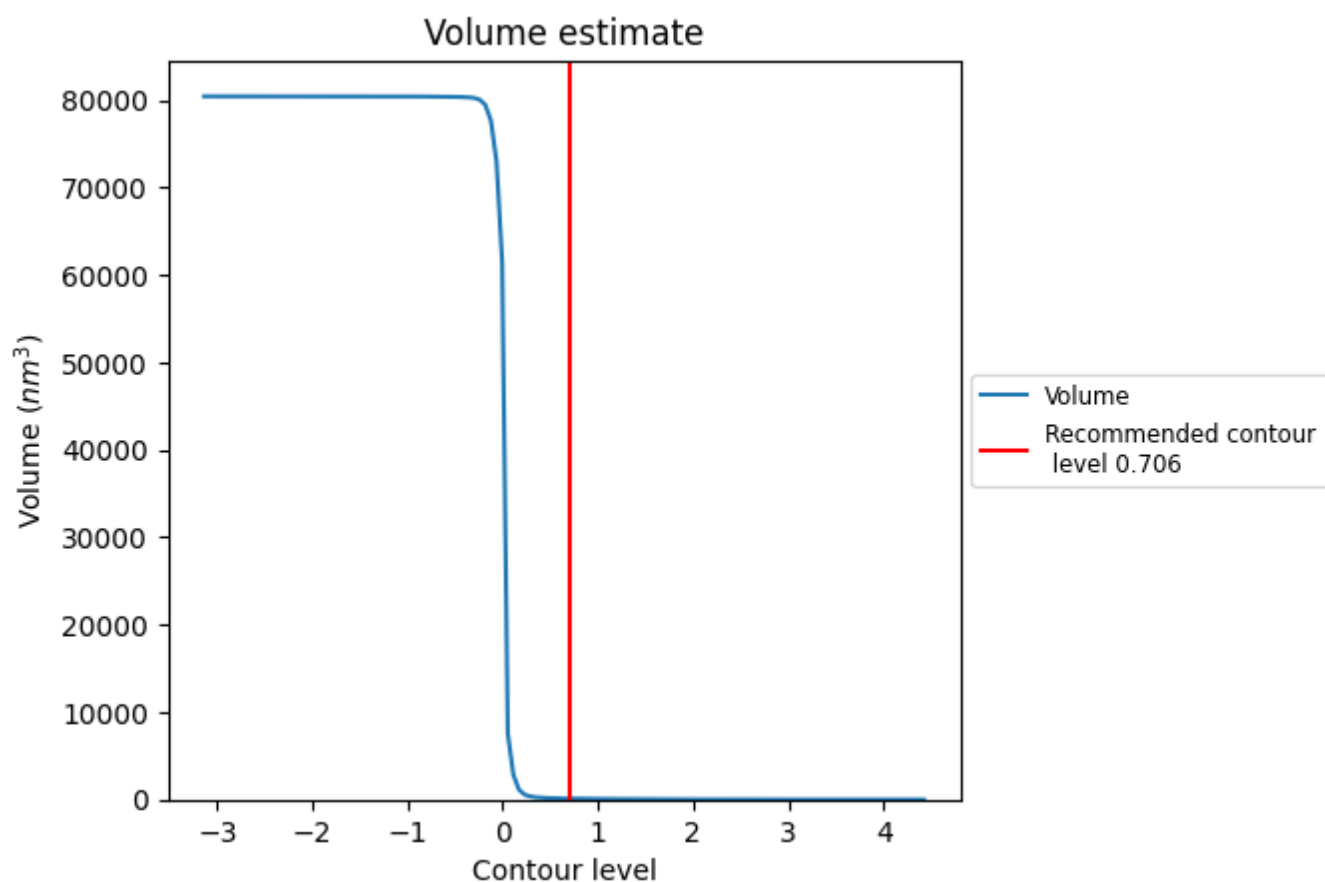
This section contains the results of statistical analysis of the map.

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.

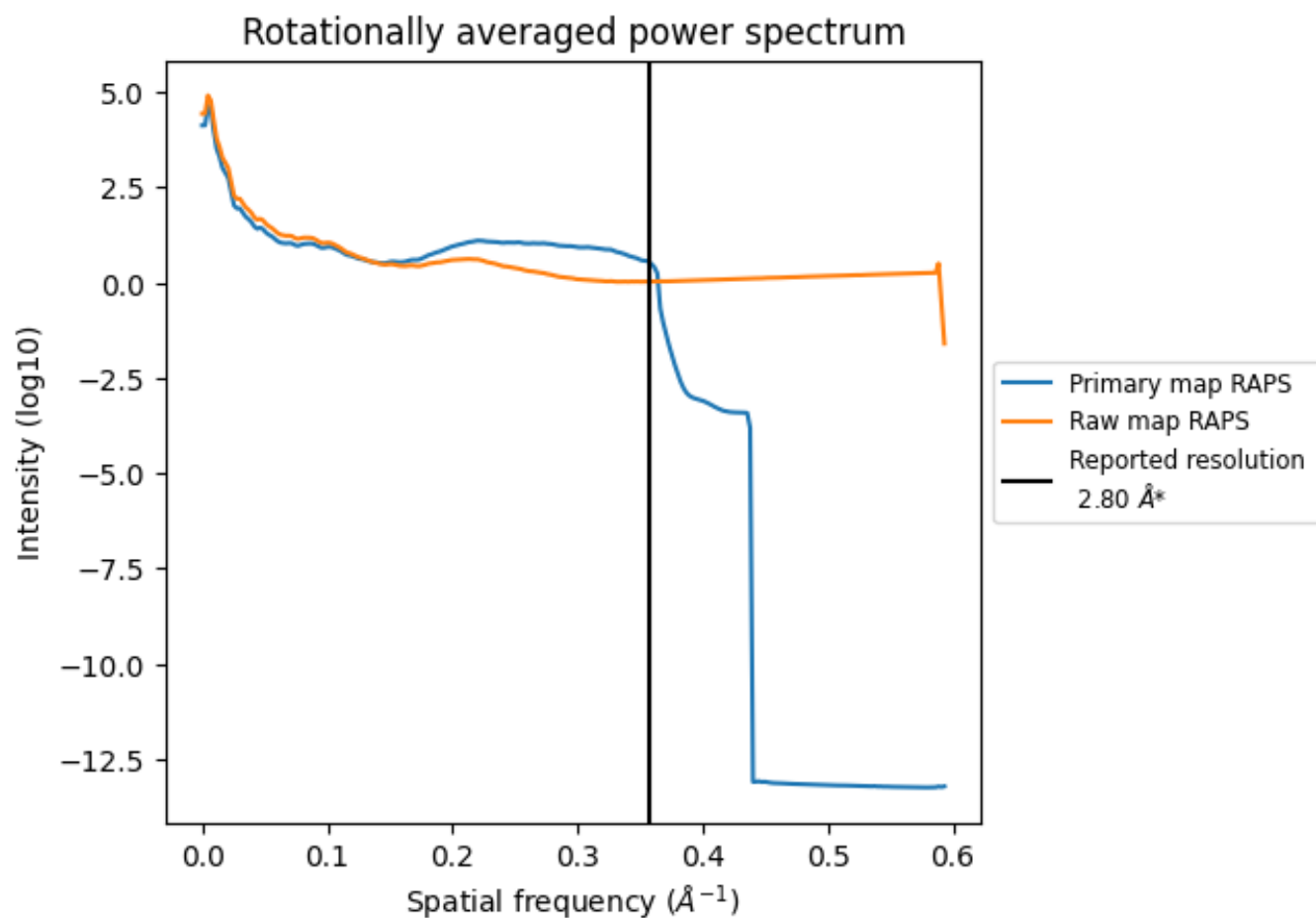
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm³; this corresponds to an approximate mass of 96 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 ⓘ

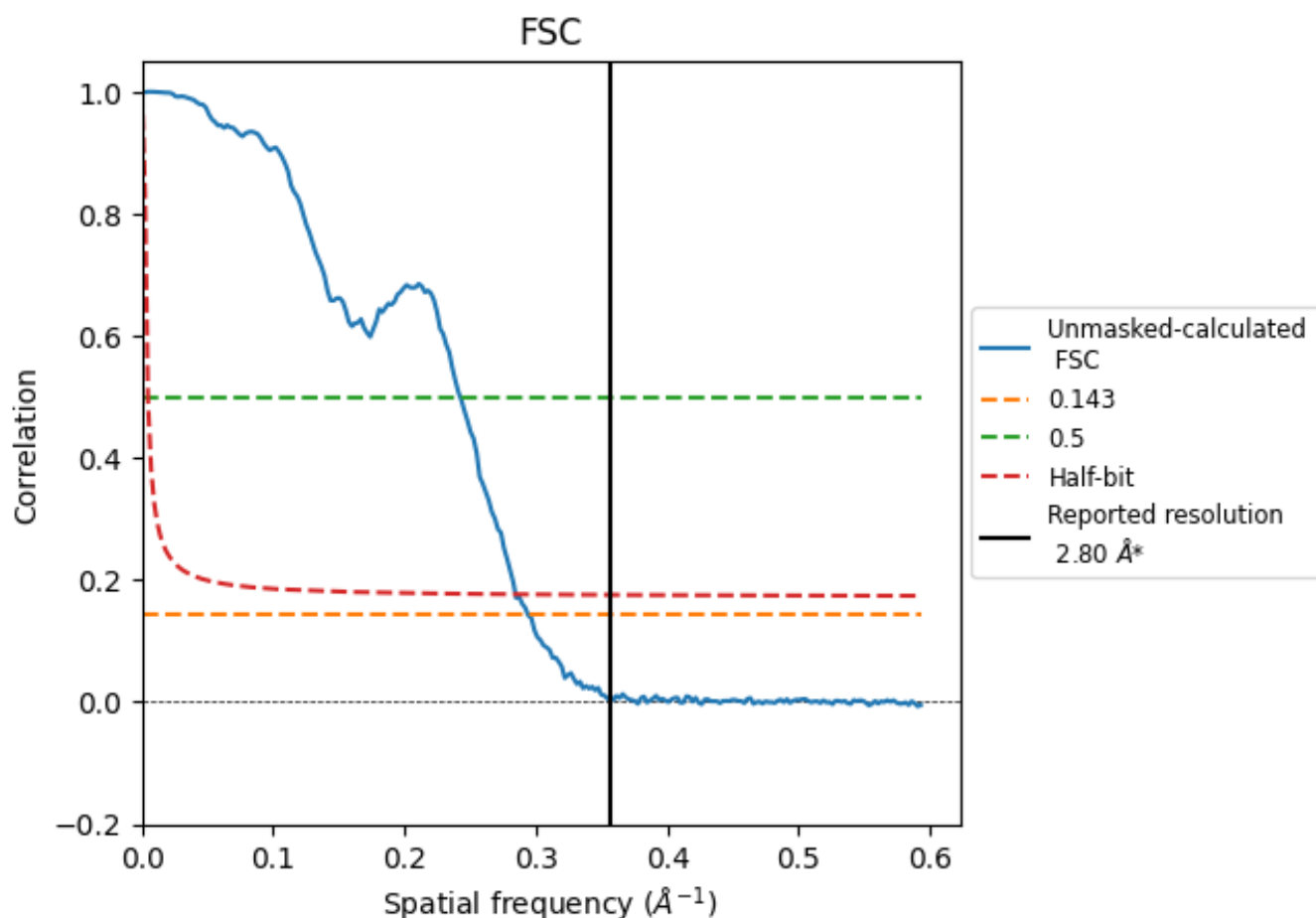


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

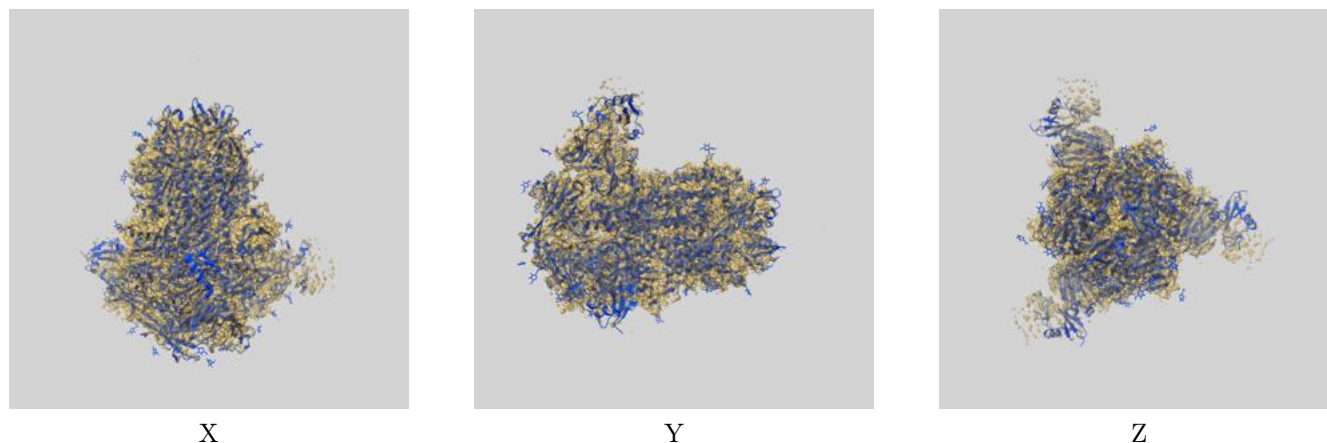
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	4.13	3.52

*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 3.40 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

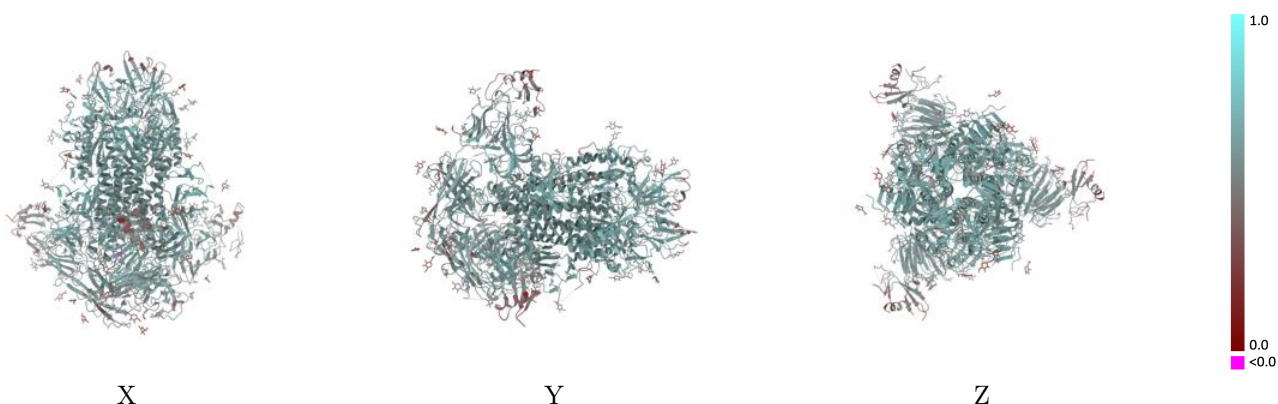
This section contains information regarding the fit between EMDB map EMD-26730 and PDB model 7USA. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



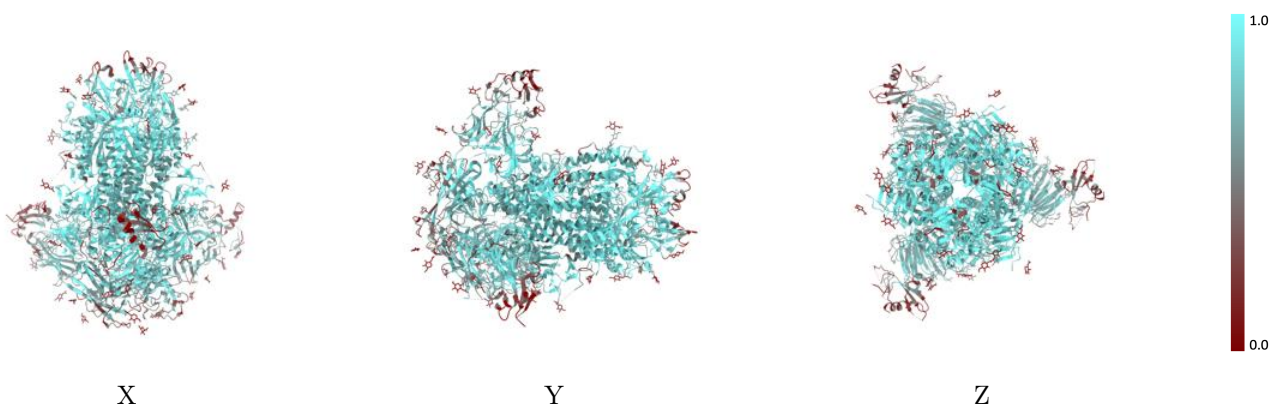
The images above show the 3D surface view of the map at the recommended contour level 0.706 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



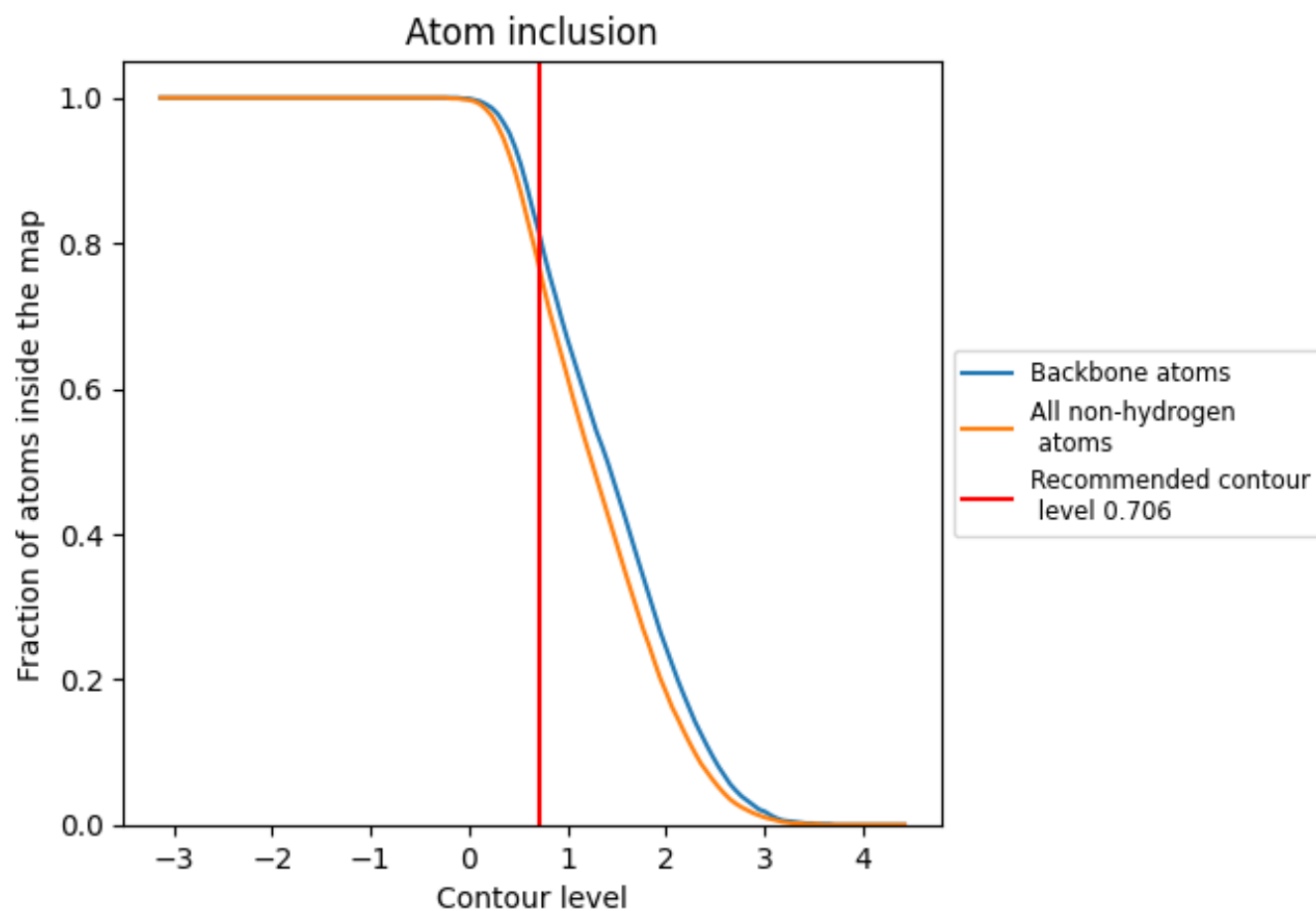
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.706).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.706) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.5820
A	 0.7820	 0.5850
B	 0.7810	 0.5860
C	 0.7830	 0.5860
D	 0.2140	 0.4540
E	 0.3570	 0.4700
F	 0.7140	 0.5650
G	 0.8570	 0.5930
H	 0.2860	 0.3330
I	 0.2500	 0.4580
J	 0.6150	 0.5110
K	 0.4290	 0.4160
L	 0.3850	 0.4530
M	 0.1790	 0.4500
N	 0.3930	 0.4700
O	 0.7140	 0.5560
P	 0.8210	 0.5940
Q	 0.2860	 0.3150
R	 0.2860	 0.4660
S	 0.6410	 0.5170
T	 0.3930	 0.4270
U	 0.4100	 0.4620
V	 0.2140	 0.4460
W	 0.3570	 0.4680
X	 0.7140	 0.5740
Y	 0.8210	 0.6030
Z	 0.2860	 0.3410
a	 0.2860	 0.4760
b	 0.6410	 0.5150
c	 0.3930	 0.4150
d	 0.4100	 0.4530

