



# wwPDB EM Validation Summary Report ⓘ

Dec 31, 2024 – 06:19 PM EST

PDB ID : 8JXE  
EMDB ID : EMD-36698  
Title : rat megalin RAP complex head  
Authors : Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.  
Deposited on : 2023-06-30  
Resolution : 3.20 Å(reported)  
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

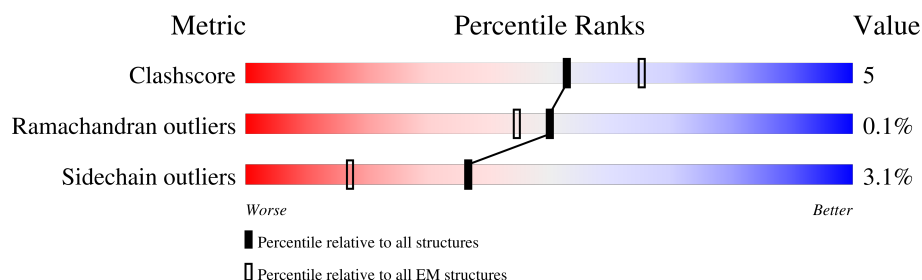
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4660	
1	B	4660	
2	C	6	
2	I	6	
3	D	3	
3	J	3	
4	G	5	
4	K	5	

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Mol	Chain	Length	Quality of chain
5	H	5	
5	L	5	
6	E	2	
6	M	2	
6	N	2	
6	P	2	
6	S	2	
6	T	2	
6	V	2	
6	W	2	
6	Y	2	
6	a	2	
6	b	2	
7	F	3	
7	U	3	
8	O	5	
8	Q	5	
8	X	5	
9	R	2	
10	Z	5	

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 23977 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 LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1469	Total	C	N	O	S	0	0
			11477	7193	2014	2187	83		
1	B	1468	Total	C	N	O	S	0	0
			11468	7187	2013	2185	83		

- Molecule 2 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	6	Total	C	N	O	0	0
			33	21	6	6		
2	C	6	Total	C	N	O	0	0
			33	21	6	6		

- Molecule 3 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	3	Total	C	N	O	S	0	0
			16	9	3	3	1		
3	D	3	Total	C	N	O	S	0	0
			16	9	3	3	1		

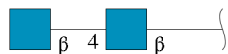
- Molecule 4 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	5	Total	C	N	O	0	0
			33	19	5	9		
4	G	5	Total	C	N	O	0	0
			33	19	5	9		

- Molecule 5 is a protein called unclear peptide.

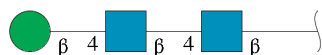
Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	5	Total	C	N	O	0	0
			28	16	6	6		
5	H	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



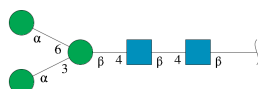
Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	M	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	W	2	Total	C	N	O	0	0
			28	16	2	10		
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		
6	b	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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
7	F	3	Total	C	N	O	0	0
			39	22	2	15		
7	U	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



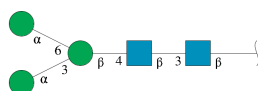
Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	5	Total	C	N	O	0	0
			61	34	2	25		
8	Q	5	Total	C	N	O	0	0
			61	34	2	25		
8	X	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



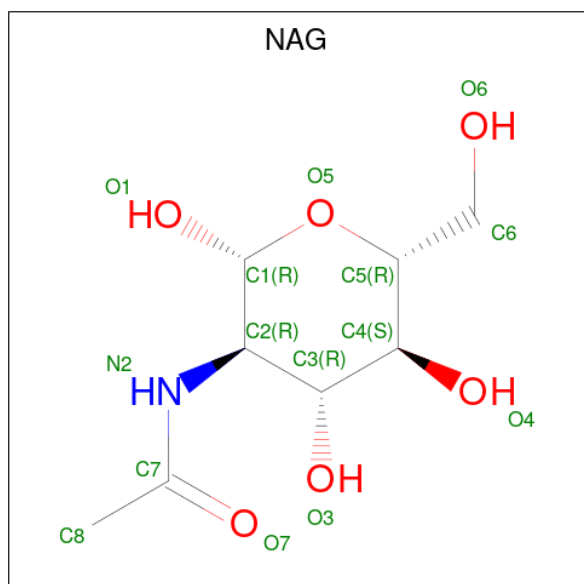
Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



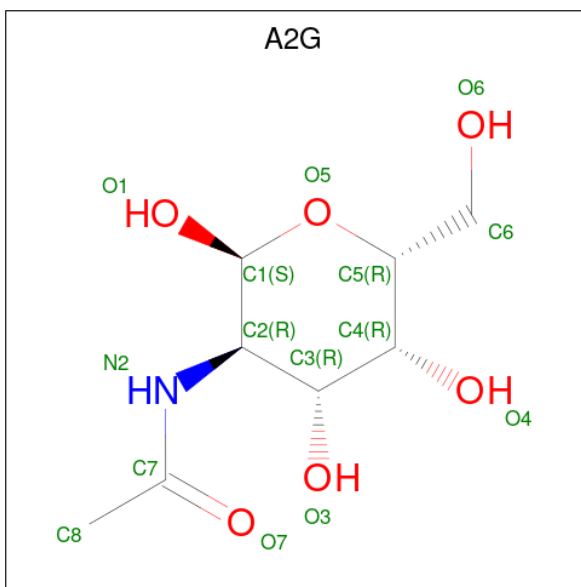
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 12 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 13 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
13	A	6	Total	Ca	0
			6	6	
13	B	6	Total	Ca	0
			6	6	

- Molecule 14 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Ni	0
			1	1	
14	B	1	Total	Ni	0
			1	1	





D2657	D2658	F2659	C2663	S2664	H2665	L2666	C2667	Q2677	Y2685	L2686	A2687	D2696	T2697	C2701	N2702	Q2703	L2704	Q2705	F2706	L2707	C2708	L2709	C2713	L2714	N2715	Q2716	L2717	L2718	K2719	N2722	D2723	N2724	D2725	C2726	G2727	D2728	G2729	S2730	H2740	T2741	C2742	R2743	S2744	T2745	A2746	F2747	R2753	C2754	V2755			
D2516	R2519	K2532	L2533	T2546	V2547	L2551	N2555	L2561	D2564	D2570	L2573	Q2574	K2575	R2578	V2589	T2600	V2601	Y2602	L2606	T2609	T2613	R2614	K2615	L2616	Y2617	R2618	D2626	L2627	M2630	R2633	T2636	Q2637	L2641	S2642	T2643	Q2648	Q2651															
R2120	R2126	V2139	R2149	A2152	Y2161	N2164	T2170	E2173	V2174	L2175	L2185	M2192	P2193	R2194	Y2204	Y2210	R2218	C2223	V2230	S2231	E2232	T2236	M2242	L2249	D2254	I2259	R2273	T2285	V2286	I2291	D2319	K2320	T2328																			
S2338	S2350	F2357	L2361	F2362	E2363	L2364	R2368	A2372	L2391	S2394	L2402	P2406	D2426	Y2427	D2428	R2433	N2441	R2444	S2456	L2463	V2468	F2474	S2484	D2485	F2486	Q2489	D2497	N2500	R2501	V2507	S2508	K2509	P2510	R2511	L2513																	
M1585	R1590	Q1595	T1598	Y1599	W1600	R1611	M1616	Y1619	I1623	Y1628	V1636	I1637	T1650	L1651	V1652	V1656	Y1657	W1658	T1659	V1666	V1680	M1681	G1689	Q1698	Q1719	A1720	P1721	C1728	P1729	L1734	S1738	R1743	G1744	D1745	R1752	V1753	D1754															
I1757	I1775	I1778	I1782	Y1782	E1797	I1802	H1803	F1815	L1827	Y1837	Y1838	E1847	G1853	R1856	T1860	F1873	H1891	M1906	D1907	E1923	T1926	Y1935	W1936	A1937	G1966	V1969	Y1981	V2002	P2003	Y2004	Q2007	L2035	M2070																			
H1404	R1409	F1412	R1413	C1414	A1415	C1416	Y1420	D1425	G1426	R1427	E1435	H1436	P1437	L1438	L1439	A1442	V1449	D1450	A1454	H1455	L1459	D1465	F1468	L1472	D1473	S1476	V1477	T1478	S1484	F1495	Q1496	M1497	T1499	I1515	H1543	K1550	L1560	M1569														
G1322	Y1323	S1324	T1325	C1326	I1327	N1328	L1329	L1332	C1333	D1334	G1335	V1336	F1337	D1338	C1339	P1340	N1341	C1342	T1343	D1344	E1345	S1346	P1347	L1348	C1349	N1350	P1351	D1352	S1353	C1354	S1355	H1356	F1357	N1358	G1359	G1360	H1363	C1364	C1365	M1366	Q1367	G1368	G1371	A1372	T1373	C1374	L1375	L1382	A1383	N1384	K1387	C1401
SER	ASP	GLU	HIS	THR	GLY	CYS	VAL	THR	CYS	ASP	THR	CYS	ASP	ASN	GLY	ILE	TYR	LYS	ALA	TRP	ILE	TRP	GLY	ASP	ASP	ASN	ASP	CYS	ARG	ASP	MET	SER	GLU	LYS	ASP	CYS	PRO	T1308	Q1309	P1310	F1311	H1312	C1313	P1314	S1315	T1316	Q1317	W1318	Q1319			
LEU	SER	ASP	GLN	TRP	PHE	ARG	LEU	PRO	ALA	THR	ASP	GLY	LEU	HIS	VAL	PHE	ASP	THR	ILE	SER	GLY	TRP	CYS	ASP	PRO	HIS	ASP	PRO	HIS	ASP	GLY	VAL	ASP	GLY	ASP	LEU	TRP	VAL	ASP	PHE	ARG	ASP	LYS	ILE	GLY	SER	HIS	THR	LEU	ASP	GLY	
ALA	TYR	ASP	ALA	ASP	LEU	GLN	GLY	ASP	THR	CYS	ASN	ASP	THR	CYS	ASP	ALA	GLY	TYR	VAL	ASP	ASP	TRP	CYS	GLY	ASP	LEU	LYS	THR	ASP	GLY	GLU	ALA	ASP	GLY	VAL	ASP	PRO	ASP	THR	THR	GLN	ALA	THR	THR	ALA	CYS	GLY	GLU	ASP	GLY	PRO	
PRO	THR	GLN	GLN	CYS	GLY	SER	LEU	PRO	ALA	THR	ASP	GLY	LEU	HIS	VAL	PHE	ASP	THR	ILE	SER	GLY	TRP	CYS	ASP	PRO	HIS	ASP	PRO	HIS	ASP	GLY	VAL	ASP	GLY	ASP	LEU	TRP	VAL	ASP	PHE	ARG	ASP	LYS	ILE	GLY	SER	HIS	THR	LEU	ASP	GLY	
PRO	GLY	TRP	HIS	CYS	CYS	ASP	ASP	LEU	ASP	GLY	ASP	GLN	ASN	ASP	GLY	ALA	THR	SER	TYR	VAL	ASP	TRP	CYS	GLY	ASP	LEU	LYS	THR	ASP	GLY	GLU	ALA	ASP	GLY	VAL	ASP	PRO	ASP	THR	THR	GLU	ASP	VAL	ASP	GLY	SER	HIS	THR	LEU	ASP	GLY	
GLU	LYS	ASN	CYS	GLN	ALA	SER	GLY	PRO	THR	GLN	PHE	CYS	ARG	GLY	ILE	PRO	TYR	VAL	ASP	ASP	CYS	TRP	CYS	GLY	ASP	LEU	LYS	THR	ASP	GLY	GLU	ALA	ASP	GLY	VAL	ASP	PRO	ASP	THR	THR	GLU	ASP	VAL	ASP	GLY	SER	HIS	THR	LEU	ASP	GLY	
CYS	ILE	ASN	SER	ARG	TYR	ARG	ARG	CYS	ASP	THR	CYS	ASP	ASN	GLY	ALA	GLY	THR	PRO	ARG	PRO	GLY	MET	CYS	ASP	ASP	GLU	PHE	GLN	CYS	GLN	GLY	ASP	GLY	VAL	ASP	PRO	ASP	THR	THR	GLU	ASP	VAL	ASP	GLY	SER	HIS	THR	LEU	ASP	GLY		











- Molecule 2: unclear peptide

Chain I:  83% 17%



- Molecule 2: unclear peptide

Chain C:  83% 17%



- Molecule 3: unclear peptide

Chain J:  33% 100%




- Molecule 3: unclear peptide

Chain D:  33% 100%




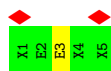
- Molecule 4: unclear peptide

Chain K:  20% 80% 20%



- Molecule 4: unclear peptide

Chain G:  40% 80% 20%



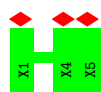
- Molecule 5: unclear peptide

Chain L:  20% 100%



- Molecule 5: unclear peptide





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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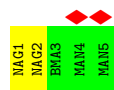
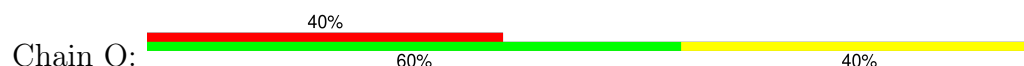
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



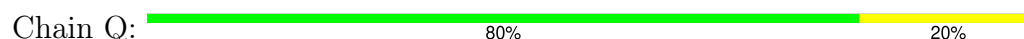
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



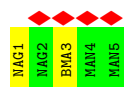
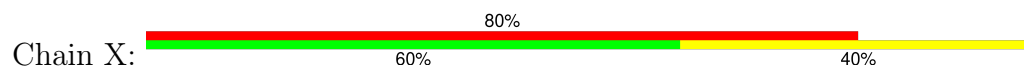
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 10:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-3)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain Z:  60% 40%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0285	Depositor
Map size ( $\text{\AA}$ )	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.411, 1.411, 1.411	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, BMA, NI, A2G, MAN

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	0.25	0/11766	0.51	0/16026
1	B	0.26	0/11757	0.52	0/16013
2	C	0.29	0/7	1.26	0/8
2	I	0.25	0/7	0.87	0/8
3	D	0.27	0/5	0.16	0/5
3	J	0.26	0/5	0.05	0/5
4	G	0.24	0/17	0.35	0/21
4	K	0.31	0/17	0.51	0/21
5	H	0.19	0/7	0.26	0/8
5	L	0.21	0/7	0.52	0/8
All	All	0.26	0/23595	0.52	0/32123

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11477	0	10926	128	0
1	B	11468	0	10914	111	0
2	C	33	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	33	0	18	1	0
3	D	16	0	8	0	0
3	J	16	0	8	0	0
4	G	33	0	17	0	0
4	K	33	0	18	1	0
5	H	28	0	13	0	0
5	L	28	0	12	0	0
6	E	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
6	P	28	0	25	0	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	V	28	0	25	0	0
6	W	28	0	25	0	0
6	Y	28	0	25	0	0
6	a	28	0	25	0	0
6	b	28	0	25	0	0
7	F	39	0	34	1	0
7	U	39	0	34	0	0
8	O	61	0	52	0	0
8	Q	61	0	52	0	0
8	X	61	0	52	0	0
9	R	28	0	25	0	0
10	Z	61	0	52	0	0
11	A	56	0	52	0	0
11	B	56	0	52	0	0
12	A	14	0	12	0	0
12	B	14	0	12	0	0
13	A	6	0	0	0	0
13	B	6	0	0	0	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
All	All	23977	0	22656	238	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 5.

The worst 5 of 238 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:2507:VAL:HG21	1:B:2524:TRP:HE1	1.52	0.74
1:A:2708:CYS:SG	1:A:2730:SER:OG	2.45	0.74
1:B:1900:LYS:HE2	1:B:1902:ALA:HB2	1.71	0.71
1:B:2203:ARG:NH1	1:B:2361:LEU:O	2.27	0.68
1:B:2651:GLN:N	1:B:2651:GLN:OE1	2.27	0.68

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	1467/4660 (32%)	1401 (96%)	66 (4%)	0	100	100
1	B	1466/4660 (32%)	1394 (95%)	70 (5%)	2 (0%)	48	80
2	C	1/6 (17%)	1 (100%)	0	0	100	100
2	I	1/6 (17%)	1 (100%)	0	0	100	100
3	D	1/3 (33%)	1 (100%)	0	0	100	100
3	J	1/3 (33%)	0	1 (100%)	0	100	100
4	G	2/5 (40%)	2 (100%)	0	0	100	100
4	K	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
5	H	1/5 (20%)	0	1 (100%)	0	100	100
5	L	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2943/9358 (31%)	2802 (95%)	139 (5%)	2 (0%)	50	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1500	ASP
1	B	2743	ARG



### 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	1274/4089 (31%)	1233 (97%)	41 (3%)	34	65
1	B	1272/4089 (31%)	1234 (97%)	38 (3%)	36	66
2	C	1/1 (100%)	1 (100%)	0	100	100
2	I	1/1 (100%)	1 (100%)	0	100	100
3	D	1/1 (100%)	1 (100%)	0	100	100
3	J	1/1 (100%)	1 (100%)	0	100	100
4	G	2/2 (100%)	1 (50%)	1 (50%)	0	0
4	K	2/2 (100%)	2 (100%)	0	100	100
5	H	1/1 (100%)	1 (100%)	0	100	100
5	L	1/1 (100%)	1 (100%)	0	100	100
All	All	2556/8188 (31%)	2476 (97%)	80 (3%)	37	66

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1967	LEU
1	B	2519	ARG
1	B	2041	MET
1	B	2297	ASN
1	B	2706	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2765	ASN
1	B	2665	HIS
1	B	1891	HIS
1	B	2710	ASN
1	B	2378	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 ⓘ

50 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	$\# Z  > 2$
6	NAG	E	1	1,6	14,14,15	0.43	0	17,19,21	1.52	2 (11%)
6	NAG	E	2	6	14,14,15	0.34	0	17,19,21	0.74	1 (5%)
7	NAG	F	1	1,7	14,14,15	0.44	0	17,19,21	0.94	1 (5%)
7	NAG	F	2	7	14,14,15	0.31	0	17,19,21	0.73	0
7	BMA	F	3	7	11,11,12	0.24	0	15,15,17	1.01	1 (6%)
6	NAG	M	1	1,6	14,14,15	0.32	0	17,19,21	0.75	1 (5%)
6	NAG	M	2	6	14,14,15	0.32	0	17,19,21	0.67	0
6	NAG	N	1	1,6	14,14,15	0.30	0	17,19,21	0.52	0
6	NAG	N	2	6	14,14,15	0.32	0	17,19,21	0.79	0
8	NAG	O	1	8,1	14,14,15	0.42	0	17,19,21	1.51	5 (29%)
8	NAG	O	2	8	14,14,15	0.28	0	17,19,21	1.14	2 (11%)
8	BMA	O	3	8	11,11,12	0.23	0	15,15,17	0.77	0
8	MAN	O	4	8	11,11,12	0.24	0	15,15,17	0.51	0
8	MAN	O	5	8	11,11,12	0.22	0	15,15,17	0.50	0
6	NAG	P	1	1,6	14,14,15	0.31	0	17,19,21	0.86	1 (5%)
6	NAG	P	2	6	14,14,15	0.35	0	17,19,21	0.58	0
8	NAG	Q	1	8,1	14,14,15	0.32	0	17,19,21	0.56	0
8	NAG	Q	2	8	14,14,15	0.29	0	17,19,21	0.66	0
8	BMA	Q	3	8	11,11,12	0.22	0	15,15,17	0.96	1 (6%)
8	MAN	Q	4	8	11,11,12	0.22	0	15,15,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	Q	5	8	11,11,12	0.23	0	15,15,17	0.50	0
9	NAG	R	1	1,9	14,14,15	0.45	0	17,19,21	0.91	0
9	NAG	R	2	9	14,14,15	0.28	0	17,19,21	0.89	0
6	NAG	S	1	1,6	14,14,15	0.47	0	17,19,21	1.34	2 (11%)
6	NAG	S	2	6	14,14,15	0.30	0	17,19,21	0.91	1 (5%)
6	NAG	T	1	1,6	14,14,15	0.30	0	17,19,21	0.65	0
6	NAG	T	2	6	14,14,15	0.33	0	17,19,21	0.76	1 (5%)
7	NAG	U	1	1,7	14,14,15	0.40	0	17,19,21	0.79	1 (5%)
7	NAG	U	2	7	14,14,15	0.48	0	17,19,21	0.74	0
7	BMA	U	3	7	11,11,12	0.23	0	15,15,17	0.87	1 (6%)
6	NAG	V	1	1,6	14,14,15	0.64	0	17,19,21	1.58	1 (5%)
6	NAG	V	2	6	14,14,15	0.45	0	17,19,21	1.03	1 (5%)
6	NAG	W	1	1,6	14,14,15	0.39	0	17,19,21	0.80	0
6	NAG	W	2	6	14,14,15	0.31	0	17,19,21	0.63	0
8	NAG	X	1	8,1	14,14,15	0.39	0	17,19,21	0.81	1 (5%)
8	NAG	X	2	8	14,14,15	0.32	0	17,19,21	0.80	0
8	BMA	X	3	8	11,11,12	0.26	0	15,15,17	1.10	2 (13%)
8	MAN	X	4	8	11,11,12	0.26	0	15,15,17	0.52	0
8	MAN	X	5	8	11,11,12	0.24	0	15,15,17	0.63	0
6	NAG	Y	1	1,6	14,14,15	0.30	0	17,19,21	0.49	0
6	NAG	Y	2	6	14,14,15	0.31	0	17,19,21	0.69	0
10	NAG	Z	1	10,1	14,14,15	0.63	0	17,19,21	1.29	2 (11%)
10	NAG	Z	2	10	14,14,15	0.36	0	17,19,21	1.14	1 (5%)
10	BMA	Z	3	10	11,11,12	0.21	0	15,15,17	0.91	0
10	MAN	Z	4	10	11,11,12	0.22	0	15,15,17	0.49	0
10	MAN	Z	5	10	11,11,12	0.22	0	15,15,17	0.51	0
6	NAG	a	1	1,6	14,14,15	0.49	0	17,19,21	1.14	3 (17%)
6	NAG	a	2	6	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
6	NAG	b	1	1,6	14,14,15	0.28	0	17,19,21	0.81	0
6	NAG	b	2	6	14,14,15	0.31	0	17,19,21	0.79	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
6	NAG	E	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
7	NAG	F	1	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	F	2	7	-	2/6/23/26	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	1/6/23/26	0/1/1/1
6	NAG	N	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
8	NAG	O	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	2/6/23/26	0/1/1/1
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1
8	MAN	O	4	8	-	0/2/19/22	0/1/1/1
8	MAN	O	5	8	-	0/2/19/22	0/1/1/1
6	NAG	P	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
8	NAG	Q	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	0/2/19/22	0/1/1/1
9	NAG	R	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	R	2	9	-	0/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	T	2	6	-	1/6/23/26	0/1/1/1
7	NAG	U	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	U	2	7	-	3/6/23/26	0/1/1/1
7	BMA	U	3	7	-	1/2/19/22	0/1/1/1
6	NAG	V	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
6	NAG	W	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	W	2	6	-	0/6/23/26	0/1/1/1
8	NAG	X	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
8	MAN	X	4	8	-	0/2/19/22	0/1/1/1
8	MAN	X	5	8	-	0/2/19/22	0/1/1/1
6	NAG	Y	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	1/6/23/26	0/1/1/1
10	NAG	Z	1	10,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	Z	2	10	-	2/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	1/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	1/2/19/22	0/1/1/1
6	NAG	a	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	3/6/23/26	0/1/1/1
6	NAG	b	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	b	2	6	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	1	NAG	C1-O5-C5	6.30	120.63	112.19
6	E	1	NAG	C1-O5-C5	4.57	118.31	112.19
6	S	1	NAG	C1-O5-C5	4.35	118.01	112.19
8	O	2	NAG	C1-O5-C5	3.46	116.83	112.19
6	V	2	NAG	C1-O5-C5	3.24	116.53	112.19

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

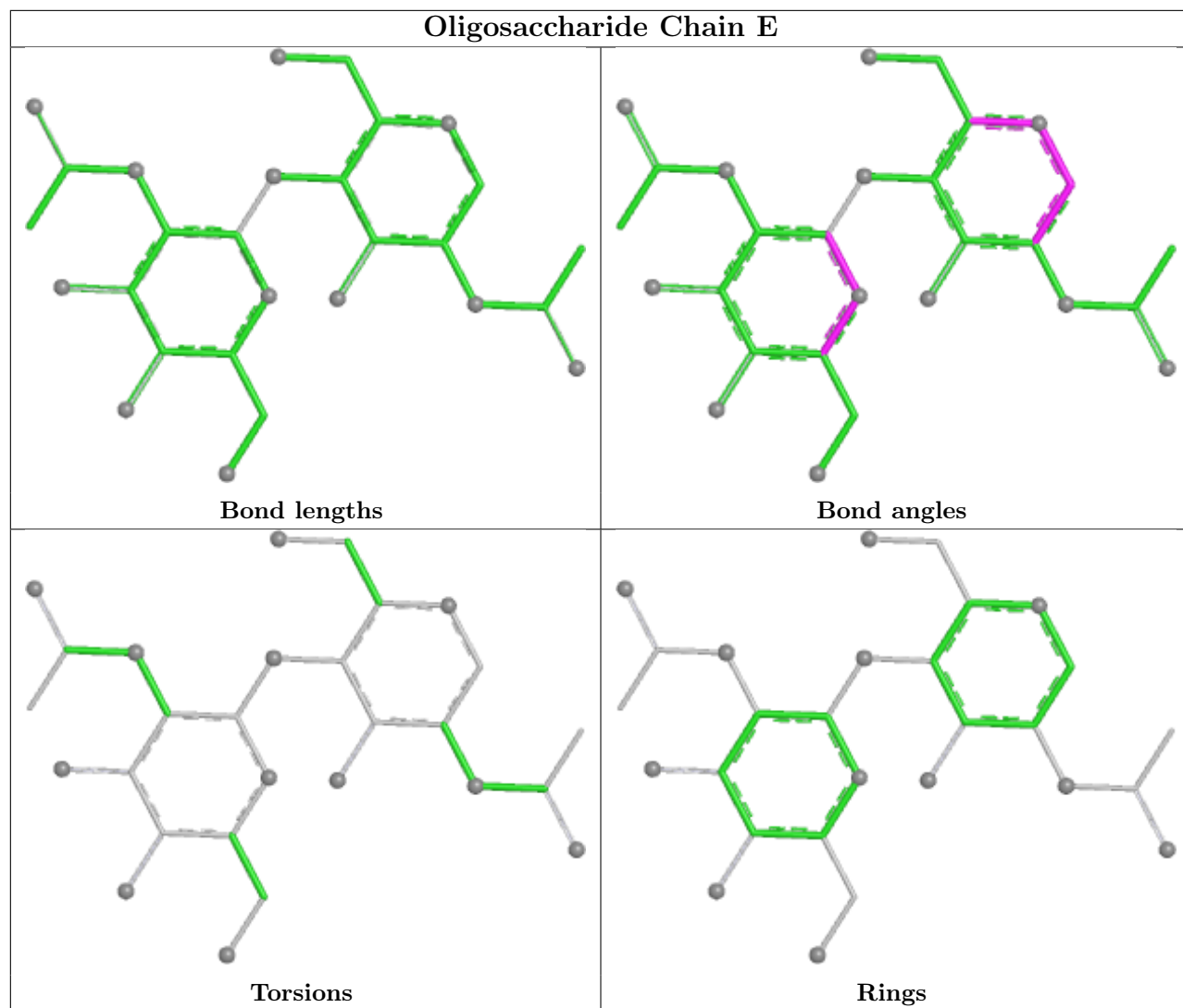
Mol	Chain	Res	Type	Atoms
6	N	2	NAG	C1-C2-N2-C7
6	W	1	NAG	C3-C2-N2-C7
6	W	1	NAG	C8-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
6	a	2	NAG	C1-C2-N2-C7

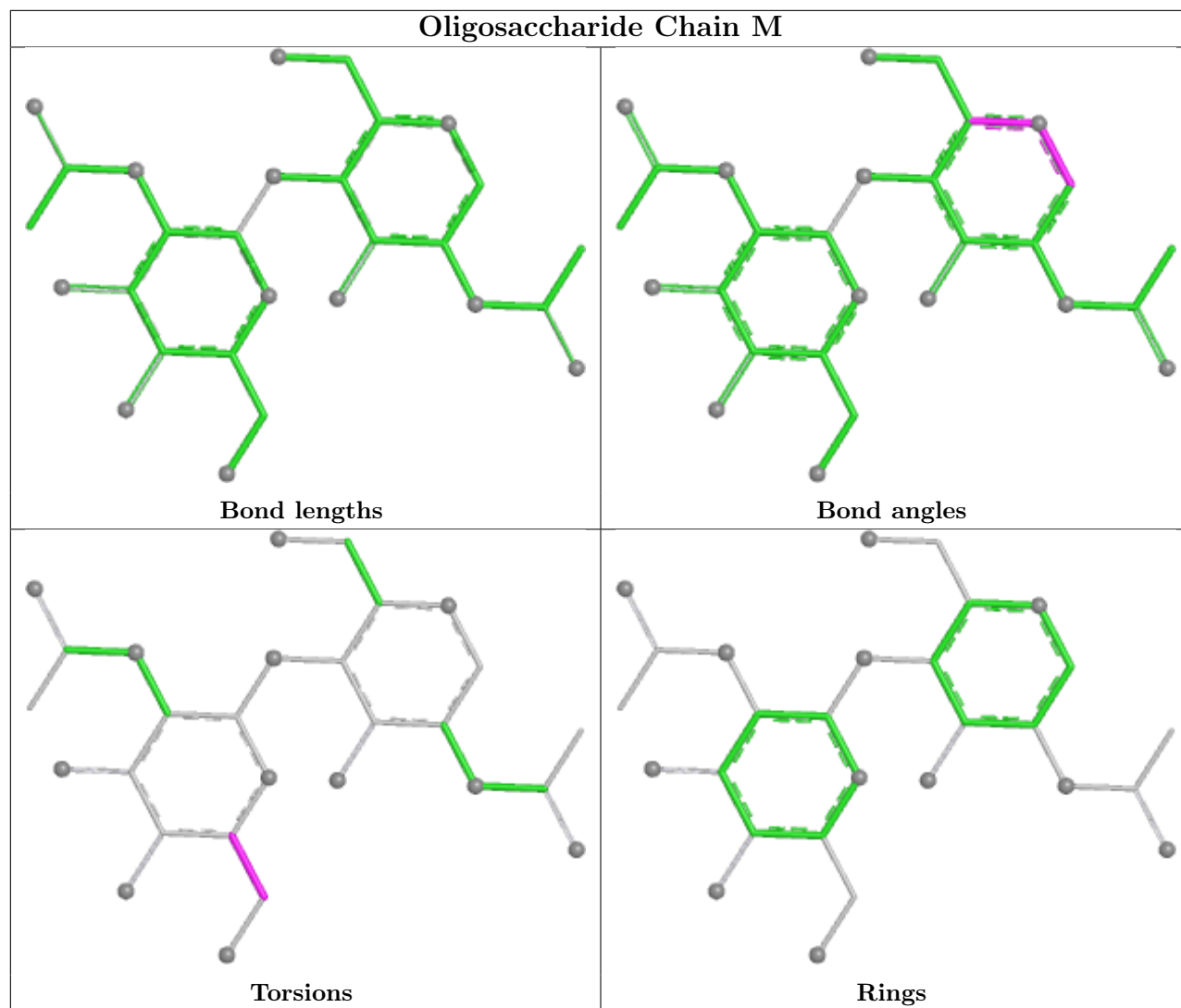
There are no ring outliers.

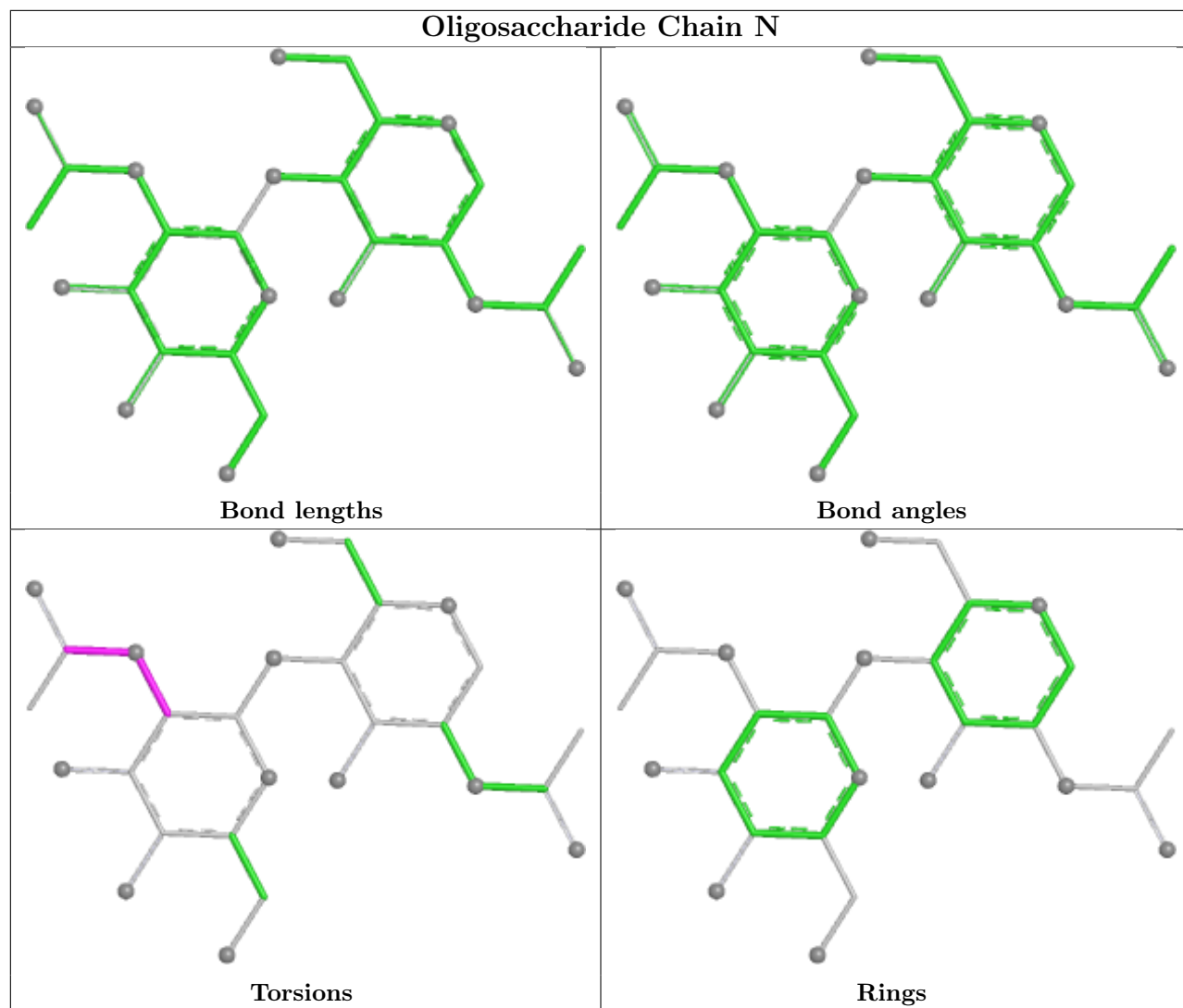
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1	NAG	1	0

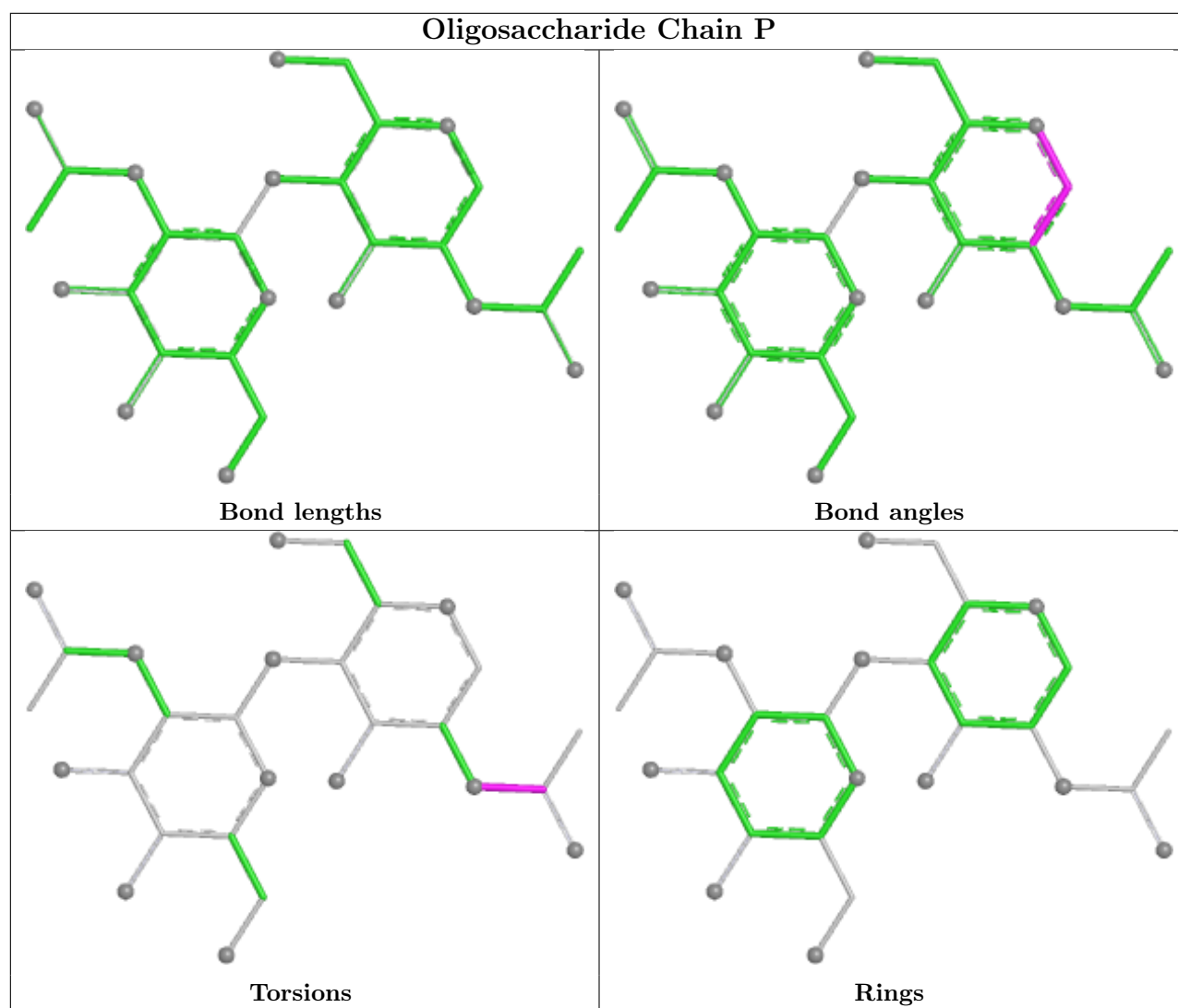
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

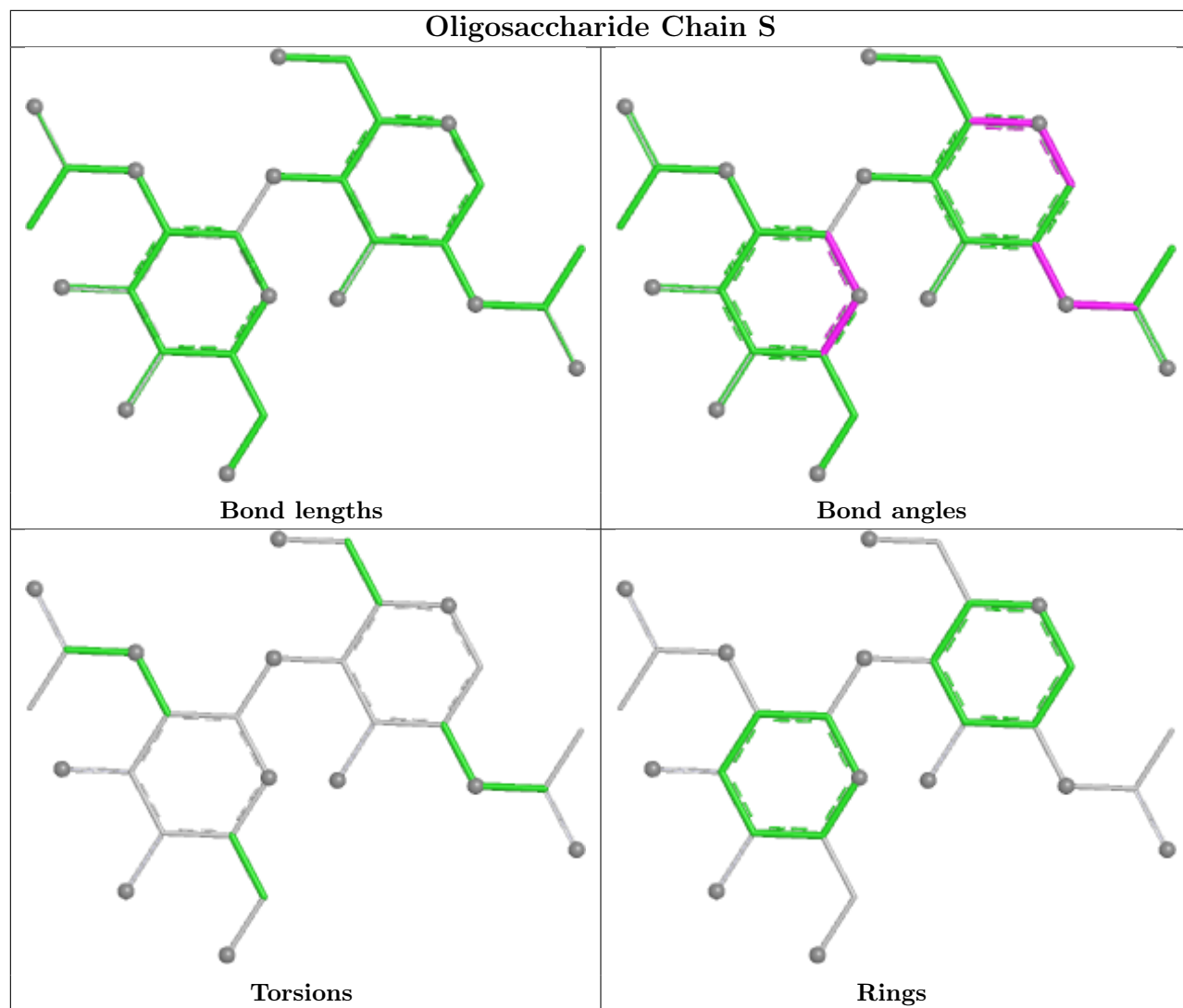


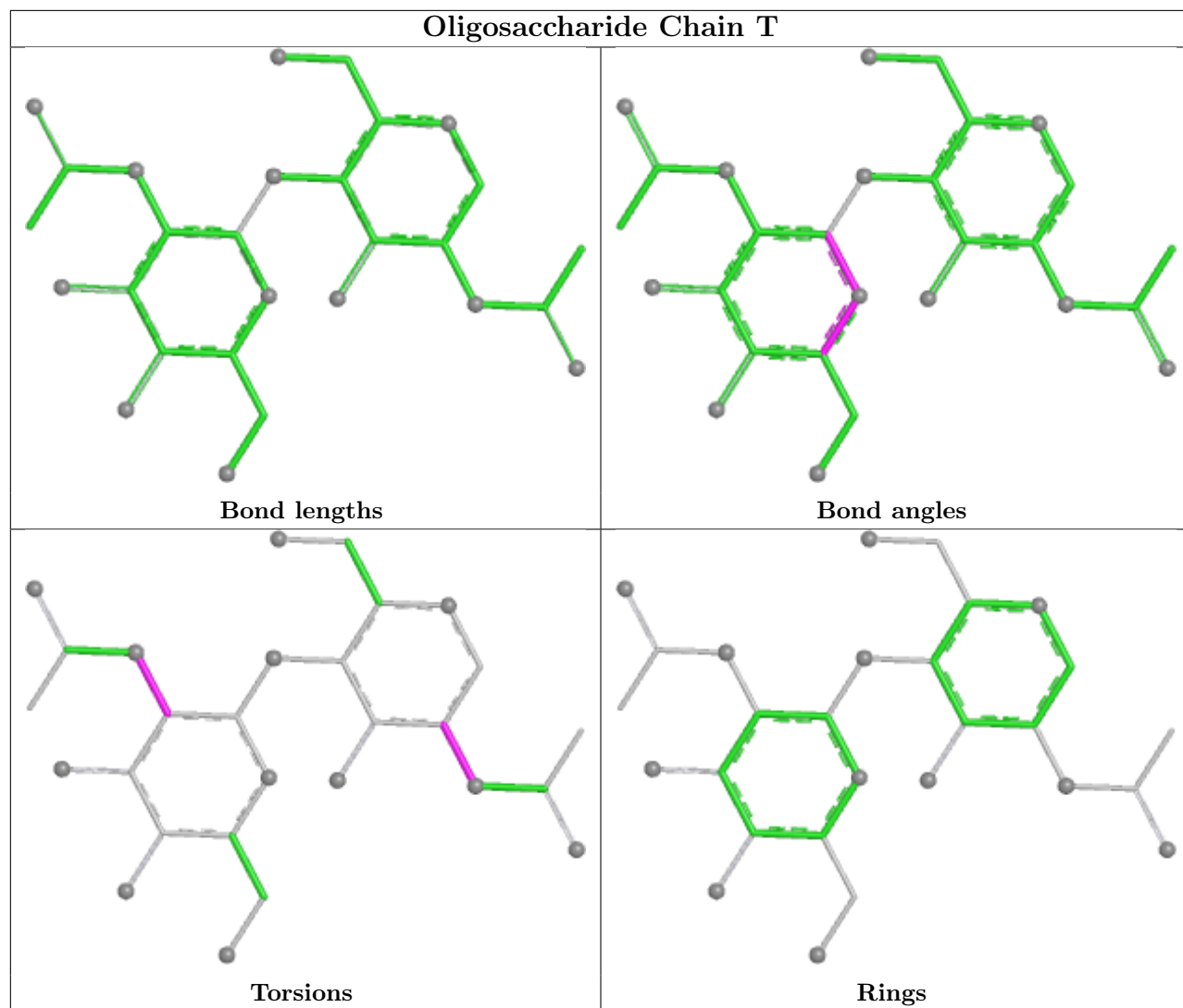


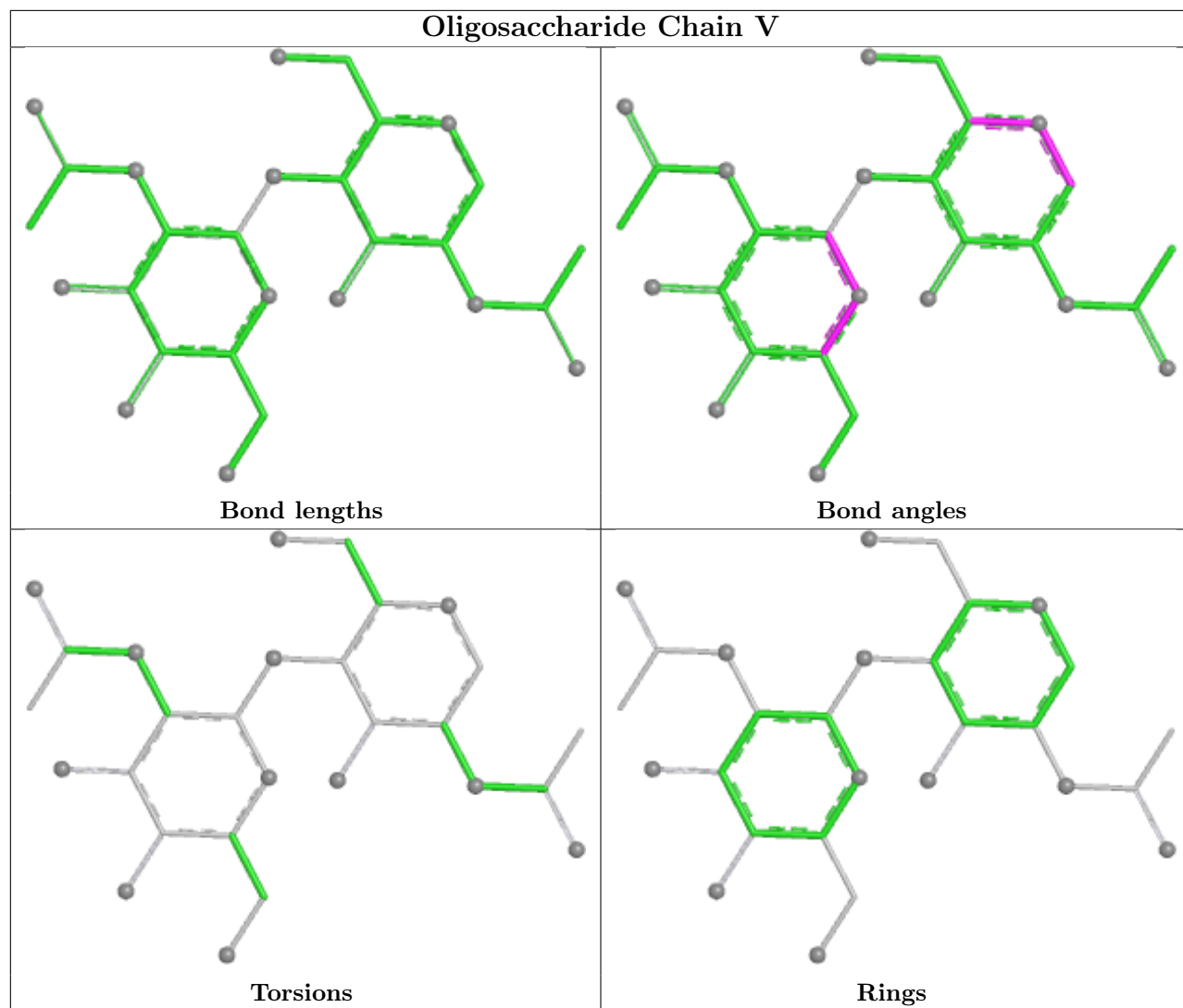


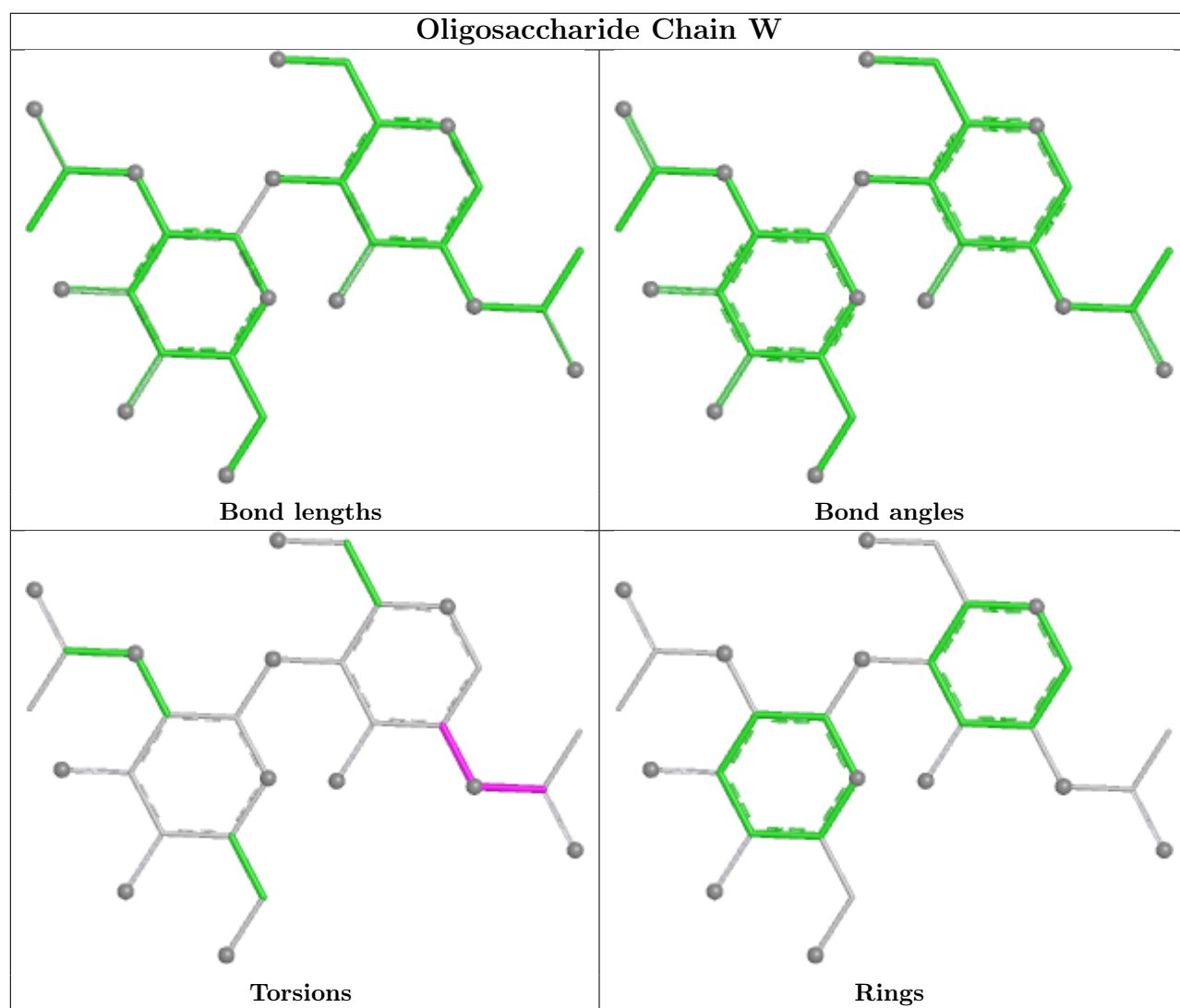


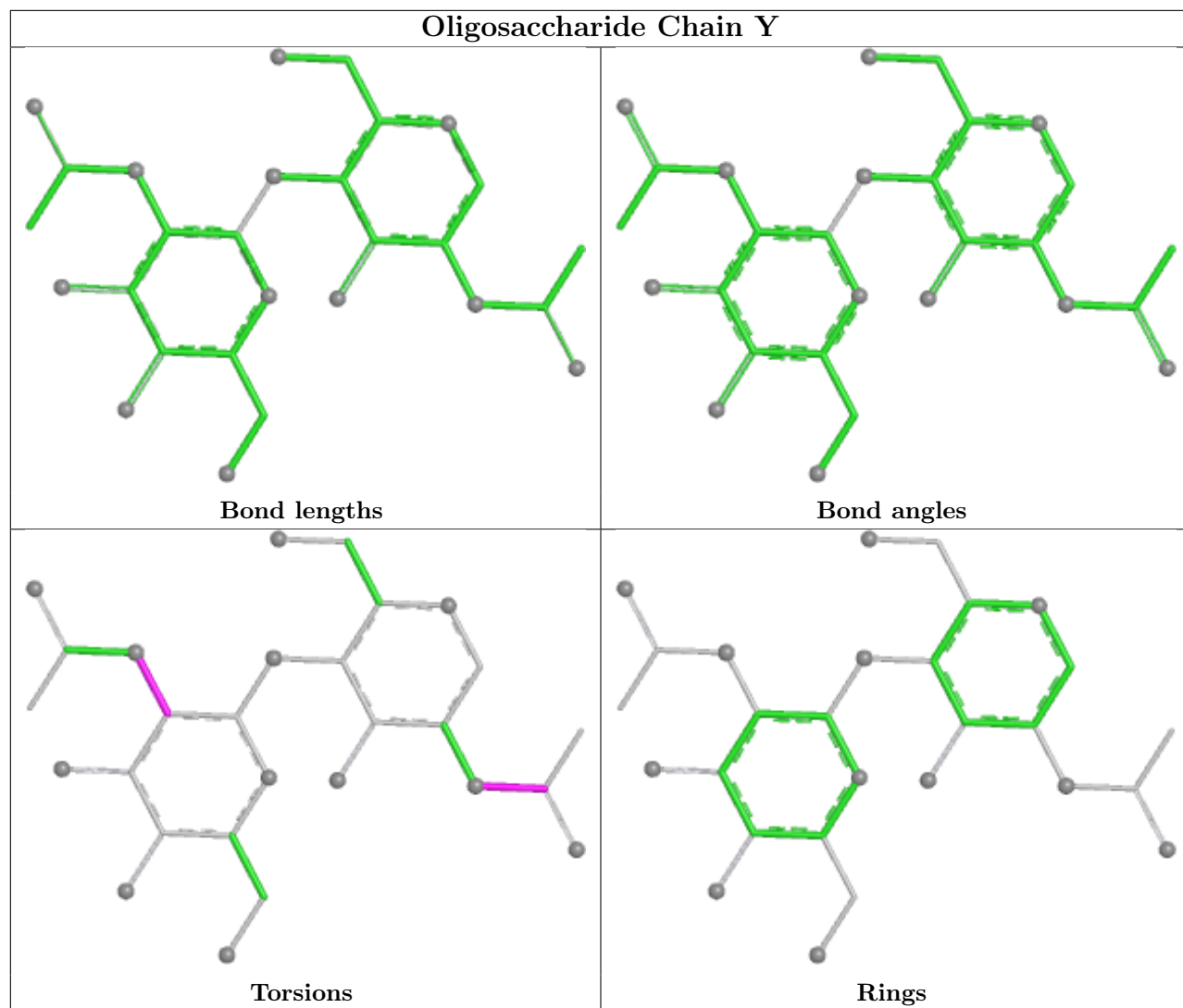


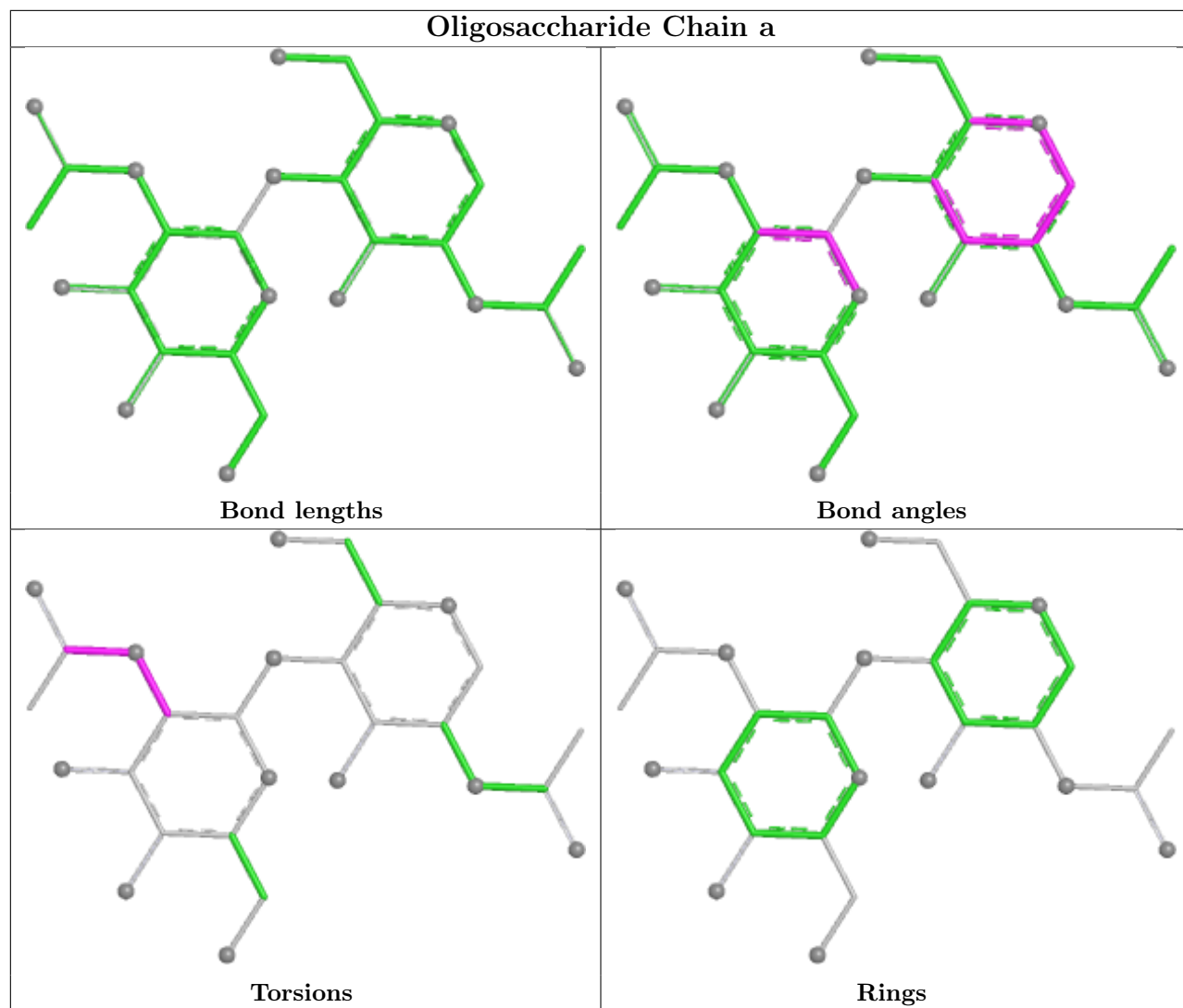


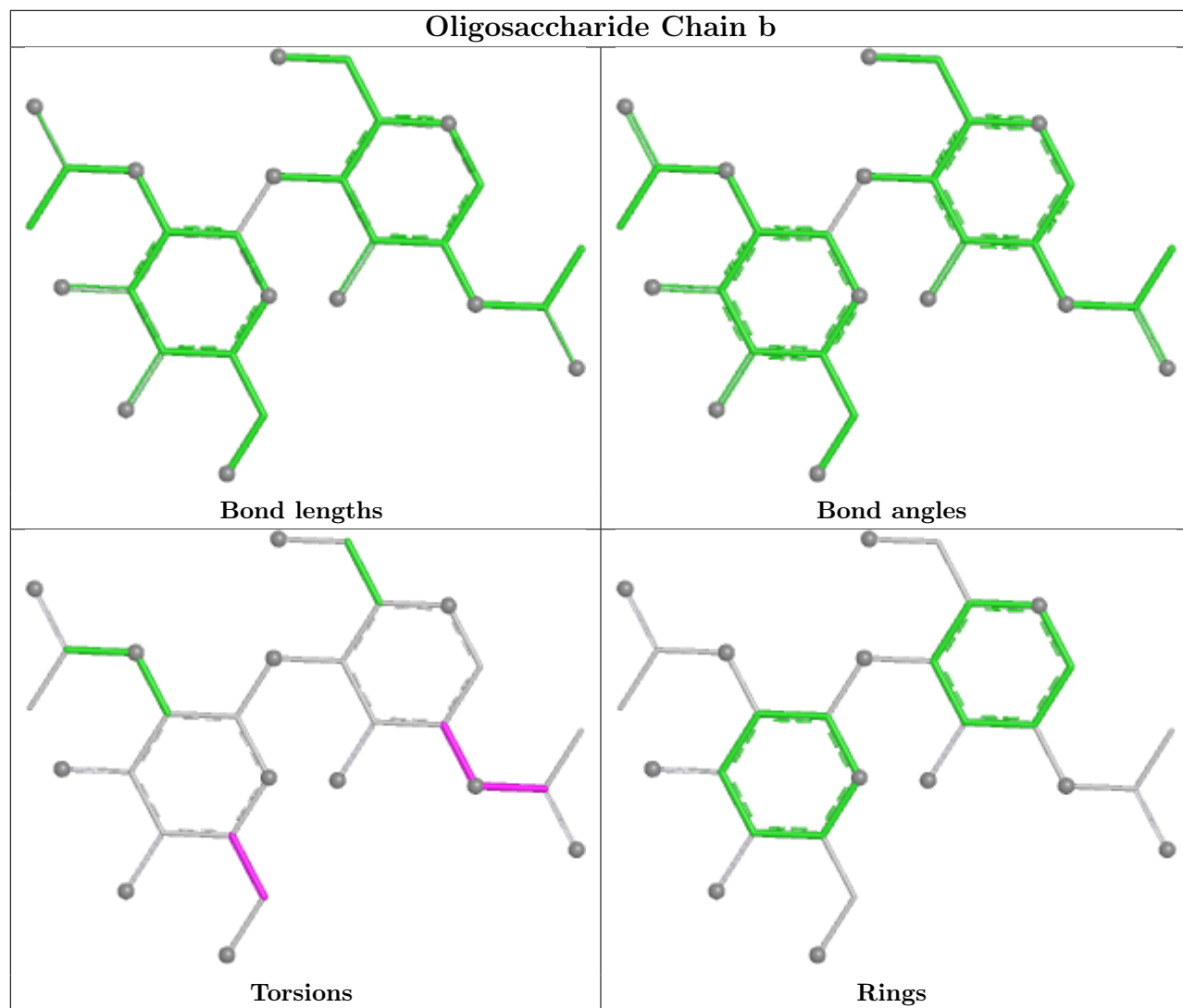




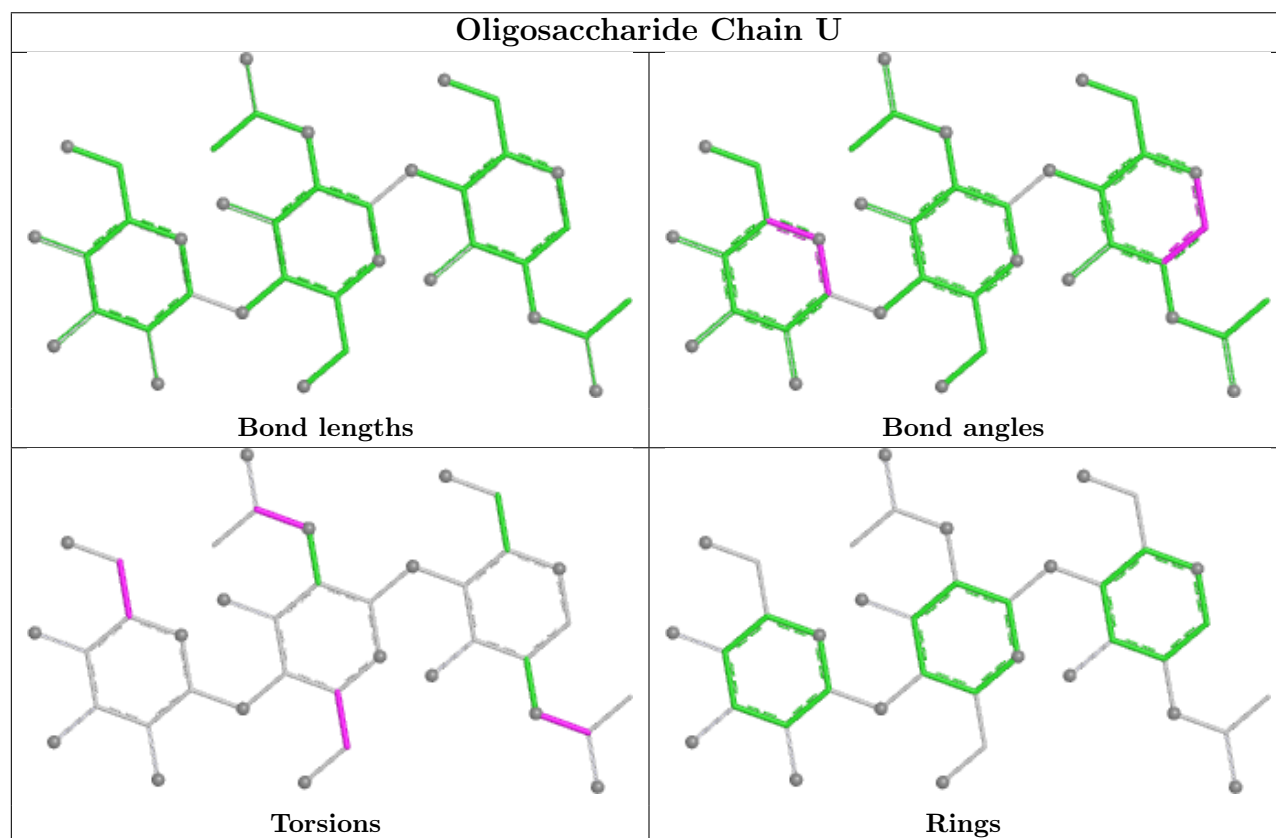
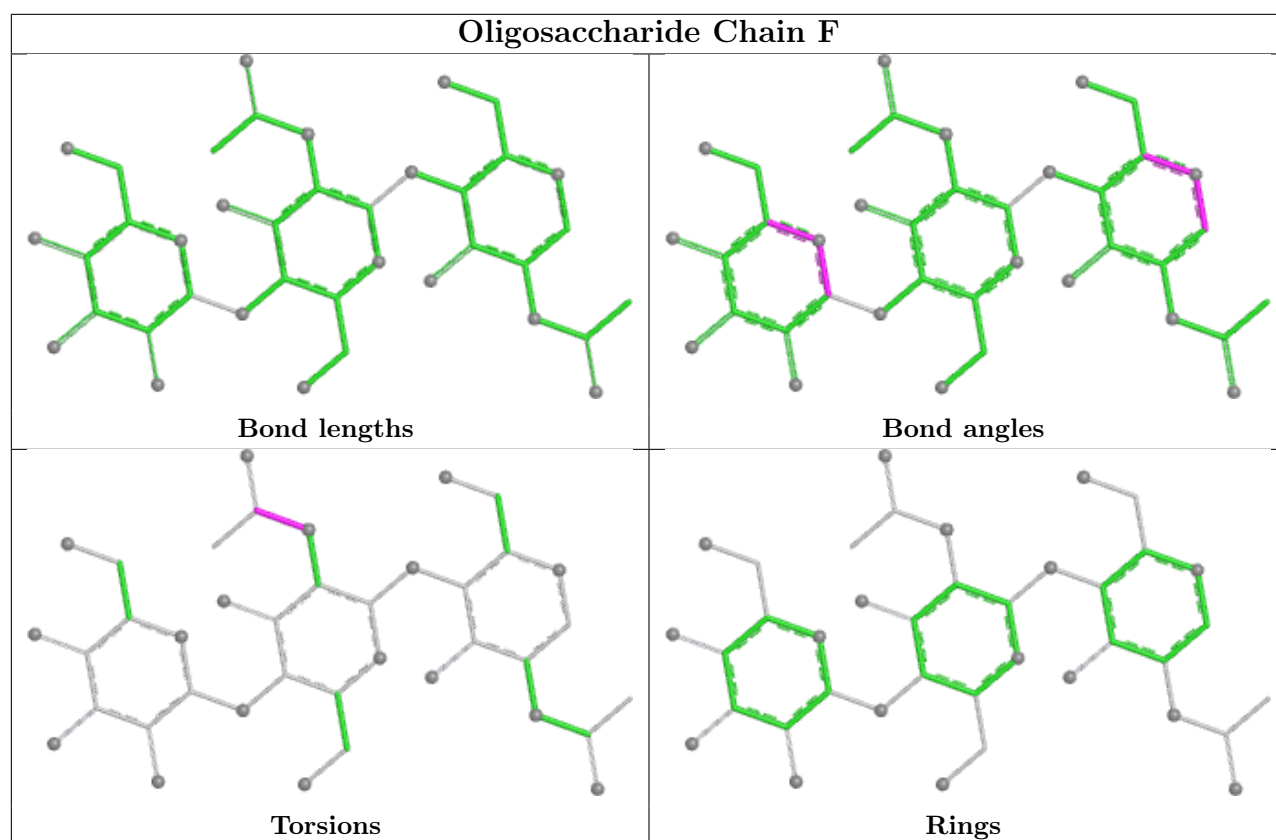


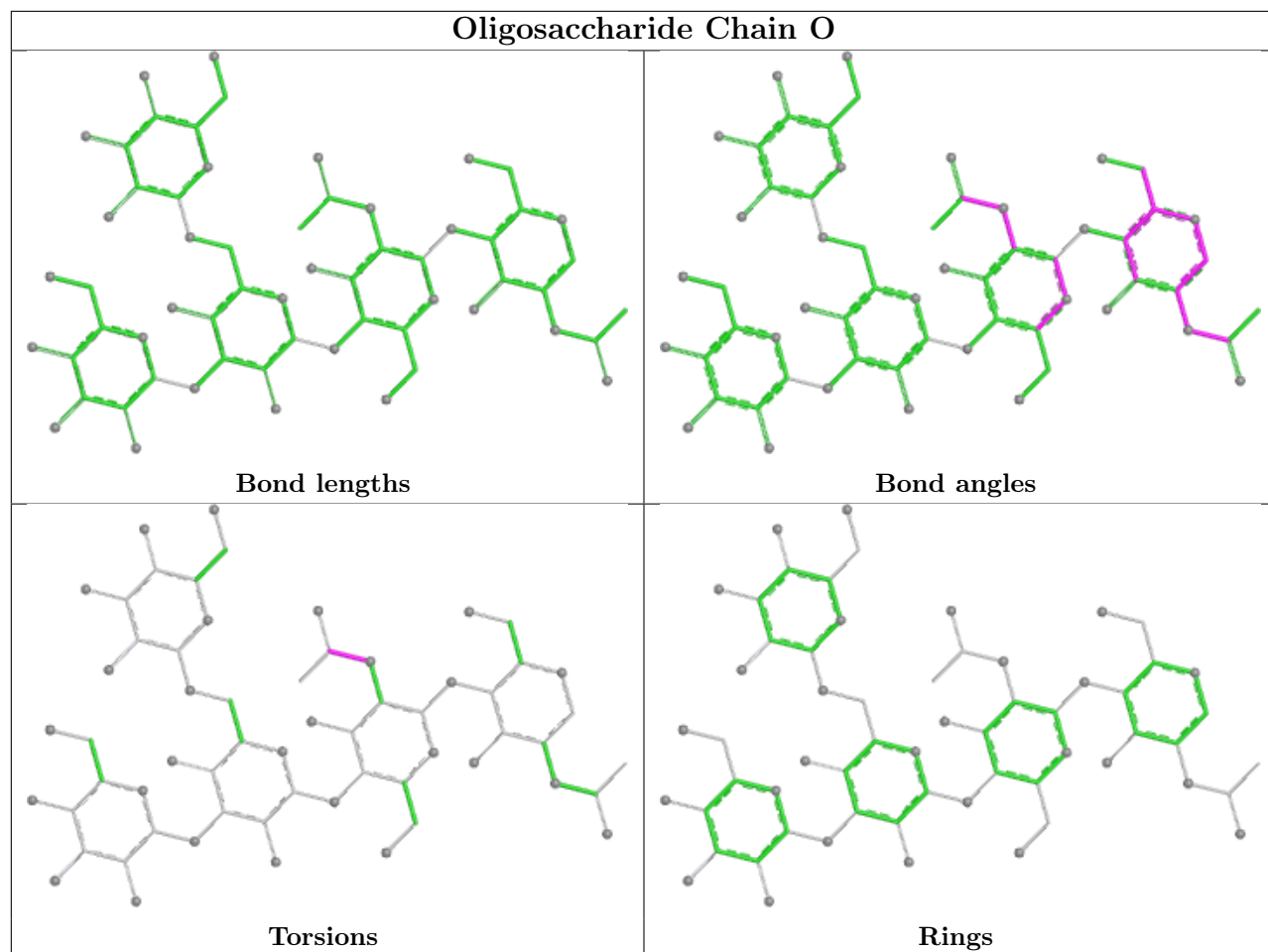


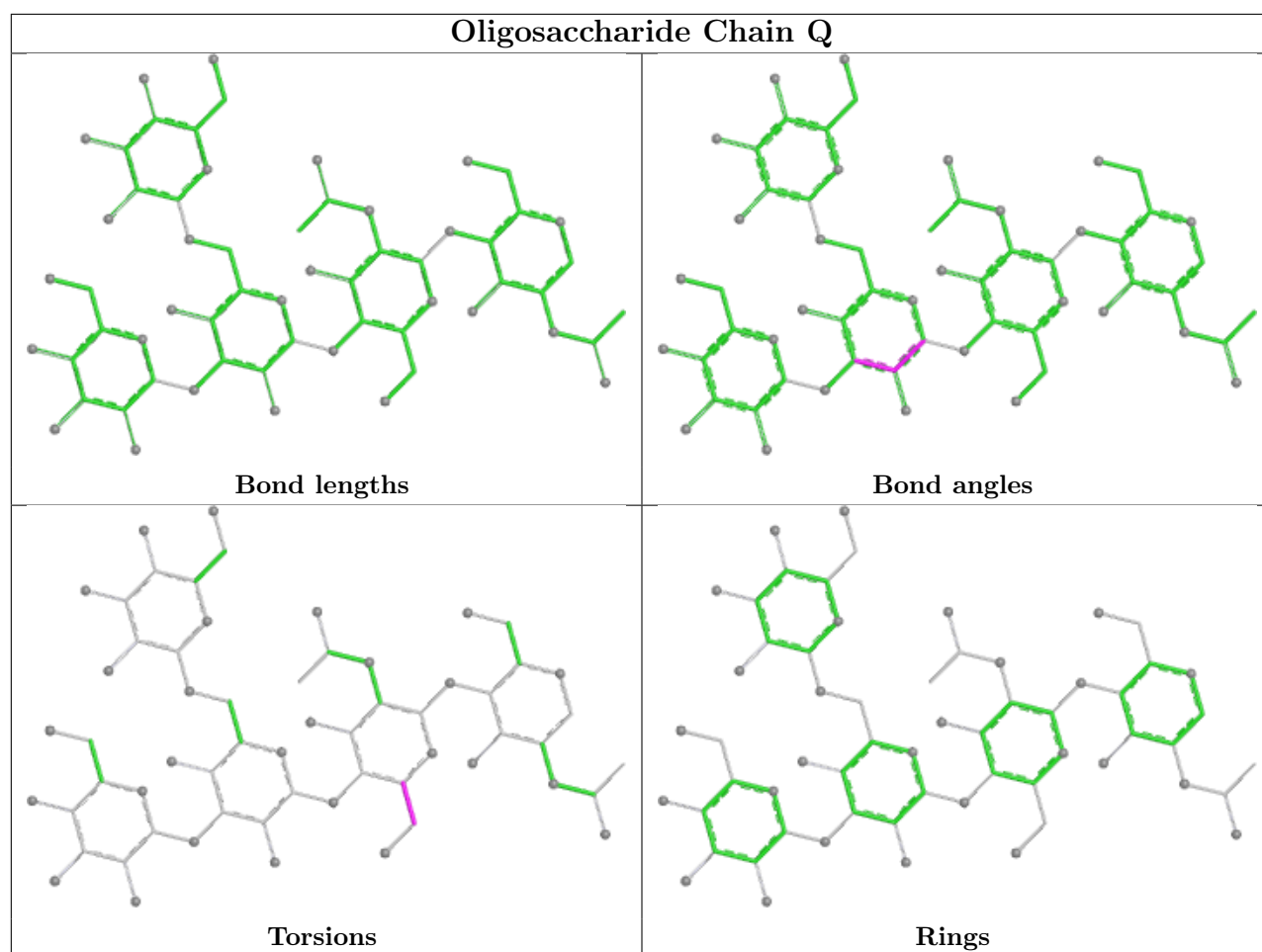


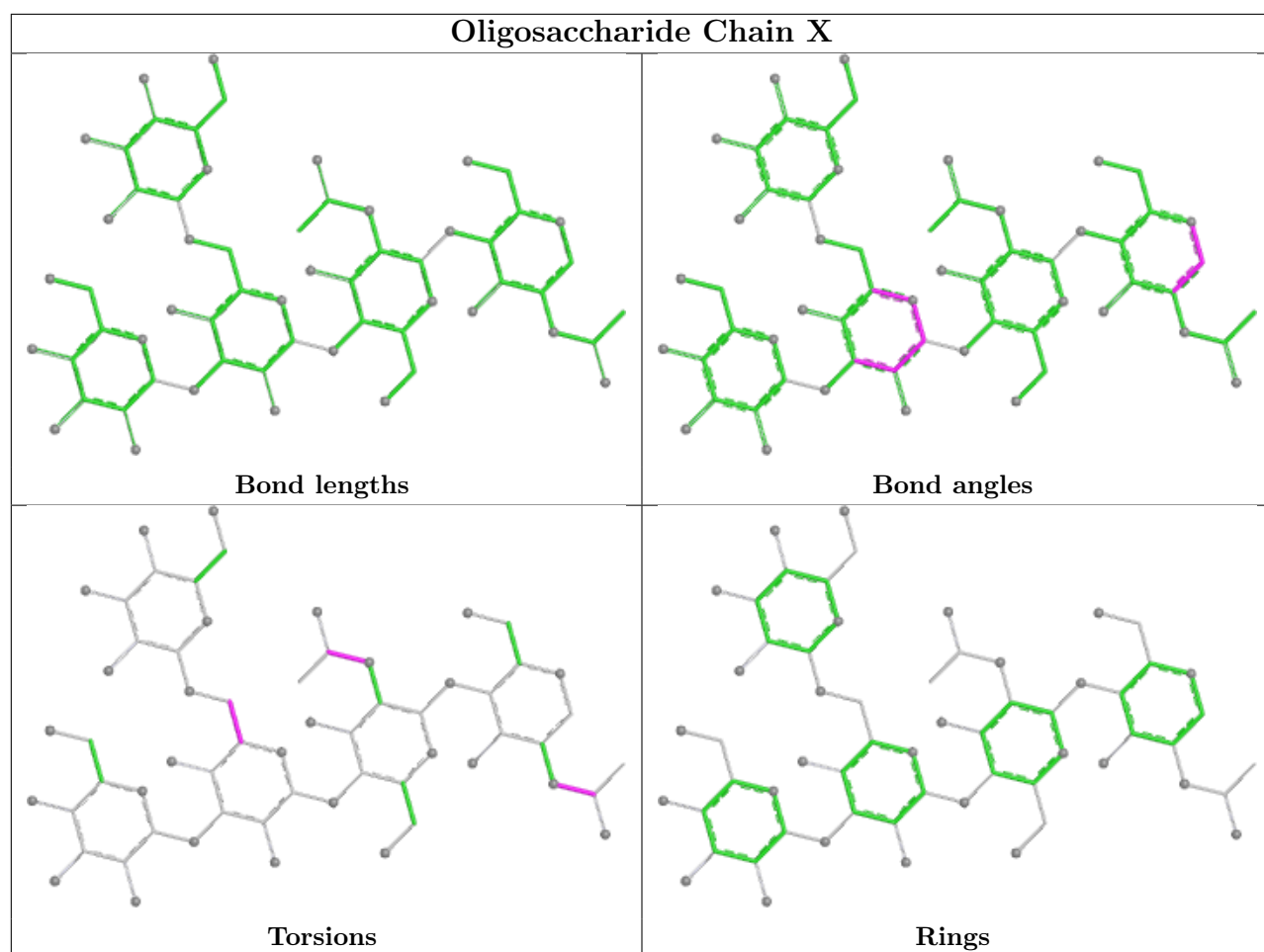


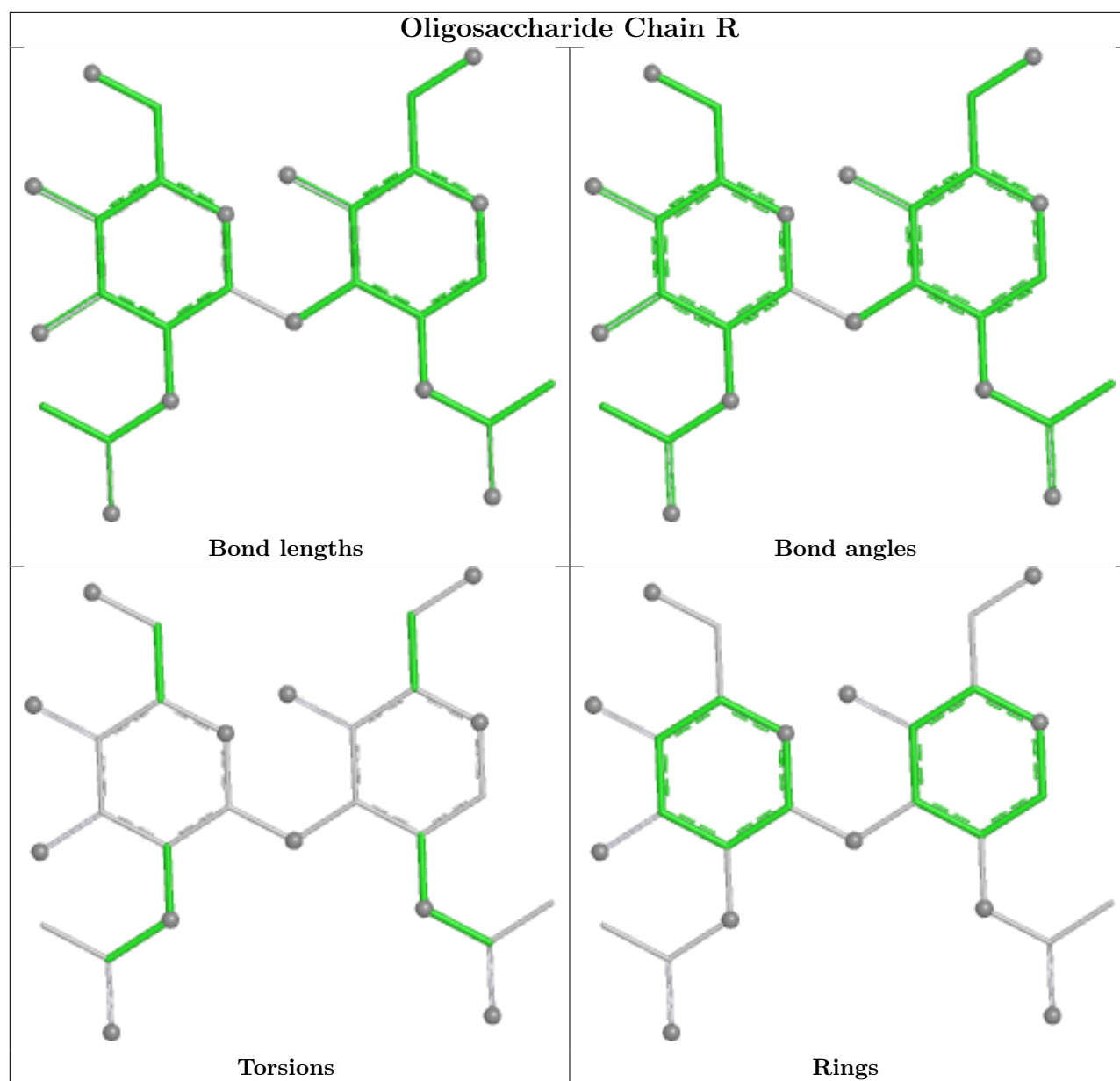


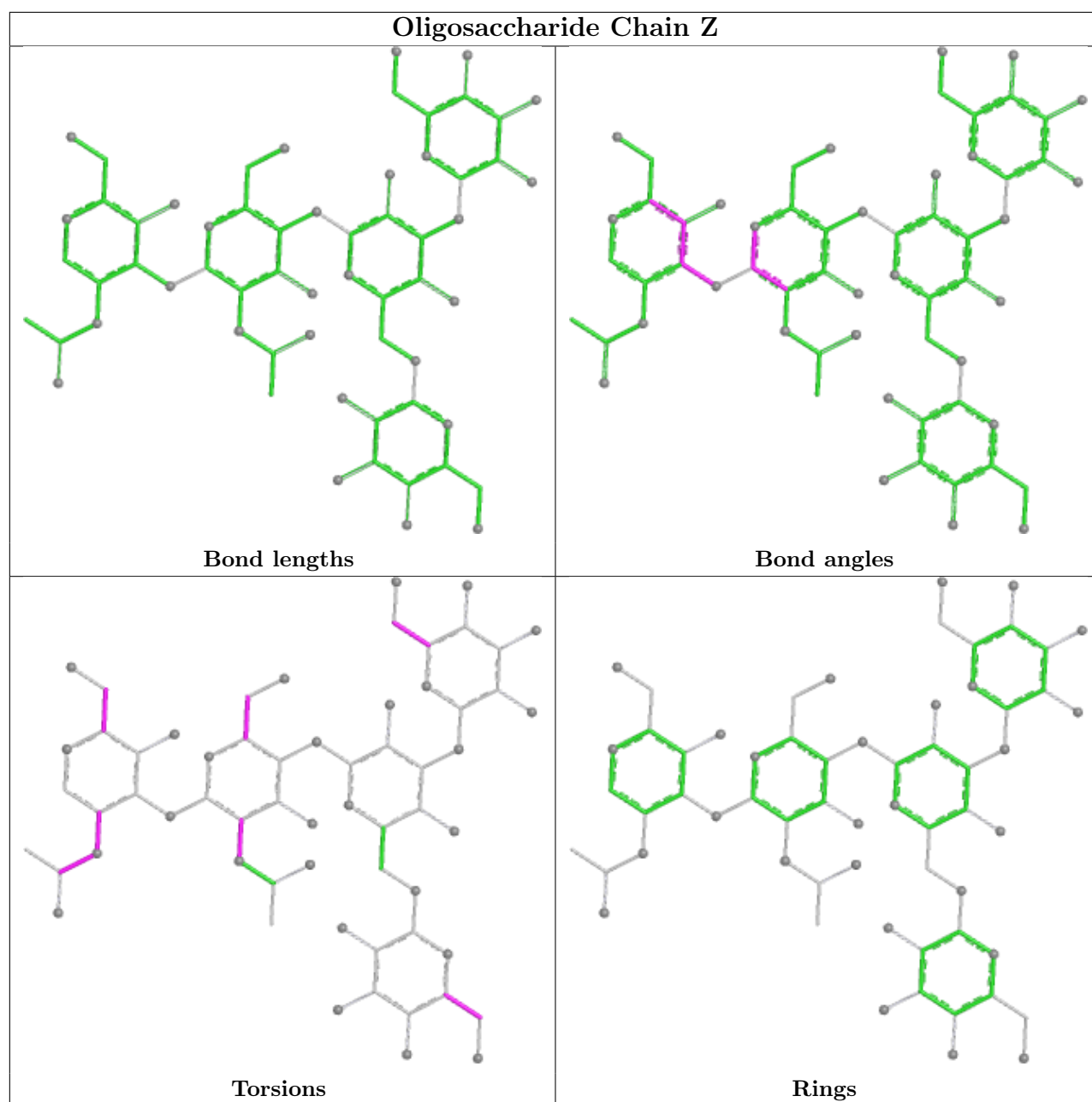












## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 for Mogul analysis.

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
11	NAG	B	4701	1	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
11	NAG	A	4703	1	14,14,15	0.30	0	17,19,21	0.71	0
11	NAG	A	4704	1	14,14,15	0.54	0	17,19,21	2.13	2 (11%)
11	NAG	B	4702	1	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
11	NAG	B	4703	1	14,14,15	0.87	1 (7%)	17,19,21	1.14	2 (11%)
11	NAG	B	4704	1	14,14,15	0.35	0	17,19,21	0.66	0
11	NAG	A	4702	1	14,14,15	0.31	0	17,19,21	0.52	0
12	A2G	B	4705	1	14,14,15	0.45	0	17,19,21	1.32	1 (5%)
12	A2G	A	4705	1	14,14,15	0.38	0	17,19,21	0.45	0
11	NAG	A	4701	1	14,14,15	0.41	0	17,19,21	1.20	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
11	NAG	B	4701	1	-	0/6/23/26	0/1/1/1
11	NAG	A	4703	1	-	3/6/23/26	0/1/1/1
11	NAG	A	4704	1	-	3/6/23/26	0/1/1/1
11	NAG	B	4702	1	-	0/6/23/26	0/1/1/1
11	NAG	B	4703	1	-	0/6/23/26	0/1/1/1
11	NAG	B	4704	1	-	3/6/23/26	0/1/1/1
11	NAG	A	4702	1	-	0/6/23/26	0/1/1/1
12	A2G	B	4705	1	-	0/6/23/26	0/1/1/1
12	A2G	A	4705	1	-	2/6/23/26	0/1/1/1
11	NAG	A	4701	1	-	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)
11	B	4703	NAG	C1-C2	2.70	1.56	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	4704	NAG	C1-O5-C5	7.34	122.02	112.19
12	B	4705	A2G	O5-C1-C2	4.70	118.57	111.29
11	A	4701	NAG	C1-O5-C5	3.84	117.33	112.19
11	A	4704	NAG	O5-C1-C2	3.83	117.21	111.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	4703	NAG	O5-C5-C4	-2.38	105.04	110.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	4703	NAG	C1-C2-N2-C7
11	A	4704	NAG	C3-C2-N2-C7
11	A	4704	NAG	C8-C7-N2-C2
11	A	4704	NAG	O7-C7-N2-C2
11	B	4704	NAG	C1-C2-N2-C7

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.



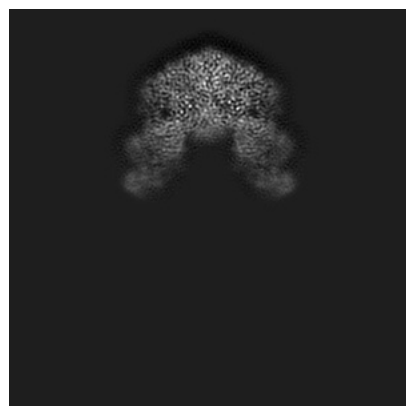
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36698. These allow visual inspection of the internal detail of the map and identification of artifacts.

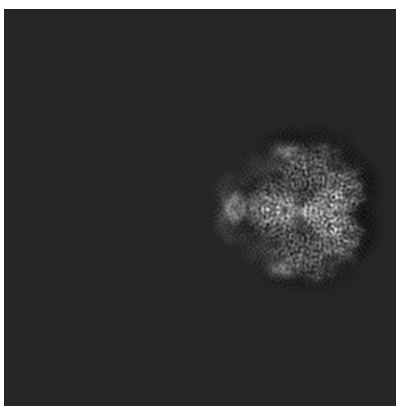
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

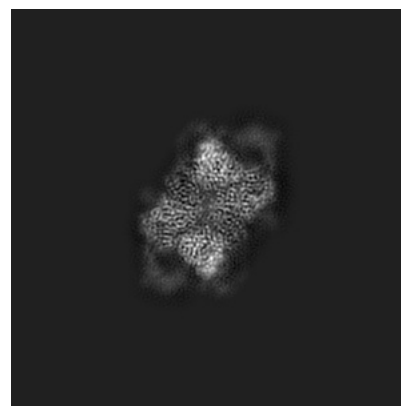
#### 6.1.1 Primary map



X

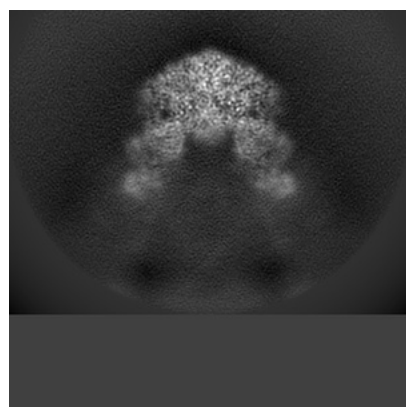


Y

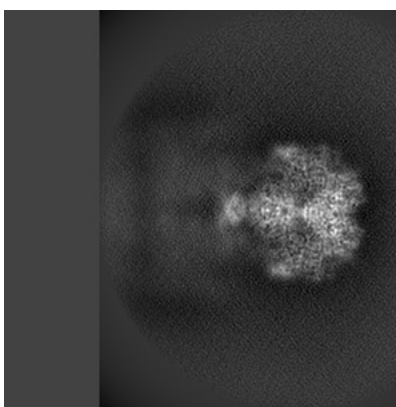


Z

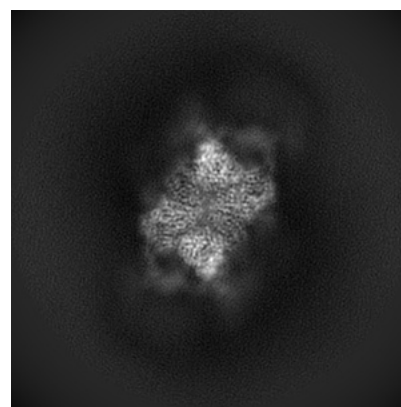
#### 6.1.2 Raw map



X



Y

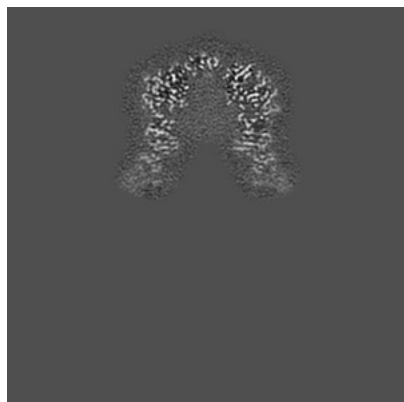


Z

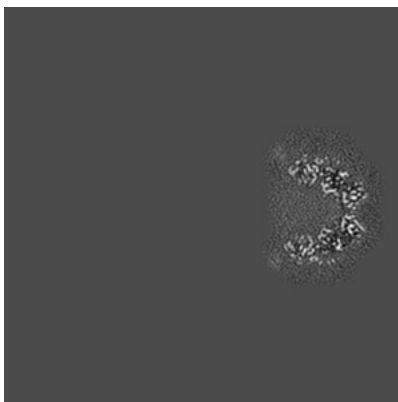
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

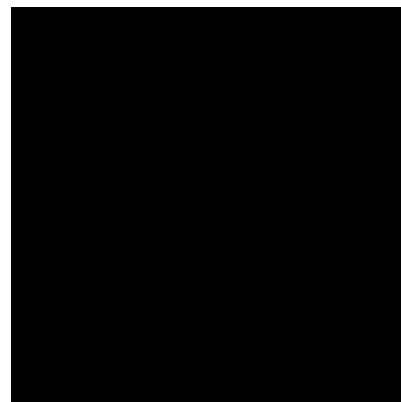
### 6.2.1 Primary map



X Index: 130

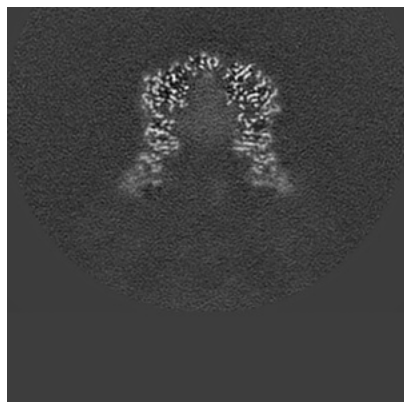


Y Index: 130

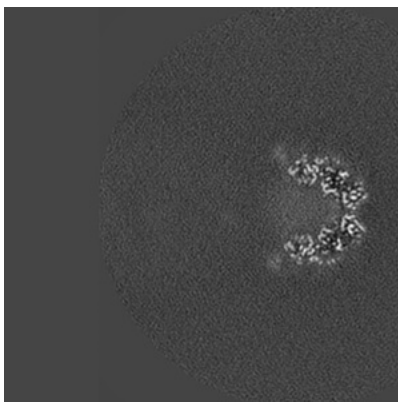


Z Index: 130

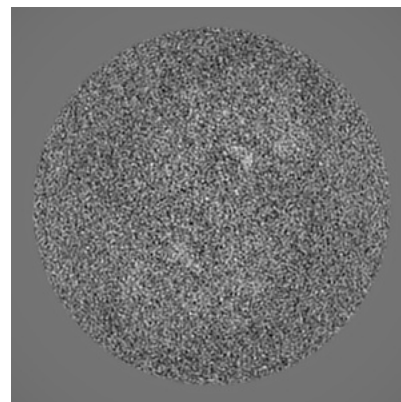
### 6.2.2 Raw map



X Index: 130



Y Index: 130

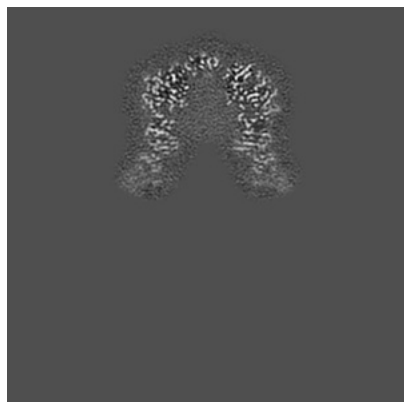


Z Index: 130

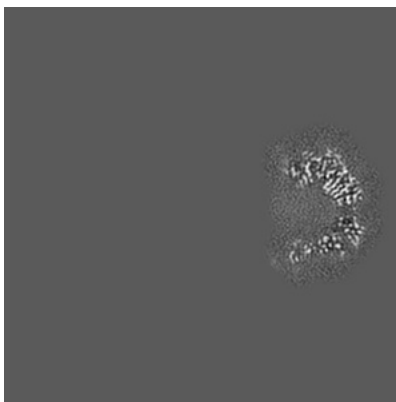
The images above show central slices of the map in three orthogonal directions.

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

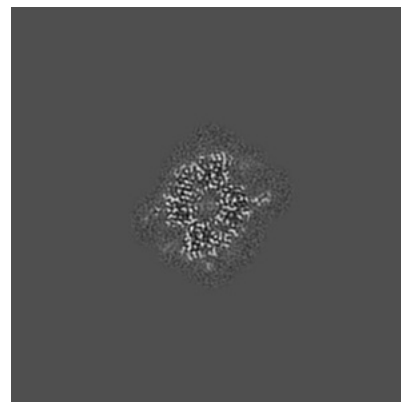
### 6.3.1 Primary map



X Index: 130

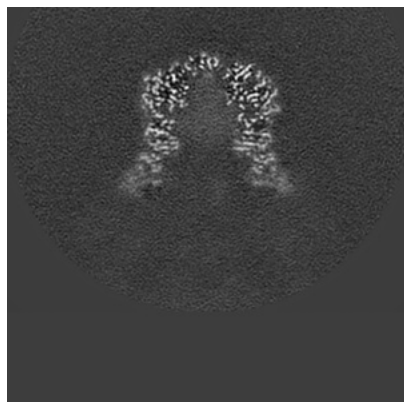


Y Index: 133

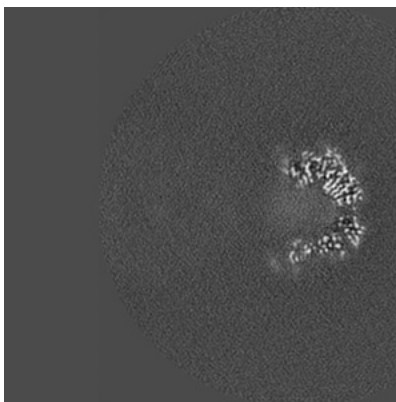


Z Index: 215

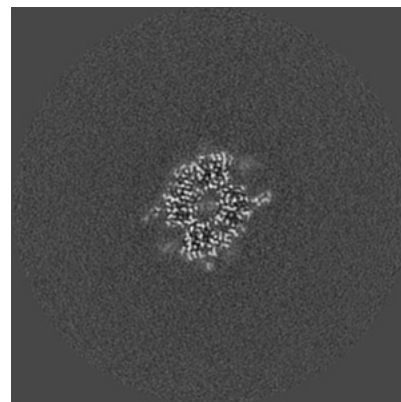
### 6.3.2 Raw map



X Index: 130



Y Index: 133

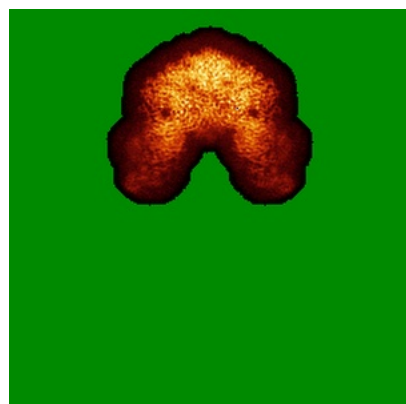


Z Index: 215

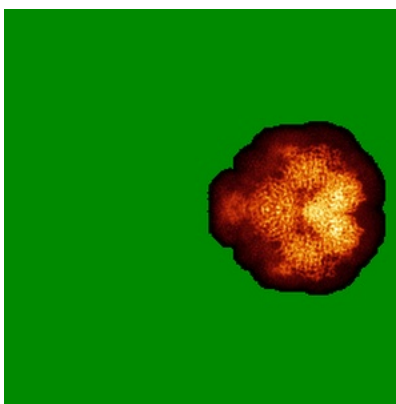
The images above show the largest variance slices of the map in three orthogonal directions.

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

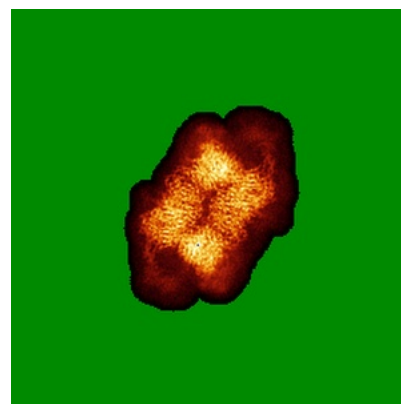
### 6.4.1 Primary map



X

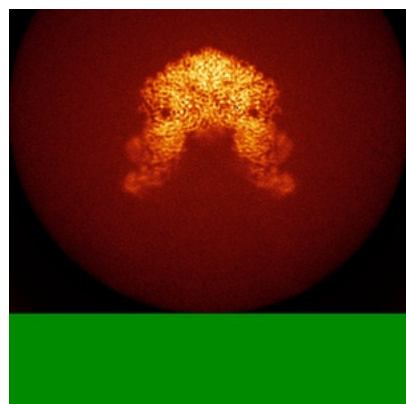


Y

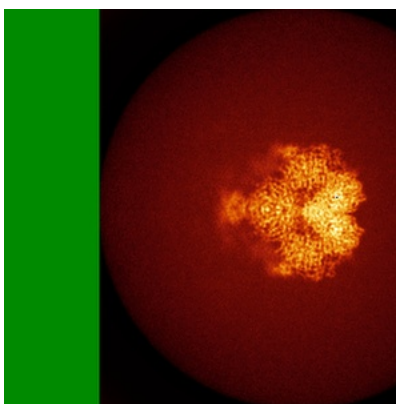


Z

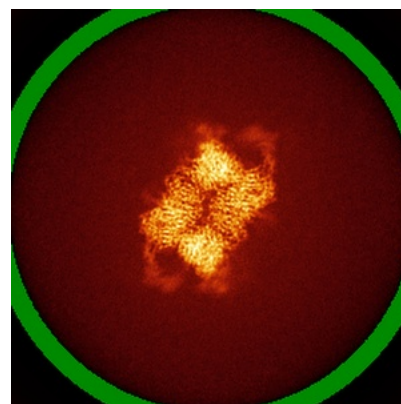
### 6.4.2 Raw map



X



Y

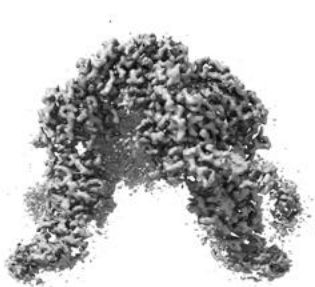


Z

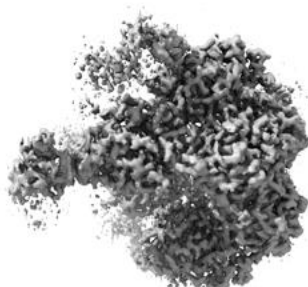
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



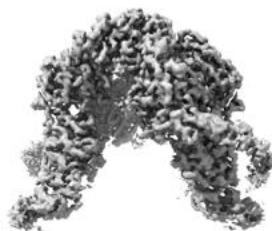
Y



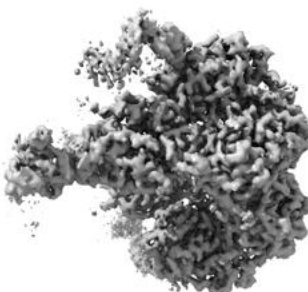
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0285. 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



X



Y



Z

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.

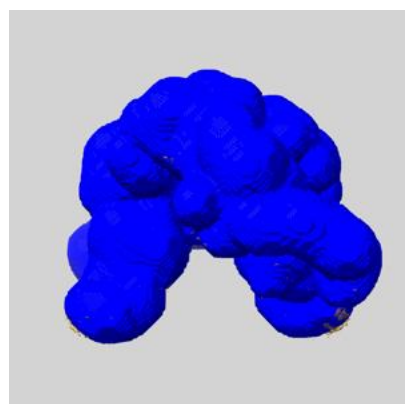
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

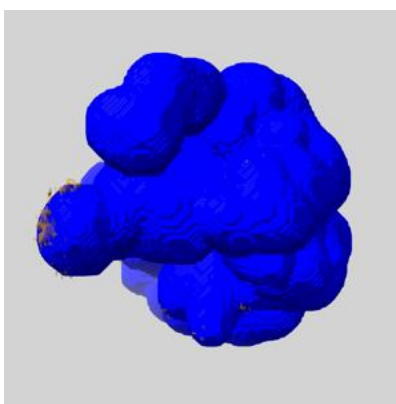
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

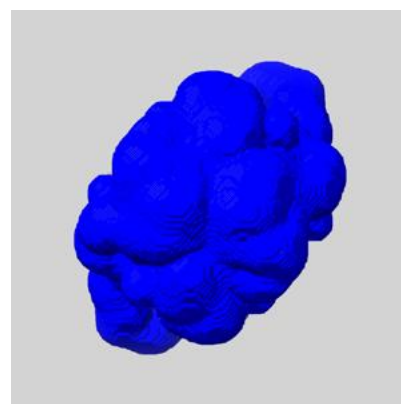
### 6.6.1 emd\_36698\_msk\_1.map [i](#)



X



Y

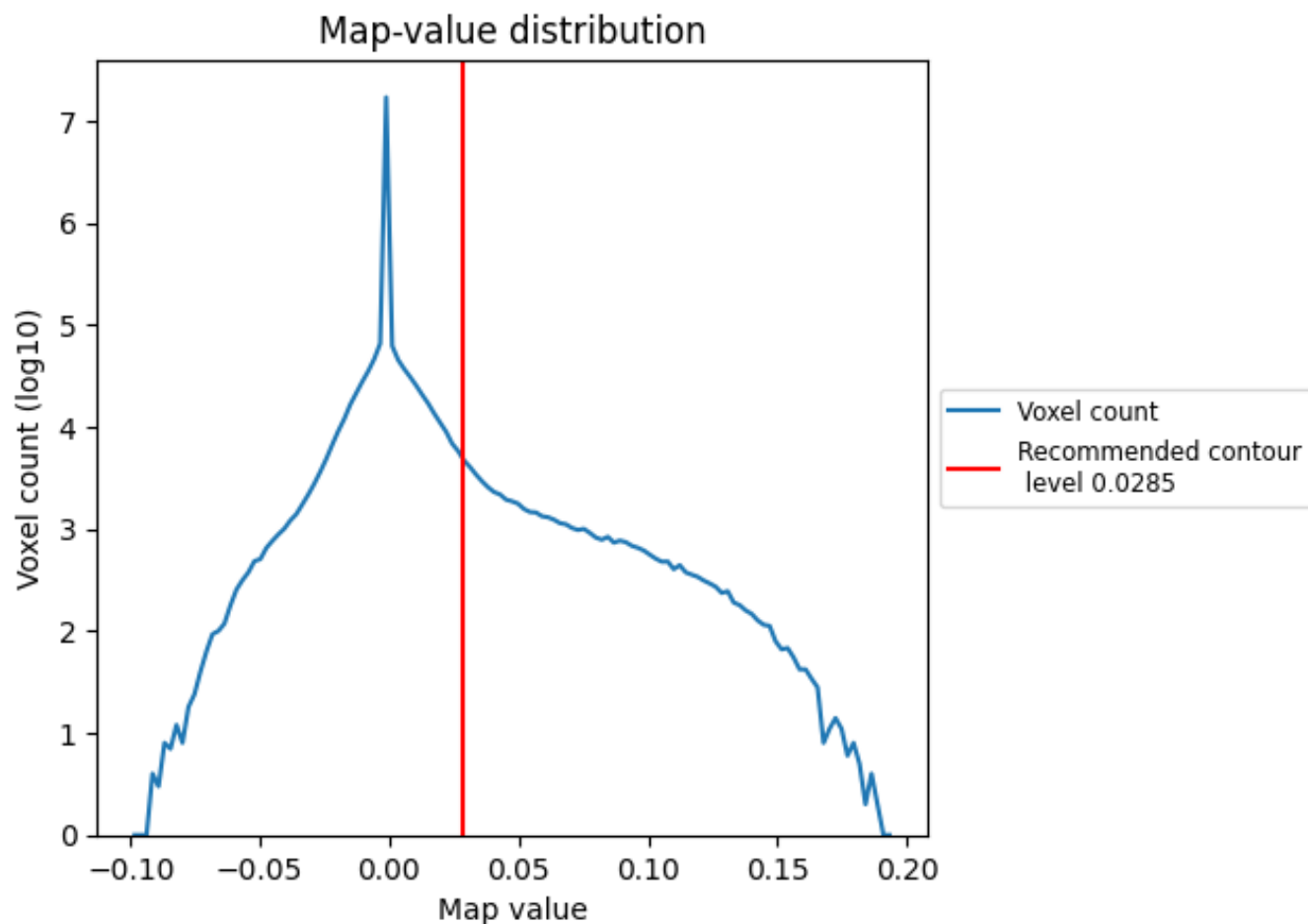


Z

## 7 Map analysis [i](#)

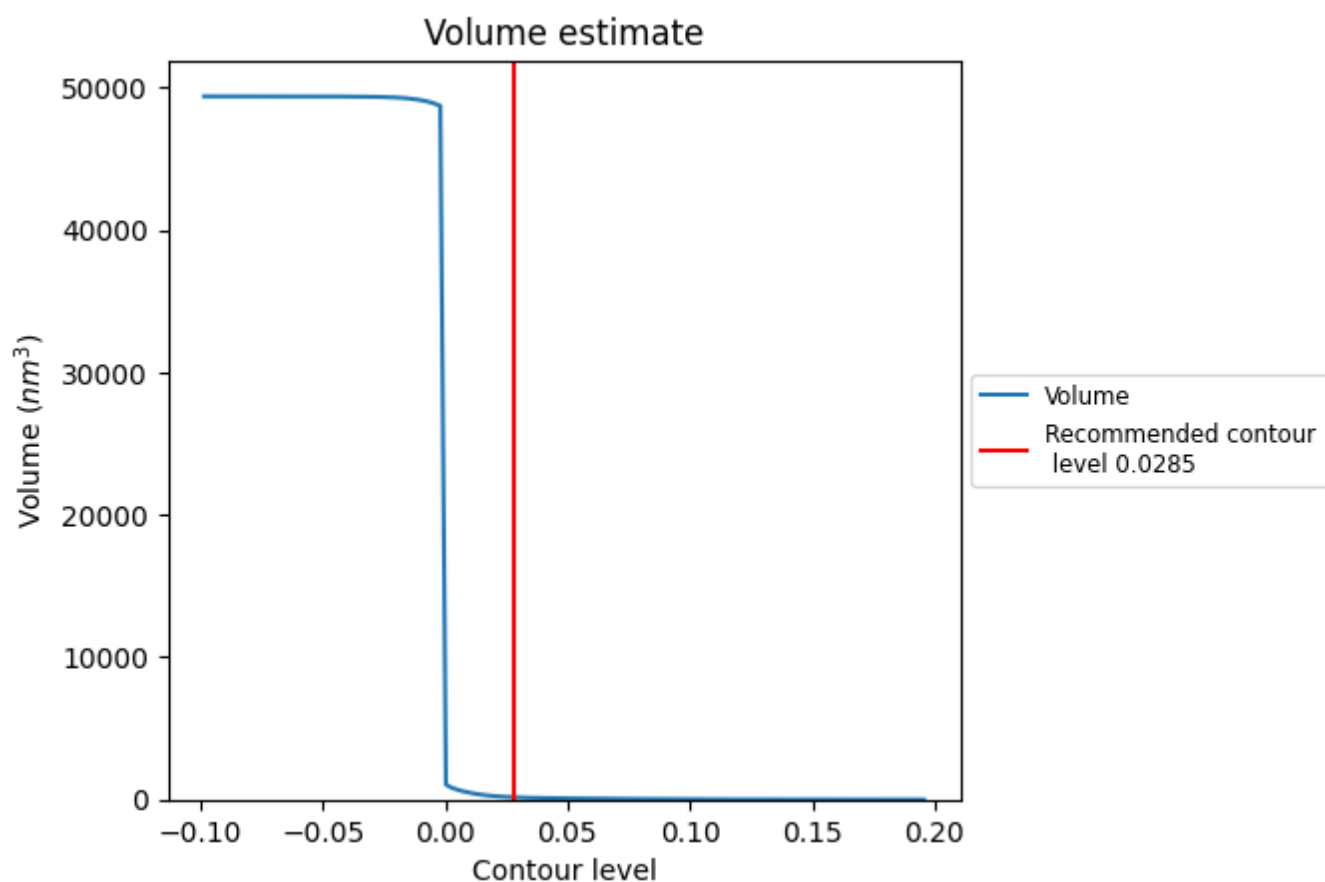
This section contains the results of statistical analysis of the map.

### 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](#)

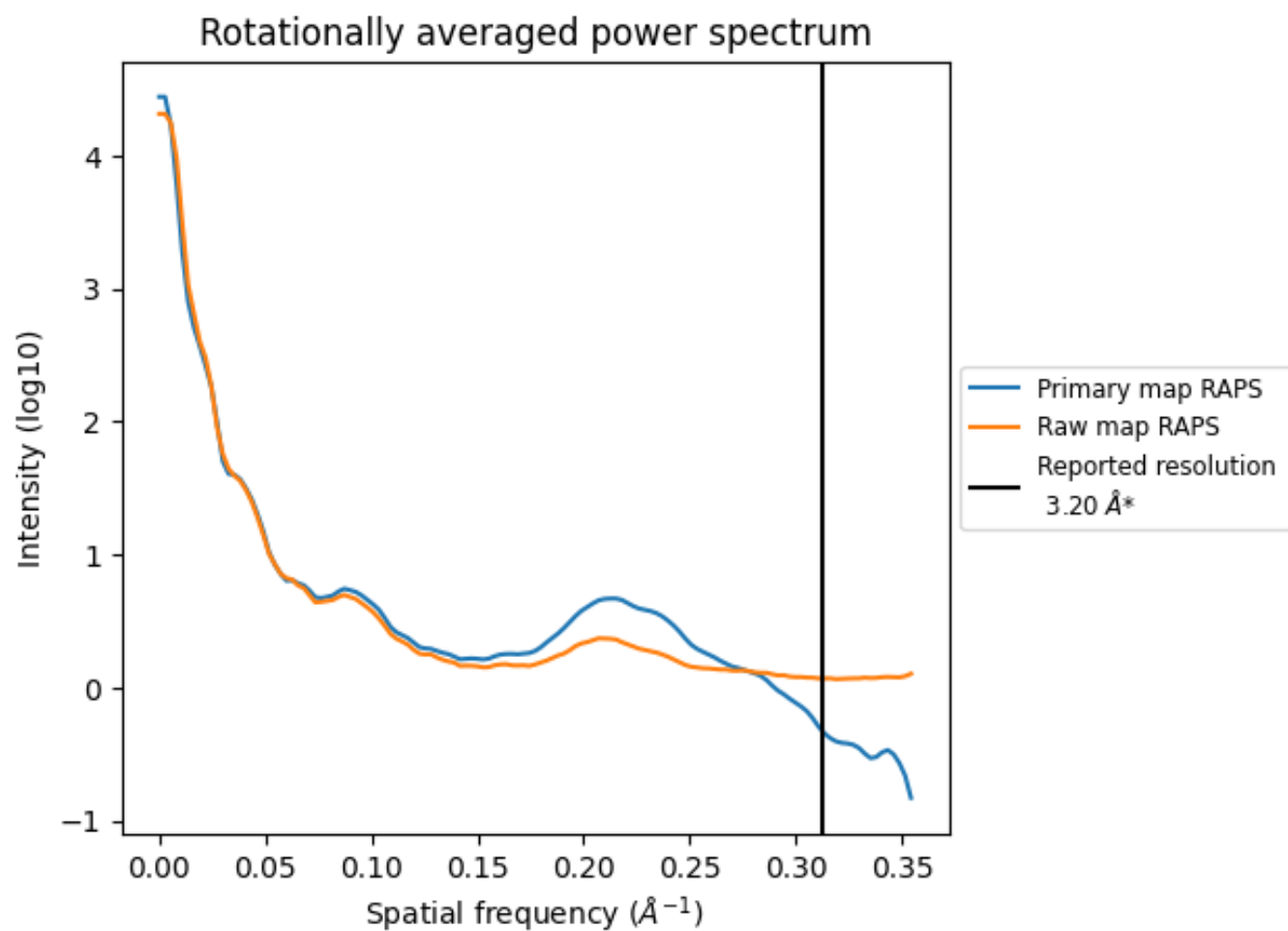


The volume at the recommended contour level is 159 nm<sup>3</sup>; this corresponds to an approximate mass of 144 kDa.

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 ⓘ

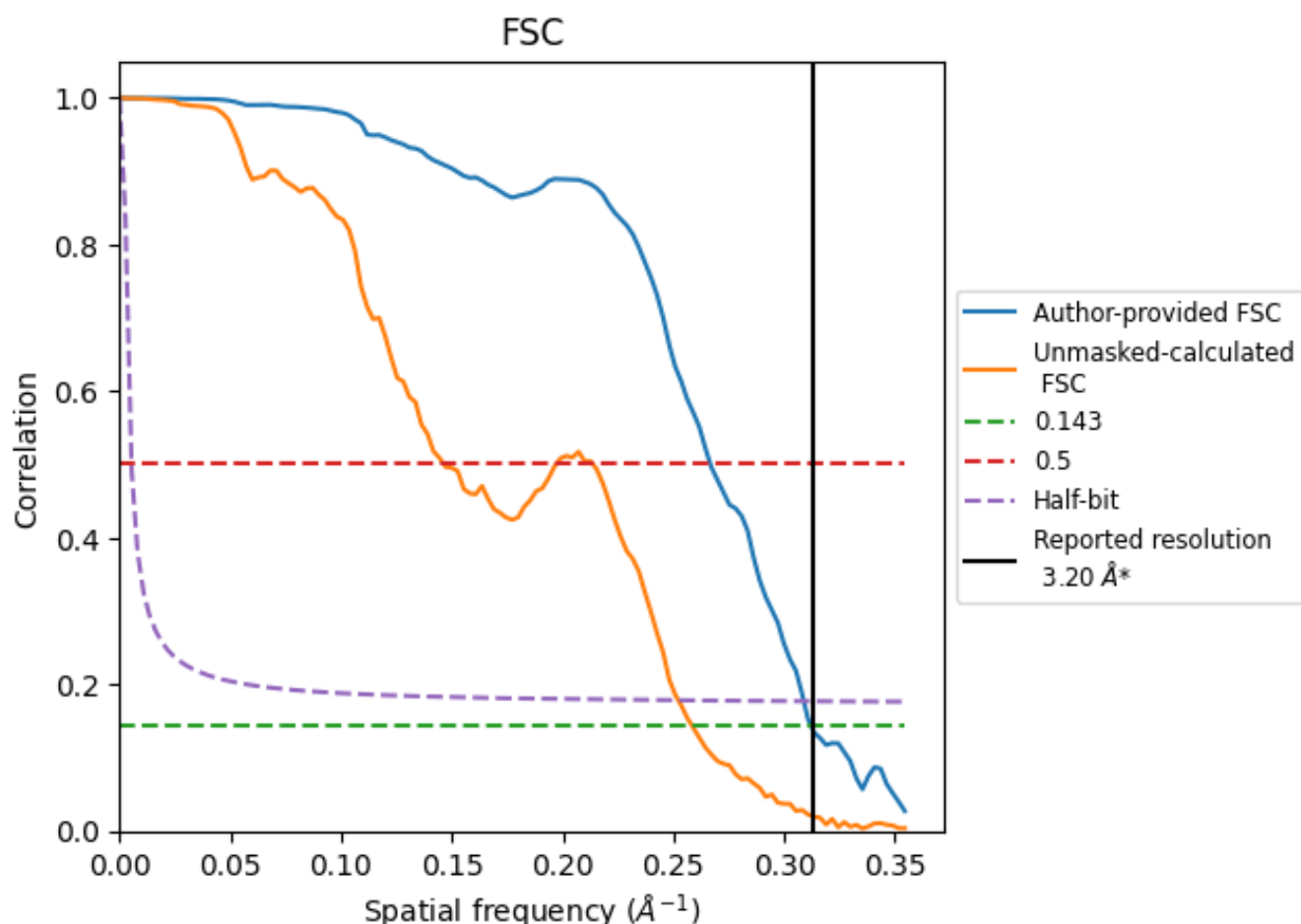


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

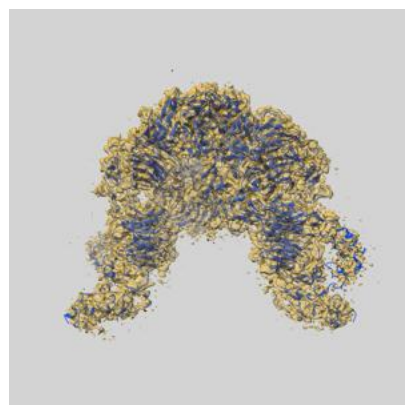
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.75	3.24
Unmasked-calculated*	3.87	6.83	3.97

\*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 3.87 differs from the reported value 3.2 by more than 10 %

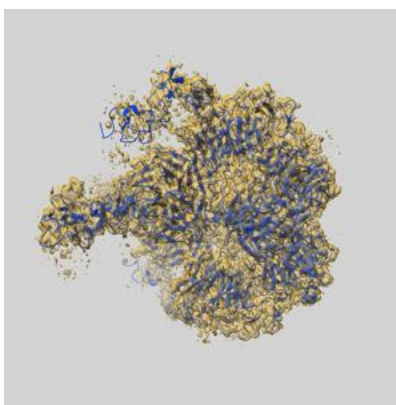
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36698 and PDB model 8JXE. Per-residue inclusion information can be found in section [3](#) on page [9](#).

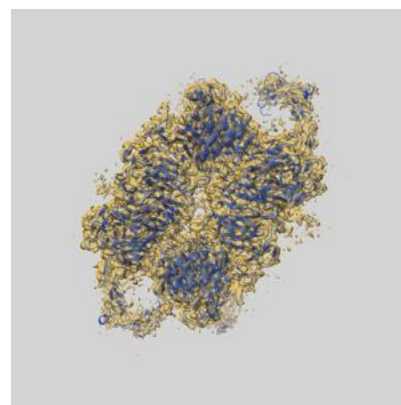
### 9.1 Map-model overlay [i](#)



X



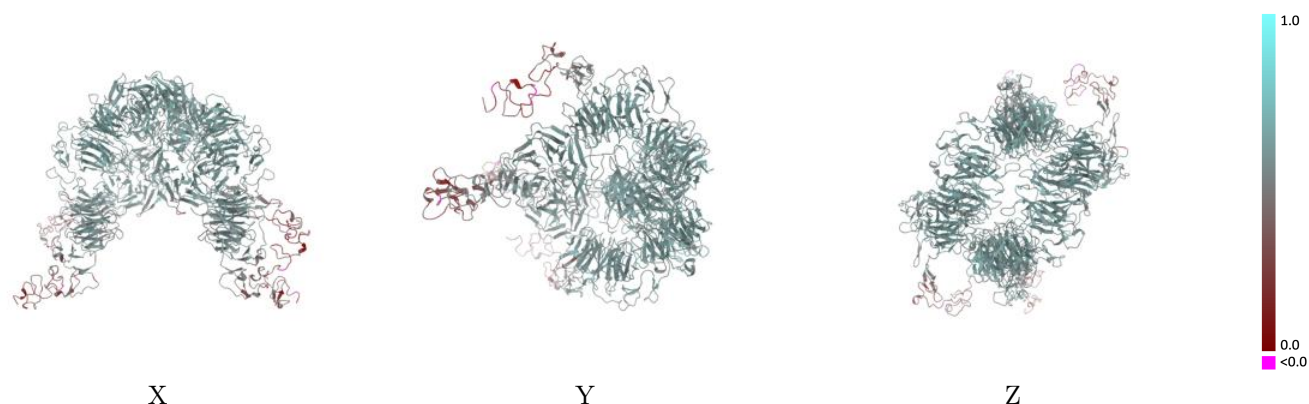
Y



Z

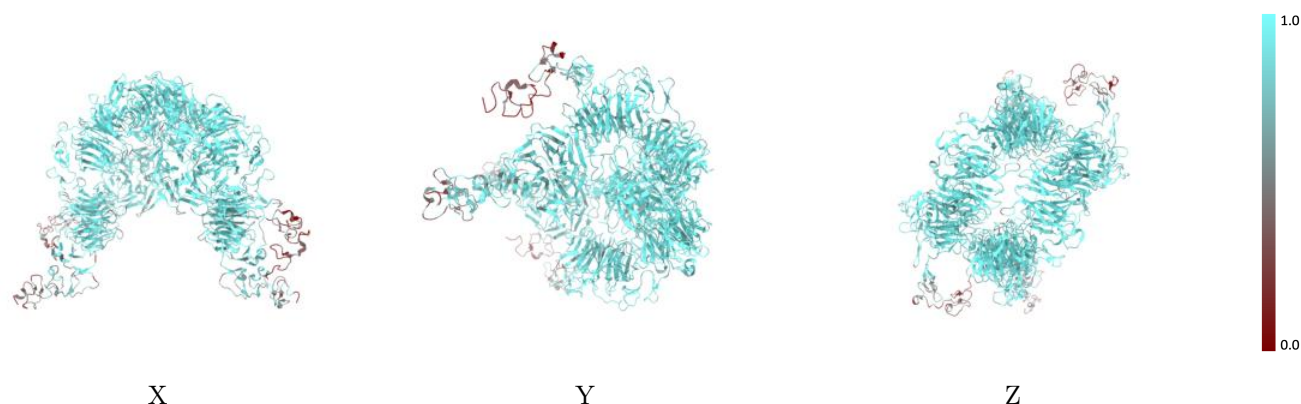
The images above show the 3D surface view of the map at the recommended contour level 0.0285 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



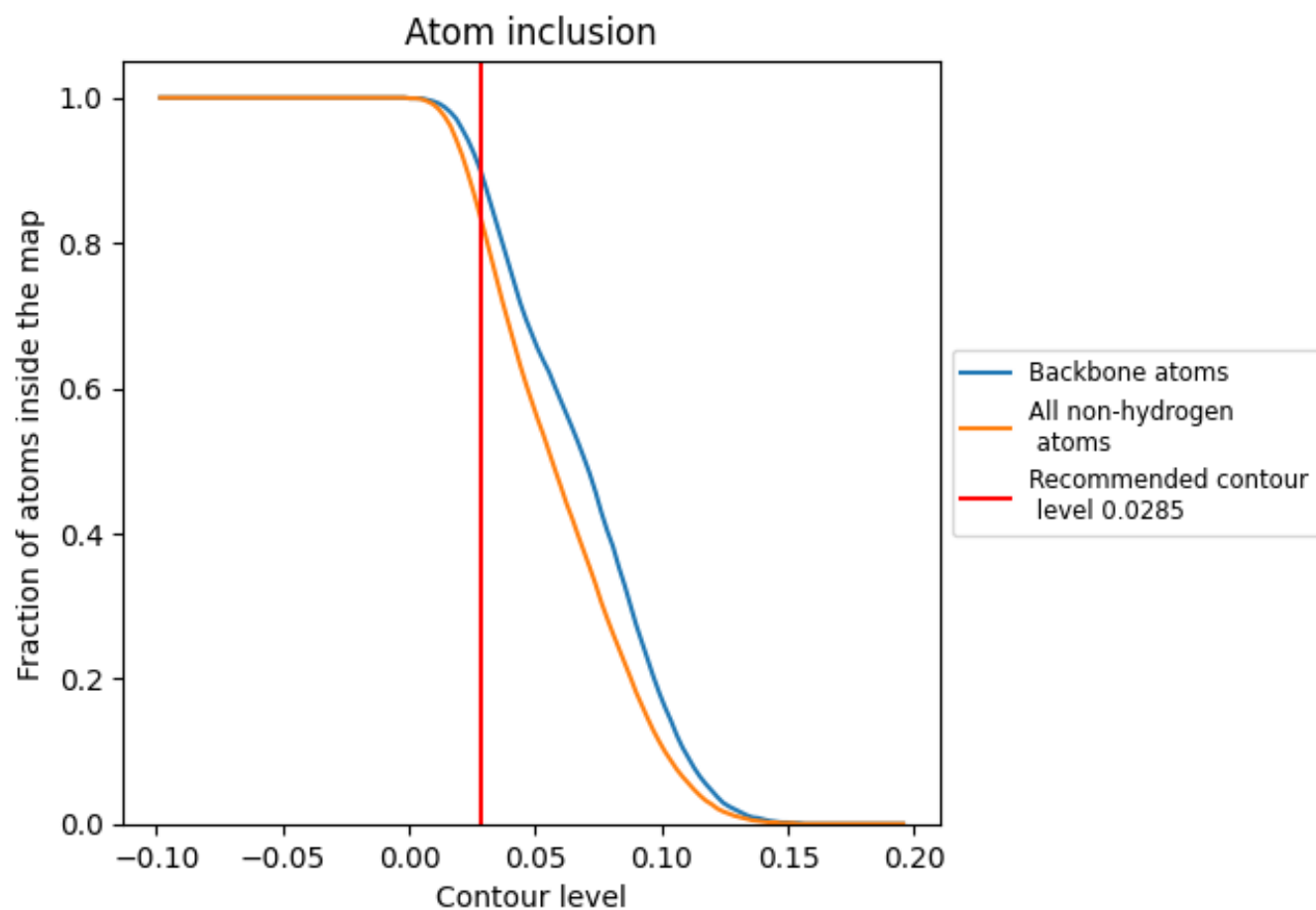
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0285).



























































## 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 (0.0285) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.5390
A	 0.8460	 0.5460
B	 0.8410	 0.5400
C	 0.9090	 0.5340
D	 0.6250	 0.3670
E	 0.4640	 0.4280
F	 0.6920	 0.4410
G	 0.4850	 0.5190
H	 0.4640	 0.4700
I	 0.8790	 0.5360
J	 0.5620	 0.4460
K	 0.6360	 0.4830
L	 0.6430	 0.5130
M	 0.5360	 0.4340
N	 0.3930	 0.4270
O	 0.4750	 0.4460
P	 0.4640	 0.4690
Q	 0.8030	 0.5310
R	 0.3930	 0.2750
S	 0.5360	 0.4280
T	 0.2140	 0.3370
U	 0.5900	 0.3980
V	 0.6430	 0.4140
W	 0.3570	 0.4020
X	 0.3610	 0.4140
Y	 0.5000	 0.4420
Z	 0.7870	 0.4670
a	 0.3570	 0.3360
b	 0.7500	 0.4560

