



# wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 04:37 PM JST

PDB ID : 8JX8  
EMDB ID : EMD-36692  
Title : rat megalin 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 : 3.30 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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

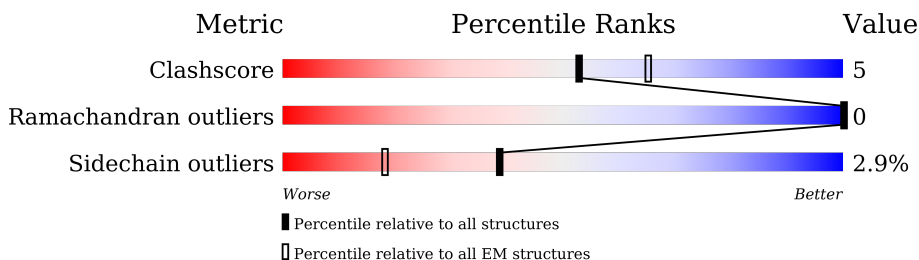
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	60% 100%
5	L	5	40% 100%
6	E	2	50% 100%
6	M	2	50% 100%
6	N	2	50% 100%
6	P	2	50% 100%
6	R	2	50% 50%
6	S	2	50% 100%
6	T	2	50% 100%
6	V	2	50% 50%
6	W	2	100% 100%
6	Y	2	50% 50%
6	a	2	50% 100%
6	b	2	50% 50%
7	F	3	67% 100%
7	U	3	33% 67% 33%
8	O	5	40% 60%
8	Q	5	20% 60% 40%
8	X	5	60% 40% 40% 20%
8	Z	5	20% 80% 20%

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 23459 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
			Total	C	N	O	S		
1	A	1436	Total	C	N	O	S	0	0
			11221	7043	1967	2133	78		
1	B	1434	Total	C	N	O	S	0	0
			11208	7035	1965	2131	77		

- Molecule 2 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	6	Total	C	N	O	0	0
			33	21	6	6		
2	I	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
			Total	C	N	O	S		
3	D	3	Total	C	N	O	S	0	0
			16	9	3	3	1		
3	J	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
			Total	C	N	O		
4	G	5	Total	C	N	O	0	0
			33	19	5	9		
4	K	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	H	5	Total	C	N	O	0	0
			28	16	6	6		
5	L	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.



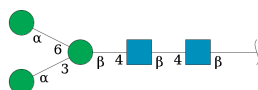
Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	M	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	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
			Total	C	N	O		
7	F	3	39	22	2	15	0	0
7	U	3	39	22	2	15	0	0

- 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.



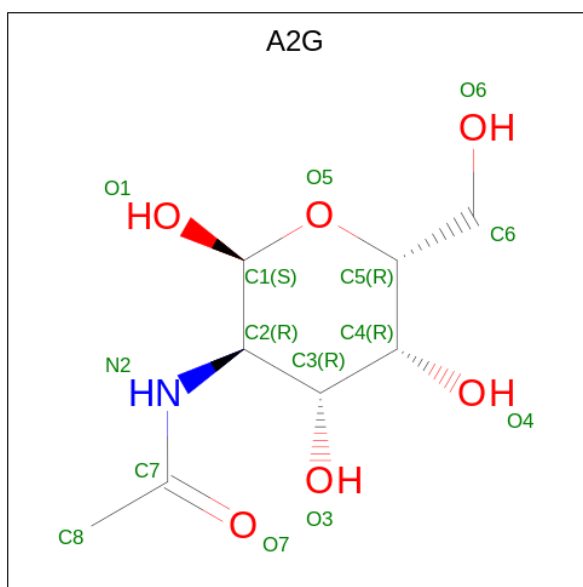
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	O	5	61	34	2	25	0	0
8	Q	5	61	34	2	25	0	0
8	X	5	61	34	2	25	0	0
8	Z	5	61	34	2	25	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 10 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
11	A	5	Total	Ca	0
			5	5	
11	B	5	Total	Ca	0
			5	5	

- Molecule 12 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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













W1574	V1752	V1997	C2223	A2512	F2706	THR	ALA	SER	PHE	THR	ILE	SER	THR	THR	ASP
R1579	R1753	L1998	T2236	I2513	T2707	THR	ASP	THR	ARG	THR	THR	THR	THR	GLU	GLU
I1580	D1754	R1999	P2237	R2519	C2708	THR	GLY	GLN	CYS	GLU	PHE	THR	THR	ASP	ALA
E1581	I1755	Y2004	M2242	W2527	N2709	THR	SER	THR	ARG	THR	THR	THR	THR	THR	ILE
R1590	S1768	R2006	E2288	G2528	N2710	THR	PRO	VAL	ASN	ARG	CYS	VAL	THR	VAL	CYS
I1591	N1769	G2007	Y2274	F2542	H2711	THR	ASP	PRO	ASP	ARG	ASN	THR	THR	THR	ASN
V1592	D1770	R2013	Y2319	L2551	H2712	THR	ALA	THR	ALA	THR	THR	THR	THR	THR	ASN
V1594	I1775	N2015	D2320	L2551	K2713	THR	GLY	LEU	GLY	ASP	THR	THR	THR	THR	ASN
Q1595	I1778	A2016	K2320	P2554	N2714	THR	VAL	SER	ASP	ASP	CYS	THR	THR	THR	THR
I1598	P2036	Y2036	L2323	E2562	D2717	THR	ASN	ASP	GLU	ASP	THR	THR	THR	THR	THR
I1599	G1781	Y2062	L2361	T2563	K2718	THR	ASN	ASP	GLU	GLU	THR	THR	THR	THR	THR
M1600	Y1782	Y2062	L2361	T2563	K2719	THR	ASN	ASP	GLU	GLU	THR	THR	THR	THR	THR
P1601	D1783	L2071	L2364	D2564	N2720	THR	GLN	GLY	THR	THR	THR	THR	THR	THR	THR
L1604	S1789	L2071	L2391	V2589	K2721	THR	SER	THR	THR	THR	THR	THR	THR	THR	THR
I1613	V1796	R2075	L2395	W2590	D2721	THR	ARG	THR	THR	THR	THR	THR	THR	THR	THR
M1616	H1803	D2083	N2396	L2599	N2722	THR	ASN	GLY	THR	THR	THR	THR	THR	THR	THR
Y1619	D1808	N2097	D2426	A2619	D2723	THR	ASN	ASN	THR	THR	THR	THR	THR	THR	THR
I1623	N1811	N2123	Y2427	G2624	N2724	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR
V1642	V1814	R2127	S2442	L2634	D2725	THR	VAL	PHE	THR	THR	THR	THR	THR	THR	THR
P1646	L1821	W2139	L2443	T2636	N2726	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L1649	L1827	I2143	S2456	T2643	D2727	THR	ASN	ALA	THR	THR	THR	THR	THR	THR	THR
D1660	W1831	N2146	Y2468	Q2648	N2728	THR	ASN	THR	THR	THR	THR	THR	THR	THR	THR
R1661	D1854	G2147	T2469	P2655	D2731	THR	VAL	VAL	THR	THR	THR	THR	THR	THR	THR
M1681	F1873	N2148	D2470	Q2651	V2736	THR	ASP	GLY	THR	THR	THR	THR	THR	THR	THR
I1693	H1891	I2148	D2470	Q2651	F2739	THR	GLY	LEU	THR	THR	THR	THR	THR	THR	THR
Q1698	K1900	R2149	N2478	N2654	H2740	THR	ASP	ASP	THR	THR	THR	THR	THR	THR	THR
M1703	I1901	R2149	R2479	P2655	T2741	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
C1714	A1902	N2178	R2480	C2656	CYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
Q1719	M1906	N2178	L2481	E2681	H2741	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
A1720	N1918	N2178	S2484	W2684	CYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
P1721	M1955	N2178	D2485	Y2685	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
P1729	M1955	N2178	S2487	L2686	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
M1733	G1966	H2202	M2492	N2688	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
L1734	L1967	H2202	S2493	A2687	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
S1735	E1985	W2207	M2494	D2689	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
D1736	R1986	Y2210	A2495	N2690	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
C1741	V1987	S2219	R2507	C2693	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
			S2507	T2697	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
			K2509	G2698	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
			P2510	T2699	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
			R2511	R2700	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR




SER LYS LYS ARG ASN LEU THR PRO GLY TYR THR ALA THR GLU ASP THR PHE LYS ASP THR ALA ASN LEU VAL LYS GLU ASP SER ASP VAL

- Molecule 2: unclear peptide

Chain C:  67% 33%

 X1 X2 L3 X6

- Molecule 2: unclear peptide

Chain I:  83% 17%

 X1 X2 L3 X6

- Molecule 3: unclear peptide

Chain D:  33% 100%

 X1 X2 X3


- Molecule 3: unclear peptide

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: unclear peptide

Chain G:  20% 60% 40%

 X1 E2 E3 X4 X5

- Molecule 4: unclear peptide

Chain K:  80% 20%

 X1 E2 X4 X5

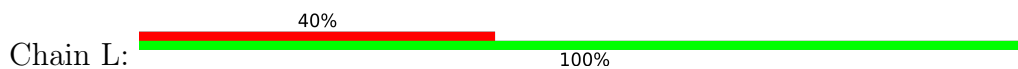
- Molecule 5: unclear peptide

Chain H:  60% 100%

 X0 X1 X4



- Molecule 5: unclear peptide



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



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



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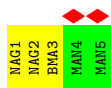
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



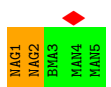
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



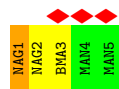
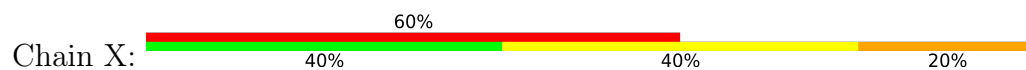
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



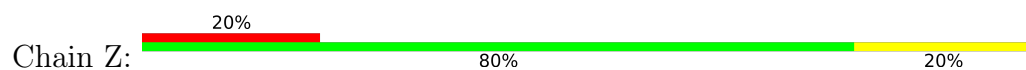
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101096	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)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.278	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0434	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: NI, MAN, A2G, BMA, CA, 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	0.26	0/11504	0.52	0/15672
1	B	0.26	0/11490	0.52	0/15652
2	C	0.31	0/7	0.59	0/8
2	I	0.42	0/7	0.54	0/8
3	D	0.32	0/5	0.25	0/5
3	J	0.22	0/5	0.14	0/5
4	G	0.24	0/17	0.29	0/21
4	K	0.23	0/17	0.40	0/21
5	H	0.22	0/7	0.41	0/8
5	L	0.27	0/7	0.30	0/8
All	All	0.26	0/23066	0.52	0/31408

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	11221	0	10723	121	0
1	B	11208	0	10709	113	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	2	0
3	D	16	0	8	0	0
3	J	16	0	8	0	0
4	G	33	0	19	1	0
4	K	33	0	18	1	0
5	H	28	0	12	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	R	28	0	25	0	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	V	28	0	25	1	0
6	W	28	0	25	0	0
6	Y	28	0	25	1	0
6	a	28	0	25	0	0
6	b	28	0	25	0	0
7	F	39	0	34	0	0
7	U	39	0	34	1	0
8	O	61	0	52	0	0
8	Q	61	0	52	2	0
8	X	61	0	52	1	0
8	Z	61	0	52	0	0
9	A	56	0	52	1	0
9	B	56	0	52	0	0
10	A	14	0	12	0	0
10	B	14	0	12	0	0
11	A	5	0	0	0	0
11	B	5	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
All	All	23459	0	22249	234	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 234 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:ASN:ND2	1:A:1451:ASN:OD1	2.25	0.70
1:A:2600:THR:HG21	1:A:2642:SER:HA	1.73	0.69
1:A:1383:ALA:HB3	1:A:1388:THR:HG23	1.77	0.67
1:A:1543:HIS:HB3	1:A:1729:PRO:HG3	1.76	0.67
1:A:1719:GLN:HG3	1:A:1721:PRO:HD2	1.76	0.66

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	1434/4660 (31%)	1338 (93%)	96 (7%)	0	100	100
1	B	1432/4660 (31%)	1366 (95%)	66 (5%)	0	100	100
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%)	2 (100%)	0	0	100	100
5	H	1/5 (20%)	1 (100%)	0	0	100	100
5	L	1/5 (20%)	1 (100%)	0	0	100	100
All	All	2876/9358 (31%)	2713 (94%)	163 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1247/4089 (30%)	1206 (97%)	41 (3%)	33	60
1	B	1245/4089 (30%)	1214 (98%)	31 (2%)	42	67
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	2502/8188 (31%)	2429 (97%)	73 (3%)	39	63

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2149	ARG
1	B	2736	VAL
1	B	2274	TYR
1	B	2564	ASP
1	A	2088	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1367	GLN
1	B	1993	ASN
1	B	2710	ASN
1	B	2097	ASN
1	A	1864	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

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	6,1	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
6	NAG	E	2	6	14,14,15	0.31	0	17,19,21	1.04	2 (11%)
7	NAG	F	1	1,7	14,14,15	0.45	0	17,19,21	1.46	4 (23%)
7	NAG	F	2	7	14,14,15	0.26	0	17,19,21	0.72	1 (5%)
7	BMA	F	3	7	11,11,12	0.24	0	15,15,17	0.86	1 (6%)
6	NAG	M	1	6,1	14,14,15	0.32	0	17,19,21	0.62	0
6	NAG	M	2	6	14,14,15	0.30	0	17,19,21	0.74	0
6	NAG	N	1	6,1	14,14,15	0.34	0	17,19,21	1.18	2 (11%)
6	NAG	N	2	6	14,14,15	0.32	0	17,19,21	0.93	1 (5%)
8	NAG	O	1	1,8	14,14,15	0.33	0	17,19,21	1.50	2 (11%)
8	NAG	O	2	8	14,14,15	0.29	0	17,19,21	0.90	1 (5%)
8	BMA	O	3	8	11,11,12	0.23	0	15,15,17	0.97	1 (6%)
8	MAN	O	4	8	11,11,12	0.25	0	15,15,17	0.64	0
8	MAN	O	5	8	11,11,12	0.27	0	15,15,17	0.71	0
6	NAG	P	1	6,1	14,14,15	0.29	0	17,19,21	0.64	0
6	NAG	P	2	6	14,14,15	0.30	0	17,19,21	0.90	0
8	NAG	Q	1	1,8	14,14,15	0.35	0	17,19,21	0.87	1 (5%)
8	NAG	Q	2	8	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
8	BMA	Q	3	8	11,11,12	0.21	0	15,15,17	0.79	0
8	MAN	Q	4	8	11,11,12	0.24	0	15,15,17	0.73	0
8	MAN	Q	5	8	11,11,12	0.21	0	15,15,17	0.65	0
6	NAG	R	1	6,1	14,14,15	0.29	0	17,19,21	0.71	0
6	NAG	R	2	6	14,14,15	0.31	0	17,19,21	0.91	1 (5%)
6	NAG	S	1	6,1	14,14,15	0.31	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	S	2	6	14,14,15	0.30	0	17,19,21	0.76	0
6	NAG	T	1	6,1	14,14,15	0.31	0	17,19,21	0.65	0
6	NAG	T	2	6	14,14,15	0.32	0	17,19,21	0.78	0
7	NAG	U	1	1,7	14,14,15	0.29	0	17,19,21	0.62	0
7	NAG	U	2	7	14,14,15	0.31	0	17,19,21	0.56	0
7	BMA	U	3	7	11,11,12	0.25	0	15,15,17	0.75	0
6	NAG	V	1	6,1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
6	NAG	V	2	6	14,14,15	0.27	0	17,19,21	0.80	0
6	NAG	W	1	6,1	14,14,15	0.28	0	17,19,21	0.71	0
6	NAG	W	2	6	14,14,15	0.29	0	17,19,21	0.67	0
8	NAG	X	1	1,8	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
8	NAG	X	2	8	14,14,15	0.34	0	17,19,21	0.96	1 (5%)
8	BMA	X	3	8	11,11,12	0.26	0	15,15,17	0.95	1 (6%)
8	MAN	X	4	8	11,11,12	0.25	0	15,15,17	0.63	0
8	MAN	X	5	8	11,11,12	0.21	0	15,15,17	0.66	0
6	NAG	Y	1	6,1	14,14,15	0.73	1 (7%)	17,19,21	1.29	1 (5%)
6	NAG	Y	2	6	14,14,15	0.39	0	17,19,21	0.84	1 (5%)
8	NAG	Z	1	1,8	14,14,15	0.38	0	17,19,21	0.84	1 (5%)
8	NAG	Z	2	8	14,14,15	0.30	0	17,19,21	0.65	0
8	BMA	Z	3	8	11,11,12	0.20	0	15,15,17	0.69	0
8	MAN	Z	4	8	11,11,12	0.23	0	15,15,17	0.66	0
8	MAN	Z	5	8	11,11,12	0.20	0	15,15,17	0.66	0
6	NAG	a	1	6,1	14,14,15	0.32	0	17,19,21	0.68	0
6	NAG	a	2	6	14,14,15	0.36	0	17,19,21	0.70	0
6	NAG	b	1	6,1	14,14,15	0.31	0	17,19,21	1.10	2 (11%)
6	NAG	b	2	6	14,14,15	0.32	0	17,19,21	0.69	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	6,1	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	3/6/23/26	0/1/1/1
7	NAG	F	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	1/6/23/26	0/1/1/1
7	BMA	F	3	7	-	0/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	1	NAG	C1-C2	2.40	1.55	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	1	NAG	C1-O5-C5	4.38	118.12	112.19
6	Y	1	NAG	C1-O5-C5	3.71	117.21	112.19
7	F	1	NAG	O5-C5-C6	3.66	112.95	107.20
8	O	1	NAG	O5-C1-C2	-3.65	105.52	111.29
6	V	1	NAG	C1-O5-C5	-3.56	107.37	112.19

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

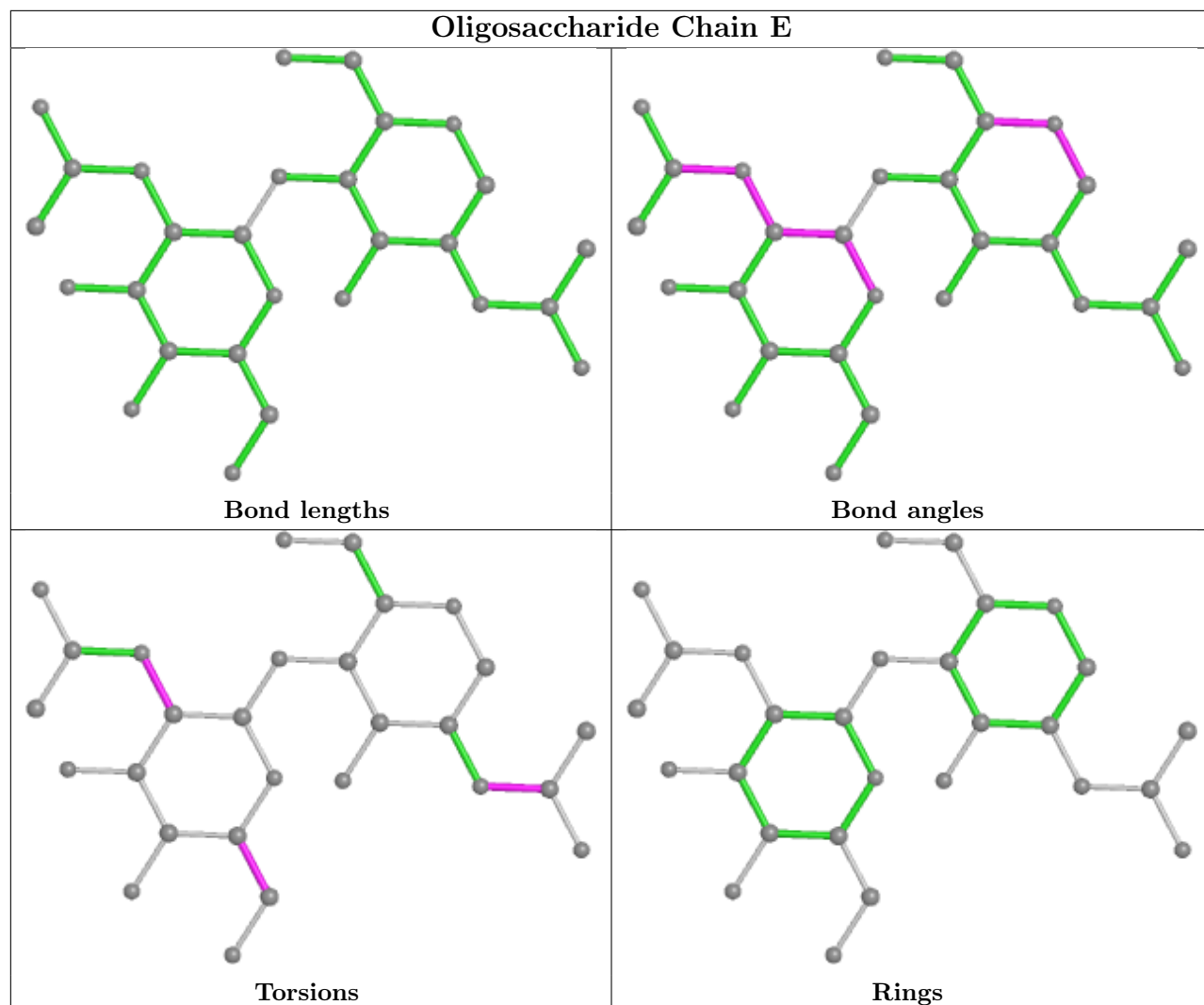
Mol	Chain	Res	Type	Atoms
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
7	F	1	NAG	C8-C7-N2-C2
7	F	1	NAG	O7-C7-N2-C2
6	E	1	NAG	C8-C7-N2-C2

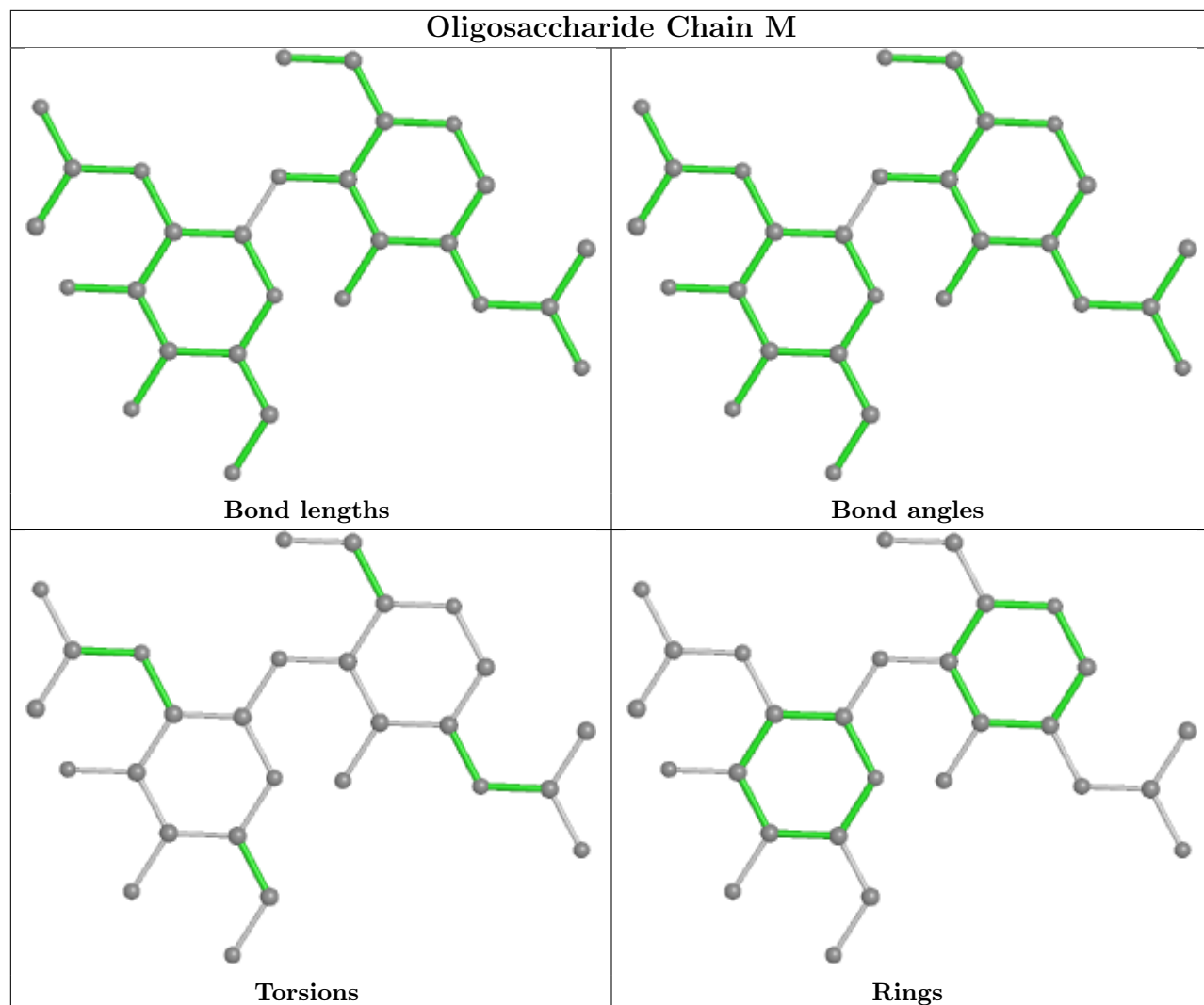
There are no ring outliers.

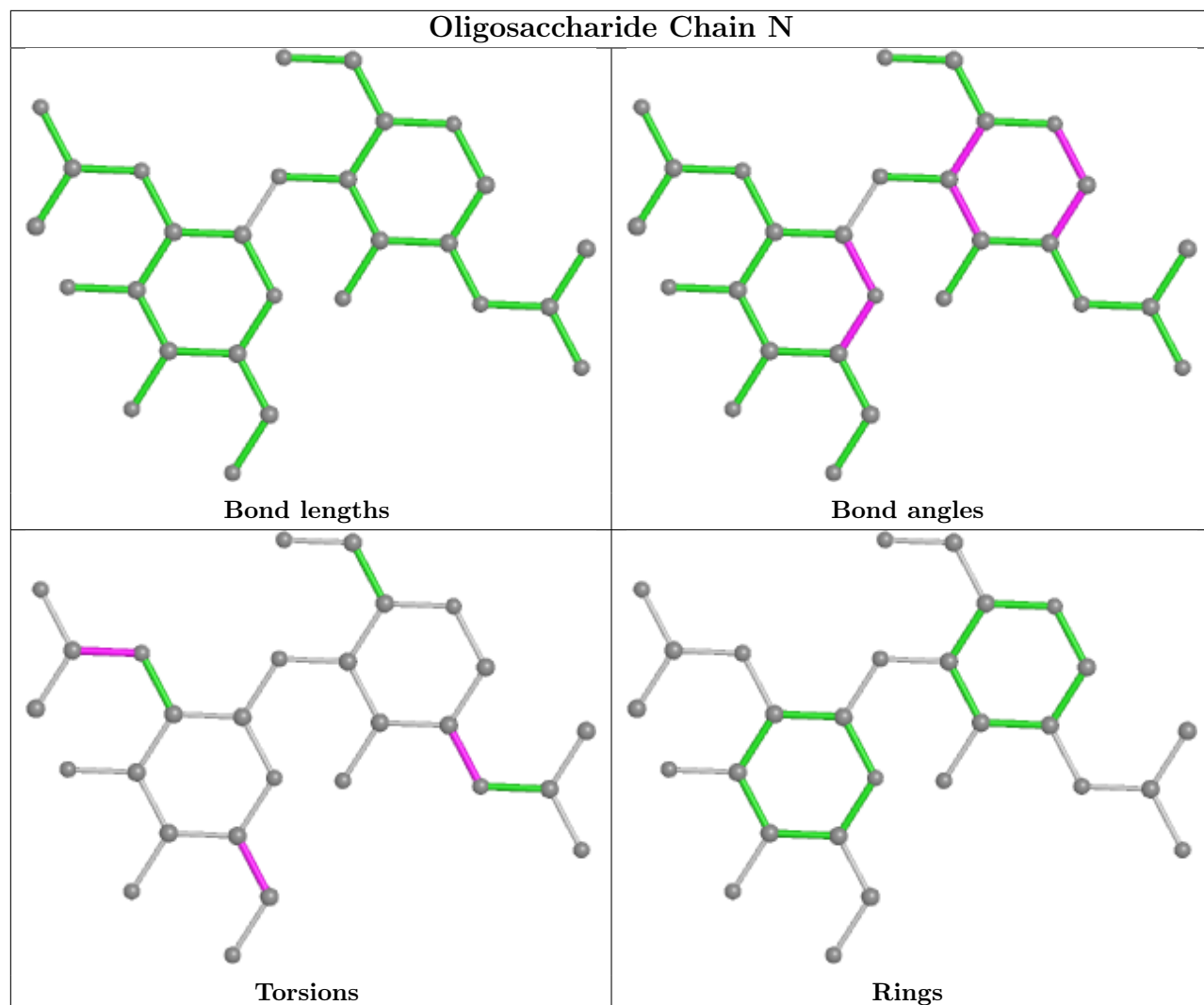
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Q	1	NAG	2	0
6	V	1	NAG	1	0
8	X	1	NAG	1	0
7	U	1	NAG	1	0
6	Y	1	NAG	1	0
8	Q	2	NAG	1	0

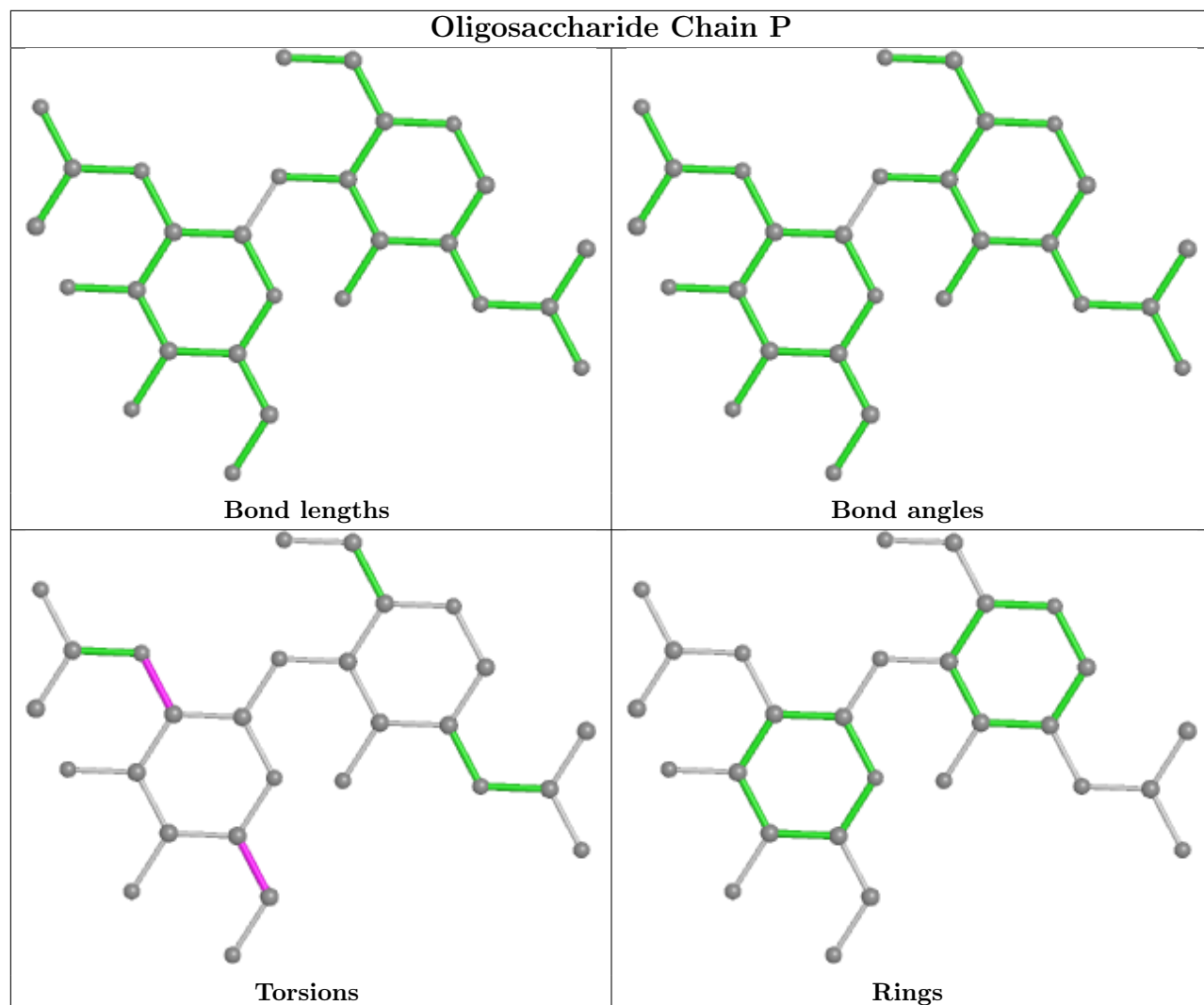
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

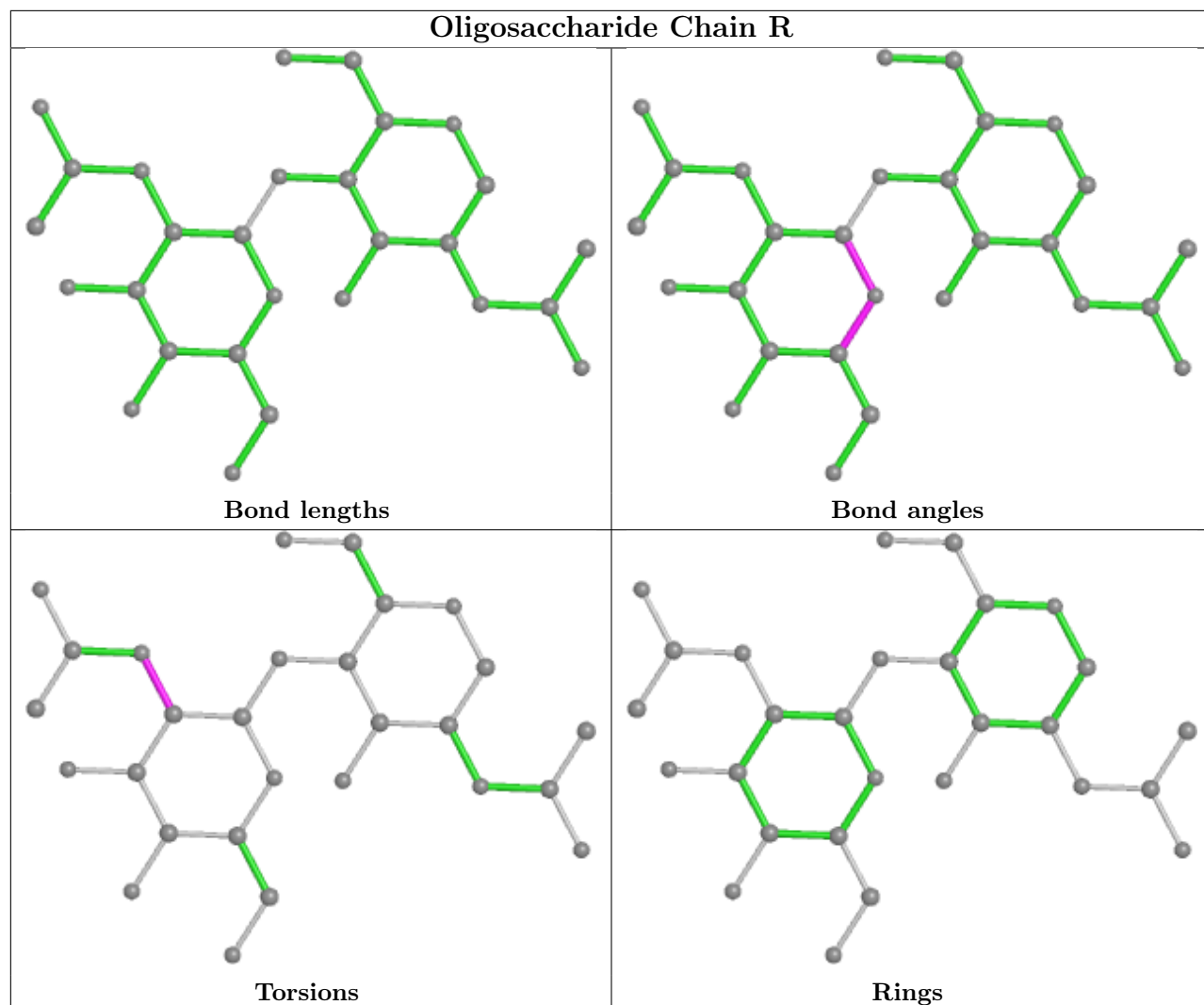


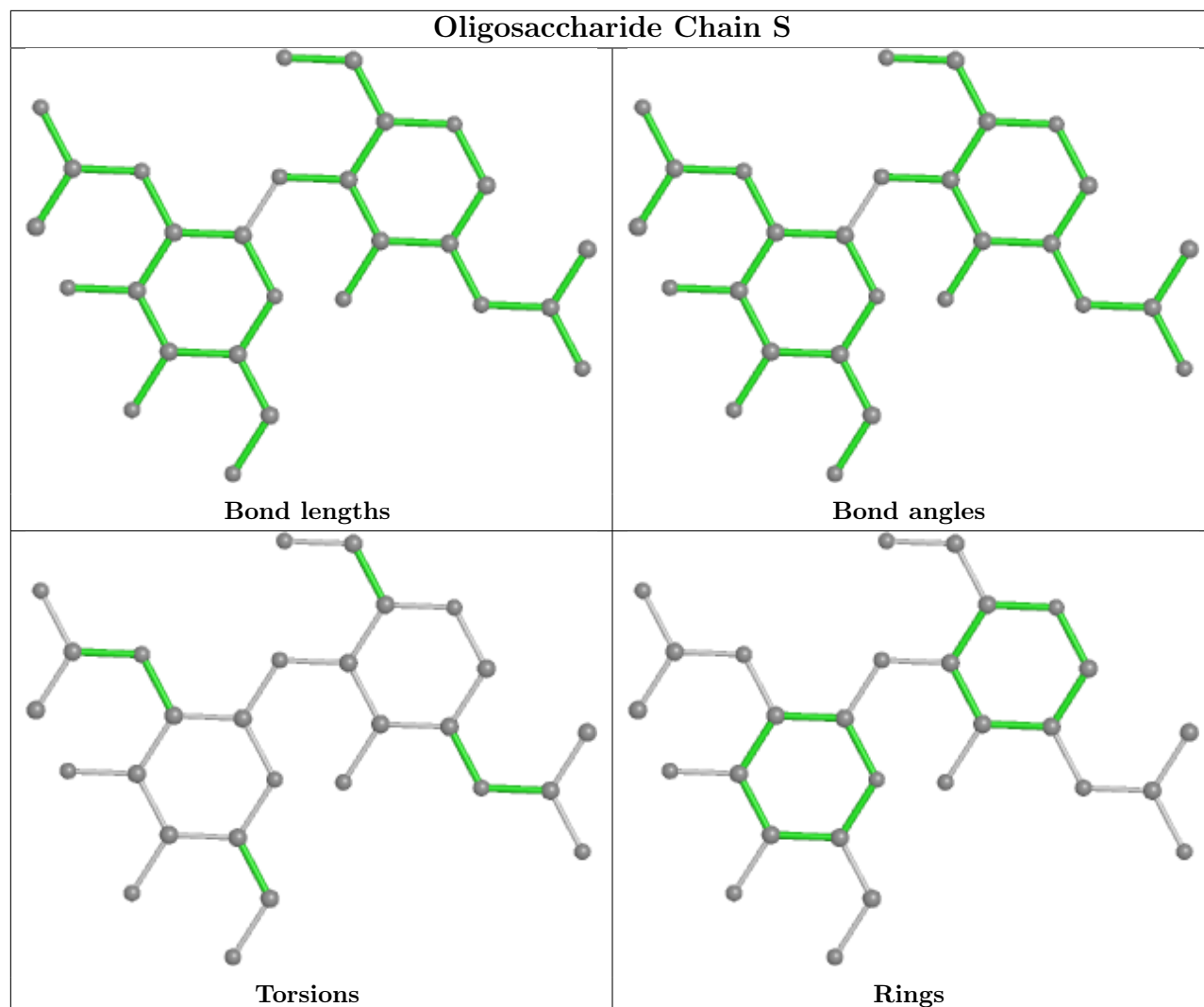


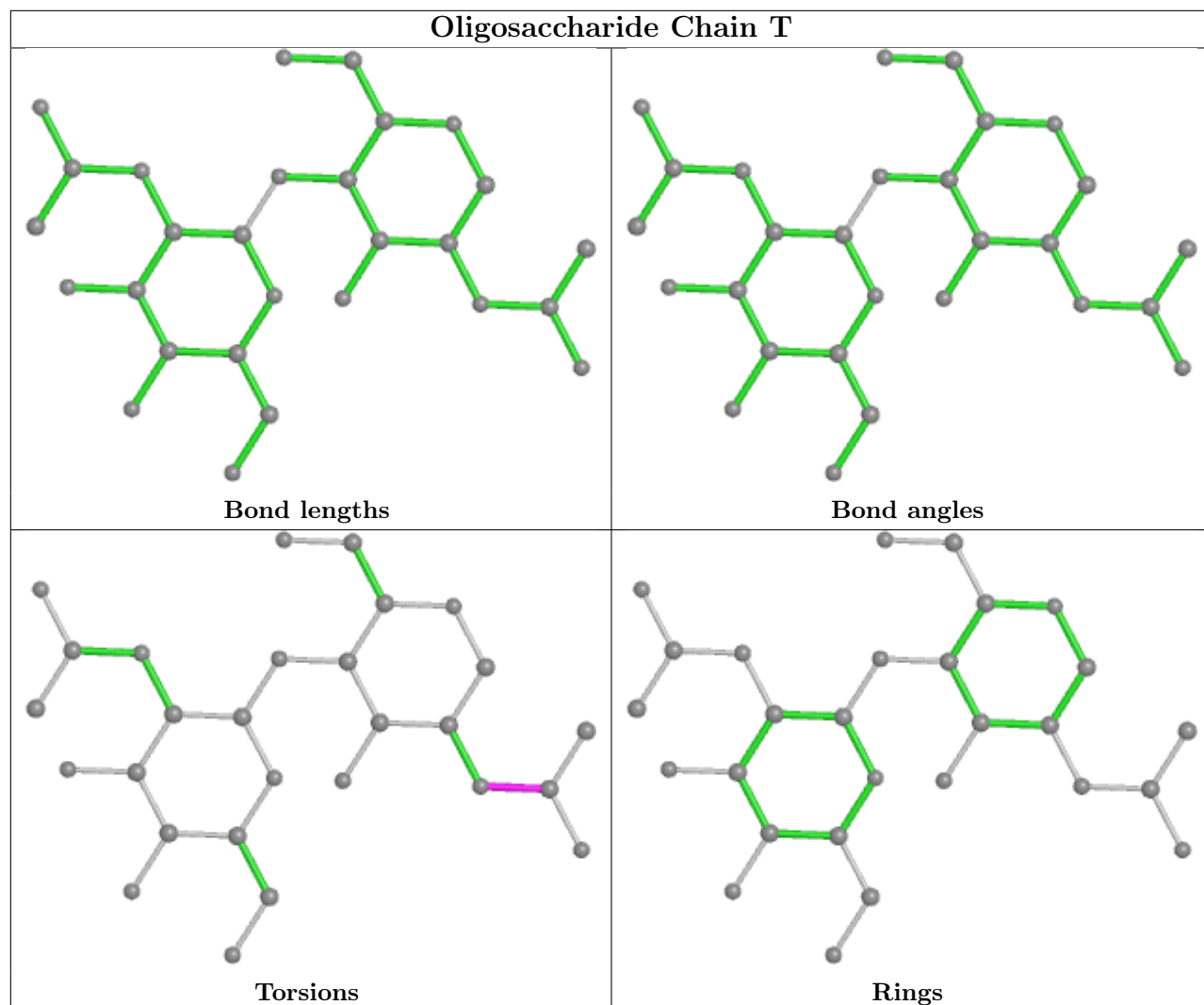


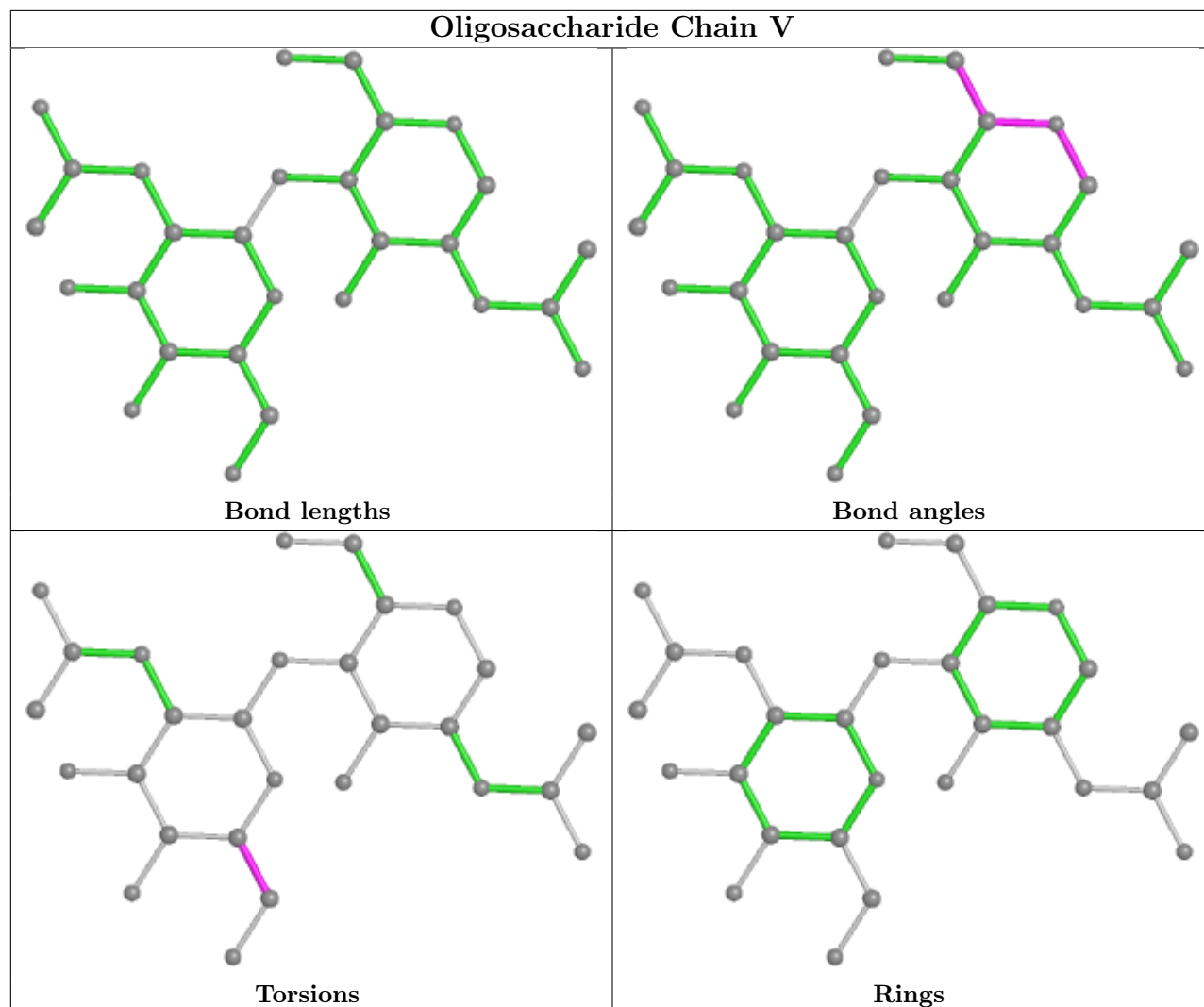


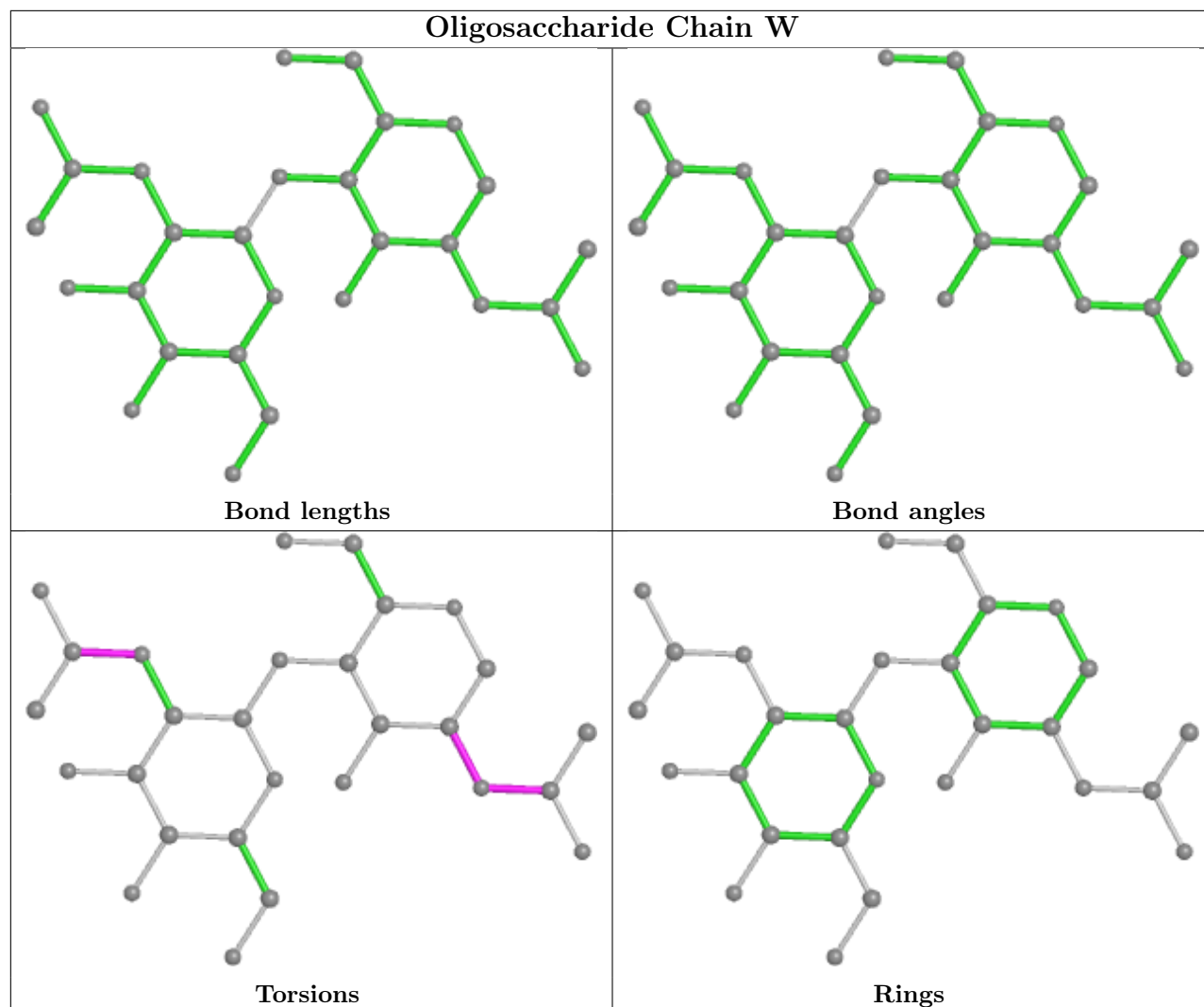


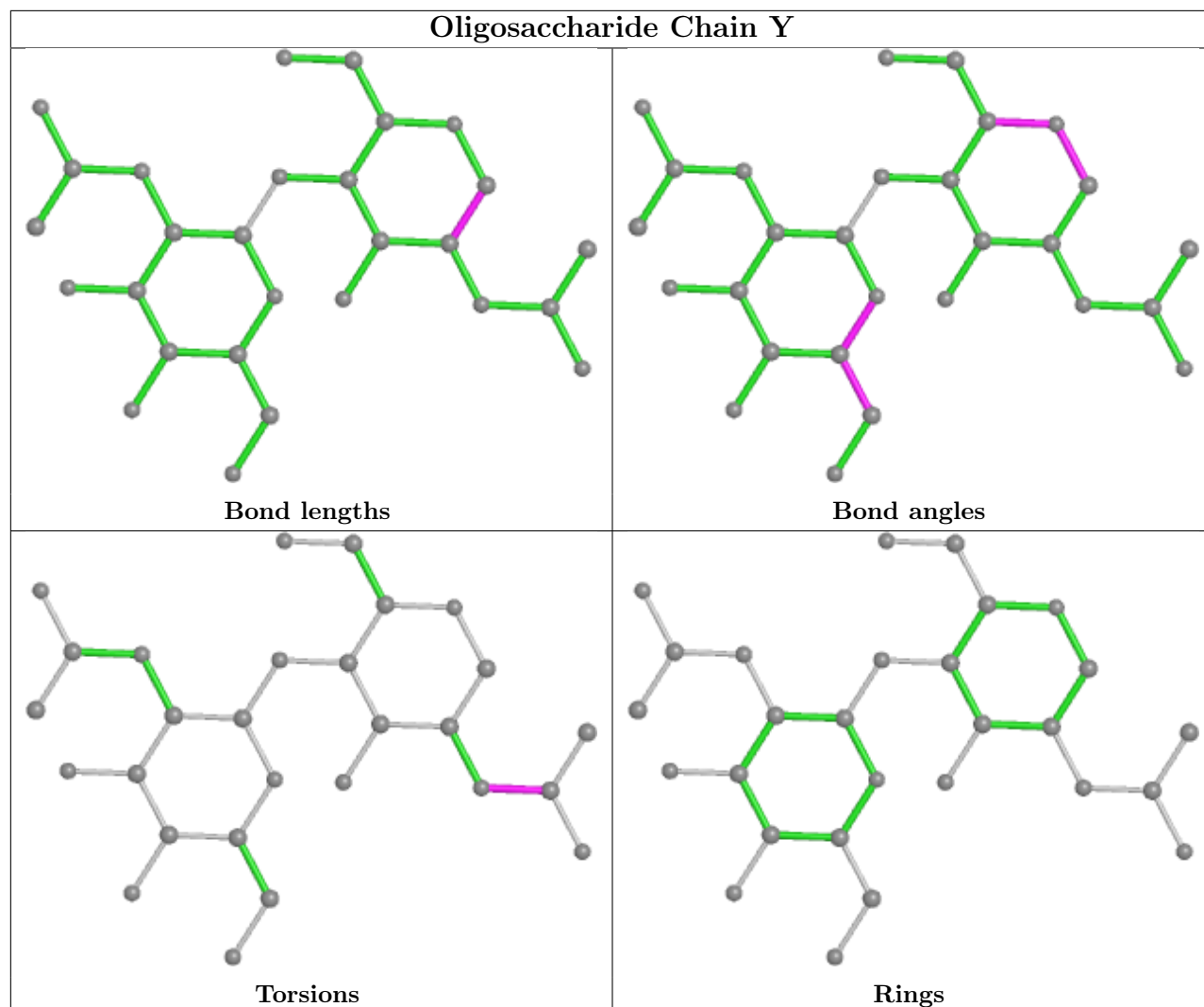


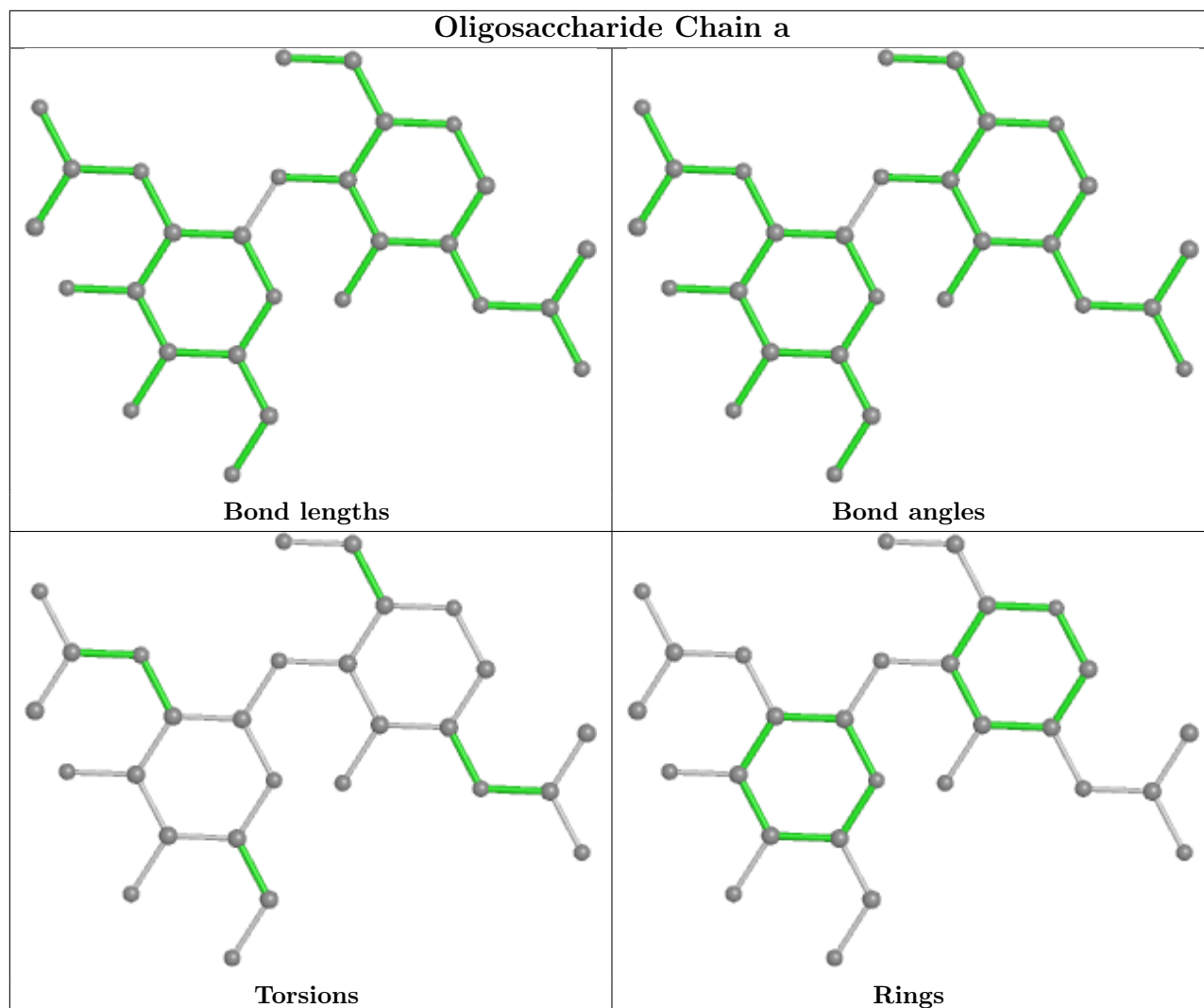




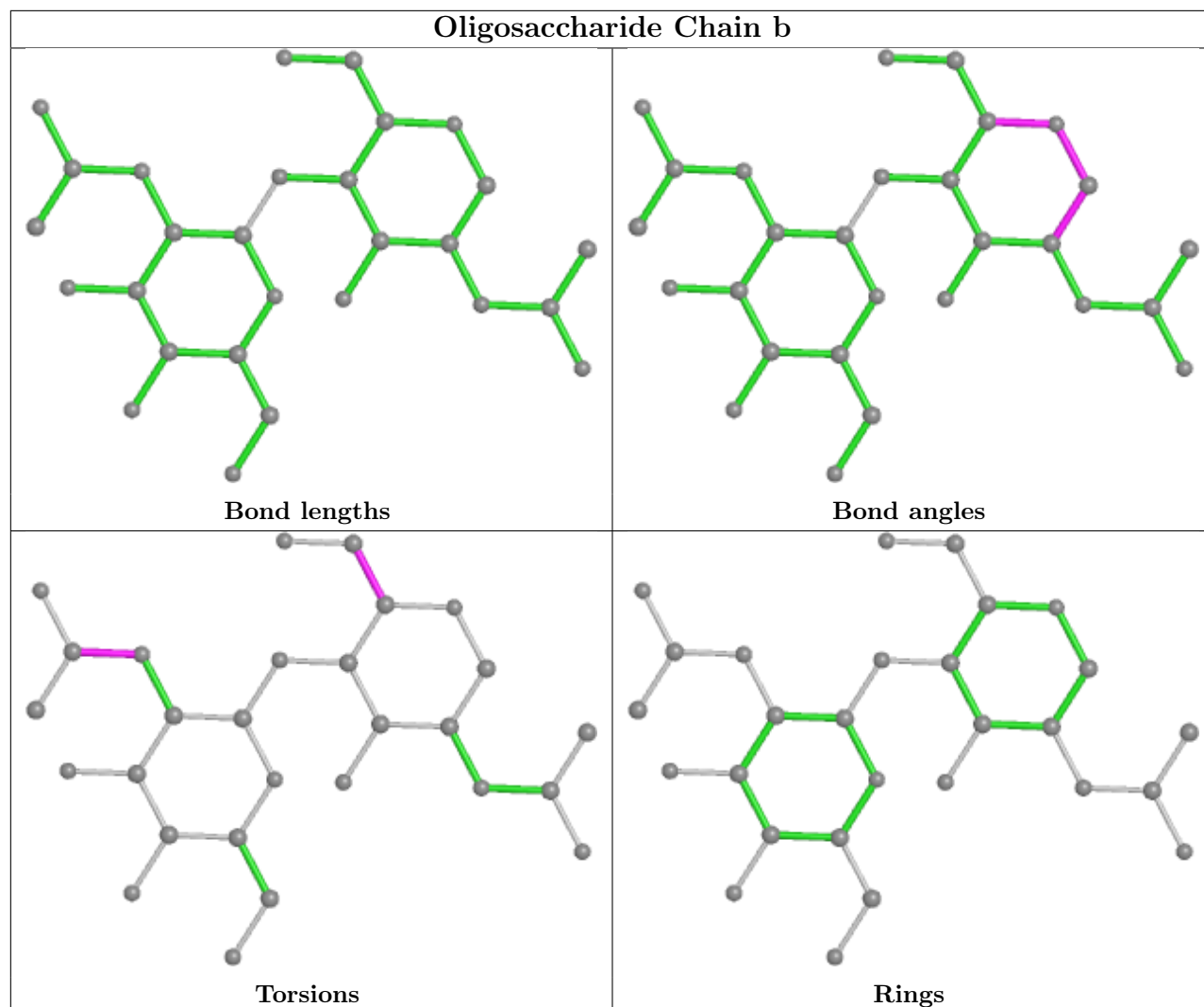


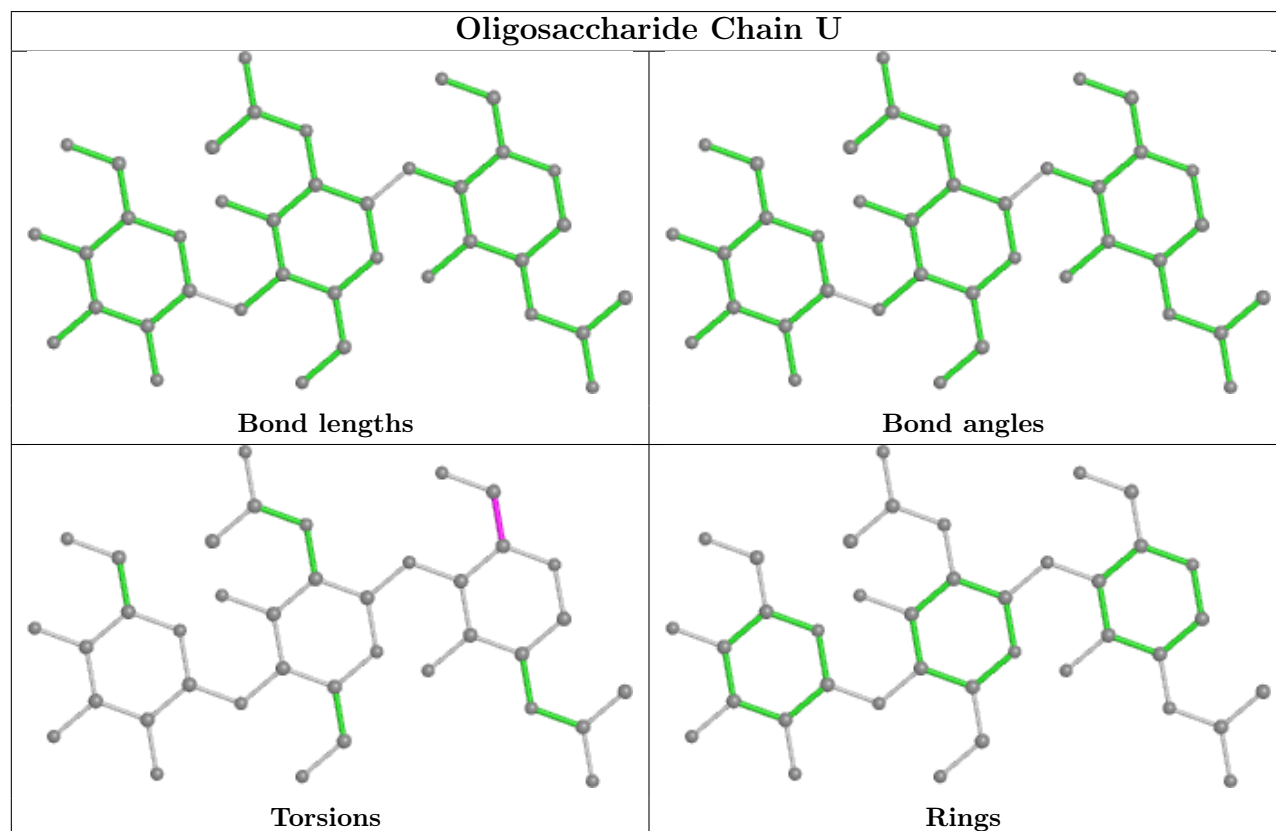
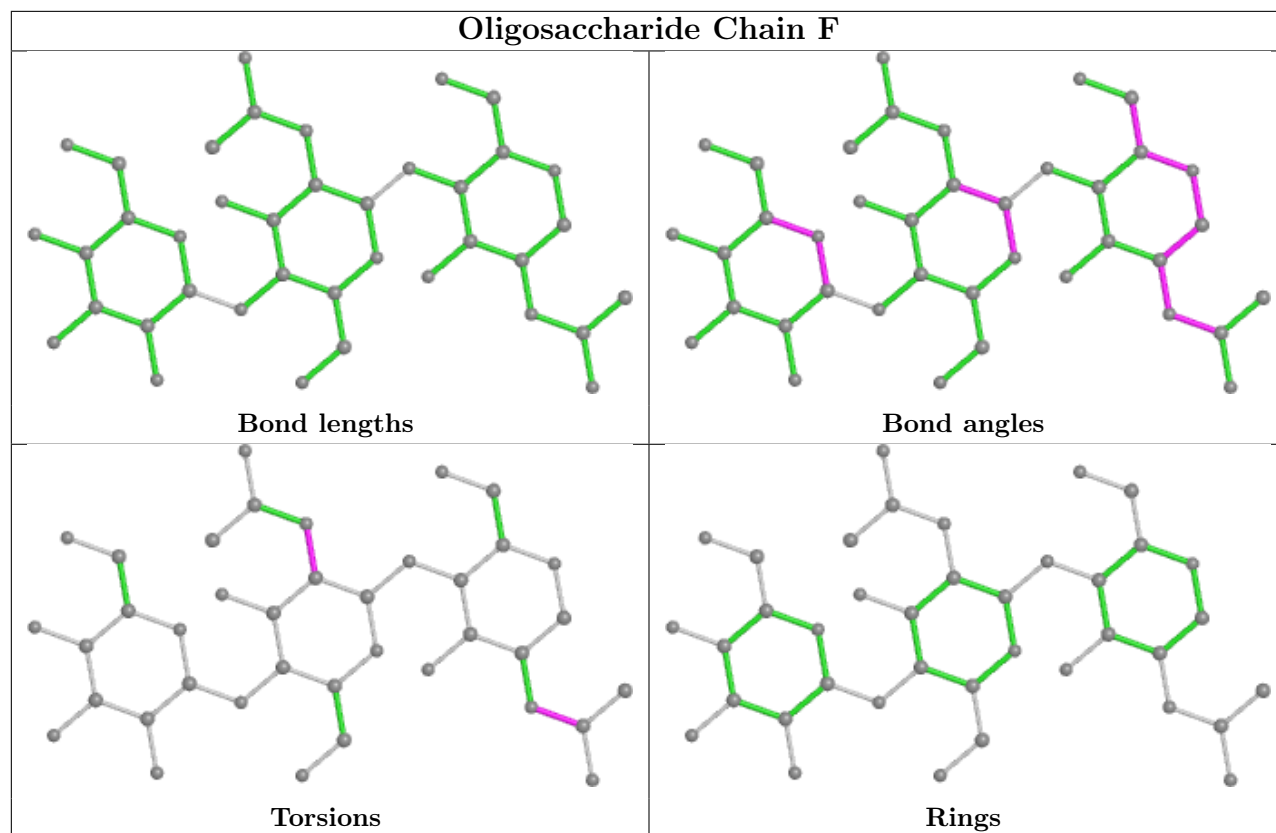


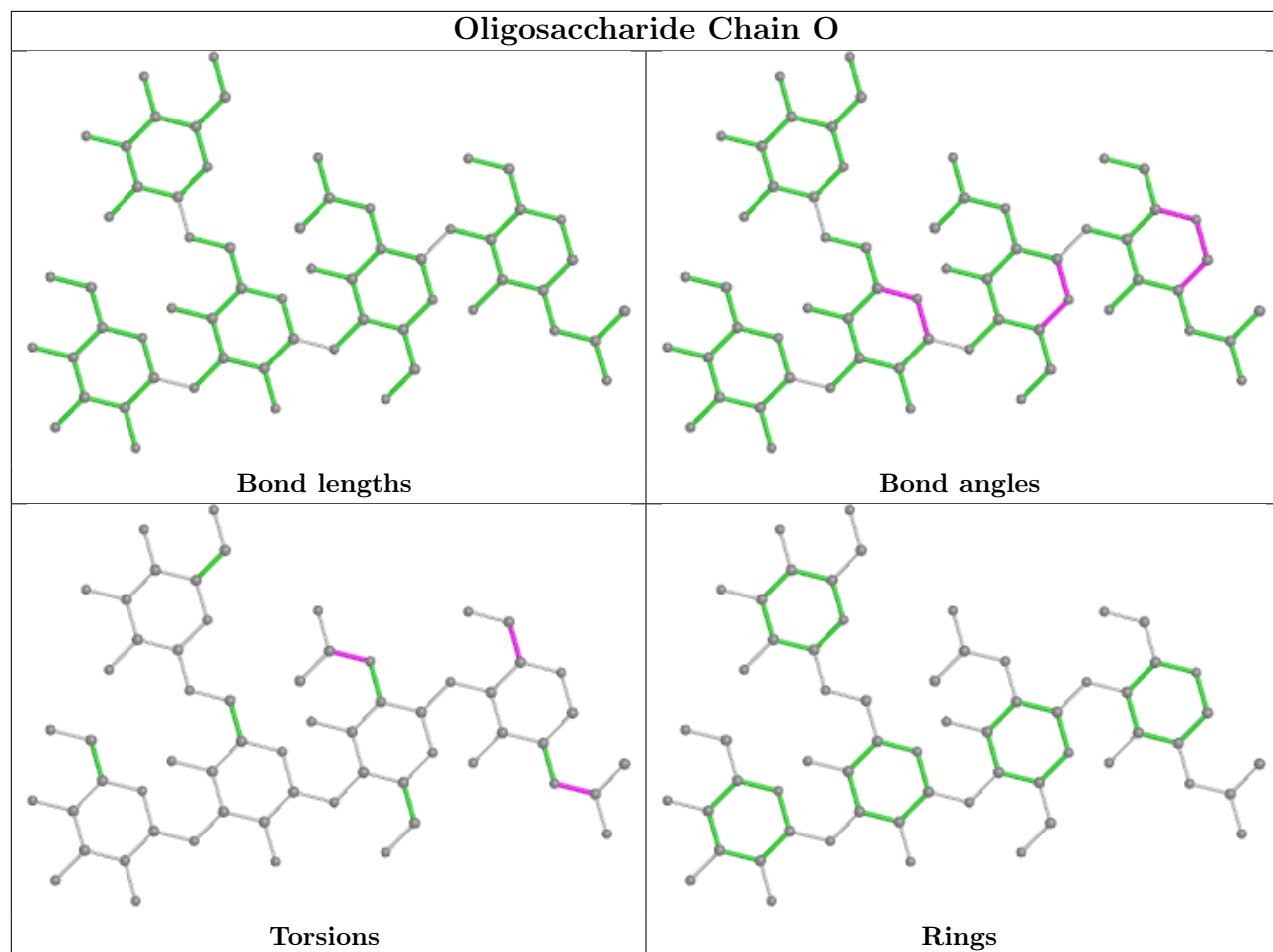


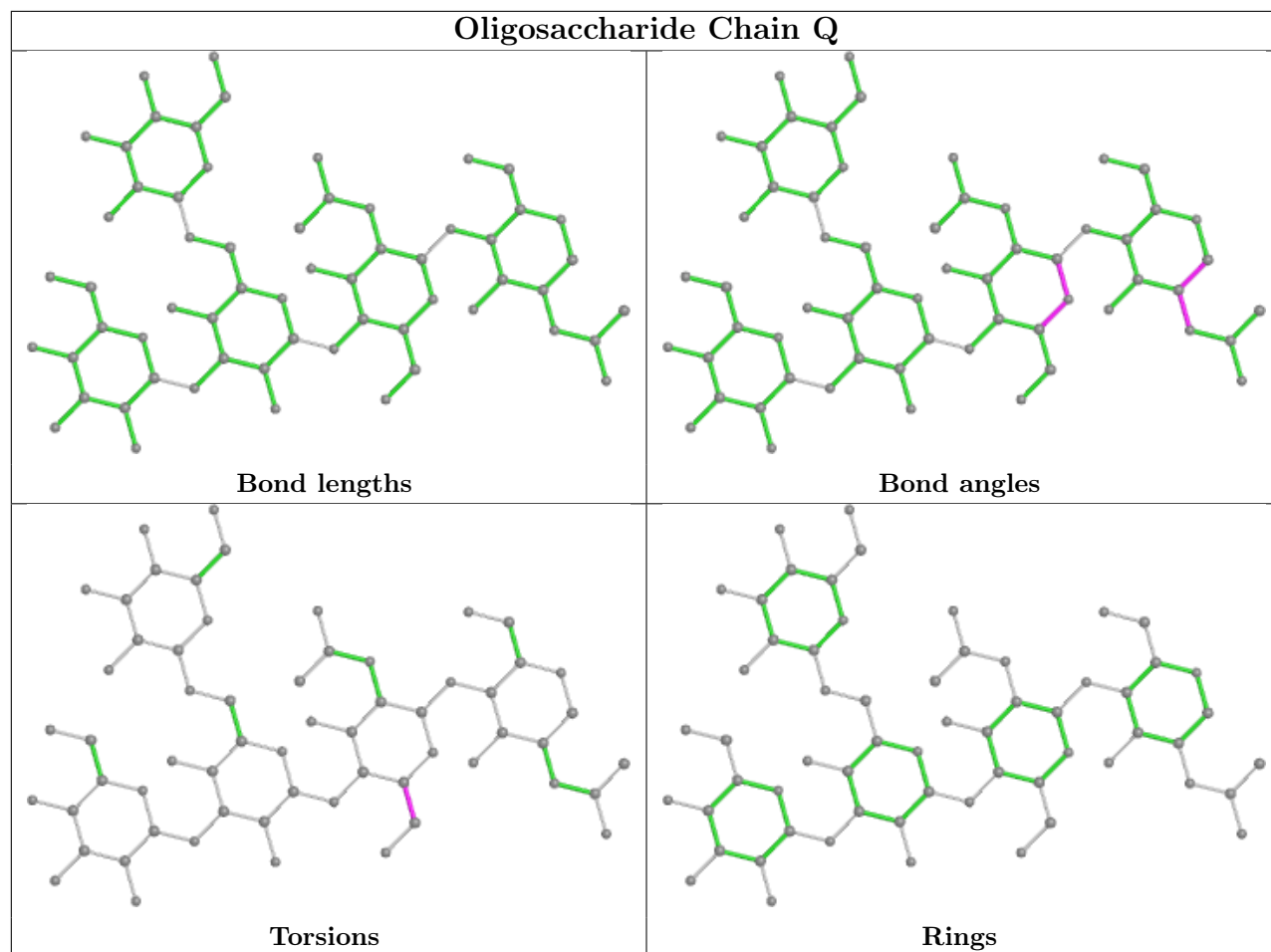


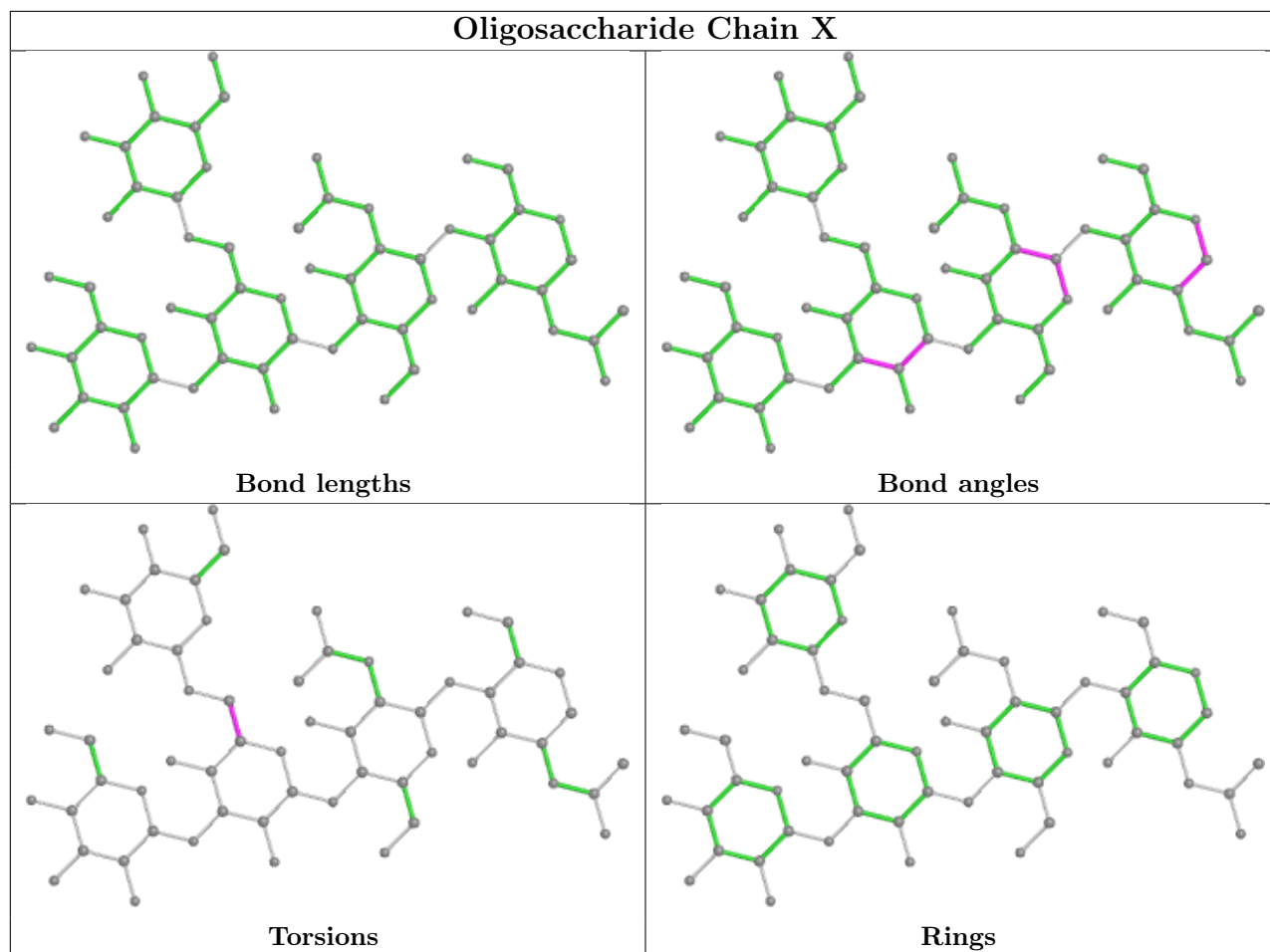


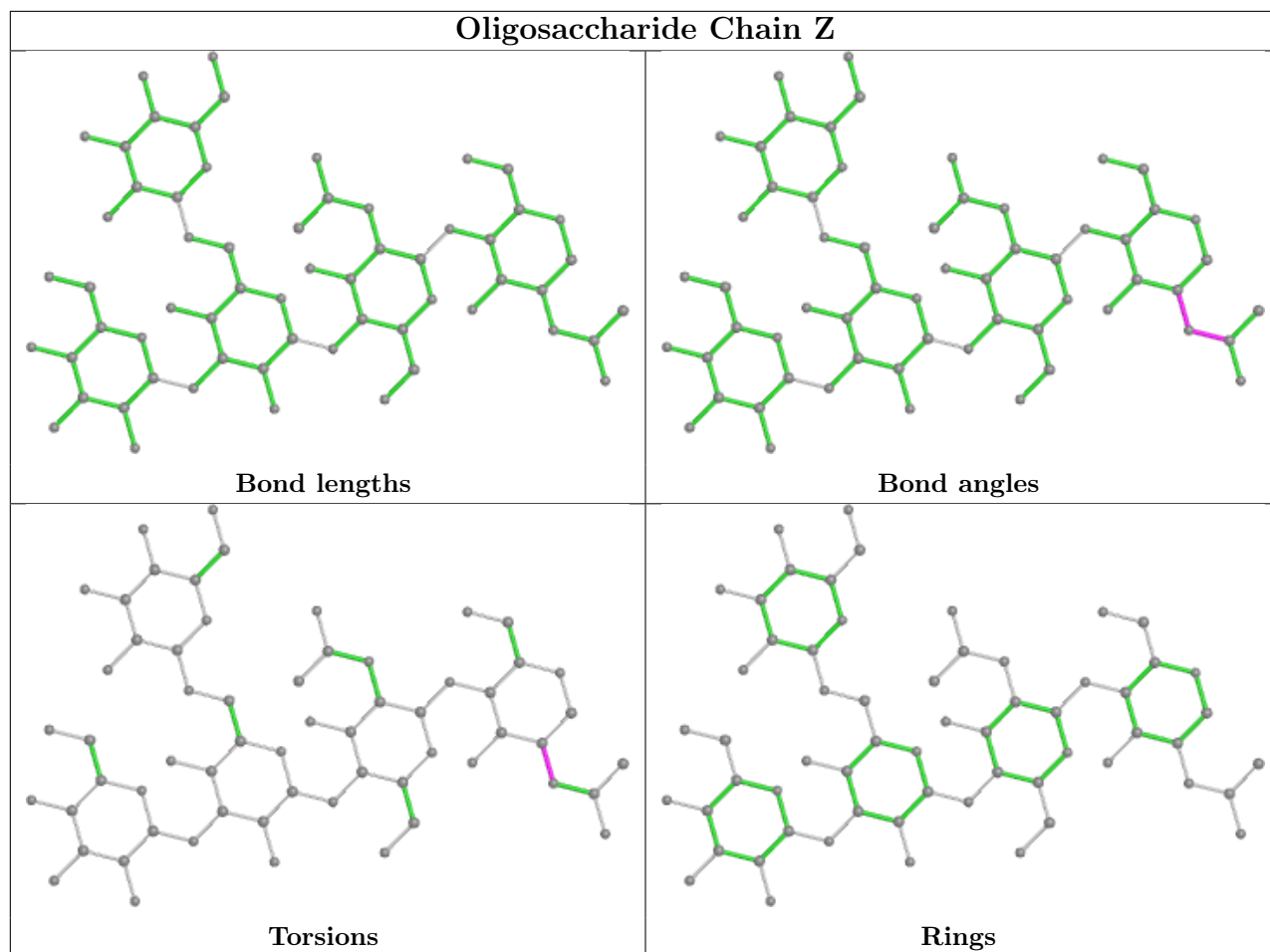












## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 12 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	$\# Z  > 2$
9	NAG	A	4704	1	14,14,15	0.38	0	17,19,21	0.85	0
9	NAG	B	4702	1	14,14,15	0.53	0	17,19,21	1.94	3 (17%)
9	NAG	A	4702	1	14,14,15	0.33	0	17,19,21	0.91	1 (5%)
9	NAG	B	4704	1	14,14,15	0.50	0	17,19,21	2.14	2 (11%)
10	A2G	A	4705	1	14,14,15	0.39	0	17,19,21	0.71	0
9	NAG	B	4703	1	14,14,15	0.29	0	17,19,21	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	A	4703	1	14,14,15	0.36	0	17,19,21	1.05	1 (5%)
9	NAG	B	4701	1	14,14,15	0.34	0	17,19,21	0.75	1 (5%)
9	NAG	A	4701	1	14,14,15	0.40	0	17,19,21	2.23	3 (17%)
10	A2G	B	4705	1	14,14,15	0.39	0	17,19,21	0.42	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
9	NAG	A	4704	1	-	4/6/23/26	0/1/1/1
9	NAG	B	4702	1	-	0/6/23/26	0/1/1/1
9	NAG	A	4702	1	-	2/6/23/26	0/1/1/1
9	NAG	B	4704	1	-	5/6/23/26	0/1/1/1
10	A2G	A	4705	1	-	1/6/23/26	0/1/1/1
9	NAG	B	4703	1	-	3/6/23/26	0/1/1/1
9	NAG	A	4703	1	-	5/6/23/26	0/1/1/1
9	NAG	B	4701	1	-	2/6/23/26	0/1/1/1
9	NAG	A	4701	1	-	3/6/23/26	0/1/1/1
10	A2G	B	4705	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	4701	NAG	C1-O5-C5	7.91	122.91	112.19
9	B	4702	NAG	C1-O5-C5	6.32	120.76	112.19
9	B	4704	NAG	C1-O5-C5	-6.25	103.72	112.19
9	B	4704	NAG	O5-C5-C6	5.52	115.86	107.20
9	A	4701	NAG	C4-C3-C2	-3.35	106.11	111.02

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	4703	NAG	C3-C2-N2-C7
9	A	4704	NAG	C3-C2-N2-C7
9	A	4704	NAG	C8-C7-N2-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
9	A	4704	NAG	O7-C7-N2-C2
9	B	4704	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	4701	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



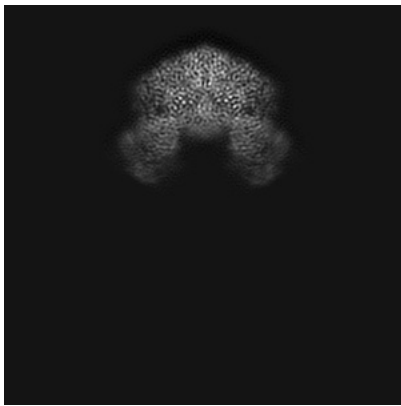
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36692. These allow visual inspection of the internal detail of the map and identification of artifacts.

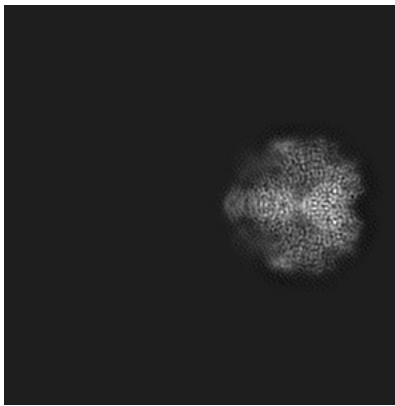
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

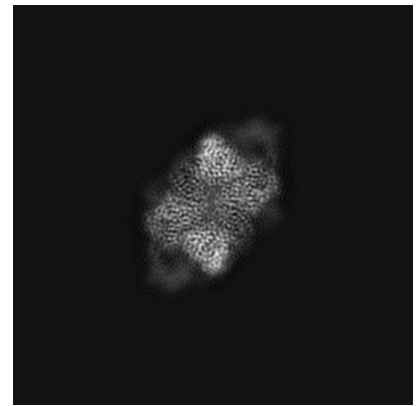
#### 6.1.1 Primary map



X

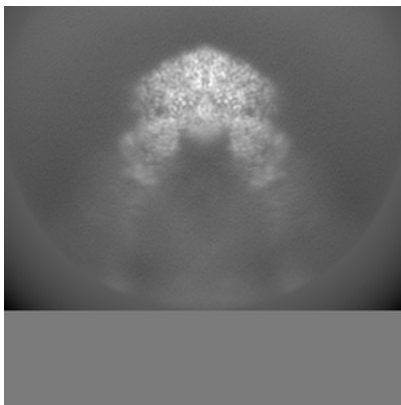


Y

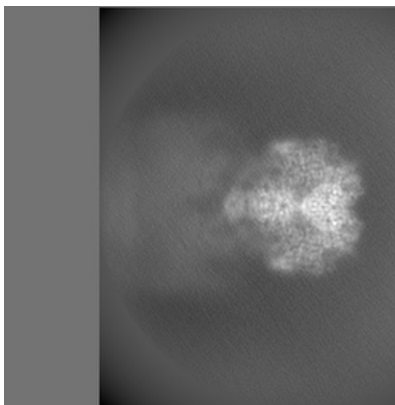


Z

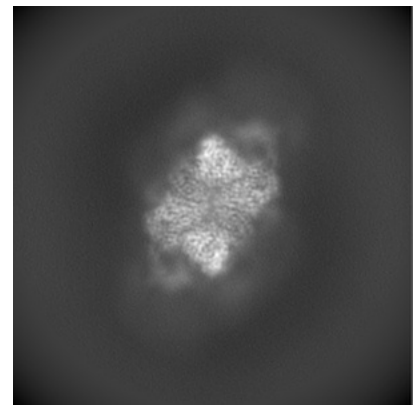
#### 6.1.2 Raw map



X



Y

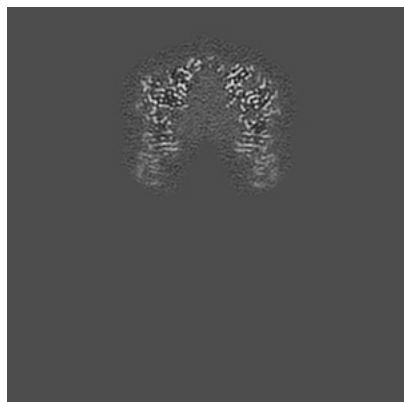


Z

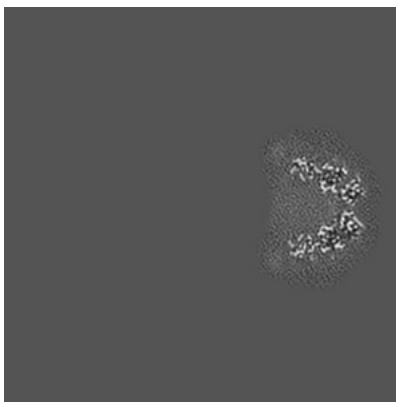
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

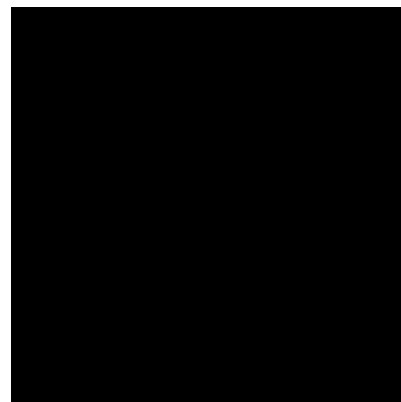
### 6.2.1 Primary map



X Index: 130

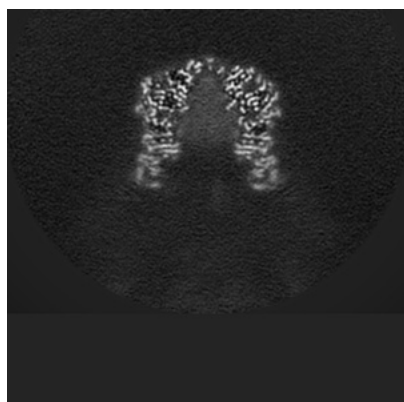


Y Index: 130

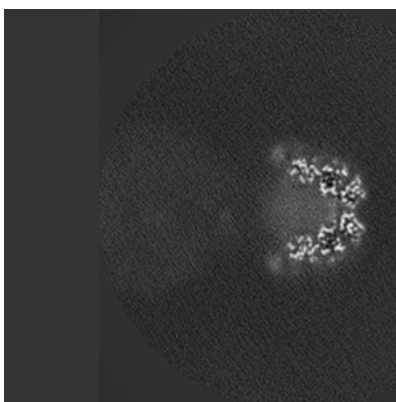


Z Index: 130

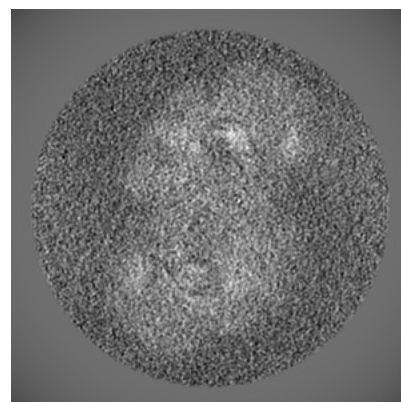
### 6.2.2 Raw map



X Index: 130



Y Index: 130

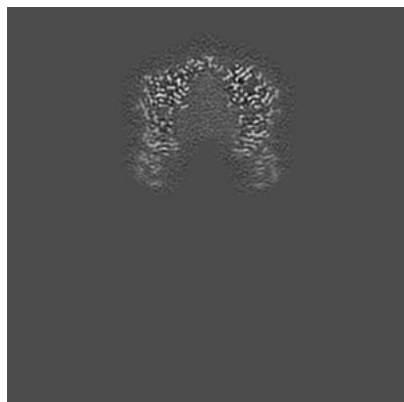


Z Index: 130

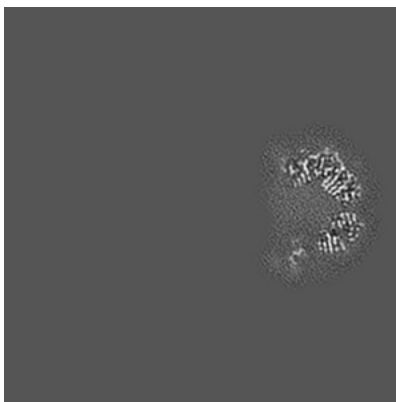
The images above show central slices of the map in three orthogonal directions.

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

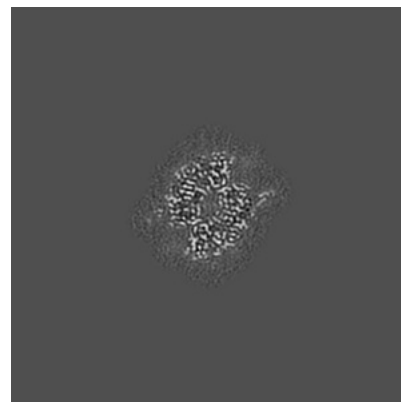
### 6.3.1 Primary map



X Index: 131

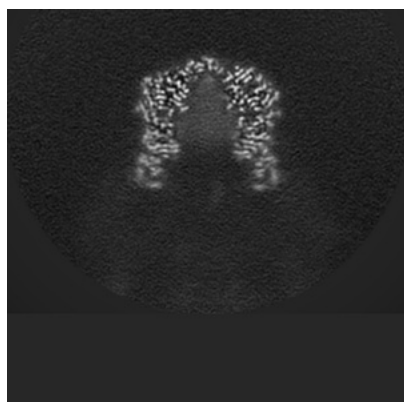


Y Index: 134

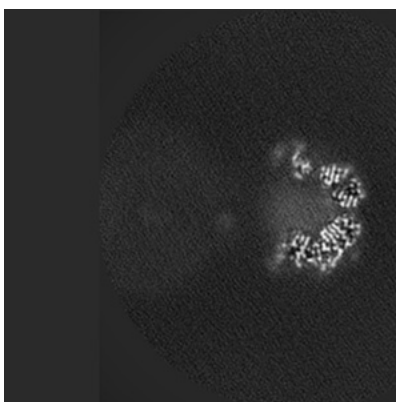


Z Index: 215

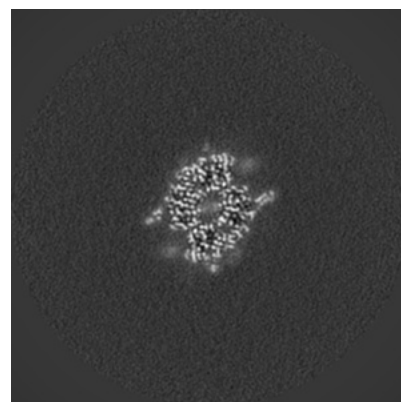
### 6.3.2 Raw map



X Index: 131



Y Index: 127

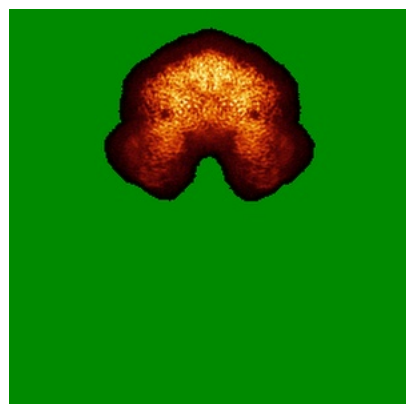


Z Index: 214

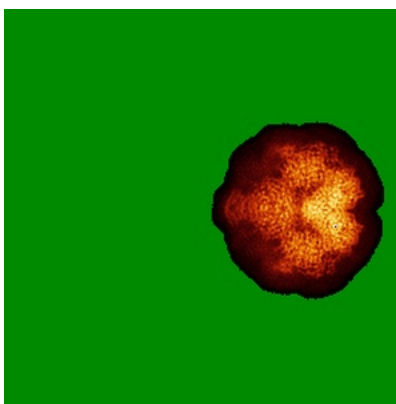
The images above show the largest variance slices of the map in three orthogonal directions.

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

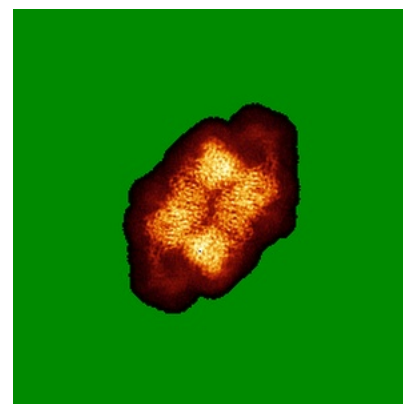
### 6.4.1 Primary map



X

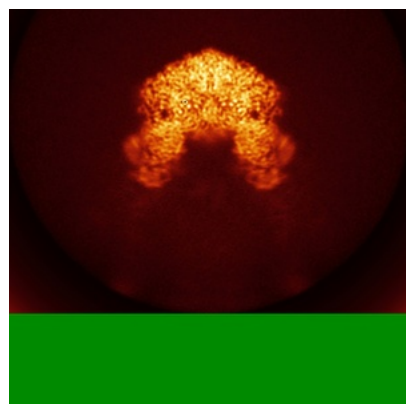


Y

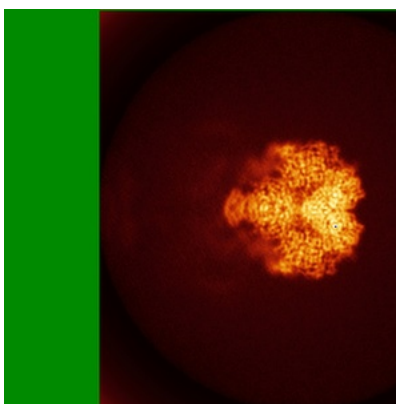


Z

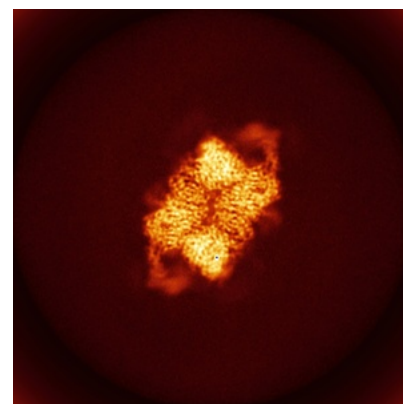
### 6.4.2 Raw map



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.

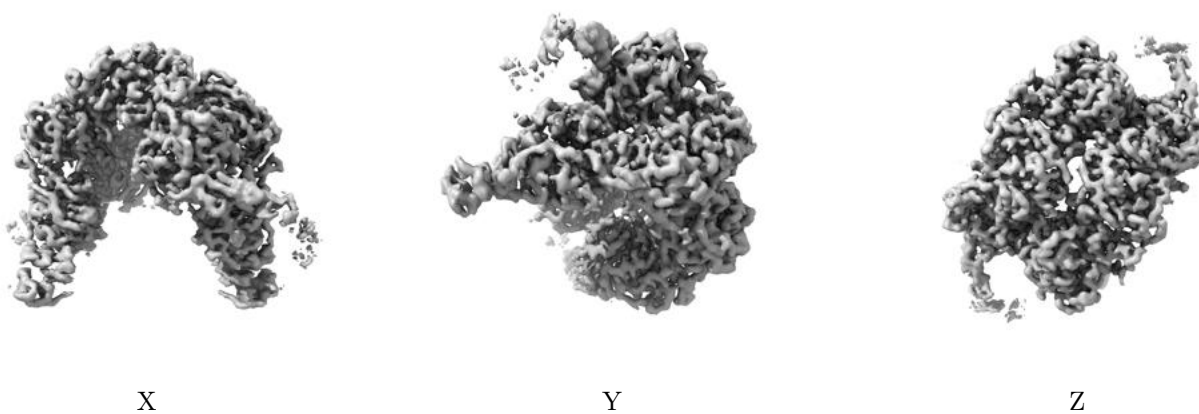
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0434. 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.

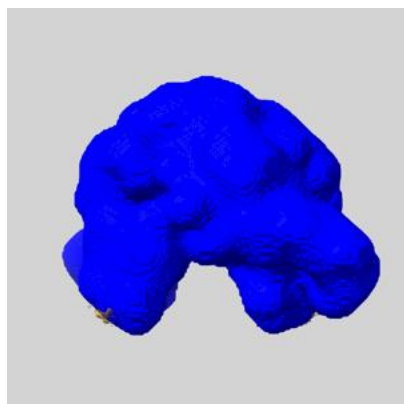
## 6.6 Mask visualisation [i](#)

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

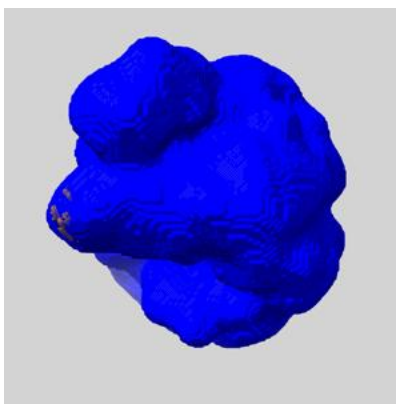
A mask typically either:

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

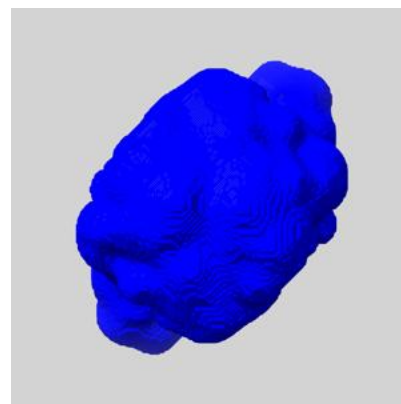
### 6.6.1 emd\_36692\_msk\_1.map [i](#)



X



Y

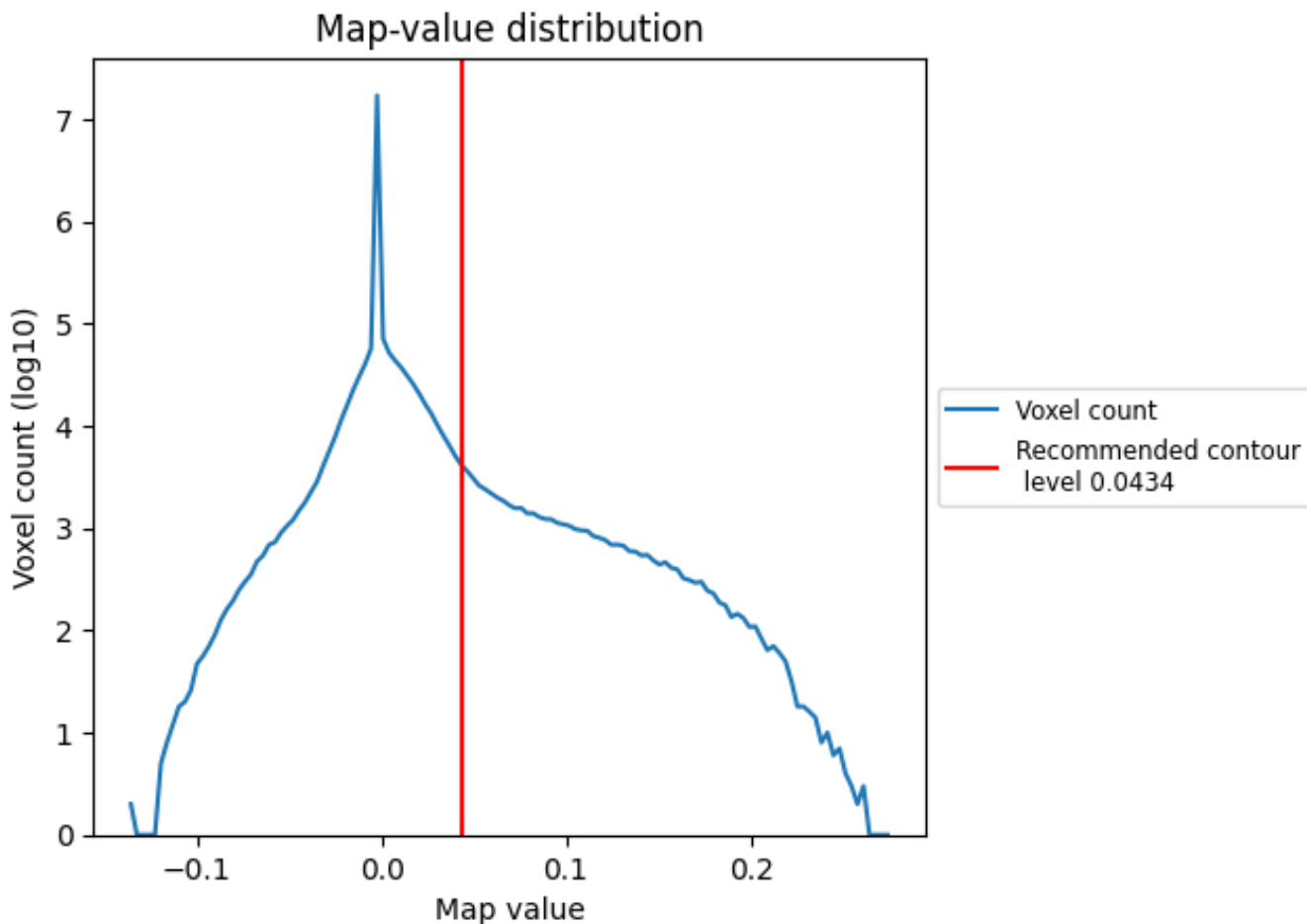


Z

## 7 Map analysis [i](#)

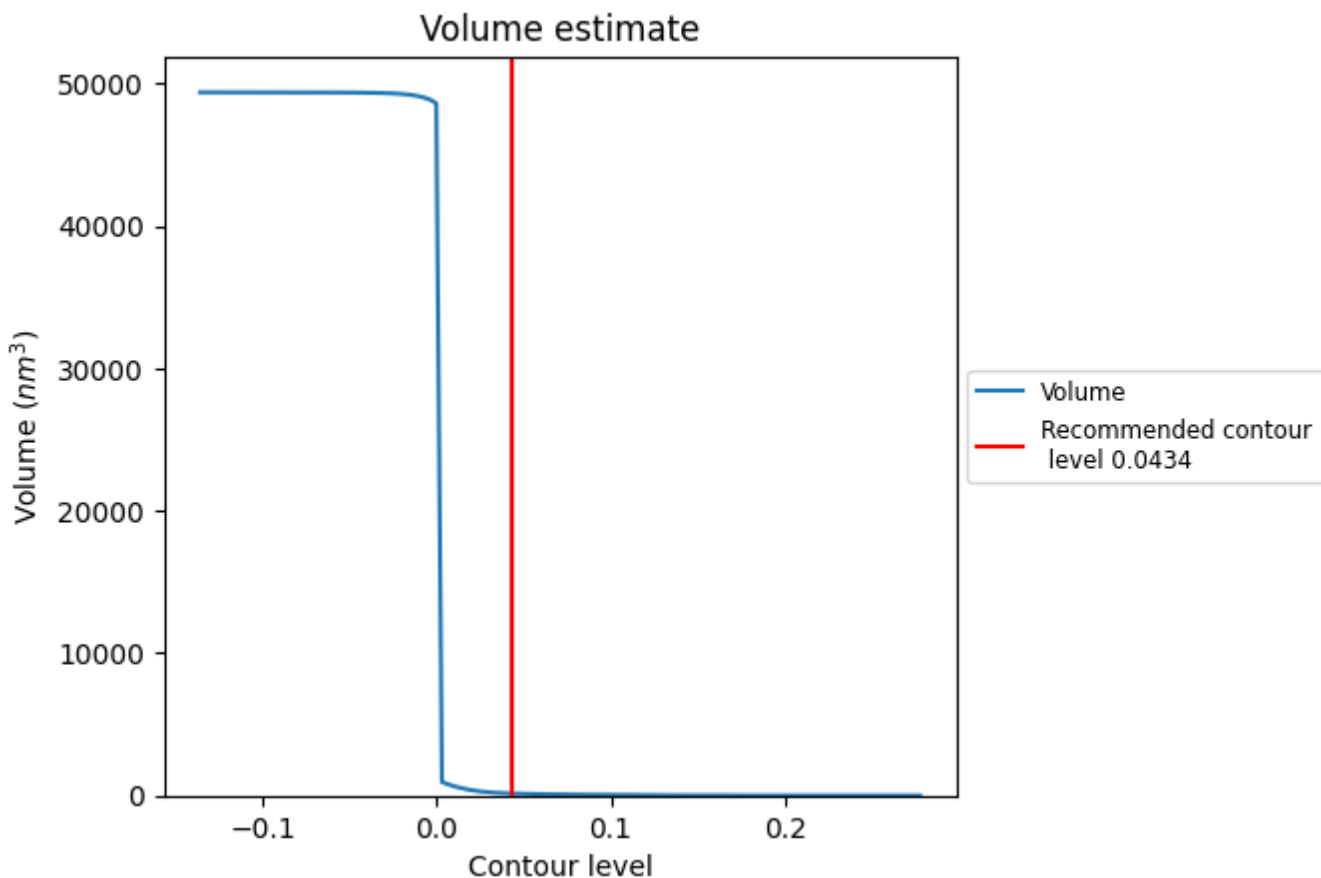
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

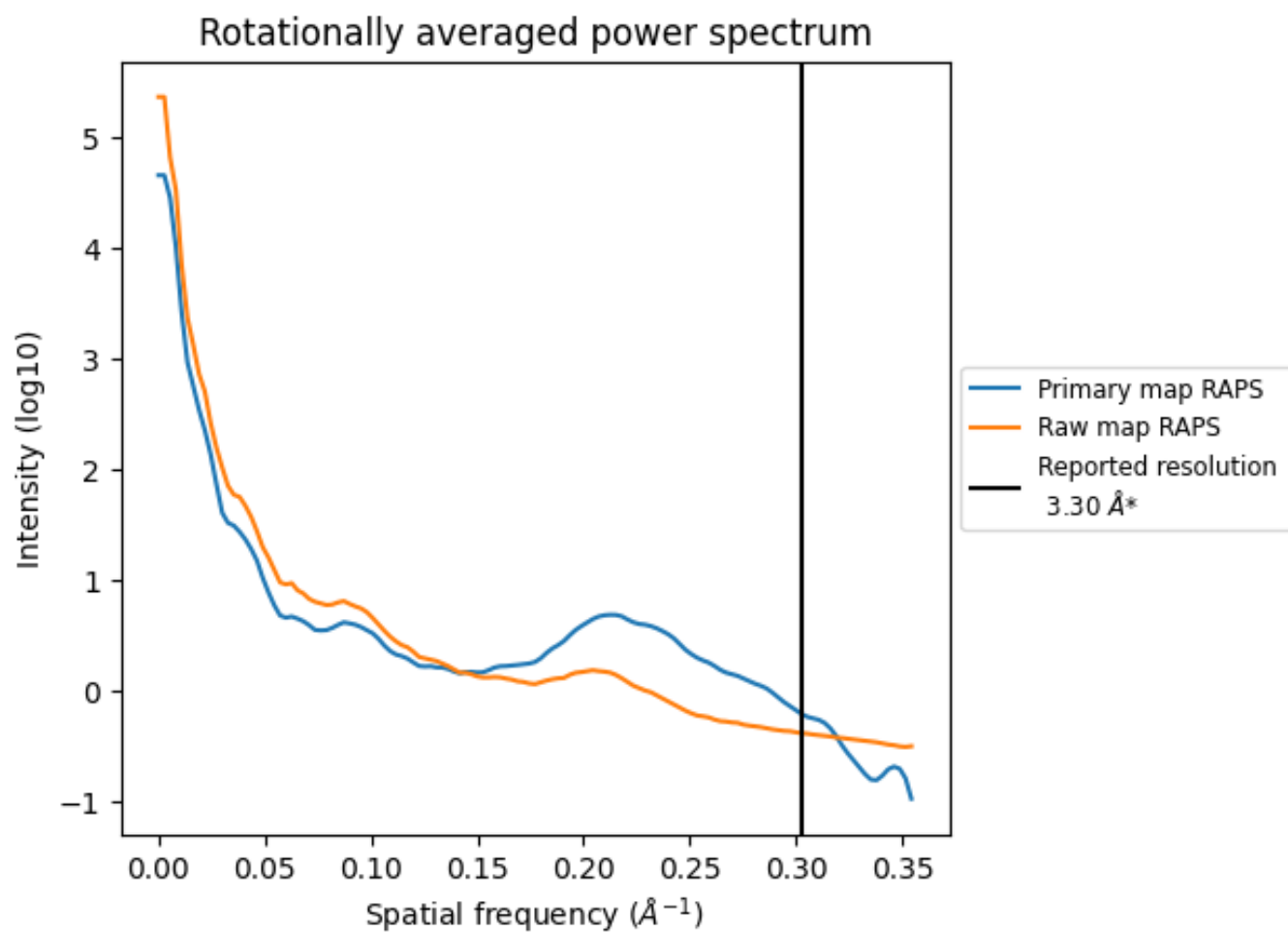


The volume at the recommended contour level is 144 nm<sup>3</sup>; this corresponds to an approximate mass of 130 kDa.

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 i

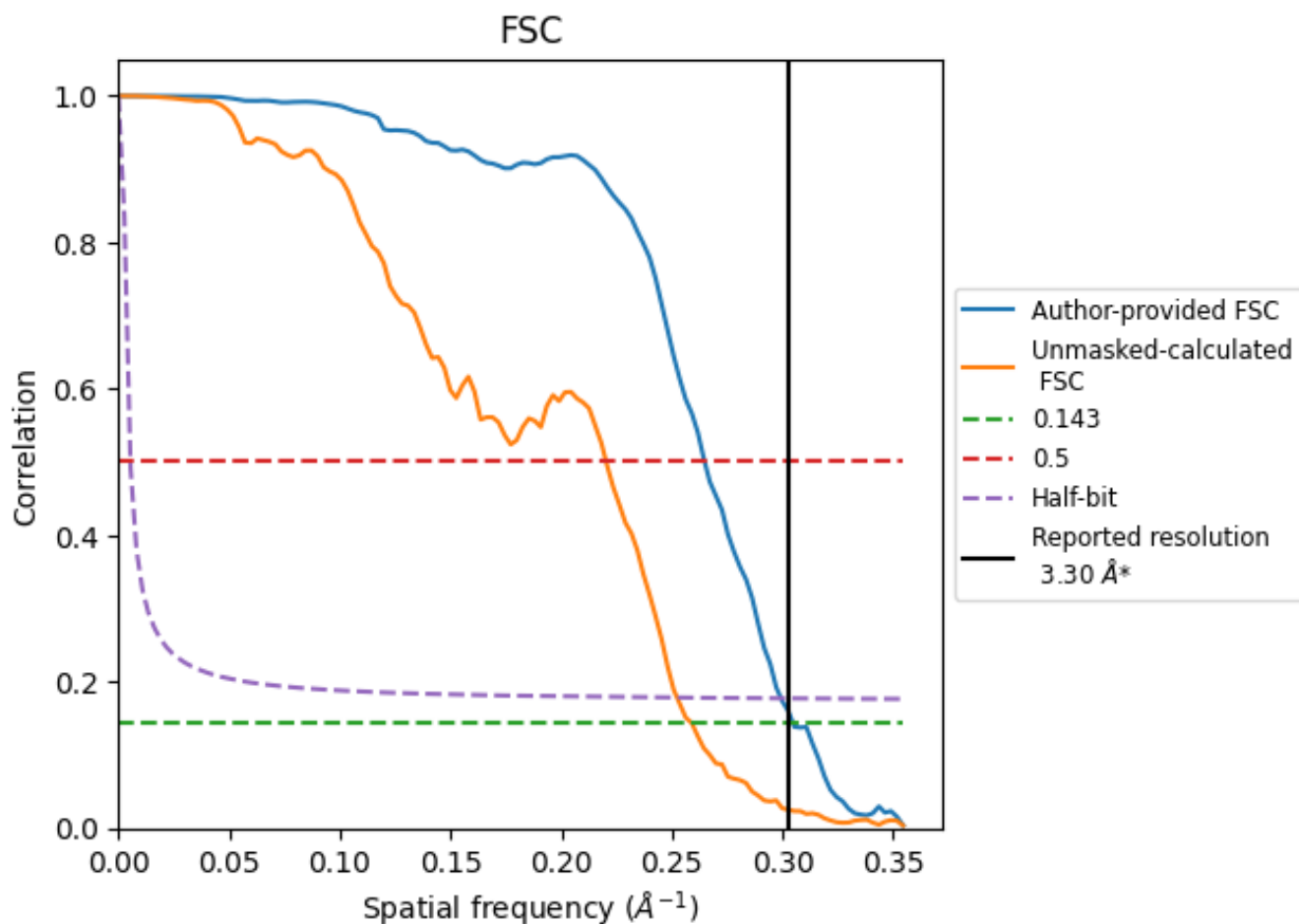


\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

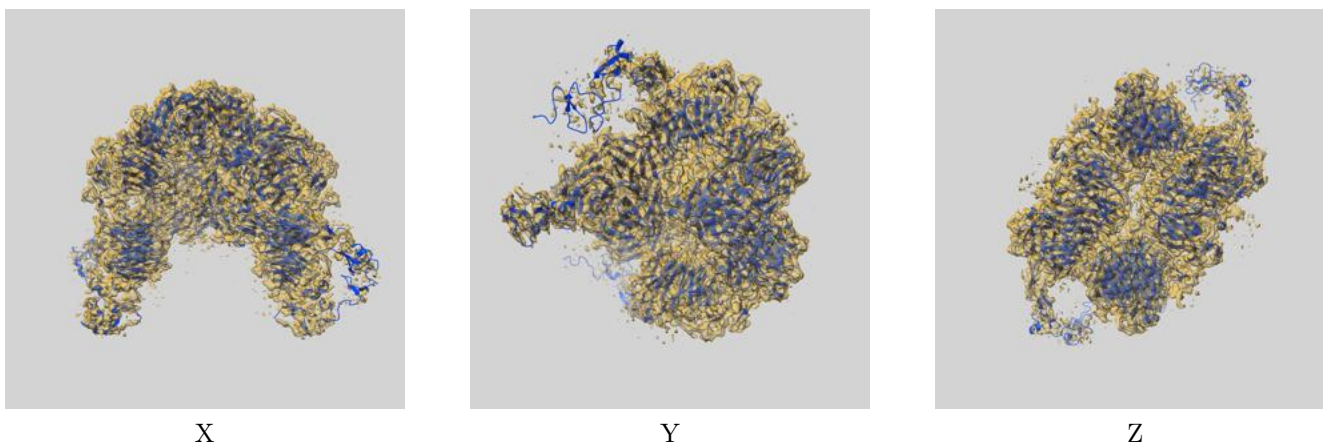
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.78	3.34
Unmasked-calculated*	3.86	4.54	3.96

\*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 3.86 differs from the reported value 3.3 by more than 10 %

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

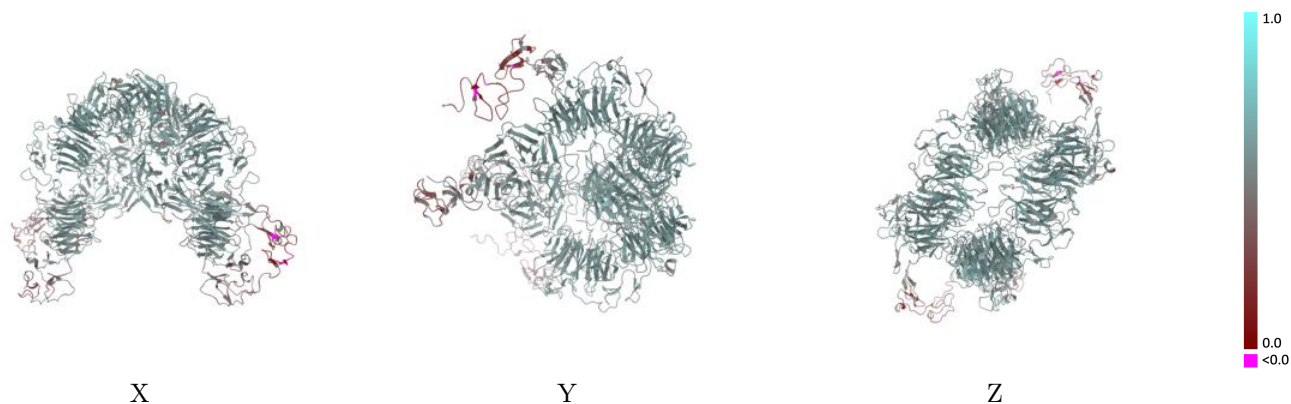
This section contains information regarding the fit between EMDB map EMD-36692 and PDB model 8JX8. Per-residue inclusion information can be found in section 3 on page 9.

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



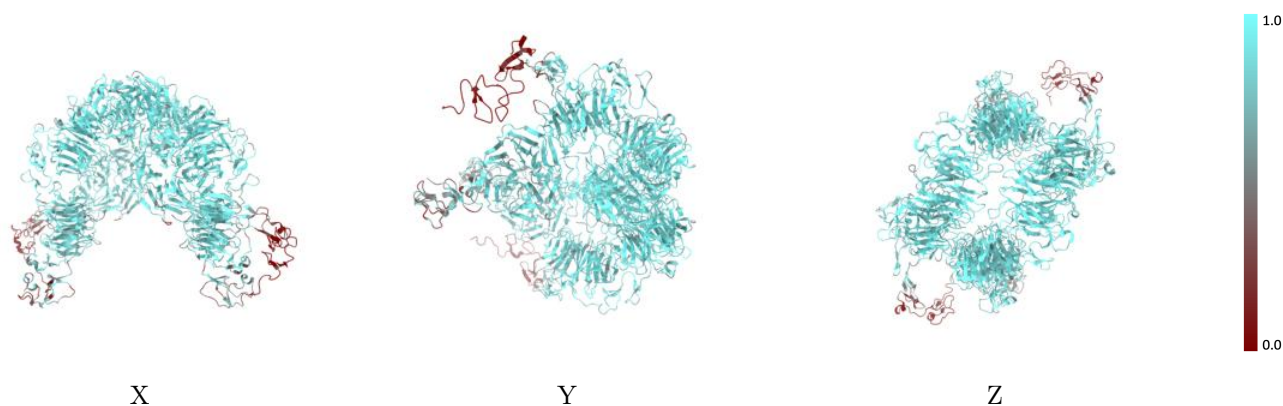
The images above show the 3D surface view of the map at the recommended contour level 0.0434 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



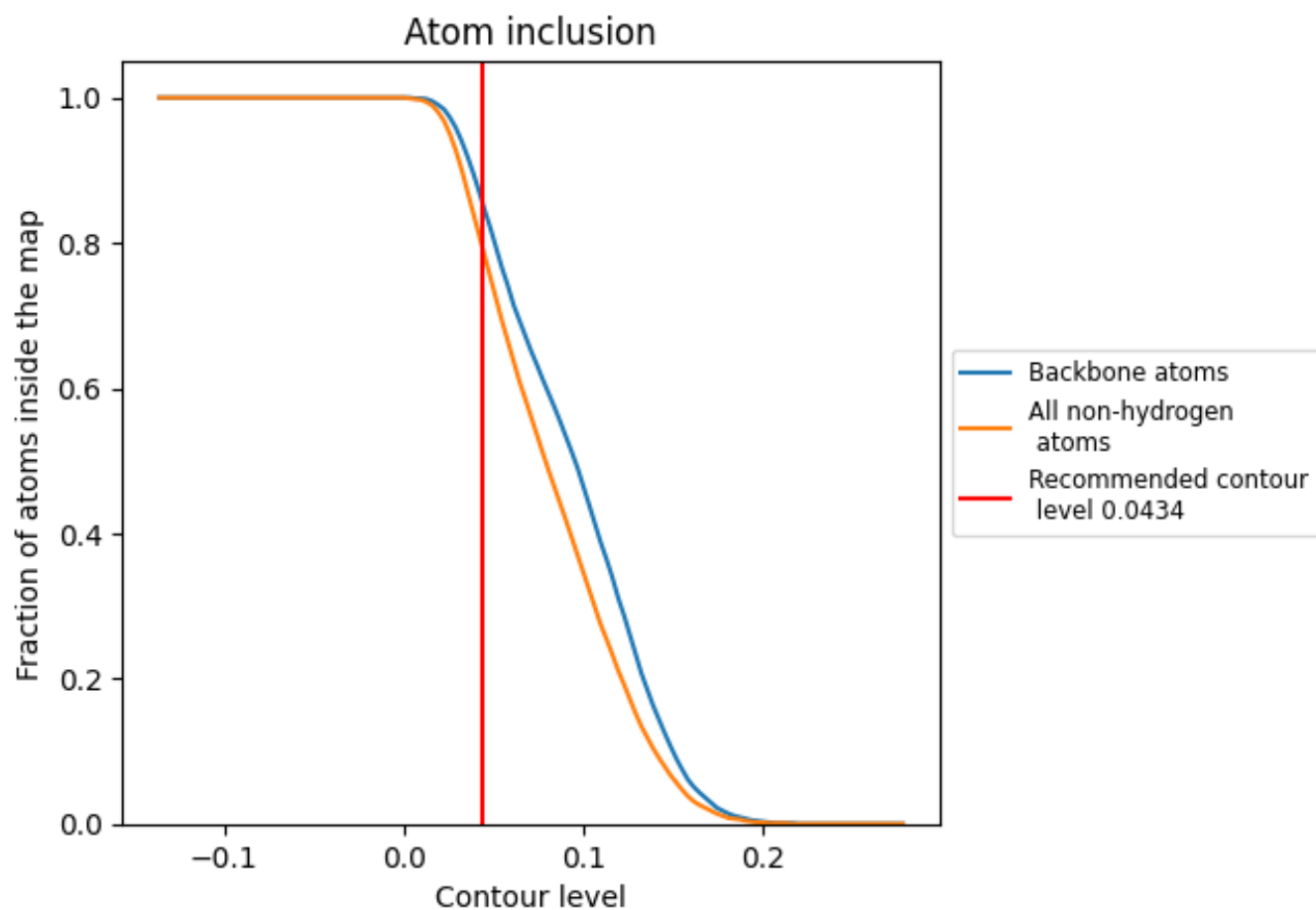
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0434).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.0434) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7970	 0.5380
A	 0.8060	 0.5410
B	 0.8070	 0.5410
C	 0.9090	 0.5370
D	 0.6250	 0.4240
E	 0.2860	 0.3370
F	 0.4100	 0.3670
G	 0.7270	 0.5130
H	 0.5000	 0.4870
I	 0.8180	 0.5400
J	 0.6880	 0.4810
K	 0.7270	 0.4210
L	 0.5710	 0.4560
M	 0.5000	 0.4690
N	 0.3570	 0.3910
O	 0.4750	 0.4530
P	 0.4290	 0.4410
Q	 0.7210	 0.5280
R	 0.4290	 0.4540
S	 0.5360	 0.4510
T	 0.4290	 0.4100
U	 0.5900	 0.4420
V	 0.5360	 0.4680
W	 0.2140	 0.3240
X	 0.3110	 0.4030
Y	 0.5000	 0.5350
Z	 0.7540	 0.5460
a	 0.3210	 0.3710
b	 0.5000	 0.4690

