



Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 09:56 AM EST

PDB ID : 7T9A
EMDB ID : EMD-25754
Title : ApexGT2 in complex with GT2-d42.16 and RM20A3 Fabs
Authors : Berndsen, Z.T.
Deposited on : 2021-12-18
Resolution : 3.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

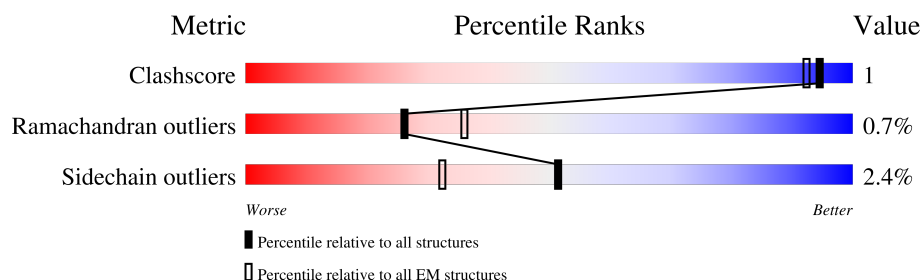
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.54 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.



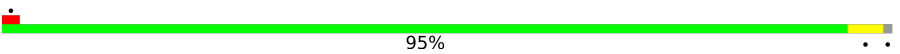

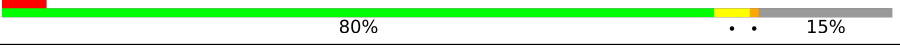



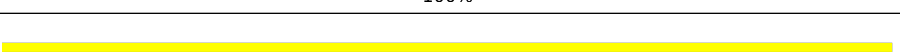

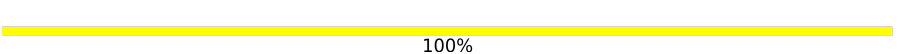
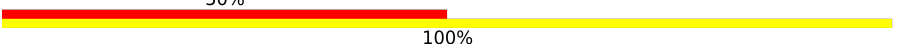

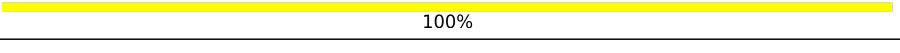
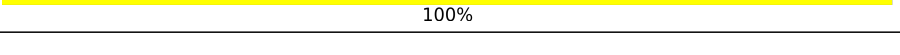
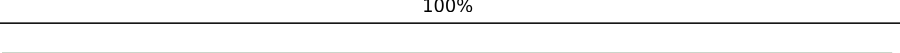
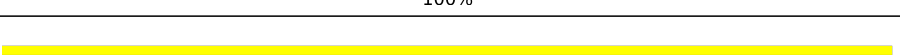
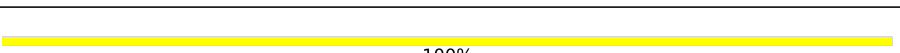
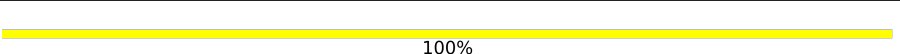

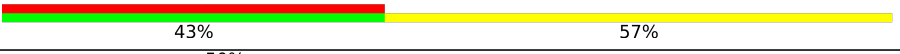
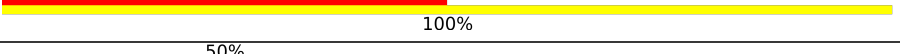
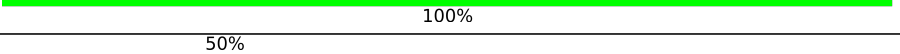
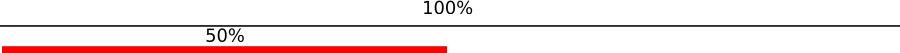
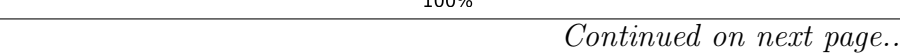


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	473	
1	C	473	
1	E	473	
2	B	162	
2	D	162	
2	F	162	
3	J	125	
3	M	125	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	O	125	 95%
4	K	128	 80% 15%
4	N	128	 80% 15%
4	P	128	 79% 5% 15%
5	H	134	 54% 91% 7%
6	L	107	 66% 91% 7%
7	G	2	 50% 100%
7	I	2	 100%
7	V	2	 50% 50%
7	W	2	 100%
7	X	2	 50% 100%
7	Z	2	 50% 50%
7	c	2	 100%
7	d	2	 100%
7	f	2	 100%
7	g	2	 100%
8	Q	4	 100%
8	Y	4	 100%
8	e	4	 100%
9	R	3	 33% 33% 67%
10	S	7	 43% 43% 57%
11	T	2	 50% 100%
11	U	2	 50% 100%
11	a	2	 50% 100%
11	b	2	 50% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	h	2	<div> <div></div> <div>50%</div> <div></div> <div>100%</div> </div>
11	i	2	<div> <div></div> <div>50%</div> <div></div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 21517 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 HIV Envelope ApexGT2 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	434	Total	C	N	O	S	0	0
			3418	2151	600	640	27		
1	C	433	Total	C	N	O	S	0	0
			3410	2147	598	638	27		
1	E	434	Total	C	N	O	S	0	0
			3418	2151	600	640	27		

- Molecule 2 is a protein called HIV Envelope ApexGT2 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			958	604	167	181	6		
2	D	120	Total	C	N	O	S	0	0
			958	604	167	181	6		
2	F	120	Total	C	N	O	S	0	0
			958	604	167	181	6		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	517	SER	PHE	conflict	UNP Q2N0S8
B	559	PRO	ILE	conflict	UNP Q2N0S8
B	561	PRO	ALA	conflict	UNP Q2N0S8
B	568	ASP	LEU	conflict	UNP Q2N0S8
B	570	HIS	VAL	conflict	UNP Q2N0S8
B	585	HIS	ARG	conflict	UNP Q2N0S8
B	605	CYS	THR	conflict	UNP Q2N0S8
B	665	GLY	-	expression tag	UNP Q2N0S8
B	666	THR	-	expression tag	UNP Q2N0S8
B	667	LYS	-	expression tag	UNP Q2N0S8
B	668	HIS	-	expression tag	UNP Q2N0S8
B	669	HIS	-	expression tag	UNP Q2N0S8
B	670	HIS	-	expression tag	UNP Q2N0S8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	671	HIS	-	expression tag	UNP Q2N0S8
B	672	HIS	-	expression tag	UNP Q2N0S8
B	673	HIS	-	expression tag	UNP Q2N0S8
D	517	SER	PHE	conflict	UNP Q2N0S8
D	559	PRO	ILE	conflict	UNP Q2N0S8
D	561	PRO	ALA	conflict	UNP Q2N0S8
D	568	ASP	LEU	conflict	UNP Q2N0S8
D	570	HIS	VAL	conflict	UNP Q2N0S8
D	585	HIS	ARG	conflict	UNP Q2N0S8
D	605	CYS	THR	conflict	UNP Q2N0S8
D	665	GLY	-	expression tag	UNP Q2N0S8
D	666	THR	-	expression tag	UNP Q2N0S8
D	667	LYS	-	expression tag	UNP Q2N0S8
D	668	HIS	-	expression tag	UNP Q2N0S8
D	669	HIS	-	expression tag	UNP Q2N0S8
D	670	HIS	-	expression tag	UNP Q2N0S8
D	671	HIS	-	expression tag	UNP Q2N0S8
D	672	HIS	-	expression tag	UNP Q2N0S8
D	673	HIS	-	expression tag	UNP Q2N0S8
F	517	SER	PHE	conflict	UNP Q2N0S8
F	559	PRO	ILE	conflict	UNP Q2N0S8
F	561	PRO	ALA	conflict	UNP Q2N0S8
F	568	ASP	LEU	conflict	UNP Q2N0S8
F	570	HIS	VAL	conflict	UNP Q2N0S8
F	585	HIS	ARG	conflict	UNP Q2N0S8
F	605	CYS	THR	conflict	UNP Q2N0S8
F	665	GLY	-	expression tag	UNP Q2N0S8
F	666	THR	-	expression tag	UNP Q2N0S8
F	667	LYS	-	expression tag	UNP Q2N0S8
F	668	HIS	-	expression tag	UNP Q2N0S8
F	669	HIS	-	expression tag	UNP Q2N0S8
F	670	HIS	-	expression tag	UNP Q2N0S8
F	671	HIS	-	expression tag	UNP Q2N0S8
F	672	HIS	-	expression tag	UNP Q2N0S8
F	673	HIS	-	expression tag	UNP Q2N0S8

- Molecule 3 is a protein called RM20A3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	124	Total	C	N	O	S	0	0
			943	595	161	182	5		
3	M	124	Total	C	N	O	S	0	0
			943	595	161	182	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	124	Total	C	N	O	S	0	0
			943	595	161	182	5		

- Molecule 4 is a protein called RM20A3 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	109	Total	C	N	O	S	0	0
			811	505	136	167	3		
4	N	109	Total	C	N	O	S	0	0
			811	505	136	167	3		
4	P	109	Total	C	N	O	S	0	0
			811	505	136	167	3		

- Molecule 5 is a protein called GT2-d42.16 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	132	Total	C	N	O	S	0	0
			1052	664	170	212	6		

- Molecule 6 is a protein called GT2-d42.16 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	106	Total	C	N	O	S	0	0
			799	502	134	161	2		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



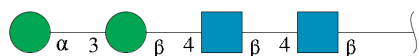
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	I	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

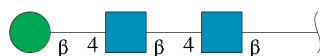
Mol	Chain	Residues	Atoms				AltConf	Trace
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	f	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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	Q	4	Total	C	N	O	0	0
			50	28	2	20		
8	Y	4	Total	C	N	O	0	0
			50	28	2	20		
8	e	4	Total	C	N	O	0	0
			50	28	2	20		

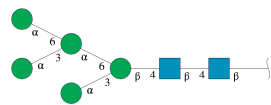
- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyra

nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



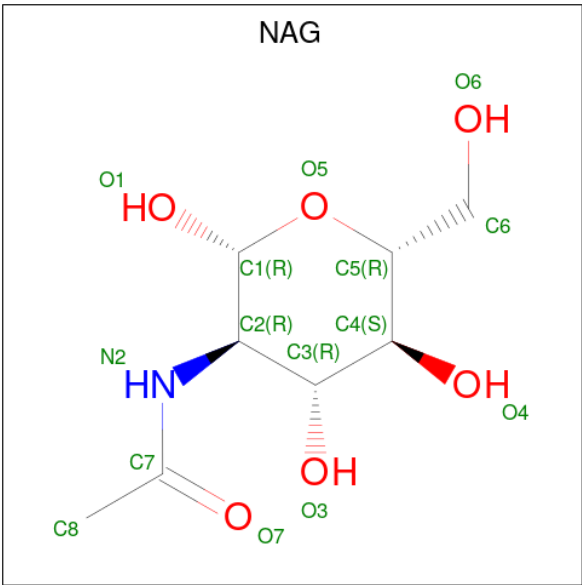
Mol	Chain	Residues	Atoms				AltConf	Trace
10	S	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	T	2	Total	C	N	O	0	0
			24	14	1	9		
11	U	2	Total	C	N	O	0	0
			24	14	1	9		
11	a	2	Total	C	N	O	0	0
			24	14	1	9		
11	b	2	Total	C	N	O	0	0
			24	14	1	9		
11	h	2	Total	C	N	O	0	0
			24	14	1	9		
11	i	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	A	1	Total	C	N	O	0
			168	96	12	60	
12	B	1	Total	C	N	O	0
			28	16	2	10	
12	B	1	Total	C	N	O	0
			28	16	2	10	

Continued on next page...

Continued from previous page...

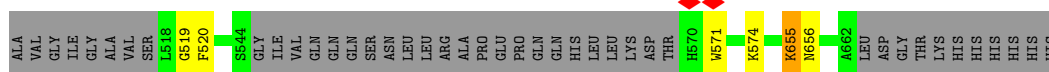
Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	C	1	Total 168	C 96	N 12	O 60	0
12	D	1	Total 28	C 16	N 2	O 10	0
12	D	1	Total 28	C 16	N 2	O 10	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0

Continued on next page...

Continued from previous page...

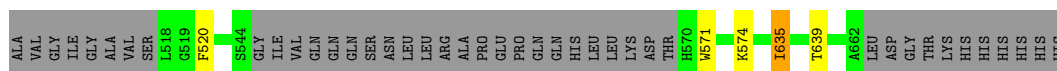
Mol	Chain	Residues	Atoms				AltConf
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	E	1	Total 168	C 96	N 12	O 60	0
12	F	1	Total 28	C 16	N 2	O 10	0
12	F	1	Total 28	C 16	N 2	O 10	0

Chain B:  70% 26%



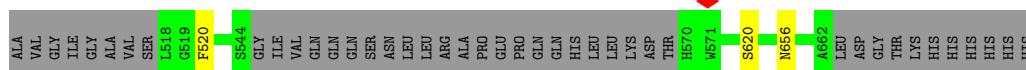
- Molecule 2: HIV Envelope ApexGT2 gp41

Chain D:  71% 26%



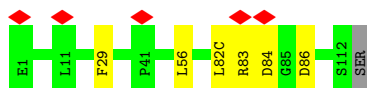
- Molecule 2: HIV Envelope ApexGT2 gp41

Chain F:  72% 26%



- Molecule 3: RM20A3 Fab Heavy Chain

Chain J:  94% 5%



- Molecule 3: RM20A3 Fab Heavy Chain

Chain M:  94% 6%




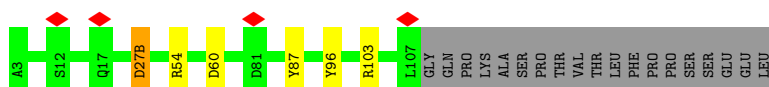
- Molecule 3: RM20A3 Fab Heavy Chain

Chain O:  95% 2%

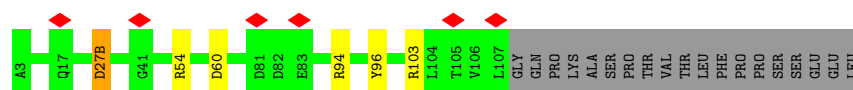
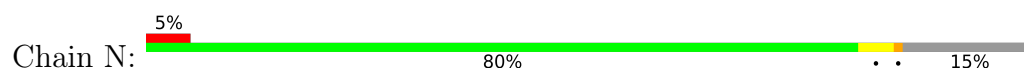


- Molecule 4: RM20A3 Fab Light Chain

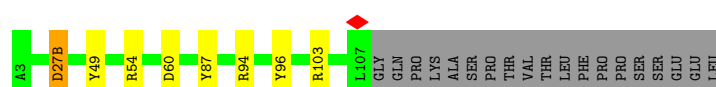
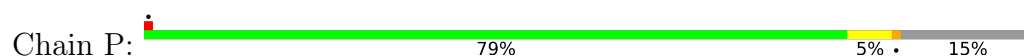
Chain K:  80% 15%



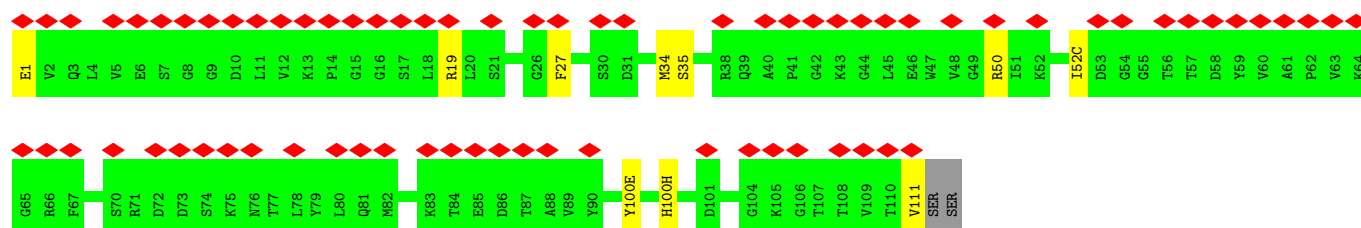
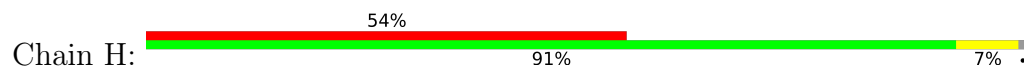
- Molecule 4: RM20A3 Fab Light Chain



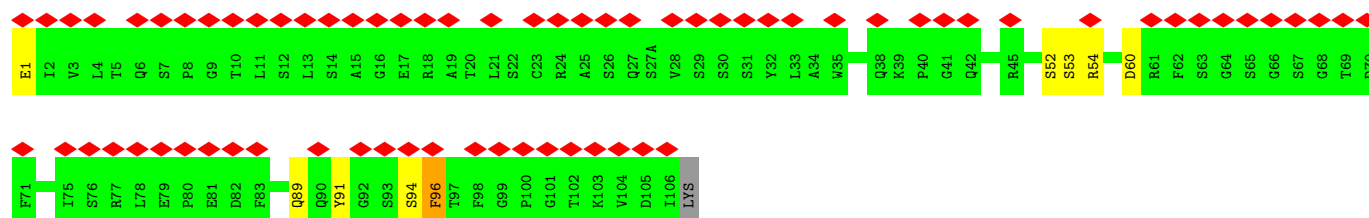
- Molecule 4: RM20A3 Fab Light Chain



- Molecule 5: GT2-d42.16 Fab Heavy Chain



- Molecule 6: GT2-d42.16 Fab Light Chain



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



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





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



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



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



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



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



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



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

Chain f:  100%

NAG1
NAG2

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

Chain g:  100%

NAG1
NAG2

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

Chain Q:  100%

NAG1
NAG2
BMA3
MAN4

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

Chain Y:  100%

NAG1
NAG2
BMA3
MAN4

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

Chain e:  100%

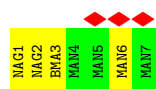
NAG1
NAG2
BMA3
MAN4

- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  33% 33% 67%

NAG1
NAG2
BMA3

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



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62971	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.155	Depositor
Minimum map value	-0.453	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.237	Depositor
Map size (Å)	360.5, 360.5, 360.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.00	4/3490 (0.1%)	0.89	8/4744 (0.2%)
1	C	1.01	0/3482	0.91	9/4733 (0.2%)
1	E	0.98	2/3489 (0.1%)	0.87	8/4741 (0.2%)
2	B	0.99	1/977 (0.1%)	0.75	0/1325
2	D	0.98	1/977 (0.1%)	0.74	0/1325
2	F	1.01	1/977 (0.1%)	0.72	0/1325
3	J	1.10	1/963 (0.1%)	0.95	2/1300 (0.2%)
3	M	1.09	1/963 (0.1%)	0.93	1/1300 (0.1%)
3	O	1.12	2/963 (0.2%)	0.94	0/1300
4	K	1.13	3/830 (0.4%)	1.00	3/1129 (0.3%)
4	N	1.11	2/830 (0.2%)	0.96	2/1129 (0.2%)
4	P	1.12	4/830 (0.5%)	0.98	2/1129 (0.2%)
5	H	1.03	4/1044 (0.4%)	0.92	2/1415 (0.1%)
6	L	0.91	1/816 (0.1%)	0.96	1/1106 (0.1%)
All	All	1.03	27/20631 (0.1%)	0.89	38/28001 (0.1%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	27(B)	ASP	CB-CG	-7.70	1.35	1.51
6	L	1	GLU	CB-CG	6.89	1.65	1.52
4	N	27(B)	ASP	CB-CG	-6.60	1.37	1.51
2	D	520	PHE	CB-CG	-6.55	1.40	1.51
5	H	111	VAL	CB-CG2	6.41	1.66	1.52
2	F	520	PHE	CB-CG	-6.40	1.40	1.51
4	K	96	TYR	CB-CG	-6.29	1.42	1.51
4	P	27(B)	ASP	CB-CG	-6.21	1.38	1.51
4	N	96	TYR	CB-CG	-6.09	1.42	1.51
2	B	520	PHE	CB-CG	-6.00	1.41	1.51
5	H	34	MET	CG-SD	-5.80	1.66	1.81
4	P	96	TYR	CB-CG	-5.68	1.43	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	27	PHE	CB-CG	-5.64	1.41	1.51
1	E	503	ARG	NE-CZ	5.57	1.40	1.33
1	A	247	CYS	CB-SG	-5.52	1.72	1.81
5	H	1	GLU	CB-CG	5.50	1.62	1.52
3	J	29	PHE	CB-CG	-5.46	1.42	1.51
3	M	1	GLU	CB-CG	5.45	1.62	1.52
3	O	1	GLU	CB-CG	5.44	1.62	1.52
4	K	87	TYR	CB-CG	-5.42	1.43	1.51
4	P	87	TYR	CB-CG	-5.41	1.43	1.51
4	P	49	TYR	CB-CG	-5.18	1.43	1.51
1	E	42	VAL	CB-CG1	-5.15	1.42	1.52
1	A	503	ARG	NE-CZ	5.11	1.39	1.33
3	O	29	PHE	CB-CG	-5.10	1.42	1.51
1	A	102	GLU	CD-OE2	-5.07	1.20	1.25
1	A	42	VAL	CB-CG1	-5.04	1.42	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	151	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	C	166	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	E	151	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	C	166	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	C	151	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	C	40	TYR	CB-CG-CD1	-7.94	116.23	121.00
1	E	151	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	C	476	ARG	NE-CZ-NH2	-7.82	116.39	120.30
6	L	54	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	C	327	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	E	469	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	476	ARG	NE-CZ-NH2	-7.15	116.73	120.30
5	H	19	ARG	NE-CZ-NH2	-6.78	116.91	120.30
4	K	27(B)	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	C	469	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	E	503	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	469	ARG	NE-CZ-NH2	-6.54	117.03	120.30
4	P	54	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	327	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	456	ARG	NE-CZ-NH2	-6.20	117.20	120.30
4	K	54	ARG	NE-CZ-NH2	-6.19	117.21	120.30
5	H	50	ARG	NE-CZ-NH2	-6.09	117.26	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	86	ASP	CB-CG-OD1	6.05	123.75	118.30
4	N	54	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	E	480	ARG	NE-CZ-NH1	5.99	123.29	120.30
3	J	83	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	503	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	M	83	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	E	273	ARG	NE-CZ-NH1	5.39	122.99	120.30
4	N	103	ARG	NE-CZ-NH2	-5.33	117.64	120.30
4	P	103	ARG	NE-CZ-NH2	-5.27	117.66	120.30
4	K	103	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	169	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	469	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	469	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	298	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	E	480	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3418	0	3355	11	0
1	C	3410	0	3351	10	0
1	E	3418	0	3357	8	0
2	B	958	0	923	5	0
2	D	958	0	923	2	0
2	F	958	0	924	2	0
3	J	943	0	915	2	0
3	M	943	0	915	3	0
3	O	943	0	915	1	0
4	K	811	0	767	1	0
4	N	811	0	767	1	0
4	P	811	0	767	1	0
5	H	1052	0	976	0	0
6	L	799	0	771	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	28	0	25	0	0
7	I	28	0	25	0	0
7	V	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0
7	Z	28	0	25	1	0
7	c	28	0	25	0	0
7	d	28	0	25	0	0
7	f	28	0	25	0	0
7	g	28	0	25	0	0
8	Q	50	0	43	0	0
8	Y	50	0	43	0	0
8	e	50	0	43	0	0
9	R	39	0	34	0	0
10	S	83	0	70	0	0
11	T	24	0	22	0	0
11	U	24	0	22	0	0
11	a	24	0	22	0	0
11	b	24	0	22	0	0
11	h	24	0	22	0	0
11	i	24	0	22	0	0
12	A	168	0	156	0	0
12	B	28	0	26	0	0
12	C	168	0	156	1	0
12	D	28	0	26	0	0
12	E	168	0	156	0	0
12	F	28	0	26	1	0
All	All	21517	0	20787	43	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 1.

All (43) 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)
6:L:94:SER:C	6:L:96:PHE:N	2.38	0.76
1:A:55:ALA:HA	1:A:76:PRO:HD2	1.68	0.73
1:C:68:VAL:N	1:C:208:VAL:HG13	2.09	0.68
1:C:69:TRP:CH2	1:C:108:ILE:HG23	2.30	0.66
1:A:123:THR:N	1:A:124:PRO:CD	2.66	0.58
1:C:198:THR:HB	12:C:611:NAG:H82	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:84:ASP:N	3:J:84:ASP:OD1	2.37	0.57
1:C:123:THR:N	1:C:124:PRO:CD	2.67	0.56
3:O:84:ASP:OD1	3:O:84:ASP:N	2.37	0.55
3:M:84:ASP:N	3:M:84:ASP:OD1	2.37	0.55
1:E:123:THR:N	1:E:124:PRO:CD	2.70	0.55
1:C:134:VAL:HG13	7:Z:1:NAG:H81	1.89	0.55
1:C:107:ASP:OD1	2:D:574:LYS:NZ	2.43	0.52
2:F:620:SER:HB3	12:F:702:NAG:H62	1.92	0.51
1:E:474:ASP:OD1	1:E:475:MET:N	2.45	0.49
2:B:656:ASN:HB3	3:M:56:LEU:HD21	1.95	0.48
1:C:69:TRP:HH2	1:C:108:ILE:HG23	1.78	0.48
1:A:56:SER:H	1:A:75:VAL:HB	1.79	0.47
1:A:74:CYS:HB2	2:B:571:TRP:HE1	1.79	0.47
3:J:56:LEU:HD21	2:F:656:ASN:HB3	1.95	0.47
1:E:69:TRP:HZ3	1:E:108:ILE:HG23	1.80	0.45
6:L:91:TYR:CG	6:L:91:TYR:O	2.69	0.45
4:N:60:ASP:OD1	4:N:60:ASP:N	2.48	0.45
1:A:106:GLU:OE2	2:B:574:LYS:NZ	2.50	0.45
2:B:655:LYS:HA	2:B:655:LYS:HD2	1.58	0.45
1:E:95:MET:HG3	1:E:96:TRP:CE3	2.54	0.42
1:C:71:THR:HG21	2:D:571:TRP:CD1	2.54	0.42
4:P:60:ASP:N	4:P:60:ASP:OD1	2.48	0.42
1:A:53:PHE:HE1	1:A:76:PRO:HG3	1.85	0.42
1:C:117:LYS:N	1:C:118:PRO:CD	2.83	0.42
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.85	0.42
1:E:77:THR:HB	1:E:79:PRO:HD3	2.00	0.42
1:A:84:ILE:HD12	2:B:519:GLY:HA3	2.01	0.42
6:L:60:ASP:N	6:L:60:ASP:OD1	2.49	0.42
1:E:117:LYS:N	1:E:118:PRO:CD	2.83	0.42
1:A:187:ASN:HD22	1:A:187:ASN:HA	1.55	0.41
3:M:61:ASP:OD1	3:M:61:ASP:N	2.52	0.41
4:K:60:ASP:N	4:K:60:ASP:OD1	2.47	0.41
1:E:100:MET:HE2	1:E:100:MET:HB3	1.92	0.41
1:A:232:LYS:NZ	1:A:269:GLU:OE2	2.52	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.90	0.40
1:E:104:MET:HG2	1:E:108:ILE:HD12	2.01	0.40
1:A:117:LYS:N	1:A:118:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/473 (90%)	403 (95%)	19 (4%)	4 (1%)	17	58
1	C	425/473 (90%)	410 (96%)	13 (3%)	2 (0%)	29	68
1	E	424/473 (90%)	401 (95%)	19 (4%)	4 (1%)	17	58
2	B	116/162 (72%)	114 (98%)	2 (2%)	0	100	100
2	D	116/162 (72%)	111 (96%)	4 (3%)	1 (1%)	17	58
2	F	116/162 (72%)	114 (98%)	2 (2%)	0	100	100
3	J	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	19	60
3	M	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	19	60
3	O	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	19	60
4	K	107/128 (84%)	101 (94%)	5 (5%)	1 (1%)	17	58
4	N	107/128 (84%)	101 (94%)	5 (5%)	1 (1%)	17	58
4	P	107/128 (84%)	101 (94%)	5 (5%)	1 (1%)	17	58
5	H	128/134 (96%)	125 (98%)	3 (2%)	0	100	100
6	L	102/107 (95%)	98 (96%)	3 (3%)	1 (1%)	15	55
All	All	2540/2905 (87%)	2431 (96%)	91 (4%)	18 (1%)	26	62

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	82(C)	LEU
3	M	82(C)	LEU
1	E	79	PRO
3	O	82(C)	LEU
4	K	27(B)	ASP
4	P	27(B)	ASP
1	A	426	MET
1	A	465	THR
1	C	426	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	N	27(B)	ASP
1	A	55	ALA
1	A	77	THR
6	L	52	SER
1	C	465	THR
1	E	81	PRO
1	E	426	MET
1	E	465	THR
2	D	635	ILE

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	389/420 (93%)	375 (96%)	14 (4%)	35	67
1	C	388/420 (92%)	378 (97%)	10 (3%)	46	75
1	E	389/420 (93%)	373 (96%)	16 (4%)	30	64
2	B	103/138 (75%)	102 (99%)	1 (1%)	76	89
2	D	103/138 (75%)	101 (98%)	2 (2%)	57	80
2	F	103/138 (75%)	103 (100%)	0	100	100
3	J	101/102 (99%)	101 (100%)	0	100	100
3	M	101/102 (99%)	100 (99%)	1 (1%)	76	89
3	O	101/102 (99%)	100 (99%)	1 (1%)	76	89
4	K	89/106 (84%)	89 (100%)	0	100	100
4	N	89/106 (84%)	88 (99%)	1 (1%)	73	88
4	P	89/106 (84%)	88 (99%)	1 (1%)	73	88
5	H	109/111 (98%)	106 (97%)	3 (3%)	43	73
6	L	87/88 (99%)	84 (97%)	3 (3%)	37	69
All	All	2241/2497 (90%)	2188 (98%)	53 (2%)	51	76

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS
1	A	57	ASP
1	A	72	HIS
1	A	115	SER
1	A	129	LEU
1	A	137	ASN
1	A	158	SER
1	A	184	MET
1	A	187	ASN
1	A	198	THR
1	A	199	SER
1	A	201	ILE
1	A	213	ILE
1	A	322	ASP
2	B	655	LYS
1	C	54	CYS
1	C	71	THR
1	C	129	LEU
1	C	137	ASN
1	C	169	ARG
1	C	184	MET
1	C	187	ASN
1	C	188	SER
1	C	201	ILE
1	C	245	VAL
2	D	635	ILE
2	D	639	THR
3	M	52	ASN
4	N	94	ARG
1	E	54	CYS
1	E	68	VAL
1	E	69	TRP
1	E	71	THR
1	E	77	THR
1	E	129	LEU
1	E	137	ASN
1	E	182	VAL
1	E	188	SER
1	E	192	ARG
1	E	199	SER
1	E	201	ILE
1	E	211	GLU
1	E	215	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	423	ILE
1	E	500	ARG
3	O	52	ASN
4	P	94	ARG
5	H	35	SER
5	H	52(C)	ILE
5	H	100(H)	HIS
6	L	53	SER
6	L	89	GLN
6	L	96	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	82	GLN
1	A	187	ASN
1	A	425	ASN
3	J	52	ASN
3	O	52	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
5	TYS	H	100(E)	5	15,16,17	2.90	7 (46%)	18,22,24	0.71	0
5	TYS	H	100(I)	5	15,16,17	0.56	0	18,22,24	0.96	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
5	TYS	H	100(E)	5	-	0/10/11/13	0/1/1/1
5	TYS	H	100(I)	5	-	0/10/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	100(E)	TYS	CD1-CG	4.97	1.49	1.38
5	H	100(E)	TYS	CE1-CZ	4.60	1.47	1.38
5	H	100(E)	TYS	CE2-CZ	4.50	1.47	1.38
5	H	100(E)	TYS	CD2-CG	4.29	1.48	1.38
5	H	100(E)	TYS	CE1-CD1	3.86	1.45	1.38
5	H	100(E)	TYS	CE2-CD2	3.83	1.45	1.38
5	H	100(E)	TYS	CB-CG	2.11	1.56	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

54 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
7	NAG	G	1	7,1	14,14,15	2.04	5 (35%)	17,19,21	0.96	0
7	NAG	G	2	7	14,14,15	1.88	5 (35%)	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	I	1	7,1	14,14,15	2.14	7 (50%)	17,19,21	3.59	6 (35%)
7	NAG	I	2	7	14,14,15	1.90	6 (42%)	17,19,21	0.95	1 (5%)
8	NAG	Q	1	8,1	14,14,15	2.01	5 (35%)	17,19,21	1.18	3 (17%)
8	NAG	Q	2	8	14,14,15	1.82	5 (35%)	17,19,21	0.88	0
8	BMA	Q	3	8	11,11,12	0.77	0	15,15,17	0.87	1 (6%)
8	MAN	Q	4	8	11,11,12	1.97	5 (45%)	15,15,17	0.72	0
9	NAG	R	1	9,1	14,14,15	0.45	0	17,19,21	1.16	2 (11%)
9	NAG	R	2	9	14,14,15	0.53	0	17,19,21	1.05	2 (11%)
9	BMA	R	3	9	11,11,12	0.24	0	15,15,17	0.68	0
10	NAG	S	1	10,1	14,14,15	0.36	0	17,19,21	1.39	1 (5%)
10	NAG	S	2	10	14,14,15	0.37	0	17,19,21	0.91	2 (11%)
10	BMA	S	3	10	11,11,12	0.22	0	15,15,17	0.86	1 (6%)
10	MAN	S	4	10	11,11,12	0.28	0	15,15,17	1.06	0
10	MAN	S	5	10	11,11,12	0.29	0	15,15,17	0.64	0
10	MAN	S	6	10	11,11,12	0.23	0	15,15,17	1.25	1 (6%)
10	MAN	S	7	10	11,11,12	0.21	0	15,15,17	0.65	0
11	NAG	T	1	11,2	14,14,15	0.48	0	17,19,21	1.06	1 (5%)
11	FUC	T	2	11	10,10,11	0.32	0	14,14,16	0.97	1 (7%)
11	NAG	U	1	11,2	14,14,15	0.33	0	17,19,21	0.74	0
11	FUC	U	2	11	10,10,11	0.24	0	14,14,16	0.60	0
7	NAG	V	1	7,1	14,14,15	0.37	0	17,19,21	0.92	0
7	NAG	V	2	7	14,14,15	0.33	0	17,19,21	0.65	1 (5%)
7	NAG	W	1	7,1	14,14,15	2.02	5 (35%)	17,19,21	1.03	0
7	NAG	W	2	7	14,14,15	1.90	5 (35%)	17,19,21	0.96	1 (5%)
7	NAG	X	1	7,1	14,14,15	2.13	7 (50%)	17,19,21	3.21	5 (29%)
7	NAG	X	2	7	14,14,15	1.91	5 (35%)	17,19,21	0.96	1 (5%)
8	NAG	Y	1	8,1	14,14,15	1.95	3 (21%)	17,19,21	1.14	3 (17%)
8	NAG	Y	2	8	14,14,15	1.85	5 (35%)	17,19,21	0.93	1 (5%)
8	BMA	Y	3	8	11,11,12	0.73	0	15,15,17	0.79	1 (6%)
8	MAN	Y	4	8	11,11,12	1.97	5 (45%)	15,15,17	0.68	0
7	NAG	Z	1	7,1	14,14,15	1.89	4 (28%)	17,19,21	1.00	1 (5%)
7	NAG	Z	2	7	14,14,15	1.87	5 (35%)	17,19,21	0.91	1 (5%)
11	NAG	a	1	11,2	14,14,15	0.37	0	17,19,21	0.73	0
11	FUC	a	2	11	10,10,11	0.31	0	14,14,16	1.04	0
11	NAG	b	1	11,2	14,14,15	0.33	0	17,19,21	0.95	1 (5%)
11	FUC	b	2	11	10,10,11	0.20	0	14,14,16	0.84	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	c	1	7,1	14,14,15	2.11	5 (35%)	17,19,21	1.01	0
7	NAG	c	2	7	14,14,15	1.93	6 (42%)	17,19,21	0.98	1 (5%)
7	NAG	d	1	7,1	14,14,15	2.09	7 (50%)	17,19,21	3.12	5 (29%)
7	NAG	d	2	7	14,14,15	1.91	5 (35%)	17,19,21	0.96	2 (11%)
8	NAG	e	1	8,1	14,14,15	1.98	4 (28%)	17,19,21	1.13	2 (11%)
8	NAG	e	2	8	14,14,15	1.89	5 (35%)	17,19,21	0.93	1 (5%)
8	BMA	e	3	8	11,11,12	0.76	0	15,15,17	0.79	1 (6%)
8	MAN	e	4	8	11,11,12	1.96	5 (45%)	15,15,17	0.70	0
7	NAG	f	1	7,1	14,14,15	1.97	4 (28%)	17,19,21	0.98	1 (5%)
7	NAG	f	2	7	14,14,15	1.85	5 (35%)	17,19,21	0.81	0
7	NAG	g	1	7,1	14,14,15	0.38	0	17,19,21	0.84	0
7	NAG	g	2	7	14,14,15	0.36	0	17,19,21	0.77	0
11	NAG	h	1	11,2	14,14,15	0.46	0	17,19,21	1.72	3 (17%)
11	FUC	h	2	11	10,10,11	2.07	6 (60%)	14,14,16	0.63	0
11	NAG	i	1	11,2	14,14,15	0.60	0	17,19,21	2.39	5 (29%)
11	FUC	i	2	11	10,10,11	0.35	0	14,14,16	1.50	3 (21%)

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
7	NAG	G	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
7	NAG	I	1	7,1	-	5/6/23/26	0/1/1/1
7	NAG	I	2	7	-	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	-	0/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	1/2/19/22	0/1/1/1
9	NAG	R	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	4/6/23/26	0/1/1/1
9	BMA	R	3	9	-	2/2/19/22	0/1/1/1
10	NAG	S	1	10,1	-	4/6/23/26	0/1/1/1
10	NAG	S	2	10	-	4/6/23/26	0/1/1/1
10	BMA	S	3	10	-	2/2/19/22	0/1/1/1
10	MAN	S	4	10	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	S	5	10	-	1/2/19/22	0/1/1/1
10	MAN	S	6	10	-	0/2/19/22	0/1/1/1
10	MAN	S	7	10	-	1/2/19/22	0/1/1/1
11	NAG	T	1	11,2	-	2/6/23/26	0/1/1/1
11	FUC	T	2	11	-	-	0/1/1/1
11	NAG	U	1	11,2	-	2/6/23/26	0/1/1/1
11	FUC	U	2	11	-	-	0/1/1/1
7	NAG	V	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1
7	NAG	W	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
8	NAG	Y	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1
7	NAG	Z	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	0/6/23/26	0/1/1/1
11	NAG	a	1	11,2	-	2/6/23/26	0/1/1/1
11	FUC	a	2	11	-	-	0/1/1/1
11	NAG	b	1	11,2	-	2/6/23/26	0/1/1/1
11	FUC	b	2	11	-	-	0/1/1/1
7	NAG	c	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	NAG	d	1	7,1	-	3/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
8	NAG	e	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	BMA	e	3	8	-	2/2/19/22	0/1/1/1
8	MAN	e	4	8	-	0/2/19/22	0/1/1/1
7	NAG	f	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	f	2	7	-	0/6/23/26	0/1/1/1
7	NAG	g	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	4/6/23/26	0/1/1/1
11	NAG	h	1	11,2	-	4/6/23/26	0/1/1/1
11	FUC	h	2	11	-	-	0/1/1/1
11	NAG	i	1	11,2	-	2/6/23/26	0/1/1/1
11	FUC	i	2	11	-	-	0/1/1/1

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	1	NAG	C1-C2	5.70	1.60	1.52
7	W	1	NAG	C1-C2	5.26	1.60	1.52
8	Q	1	NAG	C1-C2	5.25	1.60	1.52
7	G	1	NAG	C1-C2	5.04	1.59	1.52
8	Y	1	NAG	C1-C2	5.03	1.59	1.52
8	e	1	NAG	C1-C2	4.99	1.59	1.52
7	I	1	NAG	C1-C2	4.89	1.59	1.52
7	X	1	NAG	C1-C2	4.79	1.59	1.52
7	f	1	NAG	C1-C2	4.79	1.59	1.52
7	d	1	NAG	C1-C2	4.66	1.59	1.52
7	Z	1	NAG	C1-C2	4.41	1.58	1.52
7	d	2	NAG	C1-C2	4.34	1.58	1.52
8	e	2	NAG	C1-C2	4.34	1.58	1.52
7	c	2	NAG	C1-C2	4.32	1.58	1.52
7	X	2	NAG	C1-C2	4.30	1.58	1.52
7	I	2	NAG	C1-C2	4.24	1.58	1.52
7	W	2	NAG	C1-C2	4.15	1.58	1.52
8	Y	2	NAG	C1-C2	4.06	1.58	1.52
7	Z	2	NAG	C1-C2	3.98	1.58	1.52
7	G	2	NAG	C1-C2	3.95	1.58	1.52
7	f	2	NAG	C1-C2	3.94	1.58	1.52
8	Q	2	NAG	C1-C2	3.86	1.58	1.52
7	W	2	NAG	O5-C5	3.22	1.50	1.43
11	h	2	FUC	C2-C3	3.21	1.57	1.52
7	G	2	NAG	O5-C5	3.21	1.49	1.43
8	Q	4	MAN	C2-C3	3.20	1.57	1.52
8	Y	4	MAN	C2-C3	3.20	1.57	1.52
8	e	4	MAN	O5-C5	3.15	1.49	1.43
8	Y	4	MAN	O5-C5	3.14	1.49	1.43
8	Q	4	MAN	O5-C5	3.13	1.49	1.43
8	e	4	MAN	C2-C3	3.12	1.57	1.52
7	Z	2	NAG	O5-C5	3.12	1.49	1.43
7	f	2	NAG	O5-C5	3.08	1.49	1.43
7	d	2	NAG	O5-C5	3.04	1.49	1.43
7	G	1	NAG	O5-C5	3.01	1.49	1.43
7	c	2	NAG	O5-C5	3.00	1.49	1.43
7	f	1	NAG	O5-C5	2.98	1.49	1.43
7	X	2	NAG	O5-C5	2.98	1.49	1.43
7	I	2	NAG	O5-C5	2.95	1.49	1.43
7	I	1	NAG	C2-N2	2.94	1.51	1.46
11	h	2	FUC	O5-C5	2.92	1.49	1.43
8	Q	2	NAG	O5-C5	2.85	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	1	NAG	C2-N2	2.84	1.51	1.46
8	Y	2	NAG	O5-C5	2.84	1.49	1.43
8	e	2	NAG	O5-C5	2.82	1.49	1.43
7	d	1	NAG	C2-N2	2.76	1.51	1.46
7	Z	1	NAG	O5-C5	2.75	1.49	1.43
11	h	2	FUC	C1-C2	2.74	1.58	1.52
7	X	1	NAG	O5-C5	2.70	1.48	1.43
8	e	4	MAN	C1-C2	2.68	1.58	1.52
8	Q	4	MAN	C1-C2	2.67	1.58	1.52
8	Y	4	MAN	C1-C2	2.64	1.58	1.52
7	d	1	NAG	O5-C5	2.63	1.48	1.43
7	W	1	NAG	O5-C5	2.62	1.48	1.43
7	I	1	NAG	O5-C5	2.54	1.48	1.43
7	f	1	NAG	O5-C1	2.53	1.47	1.43
8	e	1	NAG	O5-C5	2.51	1.48	1.43
7	d	1	NAG	C4-C3	2.51	1.58	1.52
8	e	2	NAG	C3-C2	2.49	1.57	1.52
7	c	1	NAG	O5-C5	2.47	1.48	1.43
7	Z	1	NAG	O5-C1	2.45	1.47	1.43
7	X	1	NAG	C4-C3	2.45	1.58	1.52
8	Q	4	MAN	C4-C5	2.44	1.58	1.53
7	X	2	NAG	C4-C5	2.44	1.58	1.53
7	X	1	NAG	O5-C1	2.44	1.47	1.43
8	e	1	NAG	C3-C2	2.43	1.57	1.52
7	I	2	NAG	C3-C2	2.42	1.57	1.52
7	I	1	NAG	C3-C2	2.41	1.57	1.52
7	X	2	NAG	C3-C2	2.41	1.57	1.52
7	d	2	NAG	C3-C2	2.40	1.57	1.52
7	G	2	NAG	C4-C5	2.40	1.58	1.53
7	I	1	NAG	C4-C3	2.39	1.58	1.52
7	f	1	NAG	C4-C5	2.39	1.58	1.53
8	Q	1	NAG	O5-C5	2.38	1.48	1.43
8	Y	4	MAN	C4-C5	2.37	1.58	1.53
7	c	1	NAG	C3-C2	2.37	1.57	1.52
8	e	4	MAN	C4-C5	2.37	1.58	1.53
7	d	1	NAG	O5-C1	2.37	1.47	1.43
7	c	2	NAG	C3-C2	2.36	1.57	1.52
7	G	1	NAG	O5-C1	2.36	1.47	1.43
8	Q	1	NAG	C3-C2	2.35	1.57	1.52
7	d	1	NAG	C4-C5	2.35	1.58	1.53
7	c	2	NAG	C4-C5	2.34	1.58	1.53
7	f	2	NAG	C3-C2	2.34	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	1	NAG	O5-C5	2.33	1.48	1.43
7	I	2	NAG	C4-C5	2.33	1.57	1.53
7	d	2	NAG	C4-C5	2.32	1.57	1.53
7	W	2	NAG	C4-C5	2.32	1.57	1.53
7	X	1	NAG	C3-C2	2.30	1.57	1.52
7	G	2	NAG	C3-C2	2.30	1.57	1.52
11	h	2	FUC	O5-C1	2.30	1.47	1.43
7	I	1	NAG	O5-C1	2.29	1.47	1.43
8	Y	2	NAG	C4-C5	2.29	1.57	1.53
11	h	2	FUC	C4-C5	2.29	1.57	1.52
7	W	2	NAG	C3-C2	2.29	1.57	1.52
7	G	1	NAG	C3-C2	2.29	1.57	1.52
7	Z	2	NAG	C4-C5	2.29	1.57	1.53
8	Q	2	NAG	C4-C5	2.27	1.57	1.53
7	Z	1	NAG	C4-C5	2.26	1.57	1.53
8	Q	2	NAG	C3-C2	2.26	1.57	1.52
8	Y	4	MAN	O5-C1	2.25	1.47	1.43
8	Y	1	NAG	C3-C2	2.24	1.57	1.52
7	d	1	NAG	C3-C2	2.23	1.57	1.52
7	Z	2	NAG	C3-C2	2.23	1.57	1.52
7	W	1	NAG	O5-C1	2.22	1.47	1.43
7	W	1	NAG	C3-C2	2.22	1.57	1.52
7	f	2	NAG	C4-C5	2.21	1.57	1.53
7	I	1	NAG	C4-C5	2.21	1.57	1.53
7	X	1	NAG	C4-C5	2.21	1.57	1.53
8	Q	4	MAN	O5-C1	2.20	1.47	1.43
8	Q	1	NAG	O5-C1	2.19	1.47	1.43
8	e	4	MAN	O5-C1	2.19	1.47	1.43
8	Y	2	NAG	C3-C2	2.19	1.57	1.52
11	h	2	FUC	C4-C3	2.18	1.57	1.52
7	G	1	NAG	C4-C5	2.18	1.57	1.53
7	G	2	NAG	C4-C3	2.17	1.57	1.52
7	c	1	NAG	O5-C1	2.16	1.47	1.43
8	Q	2	NAG	C4-C3	2.16	1.57	1.52
7	c	2	NAG	C4-C3	2.14	1.57	1.52
7	W	2	NAG	C4-C3	2.12	1.57	1.52
8	e	2	NAG	C4-C5	2.11	1.57	1.53
7	I	2	NAG	C4-C3	2.10	1.57	1.52
7	X	2	NAG	C4-C3	2.08	1.57	1.52
8	Q	1	NAG	C4-C3	2.07	1.57	1.52
7	W	1	NAG	C4-C5	2.07	1.57	1.53
7	Z	2	NAG	C4-C3	2.05	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	1	NAG	C4-C3	2.05	1.57	1.52
8	e	2	NAG	C4-C3	2.04	1.57	1.52
7	c	2	NAG	C2-N2	2.04	1.49	1.46
8	e	1	NAG	O5-C1	2.04	1.47	1.43
7	I	2	NAG	C2-N2	2.02	1.49	1.46
8	Y	2	NAG	C4-C3	2.01	1.57	1.52
7	d	2	NAG	C4-C3	2.01	1.57	1.52
7	f	2	NAG	C4-C3	2.00	1.57	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	1	NAG	C8-C7-N2	9.24	131.75	116.10
7	X	1	NAG	C8-C7-N2	8.62	130.69	116.10
7	d	1	NAG	C8-C7-N2	8.44	130.40	116.10
7	I	1	NAG	C2-N2-C7	7.52	133.62	122.90
7	X	1	NAG	C2-N2-C7	6.37	131.97	122.90
11	i	1	NAG	O5-C5-C6	-6.28	97.36	107.20
7	d	1	NAG	C2-N2-C7	6.15	131.66	122.90
11	h	1	NAG	O5-C5-C6	5.84	116.36	107.20
7	I	1	NAG	O7-C7-N2	-5.44	111.94	121.95
7	I	1	NAG	C1-C2-N2	5.20	119.37	110.49
7	X	1	NAG	O7-C7-N2	-5.05	112.66	121.95
11	i	1	NAG	O4-C4-C3	-4.89	99.05	110.35
7	d	1	NAG	O7-C7-N2	-4.88	112.98	121.95
10	S	1	NAG	C1-O5-C5	4.27	117.98	112.19
7	X	1	NAG	C1-C2-N2	4.12	117.52	110.49
7	d	1	NAG	C1-C2-N2	3.87	117.10	110.49
11	i	1	NAG	C1-O5-C5	3.44	116.86	112.19
11	T	1	NAG	C1-O5-C5	3.21	116.55	112.19
11	i	2	FUC	O2-C2-C3	-3.20	103.72	110.14
7	I	1	NAG	O7-C7-C8	-3.09	116.31	122.06
9	R	1	NAG	O4-C4-C3	-3.09	103.21	110.35
7	d	1	NAG	O7-C7-C8	-2.92	116.62	122.06
7	X	1	NAG	O7-C7-C8	-2.91	116.64	122.06
10	S	6	MAN	C1-O5-C5	2.86	116.06	112.19
11	i	2	FUC	O5-C1-C2	-2.83	106.40	110.77
8	Q	1	NAG	C8-C7-N2	2.75	120.76	116.10
11	b	1	NAG	O5-C5-C6	2.74	111.51	107.20
9	R	1	NAG	C2-N2-C7	-2.62	119.18	122.90
8	Y	1	NAG	C8-C7-N2	2.49	120.31	116.10
11	i	1	NAG	C4-C3-C2	2.46	114.62	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	1	NAG	C8-C7-N2	2.45	120.25	116.10
10	S	2	NAG	O4-C4-C3	-2.37	104.87	110.35
10	S	2	NAG	C2-N2-C7	-2.36	119.54	122.90
7	G	2	NAG	C8-C7-N2	2.33	120.04	116.10
8	Q	1	NAG	O7-C7-C8	-2.29	117.80	122.06
8	Y	3	BMA	C2-C3-C4	-2.28	106.96	110.89
7	c	2	NAG	C8-C7-N2	2.26	119.92	116.10
8	e	3	BMA	C2-C3-C4	-2.25	107.01	110.89
7	Z	1	NAG	C8-C7-N2	2.24	119.90	116.10
11	h	1	NAG	C6-C5-C4	-2.21	107.82	113.00
10	S	3	BMA	O5-C5-C6	2.18	110.63	107.20
8	Y	2	NAG	C8-C7-N2	2.17	119.78	116.10
8	Q	1	NAG	C1-O5-C5	2.17	115.13	112.19
11	h	1	NAG	C4-C3-C2	-2.16	107.86	111.02
7	W	2	NAG	C8-C7-N2	2.15	119.73	116.10
11	i	1	NAG	C2-N2-C7	-2.15	119.85	122.90
8	e	2	NAG	C8-C7-N2	2.14	119.72	116.10
8	e	1	NAG	C1-O5-C5	2.14	115.09	112.19
8	Q	3	BMA	C2-C3-C4	-2.11	107.24	110.89
9	R	2	NAG	O5-C1-C2	2.10	114.61	111.29
9	R	2	NAG	C1-C2-N2	-2.10	106.89	110.49
7	d	2	NAG	C8-C7-N2	2.10	119.66	116.10
7	f	1	NAG	C8-C7-N2	2.10	119.65	116.10
8	Y	1	NAG	O7-C7-C8	-2.08	118.20	122.06
7	V	2	NAG	C1-O5-C5	2.06	114.98	112.19
7	I	2	NAG	C8-C7-N2	2.05	119.57	116.10
11	i	2	FUC	C1-O5-C5	2.04	117.39	112.78
11	b	2	FUC	O5-C1-C2	2.03	113.91	110.77
7	d	2	NAG	C1-O5-C5	2.02	114.94	112.19
7	I	1	NAG	C1-O5-C5	2.02	114.93	112.19
7	X	2	NAG	C8-C7-N2	2.02	119.52	116.10
7	Z	2	NAG	C8-C7-N2	2.02	119.51	116.10
8	Y	1	NAG	C1-O5-C5	2.00	114.91	112.19
11	T	2	FUC	O5-C1-C2	-2.00	107.68	110.77

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	1	NAG	C1-C2-N2-C7
7	g	1	NAG	C8-C7-N2-C2
7	g	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	R	1	NAG	C8-C7-N2-C2
9	R	1	NAG	O7-C7-N2-C2
9	R	2	NAG	C8-C7-N2-C2
9	R	2	NAG	O7-C7-N2-C2
10	S	2	NAG	C8-C7-N2-C2
10	S	2	NAG	O7-C7-N2-C2
11	a	1	NAG	C8-C7-N2-C2
11	a	1	NAG	O7-C7-N2-C2
9	R	2	NAG	O5-C5-C6-O6
8	e	3	BMA	C4-C5-C6-O6
7	X	1	NAG	C1-C2-N2-C7
8	e	3	BMA	O5-C5-C6-O6
9	R	3	BMA	O5-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6
7	V	1	NAG	C8-C7-N2-C2
11	U	1	NAG	C8-C7-N2-C2
11	U	1	NAG	O7-C7-N2-C2
9	R	3	BMA	C4-C5-C6-O6
10	S	3	BMA	O5-C5-C6-O6
10	S	1	NAG	O5-C5-C6-O6
11	T	1	NAG	O5-C5-C6-O6
7	V	1	NAG	O7-C7-N2-C2
11	b	1	NAG	C8-C7-N2-C2
7	d	1	NAG	C1-C2-N2-C7
11	T	1	NAG	C4-C5-C6-O6
10	S	3	BMA	C4-C5-C6-O6
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
7	X	1	NAG	C8-C7-N2-C2
7	X	1	NAG	O7-C7-N2-C2
7	d	1	NAG	C8-C7-N2-C2
7	d	1	NAG	O7-C7-N2-C2
11	b	1	NAG	O7-C7-N2-C2
10	S	1	NAG	C8-C7-N2-C2
10	S	1	NAG	C4-C5-C6-O6
10	S	2	NAG	O5-C5-C6-O6
10	S	1	NAG	O7-C7-N2-C2
8	Q	3	BMA	O5-C5-C6-O6
7	V	2	NAG	C8-C7-N2-C2
11	h	1	NAG	C4-C5-C6-O6
7	g	2	NAG	C8-C7-N2-C2
10	S	5	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

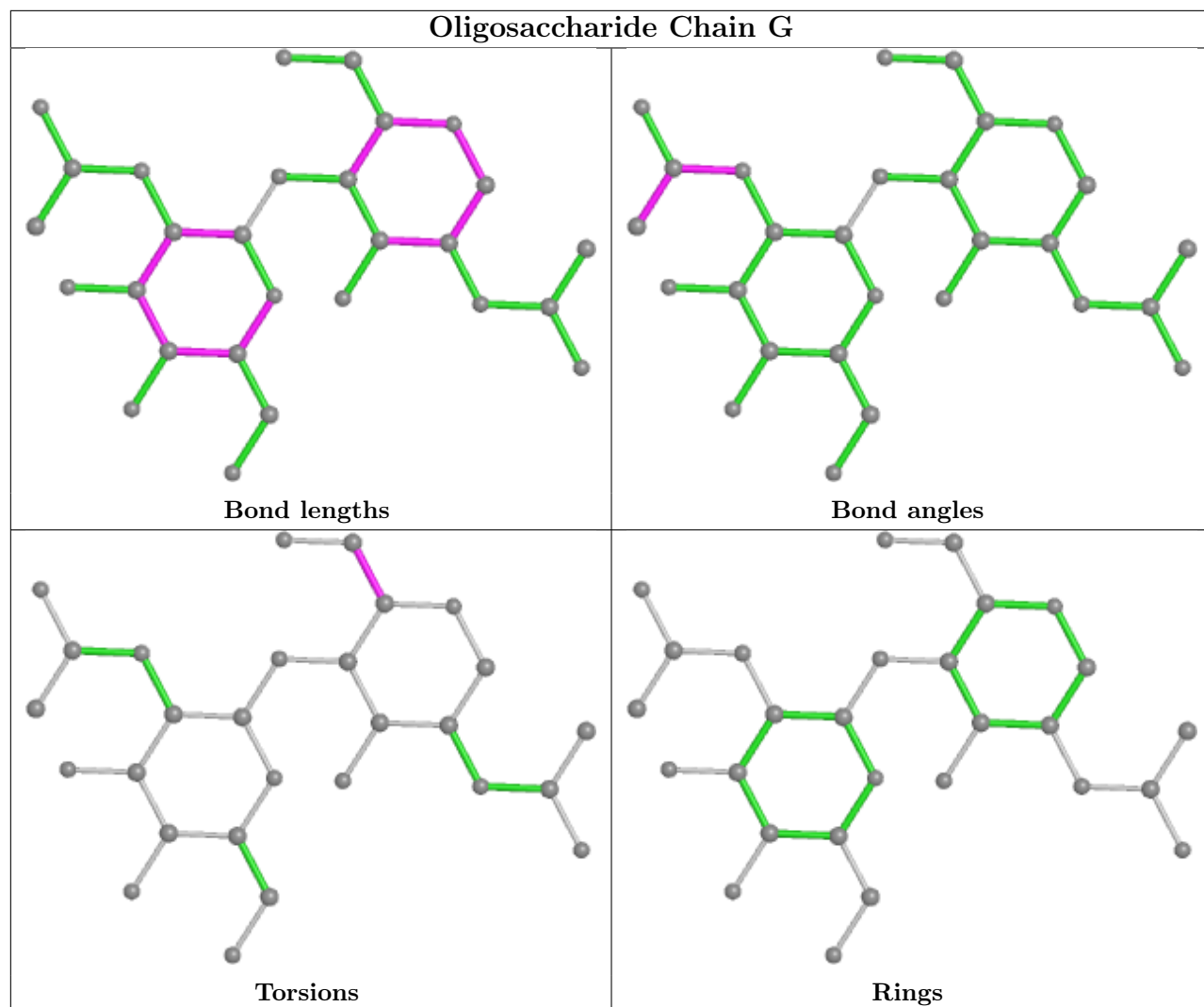
Mol	Chain	Res	Type	Atoms
8	Y	3	BMA	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
8	Q	4	MAN	O5-C5-C6-O6
7	V	2	NAG	O7-C7-N2-C2
7	g	2	NAG	C4-C5-C6-O6
7	g	2	NAG	O7-C7-N2-C2
7	G	1	NAG	C4-C5-C6-O6
10	S	7	MAN	C4-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
11	h	1	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
10	S	2	NAG	C4-C5-C6-O6
11	i	1	NAG	C8-C7-N2-C2
11	h	1	NAG	C8-C7-N2-C2
11	i	1	NAG	O7-C7-N2-C2
7	I	1	NAG	O5-C5-C6-O6
11	h	1	NAG	O7-C7-N2-C2

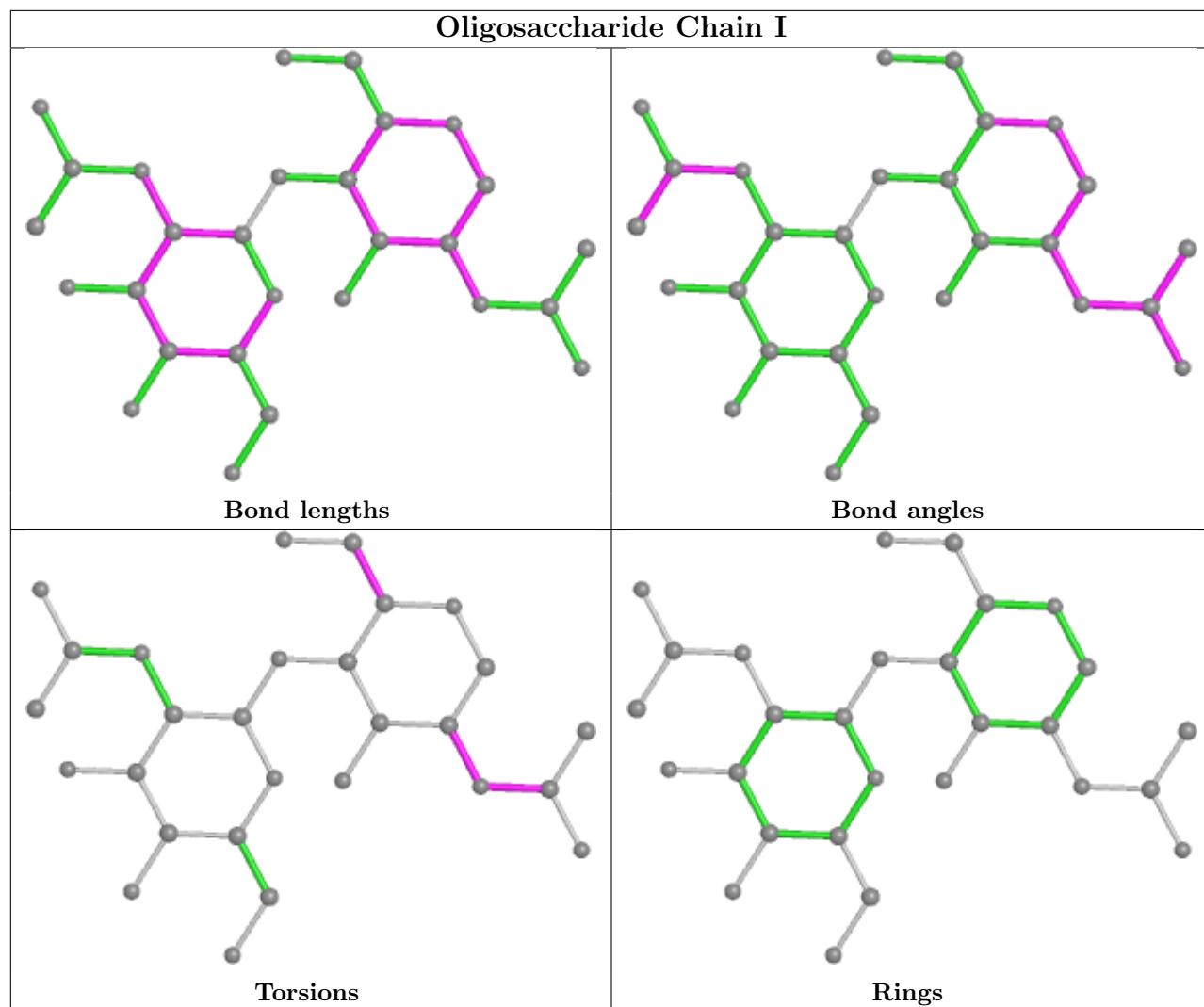
There are no ring outliers.

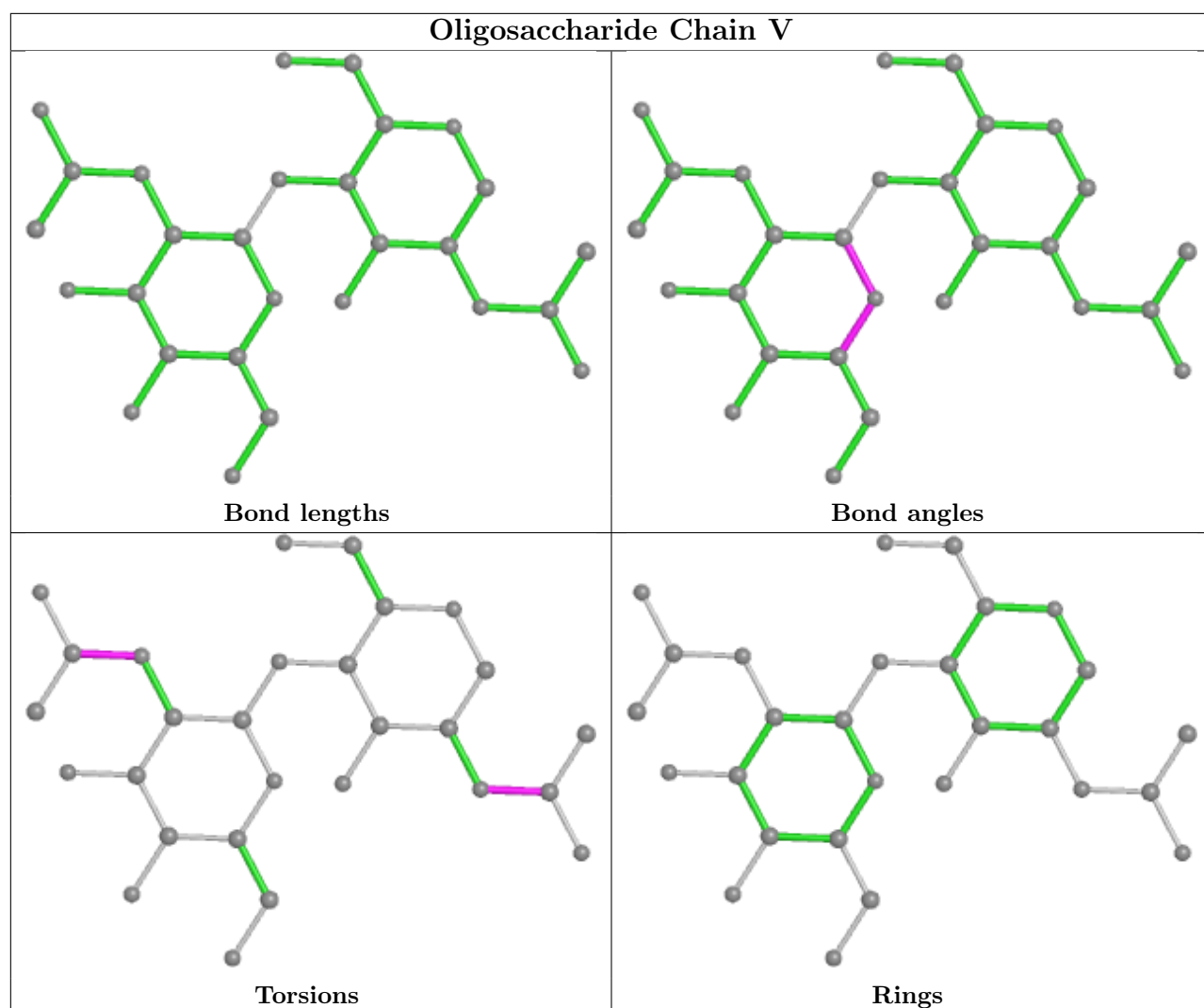
1 monomer is involved in 1 short contact:

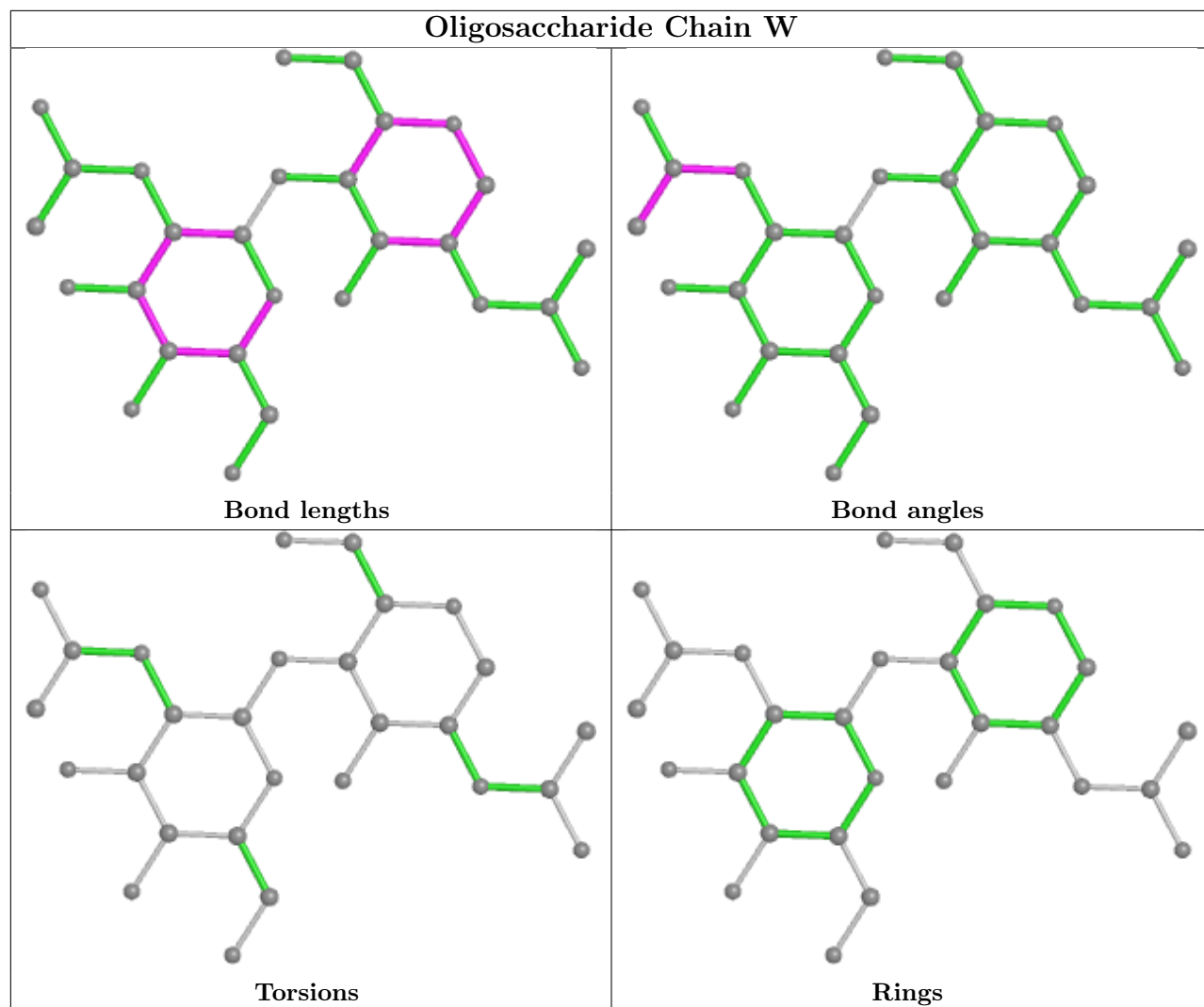
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Z	1	NAG	1	0

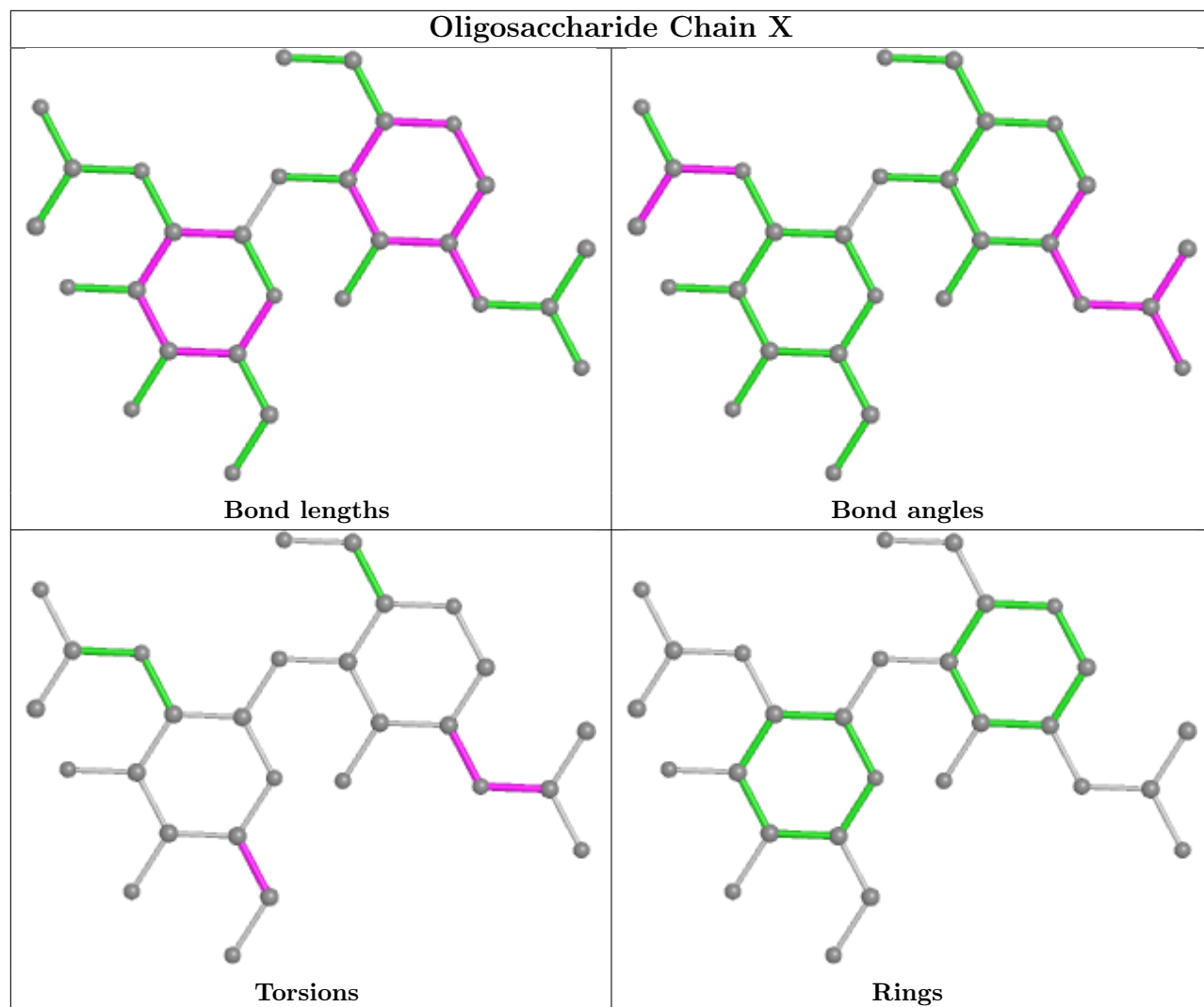
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

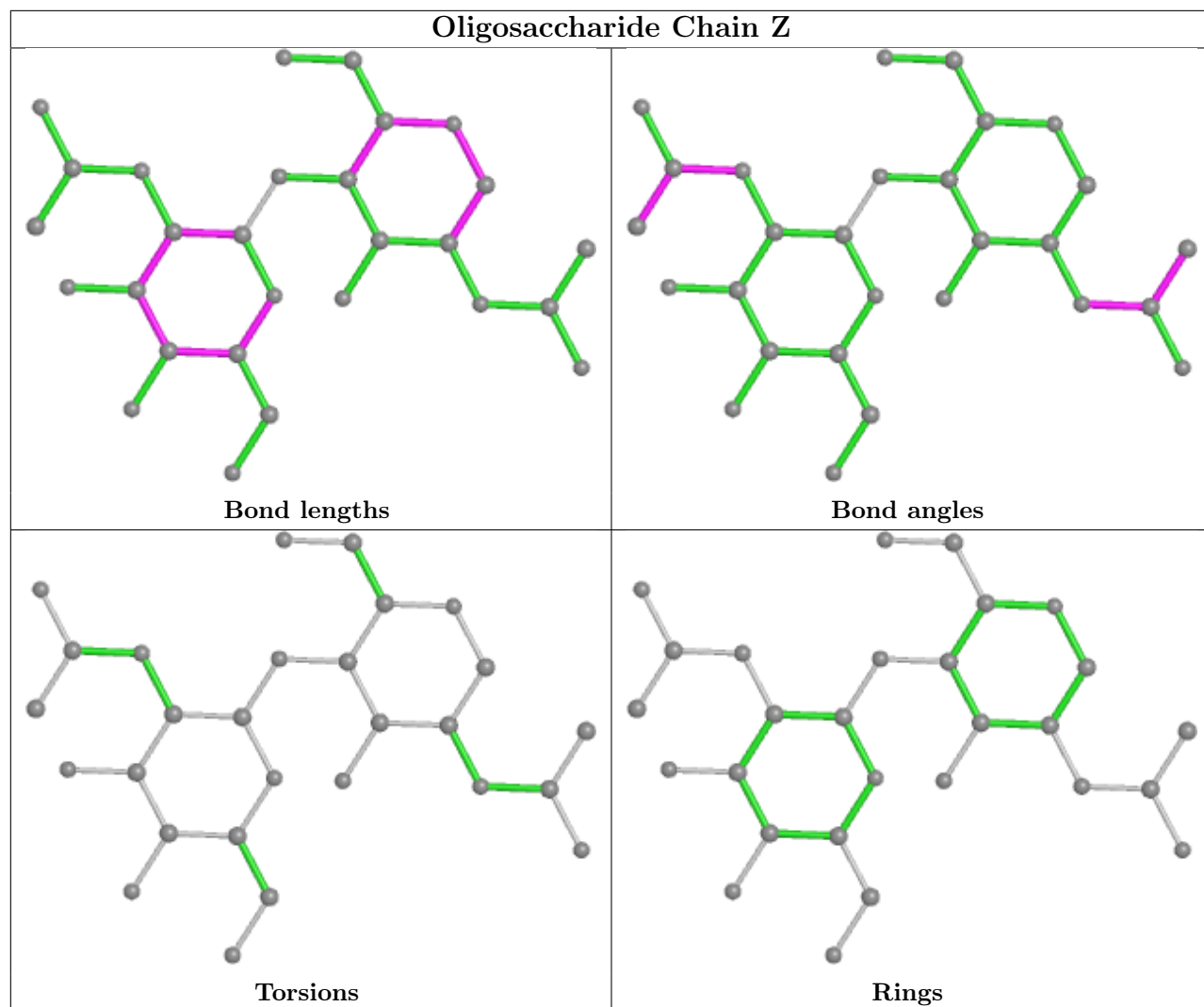


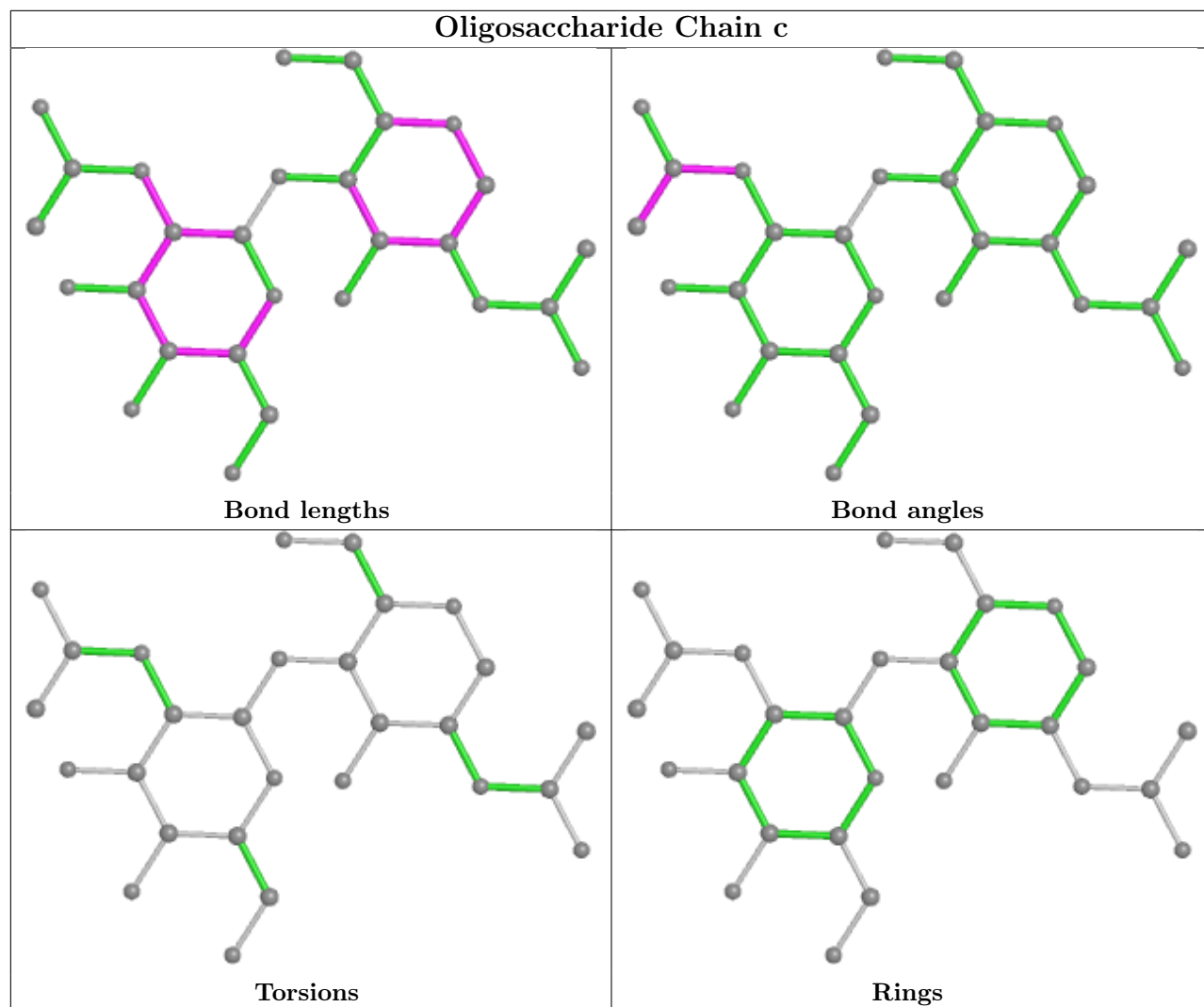


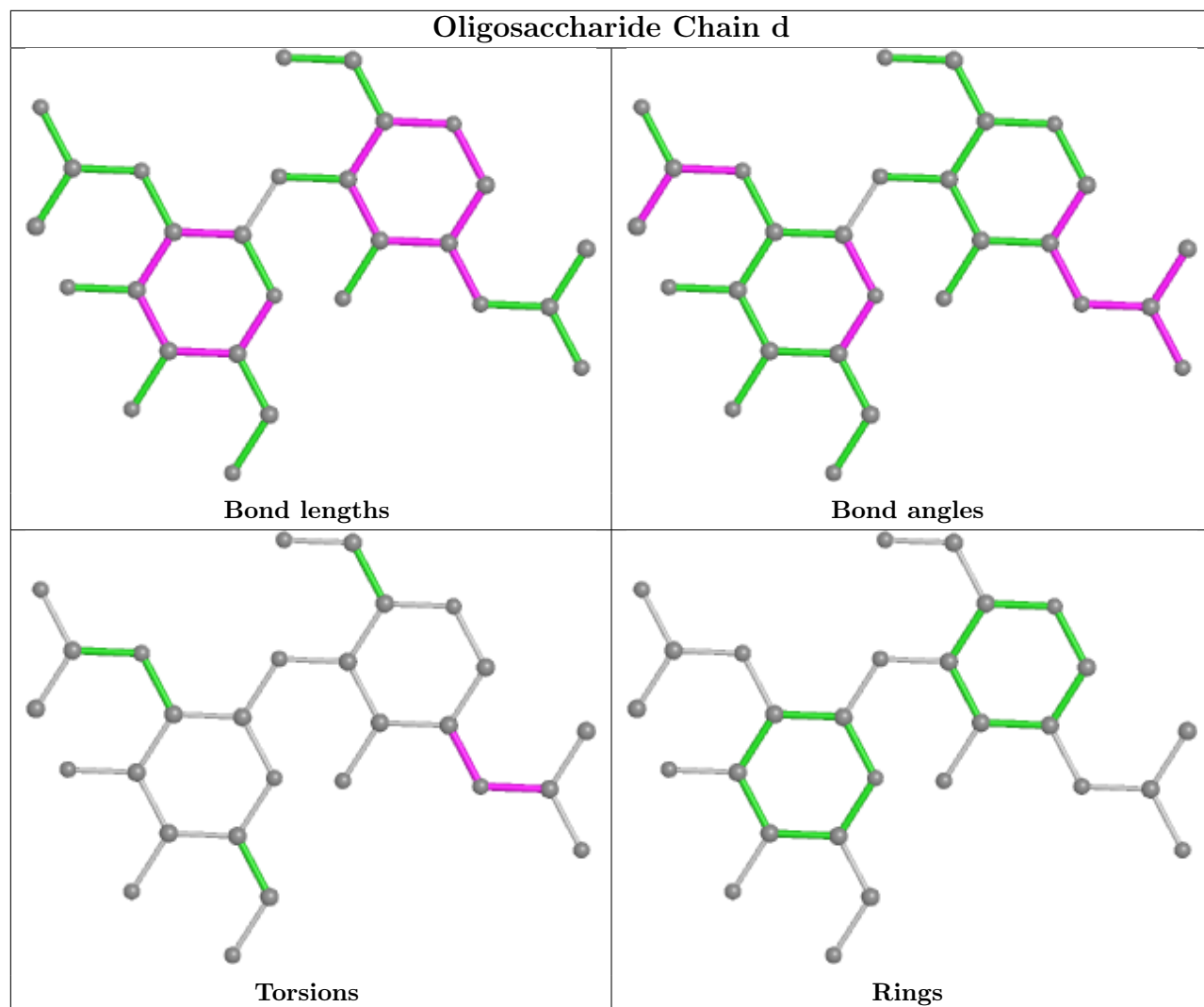


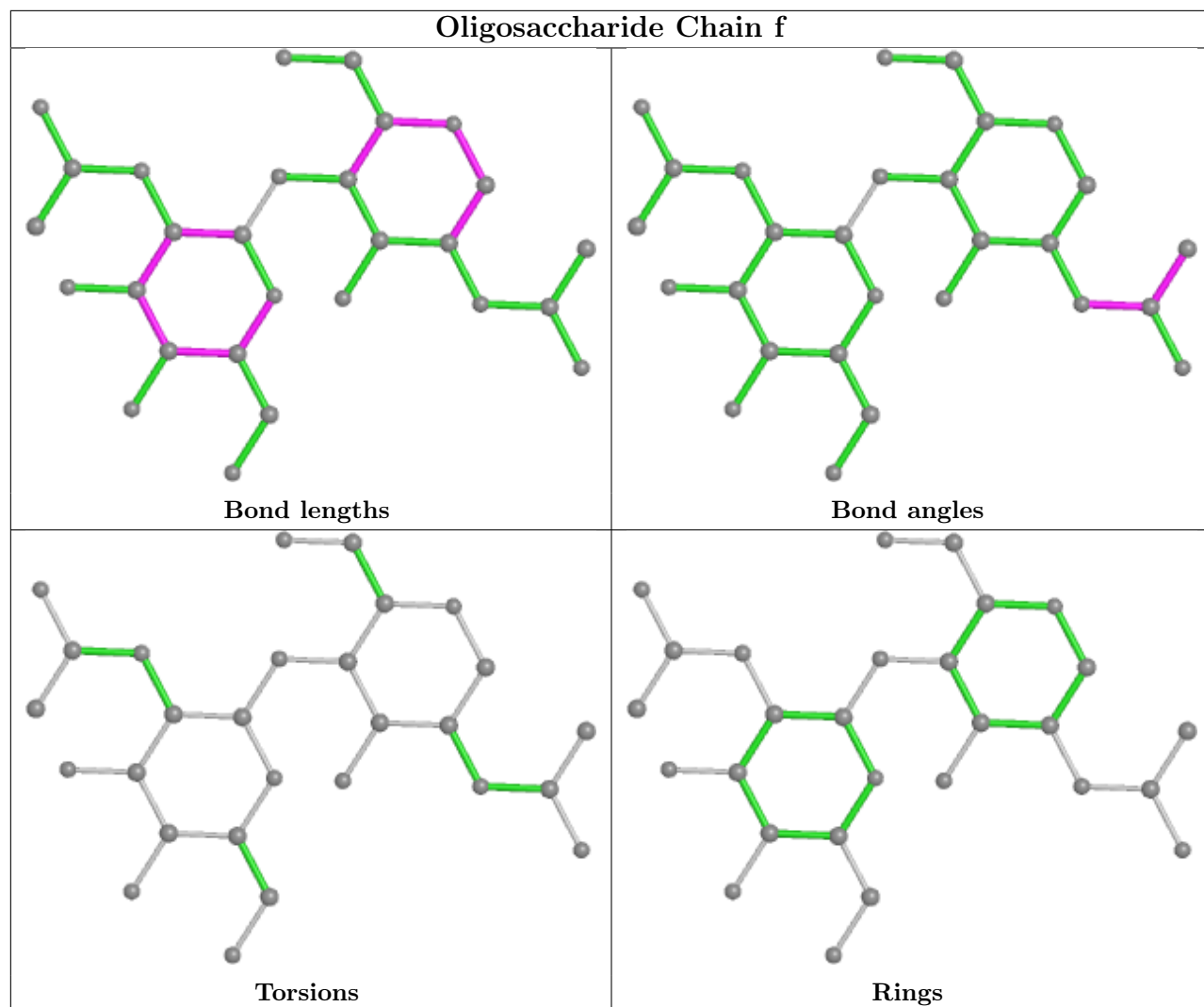


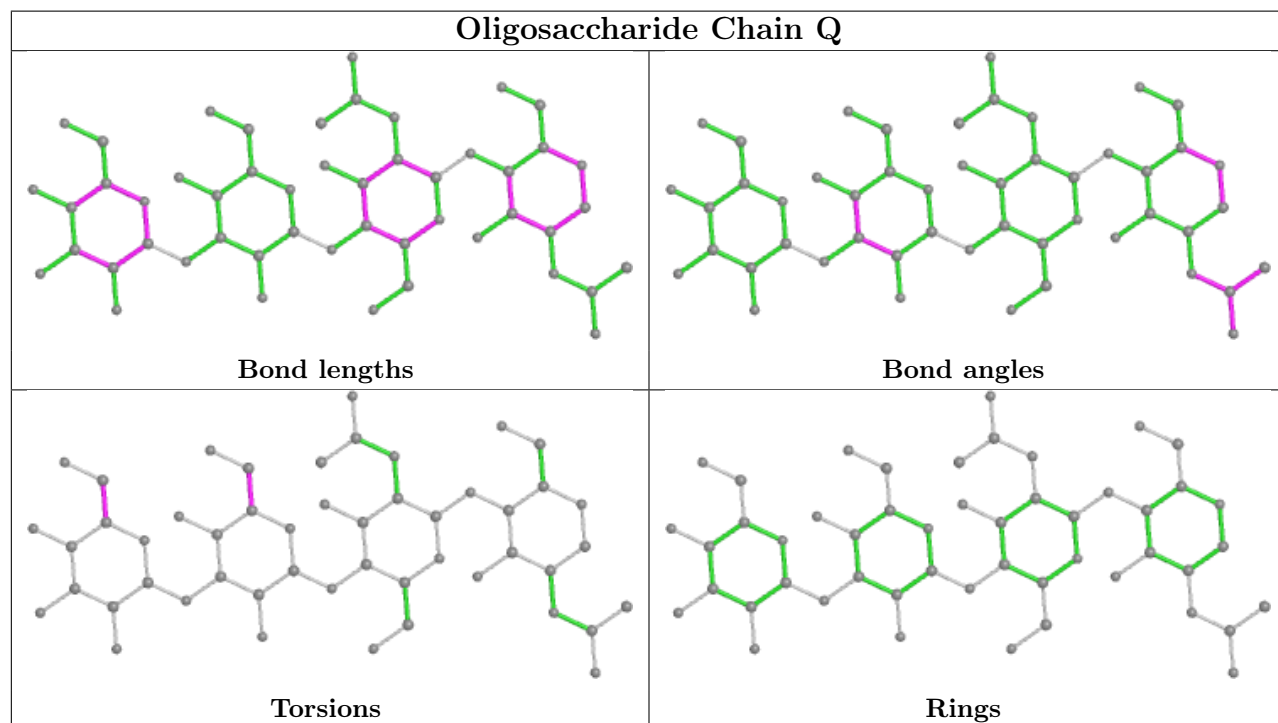
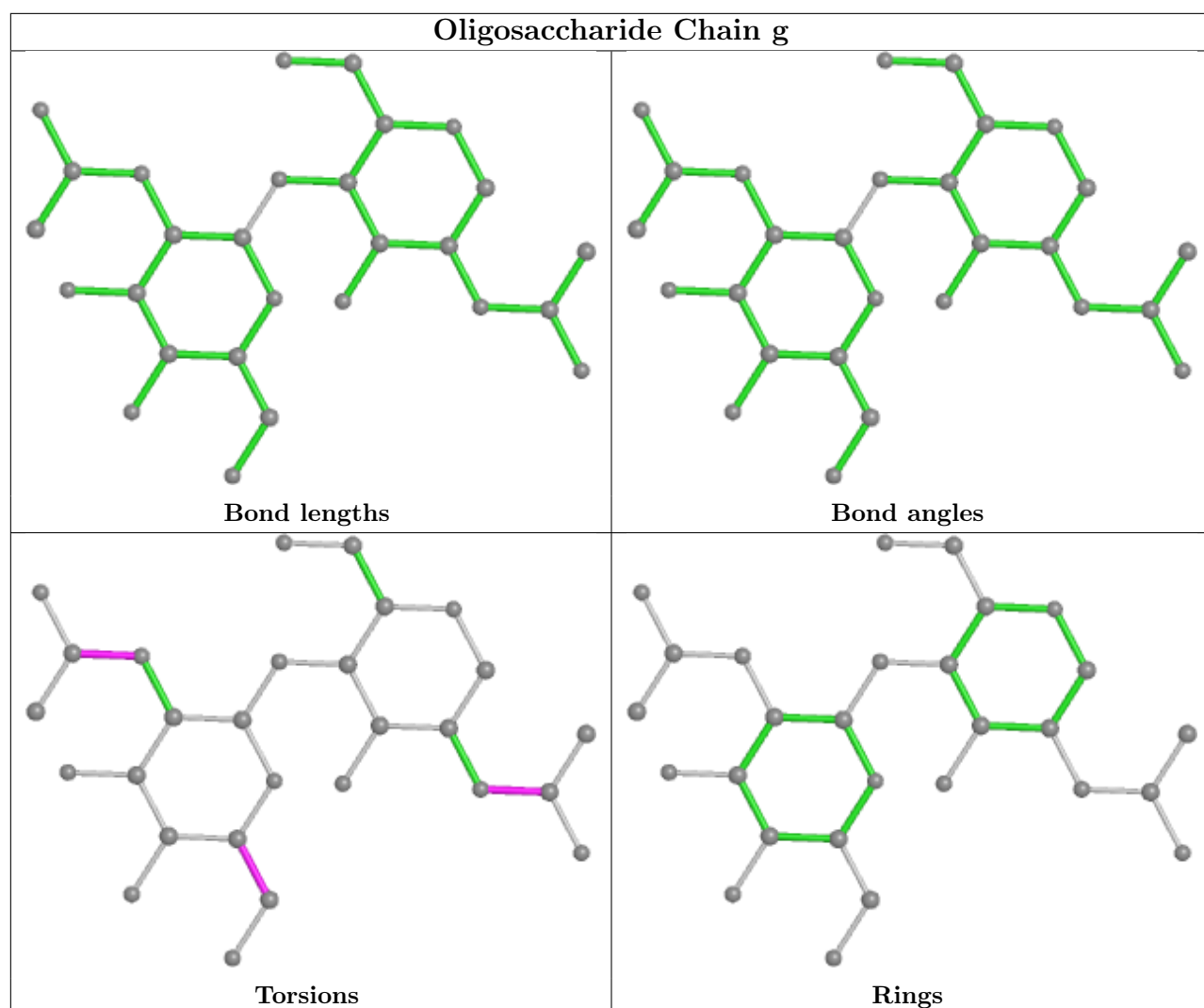


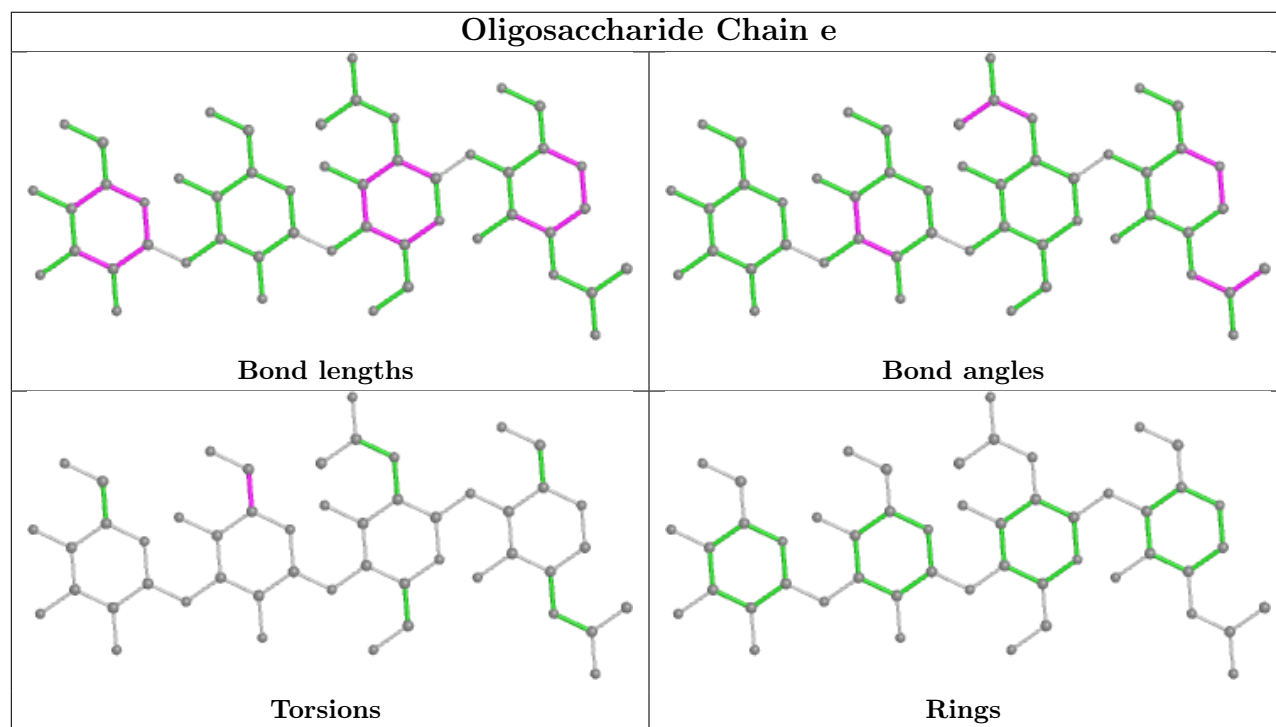
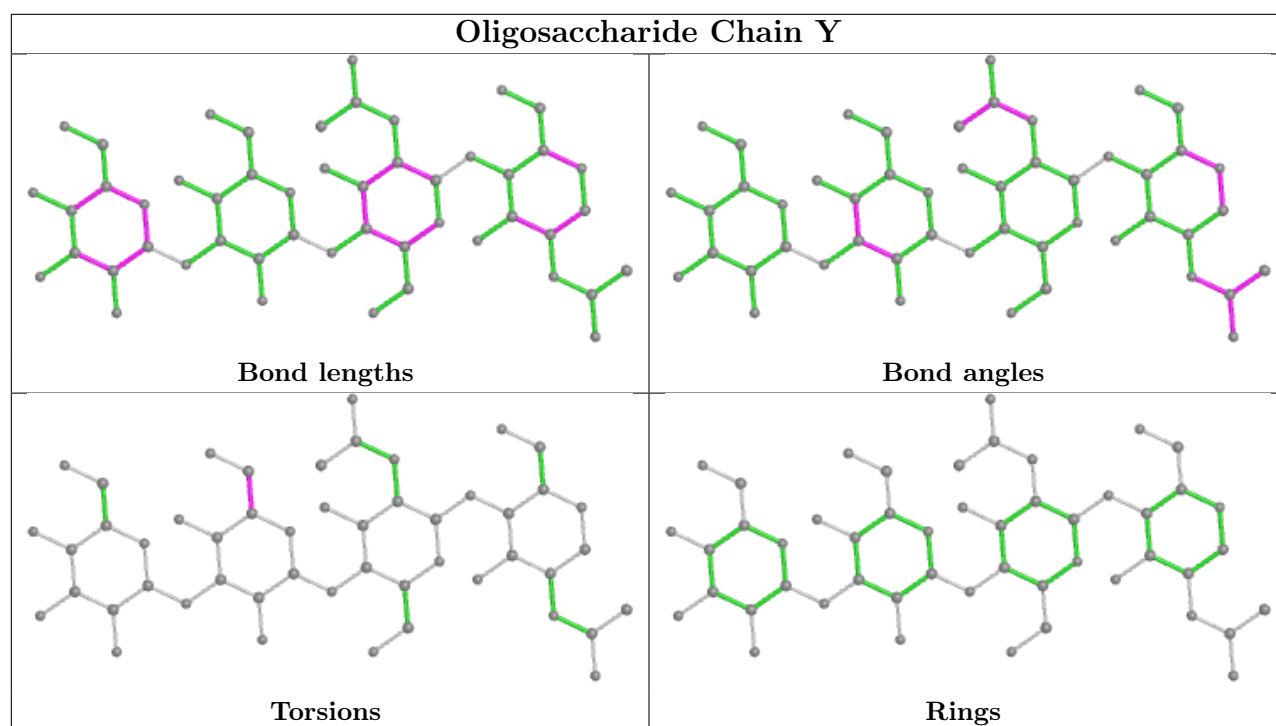


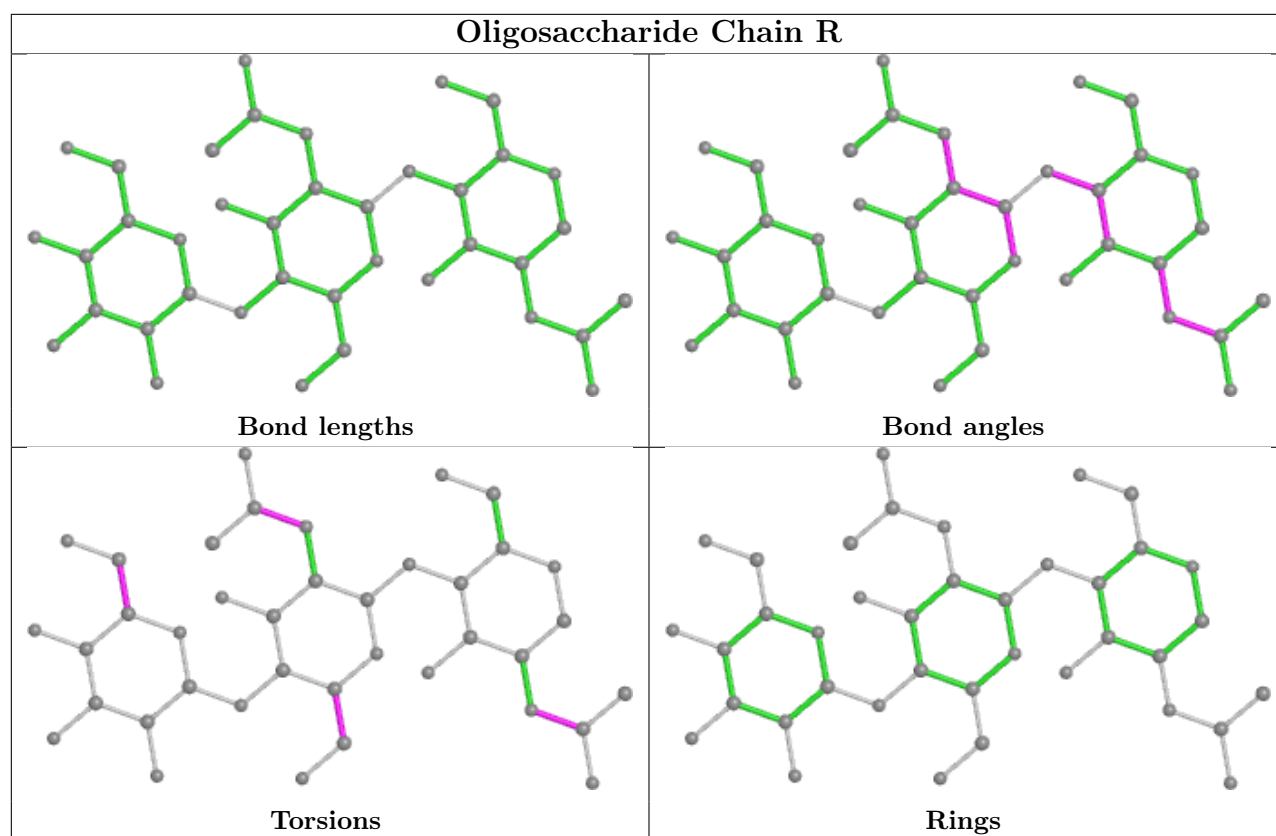


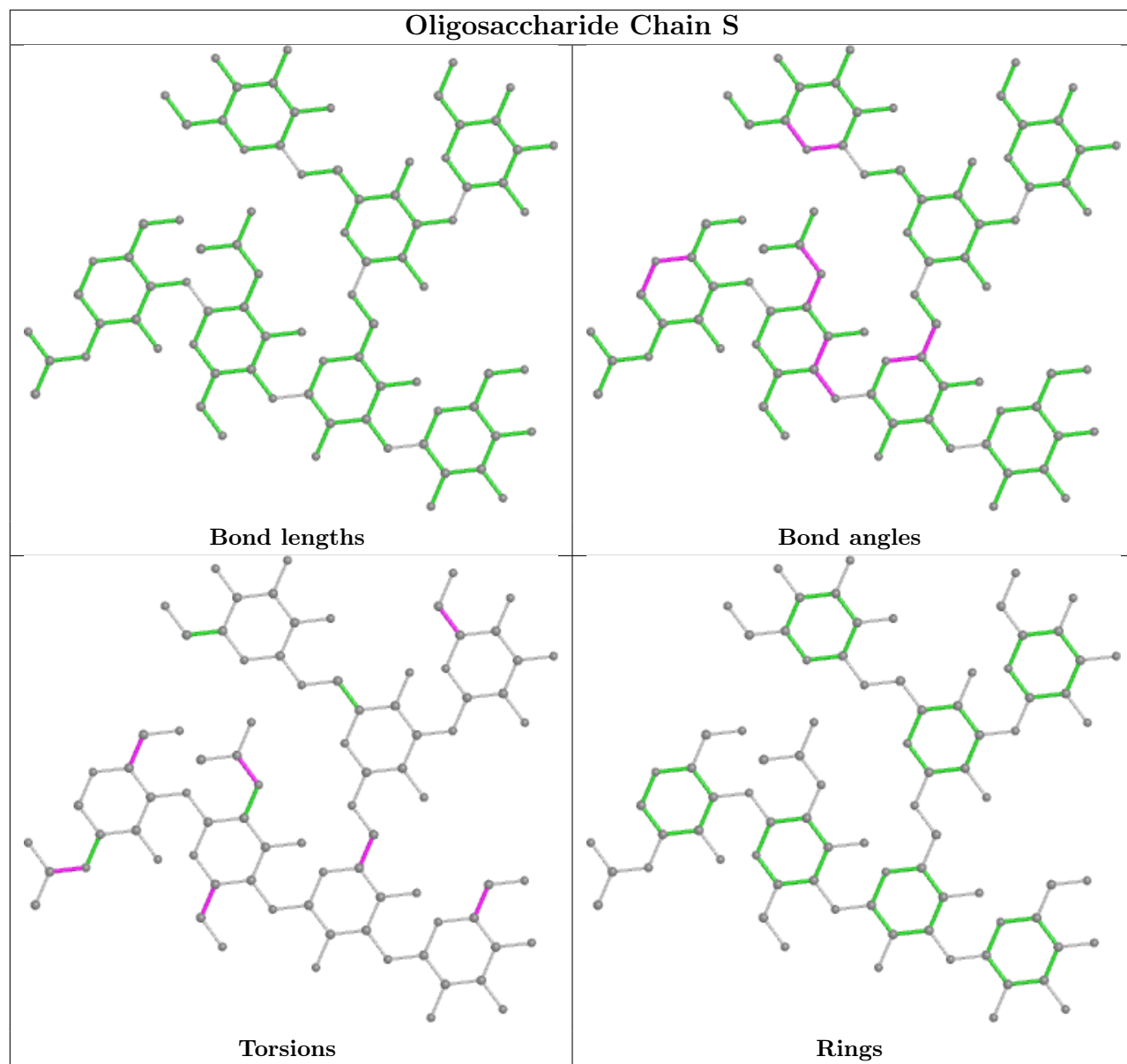


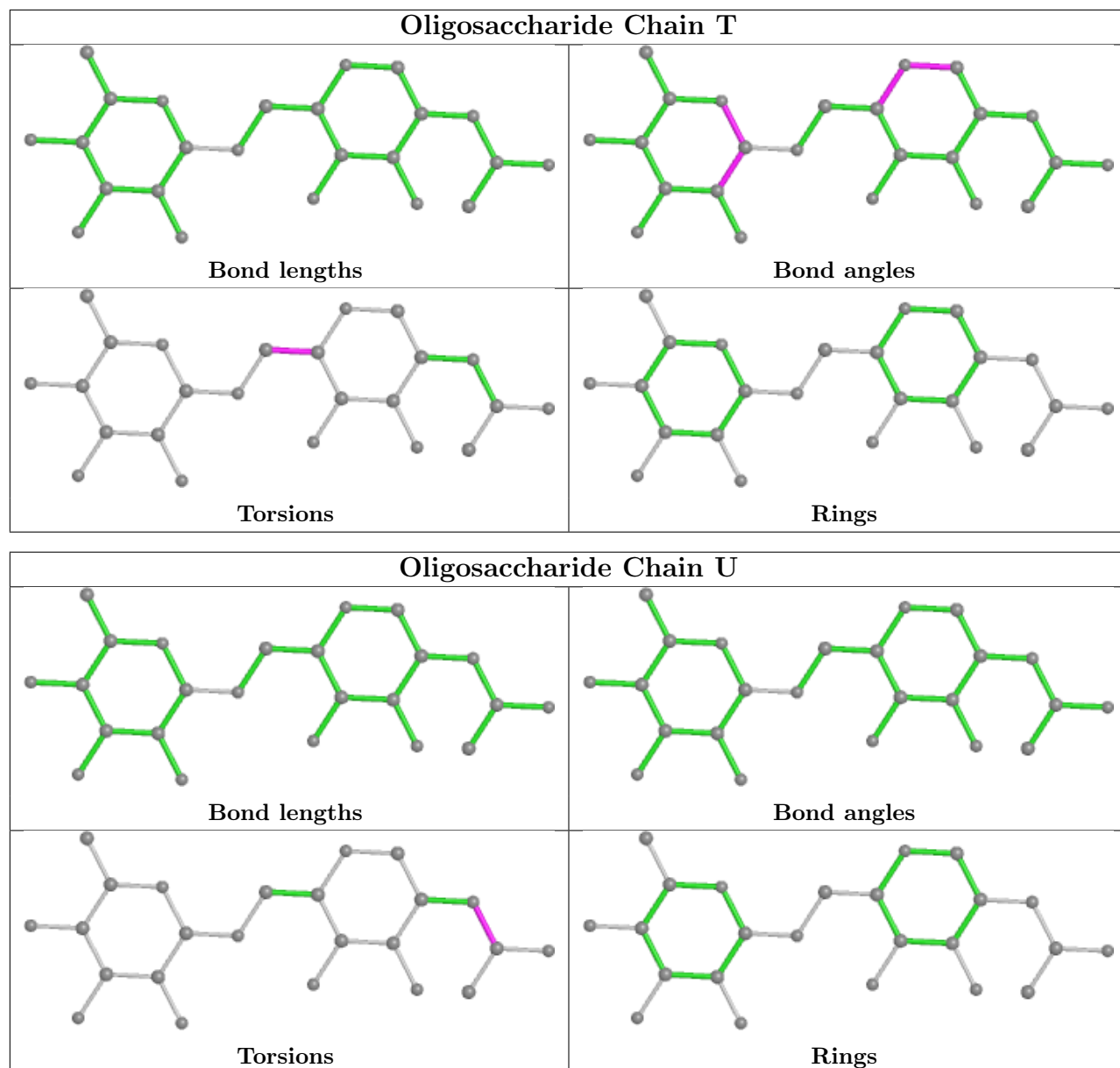


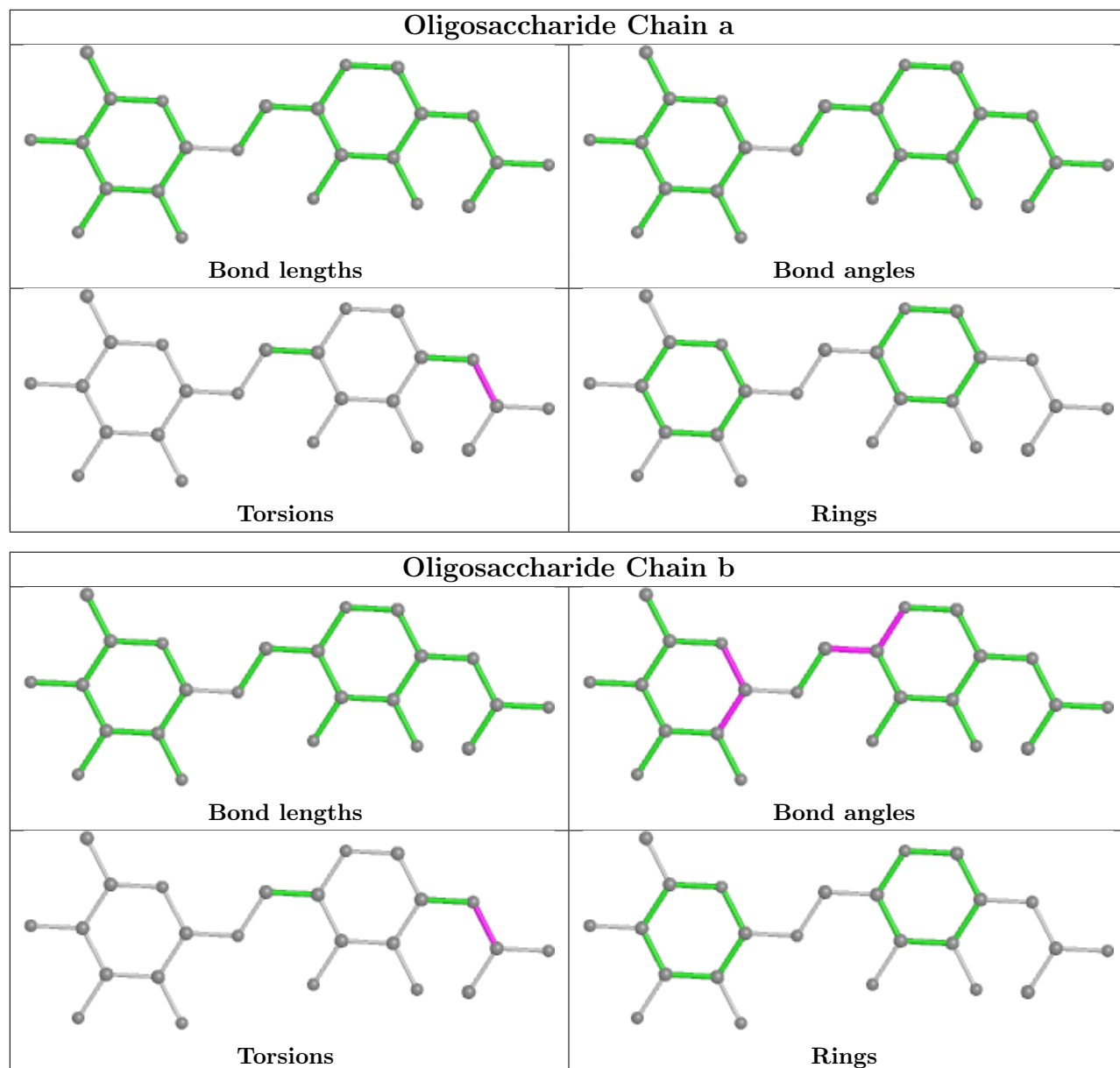


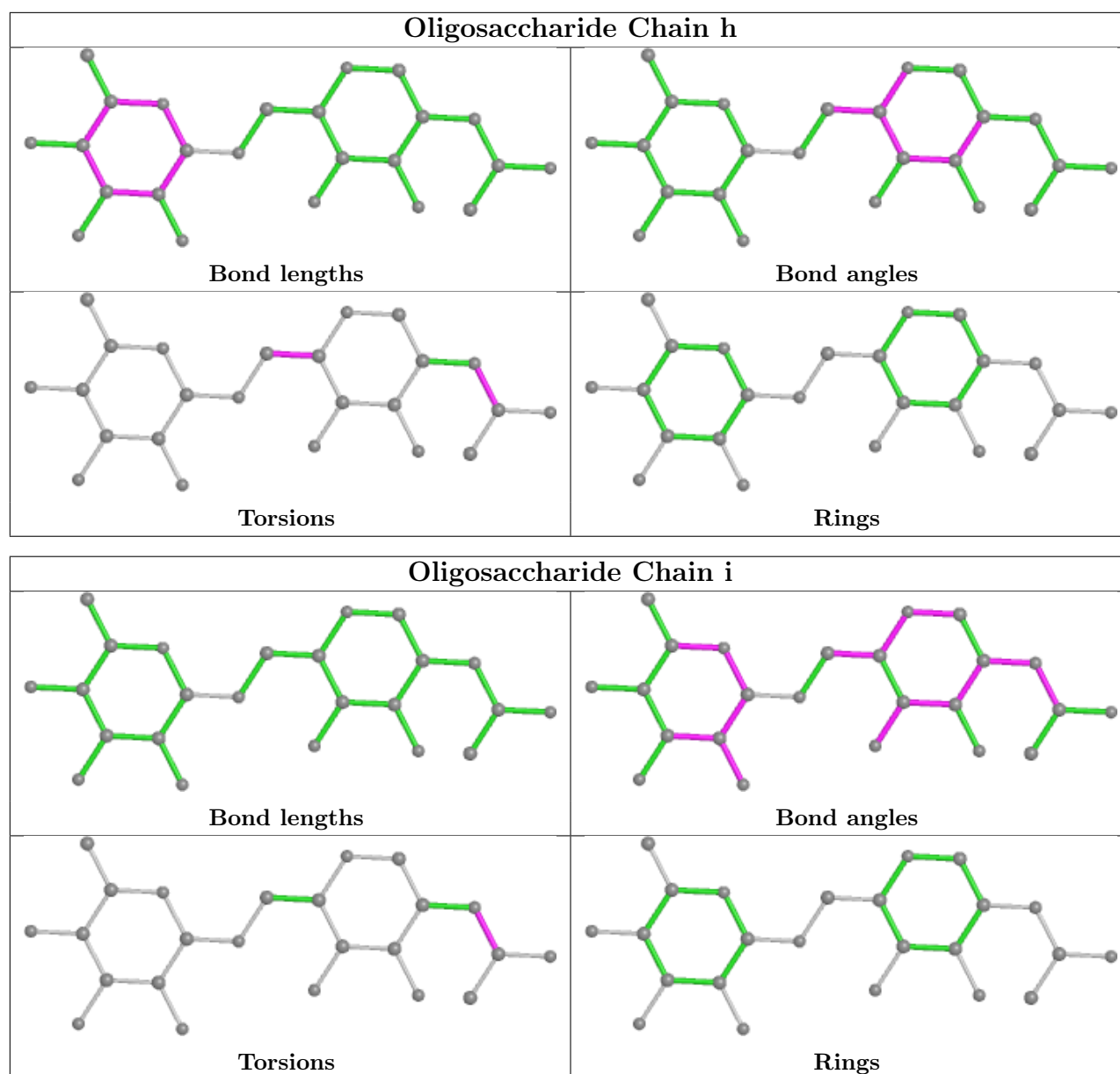












5.6 Ligand geometry [i](#)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	E	607	1	14,14,15	2.16	7 (50%)	17,19,21	1.06	1 (5%)
12	NAG	C	609	1	14,14,15	1.95	4 (28%)	17,19,21	1.06	1 (5%)
12	NAG	A	605	1	14,14,15	2.00	5 (35%)	17,19,21	1.02	1 (5%)
12	NAG	C	604	1	14,14,15	2.14	5 (35%)	17,19,21	0.94	1 (5%)
12	NAG	E	608	1	14,14,15	2.04	7 (50%)	17,19,21	1.01	1 (5%)
12	NAG	C	611	1	14,14,15	2.02	5 (35%)	17,19,21	1.15	2 (11%)
12	NAG	E	603	1	14,14,15	2.18	6 (42%)	17,19,21	0.93	1 (5%)
12	NAG	A	609	1	14,14,15	1.98	5 (35%)	17,19,21	1.00	0
12	NAG	A	601	1	14,14,15	1.94	6 (42%)	17,19,21	1.12	2 (11%)
12	NAG	C	612	1	14,14,15	2.03	5 (35%)	17,19,21	0.99	1 (5%)
12	NAG	E	602	1	14,14,15	2.02	6 (42%)	17,19,21	1.06	1 (5%)
12	NAG	E	610	1	14,14,15	2.08	5 (35%)	17,19,21	0.95	1 (5%)
12	NAG	A	608	1	14,14,15	1.96	5 (35%)	17,19,21	1.09	2 (11%)
12	NAG	F	702	2	14,14,15	0.27	0	17,19,21	0.69	0
12	NAG	E	601	1	14,14,15	1.98	6 (42%)	17,19,21	1.26	2 (11%)
12	NAG	C	602	1	14,14,15	1.98	6 (42%)	17,19,21	1.07	1 (5%)
12	NAG	A	603	1	14,14,15	2.13	6 (42%)	17,19,21	0.99	1 (5%)
12	NAG	E	604	1	14,14,15	2.17	5 (35%)	17,19,21	0.95	1 (5%)
12	NAG	C	610	1	14,14,15	2.11	5 (35%)	17,19,21	0.98	0
12	NAG	A	612	1	14,14,15	2.04	6 (42%)	17,19,21	0.98	1 (5%)
12	NAG	D	702	2	14,14,15	0.34	0	17,19,21	0.61	0
12	NAG	E	611	1	14,14,15	2.01	6 (42%)	17,19,21	1.07	1 (5%)
12	NAG	C	607	1	14,14,15	2.11	5 (35%)	17,19,21	1.05	2 (11%)
12	NAG	A	606	1	14,14,15	2.12	6 (42%)	17,19,21	1.08	1 (5%)
12	NAG	E	605	1	14,14,15	1.99	5 (35%)	17,19,21	0.99	1 (5%)
12	NAG	F	701	2	14,14,15	0.34	0	17,19,21	0.82	0
12	NAG	C	608	1	14,14,15	1.95	7 (50%)	17,19,21	1.01	1 (5%)
12	NAG	E	612	1	14,14,15	2.06	4 (28%)	17,19,21	1.02	1 (5%)
12	NAG	E	609	1	14,14,15	2.02	5 (35%)	17,19,21	1.03	1 (5%)
12	NAG	A	604	1	14,14,15	2.14	5 (35%)	17,19,21	0.95	1 (5%)
12	NAG	A	602	1	14,14,15	2.07	7 (50%)	17,19,21	1.08	2 (11%)
12	NAG	A	610	1	14,14,15	2.06	5 (35%)	17,19,21	0.90	0
12	NAG	C	603	1	14,14,15	2.14	6 (42%)	17,19,21	1.00	1 (5%)
12	NAG	C	605	1	14,14,15	2.06	5 (35%)	17,19,21	1.01	0
12	NAG	B	701	2	14,14,15	0.33	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	C	601	1	14,14,15	1.94	6 (42%)	17,19,21	1.13	2 (11%)
12	NAG	D	701	2	14,14,15	0.37	0	17,19,21	1.32	2 (11%)
12	NAG	E	606	1	14,14,15	2.09	5 (35%)	17,19,21	1.06	1 (5%)
12	NAG	A	607	1	14,14,15	2.14	6 (42%)	17,19,21	0.98	1 (5%)
12	NAG	B	702	2	14,14,15	0.27	0	17,19,21	0.70	0
12	NAG	A	611	1	14,14,15	2.00	5 (35%)	17,19,21	1.15	1 (5%)
12	NAG	C	606	1	14,14,15	2.15	7 (50%)	17,19,21	1.07	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
12	NAG	E	607	1	-	0/6/23/26	0/1/1/1
12	NAG	C	609	1	-	1/6/23/26	0/1/1/1
12	NAG	A	605	1	-	1/6/23/26	0/1/1/1
12	NAG	C	604	1	-	0/6/23/26	0/1/1/1
12	NAG	E	608	1	-	0/6/23/26	0/1/1/1
12	NAG	C	611	1	-	0/6/23/26	0/1/1/1
12	NAG	E	603	1	-	0/6/23/26	0/1/1/1
12	NAG	A	609	1	-	1/6/23/26	0/1/1/1
12	NAG	A	601	1	-	0/6/23/26	0/1/1/1
12	NAG	C	612	1	-	0/6/23/26	0/1/1/1
12	NAG	E	602	1	-	1/6/23/26	0/1/1/1
12	NAG	E	610	1	-	0/6/23/26	0/1/1/1
12	NAG	A	608	1	-	0/6/23/26	0/1/1/1
12	NAG	F	702	2	-	2/6/23/26	0/1/1/1
12	NAG	E	601	1	-	0/6/23/26	0/1/1/1
12	NAG	C	602	1	-	2/6/23/26	0/1/1/1
12	NAG	A	603	1	-	0/6/23/26	0/1/1/1
12	NAG	E	604	1	-	0/6/23/26	0/1/1/1
12	NAG	C	610	1	-	1/6/23/26	0/1/1/1
12	NAG	A	612	1	-	0/6/23/26	0/1/1/1
12	NAG	D	702	2	-	0/6/23/26	0/1/1/1
12	NAG	E	611	1	-	1/6/23/26	0/1/1/1
12	NAG	C	607	1	-	0/6/23/26	0/1/1/1
12	NAG	A	606	1	-	0/6/23/26	0/1/1/1
12	NAG	E	605	1	-	2/6/23/26	0/1/1/1
12	NAG	F	701	2	-	0/6/23/26	0/1/1/1
12	NAG	C	608	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	E	612	1	-	0/6/23/26	0/1/1/1
12	NAG	E	609	1	-	0/6/23/26	0/1/1/1
12	NAG	A	604	1	-	0/6/23/26	0/1/1/1
12	NAG	A	602	1	-	1/6/23/26	0/1/1/1
12	NAG	A	610	1	-	0/6/23/26	0/1/1/1
12	NAG	C	603	1	-	0/6/23/26	0/1/1/1
12	NAG	C	605	1	-	1/6/23/26	0/1/1/1
12	NAG	B	701	2	-	2/6/23/26	0/1/1/1
12	NAG	C	601	1	-	0/6/23/26	0/1/1/1
12	NAG	D	701	2	-	3/6/23/26	0/1/1/1
12	NAG	E	606	1	-	0/6/23/26	0/1/1/1
12	NAG	A	607	1	-	0/6/23/26	0/1/1/1
12	NAG	B	702	2	-	0/6/23/26	0/1/1/1
12	NAG	A	611	1	-	1/6/23/26	0/1/1/1
12	NAG	C	606	1	-	0/6/23/26	0/1/1/1

All (200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	610	NAG	C1-C2	5.28	1.60	1.52
12	C	607	NAG	C1-C2	5.28	1.60	1.52
12	E	603	NAG	C1-C2	5.26	1.60	1.52
12	A	606	NAG	C1-C2	5.22	1.60	1.52
12	C	606	NAG	C1-C2	5.21	1.60	1.52
12	E	610	NAG	C1-C2	5.20	1.60	1.52
12	A	603	NAG	C1-C2	5.18	1.60	1.52
12	A	604	NAG	C1-C2	5.16	1.60	1.52
12	C	603	NAG	C1-C2	5.15	1.60	1.52
12	E	606	NAG	C1-C2	5.13	1.60	1.52
12	C	604	NAG	C1-C2	5.10	1.60	1.52
12	C	605	NAG	C1-C2	5.09	1.59	1.52
12	E	604	NAG	C1-C2	5.09	1.59	1.52
12	E	608	NAG	C1-C2	5.07	1.59	1.52
12	A	602	NAG	C1-C2	5.07	1.59	1.52
12	E	609	NAG	C1-C2	5.06	1.59	1.52
12	A	607	NAG	C1-C2	5.01	1.59	1.52
12	E	612	NAG	C1-C2	4.97	1.59	1.52
12	A	610	NAG	C1-C2	4.95	1.59	1.52
12	A	612	NAG	C1-C2	4.87	1.59	1.52
12	C	609	NAG	C1-C2	4.86	1.59	1.52
12	A	608	NAG	C1-C2	4.85	1.59	1.52
12	A	611	NAG	C1-C2	4.83	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	602	NAG	C1-C2	4.83	1.59	1.52
12	C	612	NAG	C1-C2	4.82	1.59	1.52
12	A	605	NAG	C1-C2	4.81	1.59	1.52
12	E	607	NAG	C1-C2	4.79	1.59	1.52
12	A	609	NAG	C1-C2	4.74	1.59	1.52
12	C	611	NAG	C1-C2	4.74	1.59	1.52
12	E	605	NAG	C1-C2	4.67	1.59	1.52
12	C	608	NAG	C1-C2	4.59	1.59	1.52
12	E	611	NAG	C1-C2	4.56	1.59	1.52
12	A	601	NAG	C1-C2	4.41	1.58	1.52
12	C	601	NAG	C1-C2	4.31	1.58	1.52
12	E	601	NAG	C1-C2	4.31	1.58	1.52
12	C	602	NAG	C1-C2	4.18	1.58	1.52
12	E	604	NAG	O5-C5	3.48	1.50	1.43
12	E	607	NAG	O5-C5	3.48	1.50	1.43
12	A	607	NAG	O5-C5	3.39	1.50	1.43
12	E	603	NAG	O5-C5	3.33	1.50	1.43
12	C	604	NAG	O5-C5	3.30	1.50	1.43
12	A	604	NAG	O5-C5	3.21	1.49	1.43
12	E	601	NAG	O5-C5	3.19	1.49	1.43
12	E	612	NAG	O5-C5	3.19	1.49	1.43
12	A	609	NAG	O5-C5	3.16	1.49	1.43
12	C	602	NAG	O5-C5	3.15	1.49	1.43
12	C	603	NAG	O5-C5	3.14	1.49	1.43
12	A	610	NAG	O5-C5	3.13	1.49	1.43
12	E	610	NAG	O5-C5	3.10	1.49	1.43
12	C	610	NAG	O5-C5	3.10	1.49	1.43
12	C	606	NAG	O5-C5	3.09	1.49	1.43
12	C	607	NAG	O5-C5	3.09	1.49	1.43
12	E	611	NAG	O5-C5	3.07	1.49	1.43
12	C	601	NAG	O5-C5	3.06	1.49	1.43
12	C	612	NAG	O5-C5	3.06	1.49	1.43
12	A	603	NAG	O5-C5	3.06	1.49	1.43
12	E	606	NAG	O5-C5	3.06	1.49	1.43
12	E	605	NAG	O5-C5	3.05	1.49	1.43
12	A	612	NAG	O5-C5	3.05	1.49	1.43
12	A	606	NAG	O5-C5	3.04	1.49	1.43
12	C	605	NAG	O5-C5	3.02	1.49	1.43
12	C	611	NAG	O5-C5	3.01	1.49	1.43
12	E	607	NAG	O5-C1	3.00	1.48	1.43
12	A	601	NAG	O5-C5	2.99	1.49	1.43
12	E	609	NAG	O5-C5	2.99	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	608	NAG	O5-C5	2.98	1.49	1.43
12	E	604	NAG	O5-C1	2.96	1.48	1.43
12	E	602	NAG	O5-C5	2.92	1.49	1.43
12	A	604	NAG	O5-C1	2.89	1.48	1.43
12	A	607	NAG	O5-C1	2.88	1.48	1.43
12	A	605	NAG	O5-C5	2.87	1.49	1.43
12	C	604	NAG	O5-C1	2.87	1.48	1.43
12	E	603	NAG	O5-C1	2.86	1.48	1.43
12	E	611	NAG	O5-C1	2.83	1.48	1.43
12	C	609	NAG	O5-C5	2.83	1.49	1.43
12	A	611	NAG	O5-C5	2.82	1.49	1.43
12	C	608	NAG	O5-C5	2.81	1.49	1.43
12	C	606	NAG	O5-C1	2.80	1.48	1.43
12	C	603	NAG	O5-C1	2.79	1.48	1.43
12	E	608	NAG	O5-C5	2.78	1.49	1.43
12	A	602	NAG	O5-C5	2.77	1.49	1.43
12	E	601	NAG	O5-C1	2.74	1.48	1.43
12	A	605	NAG	O5-C1	2.73	1.48	1.43
12	A	603	NAG	O5-C1	2.72	1.48	1.43
12	A	610	NAG	O5-C1	2.72	1.48	1.43
12	C	602	NAG	O5-C1	2.71	1.48	1.43
12	C	610	NAG	O5-C1	2.71	1.48	1.43
12	C	611	NAG	O5-C1	2.68	1.48	1.43
12	E	605	NAG	O5-C1	2.67	1.48	1.43
12	C	601	NAG	O5-C1	2.65	1.48	1.43
12	A	609	NAG	O5-C1	2.65	1.47	1.43
12	A	606	NAG	O5-C1	2.64	1.47	1.43
12	C	607	NAG	O5-C1	2.63	1.47	1.43
12	C	605	NAG	O5-C1	2.63	1.47	1.43
12	E	606	NAG	O5-C1	2.62	1.47	1.43
12	E	610	NAG	O5-C1	2.61	1.47	1.43
12	E	612	NAG	O5-C1	2.59	1.47	1.43
12	A	601	NAG	O5-C1	2.57	1.47	1.43
12	C	609	NAG	O5-C1	2.56	1.47	1.43
12	A	612	NAG	O5-C1	2.54	1.47	1.43
12	E	602	NAG	O5-C1	2.53	1.47	1.43
12	A	602	NAG	O5-C1	2.53	1.47	1.43
12	C	612	NAG	O5-C1	2.52	1.47	1.43
12	A	611	NAG	O5-C1	2.50	1.47	1.43
12	E	609	NAG	O5-C1	2.50	1.47	1.43
12	A	603	NAG	C3-C2	2.49	1.57	1.52
12	C	603	NAG	C3-C2	2.49	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	608	NAG	O5-C1	2.45	1.47	1.43
12	C	606	NAG	C2-N2	2.40	1.50	1.46
12	A	610	NAG	C3-C2	2.40	1.57	1.52
12	C	602	NAG	C4-C5	2.39	1.58	1.53
12	A	608	NAG	O5-C1	2.37	1.47	1.43
12	E	612	NAG	C3-C2	2.36	1.57	1.52
12	E	602	NAG	C3-C2	2.35	1.57	1.52
12	A	612	NAG	C3-C2	2.34	1.57	1.52
12	E	610	NAG	C3-C2	2.33	1.57	1.52
12	C	610	NAG	C3-C2	2.33	1.57	1.52
12	E	603	NAG	C4-C5	2.32	1.57	1.53
12	C	602	NAG	C3-C2	2.32	1.57	1.52
12	E	604	NAG	C3-C2	2.31	1.57	1.52
12	A	602	NAG	C3-C2	2.31	1.57	1.52
12	C	611	NAG	C3-C2	2.31	1.57	1.52
12	C	612	NAG	C3-C2	2.30	1.57	1.52
12	A	602	NAG	C4-C5	2.30	1.57	1.53
12	A	604	NAG	C3-C2	2.30	1.57	1.52
12	C	608	NAG	O5-C1	2.29	1.47	1.43
12	A	604	NAG	C4-C5	2.29	1.57	1.53
12	C	603	NAG	C4-C5	2.29	1.57	1.53
12	A	606	NAG	C3-C2	2.29	1.57	1.52
12	E	603	NAG	C3-C2	2.29	1.57	1.52
12	A	611	NAG	C3-C2	2.29	1.57	1.52
12	C	607	NAG	C3-C2	2.29	1.57	1.52
12	C	608	NAG	C3-C2	2.29	1.57	1.52
12	E	604	NAG	C4-C5	2.28	1.57	1.53
12	E	607	NAG	C4-C5	2.28	1.57	1.53
12	C	605	NAG	C4-C5	2.28	1.57	1.53
12	C	606	NAG	C3-C2	2.28	1.57	1.52
12	E	608	NAG	C3-C2	2.27	1.57	1.52
12	A	608	NAG	C3-C2	2.27	1.57	1.52
12	A	603	NAG	C4-C5	2.26	1.57	1.53
12	C	604	NAG	C4-C5	2.26	1.57	1.53
12	C	604	NAG	C3-C2	2.25	1.57	1.52
12	A	601	NAG	C3-C2	2.24	1.57	1.52
12	A	601	NAG	C4-C5	2.24	1.57	1.53
12	E	607	NAG	C2-N2	2.23	1.50	1.46
12	E	601	NAG	C2-N2	2.23	1.50	1.46
12	A	602	NAG	C2-N2	2.22	1.50	1.46
12	E	605	NAG	C3-C2	2.22	1.57	1.52
12	E	602	NAG	C4-C5	2.22	1.57	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	612	NAG	C4-C5	2.21	1.57	1.53
12	E	601	NAG	C4-C5	2.21	1.57	1.53
12	E	607	NAG	C3-C2	2.20	1.57	1.52
12	C	605	NAG	C3-C2	2.19	1.57	1.52
12	E	611	NAG	C4-C5	2.19	1.57	1.53
12	E	609	NAG	C3-C2	2.19	1.57	1.52
12	C	601	NAG	C4-C5	2.18	1.57	1.53
12	A	605	NAG	C3-C2	2.18	1.57	1.52
12	A	606	NAG	C2-N2	2.18	1.50	1.46
12	E	608	NAG	C2-N2	2.18	1.50	1.46
12	A	609	NAG	C4-C5	2.18	1.57	1.53
12	A	607	NAG	C3-C2	2.17	1.57	1.52
12	A	611	NAG	C4-C5	2.17	1.57	1.53
12	E	606	NAG	C3-C2	2.16	1.57	1.52
12	C	608	NAG	C4-C5	2.16	1.57	1.53
12	E	606	NAG	C4-C5	2.16	1.57	1.53
12	E	611	NAG	C3-C2	2.15	1.57	1.52
12	C	601	NAG	C3-C2	2.15	1.57	1.52
12	E	607	NAG	C4-C3	2.14	1.57	1.52
12	C	610	NAG	C4-C5	2.13	1.57	1.53
12	C	611	NAG	C4-C5	2.13	1.57	1.53
12	A	607	NAG	C4-C5	2.13	1.57	1.53
12	C	609	NAG	C4-C5	2.11	1.57	1.53
12	C	602	NAG	C4-C3	2.11	1.57	1.52
12	A	606	NAG	C4-C5	2.10	1.57	1.53
12	E	605	NAG	C4-C5	2.10	1.57	1.53
12	A	612	NAG	C4-C5	2.08	1.57	1.53
12	A	608	NAG	C4-C5	2.08	1.57	1.53
12	A	609	NAG	C3-C2	2.07	1.56	1.52
12	A	605	NAG	C4-C5	2.07	1.57	1.53
12	A	612	NAG	C4-C3	2.07	1.57	1.52
12	E	611	NAG	C4-C3	2.07	1.57	1.52
12	E	603	NAG	C4-C3	2.07	1.57	1.52
12	A	601	NAG	C4-C3	2.06	1.57	1.52
12	C	607	NAG	C4-C5	2.06	1.57	1.53
12	A	607	NAG	C2-N2	2.06	1.49	1.46
12	E	610	NAG	C4-C5	2.06	1.57	1.53
12	C	601	NAG	C4-C3	2.05	1.57	1.52
12	E	601	NAG	C3-C2	2.04	1.56	1.52
12	C	603	NAG	C4-C3	2.04	1.57	1.52
12	A	603	NAG	C4-C3	2.04	1.57	1.52
12	C	608	NAG	C2-N2	2.04	1.49	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	608	NAG	C4-C3	2.03	1.57	1.52
12	E	602	NAG	C2-N2	2.02	1.49	1.46
12	E	608	NAG	C4-C3	2.02	1.57	1.52
12	A	610	NAG	C4-C5	2.02	1.57	1.53
12	C	606	NAG	C4-C5	2.02	1.57	1.53
12	E	609	NAG	C4-C5	2.02	1.57	1.53
12	C	606	NAG	C4-C3	2.01	1.57	1.52
12	A	602	NAG	C4-C3	2.01	1.57	1.52
12	E	608	NAG	C4-C5	2.01	1.57	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	701	NAG	C2-N2-C7	3.65	128.10	122.90
12	E	601	NAG	C8-C7-N2	3.53	122.08	116.10
12	A	602	NAG	C8-C7-N2	2.84	120.91	116.10
12	E	602	NAG	C8-C7-N2	2.83	120.90	116.10
12	C	611	NAG	C8-C7-N2	2.78	120.80	116.10
12	C	606	NAG	C8-C7-N2	2.75	120.75	116.10
12	E	607	NAG	C8-C7-N2	2.74	120.74	116.10
12	A	606	NAG	C8-C7-N2	2.71	120.68	116.10
12	C	607	NAG	C8-C7-N2	2.68	120.64	116.10
12	C	602	NAG	C8-C7-N2	2.67	120.62	116.10
12	C	601	NAG	C8-C7-N2	2.64	120.57	116.10
12	E	606	NAG	C8-C7-N2	2.62	120.53	116.10
12	E	611	NAG	C8-C7-N2	2.61	120.52	116.10
12	A	611	NAG	C8-C7-N2	2.60	120.50	116.10
12	A	601	NAG	C8-C7-N2	2.57	120.45	116.10
12	E	601	NAG	O7-C7-C8	-2.42	117.55	122.06
12	A	607	NAG	C8-C7-N2	2.39	120.15	116.10
12	E	608	NAG	C8-C7-N2	2.39	120.15	116.10
12	A	608	NAG	C8-C7-N2	2.31	120.02	116.10
12	E	604	NAG	C8-C7-N2	2.25	119.92	116.10
12	A	604	NAG	C8-C7-N2	2.24	119.89	116.10
12	C	611	NAG	O7-C7-C8	-2.24	117.90	122.06
12	C	608	NAG	C8-C7-N2	2.21	119.84	116.10
12	C	612	NAG	C8-C7-N2	2.21	119.84	116.10
12	A	612	NAG	C8-C7-N2	2.20	119.82	116.10
12	B	701	NAG	C4-C3-C2	-2.20	107.80	111.02
12	D	701	NAG	C1-O5-C5	2.19	115.16	112.19
12	C	604	NAG	C8-C7-N2	2.18	119.80	116.10
12	A	605	NAG	C8-C7-N2	2.16	119.76	116.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	E	609	NAG	C8-C7-N2	2.16	119.75	116.10
12	C	607	NAG	O7-C7-C8	-2.16	118.05	122.06
12	E	603	NAG	C8-C7-N2	2.13	119.70	116.10
12	C	603	NAG	C8-C7-N2	2.12	119.68	116.10
12	A	608	NAG	C1-C2-N2	-2.11	106.88	110.49
12	C	609	NAG	C8-C7-N2	2.11	119.67	116.10
12	E	612	NAG	C8-C7-N2	2.05	119.57	116.10
12	A	601	NAG	C1-C2-N2	-2.05	106.99	110.49
12	A	602	NAG	O7-C7-C8	-2.05	118.26	122.06
12	C	601	NAG	C1-C2-N2	-2.03	107.02	110.49
12	A	603	NAG	C8-C7-N2	2.03	119.53	116.10
12	E	605	NAG	C8-C7-N2	2.01	119.50	116.10
12	E	610	NAG	C8-C7-N2	2.00	119.49	116.10

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	701	NAG	C3-C2-N2-C7
12	D	701	NAG	C8-C7-N2-C2
12	D	701	NAG	O7-C7-N2-C2
12	F	702	NAG	C8-C7-N2-C2
12	F	702	NAG	O7-C7-N2-C2
12	B	701	NAG	C8-C7-N2-C2
12	B	701	NAG	O7-C7-N2-C2
12	C	602	NAG	O5-C5-C6-O6
12	E	605	NAG	O5-C5-C6-O6
12	A	605	NAG	O5-C5-C6-O6
12	E	611	NAG	O5-C5-C6-O6
12	E	602	NAG	O5-C5-C6-O6
12	A	602	NAG	O5-C5-C6-O6
12	C	609	NAG	O5-C5-C6-O6
12	A	611	NAG	O5-C5-C6-O6
12	A	609	NAG	O5-C5-C6-O6
12	C	610	NAG	O5-C5-C6-O6
12	C	605	NAG	O5-C5-C6-O6
12	C	602	NAG	C4-C5-C6-O6
12	E	605	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	611	NAG	1	0
12	F	702	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1
6	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	151:ARG	C	152:GLY	N	4.05
1	L	94:SER	C	96:PHE	N	2.38

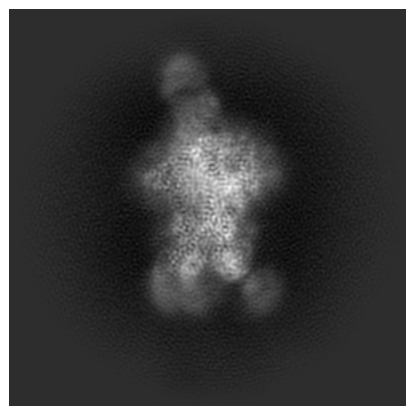
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25754. These allow visual inspection of the internal detail of the map and identification of artifacts.

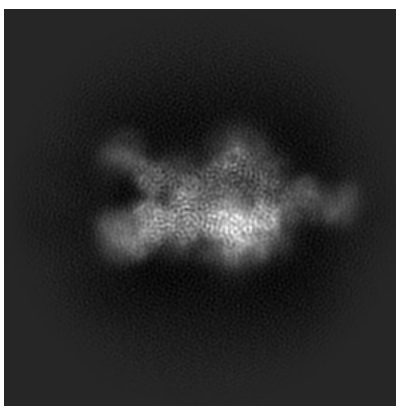
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

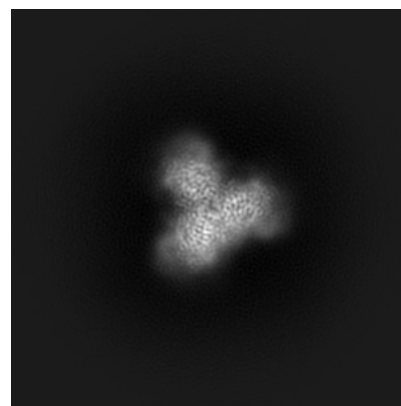
6.1.1 Primary map



X

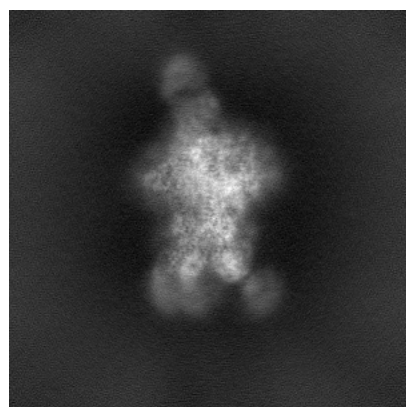


Y

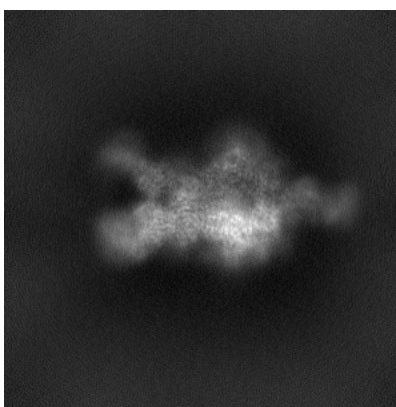


Z

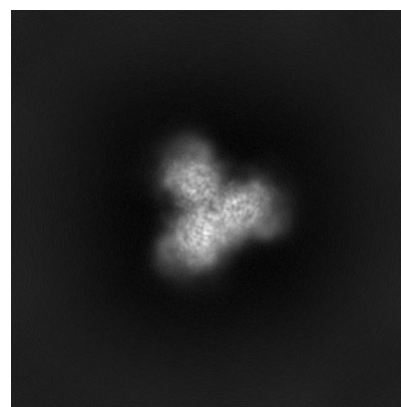
6.1.2 Raw map



X



Y

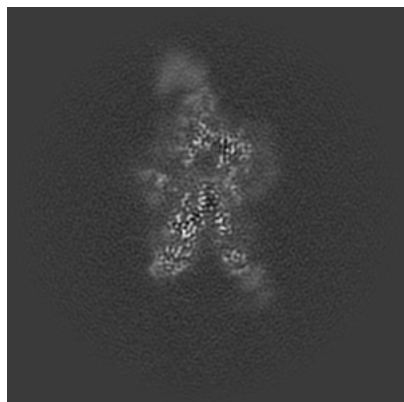


Z

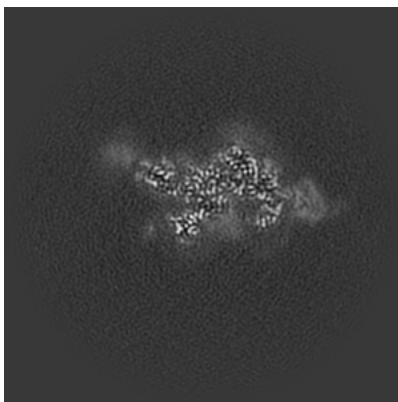
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

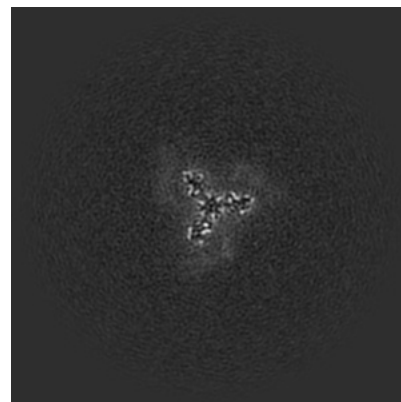
6.2.1 Primary map



X Index: 175

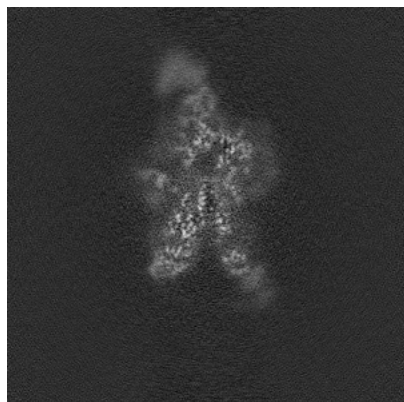


Y Index: 175

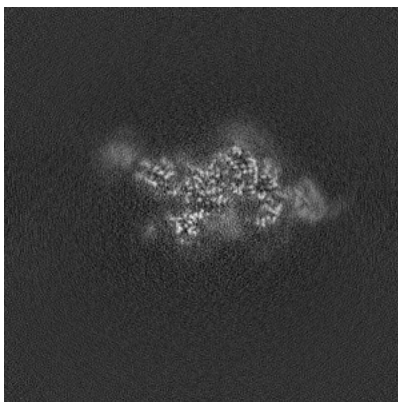


Z Index: 175

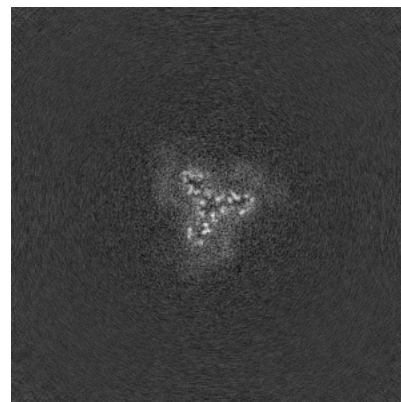
6.2.2 Raw map



X Index: 175



Y Index: 175

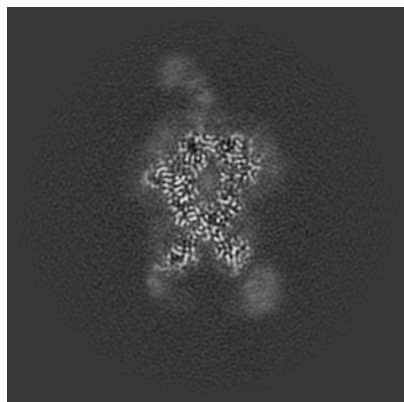


Z Index: 175

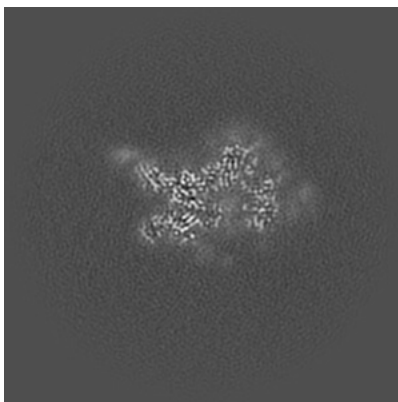
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

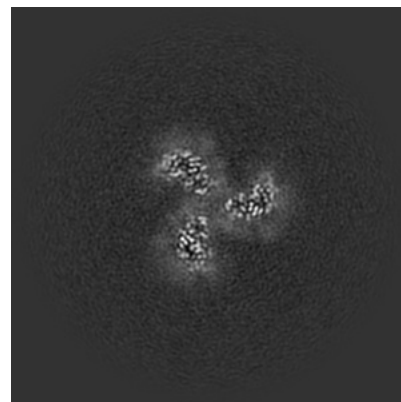
6.3.1 Primary map



X Index: 164

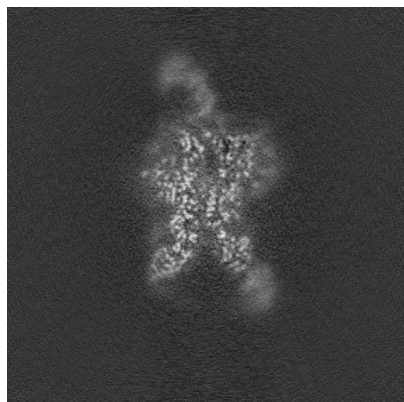


Y Index: 184

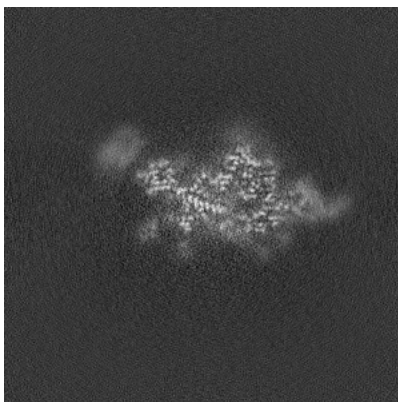


Z Index: 203

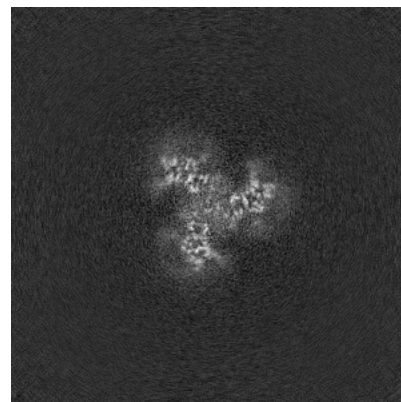
6.3.2 Raw map



X Index: 169



Y Index: 170

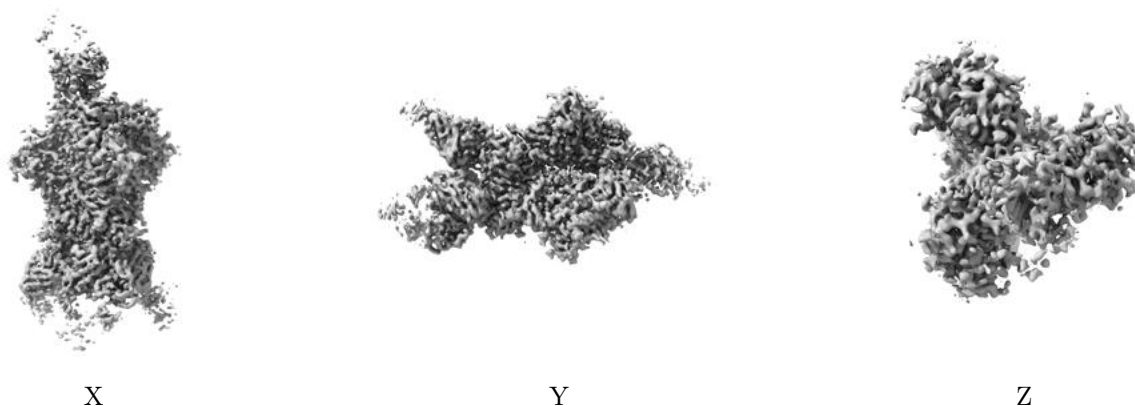


Z Index: 194

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.237. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

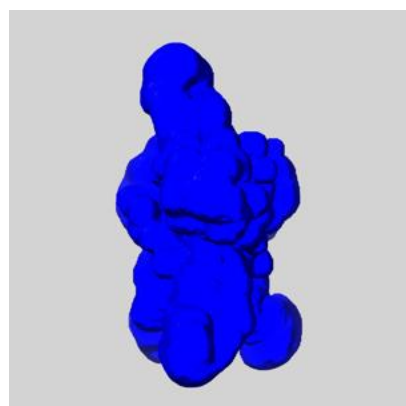
6.5 Mask visualisation [i](#)

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

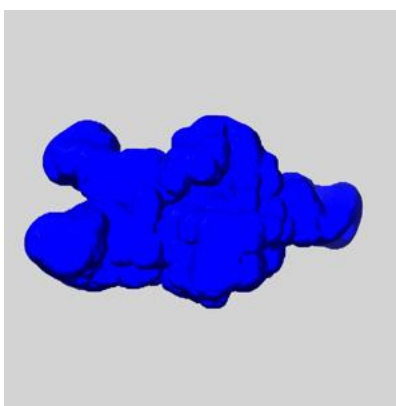
A mask typically either:

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

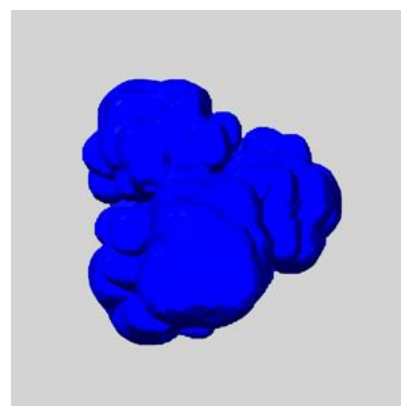
6.5.1 emd_25754_msk_1.map [i](#)



X



Y

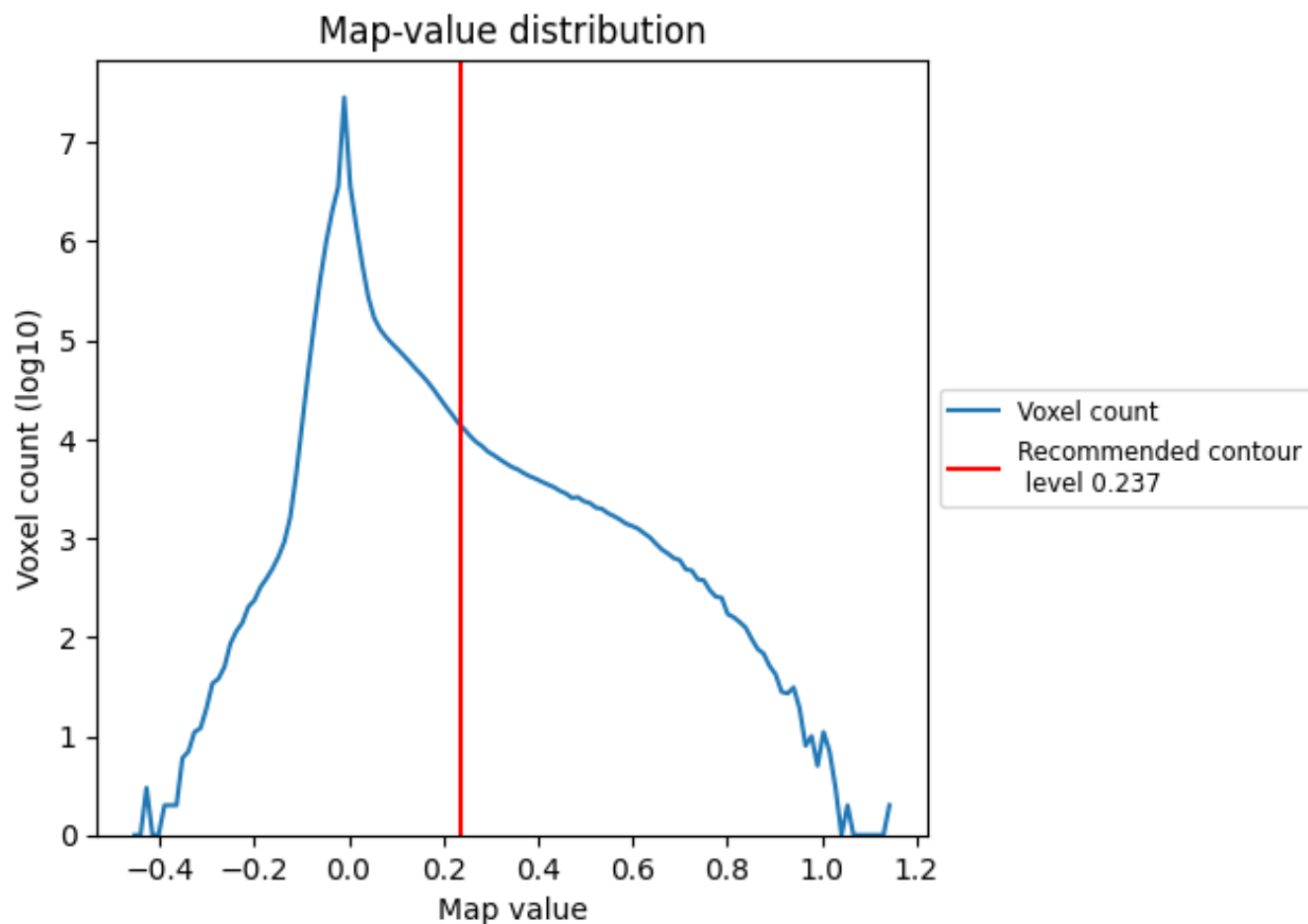


Z

7 Map analysis [i](#)

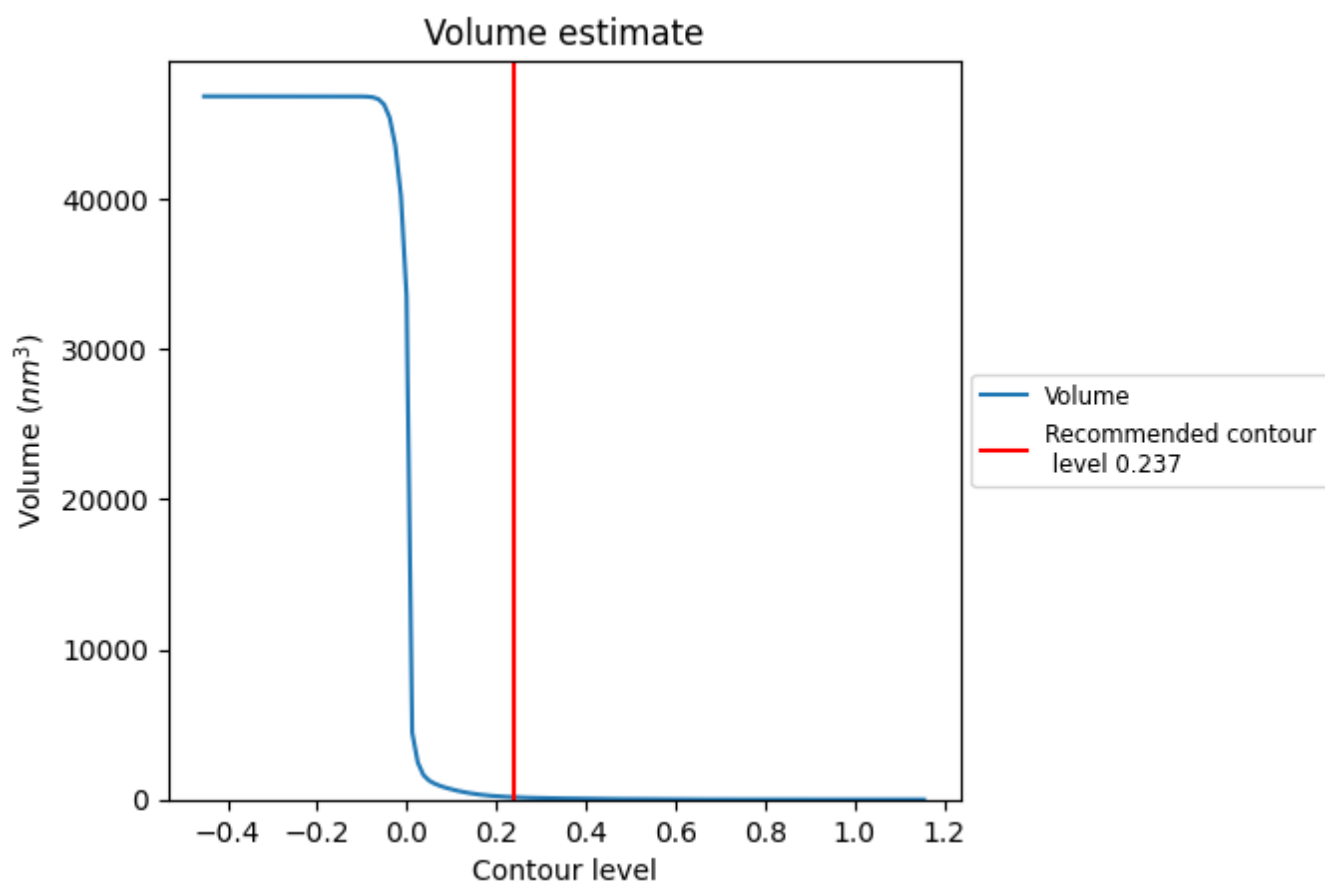
This section contains the results of statistical analysis of the map.

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.

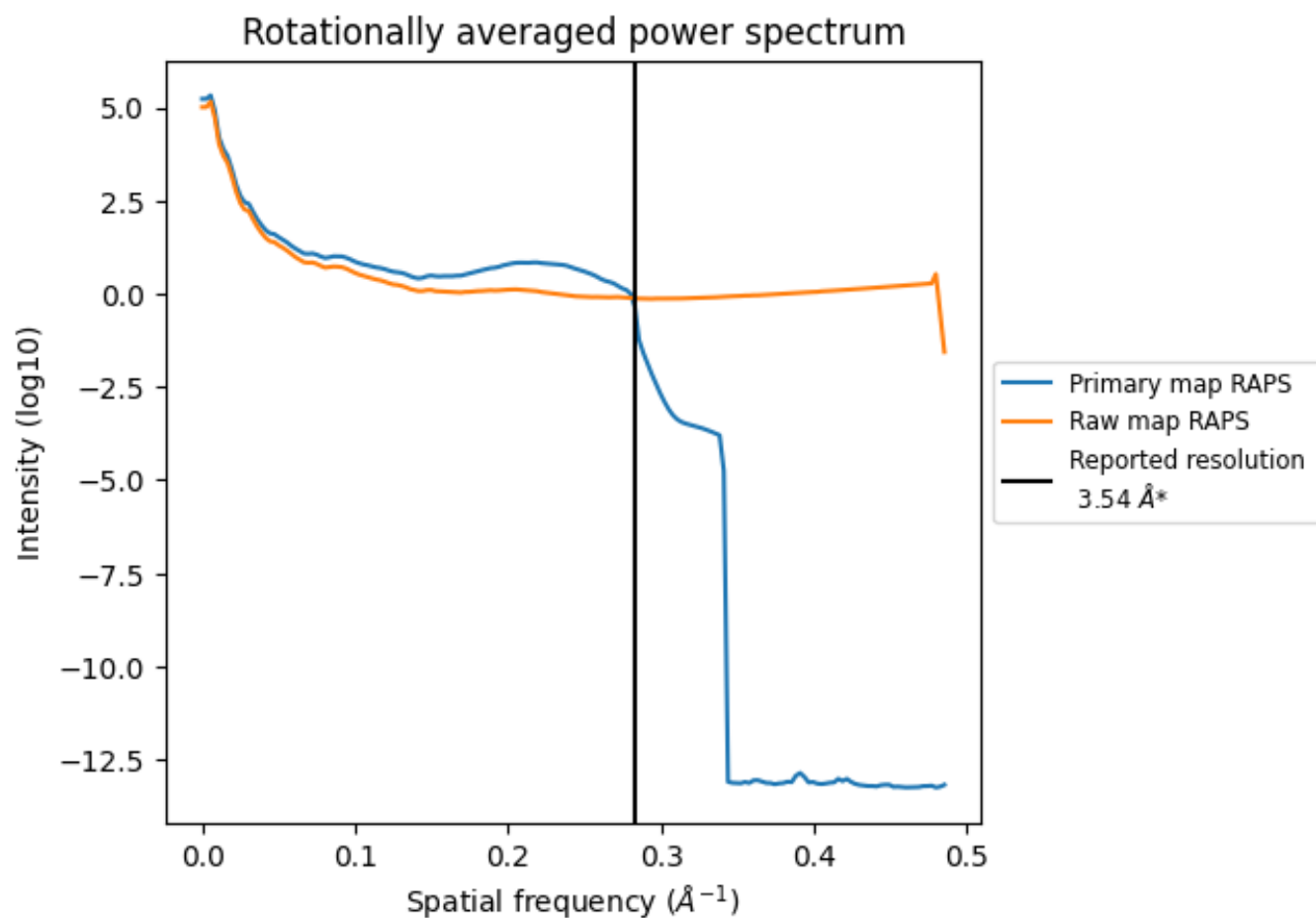
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160 nm³; this corresponds to an approximate mass of 145 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 ⓘ

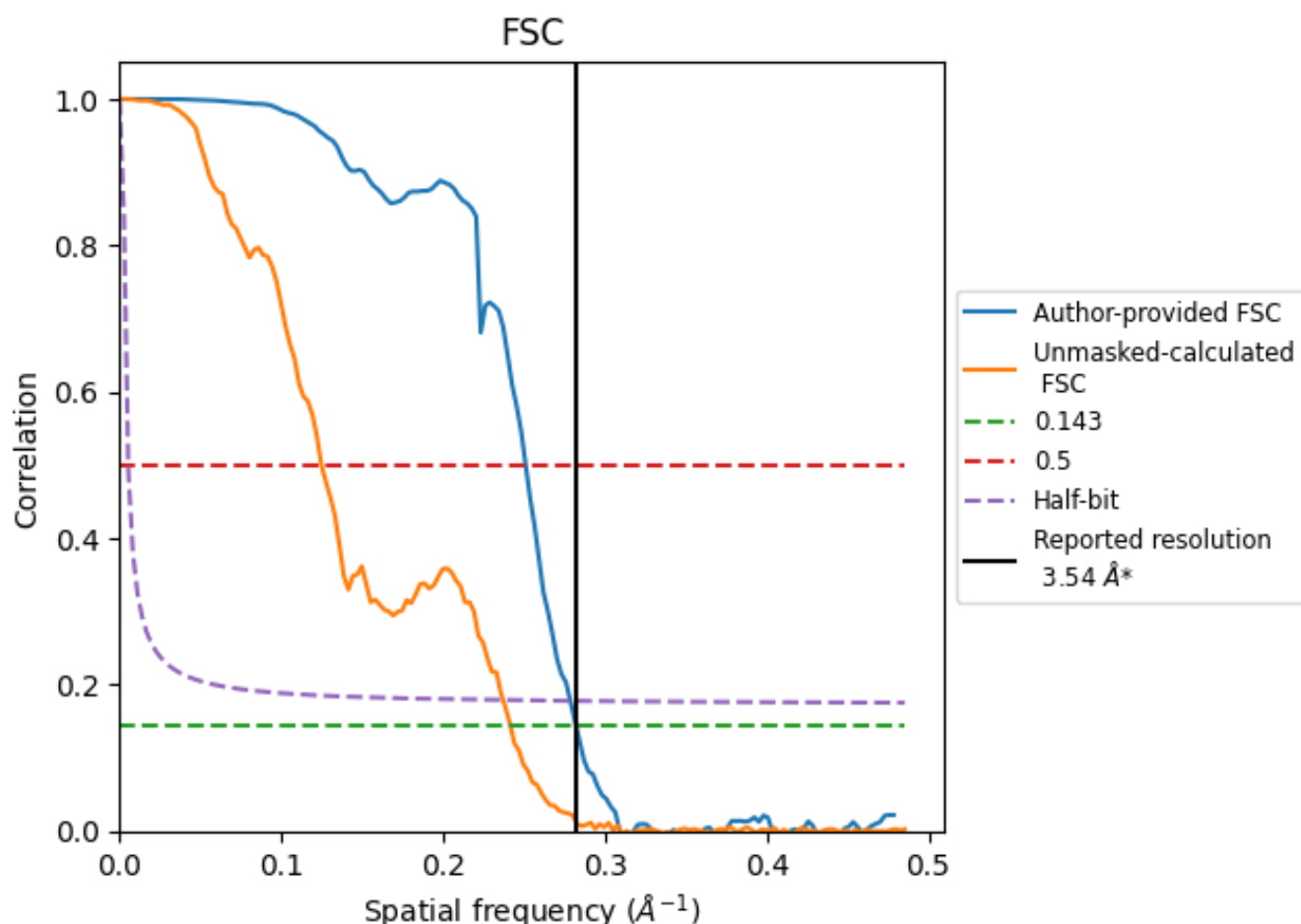


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

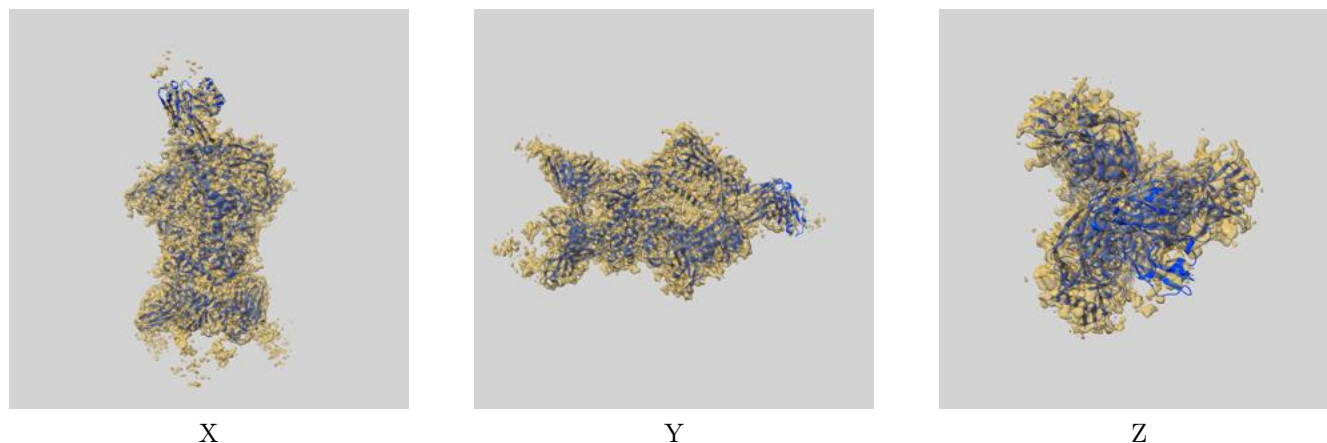
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.54	3.98	3.59
Unmasked-calculated*	4.14	8.01	4.22

*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 4.14 differs from the reported value 3.54 by more than 10 %

9 Map-model fit [i](#)

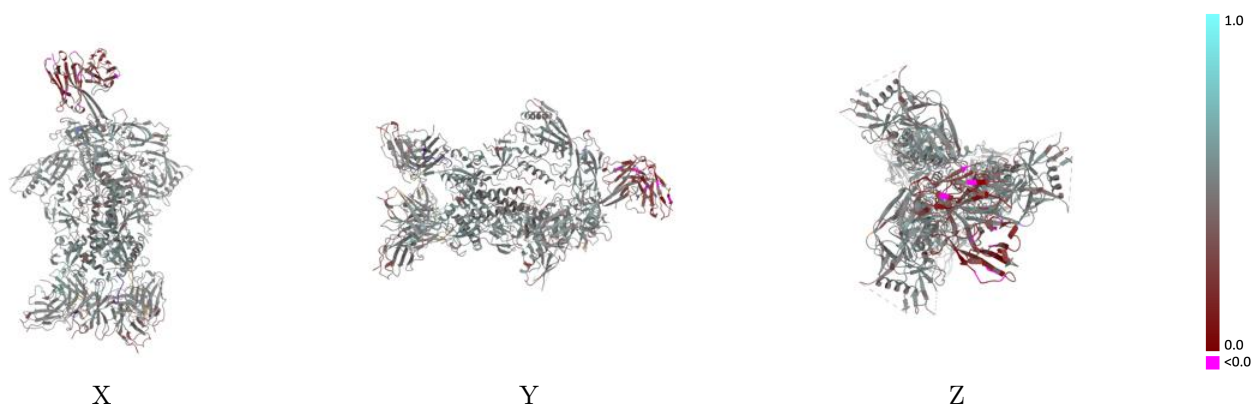
This section contains information regarding the fit between EMDB map EMD-25754 and PDB model 7T9A. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



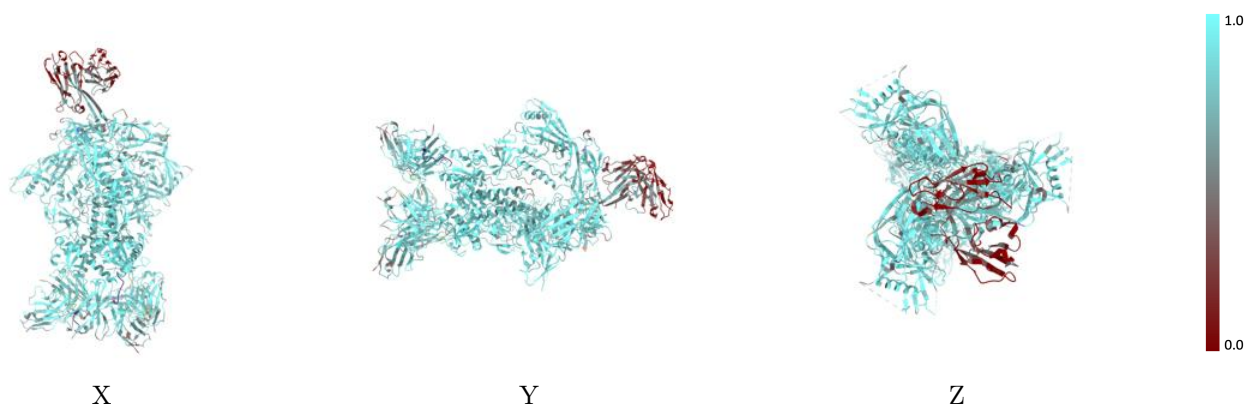
The images above show the 3D surface view of the map at the recommended contour level 0.237 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



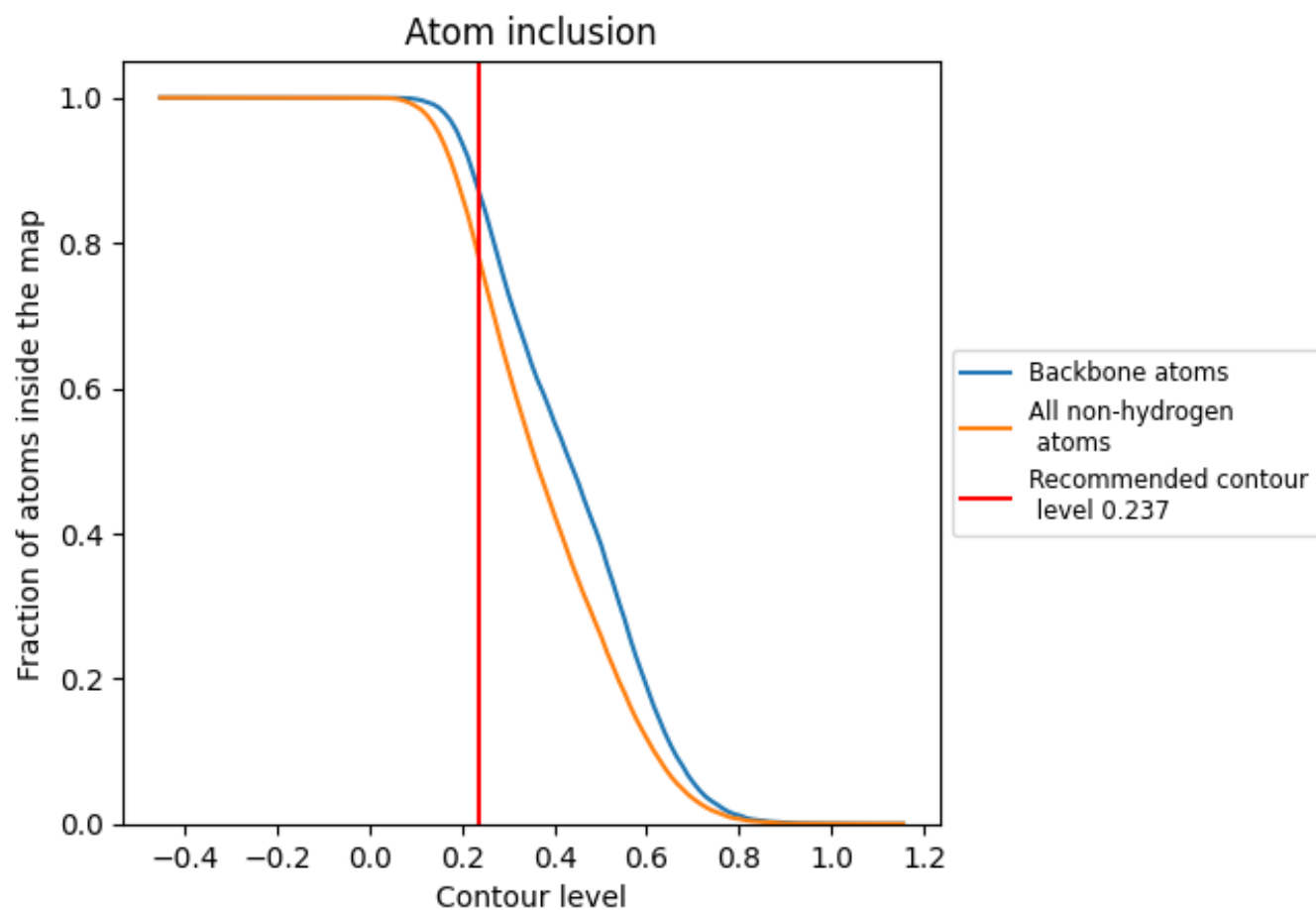
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.237).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.237) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7786	 0.4560
A	 0.8255	 0.4820
B	 0.8667	 0.4950
C	 0.8237	 0.4780
D	 0.8678	 0.4990
E	 0.8349	 0.4820
F	 0.8719	 0.4980
G	 0.5357	 0.3530
H	 0.4088	 0.2710
I	 0.6786	 0.4000
J	 0.8124	 0.4610
K	 0.7695	 0.4460
L	 0.2885	 0.2590
M	 0.8210	 0.4700
N	 0.7670	 0.4450
O	 0.8124	 0.4680
P	 0.8073	 0.4510
Q	 0.7200	 0.4600
R	 0.4359	 0.3000
S	 0.5542	 0.4100
T	 0.4583	 0.3890
U	 0.2917	 0.4360
V	 0.5714	 0.4730
W	 0.6429	 0.3760
X	 0.6071	 0.3910
Y	 0.7200	 0.4690
Z	 0.5714	 0.3620
a	 0.4167	 0.3090
b	 0.4583	 0.2900
c	 0.6429	 0.3850
d	 0.7500	 0.4890
e	 0.7600	 0.4360
f	 0.5714	 0.3520
g	 0.7500	 0.4570
h	 0.4583	 0.4220
i	 0.5000	 0.4070

