



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:29 AM UTC

PDB ID : 6VO3 / pdb_00006vo3
EMDB ID : EMD-21258
Title : AMC009 SOSIP.v4.2 in complex with PGV04 Fab
Authors : Cottrell, C.A.; de Val, N.; Ward, A.B.
Deposited on : 2020-01-29
Resolution : 4.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

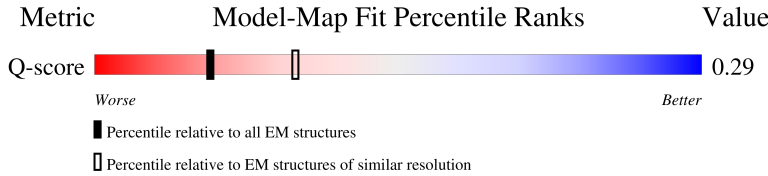
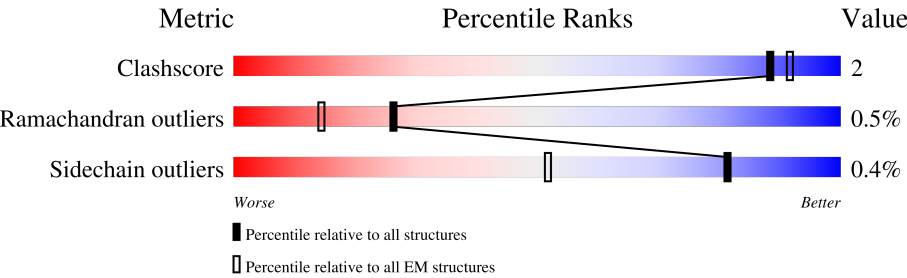
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.25 Å.

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



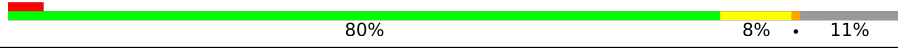
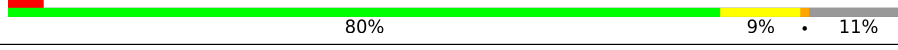
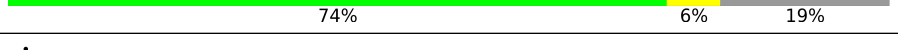
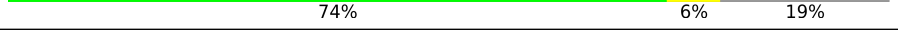
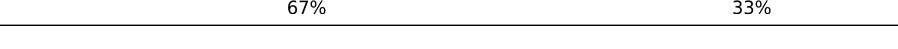
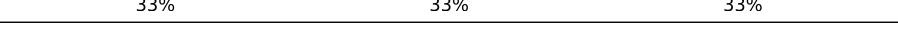
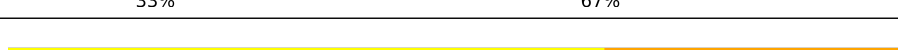
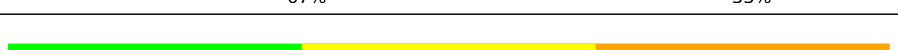
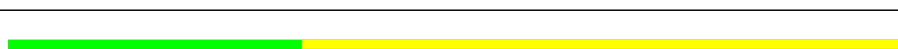
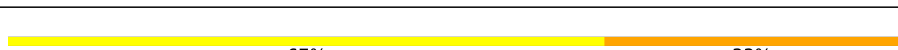
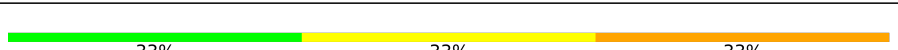
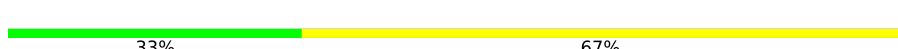
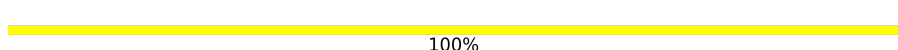
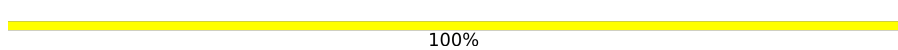
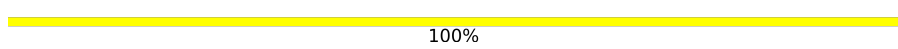
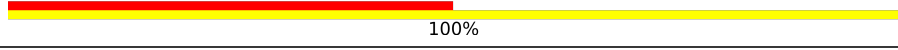
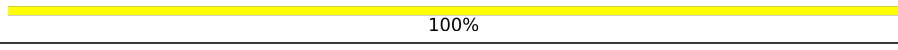
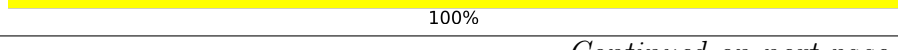
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4654 (3.75 - 4.75)

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	G	228	
1	H	228	
1	I	228	
2	J	208	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	208	
2	L	208	
3	A	482	
3	C	482	
3	D	482	
4	B	154	
4	E	154	
4	F	154	
5	M	3	
5	O	3	
5	Q	3	
5	T	3	
5	V	3	
5	X	3	
5	a	3	
5	c	3	
5	e	3	
6	N	5	
6	U	5	
6	b	5	
7	P	2	
7	R	2	
7	S	2	
7	W	2	
7	Y	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	Z	2	100%
7	d	2	50% 50%
7	f	2	50% 100%
7	g	2	100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19554 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 PGV04 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	125	Total	C	N	O	S	0	0
			994	632	179	180	3		
1	G	125	Total	C	N	O	S	0	0
			994	632	179	180	3		
1	I	125	Total	C	N	O	S	0	0
			994	632	179	180	3		

- Molecule 2 is a protein called PGV04 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	100	Total	C	N	O	S	0	0
			784	500	131	149	4		
2	J	100	Total	C	N	O	S	0	0
			784	500	131	149	4		
2	K	100	Total	C	N	O	S	0	0
			784	500	131	149	4		

- Molecule 3 is a protein called AMC009 SOSIP.v4.2 envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	429	Total	C	N	O	S	0	0
			3402	2149	598	629	26		
3	C	429	Total	C	N	O	S	0	0
			3402	2149	598	629	26		
3	D	429	Total	C	N	O	S	0	0
			3402	2149	598	629	26		

- Molecule 4 is a protein called AMC009 SOSIP.v4.2 envelope glycoprotein gp41.

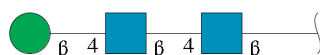
Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	124	Total	C	N	O	S	0	0
			992	623	172	190	7		

Continued on next page...

Continued from previous page...

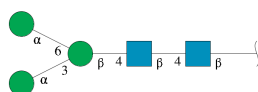
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	124	Total	C	N	O	S	0	0
			992	623	172	190	7		
4	F	124	Total	C	N	O	S	0	0
			992	623	172	190	7		

- Molecule 5 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.



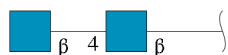
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	Q	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		
5	V	3	Total	C	N	O	0	0
			39	22	2	15		
5	X	3	Total	C	N	O	0	0
			39	22	2	15		
5	a	3	Total	C	N	O	0	0
			39	22	2	15		
5	c	3	Total	C	N	O	0	0
			39	22	2	15		
5	e	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 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.



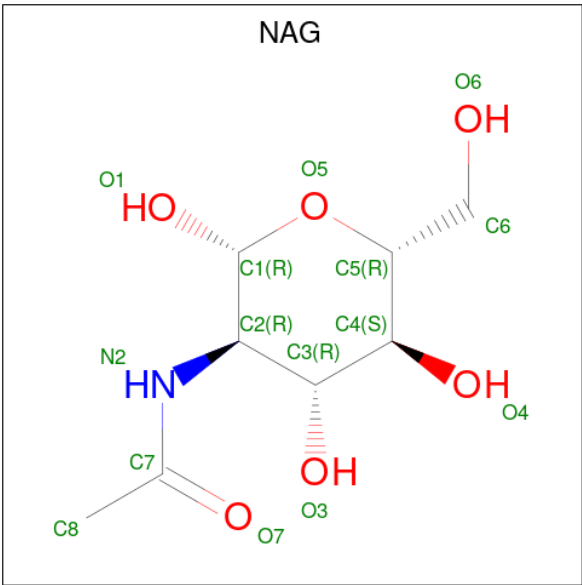
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	5	Total	C	N	O	0	0
			61	34	2	25		
6	U	5	Total	C	N	O	0	0
			61	34	2	25		
6	b	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	P	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	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	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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

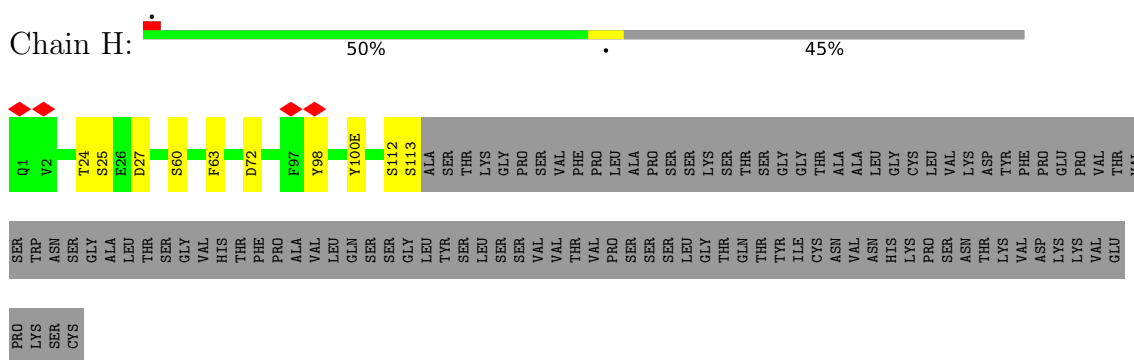
Continued from previous page...

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

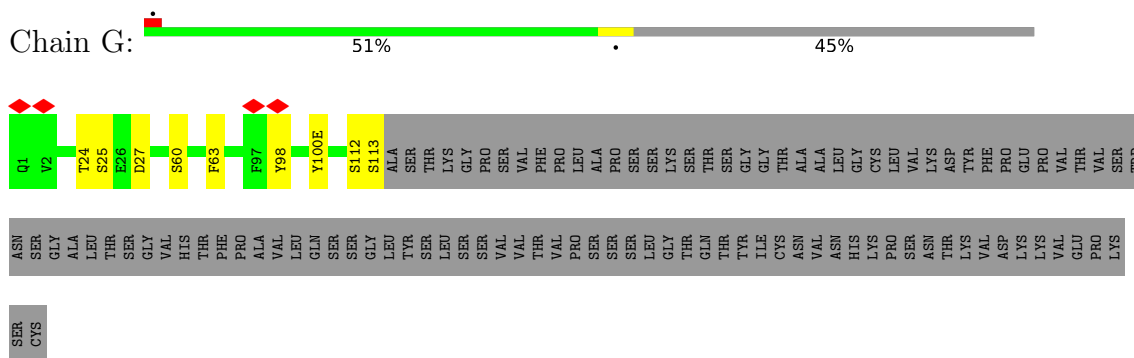
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

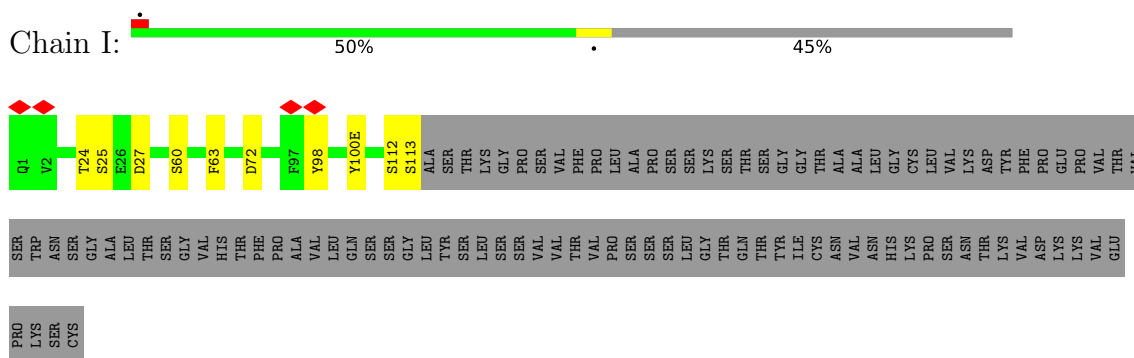
- Molecule 1: PGV04 heavy chain

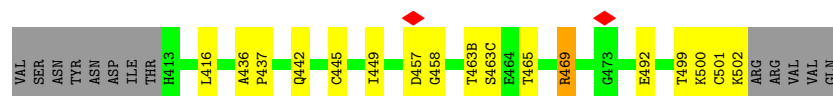


- Molecule 1: PGV04 heavy chain



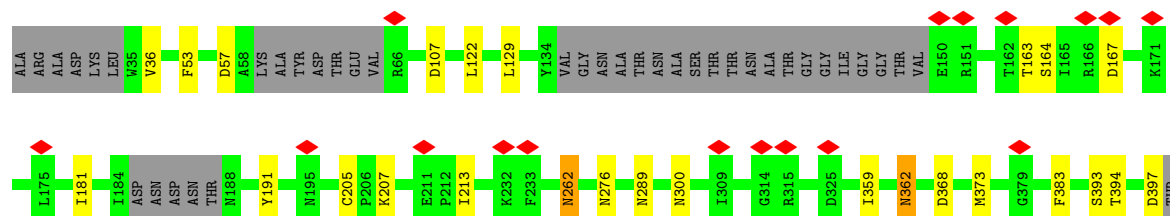
- Molecule 1: PGV04 heavy chain





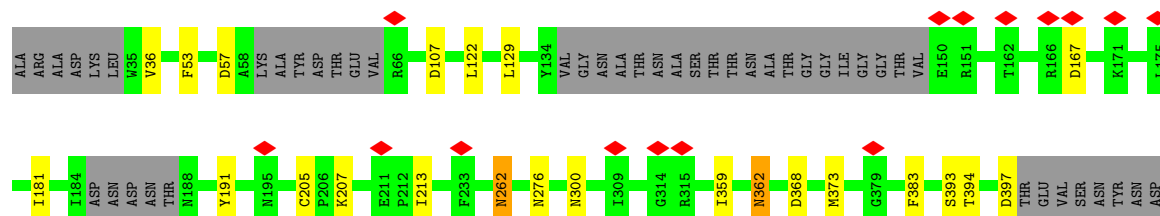
- Molecule 3: AMC009 SOSIP.v4.2 envelope glycoprotein gp120

Chain C: 80% 9% 11%



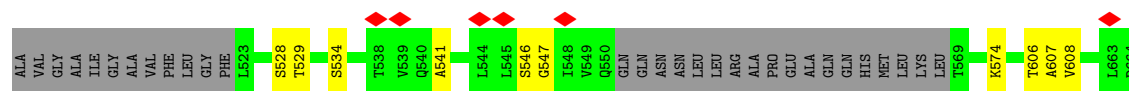
- Molecule 3: AMC009 SOSIP.v4.2 envelope glycoprotein gp120

Chain D: 80% 8% 11%



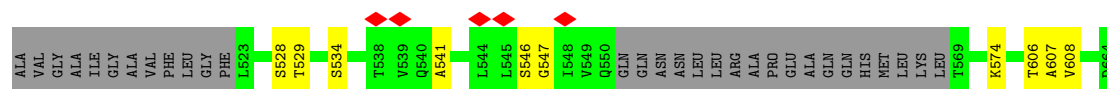
- Molecule 4: AMC009 SOSIP.v4.2 envelope glycoprotein gp41

Chain B: 74% 6% 19%

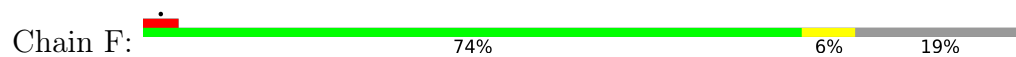


- Molecule 4: AMC009 SOSIP.v4.2 envelope glycoprotein gp41

Chain E: 74% 6% 19%



- Molecule 4: AMC009 SOSIP.v4.2 envelope glycoprotein gp41



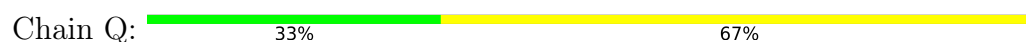
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 67% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 33% 33% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 33% 67%



- Molecule 6: 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

Chain N: 100%



- Molecule 6: 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

Chain U: 100%



- Molecule 6: 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

Chain b: 100%



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

Chain P:  50% 50%

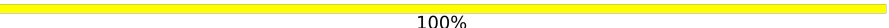


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 100%



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

Chain S:  100%

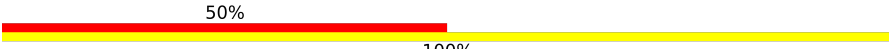


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%

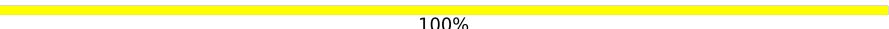


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50% 100%



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

Chain Z:  100%



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

Chain d:  50% 50%

NAG1
NAG2

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

Chain f:  50% 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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	128752	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 ($e^-/\text{\AA}^2$)	32	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	1.361	Depositor
Minimum map value	-0.778	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.33	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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: MAN, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	0.98	0/1020	1.22	5/1383 (0.4%)
1	H	0.98	0/1020	1.22	5/1383 (0.4%)
1	I	0.98	0/1020	1.22	5/1383 (0.4%)
2	J	0.97	1/804 (0.1%)	1.35	7/1087 (0.6%)
2	K	0.97	1/804 (0.1%)	1.35	7/1087 (0.6%)
2	L	0.97	1/804 (0.1%)	1.35	7/1087 (0.6%)
3	A	0.95	0/3475	1.27	26/4717 (0.6%)
3	C	0.95	0/3475	1.27	26/4717 (0.6%)
3	D	0.95	0/3475	1.27	26/4717 (0.6%)
4	B	1.03	0/1008	1.13	3/1367 (0.2%)
4	E	1.03	0/1008	1.13	3/1367 (0.2%)
4	F	1.03	0/1008	1.13	3/1367 (0.2%)
All	All	0.97	3/18921 (0.0%)	1.25	123/25662 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	88	CYS	CB-SG	-5.24	1.64	1.81
2	J	88	CYS	CB-SG	-5.24	1.64	1.81
2	K	88	CYS	CB-SG	-5.23	1.64	1.81

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	53	PHE	CA-CB-CG	8.12	121.92	113.80
3	D	53	PHE	CA-CB-CG	8.11	121.91	113.80
3	C	53	PHE	CA-CB-CG	8.10	121.90	113.80
3	A	181	ILE	N-CA-C	7.78	119.06	108.17
3	C	181	ILE	N-CA-C	7.78	119.06	108.17
3	D	181	ILE	N-CA-C	7.77	119.05	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	79	GLU	CA-C-N	7.56	127.27	119.56
2	L	79	GLU	C-N-CA	7.56	127.27	119.56
2	K	79	GLU	CA-C-N	7.52	127.23	119.56
2	K	79	GLU	C-N-CA	7.52	127.23	119.56
2	J	79	GLU	CA-C-N	7.50	127.22	119.56
2	J	79	GLU	C-N-CA	7.50	127.22	119.56
4	F	608	VAL	CA-C-N	6.90	126.89	119.78
4	F	608	VAL	C-N-CA	6.90	126.89	119.78
4	B	608	VAL	CA-C-N	6.90	126.89	119.78
4	B	608	VAL	C-N-CA	6.90	126.89	119.78
4	E	608	VAL	CA-C-N	6.88	126.87	119.78
4	E	608	VAL	C-N-CA	6.88	126.87	119.78
3	D	469	ARG	CA-C-N	6.81	126.79	119.78
3	D	469	ARG	C-N-CA	6.81	126.79	119.78
3	C	469	ARG	CA-C-N	6.79	126.78	119.78
3	C	469	ARG	C-N-CA	6.79	126.78	119.78
3	A	469	ARG	CA-C-N	6.78	126.77	119.78
3	A	469	ARG	C-N-CA	6.78	126.77	119.78
3	A	492	GLU	CA-C-N	6.37	126.50	119.87
3	A	492	GLU	C-N-CA	6.37	126.50	119.87
3	C	492	GLU	CA-C-N	6.35	126.47	119.87
3	C	492	GLU	C-N-CA	6.35	126.47	119.87
3	D	492	GLU	CA-C-N	6.35	126.47	119.87
3	D	492	GLU	C-N-CA	6.35	126.47	119.87
3	D	205	CYS	CA-C-N	6.31	126.00	119.56
3	D	205	CYS	C-N-CA	6.31	126.00	119.56
3	D	368	ASP	CA-C-N	6.31	126.00	119.56
3	D	368	ASP	C-N-CA	6.31	126.00	119.56
3	A	205	CYS	CA-C-N	6.31	125.99	119.56
3	A	205	CYS	C-N-CA	6.31	125.99	119.56
3	C	205	CYS	CA-C-N	6.30	125.99	119.56
3	C	205	CYS	C-N-CA	6.30	125.99	119.56
3	C	368	ASP	CA-C-N	6.30	125.98	119.56
3	C	368	ASP	C-N-CA	6.30	125.98	119.56
3	A	368	ASP	CA-C-N	6.30	125.98	119.56
3	A	368	ASP	C-N-CA	6.30	125.98	119.56
3	C	457	ASP	N-CA-C	6.10	119.92	112.23
3	A	457	ASP	N-CA-C	6.10	119.91	112.23
3	D	457	ASP	N-CA-C	6.08	119.89	112.23
3	D	437	PRO	CA-C-N	6.05	125.96	119.85
3	D	437	PRO	C-N-CA	6.05	125.96	119.85
3	C	437	PRO	CA-C-N	6.05	125.96	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	437	PRO	C-N-CA	6.05	125.96	119.85
3	A	437	PRO	CA-C-N	6.04	125.95	119.85
3	A	437	PRO	C-N-CA	6.04	125.95	119.85
2	K	30	TYR	CB-CA-C	-6.04	107.89	116.34
2	L	30	TYR	CB-CA-C	-6.02	107.91	116.34
2	J	30	TYR	CB-CA-C	-6.02	107.92	116.34
3	C	436	ALA	CA-C-N	5.91	126.47	120.38
3	C	436	ALA	C-N-CA	5.91	126.47	120.38
3	A	436	ALA	CA-C-N	5.90	126.45	120.38
3	A	436	ALA	C-N-CA	5.90	126.45	120.38
3	D	436	ALA	CA-C-N	5.89	126.44	120.38
3	D	436	ALA	C-N-CA	5.89	126.44	120.38
1	I	60	SER	CA-C-N	5.80	125.48	119.56
1	I	60	SER	C-N-CA	5.80	125.48	119.56
1	G	60	SER	CA-C-N	5.79	125.47	119.56
1	G	60	SER	C-N-CA	5.79	125.47	119.56
1	H	60	SER	CA-C-N	5.75	125.42	119.56
1	H	60	SER	C-N-CA	5.75	125.42	119.56
2	J	42	GLN	CA-C-N	5.72	123.78	119.66
2	J	42	GLN	C-N-CA	5.72	123.78	119.66
2	K	42	GLN	CA-C-N	5.70	123.77	119.66
2	K	42	GLN	C-N-CA	5.70	123.77	119.66
2	L	42	GLN	CA-C-N	5.70	123.76	119.66
2	L	42	GLN	C-N-CA	5.70	123.76	119.66
2	J	43	PRO	CA-C-N	5.47	125.37	119.85
2	J	43	PRO	C-N-CA	5.47	125.37	119.85
2	K	43	PRO	CA-C-N	5.46	125.36	119.85
2	K	43	PRO	C-N-CA	5.46	125.36	119.85
2	L	43	PRO	CA-C-N	5.43	125.34	119.85
2	L	43	PRO	C-N-CA	5.43	125.34	119.85
3	C	458	GLY	N-CA-C	5.37	118.09	110.74
3	A	458	GLY	N-CA-C	5.37	118.09	110.74
3	D	442	GLN	CA-C-N	-5.37	115.45	122.37
3	D	442	GLN	C-N-CA	-5.37	115.45	122.37
3	C	442	GLN	CA-C-N	-5.36	115.46	122.37
3	C	442	GLN	C-N-CA	-5.36	115.46	122.37
3	D	458	GLY	N-CA-C	5.36	118.08	110.74
3	A	442	GLN	CA-C-N	-5.35	115.47	122.37
3	A	442	GLN	C-N-CA	-5.35	115.47	122.37
3	D	359	ILE	N-CA-C	5.35	115.60	108.11
3	C	359	ILE	N-CA-C	5.34	115.59	108.11
3	A	359	ILE	N-CA-C	5.32	115.56	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	122	LEU	N-CA-C	-5.21	105.21	112.45
1	G	100(E)	TYR	N-CA-C	5.21	117.73	109.50
3	D	122	LEU	N-CA-C	-5.21	105.21	112.45
1	I	100(E)	TYR	N-CA-C	5.20	117.72	109.50
3	C	122	LEU	N-CA-C	-5.19	105.23	112.45
1	H	100(E)	TYR	N-CA-C	5.19	117.70	109.50
3	A	300	ASN	CA-CB-CG	5.16	117.76	112.60
3	C	416	LEU	CB-CA-C	-5.16	104.44	110.17
3	D	416	LEU	CB-CA-C	-5.16	104.44	110.17
3	D	300	ASN	CA-CB-CG	5.16	117.76	112.60
3	C	300	ASN	CA-CB-CG	5.15	117.75	112.60
3	A	416	LEU	CB-CA-C	-5.15	104.45	110.17
3	C	36	VAL	CB-CA-C	-5.13	105.69	111.23
3	D	36	VAL	CB-CA-C	-5.13	105.69	111.23
1	G	63	PHE	N-CA-C	-5.11	105.41	111.69
3	A	36	VAL	CB-CA-C	-5.10	105.72	111.23
1	I	98	TYR	N-CA-C	5.08	121.92	113.89
1	H	98	TYR	N-CA-C	5.08	121.92	113.89
1	H	63	PHE	N-CA-C	-5.08	105.44	111.69
1	I	63	PHE	N-CA-C	-5.07	105.46	111.69
4	B	534	SER	N-CA-C	-5.07	105.88	111.71
1	G	98	TYR	N-CA-C	5.06	121.89	113.89
4	F	534	SER	N-CA-C	-5.05	105.90	111.71
4	E	534	SER	N-CA-C	-5.05	105.90	111.71
3	C	383	PHE	CA-CB-CG	5.04	118.84	113.80
3	D	383	PHE	CA-CB-CG	5.04	118.84	113.80
3	A	383	PHE	CA-CB-CG	5.04	118.84	113.80
3	C	457	ASP	CA-C-N	-5.03	114.03	120.72
3	C	457	ASP	C-N-CA	-5.03	114.03	120.72
3	D	457	ASP	CA-C-N	-5.03	114.03	120.72
3	D	457	ASP	C-N-CA	-5.03	114.03	120.72
3	A	457	ASP	CA-C-N	-5.00	114.07	120.72
3	A	457	ASP	C-N-CA	-5.00	114.07	120.72

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	G	994	0	964	3	0
1	H	994	0	964	4	0
1	I	994	0	964	4	0
2	J	784	0	771	2	0
2	K	784	0	771	2	0
2	L	784	0	771	2	0
3	A	3402	0	3358	16	0
3	C	3402	0	3358	17	0
3	D	3402	0	3358	15	0
4	B	992	0	970	4	0
4	E	992	0	970	4	0
4	F	992	0	970	4	0
5	M	39	0	33	1	0
5	O	39	0	33	1	0
5	Q	39	0	33	0	0
5	T	39	0	33	1	0
5	V	39	0	33	1	0
5	X	39	0	33	0	0
5	a	39	0	33	1	0
5	c	39	0	33	1	0
5	e	39	0	33	0	0
6	N	61	0	49	0	0
6	U	61	0	49	0	0
6	b	61	0	49	0	0
7	P	28	0	25	0	0
7	R	28	0	25	0	0
7	S	28	0	25	0	0
7	W	28	0	25	0	0
7	Y	28	0	25	0	0
7	Z	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	A	70	0	65	1	0
8	B	14	0	13	0	0
8	C	70	0	65	1	0
8	D	70	0	65	1	0
8	E	14	0	13	0	0
8	F	14	0	13	0	0
All	All	19554	0	19092	74	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (74) 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)
3:A:207:LYS:NZ	1:I:27:ASP:OD1	2.39	0.56
1:G:27:ASP:OD1	3:D:207:LYS:NZ	2.39	0.56
3:C:57:ASP:N	3:C:57:ASP:OD1	2.38	0.56
3:D:57:ASP:N	3:D:57:ASP:OD1	2.39	0.56
1:H:27:ASP:OD1	3:C:207:LYS:NZ	2.39	0.56
3:A:57:ASP:N	3:A:57:ASP:OD1	2.38	0.55
3:A:167:ASP:OD1	3:A:167:ASP:N	2.40	0.54
3:A:107:ASP:OD1	4:B:574:LYS:NZ	2.40	0.54
3:C:107:ASP:OD1	4:E:574:LYS:NZ	2.40	0.54
4:E:606:THR:OG1	4:E:607:ALA:N	2.41	0.54
3:C:167:ASP:N	3:C:167:ASP:OD1	2.40	0.53
3:D:107:ASP:OD1	4:F:574:LYS:NZ	2.40	0.53
3:A:501:CYS:O	3:A:502:LYS:C	2.52	0.53
3:C:362:ASN:O	3:C:469:ARG:NH1	2.42	0.53
3:C:501:CYS:O	3:C:502:LYS:C	2.52	0.52
4:F:606:THR:OG1	4:F:607:ALA:N	2.41	0.52
4:B:606:THR:OG1	4:B:607:ALA:N	2.41	0.52
3:A:362:ASN:O	3:A:469:ARG:NH1	2.42	0.52
3:D:362:ASN:O	3:D:469:ARG:NH1	2.42	0.51
3:D:501:CYS:O	3:D:502:LYS:C	2.52	0.51
3:A:262:ASN:OD1	3:A:262:ASN:N	2.44	0.50
3:D:167:ASP:N	3:D:167:ASP:OD1	2.40	0.49
2:L:32:HIS:HB3	2:L:50:ALA:HB1	1.96	0.48
2:J:32:HIS:HB3	2:J:50:ALA:HB1	1.96	0.48
2:K:32:HIS:HB3	2:K:50:ALA:HB1	1.96	0.47
3:C:262:ASN:OD1	3:C:262:ASN:N	2.44	0.47
3:D:499:THR:OG1	3:D:500:LYS:N	2.48	0.47
3:D:129:LEU:HB2	3:D:191:TYR:CE2	2.51	0.46
3:C:129:LEU:HB2	3:C:191:TYR:CE2	2.51	0.46
3:A:499:THR:OG1	3:A:500:LYS:N	2.48	0.46
3:A:129:LEU:HB2	3:A:191:TYR:CE2	2.51	0.46
3:C:499:THR:OG1	3:C:500:LYS:N	2.48	0.46
3:D:262:ASN:OD1	3:D:262:ASN:N	2.44	0.45
4:E:546:SER:OG	4:E:547:GLY:N	2.50	0.45
3:C:397:ASP:C	3:C:397:ASP:OD1	2.59	0.45
4:E:528:SER:OG	4:E:529:THR:N	2.49	0.45
3:A:393:SER:OG	3:A:394:THR:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:393:SER:OG	3:C:394:THR:N	2.50	0.45
3:D:397:ASP:OD1	3:D:397:ASP:C	2.59	0.44
4:F:546:SER:OG	4:F:547:GLY:N	2.50	0.44
4:F:528:SER:OG	4:F:529:THR:N	2.49	0.44
1:H:112:SER:O	1:H:113:SER:C	2.61	0.44
4:B:546:SER:OG	4:B:547:GLY:N	2.50	0.43
1:I:112:SER:O	1:I:113:SER:C	2.61	0.43
3:A:189:ASN:OD1	3:A:189:ASN:N	2.51	0.43
3:A:397:ASP:OD1	3:A:397:ASP:C	2.59	0.43
1:G:112:SER:O	1:G:113:SER:C	2.61	0.43
3:D:393:SER:OG	3:D:394:THR:N	2.50	0.43
3:D:463(B):THR:OG1	3:D:463(C):SER:N	2.52	0.43
3:D:445:CYS:HB3	5:a:2:NAG:H83	2.01	0.43
3:D:373:MET:HG2	5:c:1:NAG:H81	2.01	0.42
2:K:77:ARG:O	2:K:78:MET:C	2.62	0.42
3:C:445:CYS:HB3	5:T:2:NAG:H83	2.01	0.42
3:C:463(B):THR:OG1	3:C:463(C):SER:N	2.52	0.42
3:A:373:MET:HG2	5:O:1:NAG:H81	2.01	0.42
3:C:289:ASN:OD1	3:C:289:ASN:N	2.52	0.42
3:C:373:MET:HG2	5:V:1:NAG:H81	2.01	0.42
3:D:463(C):SER:OG	3:D:464:GLU:N	2.53	0.42
1:H:24:THR:OG1	1:H:25:SER:N	2.53	0.42
3:A:463(B):THR:OG1	3:A:463(C):SER:N	2.52	0.42
3:A:163:THR:OG1	3:A:164:SER:N	2.50	0.42
3:C:163:THR:OG1	3:C:164:SER:N	2.50	0.41
1:I:24:THR:OG1	1:I:25:SER:N	2.53	0.41
3:A:445:CYS:HB3	5:M:2:NAG:H83	2.01	0.41
2:J:77:ARG:O	2:J:78:MET:C	2.62	0.41
1:G:24:THR:OG1	1:G:25:SER:N	2.53	0.41
4:B:528:SER:OG	4:B:529:THR:N	2.49	0.41
8:C:619:NAG:O7	8:C:619:NAG:C3	2.69	0.41
2:L:77:ARG:O	2:L:78:MET:C	2.62	0.41
3:C:463(C):SER:OG	3:C:464:GLU:N	2.53	0.40
8:A:619:NAG:O7	8:A:619:NAG:C3	2.69	0.40
1:H:72:ASP:OD1	1:H:72:ASP:C	2.65	0.40
1:I:72:ASP:C	1:I:72:ASP:OD1	2.65	0.40
8:D:619:NAG:O7	8:D:619:NAG:C3	2.69	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	G	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
1	H	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
1	I	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
2	J	98/208 (47%)	94 (96%)	4 (4%)	0	100	100
2	K	98/208 (47%)	94 (96%)	4 (4%)	0	100	100
2	L	98/208 (47%)	94 (96%)	4 (4%)	0	100	100
3	A	419/482 (87%)	397 (95%)	19 (4%)	3 (1%)	18	55
3	C	419/482 (87%)	397 (95%)	19 (4%)	3 (1%)	18	55
3	D	419/482 (87%)	397 (95%)	19 (4%)	3 (1%)	18	55
4	B	120/154 (78%)	114 (95%)	5 (4%)	1 (1%)	16	52
4	E	120/154 (78%)	114 (95%)	5 (4%)	1 (1%)	16	52
4	F	120/154 (78%)	114 (95%)	5 (4%)	1 (1%)	16	52
All	All	2280/3216 (71%)	2181 (96%)	87 (4%)	12 (0%)	26	62

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	465	THR
3	C	465	THR
3	D	465	THR
3	A	213	ILE
3	C	213	ILE
3	D	213	ILE
3	A	449	ILE
4	B	541	ALA
3	C	449	ILE
4	E	541	ALA
3	D	449	ILE
4	F	541	ALA

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	G	104/193 (54%)	104 (100%)	0	100	100
1	H	104/193 (54%)	104 (100%)	0	100	100
1	I	104/193 (54%)	104 (100%)	0	100	100
2	J	85/182 (47%)	85 (100%)	0	100	100
2	K	85/182 (47%)	85 (100%)	0	100	100
2	L	85/182 (47%)	85 (100%)	0	100	100
3	A	386/428 (90%)	383 (99%)	3 (1%)	73	77
3	C	386/428 (90%)	383 (99%)	3 (1%)	73	77
3	D	386/428 (90%)	383 (99%)	3 (1%)	73	77
4	B	107/129 (83%)	107 (100%)	0	100	100
4	E	107/129 (83%)	107 (100%)	0	100	100
4	F	107/129 (83%)	107 (100%)	0	100	100
All	All	2046/2796 (73%)	2037 (100%)	9 (0%)	81	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	262	ASN
3	A	276	ASN
3	A	362	ASN
3	C	262	ASN
3	C	276	ASN
3	C	362	ASN
3	D	262	ASN
3	D	276	ASN
3	D	362	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	195	ASN
3	A	229	ASN
3	A	352	GLN
3	A	428	GLN
3	A	442	GLN
3	C	195	ASN
3	C	229	ASN
3	C	352	GLN
3	C	428	GLN
3	C	442	GLN
3	D	195	ASN
3	D	229	ASN
3	D	352	GLN
3	D	428	GLN
3	D	442	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

60 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	M	1	5,3	14,14,15	0.89	1 (7%)	17,19,21	2.06	4 (23%)
5	NAG	M	2	5	14,14,15	0.81	0	17,19,21	1.33	2 (11%)
5	BMA	M	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.85	0
6	NAG	N	1	6,3	14,14,15	0.87	0	17,19,21	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	N	2	6	14,14,15	1.08	1 (7%)	17,19,21	1.30	2 (11%)
6	BMA	N	3	6	11,11,12	1.96	3 (27%)	15,15,17	1.08	1 (6%)
6	MAN	N	4	6	11,11,12	1.84	3 (27%)	15,15,17	1.01	2 (13%)
6	MAN	N	5	6	11,11,12	1.83	2 (18%)	15,15,17	1.10	2 (13%)
5	NAG	O	1	5,3	14,14,15	0.87	1 (7%)	17,19,21	2.27	5 (29%)
5	NAG	O	2	5	14,14,15	0.78	0	17,19,21	0.92	0
5	BMA	O	3	5	11,11,12	1.80	2 (18%)	15,15,17	0.83	1 (6%)
7	NAG	P	1	7,3	14,14,15	0.79	0	17,19,21	0.93	0
7	NAG	P	2	7	14,14,15	0.80	0	17,19,21	0.90	1 (5%)
5	NAG	Q	1	5,3	14,14,15	0.80	0	17,19,21	0.91	0
5	NAG	Q	2	5	14,14,15	0.82	0	17,19,21	0.96	1 (5%)
5	BMA	Q	3	5	11,11,12	1.79	2 (18%)	15,15,17	0.82	1 (6%)
7	NAG	R	1	7,3	14,14,15	0.81	0	17,19,21	1.44	3 (17%)
7	NAG	R	2	7	14,14,15	0.83	0	17,19,21	1.12	1 (5%)
7	NAG	S	1	7,3	14,14,15	0.83	0	17,19,21	1.30	2 (11%)
7	NAG	S	2	7	14,14,15	0.81	0	17,19,21	0.96	1 (5%)
5	NAG	T	1	5,3	14,14,15	0.89	1 (7%)	17,19,21	2.07	4 (23%)
5	NAG	T	2	5	14,14,15	0.81	0	17,19,21	1.32	2 (11%)
5	BMA	T	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.85	0
6	NAG	U	1	6,3	14,14,15	0.87	0	17,19,21	1.12	2 (11%)
6	NAG	U	2	6	14,14,15	1.08	1 (7%)	17,19,21	1.30	2 (11%)
6	BMA	U	3	6	11,11,12	1.96	3 (27%)	15,15,17	1.08	1 (6%)
6	MAN	U	4	6	11,11,12	1.84	3 (27%)	15,15,17	1.02	2 (13%)
6	MAN	U	5	6	11,11,12	1.82	2 (18%)	15,15,17	1.10	2 (13%)
5	NAG	V	1	5,3	14,14,15	0.86	1 (7%)	17,19,21	2.27	5 (29%)
5	NAG	V	2	5	14,14,15	0.78	0	17,19,21	0.92	0
5	BMA	V	3	5	11,11,12	1.80	2 (18%)	15,15,17	0.83	1 (6%)
7	NAG	W	1	7,3	14,14,15	0.78	0	17,19,21	0.93	0
7	NAG	W	2	7	14,14,15	0.80	0	17,19,21	0.90	1 (5%)
5	NAG	X	1	5,3	14,14,15	0.79	0	17,19,21	0.91	0
5	NAG	X	2	5	14,14,15	0.82	0	17,19,21	0.95	1 (5%)
5	BMA	X	3	5	11,11,12	1.80	2 (18%)	15,15,17	0.82	1 (6%)
7	NAG	Y	1	7,3	14,14,15	0.81	0	17,19,21	1.44	3 (17%)
7	NAG	Y	2	7	14,14,15	0.83	0	17,19,21	1.12	1 (5%)
7	NAG	Z	1	7,3	14,14,15	0.83	0	17,19,21	1.30	2 (11%)
7	NAG	Z	2	7	14,14,15	0.80	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	a	1	5,3	14,14,15	0.89	1 (7%)	17,19,21	2.07	4 (23%)
5	NAG	a	2	5	14,14,15	0.81	0	17,19,21	1.32	2 (11%)
5	BMA	a	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.85	0
6	NAG	b	1	6,3	14,14,15	0.87	0	17,19,21	1.12	2 (11%)
6	NAG	b	2	6	14,14,15	1.09	1 (7%)	17,19,21	1.30	2 (11%)
6	BMA	b	3	6	11,11,12	1.96	3 (27%)	15,15,17	1.08	1 (6%)
6	MAN	b	4	6	11,11,12	1.84	3 (27%)	15,15,17	1.02	2 (13%)
6	MAN	b	5	6	11,11,12	1.83	2 (18%)	15,15,17	1.10	2 (13%)
5	NAG	c	1	5,3	14,14,15	0.86	1 (7%)	17,19,21	2.27	5 (29%)
5	NAG	c	2	5	14,14,15	0.78	0	17,19,21	0.92	0
5	BMA	c	3	5	11,11,12	1.80	2 (18%)	15,15,17	0.82	1 (6%)
7	NAG	d	1	7,3	14,14,15	0.79	0	17,19,21	0.93	0
7	NAG	d	2	7	14,14,15	0.80	0	17,19,21	0.90	1 (5%)
5	NAG	e	1	5,3	14,14,15	0.80	0	17,19,21	0.91	0
5	NAG	e	2	5	14,14,15	0.82	0	17,19,21	0.95	1 (5%)
5	BMA	e	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.82	1 (6%)
7	NAG	f	1	7,3	14,14,15	0.81	0	17,19,21	1.44	3 (17%)
7	NAG	f	2	7	14,14,15	0.83	0	17,19,21	1.12	1 (5%)
7	NAG	g	1	7,3	14,14,15	0.84	0	17,19,21	1.30	2 (11%)
7	NAG	g	2	7	14,14,15	0.81	0	17,19,21	0.96	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
5	NAG	M	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
6	NAG	N	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	1/2/19/22	0/1/1/1
6	MAN	N	5	6	-	1/2/19/22	0/1/1/1
5	NAG	O	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	c	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	1/2/19/22	0/1/1/1
7	NAG	d	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	1/6/23/26	0/1/1/1
5	NAG	e	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
5	BMA	e	3	5	-	1/2/19/22	0/1/1/1
7	NAG	f	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	f	2	7	-	1/6/23/26	0/1/1/1
7	NAG	g	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	2/6/23/26	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	3	BMA	O2-C2	-4.23	1.34	1.43
5	X	3	BMA	O2-C2	-4.21	1.34	1.43
5	Q	3	BMA	O2-C2	-4.20	1.34	1.43
6	b	5	MAN	O2-C2	-4.19	1.34	1.43
6	U	5	MAN	O2-C2	-4.18	1.34	1.43
6	N	5	MAN	O2-C2	-4.17	1.34	1.43
6	N	3	BMA	O2-C2	-4.14	1.34	1.43
6	U	3	BMA	O2-C2	-4.13	1.34	1.43
6	b	3	BMA	O2-C2	-4.13	1.34	1.43
6	N	4	MAN	O2-C2	-4.11	1.34	1.43
6	b	4	MAN	O2-C2	-4.11	1.34	1.43
6	U	4	MAN	O2-C2	-4.10	1.34	1.43
5	M	3	BMA	O2-C2	-4.10	1.34	1.43
5	V	3	BMA	O2-C2	-4.10	1.34	1.43
5	O	3	BMA	O2-C2	-4.10	1.34	1.43
5	c	3	BMA	O2-C2	-4.09	1.34	1.43
5	T	3	BMA	O2-C2	-4.08	1.34	1.43
5	a	3	BMA	O2-C2	-4.07	1.34	1.43
5	V	3	BMA	C2-C3	-2.31	1.48	1.52
6	b	3	BMA	C2-C3	-2.29	1.49	1.52
5	O	3	BMA	C2-C3	-2.29	1.49	1.52
6	N	5	MAN	C2-C3	-2.29	1.49	1.52
5	M	1	NAG	C3-C2	-2.28	1.47	1.52
5	c	3	BMA	C2-C3	-2.28	1.49	1.52
5	T	1	NAG	C3-C2	-2.28	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	1	NAG	C3-C2	-2.28	1.47	1.52
6	U	3	BMA	C2-C3	-2.28	1.49	1.52
6	b	5	MAN	C2-C3	-2.26	1.49	1.52
6	N	3	BMA	C2-C3	-2.26	1.49	1.52
6	U	5	MAN	C2-C3	-2.26	1.49	1.52
6	b	2	NAG	C3-C2	-2.23	1.47	1.52
6	N	2	NAG	C3-C2	-2.23	1.47	1.52
6	U	2	NAG	C3-C2	-2.23	1.47	1.52
6	N	4	MAN	O5-C1	2.18	1.47	1.43
6	b	4	MAN	O5-C1	2.17	1.47	1.43
5	a	3	BMA	C2-C3	-2.17	1.49	1.52
6	U	4	MAN	O5-C1	2.17	1.47	1.43
5	X	3	BMA	C2-C3	-2.15	1.49	1.52
5	e	3	BMA	C2-C3	-2.14	1.49	1.52
5	M	3	BMA	C2-C3	-2.14	1.49	1.52
5	Q	3	BMA	C2-C3	-2.13	1.49	1.52
5	T	3	BMA	C2-C3	-2.12	1.49	1.52
6	N	3	BMA	C6-C5	2.11	1.58	1.51
6	U	3	BMA	C6-C5	2.11	1.58	1.51
6	b	3	BMA	C6-C5	2.09	1.58	1.51
6	U	4	MAN	C2-C3	-2.09	1.49	1.52
6	N	4	MAN	C2-C3	-2.08	1.49	1.52
6	b	4	MAN	C2-C3	-2.07	1.49	1.52
5	O	1	NAG	C3-C2	-2.02	1.48	1.52
5	V	1	NAG	C3-C2	-2.01	1.48	1.52
5	c	1	NAG	C3-C2	-2.00	1.48	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	1	NAG	O4-C4-C3	-5.23	98.04	110.38
5	V	1	NAG	O4-C4-C3	-5.22	98.06	110.38
5	O	1	NAG	O4-C4-C3	-5.21	98.08	110.38
5	T	1	NAG	O4-C4-C3	-5.10	98.36	110.38
5	M	1	NAG	O4-C4-C3	-5.09	98.37	110.38
5	a	1	NAG	O4-C4-C3	-5.09	98.37	110.38
5	c	1	NAG	O5-C5-C6	-4.96	98.01	107.66
5	V	1	NAG	O5-C5-C6	-4.96	98.01	107.66
5	O	1	NAG	O5-C5-C6	-4.94	98.04	107.66
5	T	1	NAG	O5-C5-C6	-3.89	100.08	107.66
5	a	1	NAG	O5-C5-C6	-3.89	100.10	107.66
5	M	1	NAG	O5-C5-C6	-3.88	100.12	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	b	1	NAG	C3-C4-C5	-3.53	103.83	110.23
6	U	1	NAG	C3-C4-C5	-3.53	103.83	110.23
6	N	1	NAG	C3-C4-C5	-3.53	103.83	110.23
7	g	1	NAG	C4-C3-C2	-3.42	106.00	111.02
5	M	2	NAG	C4-C3-C2	-3.40	106.03	111.02
7	Z	1	NAG	C4-C3-C2	-3.40	106.04	111.02
7	S	1	NAG	C4-C3-C2	-3.40	106.04	111.02
5	a	2	NAG	C4-C3-C2	-3.40	106.04	111.02
5	V	1	NAG	C3-C4-C5	-3.39	104.08	110.23
5	T	2	NAG	C4-C3-C2	-3.39	106.05	111.02
5	O	1	NAG	C3-C4-C5	-3.39	104.08	110.23
5	c	1	NAG	C3-C4-C5	-3.38	104.10	110.23
5	T	1	NAG	O4-C4-C5	3.33	117.53	109.32
5	a	1	NAG	O4-C4-C5	3.33	117.53	109.32
5	M	1	NAG	O4-C4-C5	3.33	117.52	109.32
7	f	2	NAG	C4-C3-C2	-3.33	106.14	111.02
7	Y	2	NAG	C4-C3-C2	-3.32	106.15	111.02
7	R	2	NAG	C4-C3-C2	-3.32	106.16	111.02
5	c	1	NAG	O4-C4-C5	3.22	117.26	109.32
5	O	1	NAG	O4-C4-C5	3.22	117.26	109.32
5	V	1	NAG	O4-C4-C5	3.21	117.23	109.32
5	M	2	NAG	C1-C2-N2	-3.16	105.45	110.43
5	a	2	NAG	C1-C2-N2	-3.16	105.45	110.43
5	T	2	NAG	C1-C2-N2	-3.15	105.47	110.43
6	N	2	NAG	O5-C1-C2	-3.05	106.57	111.29
6	U	2	NAG	O5-C1-C2	-3.05	106.57	111.29
6	b	2	NAG	O5-C1-C2	-3.05	106.58	111.29
7	f	1	NAG	O4-C4-C3	-3.00	103.31	110.38
7	Y	1	NAG	O4-C4-C3	-3.00	103.31	110.38
7	R	1	NAG	O4-C4-C3	-3.00	103.32	110.38
7	f	1	NAG	O5-C5-C6	-2.80	102.22	107.66
7	R	1	NAG	O5-C5-C6	-2.80	102.22	107.66
7	Y	1	NAG	O5-C5-C6	-2.80	102.22	107.66
7	Y	1	NAG	C3-C4-C5	-2.79	105.17	110.23
7	R	1	NAG	C3-C4-C5	-2.78	105.19	110.23
7	f	1	NAG	C3-C4-C5	-2.78	105.20	110.23
5	T	1	NAG	C3-C4-C5	-2.68	105.37	110.23
5	a	1	NAG	C3-C4-C5	-2.68	105.37	110.23
5	M	1	NAG	C3-C4-C5	-2.68	105.38	110.23
7	S	2	NAG	C4-C3-C2	-2.65	107.13	111.02
7	g	2	NAG	C4-C3-C2	-2.65	107.13	111.02
7	Z	2	NAG	C4-C3-C2	-2.64	107.14	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C4-C3-C2	2.54	114.75	111.02
5	V	1	NAG	C4-C3-C2	2.53	114.73	111.02
7	S	1	NAG	O5-C1-C2	-2.53	107.37	111.29
7	Z	1	NAG	O5-C1-C2	-2.53	107.38	111.29
7	g	1	NAG	O5-C1-C2	-2.53	107.38	111.29
5	c	1	NAG	C4-C3-C2	2.52	114.70	111.02
7	d	2	NAG	C4-C3-C2	-2.46	107.41	111.02
7	W	2	NAG	C4-C3-C2	-2.45	107.42	111.02
7	P	2	NAG	C4-C3-C2	-2.45	107.43	111.02
6	b	3	BMA	O3-C3-C4	2.34	115.90	110.38
6	N	3	BMA	O3-C3-C4	2.34	115.90	110.38
6	U	3	BMA	O3-C3-C4	2.34	115.90	110.38
5	X	2	NAG	C4-C3-C2	-2.29	107.66	111.02
5	Q	2	NAG	C4-C3-C2	-2.29	107.66	111.02
5	e	2	NAG	C4-C3-C2	-2.29	107.66	111.02
6	N	1	NAG	O5-C1-C2	-2.27	107.77	111.29
6	U	1	NAG	O5-C1-C2	-2.27	107.77	111.29
6	b	1	NAG	O5-C1-C2	-2.27	107.78	111.29
6	N	5	MAN	C2-C3-C4	-2.23	106.94	110.86
6	U	5	MAN	C2-C3-C4	-2.23	106.94	110.86
6	b	5	MAN	C2-C3-C4	-2.22	106.95	110.86
6	U	4	MAN	C2-C3-C4	-2.18	107.02	110.86
6	b	4	MAN	C2-C3-C4	-2.18	107.03	110.86
6	U	2	NAG	C4-C3-C2	-2.17	107.84	111.02
6	N	5	MAN	C1-C2-C3	2.17	112.80	109.64
6	N	4	MAN	C2-C3-C4	-2.16	107.06	110.86
6	U	5	MAN	C1-C2-C3	2.16	112.79	109.64
6	b	2	NAG	C4-C3-C2	-2.16	107.86	111.02
6	N	2	NAG	C4-C3-C2	-2.15	107.86	111.02
6	b	5	MAN	C1-C2-C3	2.14	112.77	109.64
6	b	4	MAN	C1-C2-C3	2.09	112.69	109.64
6	U	4	MAN	C1-C2-C3	2.09	112.69	109.64
6	N	4	MAN	C1-C2-C3	2.08	112.67	109.64
5	Q	3	BMA	C2-C3-C4	-2.05	107.25	110.86
5	X	3	BMA	C2-C3-C4	-2.05	107.26	110.86
5	e	3	BMA	C2-C3-C4	-2.03	107.28	110.86
5	O	3	BMA	C2-C3-C4	-2.03	107.30	110.86
5	V	3	BMA	C2-C3-C4	-2.02	107.30	110.86
5	c	3	BMA	C2-C3-C4	-2.02	107.31	110.86

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	1	NAG	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	a	3	BMA	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	b	3	BMA	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
6	b	3	BMA	C4-C5-C6-O6
5	Q	3	BMA	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
7	Y	2	NAG	O5-C5-C6-O6
7	f	2	NAG	O5-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
7	Y	1	NAG	C4-C5-C6-O6
7	f	1	NAG	C4-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

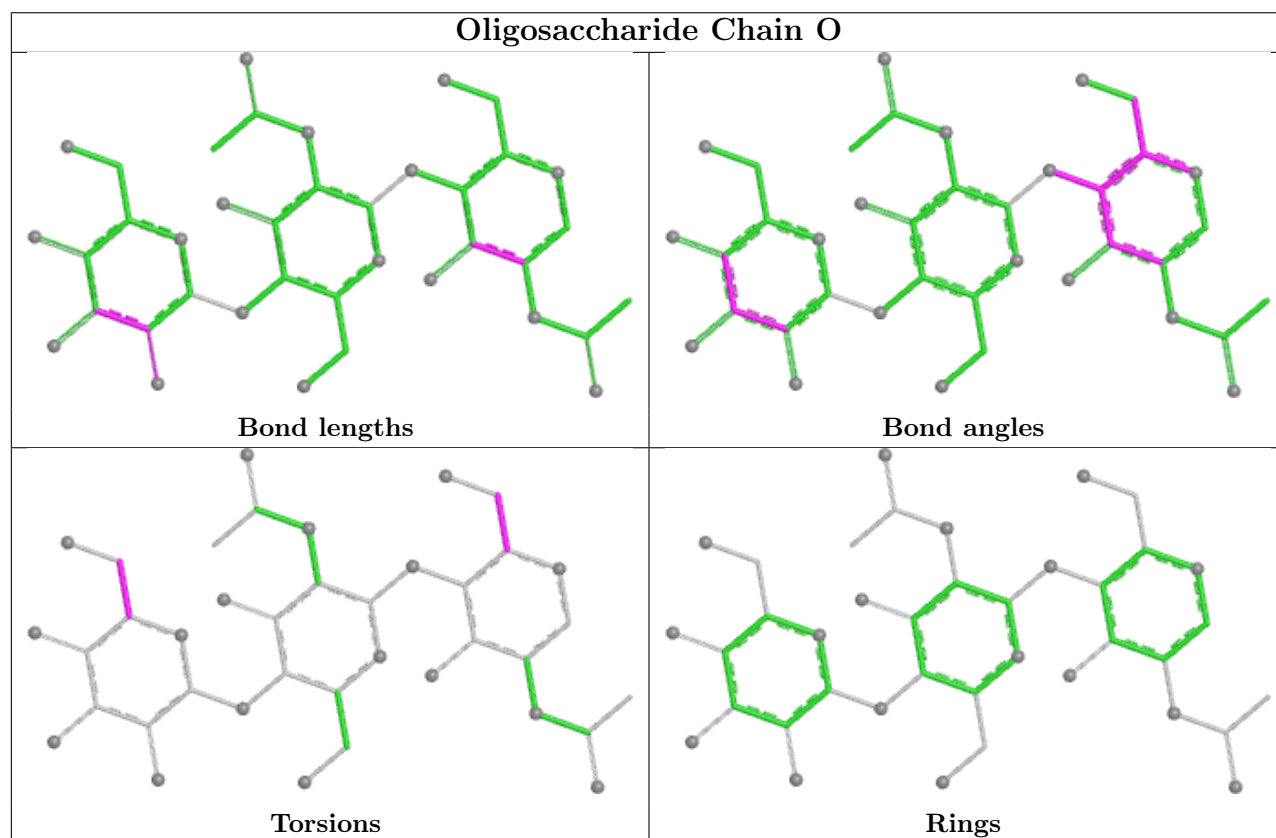
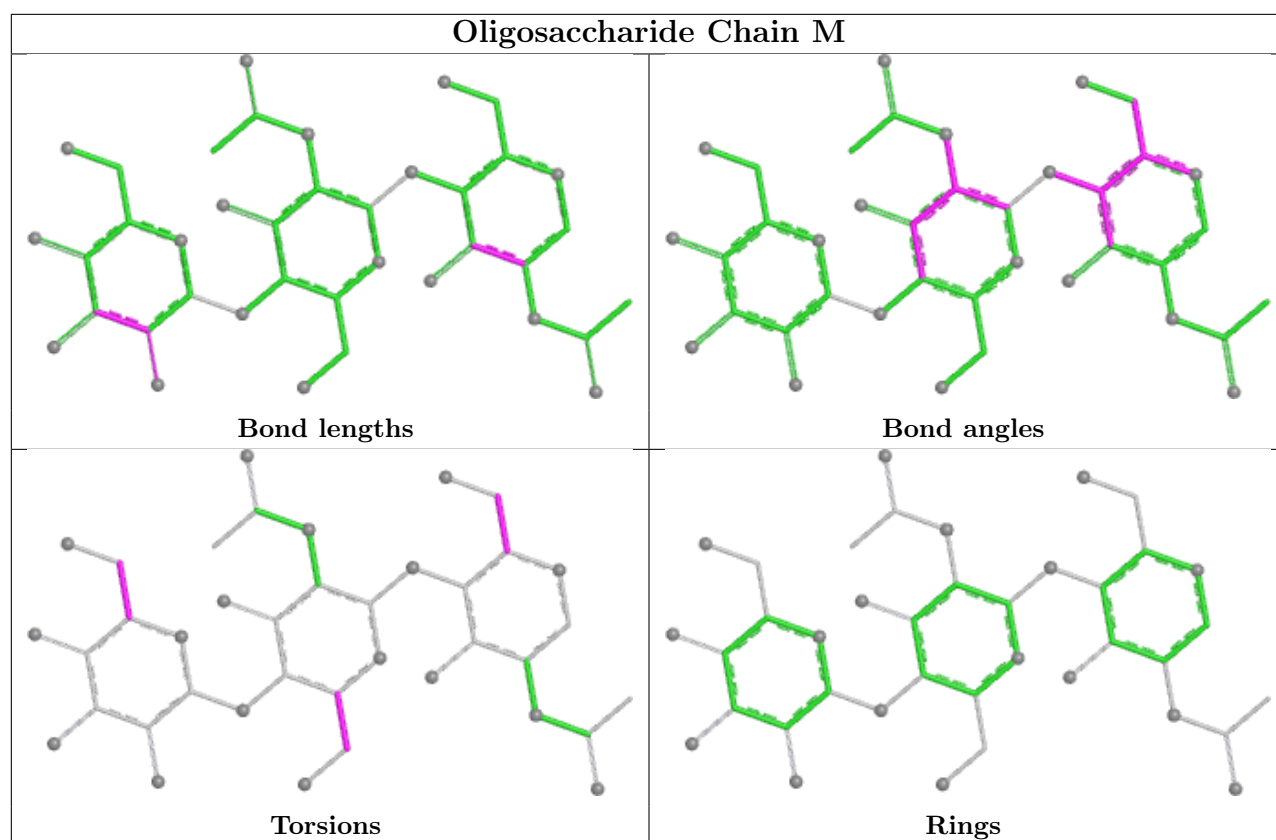
Mol	Chain	Res	Type	Atoms
6	U	4	MAN	O5-C5-C6-O6
6	b	4	MAN	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
6	U	5	MAN	O5-C5-C6-O6
6	b	5	MAN	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	M	3	BMA	C4-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	a	3	BMA	C4-C5-C6-O6

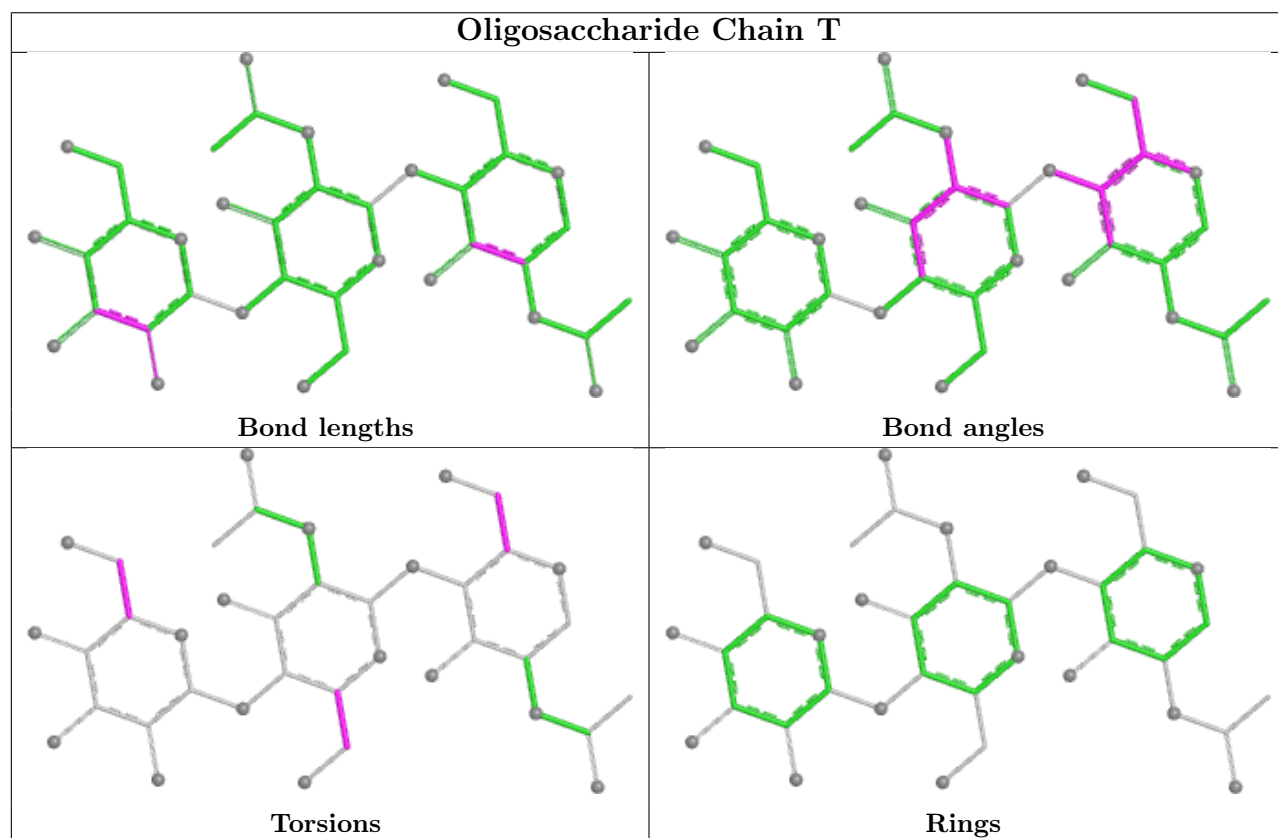
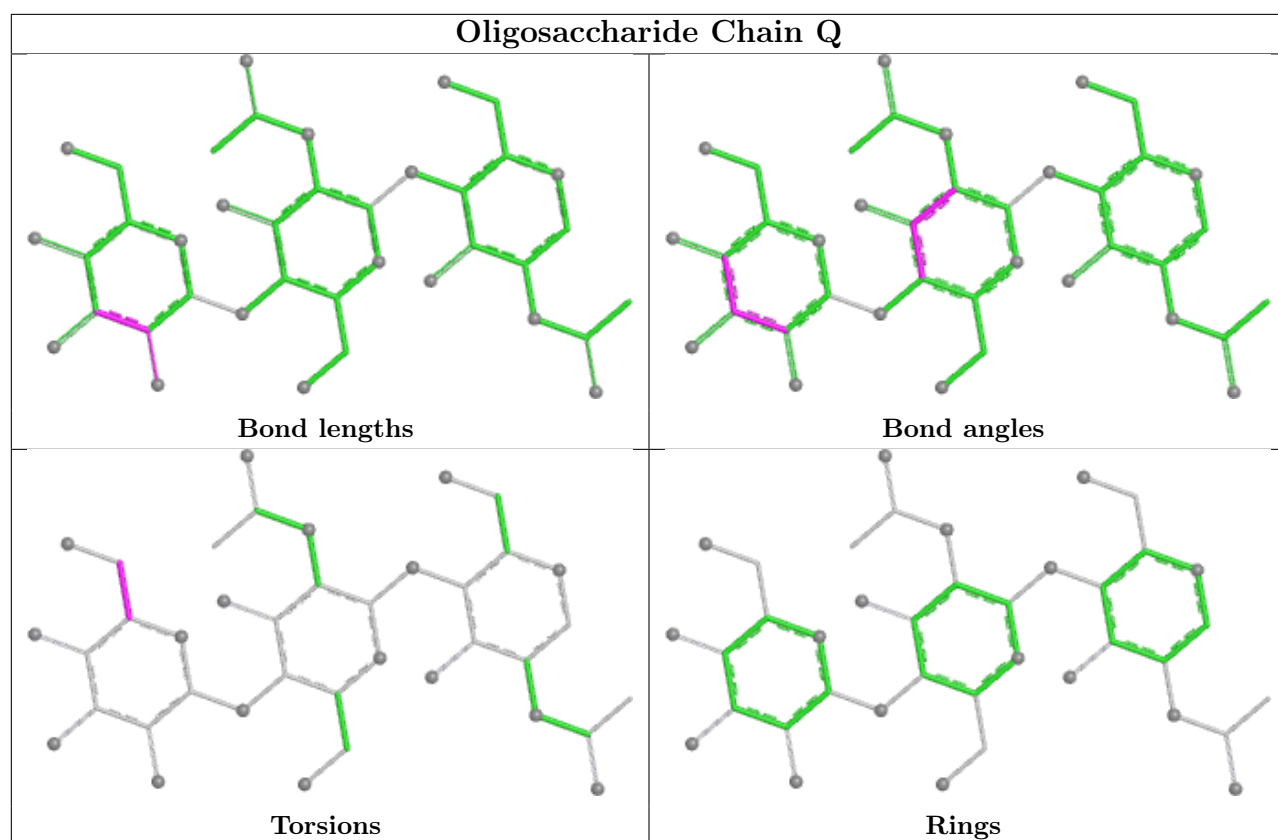
There are no ring outliers.

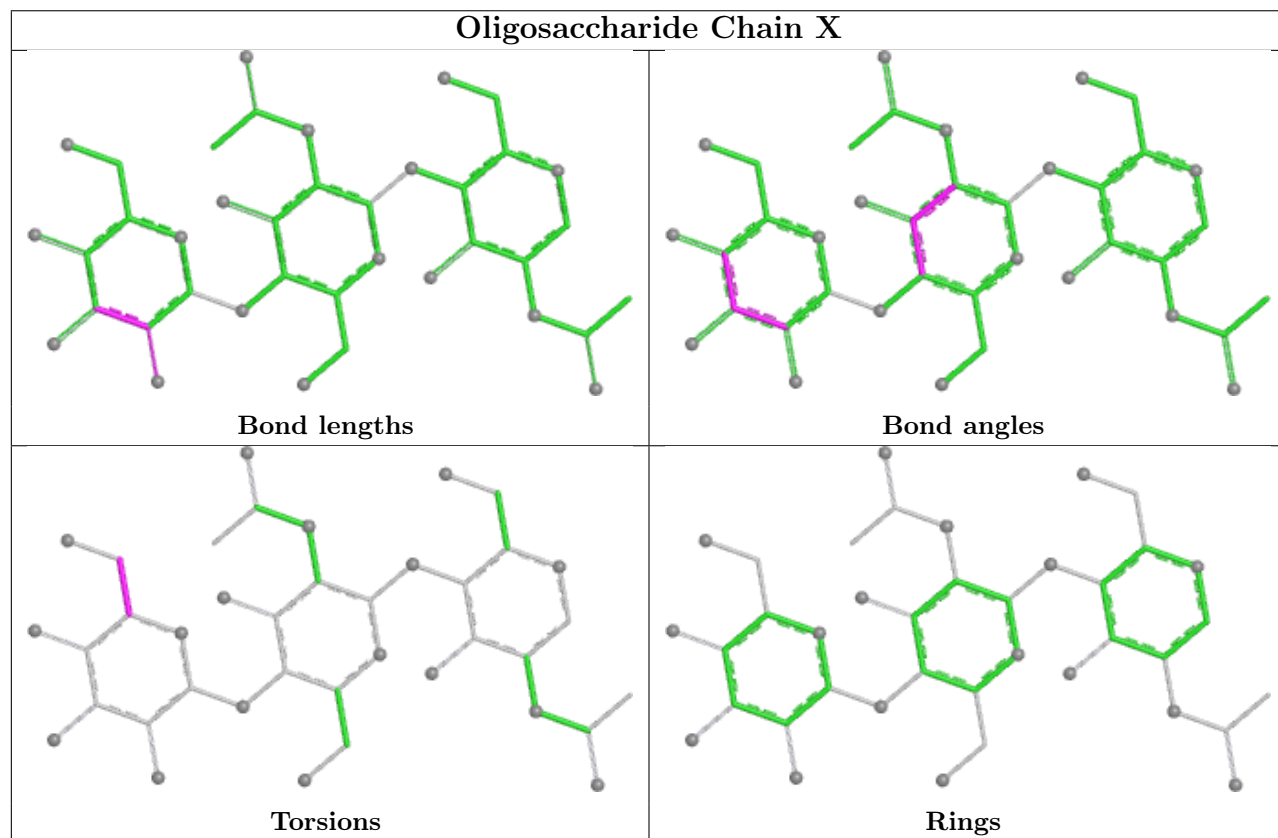
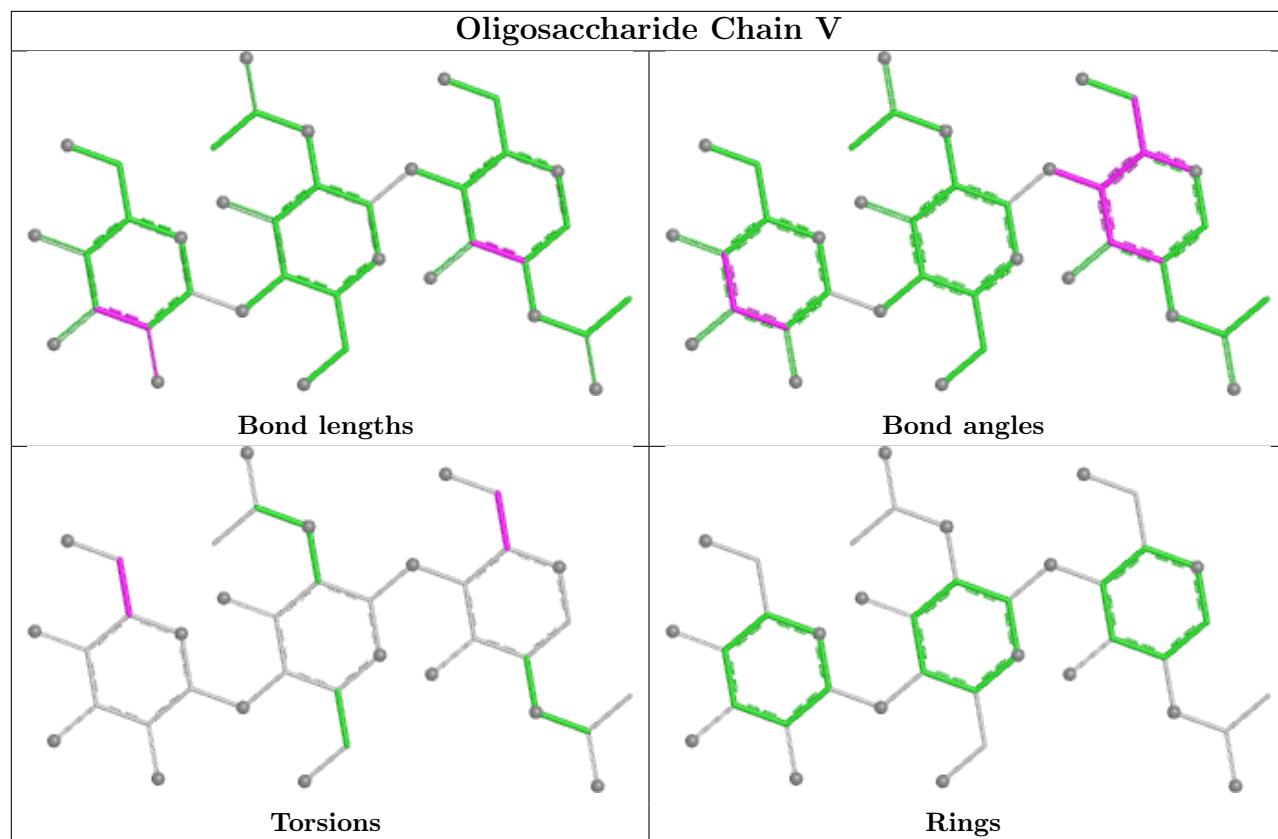
6 monomers are involved in 6 short contacts:

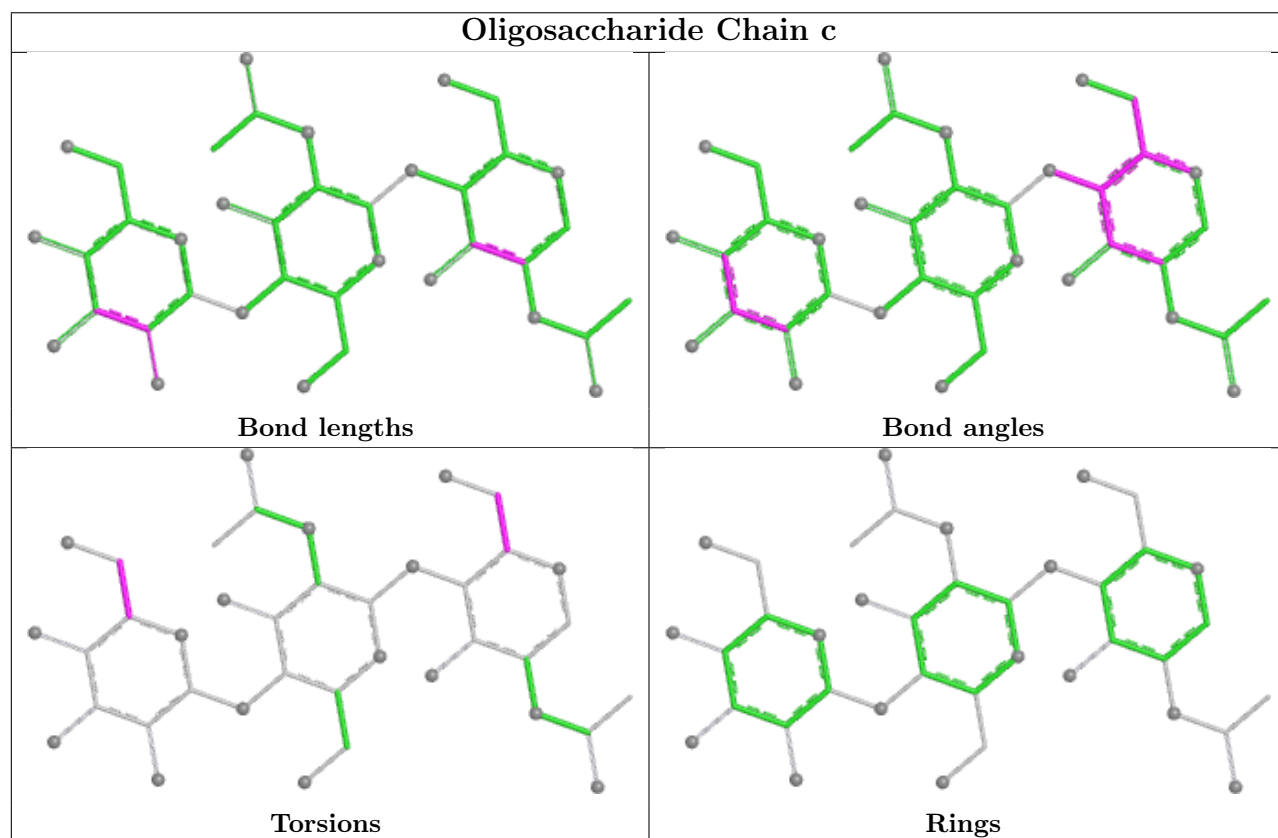
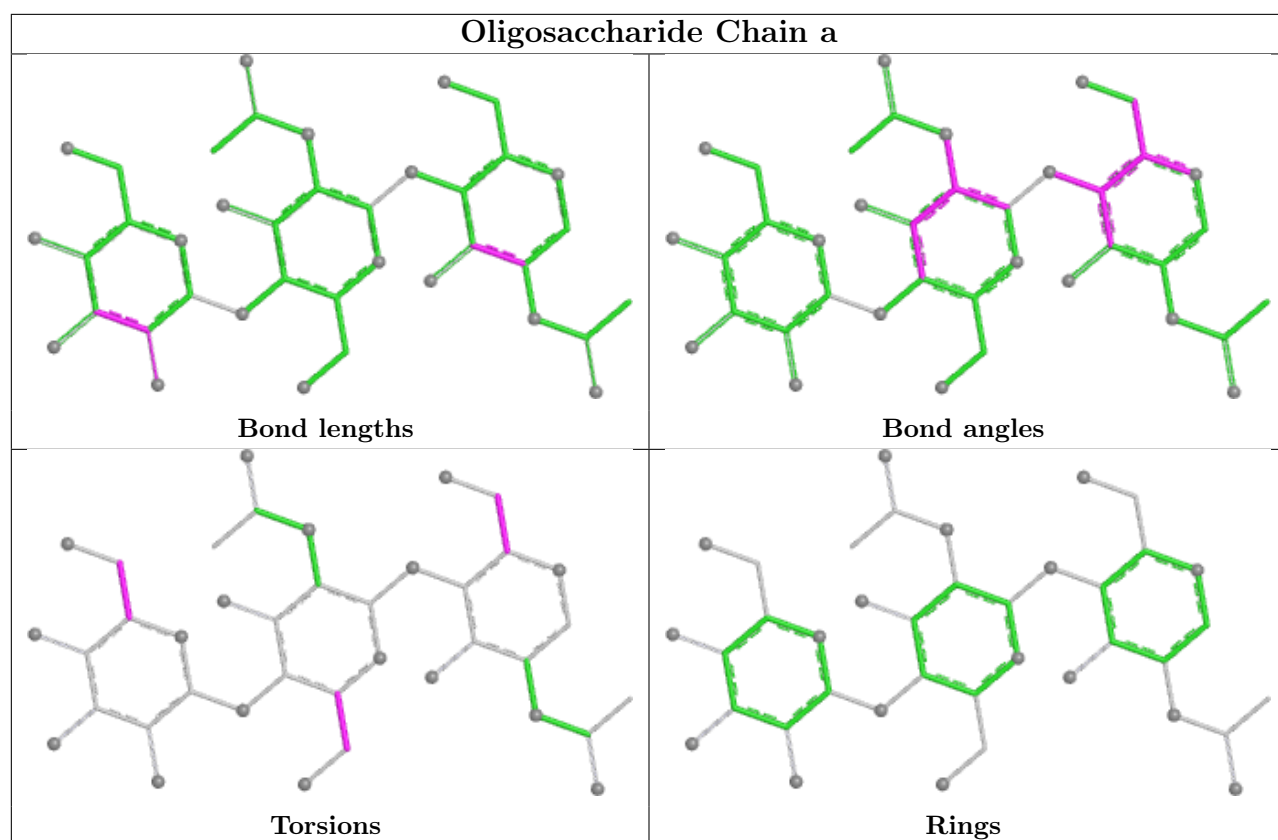
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	2	NAG	1	0
5	T	2	NAG	1	0
5	c	1	NAG	1	0
5	V	1	NAG	1	0
5	O	1	NAG	1	0
5	a	2	NAG	1	0

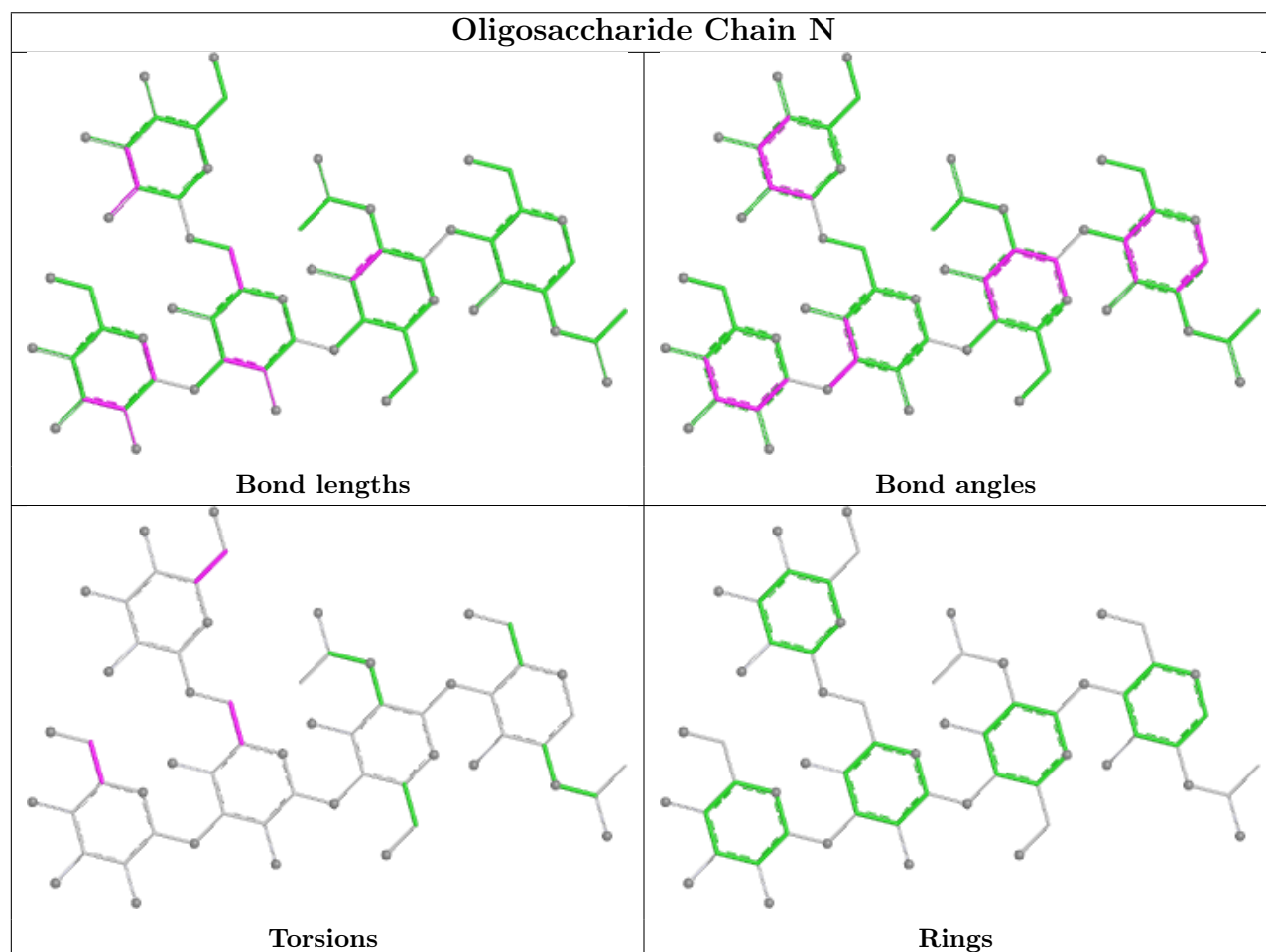
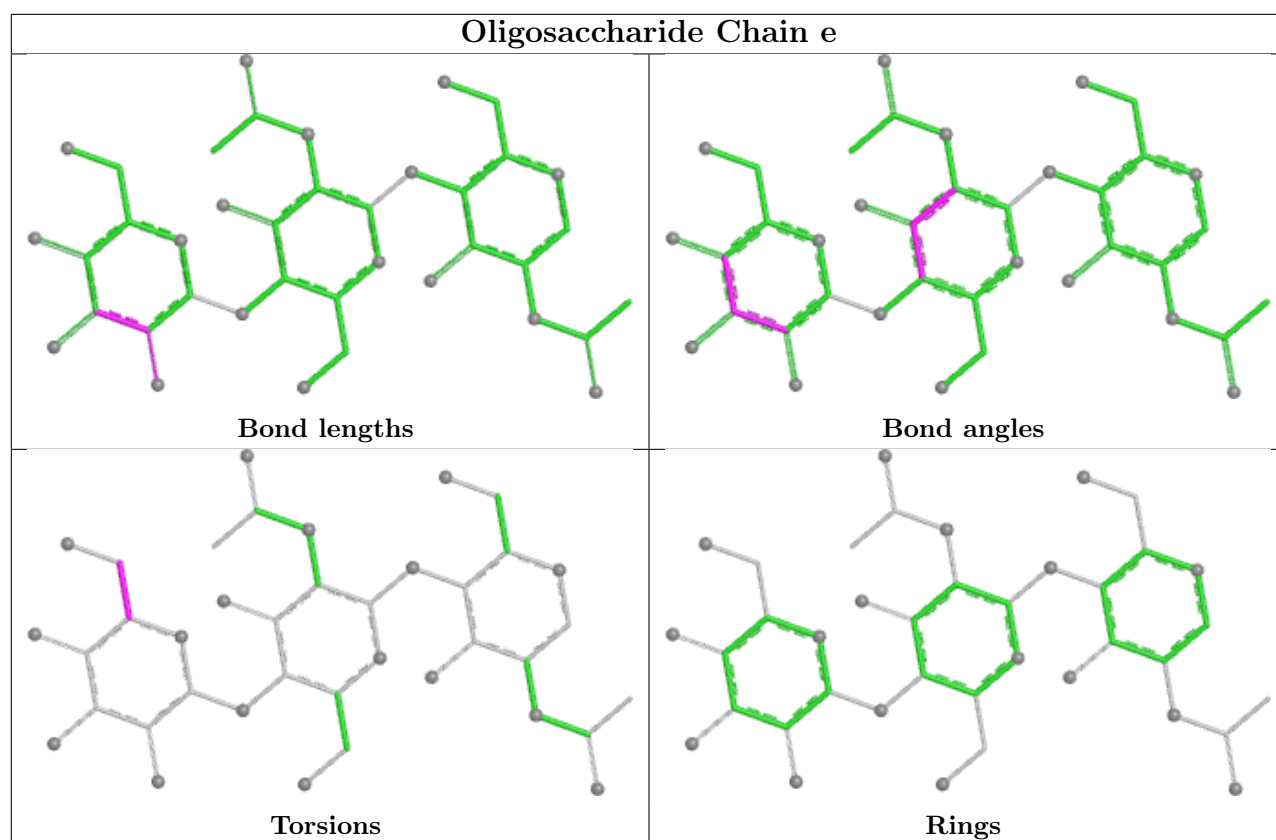
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

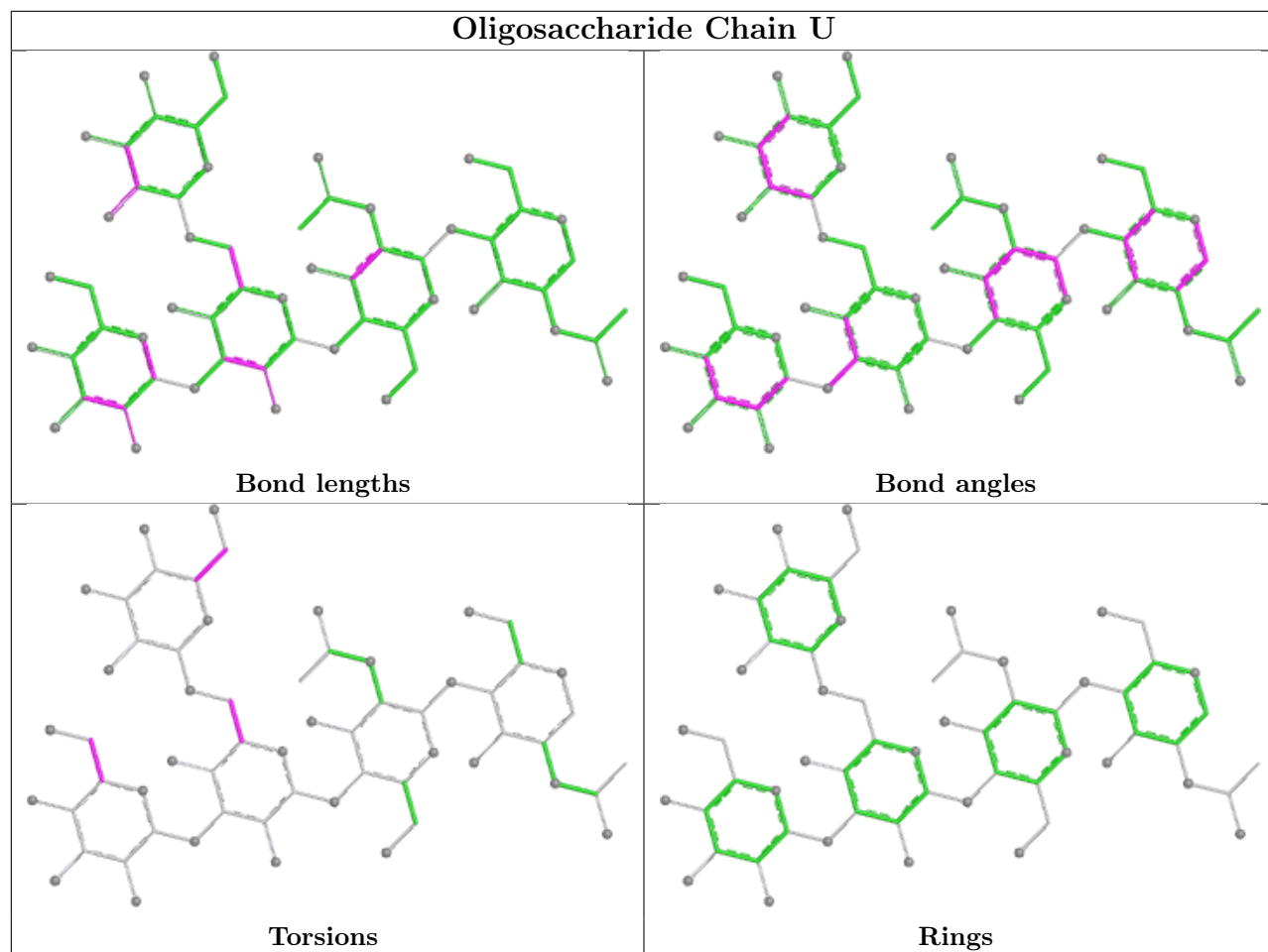


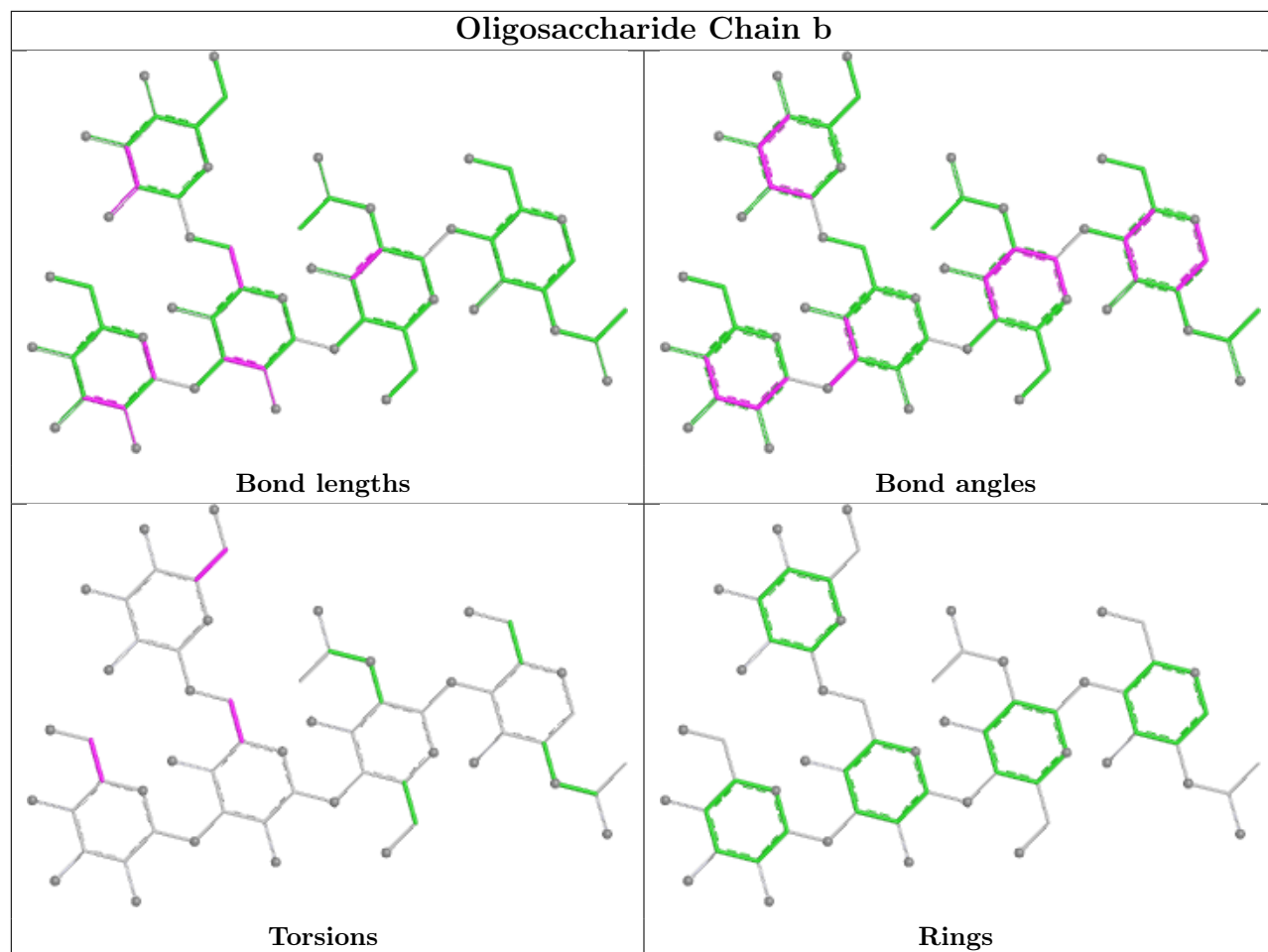


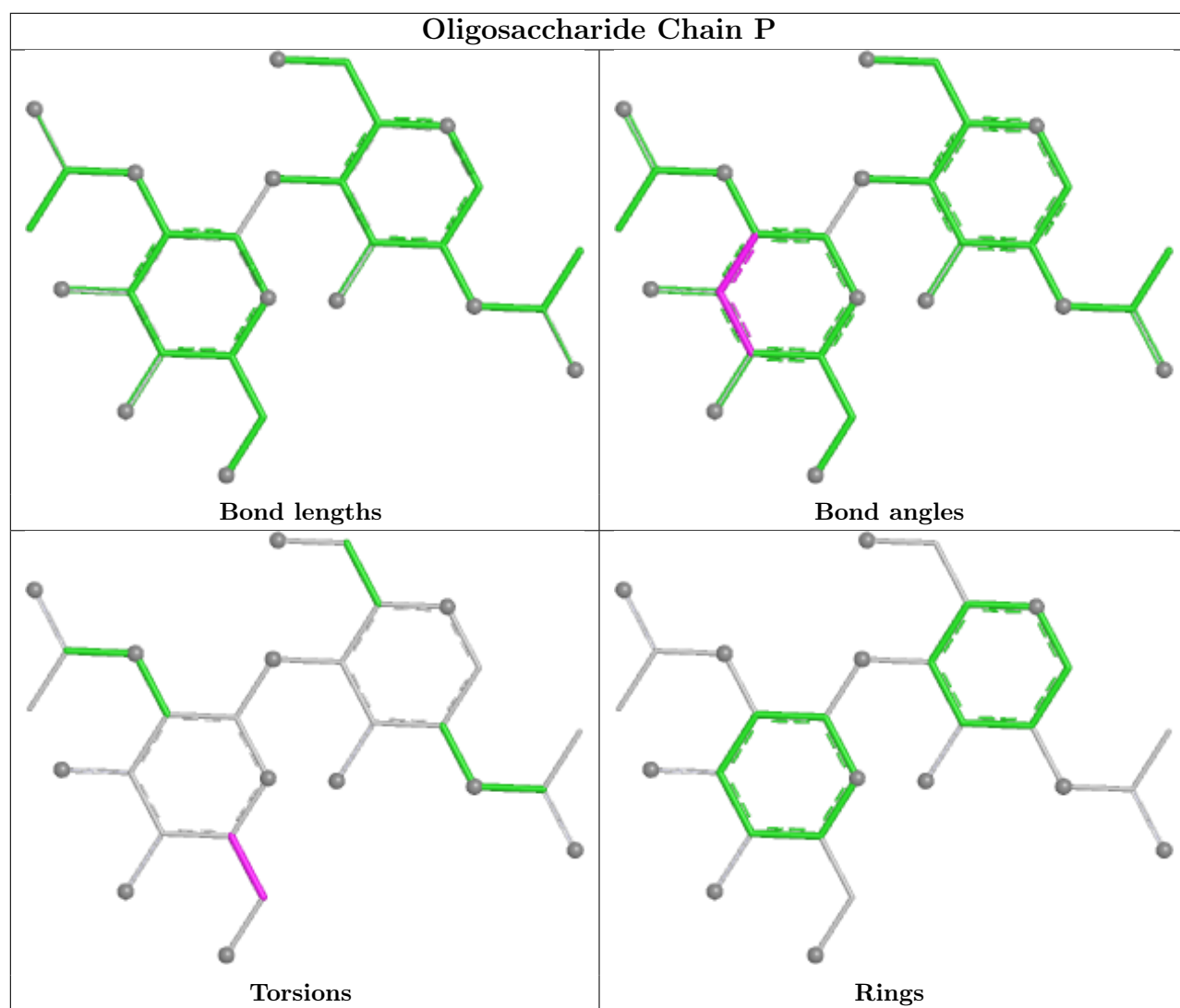


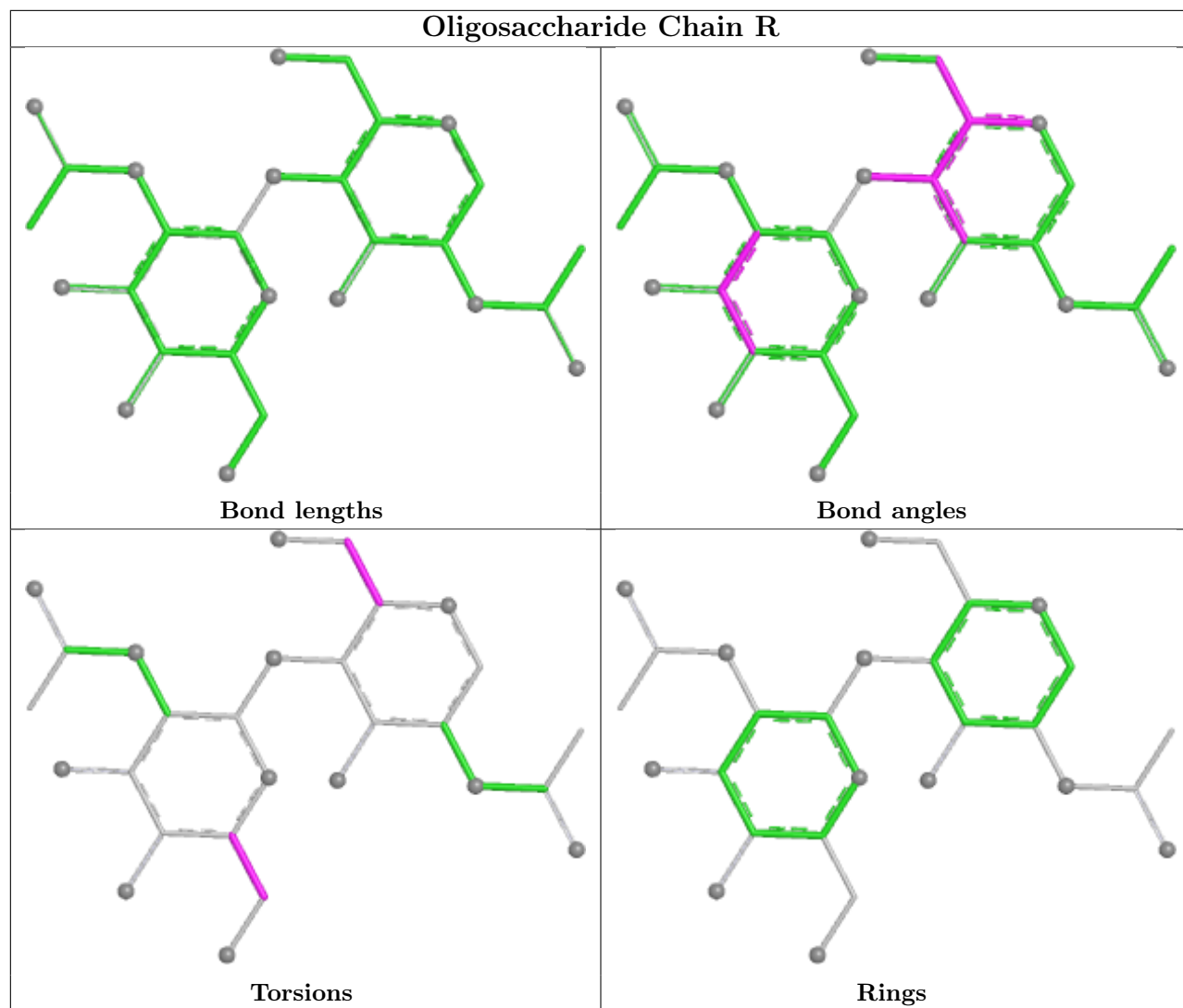


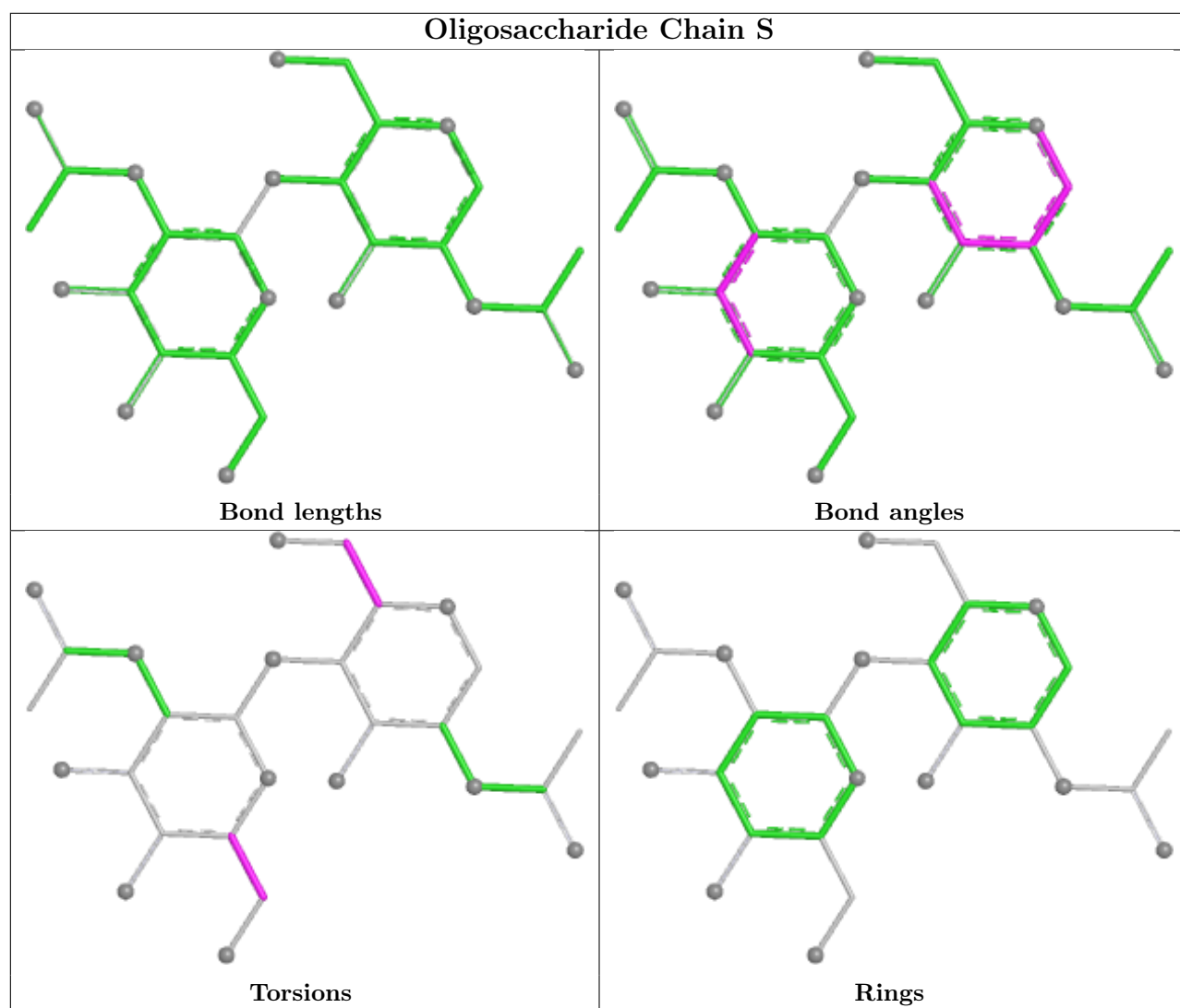


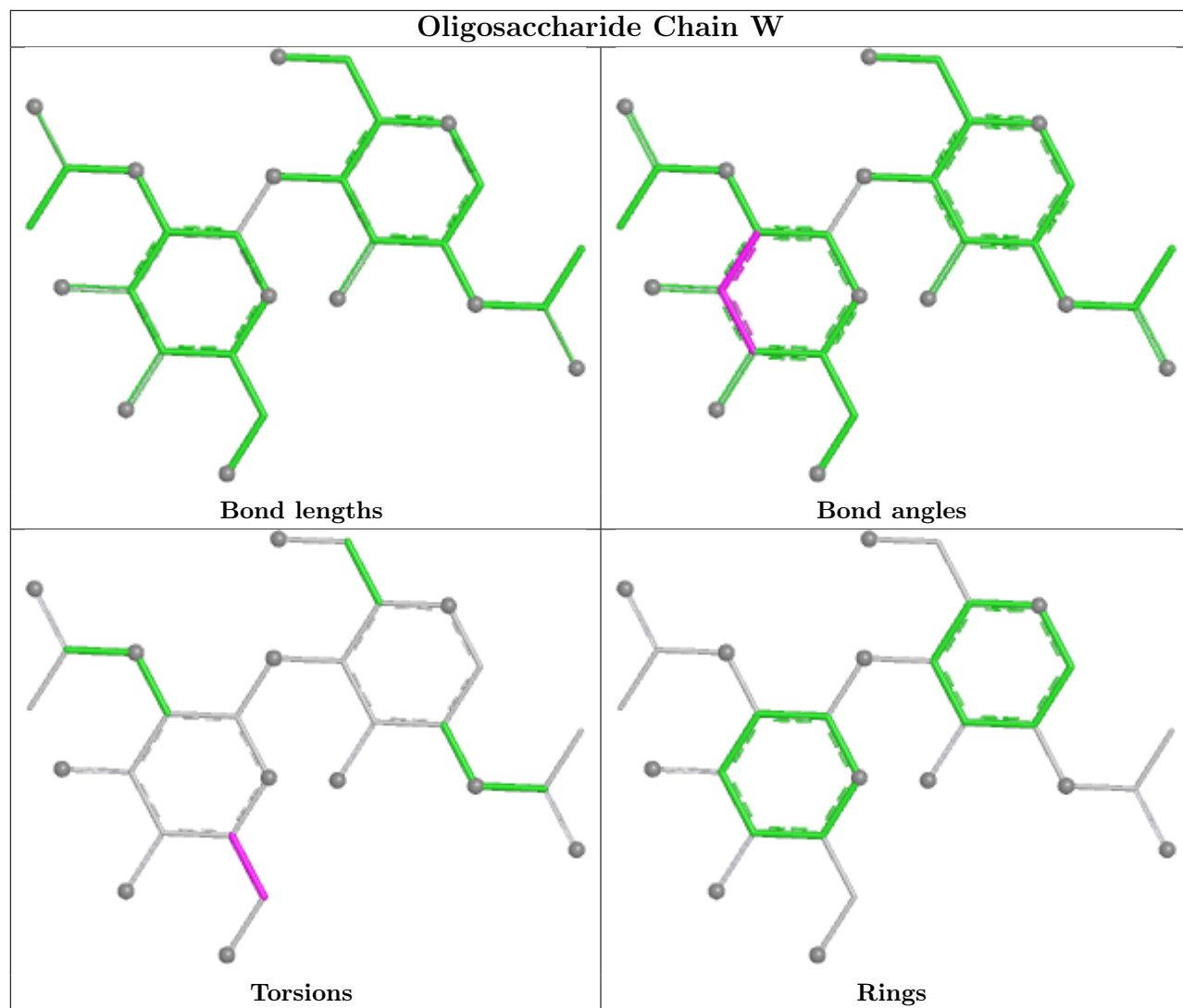


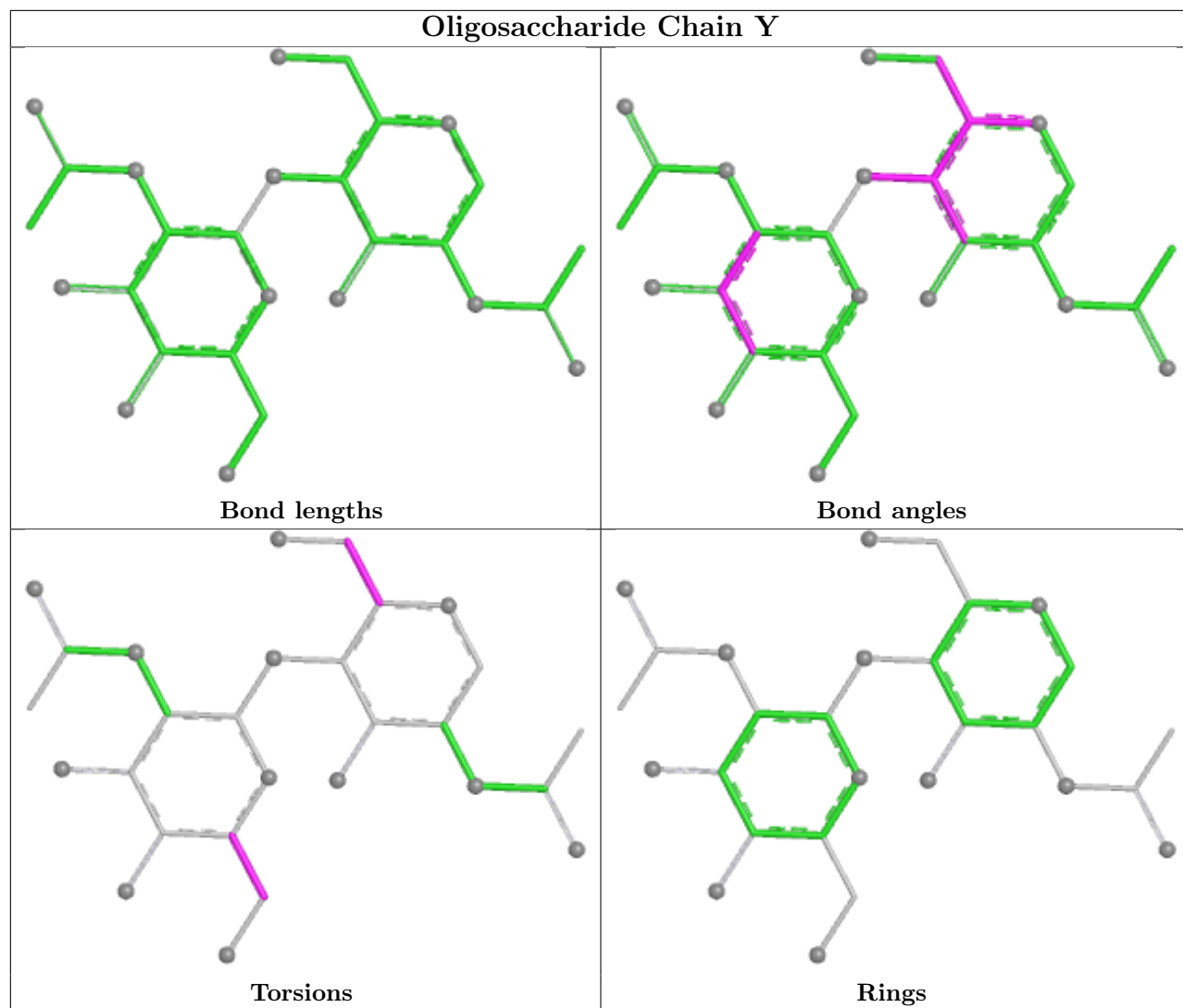


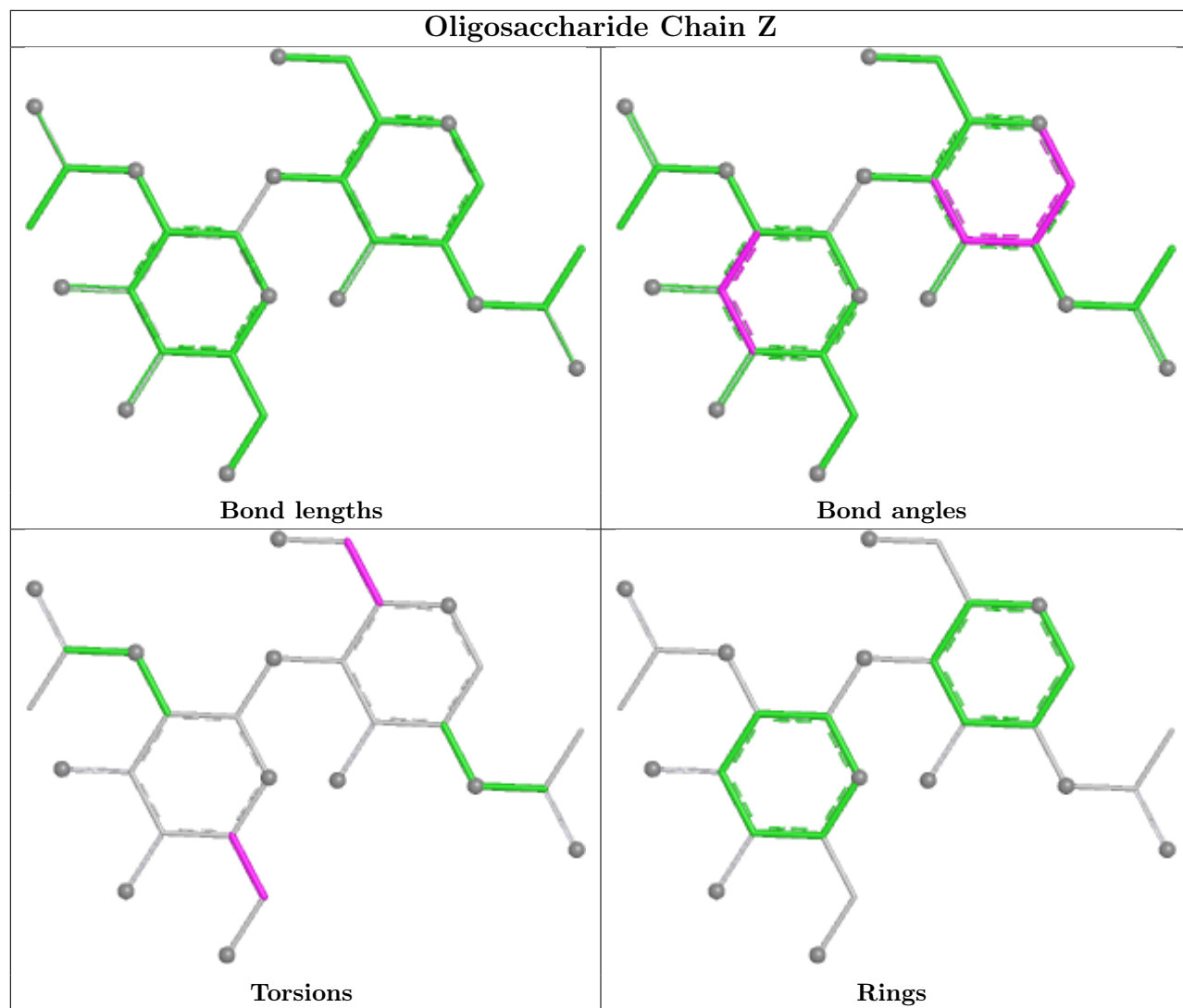


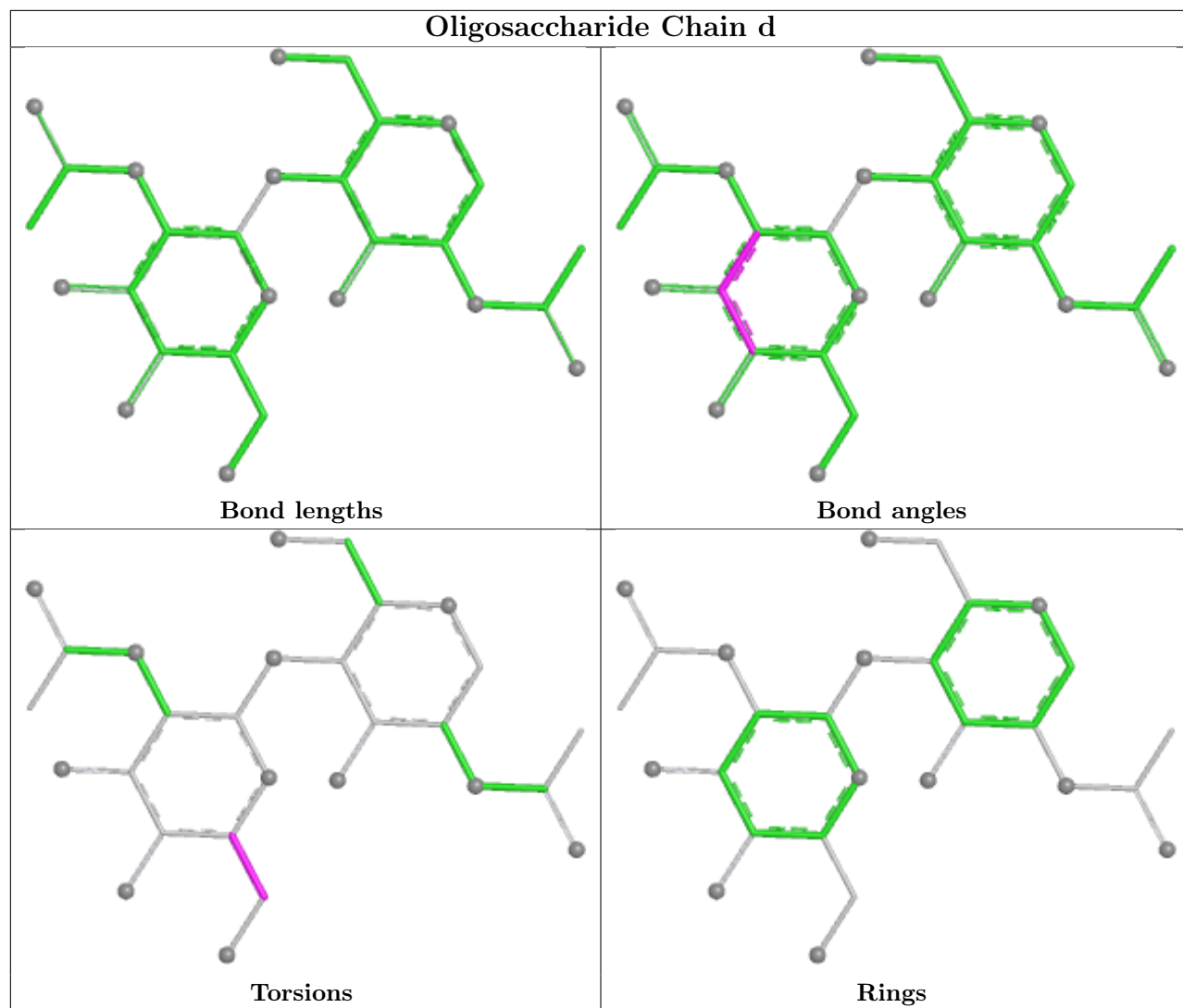


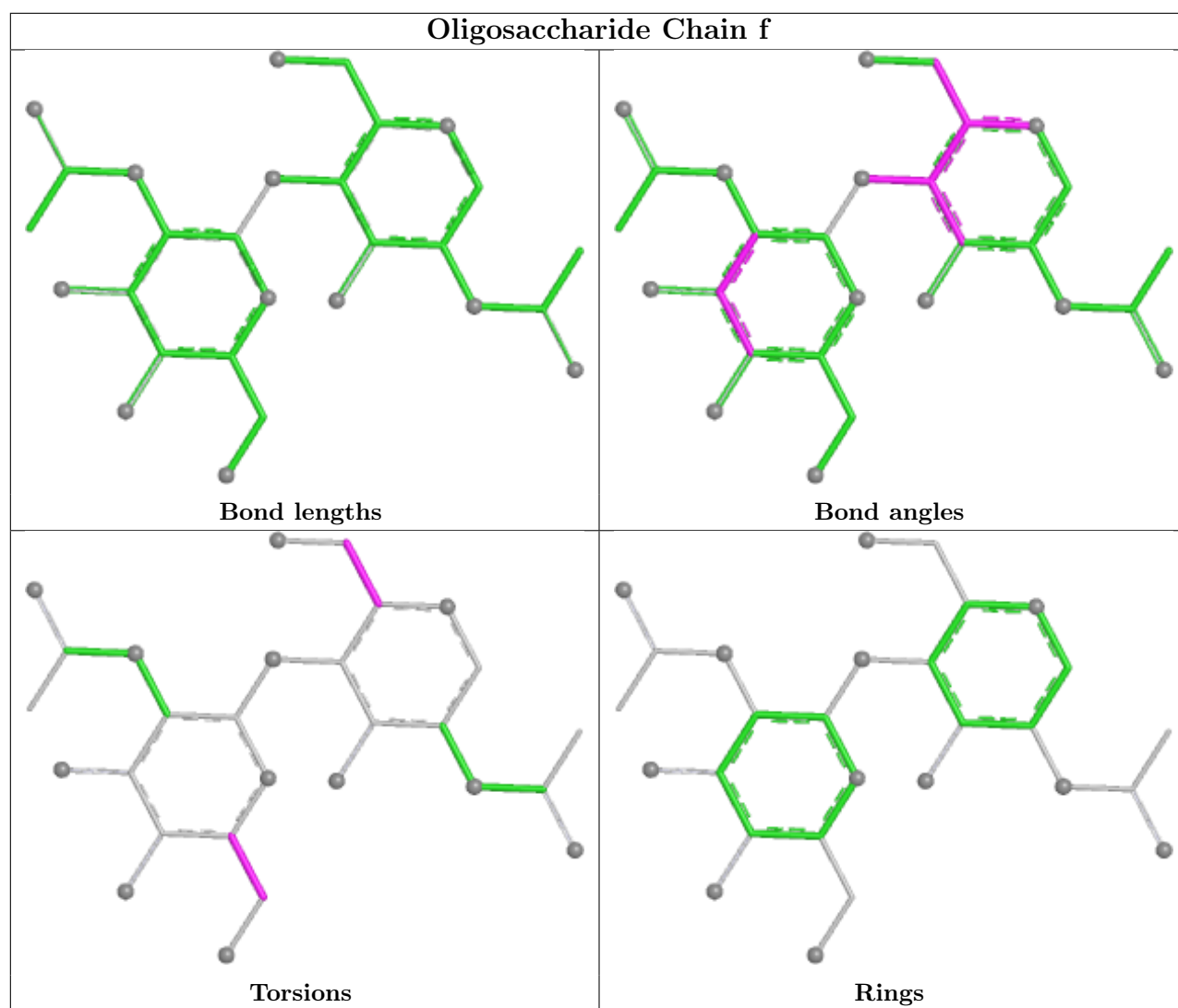


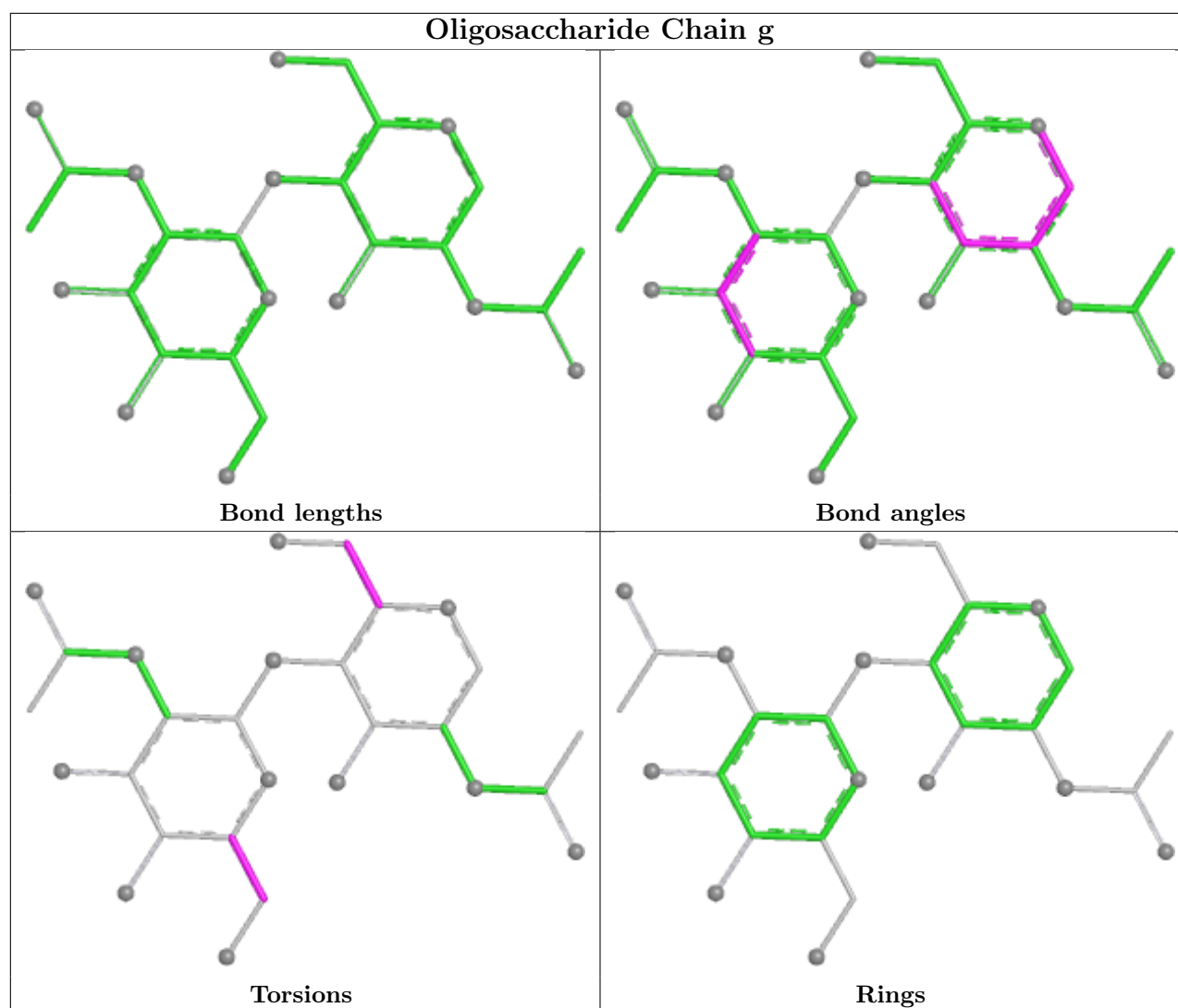












5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
8	NAG	C	619	3	14,14,15	0.83	0	17,19,21	1.57	2 (11%)
8	NAG	D	622	3	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
8	NAG	A	623	3	14,14,15	0.87	0	17,19,21	1.22	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	D	614	3	14,14,15	0.84	0	17,19,21	0.83	1 (5%)
8	NAG	D	623	3	14,14,15	0.87	0	17,19,21	1.22	1 (5%)
8	NAG	A	614	3	14,14,15	0.84	0	17,19,21	0.83	1 (5%)
8	NAG	B	701	4	14,14,15	0.85	0	17,19,21	0.77	1 (5%)
8	NAG	C	615	3	14,14,15	0.73	0	17,19,21	1.14	1 (5%)
8	NAG	A	619	3	14,14,15	0.83	0	17,19,21	1.57	2 (11%)
8	NAG	C	622	3	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
8	NAG	C	614	3	14,14,15	0.84	0	17,19,21	0.83	1 (5%)
8	NAG	E	701	4	14,14,15	0.85	0	17,19,21	0.78	1 (5%)
8	NAG	A	622	3	14,14,15	0.71	0	17,19,21	0.95	1 (5%)
8	NAG	F	701	4	14,14,15	0.84	0	17,19,21	0.77	1 (5%)
8	NAG	D	619	3	14,14,15	0.82	0	17,19,21	1.57	2 (11%)
8	NAG	D	615	3	14,14,15	0.74	0	17,19,21	1.14	1 (5%)
8	NAG	A	615	3	14,14,15	0.73	0	17,19,21	1.14	1 (5%)
8	NAG	C	623	3	14,14,15	0.87	0	17,19,21	1.22	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
8	NAG	C	619	3	-	2/6/23/26	0/1/1/1
8	NAG	D	622	3	-	1/6/23/26	0/1/1/1
8	NAG	A	623	3	-	2/6/23/26	0/1/1/1
8	NAG	D	614	3	-	1/6/23/26	0/1/1/1
8	NAG	D	623	3	-	2/6/23/26	0/1/1/1
8	NAG	A	614	3	-	1/6/23/26	0/1/1/1
8	NAG	B	701	4	-	1/6/23/26	0/1/1/1
8	NAG	C	615	3	-	3/6/23/26	0/1/1/1
8	NAG	A	619	3	-	2/6/23/26	0/1/1/1
8	NAG	C	622	3	-	1/6/23/26	0/1/1/1
8	NAG	C	614	3	-	1/6/23/26	0/1/1/1
8	NAG	E	701	4	-	1/6/23/26	0/1/1/1
8	NAG	A	622	3	-	1/6/23/26	0/1/1/1
8	NAG	F	701	4	-	1/6/23/26	0/1/1/1
8	NAG	D	619	3	-	2/6/23/26	0/1/1/1
8	NAG	D	615	3	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	615	3	-	3/6/23/26	0/1/1/1
8	NAG	C	623	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	619	NAG	C2-N2-C7	4.48	128.91	122.90
8	A	619	NAG	C2-N2-C7	4.47	128.88	122.90
8	D	619	NAG	C2-N2-C7	4.45	128.86	122.90
8	C	615	NAG	C4-C3-C2	-3.61	105.73	111.02
8	A	615	NAG	C4-C3-C2	-3.61	105.73	111.02
8	D	615	NAG	C4-C3-C2	-3.59	105.75	111.02
8	D	623	NAG	C4-C3-C2	-3.42	106.01	111.02
8	C	623	NAG	C4-C3-C2	-3.41	106.02	111.02
8	A	623	NAG	C4-C3-C2	-3.41	106.03	111.02
8	C	619	NAG	C4-C3-C2	-3.29	106.20	111.02
8	A	619	NAG	C4-C3-C2	-3.27	106.22	111.02
8	D	619	NAG	C4-C3-C2	-3.27	106.23	111.02
8	D	622	NAG	C4-C3-C2	-2.92	106.74	111.02
8	A	622	NAG	C4-C3-C2	-2.91	106.76	111.02
8	C	622	NAG	C4-C3-C2	-2.89	106.79	111.02
8	D	614	NAG	C4-C3-C2	-2.37	107.54	111.02
8	C	614	NAG	C4-C3-C2	-2.37	107.55	111.02
8	A	614	NAG	C4-C3-C2	-2.36	107.56	111.02
8	E	701	NAG	C4-C3-C2	-2.23	107.74	111.02
8	F	701	NAG	C4-C3-C2	-2.22	107.76	111.02
8	B	701	NAG	C4-C3-C2	-2.22	107.77	111.02

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	619	NAG	C3-C2-N2-C7
8	C	619	NAG	C3-C2-N2-C7
8	D	619	NAG	C3-C2-N2-C7
8	A	623	NAG	O5-C5-C6-O6
8	C	623	NAG	O5-C5-C6-O6
8	D	623	NAG	O5-C5-C6-O6
8	C	614	NAG	O5-C5-C6-O6
8	A	614	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	D	614	NAG	O5-C5-C6-O6
8	A	623	NAG	C4-C5-C6-O6
8	C	623	NAG	C4-C5-C6-O6
8	D	623	NAG	C4-C5-C6-O6
8	A	619	NAG	O5-C5-C6-O6
8	C	619	NAG	O5-C5-C6-O6
8	D	619	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	F	701	NAG	O5-C5-C6-O6
8	E	701	NAG	O5-C5-C6-O6
8	A	615	NAG	O5-C5-C6-O6
8	C	615	NAG	O5-C5-C6-O6
8	D	615	NAG	O5-C5-C6-O6
8	A	622	NAG	O5-C5-C6-O6
8	C	622	NAG	O5-C5-C6-O6
8	D	622	NAG	O5-C5-C6-O6
8	A	615	NAG	C1-C2-N2-C7
8	C	615	NAG	C1-C2-N2-C7
8	D	615	NAG	C1-C2-N2-C7
8	A	615	NAG	C3-C2-N2-C7
8	C	615	NAG	C3-C2-N2-C7
8	D	615	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	619	NAG	1	0
8	A	619	NAG	1	0
8	D	619	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.

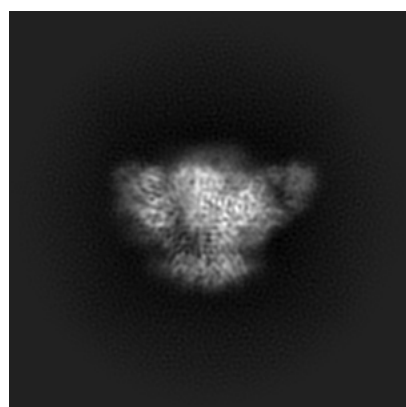
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21258. These allow visual inspection of the internal detail of the map and identification of artifacts.

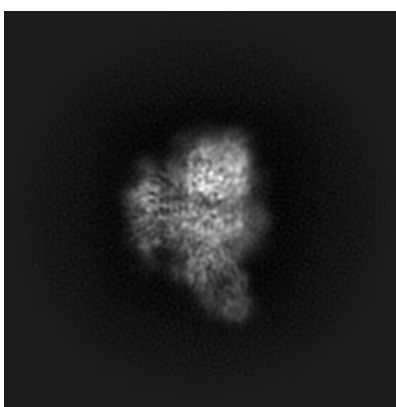
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

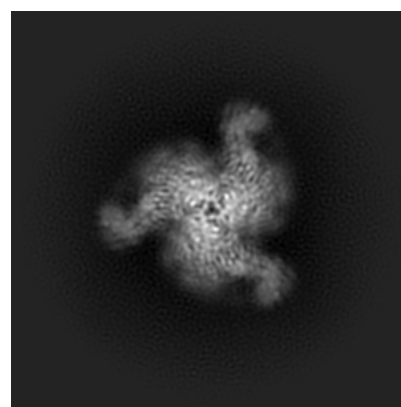
6.1.1 Primary map



X



Y

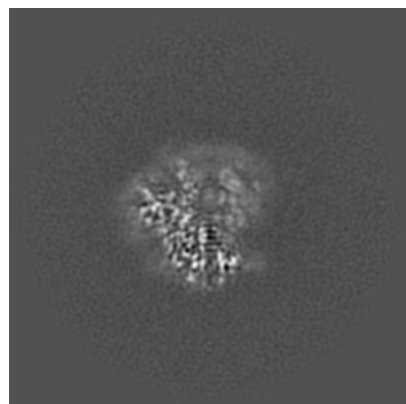


Z

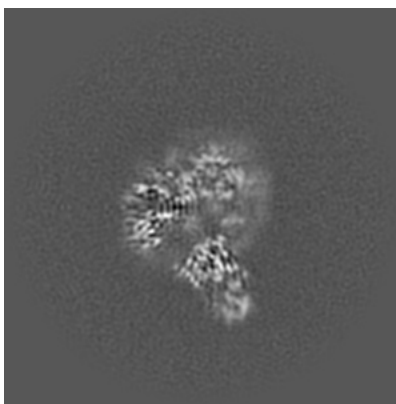
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

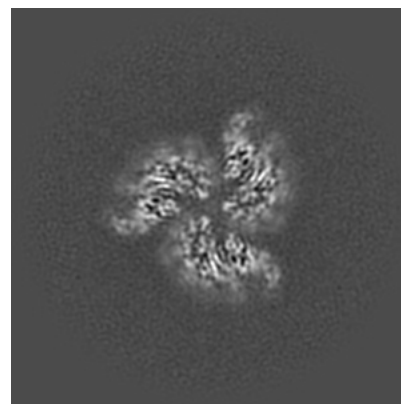
6.2.1 Primary map



X Index: 128



Y Index: 128

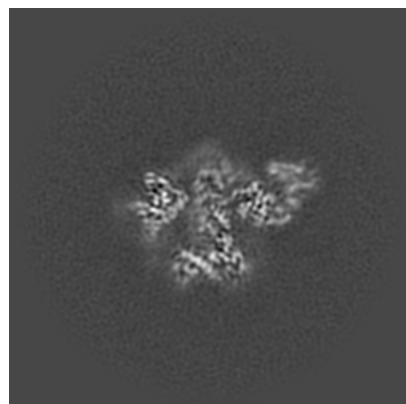


Z Index: 128

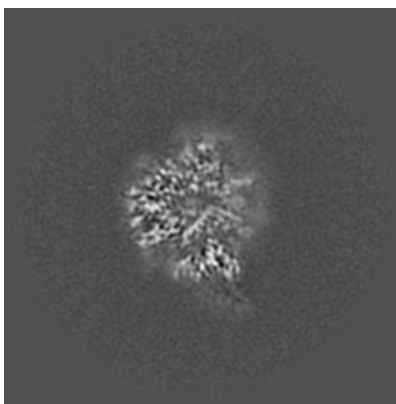
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

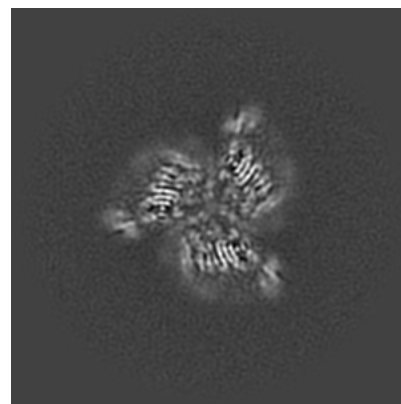
6.3.1 Primary map



X Index: 141



Y Index: 135



Z Index: 133

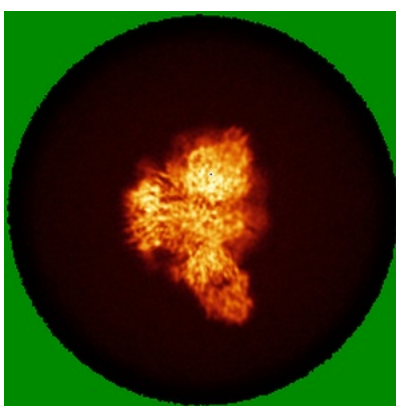
The images above show the largest variance slices of the map in three orthogonal directions.

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

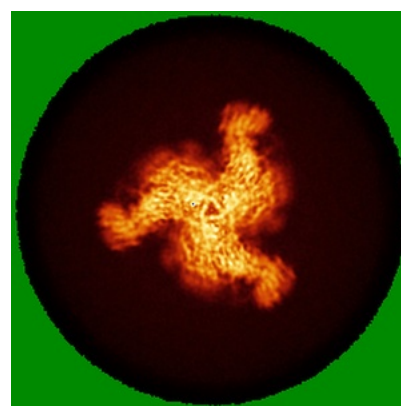
6.4.1 Primary map



X



Y

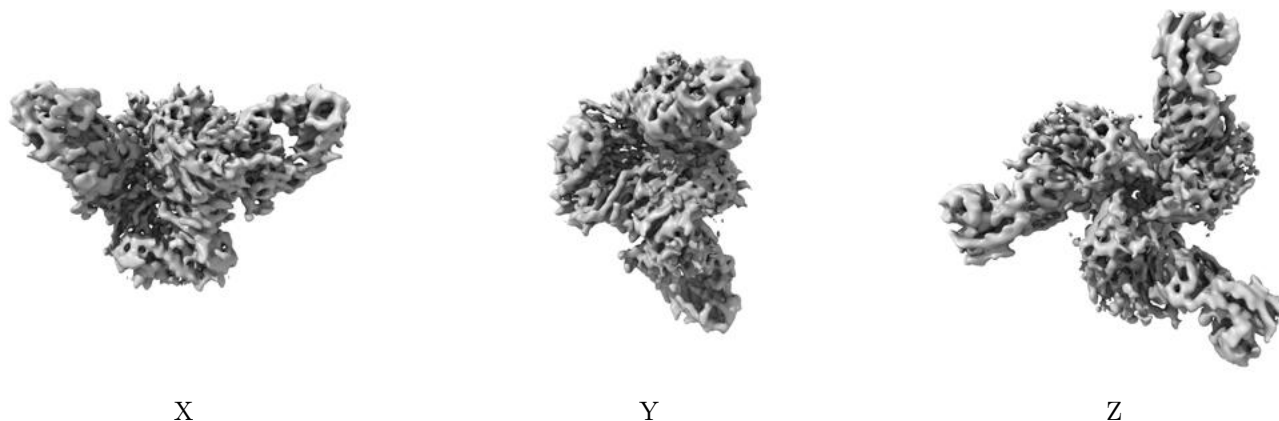


Z

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 0.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

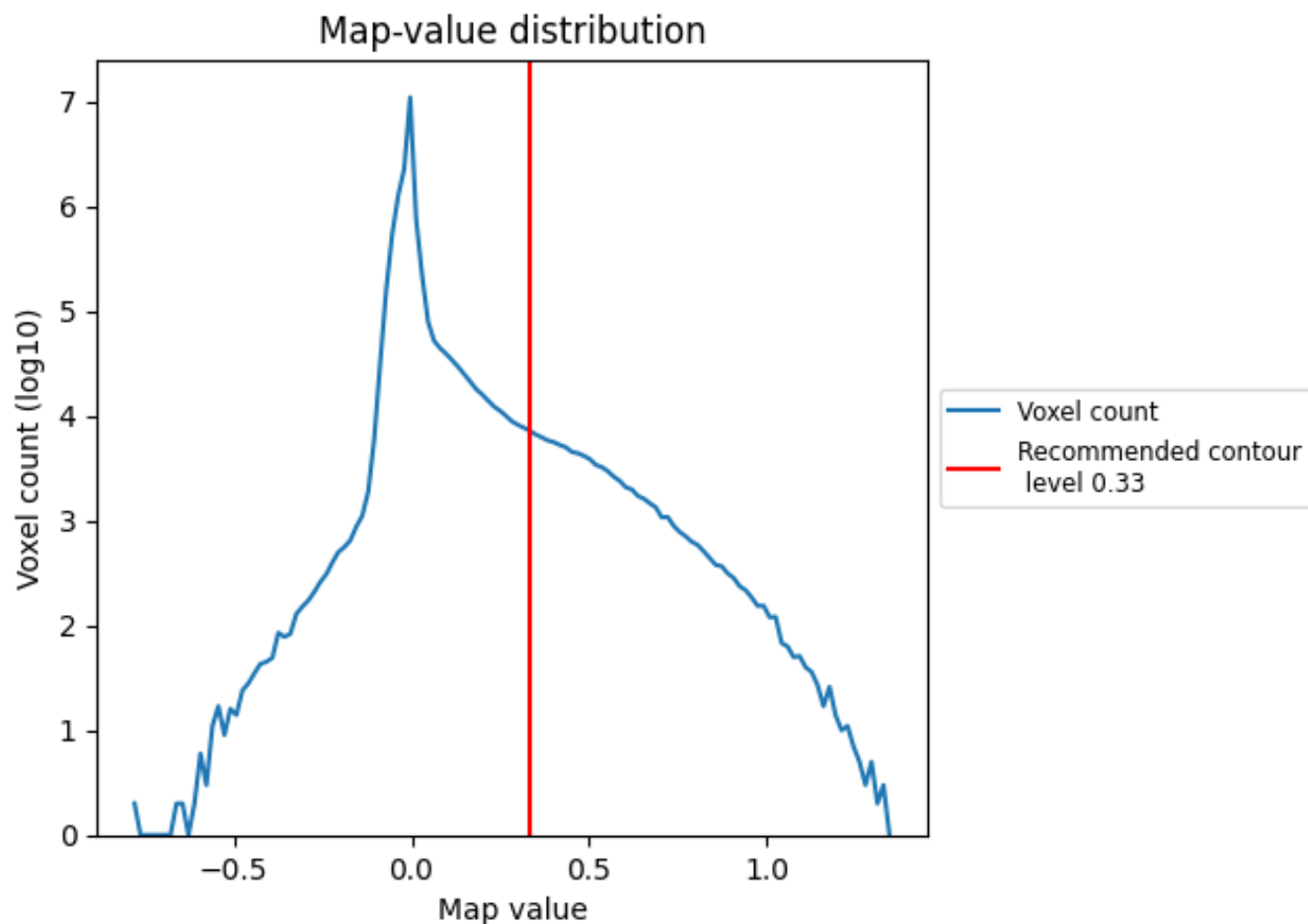
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

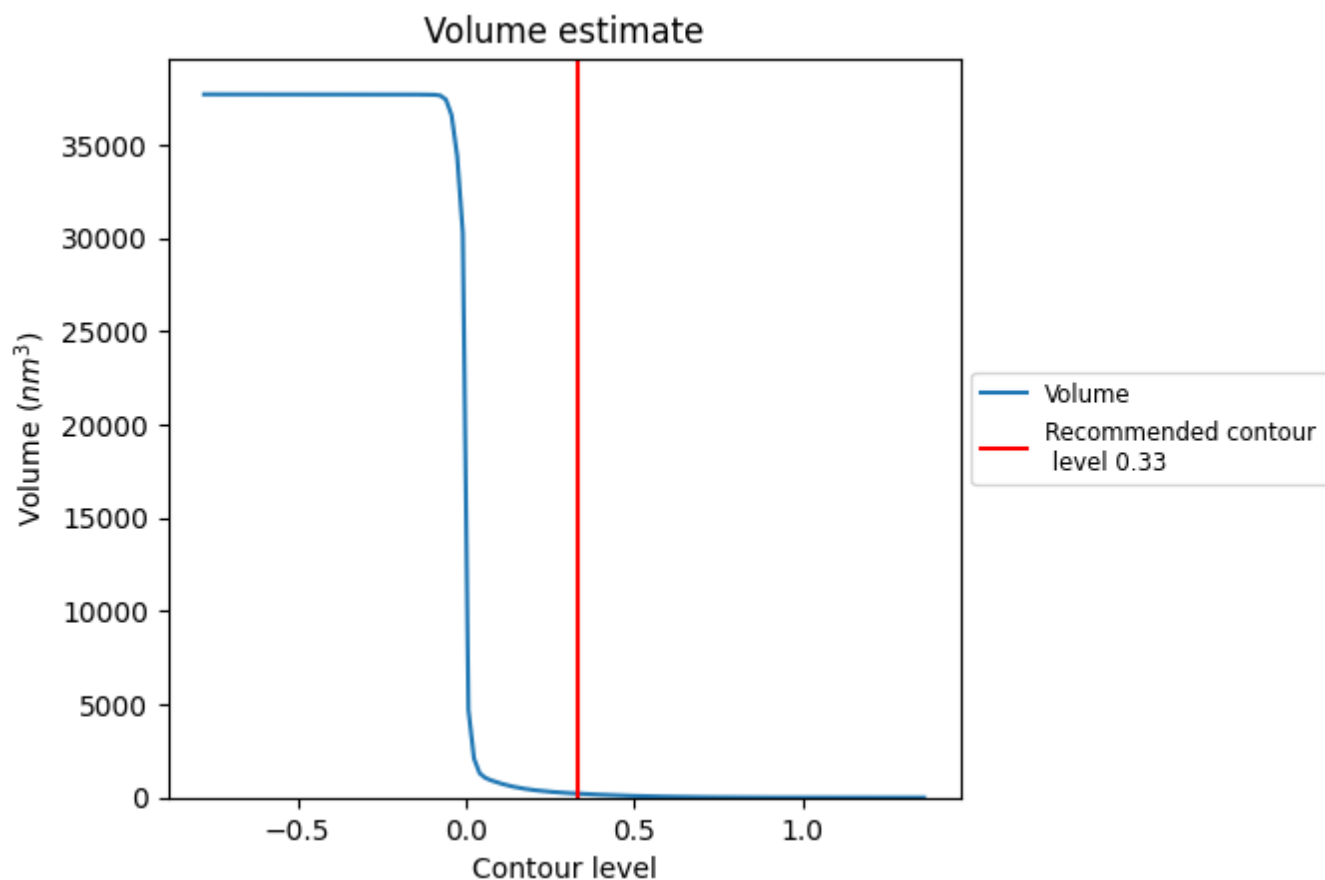
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

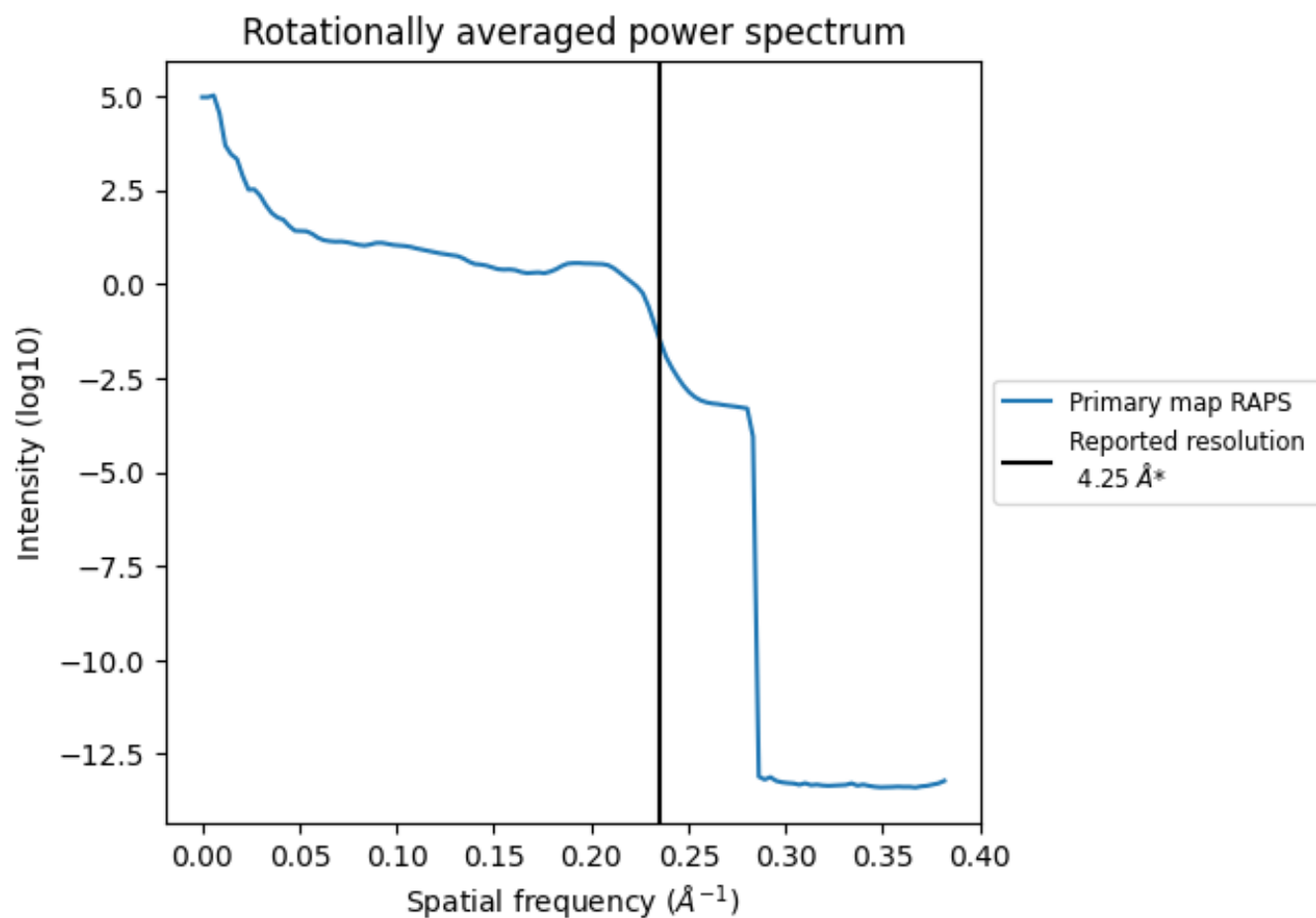
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm³; this corresponds to an approximate mass of 192 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 ⓘ

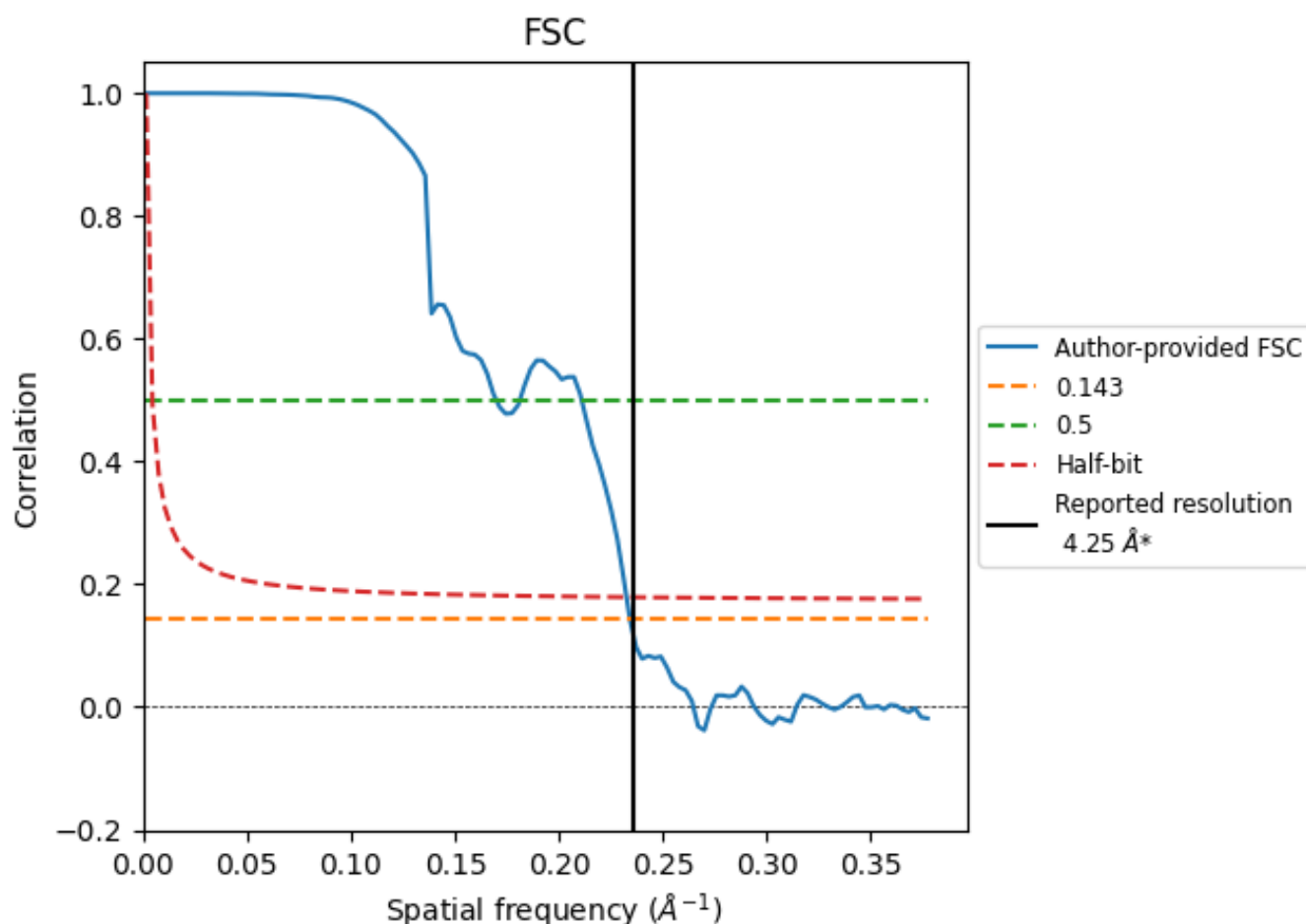


*Reported resolution corresponds to spatial frequency of 0.235 Å⁻¹

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 0.235 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

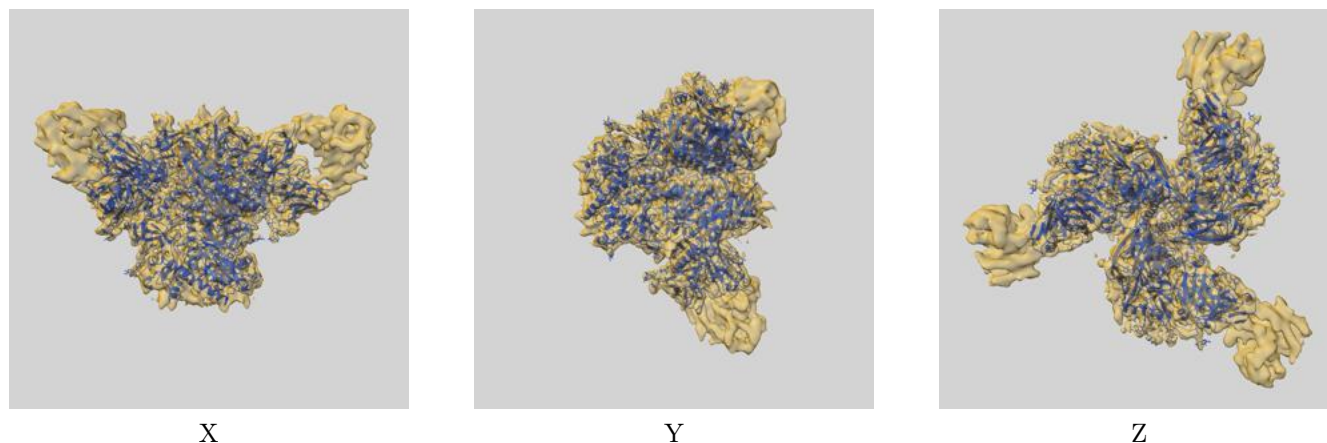
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.27	5.89	4.30
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

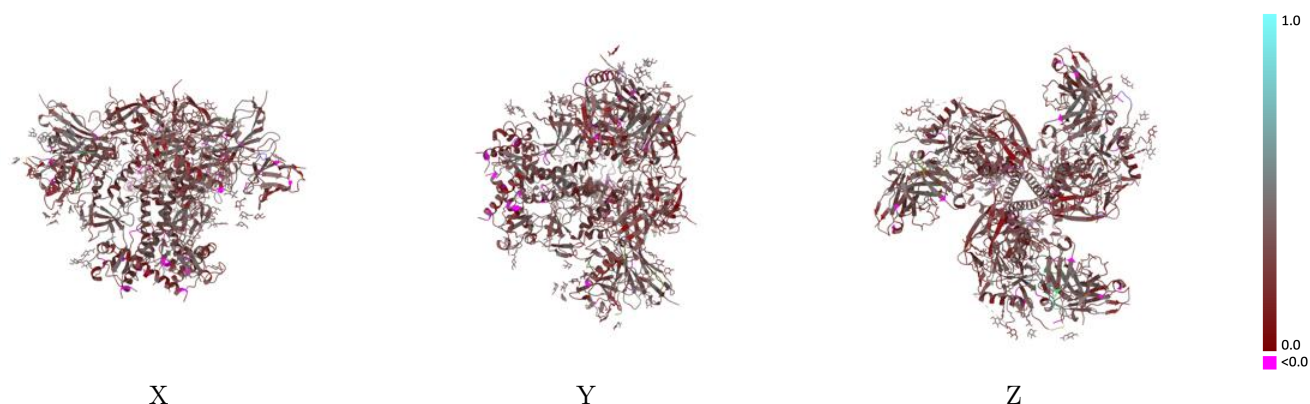
This section contains information regarding the fit between EMDB map EMD-21258 and PDB model 6VO3. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



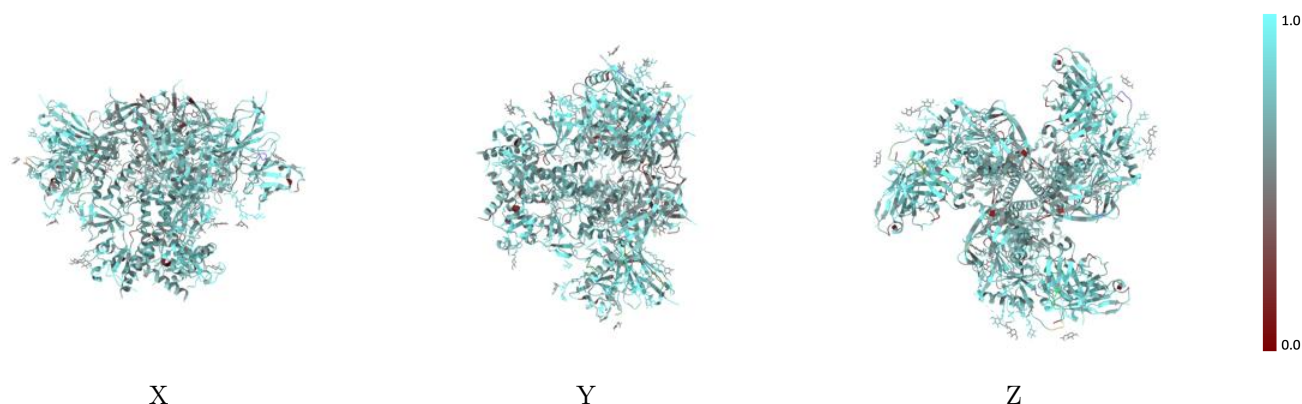
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



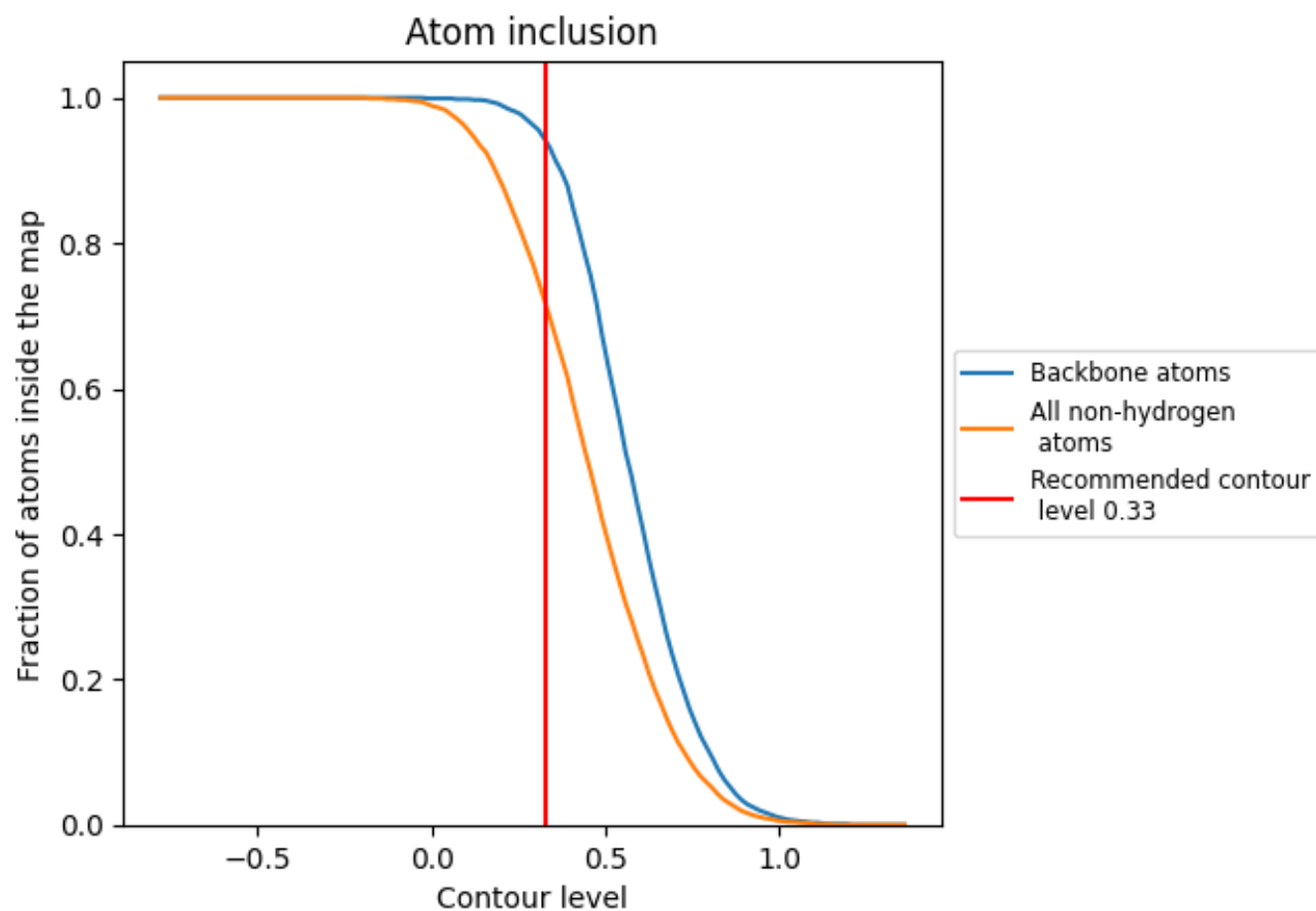
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 72% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.2900
A	 0.7040	 0.2950
B	 0.7230	 0.2510
C	 0.7040	 0.2940
D	 0.7040	 0.2930
E	 0.7260	 0.2540
F	 0.7220	 0.2520
G	 0.7440	 0.3250
H	 0.7470	 0.3220
I	 0.7450	 0.3200
J	 0.7210	 0.2630
K	 0.7200	 0.2660
L	 0.7230	 0.2620
M	 0.5900	 0.2400
N	 0.7870	 0.3400
O	 0.6670	 0.3130
P	 0.7140	 0.3850
Q	 0.7950	 0.3800
R	 0.5360	 0.3190
S	 0.6070	 0.4020
T	 0.5900	 0.2220
U	 0.8030	 0.3350
V	 0.6670	 0.3100
W	 0.7140	 0.4000
X	 0.8210	 0.3880
Y	 0.5360	 0.3330
Z	 0.6070	 0.4220
a	 0.6150	 0.2380
b	 0.7870	 0.3530
c	 0.6670	 0.3230
d	 0.7500	 0.3870
e	 0.8210	 0.3730
f	 0.5710	 0.3290
g	 0.6070	 0.4050

