



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:04 PM UTC

PDB ID : 6NF5 / pdb_00006nf5
EMDB ID : EMD-7884
Title : BG505 MD64 N332-GT5 SOSIP trimer in complex with BG18-like precursor HMP1 fragmentantigen binding and base-binding RM20A3 fragment antigen binding
Authors : Ozorowski, G.; Torres, J.L.; Steichen, J.M.; Schief, W.R.; Ward, A.B.
Deposited on : 2018-12-18
Resolution : 3.71 Å(reported)
Based on initial model : 5CEZ

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

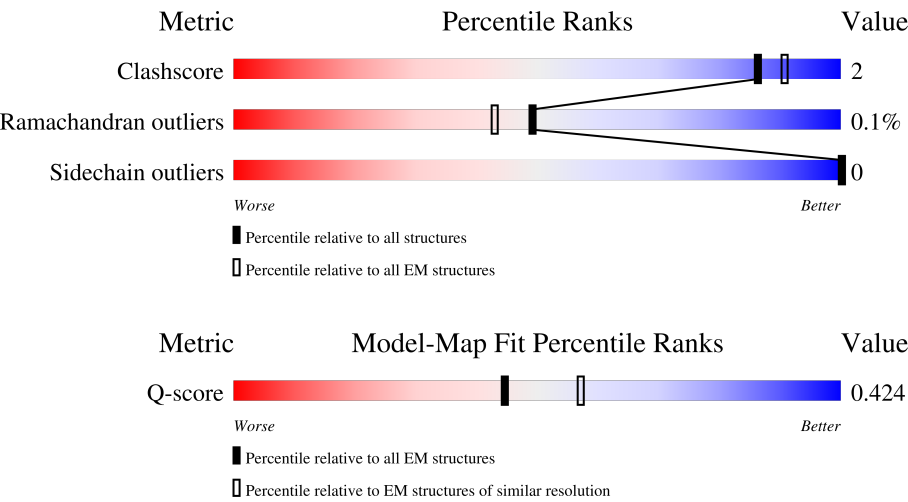
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.71 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	10534 (3.21 - 4.21)

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	481	
1	C	481	
1	J	481	
2	B	162	

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Mol	Chain	Length	Quality of chain
2	D	162	
2	M	162	
3	E	131	
3	H	131	
3	O	131	
4	F	106	
4	L	106	
4	P	106	
5	G	125	
5	K	125	
5	Q	125	
6	I	128	
6	N	128	
6	R	128	
7	S	2	
7	U	2	
7	W	2	
7	X	2	
7	Y	2	
7	Z	2	
7	b	2	
7	d	2	
7	e	2	
7	f	2	
7	g	2	

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Mol	Chain	Length	Quality of chain	
7	i	2	50%	100%
7	k	2	50%	100%
7	l	2	50%	100%
7	m	2	50%	100%
8	T	5	40%	100%
8	a	5	40%	100%
8	h	5	40%	100%
9	V	6	50%	83% 17%
9	c	6	50%	83% 17%
9	j	6	50%	83% 17%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 24933 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-1 Env BG505 MD64 N332-GT5 SOSIP gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	436	Total	C	N	O	S	0	0
			3454	2189	605	631	29		
1	C	436	Total	C	N	O	S	0	0
			3454	2189	605	631	29		
1	J	436	Total	C	N	O	S	0	0
			3454	2189	605	631	29		

- Molecule 2 is a protein called HIV-1 Env BG505 MD64 N332-GT5 SOSIP gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	122	Total	C	N	O	S	0	0
			974	614	169	185	6		
2	D	122	Total	C	N	O	S	0	0
			974	614	169	185	6		
2	M	122	Total	C	N	O	S	0	0
			974	614	169	185	6		

- Molecule 3 is a protein called BG18-like precursor HMP1 fragment antigen binding heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	128	Total	C	N	O	S	0	0
			976	623	158	192	3		
3	E	128	Total	C	N	O	S	0	0
			976	623	158	192	3		
3	O	128	Total	C	N	O	S	0	0
			976	623	158	192	3		

- Molecule 4 is a protein called BG18-like precursor HMP1 fragment antigen binding light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	99	Total	C	N	O	S	0	0
			740	463	121	154	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	99	Total	C	N	O	S	0	0
			740	463	121	154	2		
4	P	99	Total	C	N	O	S	0	0
			740	463	121	154	2		

- Molecule 5 is a protein called base-binding RM20A3 fragment antigen binding heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	123	Total	C	N	O	S	0	0
			937	592	160	180	5		
5	G	123	Total	C	N	O	S	0	0
			937	592	160	180	5		
5	Q	123	Total	C	N	O	S	0	0
			937	592	160	180	5		

- Molecule 6 is a protein called base-binding RM20A3 fragment antigen binding light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	108	Total	C	N	O	S	0	0
			803	499	135	166	3		
6	I	108	Total	C	N	O	S	0	0
			803	499	135	166	3		
6	R	108	Total	C	N	O	S	0	0
			803	499	135	166	3		

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



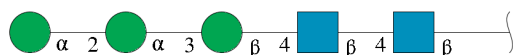
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		

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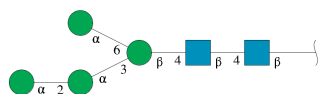
Mol	Chain	Residues	Atoms				AltConf	Trace
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	e	2	Total	C	N	O	0	0
			28	16	2	10		
7	f	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	i	2	Total	C	N	O	0	0
			28	16	2	10		
7	k	2	Total	C	N	O	0	0
			28	16	2	10		
7	l	2	Total	C	N	O	0	0
			28	16	2	10		
7	m	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



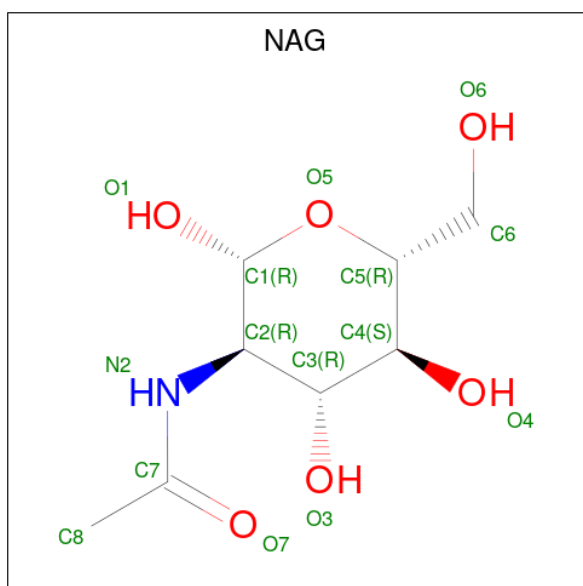
Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	5	Total	C	N	O	0	0
			61	34	2	25		
8	a	5	Total	C	N	O	0	0
			61	34	2	25		
8	h	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
9	V	6	Total	C	N	O	0	0
			72	40	2	30		
9	c	6	Total	C	N	O	0	0
			72	40	2	30		
9	j	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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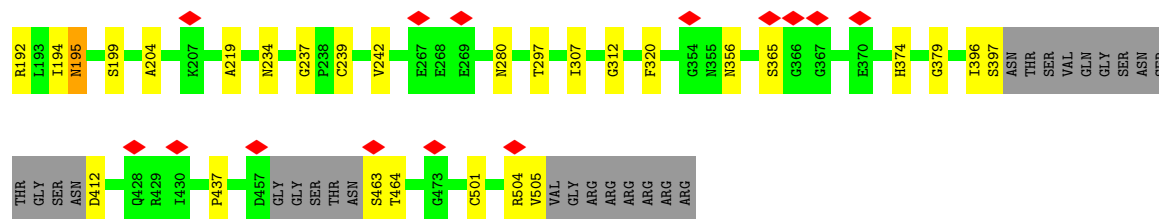
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Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total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

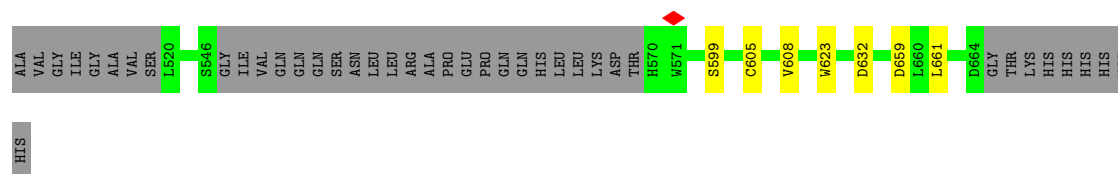
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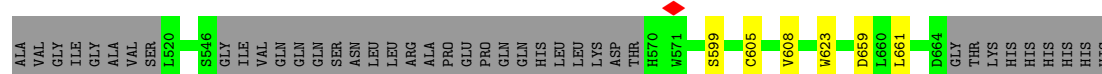
Mol	Chain	Residues	Atoms				AltConf
10	J	1	Total	C	N	O	0
			14	8	1	5	
10	J	1	Total	C	N	O	0
			14	8	1	5	
10	J	1	Total	C	N	O	0
			14	8	1	5	
10	J	1	Total	C	N	O	0
			14	8	1	5	
10	M	1	Total	C	N	O	0
			14	8	1	5	
10	M	1	Total	C	N	O	0
			14	8	1	5	



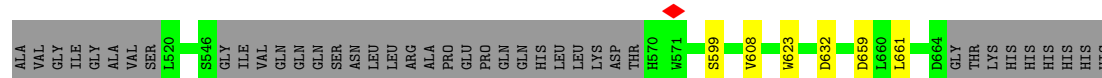
- Molecule 2: HIV-1 Env BG505 MD64 N332-GT5 SOSIP gp41



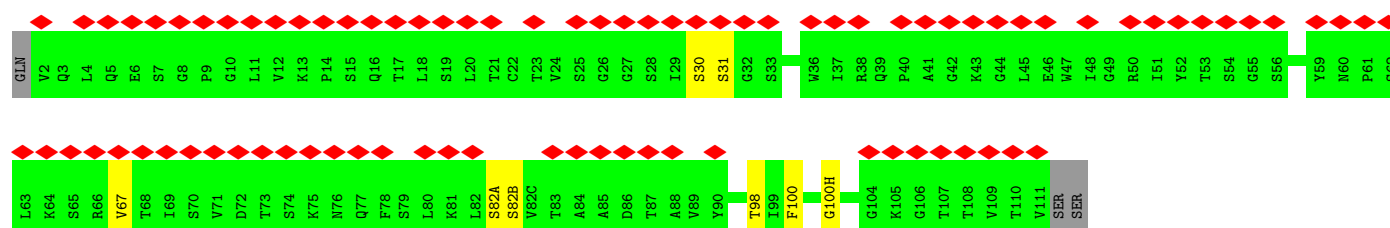
- Molecule 2: HIV-1 Env BG505 MD64 N332-GT5 SOSIP gp41



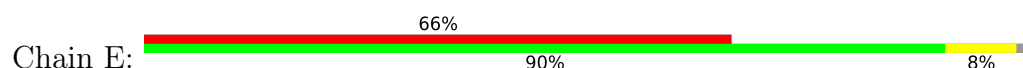
- Molecule 2: HIV-1 Env BG505 MD64 N332-GT5 SOSIP gp41

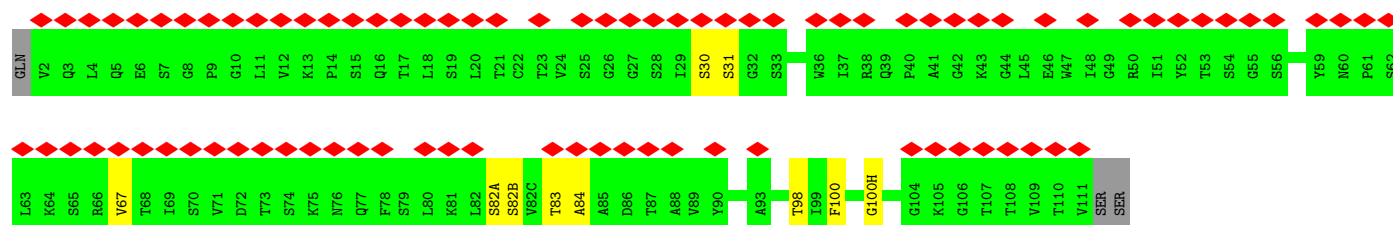


- Molecule 3: BG18-like precursor HMP1 fragment antigen binding heavy chain

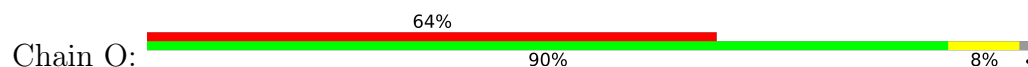


- Molecule 3: BG18-like precursor HMP1 fragment antigen binding heavy chain

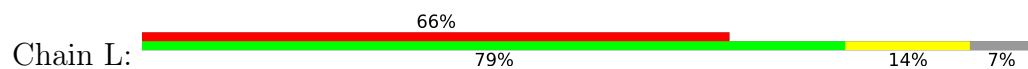




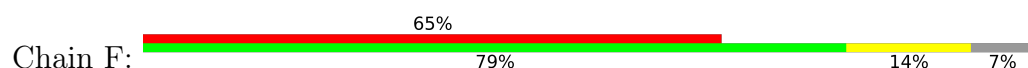
• Molecule 3: BG18-like precursor HMP1 fragment antigen binding heavy chain



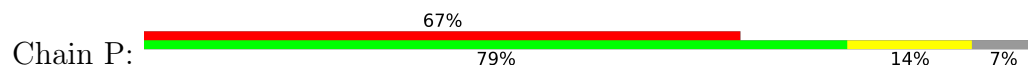
• Molecule 4: BG18-like precursor HMP1 fragment antigen binding light chain

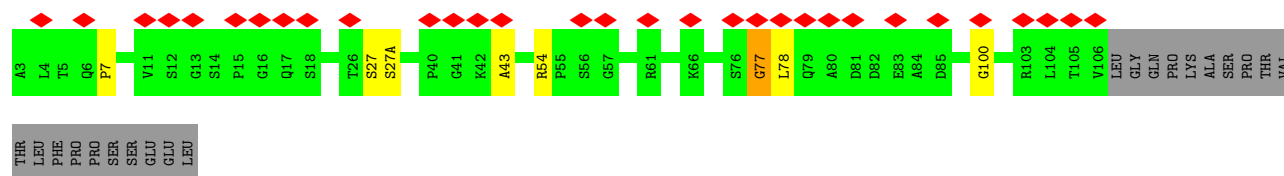


• Molecule 4: BG18-like precursor HMP1 fragment antigen binding light chain



• Molecule 4: BG18-like precursor HMP1 fragment antigen binding light chain





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



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



- Molecule 8: alpha-D-mannopyranose-(1-2)-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 8: alpha-D-mannopyranose-(1-2)-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

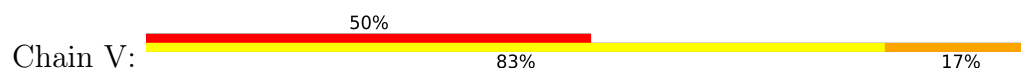
nose



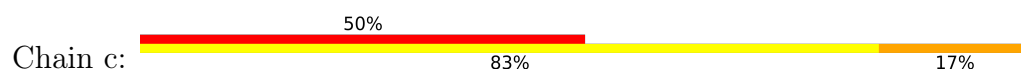
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



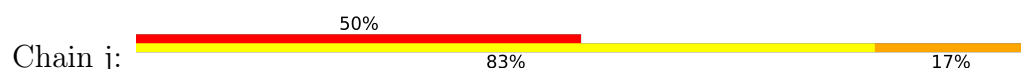
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	94466	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	0.5	Depositor
Maximum defocus (nm)	2.5	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.14	2/3531 (0.1%)	1.26	29/4792 (0.6%)
1	C	1.14	2/3531 (0.1%)	1.26	29/4792 (0.6%)
1	J	1.14	2/3531 (0.1%)	1.26	28/4792 (0.6%)
2	B	1.15	1/993 (0.1%)	1.03	4/1347 (0.3%)
2	D	1.15	1/993 (0.1%)	1.03	4/1347 (0.3%)
2	M	1.15	1/993 (0.1%)	1.03	4/1347 (0.3%)
3	E	0.98	1/1000 (0.1%)	1.26	1/1361 (0.1%)
3	H	0.98	1/1000 (0.1%)	1.26	1/1361 (0.1%)
3	O	0.98	1/1000 (0.1%)	1.26	1/1361 (0.1%)
4	F	1.02	2/756 (0.3%)	1.38	9/1030 (0.9%)
4	L	1.02	2/756 (0.3%)	1.38	9/1030 (0.9%)
4	P	1.02	2/756 (0.3%)	1.38	9/1030 (0.9%)
5	G	1.06	0/957	1.24	1/1292 (0.1%)
5	K	1.06	0/957	1.24	1/1292 (0.1%)
5	Q	1.06	0/957	1.24	1/1292 (0.1%)
6	I	1.09	0/822	1.36	10/1118 (0.9%)
6	N	1.09	0/822	1.37	10/1118 (0.9%)
6	R	1.09	0/822	1.37	10/1118 (0.9%)
All	All	1.10	18/24177 (0.1%)	1.25	161/32820 (0.5%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	100	PHE	CB-CG	-6.41	1.35	1.50
3	H	100	PHE	CB-CG	-6.41	1.35	1.50
3	O	100	PHE	CB-CG	-6.40	1.35	1.50
4	F	104	LEU	CB-CG	6.33	1.66	1.53
4	L	104	LEU	CB-CG	6.33	1.66	1.53
4	P	104	LEU	CB-CG	6.29	1.66	1.53
1	C	374	HIS	CA-C	-6.26	1.44	1.52
1	A	374	HIS	CA-C	-6.26	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	374	HIS	CA-C	-6.18	1.44	1.52
1	A	374	HIS	CB-CG	-5.78	1.42	1.50
1	C	374	HIS	CB-CG	-5.78	1.42	1.50
1	J	374	HIS	CB-CG	-5.76	1.42	1.50
2	B	623	TRP	NE1-CE2	-5.61	1.31	1.37
2	M	623	TRP	NE1-CE2	-5.61	1.31	1.37
2	D	623	TRP	NE1-CE2	-5.51	1.31	1.37
4	P	31	GLN	CG-CD	-5.06	1.39	1.52
4	L	31	GLN	CG-CD	-5.05	1.39	1.52
4	F	31	GLN	CG-CD	-5.04	1.39	1.52

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	159	PHE	CA-CB-CG	9.00	122.80	113.80
1	A	159	PHE	CA-CB-CG	8.99	122.79	113.80
1	C	159	PHE	CA-CB-CG	8.99	122.79	113.80
6	N	100	GLY	N-CA-C	-8.92	99.41	111.54
6	I	100	GLY	N-CA-C	-8.91	99.42	111.54
6	R	100	GLY	N-CA-C	-8.91	99.42	111.54
1	J	239	CYS	CA-C-N	7.50	127.17	119.82
1	J	239	CYS	C-N-CA	7.50	127.17	119.82
1	C	239	CYS	CA-C-N	7.47	127.14	119.82
1	C	239	CYS	C-N-CA	7.47	127.14	119.82
1	A	239	CYS	CA-C-N	7.45	127.12	119.82
1	A	239	CYS	C-N-CA	7.45	127.12	119.82
5	G	101	ASP	CA-CB-CG	7.08	119.68	112.60
5	K	101	ASP	CA-CB-CG	7.05	119.65	112.60
5	Q	101	ASP	CA-CB-CG	7.04	119.64	112.60
3	O	67	VAL	N-CA-C	6.76	118.53	108.46
3	H	67	VAL	N-CA-C	6.75	118.51	108.46
3	E	67	VAL	N-CA-C	6.74	118.51	108.46
1	A	237	GLY	CA-C-N	6.66	126.42	119.76
1	A	237	GLY	C-N-CA	6.66	126.42	119.76
1	C	195	ASN	CA-CB-CG	-6.63	105.97	112.60
1	J	237	GLY	CA-C-N	6.62	126.38	119.76
1	J	237	GLY	C-N-CA	6.62	126.38	119.76
4	L	90	SER	N-CA-C	-6.61	99.61	108.74
1	J	195	ASN	CA-CB-CG	-6.61	105.99	112.60
4	P	90	SER	N-CA-C	-6.61	99.62	108.74
1	A	195	ASN	CA-CB-CG	-6.59	106.01	112.60
4	F	90	SER	N-CA-C	-6.58	99.65	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	437	PRO	N-CA-C	-6.44	103.69	110.58
1	C	237	GLY	CA-C-N	6.44	126.36	119.85
1	C	237	GLY	C-N-CA	6.44	126.36	119.85
1	J	437	PRO	N-CA-C	-6.44	103.69	110.58
2	M	659	ASP	CA-CB-CG	6.44	119.04	112.60
1	J	219	ALA	CA-C-N	6.44	126.62	120.31
1	J	219	ALA	C-N-CA	6.44	126.62	120.31
2	B	659	ASP	CA-CB-CG	6.43	119.03	112.60
2	D	659	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	437	PRO	N-CA-C	-6.42	103.71	110.58
1	A	219	ALA	CA-C-N	6.41	126.59	120.31
1	A	219	ALA	C-N-CA	6.41	126.59	120.31
1	C	219	ALA	CA-C-N	6.40	126.58	120.31
1	C	219	ALA	C-N-CA	6.40	126.58	120.31
1	A	56	SER	N-CA-C	6.36	117.82	108.86
1	C	56	SER	N-CA-C	6.35	117.82	108.86
1	J	56	SER	N-CA-C	6.35	117.81	108.86
1	C	159	PHE	CB-CA-C	-6.33	96.14	109.38
1	A	159	PHE	CB-CA-C	-6.33	96.14	109.38
1	J	159	PHE	CB-CA-C	-6.33	96.15	109.38
4	P	58	ILE	CA-C-N	6.17	126.14	119.78
4	P	58	ILE	C-N-CA	6.17	126.14	119.78
4	L	58	ILE	CA-C-N	6.15	126.12	119.78
4	L	58	ILE	C-N-CA	6.15	126.12	119.78
1	J	307	ILE	N-CA-C	6.14	116.71	108.11
1	A	307	ILE	N-CA-C	6.14	116.70	108.11
1	C	307	ILE	N-CA-C	6.14	116.70	108.11
4	L	54	ARG	CA-C-N	6.12	126.08	119.78
4	L	54	ARG	C-N-CA	6.12	126.08	119.78
4	F	58	ILE	CA-C-N	6.11	126.07	119.78
4	F	58	ILE	C-N-CA	6.11	126.07	119.78
4	F	54	ARG	CA-C-N	6.10	126.07	119.78
4	F	54	ARG	C-N-CA	6.10	126.07	119.78
4	P	54	ARG	CA-C-N	6.08	126.04	119.78
4	P	54	ARG	C-N-CA	6.08	126.04	119.78
1	A	199	SER	N-CA-C	6.06	118.06	108.79
6	N	77	GLY	CA-C-N	6.05	129.35	120.82
6	N	77	GLY	C-N-CA	6.05	129.35	120.82
6	I	77	GLY	CA-C-N	6.05	129.35	120.82
6	I	77	GLY	C-N-CA	6.05	129.35	120.82
1	J	199	SER	N-CA-C	6.05	118.05	108.79
1	C	199	SER	N-CA-C	6.04	118.04	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	77	GLY	CA-C-N	6.01	129.30	120.82
6	R	77	GLY	C-N-CA	6.01	129.30	120.82
4	P	43	ALA	CA-C-N	5.98	125.92	119.76
4	P	43	ALA	C-N-CA	5.98	125.92	119.76
4	L	43	ALA	CA-C-N	5.97	125.91	119.76
4	L	43	ALA	C-N-CA	5.97	125.91	119.76
4	F	43	ALA	CA-C-N	5.92	125.86	119.76
4	F	43	ALA	C-N-CA	5.92	125.86	119.76
1	C	78	ASP	CA-C-N	5.92	125.60	119.56
1	C	78	ASP	C-N-CA	5.92	125.60	119.56
1	J	78	ASP	CA-C-N	5.89	125.56	119.56
1	J	78	ASP	C-N-CA	5.89	125.56	119.56
1	A	78	ASP	CA-C-N	5.83	125.53	119.82
1	A	78	ASP	C-N-CA	5.83	125.53	119.82
1	J	123	THR	CA-C-N	5.82	125.50	119.56
1	J	123	THR	C-N-CA	5.82	125.50	119.56
1	A	123	THR	CA-C-N	5.78	125.46	119.56
1	A	123	THR	C-N-CA	5.78	125.46	119.56
1	C	123	THR	CA-C-N	5.78	125.45	119.56
1	C	123	THR	C-N-CA	5.78	125.45	119.56
2	B	599	SER	N-CA-C	5.78	119.58	112.54
2	M	599	SER	N-CA-C	5.76	119.57	112.54
2	D	599	SER	N-CA-C	5.76	119.56	112.54
1	C	320	PHE	CA-CB-CG	5.75	119.55	113.80
6	N	54	ARG	CA-C-N	5.73	125.71	120.03
6	N	54	ARG	C-N-CA	5.73	125.71	120.03
1	A	320	PHE	CA-CB-CG	5.72	119.52	113.80
6	I	54	ARG	CA-C-N	5.71	125.68	120.03
6	I	54	ARG	C-N-CA	5.71	125.68	120.03
6	R	54	ARG	CA-C-N	5.70	125.67	120.03
6	R	54	ARG	C-N-CA	5.70	125.67	120.03
1	J	320	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	437	PRO	CA-C-N	5.64	125.61	120.03
1	A	437	PRO	C-N-CA	5.64	125.61	120.03
1	C	437	PRO	CA-C-N	5.62	125.60	120.03
1	C	437	PRO	C-N-CA	5.62	125.60	120.03
1	J	437	PRO	CA-C-N	5.62	125.59	120.03
1	J	437	PRO	C-N-CA	5.62	125.59	120.03
2	M	608	VAL	CA-C-N	5.58	125.48	119.85
2	M	608	VAL	C-N-CA	5.58	125.48	119.85
2	D	608	VAL	CA-C-N	5.56	125.46	119.85
2	D	608	VAL	C-N-CA	5.56	125.46	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	608	VAL	CA-C-N	5.52	125.42	119.85
2	B	608	VAL	C-N-CA	5.52	125.42	119.85
6	N	7	PRO	CA-C-N	5.41	125.17	119.76
6	N	7	PRO	C-N-CA	5.41	125.17	119.76
6	R	7	PRO	CA-C-N	5.41	125.17	119.76
6	R	7	PRO	C-N-CA	5.41	125.17	119.76
1	C	365	SER	N-CA-C	5.38	119.56	112.89
1	A	365	SER	N-CA-C	5.37	119.55	112.89
1	J	365	SER	N-CA-C	5.36	119.53	112.89
6	I	7	PRO	CA-C-N	5.34	125.10	119.76
6	I	7	PRO	C-N-CA	5.34	125.10	119.76
4	F	26	ASP	N-CA-C	5.29	117.80	111.71
4	P	7	PRO	N-CA-C	-5.29	104.92	110.58
4	F	7	PRO	N-CA-C	-5.28	104.93	110.58
4	L	26	ASP	N-CA-C	5.28	117.78	111.71
4	P	26	ASP	N-CA-C	5.25	117.75	111.71
4	L	7	PRO	N-CA-C	-5.24	104.98	110.58
1	A	53	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	53	PHE	CA-CB-CG	5.23	119.03	113.80
1	J	53	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	312	GLY	CA-C-N	5.16	126.29	119.84
1	A	312	GLY	C-N-CA	5.16	126.29	119.84
1	J	312	GLY	CA-C-N	5.14	126.26	119.84
1	J	312	GLY	C-N-CA	5.14	126.26	119.84
1	C	312	GLY	CA-C-N	5.11	126.23	119.84
1	C	312	GLY	C-N-CA	5.11	126.23	119.84
6	R	43	ALA	CA-C-N	5.10	125.00	119.85
6	R	43	ALA	C-N-CA	5.10	125.00	119.85
1	C	242	VAL	N-CA-C	5.09	116.79	109.51
1	J	242	VAL	N-CA-C	5.09	116.79	109.51
1	J	204	ALA	N-CA-C	5.09	117.48	109.39
1	A	242	VAL	N-CA-C	5.09	116.79	109.51
1	C	379	GLY	N-CA-C	-5.08	108.60	115.36
1	J	379	GLY	N-CA-C	-5.07	108.61	115.36
1	A	204	ALA	N-CA-C	5.07	117.45	109.39
1	C	204	ALA	N-CA-C	5.07	117.45	109.39
6	N	43	ALA	CA-C-N	5.07	124.97	119.85
6	N	43	ALA	C-N-CA	5.07	124.97	119.85
6	I	43	ALA	CA-C-N	5.07	124.97	119.85
6	I	43	ALA	C-N-CA	5.07	124.97	119.85
1	A	379	GLY	N-CA-C	-5.06	108.64	115.36
6	R	78	LEU	N-CA-C	5.05	117.63	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	78	LEU	N-CA-C	5.05	117.62	110.10
1	J	87	GLU	N-CA-C	5.04	116.77	111.28
6	N	78	LEU	N-CA-C	5.03	117.59	110.10
1	A	87	GLU	N-CA-C	5.03	116.76	111.28
1	A	415	ILE	N-CA-C	5.02	115.14	108.11
1	C	87	GLU	N-CA-C	5.02	116.75	111.28
1	C	415	ILE	N-CA-C	5.01	115.13	108.11

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	3454	0	3413	26	0
1	C	3454	0	3413	21	0
1	J	3454	0	3413	23	0
2	B	974	0	940	6	0
2	D	974	0	940	4	0
2	M	974	0	940	4	0
3	E	976	0	950	4	0
3	H	976	0	950	3	0
3	O	976	0	950	4	0
4	F	740	0	708	4	0
4	L	740	0	708	4	0
4	P	740	0	708	4	0
5	G	937	0	910	1	0
5	K	937	0	910	2	0
5	Q	937	0	910	1	0
6	I	803	0	756	1	0
6	N	803	0	756	1	0
6	R	803	0	756	1	0
7	S	28	0	25	0	0
7	U	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Y	28	0	25	0	0
7	Z	28	0	25	0	0
7	b	28	0	25	0	0
7	d	28	0	25	0	0
7	e	28	0	25	0	0
7	f	28	0	25	0	0
7	g	28	0	25	0	0
7	i	28	0	25	0	0
7	k	28	0	25	0	0
7	l	28	0	25	0	0
7	m	28	0	25	0	0
8	T	61	0	50	0	0
8	a	61	0	50	0	0
8	h	61	0	50	0	0
9	V	72	0	58	1	0
9	c	72	0	58	1	0
9	j	72	0	58	1	0
10	A	126	0	117	2	0
10	B	28	0	26	0	0
10	C	126	0	117	2	0
10	D	28	0	26	0	0
10	J	126	0	117	2	0
10	M	28	0	26	0	0
All	All	24933	0	24159	100	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 (100) 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)
2:B:661:LEU:HB2	1:J:501:CYS:SG	2.05	0.96
1:A:501:CYS:SG	2:D:661:LEU:HB2	2.05	0.96
1:C:501:CYS:SG	2:M:661:LEU:HB2	2.05	0.95
1:A:501:CYS:SG	2:D:661:LEU:CB	2.64	0.86
2:B:661:LEU:CB	1:J:501:CYS:SG	2.64	0.86
1:C:501:CYS:SG	2:M:661:LEU:CB	2.64	0.85
1:A:501:CYS:HG	2:B:605:CYS:HG	0.80	0.79
1:A:501:CYS:SG	2:D:661:LEU:HB3	2.39	0.63
1:C:501:CYS:SG	2:M:661:LEU:HB3	2.39	0.62
2:B:661:LEU:HB3	1:J:501:CYS:SG	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:84:ASP:N	5:K:84:ASP:OD1	2.33	0.60
5:G:84:ASP:N	5:G:84:ASP:OD1	2.33	0.59
5:Q:84:ASP:N	5:Q:84:ASP:OD1	2.33	0.59
1:C:504:ARG:O	1:C:505:VAL:C	2.46	0.58
1:A:504:ARG:O	1:A:505:VAL:C	2.46	0.58
1:J:504:ARG:O	1:J:505:VAL:C	2.46	0.57
1:C:396:ILE:O	1:C:397:SER:C	2.48	0.57
1:J:396:ILE:O	1:J:397:SER:C	2.48	0.57
1:A:396:ILE:O	1:A:397:SER:C	2.48	0.56
3:E:30:SER:OG	3:E:31:SER:N	2.40	0.55
1:C:501:CYS:CB	2:D:605:CYS:HG	2.18	0.54
3:O:30:SER:OG	3:O:31:SER:N	2.40	0.53
3:H:30:SER:OG	3:H:31:SER:N	2.40	0.53
1:C:77:THR:OG1	1:C:78:ASP:N	2.43	0.52
1:A:77:THR:OG1	1:A:78:ASP:N	2.43	0.52
1:A:501:CYS:CB	2:B:605:CYS:HG	2.17	0.52
1:A:463:SER:OG	1:A:464:THR:N	2.44	0.51
1:J:77:THR:OG1	1:J:78:ASP:N	2.42	0.51
1:J:463:SER:OG	1:J:464:THR:N	2.44	0.50
1:A:167:ASP:OD2	1:A:168:LYS:NZ	2.45	0.50
6:N:27:SER:OG	6:N:27(A):SER:N	2.45	0.49
1:C:463:SER:OG	1:C:464:THR:N	2.44	0.49
1:J:167:ASP:OD2	1:J:168:LYS:NZ	2.45	0.49
1:A:123:THR:N	1:A:124:PRO:CD	2.76	0.49
1:J:280:ASN:N	1:J:280:ASN:OD1	2.46	0.49
3:E:82(A):SER:OG	3:E:82(B):SER:N	2.46	0.49
1:C:123:THR:N	1:C:124:PRO:CD	2.76	0.48
1:J:123:THR:N	1:J:124:PRO:CD	2.76	0.48
1:C:280:ASN:OD1	1:C:280:ASN:N	2.46	0.48
3:O:82(A):SER:OG	3:O:82(B):SER:N	2.46	0.48
6:R:27:SER:OG	6:R:27(A):SER:N	2.45	0.48
1:C:167:ASP:OD2	1:C:168:LYS:NZ	2.45	0.47
1:J:356:ASN:OD1	1:J:356:ASN:N	2.47	0.47
4:P:91:ALA:O	4:P:92:ASP:C	2.58	0.47
1:A:280:ASN:N	1:A:280:ASN:OD1	2.46	0.46
1:A:79:PRO:O	1:A:80:ASN:C	2.59	0.46
4:F:91:ALA:O	4:F:92:ASP:C	2.58	0.46
1:A:356:ASN:OD1	1:A:356:ASN:N	2.47	0.45
1:C:79:PRO:O	1:C:80:ASN:C	2.59	0.45
4:L:91:ALA:O	4:L:92:ASP:C	2.58	0.45
1:J:57:ASP:O	1:J:58:ALA:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:79:PRO:O	1:J:80:ASN:C	2.59	0.45
1:A:57:ASP:O	1:A:58:ALA:CB	2.64	0.45
1:C:57:ASP:O	1:C:58:ALA:CB	2.64	0.45
6:I:27:SER:OG	6:I:27(A):SER:N	2.45	0.45
4:L:50:LYS:O	4:L:50:LYS:HG2	2.17	0.45
1:A:46:LYS:NZ	2:B:632:ASP:OD2	2.41	0.44
1:J:192:ARG:HD2	10:J:604:NAG:H83	1.99	0.44
4:P:50:LYS:O	4:P:50:LYS:HG2	2.17	0.44
1:J:194:ILE:HA	10:J:604:NAG:H81	2.00	0.44
1:A:194:ILE:HA	10:A:604:NAG:H81	2.00	0.43
4:L:37:GLN:NE2	4:L:86:TYR:OH	2.51	0.43
4:P:98:PHE:CG	4:P:99:GLY:N	2.87	0.43
4:F:50:LYS:HG2	4:F:50:LYS:O	2.17	0.43
1:A:184:ILE:O	1:A:185:ASN:C	2.61	0.43
1:C:192:ARG:HD2	10:C:604:NAG:H83	2.00	0.43
4:P:37:GLN:NE2	4:P:86:TYR:OH	2.51	0.43
4:L:98:PHE:CG	4:L:99:GLY:N	2.87	0.43
1:A:192:ARG:HD2	10:A:604:NAG:H83	2.00	0.43
1:C:195:ASN:OD1	1:C:195:ASN:N	2.49	0.43
1:C:194:ILE:HA	10:C:604:NAG:H81	2.00	0.43
4:F:98:PHE:CG	4:F:99:GLY:N	2.87	0.43
1:J:184:ILE:O	1:J:185:ASN:C	2.61	0.43
3:E:98:THR:O	3:E:100(H):GLY:HA3	2.19	0.42
3:O:98:THR:O	3:O:100(H):GLY:HA3	2.19	0.42
1:C:184:ILE:O	1:C:185:ASN:C	2.61	0.42
4:F:37:GLN:NE2	4:F:86:TYR:OH	2.51	0.42
1:J:297:THR:HG22	9:j:1:NAG:H83	2.01	0.42
1:A:50:THR:OG1	1:A:51:THR:N	2.53	0.42
1:C:50:THR:OG1	1:C:51:THR:N	2.53	0.42
1:A:297:THR:HG22	9:V:1:NAG:H83	2.01	0.42
3:H:98:THR:O	3:H:100(H):GLY:HA3	2.19	0.42
1:J:50:THR:OG1	1:J:51:THR:N	2.53	0.42
1:A:66:HIS:CG	1:A:67:ASN:H	2.39	0.41
5:K:25:SER:OG	5:K:26:GLY:N	2.53	0.41
3:H:82(A):SER:OG	3:H:82(B):SER:N	2.46	0.41
1:C:297:THR:HG22	9:c:1:NAG:H83	2.01	0.41
1:J:195:ASN:OD1	1:J:195:ASN:N	2.49	0.41
1:A:66:HIS:ND1	1:A:67:ASN:N	2.69	0.41
1:A:195:ASN:OD1	1:A:195:ASN:N	2.49	0.41
1:A:412:ASP:N	1:A:412:ASP:OD1	2.51	0.41
1:J:66:HIS:CG	1:J:67:ASN:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:412:ASP:OD1	1:J:412:ASP:N	2.51	0.41
1:C:33:ASN:N	1:C:33:ASN:OD1	2.54	0.40
1:C:234:ASN:OD1	1:C:234:ASN:C	2.63	0.40
1:J:46:LYS:NZ	2:M:632:ASP:OD2	2.41	0.40
3:E:83:THR:OG1	3:E:84:ALA:N	2.55	0.40
1:J:234:ASN:OD1	1:J:234:ASN:C	2.63	0.40
1:A:33:ASN:OD1	1:A:33:ASN:N	2.54	0.40
3:O:83:THR:OG1	3:O:84:ALA:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/481 (89%)	415 (97%)	11 (3%)	0	100	100
1	C	426/481 (89%)	415 (97%)	11 (3%)	0	100	100
1	J	426/481 (89%)	415 (97%)	11 (3%)	0	100	100
2	B	118/162 (73%)	115 (98%)	3 (2%)	0	100	100
2	D	118/162 (73%)	115 (98%)	3 (2%)	0	100	100
2	M	118/162 (73%)	115 (98%)	3 (2%)	0	100	100
3	E	126/131 (96%)	119 (94%)	7 (6%)	0	100	100
3	H	126/131 (96%)	119 (94%)	7 (6%)	0	100	100
3	O	126/131 (96%)	119 (94%)	7 (6%)	0	100	100
4	F	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
4	L	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
4	P	95/106 (90%)	94 (99%)	1 (1%)	0	100	100
5	G	121/125 (97%)	118 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
5	Q	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
6	I	106/128 (83%)	98 (92%)	7 (7%)	1 (1%)	14	45
6	N	106/128 (83%)	98 (92%)	7 (7%)	1 (1%)	14	45
6	R	106/128 (83%)	98 (92%)	7 (7%)	1 (1%)	14	45
All	All	2976/3399 (88%)	2877 (97%)	96 (3%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	77	GLY
6	I	77	GLY
6	R	77	GLY

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	391/428 (91%)	391 (100%)	0	100	100
1	C	391/428 (91%)	391 (100%)	0	100	100
1	J	391/428 (91%)	391 (100%)	0	100	100
2	B	105/138 (76%)	105 (100%)	0	100	100
2	D	105/138 (76%)	105 (100%)	0	100	100
2	M	105/138 (76%)	105 (100%)	0	100	100
3	E	108/111 (97%)	108 (100%)	0	100	100
3	H	108/111 (97%)	108 (100%)	0	100	100
3	O	108/111 (97%)	108 (100%)	0	100	100
4	F	82/88 (93%)	82 (100%)	0	100	100
4	L	82/88 (93%)	82 (100%)	0	100	100
4	P	82/88 (93%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	100/102 (98%)	100 (100%)	0	100	100
5	K	100/102 (98%)	100 (100%)	0	100	100
5	Q	100/102 (98%)	100 (100%)	0	100	100
6	I	88/106 (83%)	88 (100%)	0	100	100
6	N	88/106 (83%)	88 (100%)	0	100	100
6	R	88/106 (83%)	88 (100%)	0	100	100
All	All	2622/2919 (90%)	2622 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	325	HIS
3	H	77	GLN
4	L	89	GLN
5	K	39	GLN
5	K	81	GLN
5	K	82(A)	HIS
1	C	33	ASN
1	C	105	HIS
1	C	325	HIS
3	E	77	GLN
4	F	89	GLN
5	G	39	GLN
5	G	81	GLN
5	G	82(A)	HIS
1	J	33	ASN
1	J	325	HIS
3	O	77	GLN
4	P	79	GLN
4	P	89	GLN
5	Q	82(A)	HIS

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 ⓘ

63 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	S	1	7,1	14,14,15	2.01	3 (21%)	17,19,21	1.25	1 (5%)
7	NAG	S	2	7	14,14,15	2.17	2 (14%)	17,19,21	0.80	0
8	NAG	T	1	8,1	14,14,15	1.97	2 (14%)	17,19,21	0.96	1 (5%)
8	NAG	T	2	8	14,14,15	2.10	3 (21%)	17,19,21	1.00	0
8	BMA	T	3	8	11,11,12	1.84	2 (18%)	15,15,17	1.03	1 (6%)
8	MAN	T	4	8	11,11,12	1.59	2 (18%)	15,15,17	0.86	1 (6%)
8	MAN	T	5	8	11,11,12	1.80	2 (18%)	15,15,17	0.98	1 (6%)
7	NAG	U	1	7,1	14,14,15	2.02	3 (21%)	17,19,21	1.05	2 (11%)
7	NAG	U	2	7	14,14,15	2.13	2 (14%)	17,19,21	0.83	1 (5%)
9	NAG	V	1	9,1	14,14,15	1.87	2 (14%)	17,19,21	1.21	3 (17%)
9	NAG	V	2	9	14,14,15	2.05	3 (21%)	17,19,21	1.20	1 (5%)
9	BMA	V	3	9	11,11,12	1.88	2 (18%)	15,15,17	1.03	1 (6%)
9	MAN	V	4	9	11,11,12	1.55	1 (9%)	15,15,17	0.91	0
9	MAN	V	5	9	11,11,12	1.90	2 (18%)	15,15,17	1.00	0
9	MAN	V	6	9	11,11,12	1.84	2 (18%)	15,15,17	0.99	1 (6%)
7	NAG	W	1	7,1	14,14,15	2.02	3 (21%)	17,19,21	1.02	2 (11%)
7	NAG	W	2	7	14,14,15	2.15	2 (14%)	17,19,21	0.86	1 (5%)
7	NAG	X	1	7,1	14,14,15	2.09	4 (28%)	17,19,21	2.45	5 (29%)
7	NAG	X	2	7	14,14,15	2.11	2 (14%)	17,19,21	0.80	0
7	NAG	Y	1	2,7	14,14,15	2.09	3 (21%)	17,19,21	0.96	1 (5%)
7	NAG	Y	2	7	14,14,15	2.13	3 (21%)	17,19,21	0.86	1 (5%)
7	NAG	Z	1	7,1	14,14,15	2.01	3 (21%)	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	Z	2	7	14,14,15	2.17	2 (14%)	17,19,21	0.80	0
8	NAG	a	1	8,1	14,14,15	1.97	2 (14%)	17,19,21	0.95	1 (5%)
8	NAG	a	2	8	14,14,15	2.11	3 (21%)	17,19,21	1.00	0
8	BMA	a	3	8	11,11,12	1.84	2 (18%)	15,15,17	1.02	1 (6%)
8	MAN	a	4	8	11,11,12	1.59	2 (18%)	15,15,17	0.87	1 (6%)
8	MAN	a	5	8	11,11,12	1.80	2 (18%)	15,15,17	0.97	1 (6%)
7	NAG	b	1	7,1	14,14,15	2.02	3 (21%)	17,19,21	1.05	2 (11%)
7	NAG	b	2	7	14,14,15	2.12	2 (14%)	17,19,21	0.82	1 (5%)
9	NAG	c	1	9,1	14,14,15	1.87	2 (14%)	17,19,21	1.22	3 (17%)
9	NAG	c	2	9	14,14,15	2.05	3 (21%)	17,19,21	1.20	1 (5%)
9	BMA	c	3	9	11,11,12	1.87	2 (18%)	15,15,17	1.04	1 (6%)
9	MAN	c	4	9	11,11,12	1.55	1 (9%)	15,15,17	0.91	0
9	MAN	c	5	9	11,11,12	1.91	2 (18%)	15,15,17	1.00	0
9	MAN	c	6	9	11,11,12	1.84	2 (18%)	15,15,17	0.99	1 (6%)
7	NAG	d	1	7,1	14,14,15	2.01	3 (21%)	17,19,21	1.02	2 (11%)
7	NAG	d	2	7	14,14,15	2.17	2 (14%)	17,19,21	0.87	1 (5%)
7	NAG	e	1	7,1	14,14,15	2.08	4 (28%)	17,19,21	2.45	5 (29%)
7	NAG	e	2	7	14,14,15	2.12	2 (14%)	17,19,21	0.80	0
7	NAG	f	1	2,7	14,14,15	2.09	3 (21%)	17,19,21	0.95	1 (5%)
7	NAG	f	2	7	14,14,15	2.13	3 (21%)	17,19,21	0.85	1 (5%)
7	NAG	g	1	7,1	14,14,15	2.01	3 (21%)	17,19,21	1.26	1 (5%)
7	NAG	g	2	7	14,14,15	2.17	2 (14%)	17,19,21	0.80	0
8	NAG	h	1	8,1	14,14,15	1.97	2 (14%)	17,19,21	0.95	1 (5%)
8	NAG	h	2	8	14,14,15	2.10	3 (21%)	17,19,21	1.00	0
8	BMA	h	3	8	11,11,12	1.84	2 (18%)	15,15,17	1.03	1 (6%)
8	MAN	h	4	8	11,11,12	1.60	2 (18%)	15,15,17	0.86	1 (6%)
8	MAN	h	5	8	11,11,12	1.81	2 (18%)	15,15,17	0.97	1 (6%)
7	NAG	i	1	7,1	14,14,15	2.02	3 (21%)	17,19,21	1.05	2 (11%)
7	NAG	i	2	7	14,14,15	2.12	2 (14%)	17,19,21	0.81	1 (5%)
9	NAG	j	1	9,1	14,14,15	1.86	2 (14%)	17,19,21	1.21	3 (17%)
9	NAG	j	2	9	14,14,15	2.06	3 (21%)	17,19,21	1.20	1 (5%)
9	BMA	j	3	9	11,11,12	1.88	2 (18%)	15,15,17	1.03	1 (6%)
9	MAN	j	4	9	11,11,12	1.56	1 (9%)	15,15,17	0.91	0
9	MAN	j	5	9	11,11,12	1.91	2 (18%)	15,15,17	1.00	0
9	MAN	j	6	9	11,11,12	1.83	2 (18%)	15,15,17	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	k	1	7,1	14,14,15	2.02	3 (21%)	17,19,21	1.02	2 (11%)
7	NAG	k	2	7	14,14,15	2.16	2 (14%)	17,19,21	0.87	1 (5%)
7	NAG	l	1	7,1	14,14,15	2.09	4 (28%)	17,19,21	2.46	5 (29%)
7	NAG	l	2	7	14,14,15	2.12	2 (14%)	17,19,21	0.80	0
7	NAG	m	1	2,7	14,14,15	2.10	3 (21%)	17,19,21	0.95	1 (5%)
7	NAG	m	2	7	14,14,15	2.14	3 (21%)	17,19,21	0.85	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
7	NAG	S	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	1/6/23/26	0/1/1/1
8	NAG	T	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	1/2/19/22	0/1/1/1
8	MAN	T	4	8	-	1/2/19/22	0/1/1/1
8	MAN	T	5	8	-	2/2/19/22	0/1/1/1
7	NAG	U	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	2/6/23/26	0/1/1/1
9	NAG	V	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	V	2	9	-	1/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1
9	MAN	V	4	9	-	1/2/19/22	0/1/1/1
9	MAN	V	5	9	-	2/2/19/22	0/1/1/1
9	MAN	V	6	9	-	1/2/19/22	0/1/1/1
7	NAG	W	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	2/6/23/26	0/1/1/1
7	NAG	X	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
7	NAG	Y	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	2/6/23/26	0/1/1/1
7	NAG	Z	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	1/6/23/26	0/1/1/1
8	NAG	a	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1
8	BMA	a	3	8	-	1/2/19/22	0/1/1/1
8	MAN	a	4	8	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	a	5	8	-	2/2/19/22	0/1/1/1
7	NAG	b	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	2/6/23/26	0/1/1/1
9	NAG	c	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	c	2	9	-	1/6/23/26	0/1/1/1
9	BMA	c	3	9	-	2/2/19/22	0/1/1/1
9	MAN	c	4	9	-	1/2/19/22	0/1/1/1
9	MAN	c	5	9	-	2/2/19/22	0/1/1/1
9	MAN	c	6	9	-	1/2/19/22	0/1/1/1
7	NAG	d	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	2/6/23/26	0/1/1/1
7	NAG	e	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	e	2	7	-	1/6/23/26	0/1/1/1
7	NAG	f	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	f	2	7	-	2/6/23/26	0/1/1/1
7	NAG	g	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	g	2	7	-	1/6/23/26	0/1/1/1
8	NAG	h	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1
8	BMA	h	3	8	-	1/2/19/22	0/1/1/1
8	MAN	h	4	8	-	1/2/19/22	0/1/1/1
8	MAN	h	5	8	-	2/2/19/22	0/1/1/1
7	NAG	i	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	2/6/23/26	0/1/1/1
9	NAG	j	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	j	2	9	-	1/6/23/26	0/1/1/1
9	BMA	j	3	9	-	2/2/19/22	0/1/1/1
9	MAN	j	4	9	-	1/2/19/22	0/1/1/1
9	MAN	j	5	9	-	2/2/19/22	0/1/1/1
9	MAN	j	6	9	-	1/2/19/22	0/1/1/1
7	NAG	k	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	k	2	7	-	2/6/23/26	0/1/1/1
7	NAG	l	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	l	2	7	-	1/6/23/26	0/1/1/1
7	NAG	m	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	m	2	7	-	2/6/23/26	0/1/1/1

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	2	NAG	O5-C1	6.86	1.55	1.43
7	g	2	NAG	O5-C1	6.86	1.55	1.43
7	S	2	NAG	O5-C1	6.85	1.55	1.43
7	l	2	NAG	O5-C1	6.80	1.55	1.43
7	d	2	NAG	O5-C1	6.78	1.55	1.43
7	e	2	NAG	O5-C1	6.77	1.55	1.43
7	X	2	NAG	O5-C1	6.76	1.55	1.43
7	k	2	NAG	O5-C1	6.76	1.55	1.43
7	U	2	NAG	O5-C1	6.75	1.55	1.43
7	W	2	NAG	O5-C1	6.73	1.55	1.43
7	i	2	NAG	O5-C1	6.71	1.55	1.43
7	b	2	NAG	O5-C1	6.70	1.55	1.43
7	Y	2	NAG	O5-C1	6.62	1.54	1.43
7	m	2	NAG	O5-C1	6.62	1.54	1.43
7	f	2	NAG	O5-C1	6.59	1.54	1.43
8	a	2	NAG	O5-C1	6.49	1.54	1.43
8	h	2	NAG	O5-C1	6.48	1.54	1.43
8	T	2	NAG	O5-C1	6.47	1.54	1.43
7	m	1	NAG	O5-C1	6.38	1.54	1.43
7	f	1	NAG	O5-C1	6.36	1.54	1.43
7	Y	1	NAG	O5-C1	6.35	1.54	1.43
9	j	2	NAG	O5-C1	6.35	1.54	1.43
9	V	2	NAG	O5-C1	6.30	1.54	1.43
9	c	2	NAG	O5-C1	6.28	1.54	1.43
7	b	1	NAG	O5-C1	6.16	1.54	1.43
8	h	1	NAG	O5-C1	6.15	1.54	1.43
8	T	1	NAG	O5-C1	6.14	1.54	1.43
7	g	1	NAG	O5-C1	6.14	1.54	1.43
7	Z	1	NAG	O5-C1	6.14	1.54	1.43
7	U	1	NAG	O5-C1	6.14	1.54	1.43
7	S	1	NAG	O5-C1	6.14	1.54	1.43
8	a	1	NAG	O5-C1	6.12	1.54	1.43
7	i	1	NAG	O5-C1	6.12	1.54	1.43
7	k	1	NAG	O5-C1	5.99	1.53	1.43
7	W	1	NAG	O5-C1	5.99	1.53	1.43
7	d	1	NAG	O5-C1	5.96	1.53	1.43
7	X	1	NAG	O5-C1	5.91	1.53	1.43
7	l	1	NAG	O5-C1	5.88	1.53	1.43
7	e	1	NAG	O5-C1	5.87	1.53	1.43
9	c	1	NAG	O5-C1	5.58	1.53	1.43
9	V	1	NAG	O5-C1	5.57	1.53	1.43
9	j	1	NAG	O5-C1	5.53	1.53	1.43
9	j	5	MAN	O2-C2	-4.37	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	5	MAN	O2-C2	-4.36	1.34	1.43
9	V	5	MAN	O2-C2	-4.35	1.34	1.43
8	h	3	BMA	O2-C2	-4.26	1.34	1.43
8	T	3	BMA	O2-C2	-4.25	1.34	1.43
8	a	3	BMA	O2-C2	-4.24	1.34	1.43
9	V	6	MAN	O2-C2	-4.24	1.34	1.43
9	j	6	MAN	O2-C2	-4.24	1.34	1.43
9	c	6	MAN	O2-C2	-4.20	1.34	1.43
9	j	3	BMA	O2-C2	-4.18	1.34	1.43
9	V	3	BMA	O2-C2	-4.17	1.34	1.43
9	c	3	BMA	O2-C2	-4.15	1.34	1.43
8	h	5	MAN	O2-C2	-4.09	1.34	1.43
8	a	5	MAN	O2-C2	-4.08	1.34	1.43
8	T	5	MAN	O2-C2	-4.08	1.34	1.43
9	j	4	MAN	O2-C2	-3.28	1.36	1.43
9	V	4	MAN	O2-C2	-3.28	1.36	1.43
9	c	4	MAN	O2-C2	-3.27	1.36	1.43
8	T	4	MAN	O2-C2	-3.16	1.36	1.43
8	a	4	MAN	O2-C2	-3.15	1.36	1.43
8	h	4	MAN	O2-C2	-3.15	1.36	1.43
7	l	1	NAG	C4-C5	2.91	1.59	1.53
7	e	1	NAG	C4-C5	2.89	1.59	1.53
7	X	1	NAG	C4-C5	2.88	1.59	1.53
9	j	1	NAG	C3-C2	-2.73	1.46	1.52
9	c	1	NAG	C3-C2	-2.73	1.46	1.52
9	V	1	NAG	C3-C2	-2.73	1.46	1.52
7	f	1	NAG	C3-C2	-2.72	1.46	1.52
7	m	1	NAG	C3-C2	-2.72	1.46	1.52
7	Y	1	NAG	C3-C2	-2.68	1.46	1.52
8	a	2	NAG	C3-C2	-2.65	1.47	1.52
8	h	2	NAG	C3-C2	-2.64	1.47	1.52
8	T	2	NAG	C3-C2	-2.63	1.47	1.52
9	j	3	BMA	C2-C3	-2.60	1.48	1.52
9	c	3	BMA	C2-C3	-2.59	1.48	1.52
9	V	3	BMA	C2-C3	-2.58	1.48	1.52
9	j	2	NAG	C3-C2	-2.55	1.47	1.52
9	c	2	NAG	C3-C2	-2.55	1.47	1.52
9	V	2	NAG	C3-C2	-2.52	1.47	1.52
7	d	1	NAG	C3-C2	-2.51	1.47	1.52
7	W	1	NAG	C3-C2	-2.50	1.47	1.52
7	i	1	NAG	C3-C2	-2.49	1.47	1.52
7	k	1	NAG	C3-C2	-2.48	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	2	NAG	C3-C2	-2.48	1.47	1.52
8	a	3	BMA	C2-C3	-2.47	1.48	1.52
7	l	1	NAG	C3-C2	-2.47	1.47	1.52
7	S	2	NAG	C3-C2	-2.47	1.47	1.52
7	b	1	NAG	C3-C2	-2.47	1.47	1.52
7	Z	2	NAG	C3-C2	-2.46	1.47	1.52
7	U	1	NAG	C3-C2	-2.45	1.47	1.52
8	h	3	BMA	C2-C3	-2.45	1.48	1.52
8	T	3	BMA	C2-C3	-2.45	1.48	1.52
7	X	1	NAG	C3-C2	-2.44	1.47	1.52
7	e	1	NAG	C3-C2	-2.43	1.47	1.52
7	W	2	NAG	C3-C2	-2.42	1.47	1.52
7	k	2	NAG	C3-C2	-2.42	1.47	1.52
7	Z	1	NAG	C3-C2	-2.42	1.47	1.52
7	d	2	NAG	C3-C2	-2.41	1.47	1.52
7	g	1	NAG	C3-C2	-2.39	1.47	1.52
7	S	1	NAG	C3-C2	-2.38	1.47	1.52
9	c	5	MAN	C2-C3	-2.36	1.48	1.52
9	j	5	MAN	C2-C3	-2.35	1.48	1.52
8	h	1	NAG	C3-C2	-2.34	1.47	1.52
7	X	2	NAG	C3-C2	-2.33	1.47	1.52
7	m	2	NAG	C3-C2	-2.33	1.47	1.52
8	T	1	NAG	C3-C2	-2.33	1.47	1.52
9	V	5	MAN	C2-C3	-2.32	1.48	1.52
7	l	2	NAG	C3-C2	-2.32	1.47	1.52
8	a	1	NAG	C3-C2	-2.31	1.47	1.52
7	e	2	NAG	C3-C2	-2.31	1.47	1.52
9	c	6	MAN	C2-C3	-2.30	1.49	1.52
7	Y	2	NAG	C3-C2	-2.30	1.47	1.52
7	f	2	NAG	C3-C2	-2.30	1.47	1.52
7	k	1	NAG	C1-C2	-2.28	1.49	1.52
7	l	1	NAG	C4-C3	2.28	1.58	1.52
7	d	1	NAG	C1-C2	-2.27	1.49	1.52
9	V	6	MAN	C2-C3	-2.26	1.49	1.52
7	W	1	NAG	C1-C2	-2.24	1.49	1.52
9	j	6	MAN	C2-C3	-2.23	1.49	1.52
7	X	1	NAG	C4-C3	2.23	1.58	1.52
7	e	1	NAG	C4-C3	2.23	1.58	1.52
7	U	2	NAG	C3-C2	-2.19	1.47	1.52
8	a	2	NAG	C1-C2	-2.18	1.49	1.52
7	i	2	NAG	C3-C2	-2.18	1.47	1.52
8	a	5	MAN	C2-C3	-2.15	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	2	NAG	C1-C2	-2.15	1.49	1.52
7	m	2	NAG	C1-C2	-2.14	1.49	1.52
7	Y	2	NAG	C1-C2	-2.14	1.49	1.52
8	T	5	MAN	C2-C3	-2.13	1.49	1.52
8	h	5	MAN	C2-C3	-2.12	1.49	1.52
7	b	1	NAG	C1-C2	-2.12	1.49	1.52
8	h	2	NAG	C1-C2	-2.12	1.49	1.52
7	U	1	NAG	C1-C2	-2.12	1.49	1.52
7	b	2	NAG	C3-C2	-2.12	1.48	1.52
7	f	2	NAG	C1-C2	-2.08	1.49	1.52
7	i	1	NAG	C1-C2	-2.08	1.49	1.52
9	j	2	NAG	C4-C3	2.07	1.57	1.52
8	a	4	MAN	C2-C3	-2.04	1.49	1.52
9	V	2	NAG	C4-C3	2.04	1.57	1.52
8	h	4	MAN	C2-C3	-2.03	1.49	1.52
7	f	1	NAG	C4-C3	2.02	1.57	1.52
7	m	1	NAG	C4-C3	2.01	1.57	1.52
8	T	4	MAN	C2-C3	-2.01	1.49	1.52
7	g	1	NAG	C1-C2	-2.01	1.49	1.52
7	Y	1	NAG	C4-C3	2.01	1.57	1.52
9	c	2	NAG	C4-C3	2.01	1.57	1.52
7	Z	1	NAG	C1-C2	-2.00	1.49	1.52
7	S	1	NAG	C1-C2	-2.00	1.49	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	1	NAG	O4-C4-C3	-5.01	98.57	110.38
7	l	1	NAG	O4-C4-C3	-5.00	98.58	110.38
7	e	1	NAG	O4-C4-C3	-5.00	98.59	110.38
7	l	1	NAG	O5-C5-C6	-4.61	98.69	107.66
7	e	1	NAG	O5-C5-C6	-4.60	98.71	107.66
7	X	1	NAG	O5-C5-C6	-4.60	98.72	107.66
7	l	1	NAG	O4-C4-C5	4.24	119.78	109.32
7	e	1	NAG	O4-C4-C5	4.24	119.76	109.32
7	X	1	NAG	O4-C4-C5	4.24	119.76	109.32
7	e	1	NAG	C4-C3-C2	3.95	116.81	111.02
7	l	1	NAG	C3-C4-C5	-3.95	103.07	110.23
7	X	1	NAG	C4-C3-C2	3.95	116.80	111.02
7	l	1	NAG	C4-C3-C2	3.94	116.79	111.02
7	e	1	NAG	C3-C4-C5	-3.90	103.16	110.23
7	X	1	NAG	C3-C4-C5	-3.90	103.17	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	1	NAG	C3-C4-C5	-3.77	103.40	110.23
7	S	1	NAG	C3-C4-C5	-3.75	103.44	110.23
7	Z	1	NAG	C3-C4-C5	-3.74	103.44	110.23
7	Y	1	NAG	C1-O5-C5	-2.73	108.53	112.19
9	V	1	NAG	O5-C5-C6	-2.73	102.36	107.66
7	f	1	NAG	C1-O5-C5	-2.72	108.53	112.19
9	c	1	NAG	O5-C5-C6	-2.72	102.36	107.66
8	T	3	BMA	C2-C3-C4	-2.72	106.07	110.86
8	h	3	BMA	C2-C3-C4	-2.71	106.09	110.86
9	j	1	NAG	O5-C5-C6	-2.71	102.38	107.66
7	m	1	NAG	C1-O5-C5	-2.71	108.56	112.19
8	a	3	BMA	C2-C3-C4	-2.70	106.11	110.86
9	c	3	BMA	C2-C3-C4	-2.62	106.26	110.86
9	V	3	BMA	C2-C3-C4	-2.60	106.29	110.86
9	j	3	BMA	C2-C3-C4	-2.60	106.29	110.86
7	k	1	NAG	C1-O5-C5	-2.59	108.71	112.19
7	W	1	NAG	C1-O5-C5	-2.59	108.72	112.19
7	d	1	NAG	C1-O5-C5	-2.57	108.74	112.19
9	V	1	NAG	C1-O5-C5	-2.55	108.77	112.19
9	c	1	NAG	C1-O5-C5	-2.54	108.78	112.19
8	T	1	NAG	C3-C4-C5	-2.53	105.64	110.23
9	j	1	NAG	C1-O5-C5	-2.52	108.80	112.19
8	a	1	NAG	C3-C4-C5	-2.51	105.68	110.23
8	h	1	NAG	C3-C4-C5	-2.51	105.69	110.23
7	d	1	NAG	C3-C4-C5	-2.50	105.70	110.23
7	k	1	NAG	C3-C4-C5	-2.49	105.71	110.23
7	W	1	NAG	C3-C4-C5	-2.48	105.73	110.23
7	U	1	NAG	C1-O5-C5	-2.32	109.08	112.19
7	U	1	NAG	C3-C4-C5	-2.32	106.03	110.23
7	b	1	NAG	C1-O5-C5	-2.31	109.08	112.19
7	U	2	NAG	C4-C3-C2	-2.31	107.63	111.02
7	Y	2	NAG	C4-C3-C2	-2.31	107.64	111.02
7	b	2	NAG	C4-C3-C2	-2.30	107.64	111.02
7	m	2	NAG	C4-C3-C2	-2.30	107.65	111.02
7	i	1	NAG	C3-C4-C5	-2.29	106.07	110.23
7	i	1	NAG	C1-O5-C5	-2.29	109.12	112.19
7	f	2	NAG	C4-C3-C2	-2.28	107.67	111.02
7	b	1	NAG	C3-C4-C5	-2.28	106.09	110.23
7	i	2	NAG	C4-C3-C2	-2.27	107.69	111.02
7	k	2	NAG	C4-C3-C2	-2.25	107.71	111.02
8	T	5	MAN	C2-C3-C4	-2.25	106.90	110.86
7	d	2	NAG	C4-C3-C2	-2.25	107.73	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	5	MAN	C2-C3-C4	-2.23	106.94	110.86
7	W	2	NAG	C4-C3-C2	-2.23	107.75	111.02
8	h	5	MAN	C2-C3-C4	-2.22	106.95	110.86
9	V	6	MAN	C2-C3-C4	-2.21	106.97	110.86
9	j	6	MAN	C2-C3-C4	-2.21	106.97	110.86
9	c	6	MAN	C2-C3-C4	-2.20	106.99	110.86
9	j	2	NAG	C3-C4-C5	-2.15	106.34	110.23
9	c	2	NAG	C3-C4-C5	-2.14	106.35	110.23
9	V	2	NAG	C3-C4-C5	-2.12	106.38	110.23
9	c	1	NAG	C3-C4-C5	-2.04	106.54	110.23
9	V	1	NAG	C3-C4-C5	-2.03	106.55	110.23
8	T	4	MAN	C2-C3-C4	-2.03	107.29	110.86
9	j	1	NAG	C3-C4-C5	-2.03	106.55	110.23
8	a	4	MAN	C2-C3-C4	-2.02	107.31	110.86
8	h	4	MAN	C2-C3-C4	-2.01	107.32	110.86

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	3	BMA	C4-C5-C6-O6
9	c	3	BMA	C4-C5-C6-O6
9	j	3	BMA	C4-C5-C6-O6
9	V	5	MAN	O5-C5-C6-O6
9	c	5	MAN	O5-C5-C6-O6
9	j	5	MAN	O5-C5-C6-O6
8	T	5	MAN	C4-C5-C6-O6
8	h	5	MAN	C4-C5-C6-O6
8	a	5	MAN	C4-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
9	V	3	BMA	O5-C5-C6-O6
9	c	3	BMA	O5-C5-C6-O6
9	j	3	BMA	O5-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6
7	l	1	NAG	O5-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
7	l	1	NAG	C4-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	Y	2	NAG	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
7	f	2	NAG	O5-C5-C6-O6
7	k	2	NAG	O5-C5-C6-O6
7	m	2	NAG	O5-C5-C6-O6
8	T	5	MAN	O5-C5-C6-O6
8	a	5	MAN	O5-C5-C6-O6
8	h	5	MAN	O5-C5-C6-O6
8	T	3	BMA	O5-C5-C6-O6
8	a	3	BMA	O5-C5-C6-O6
8	h	3	BMA	O5-C5-C6-O6
9	V	5	MAN	C4-C5-C6-O6
9	c	5	MAN	C4-C5-C6-O6
9	j	5	MAN	C4-C5-C6-O6
9	V	6	MAN	O5-C5-C6-O6
9	c	6	MAN	O5-C5-C6-O6
9	j	6	MAN	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	e	2	NAG	O5-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
7	X	2	NAG	O5-C5-C6-O6
8	T	4	MAN	O5-C5-C6-O6
8	a	4	MAN	O5-C5-C6-O6
8	h	4	MAN	O5-C5-C6-O6
9	V	4	MAN	O5-C5-C6-O6
9	c	4	MAN	O5-C5-C6-O6
9	j	4	MAN	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	c	2	NAG	O5-C5-C6-O6
9	j	2	NAG	O5-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
7	k	2	NAG	C4-C5-C6-O6
7	d	2	NAG	C4-C5-C6-O6
7	f	2	NAG	C4-C5-C6-O6
7	m	2	NAG	C4-C5-C6-O6
7	Y	2	NAG	C4-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
7	i	2	NAG	C4-C5-C6-O6
9	c	1	NAG	C4-C5-C6-O6

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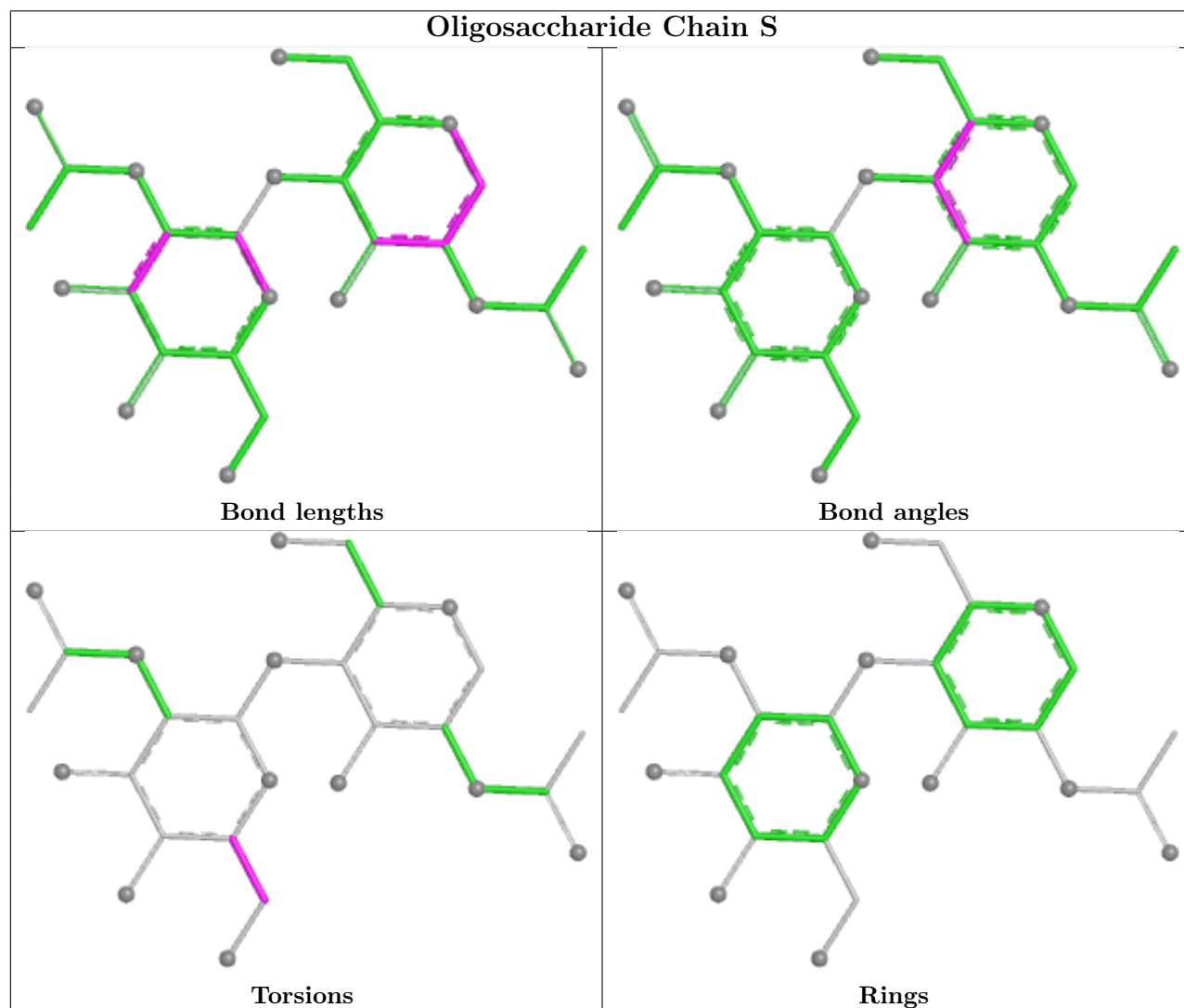
Mol	Chain	Res	Type	Atoms
9	V	1	NAG	C4-C5-C6-O6
9	j	1	NAG	C4-C5-C6-O6

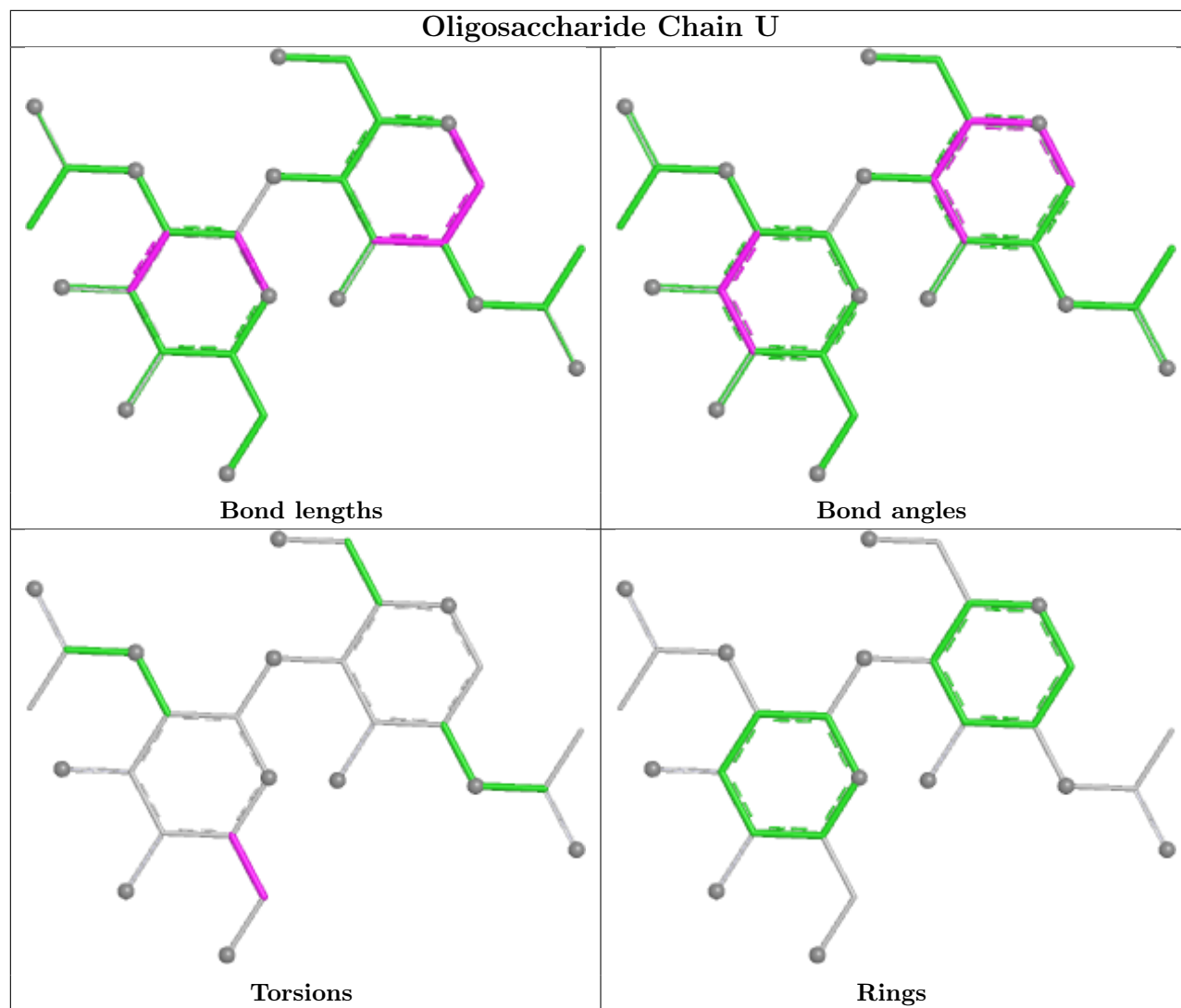
There are no ring outliers.

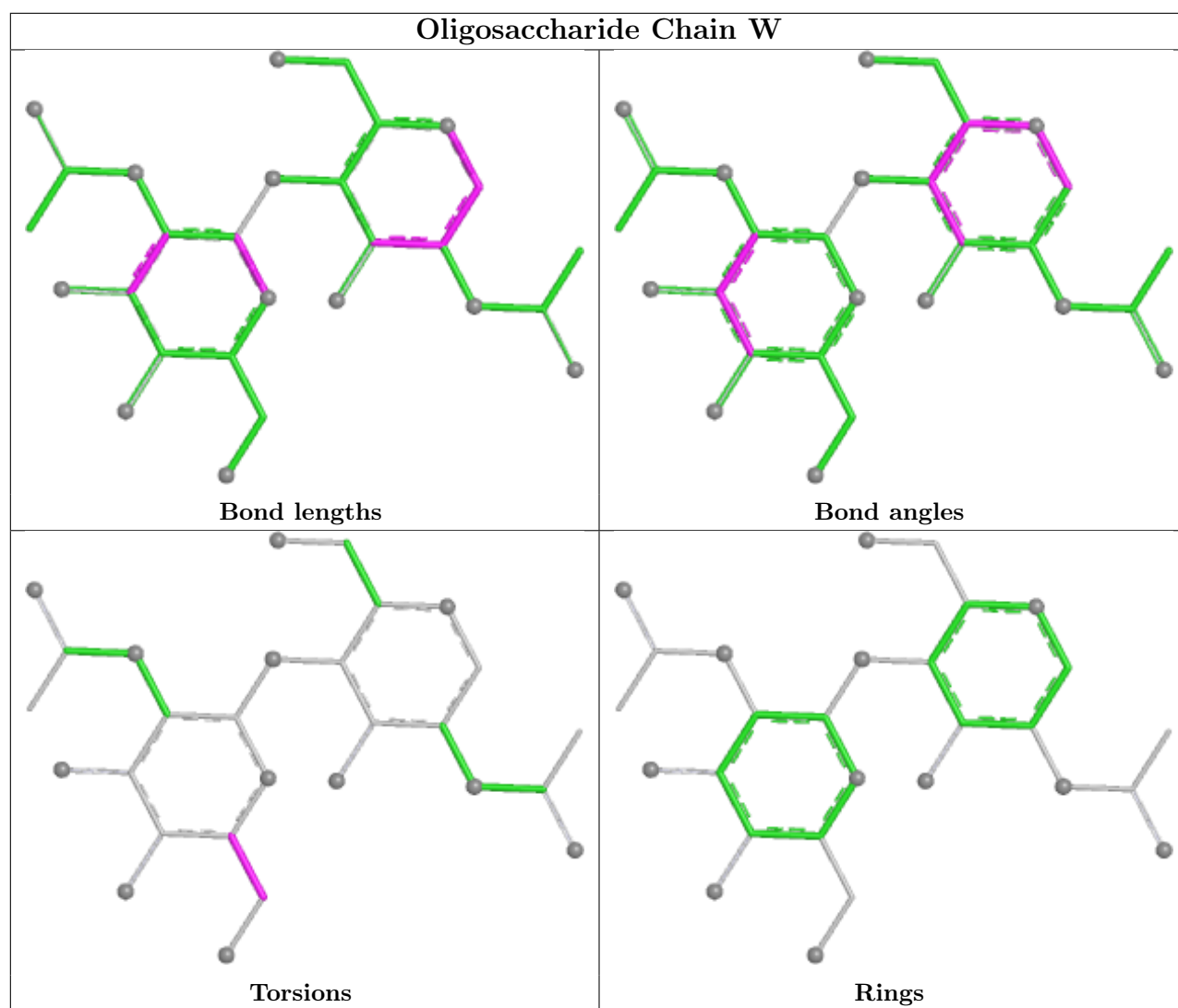
3 monomers are involved in 3 short contacts:

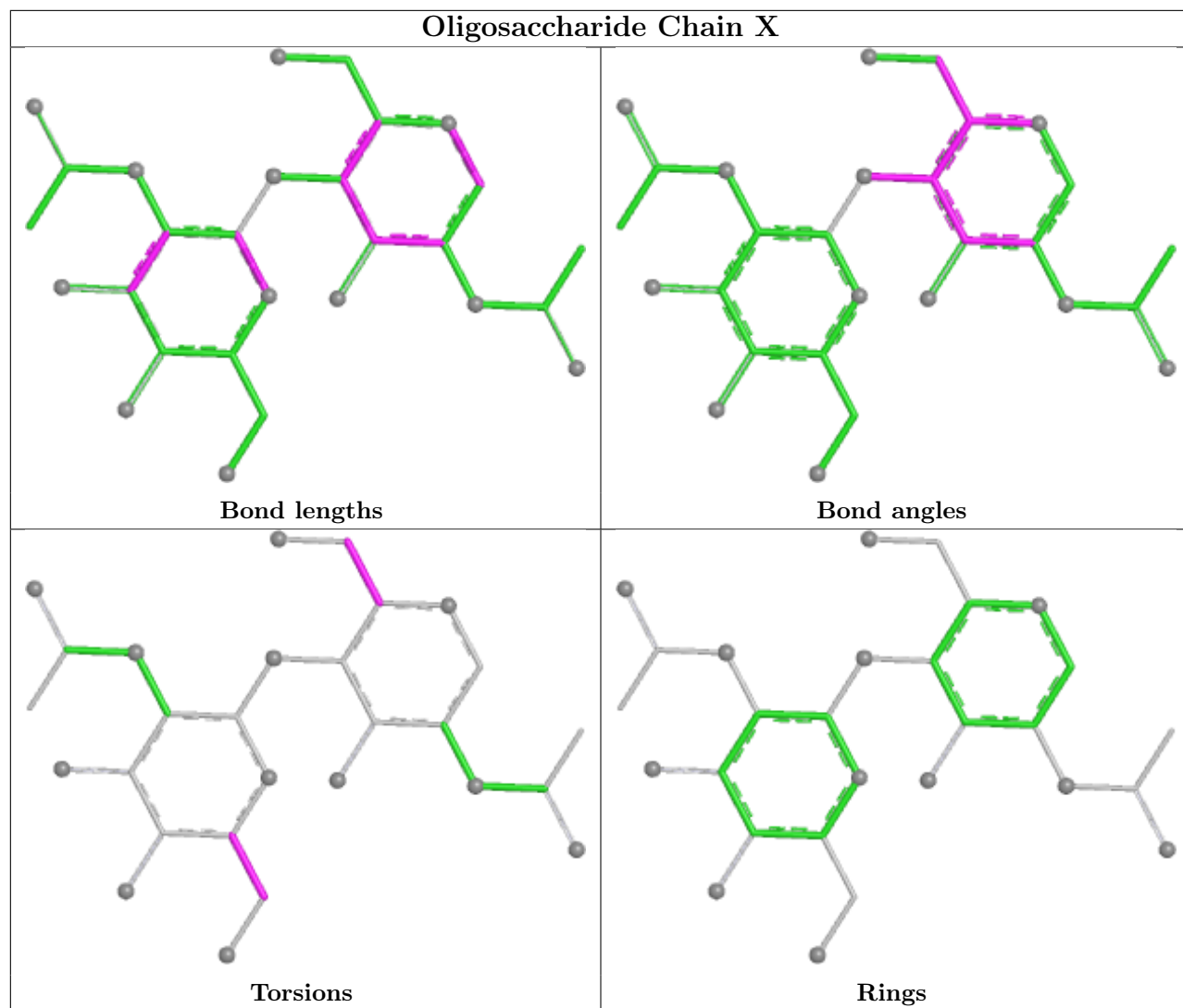
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	j	1	NAG	1	0
9	c	1	NAG	1	0
9	V	1	NAG	1	0

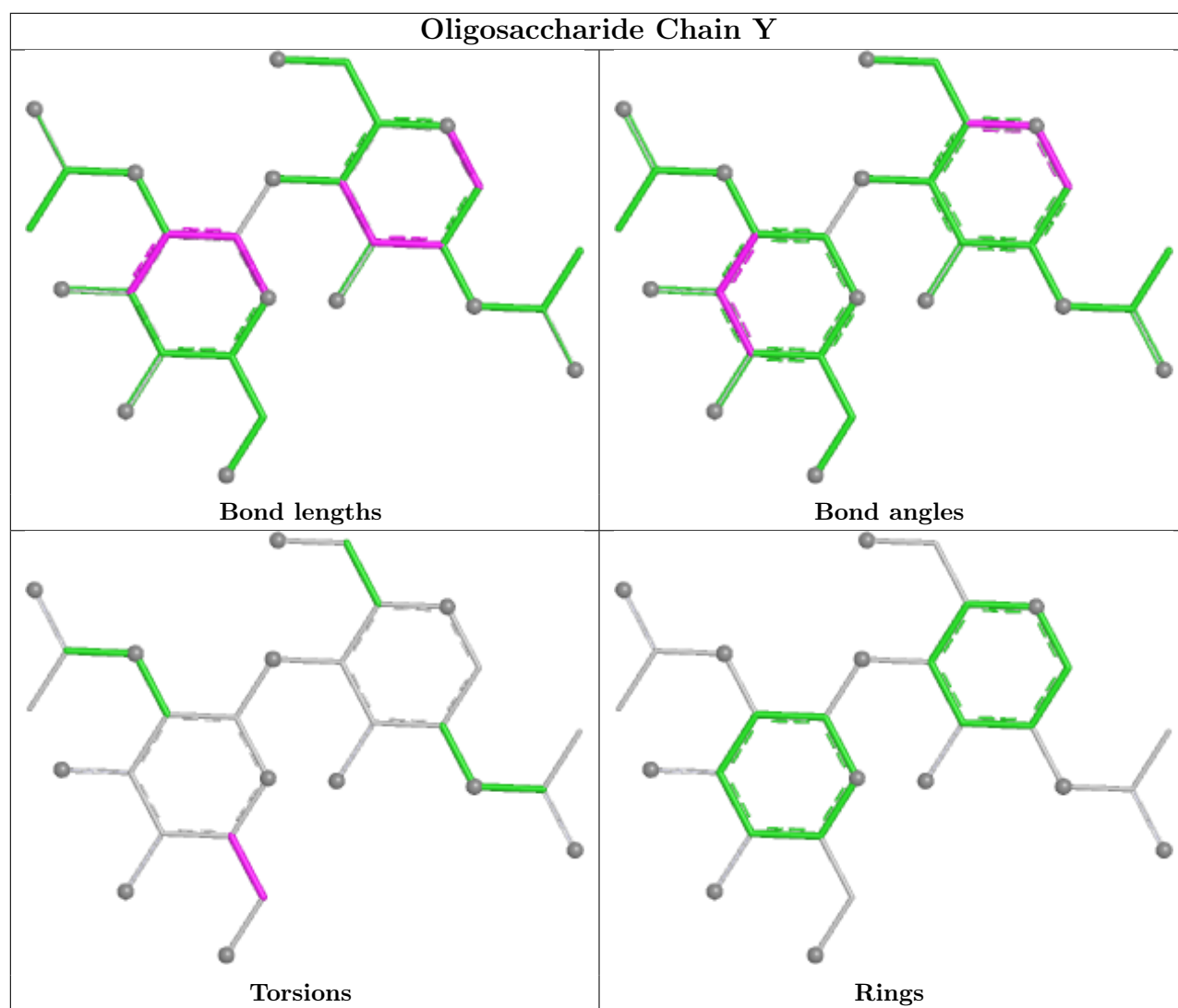
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

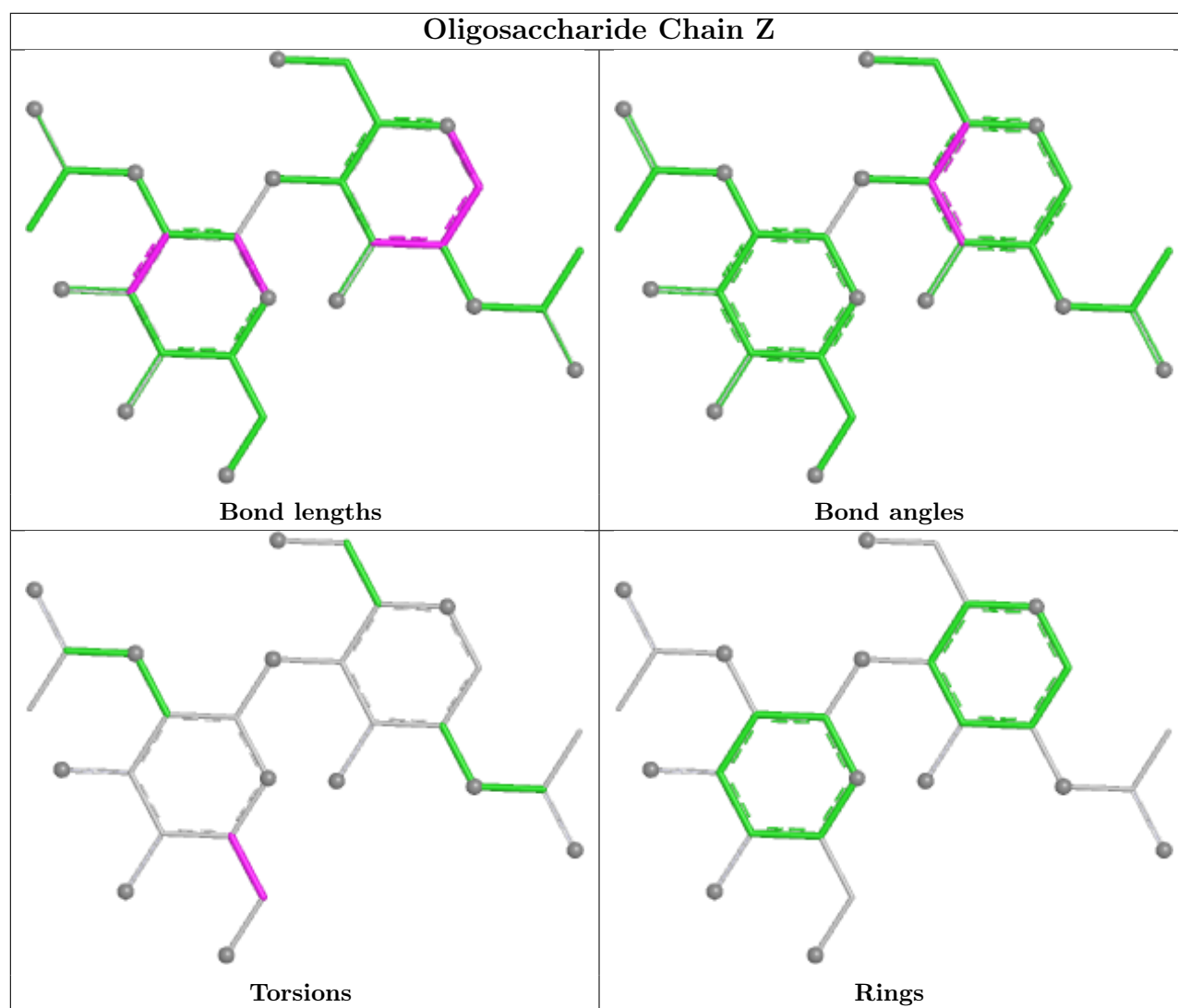


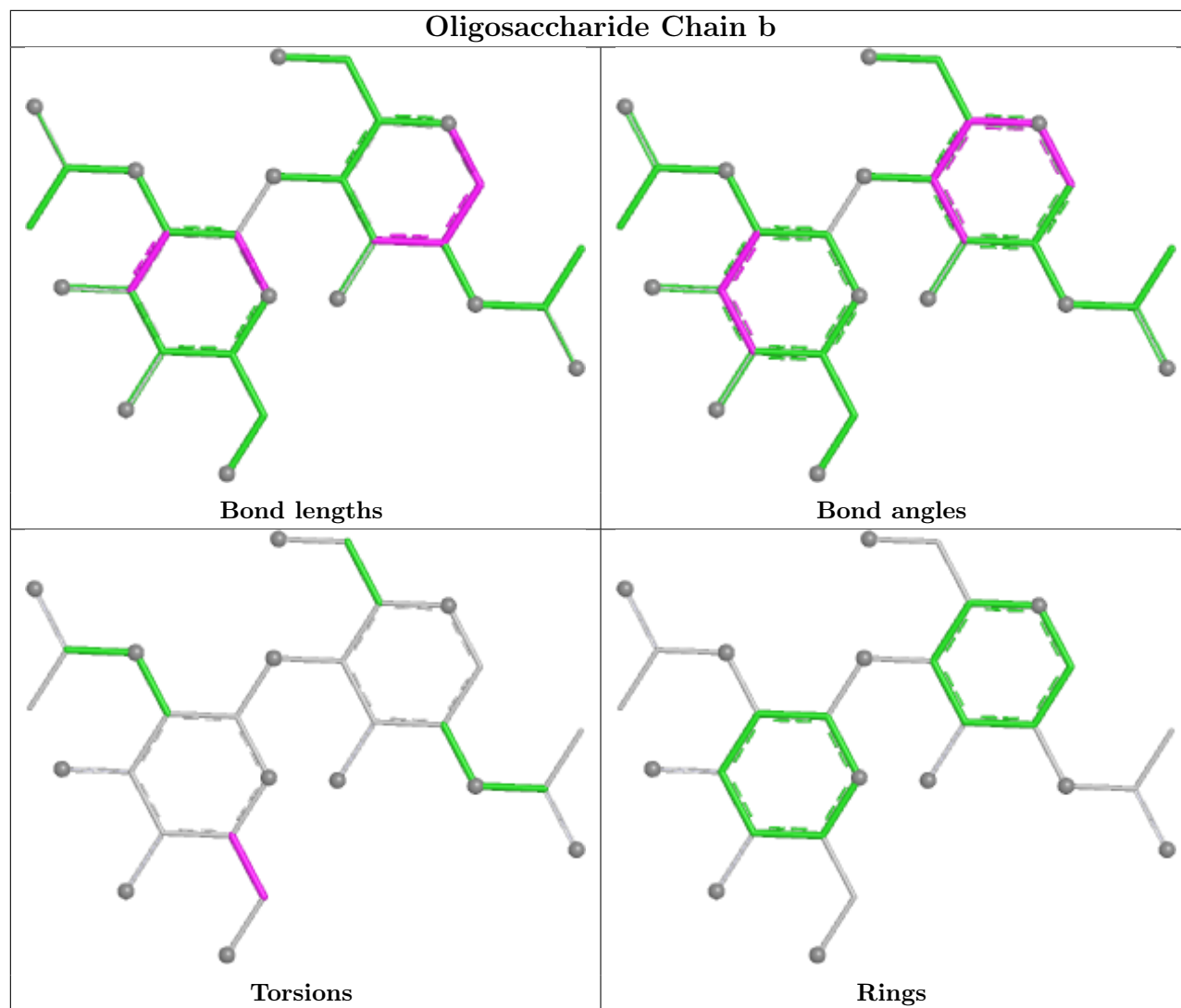


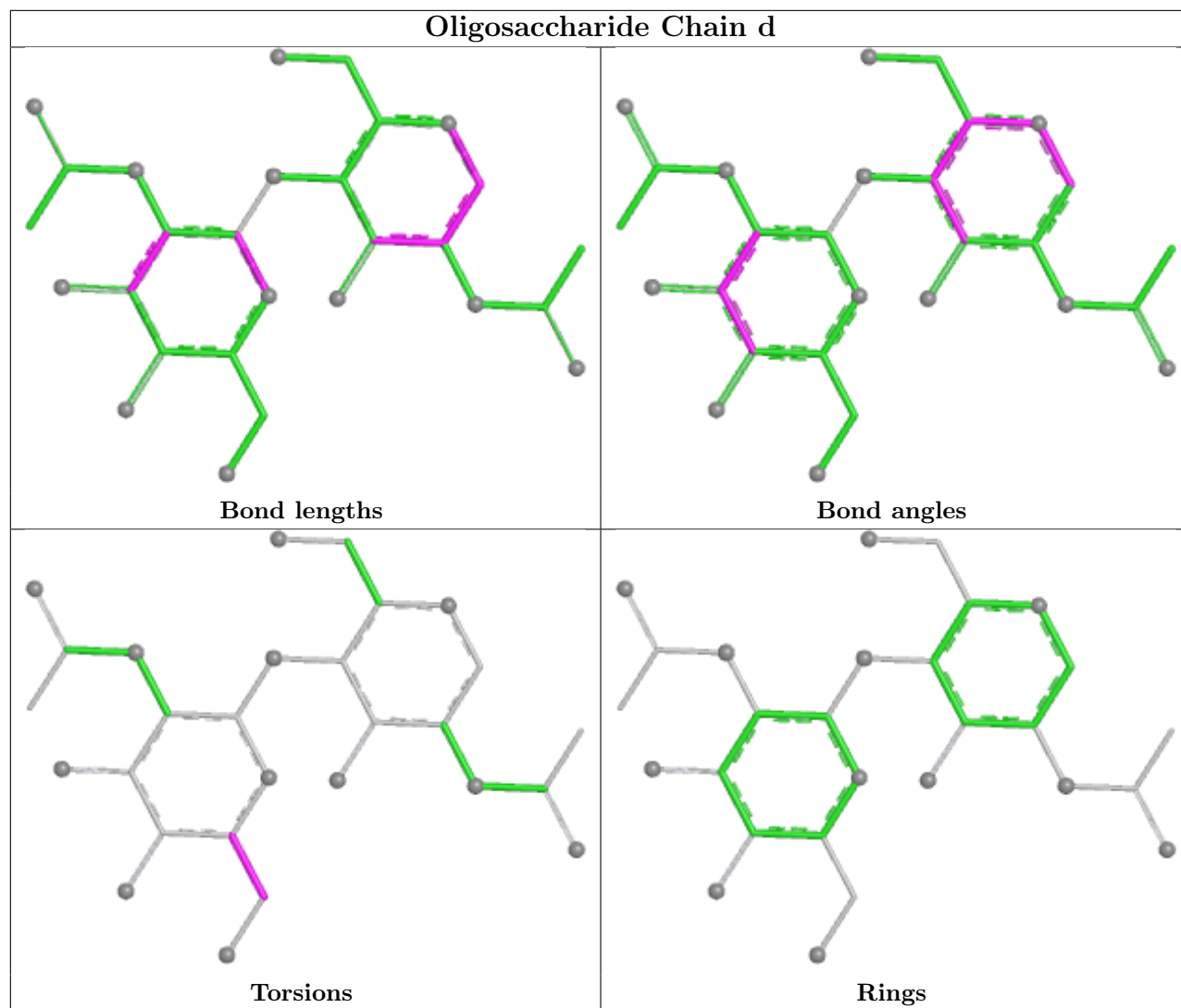


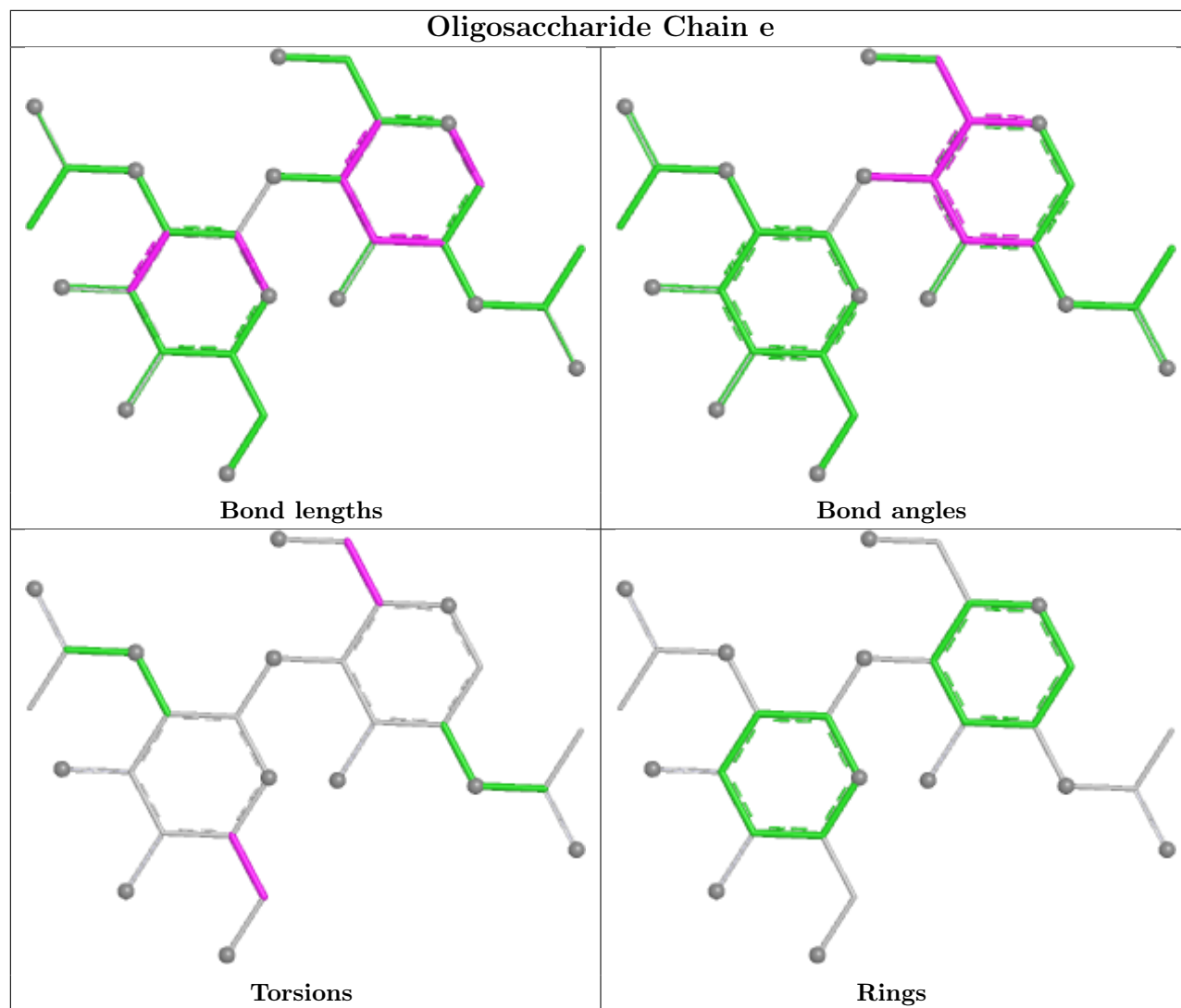


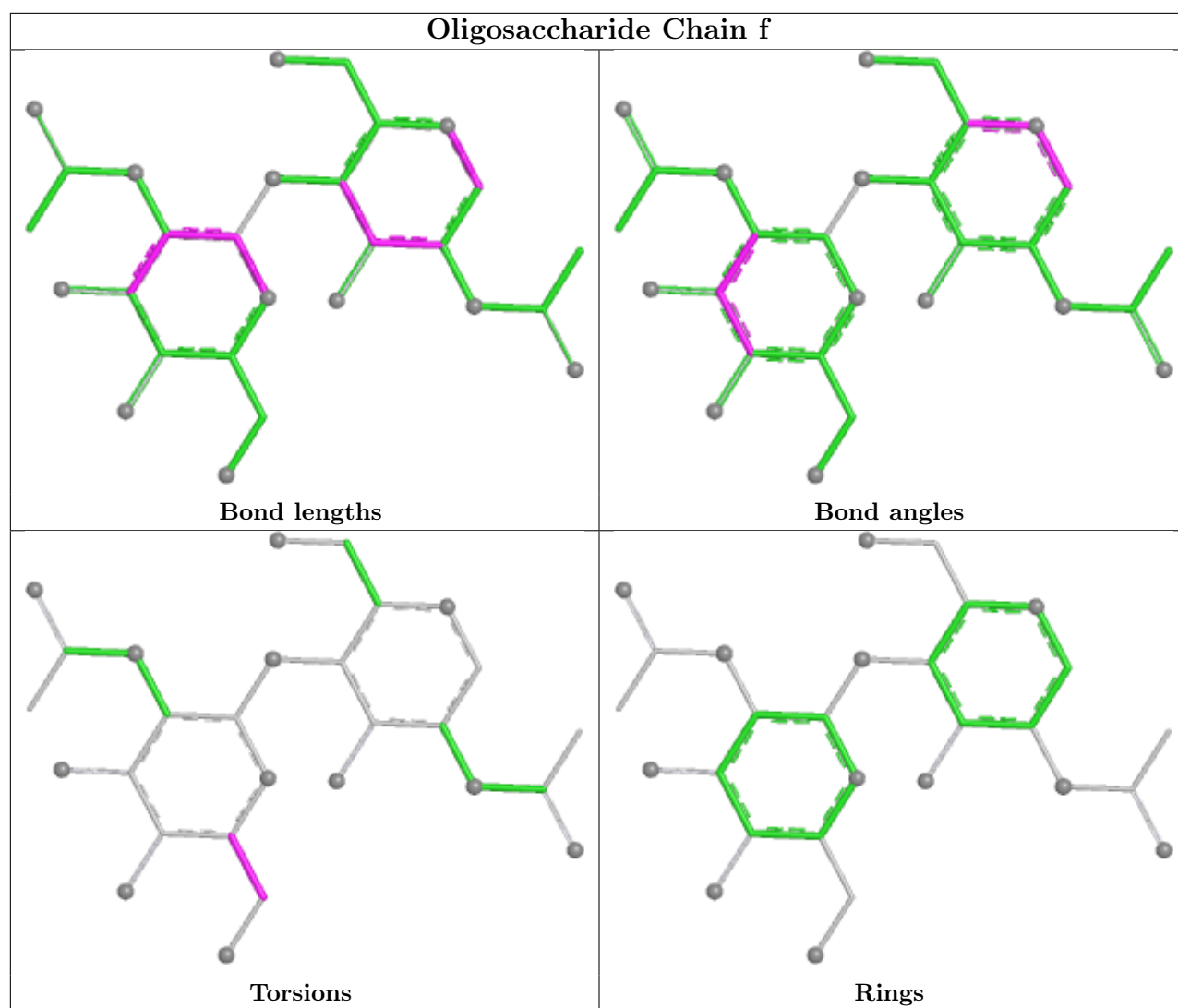


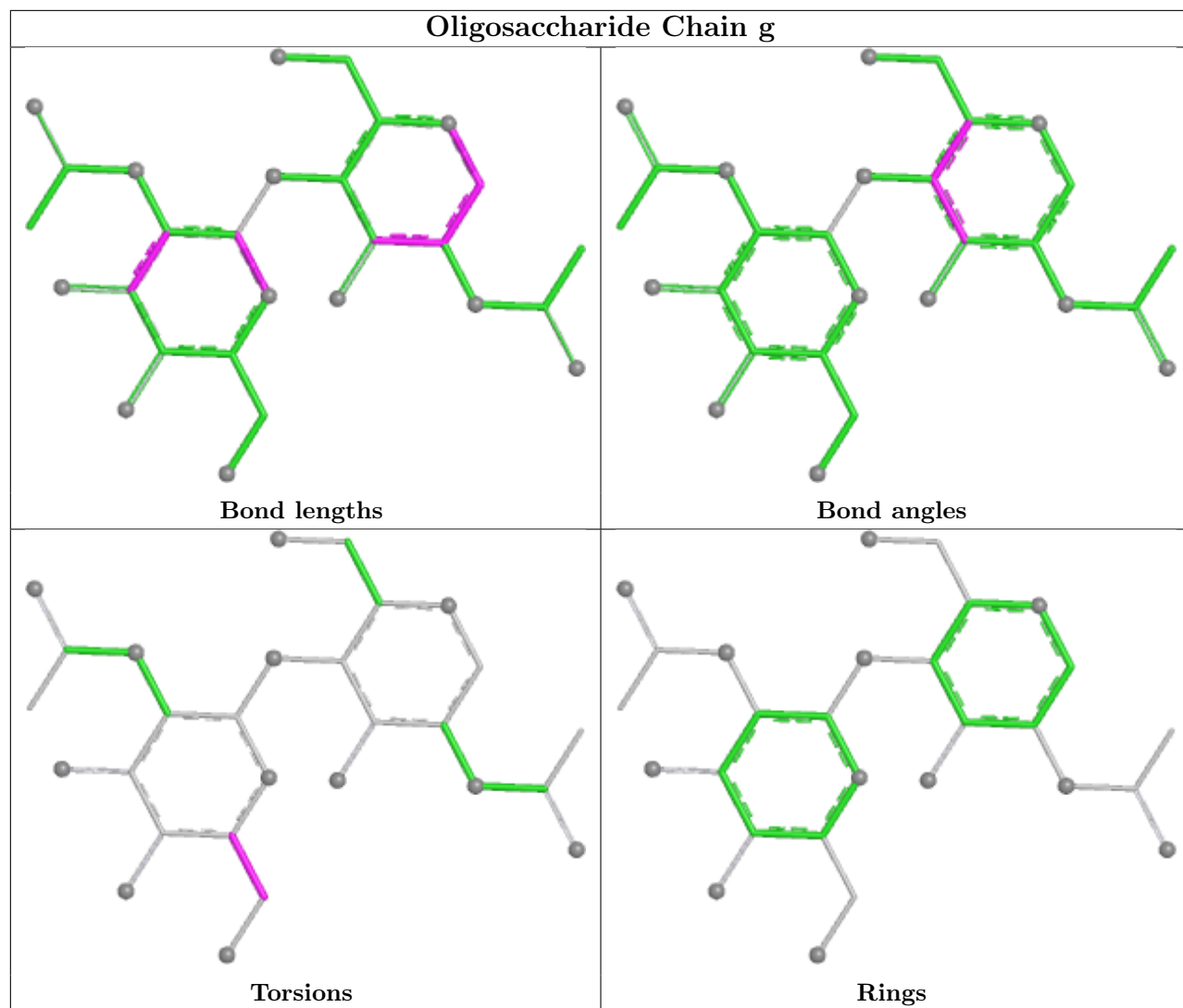


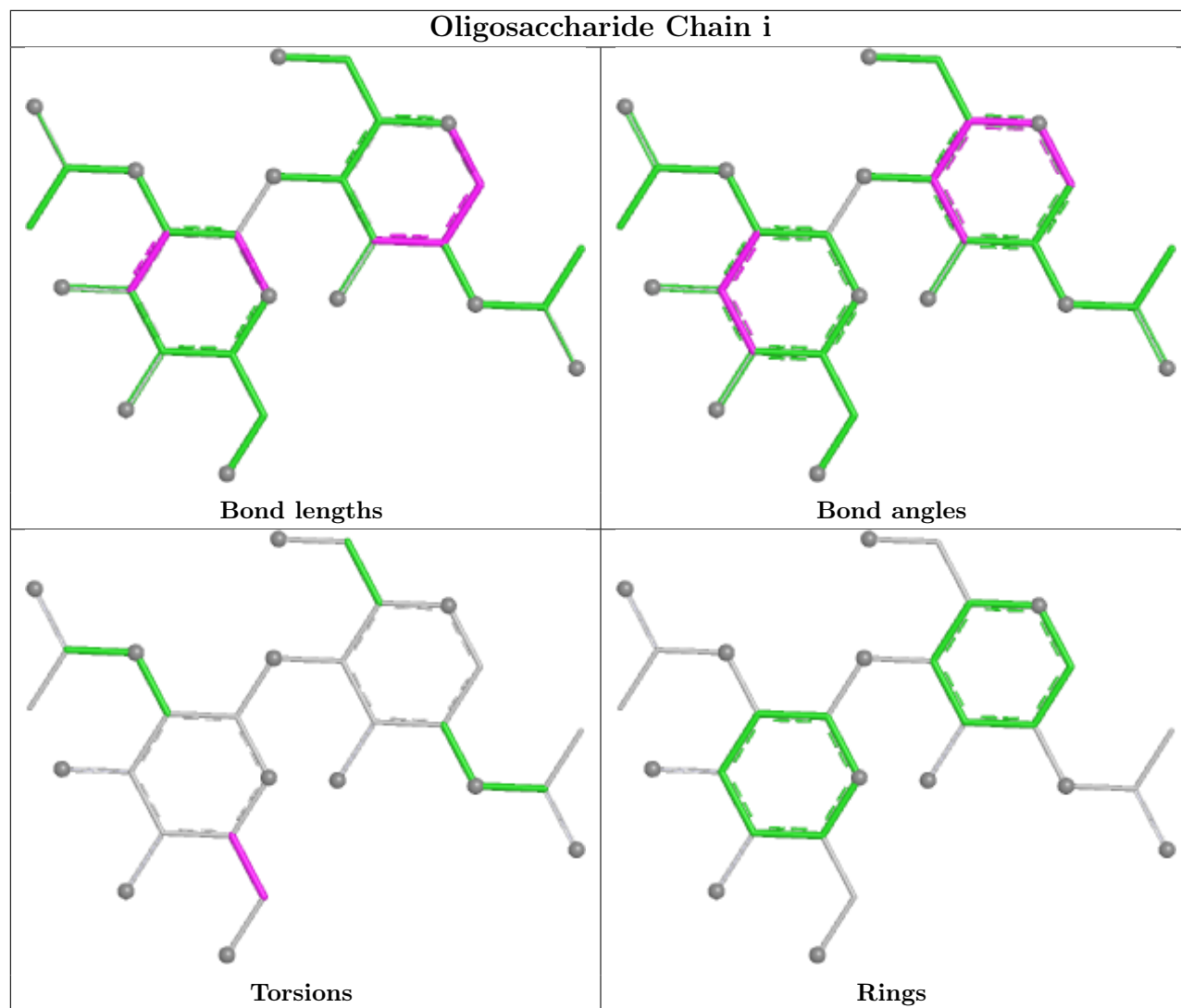


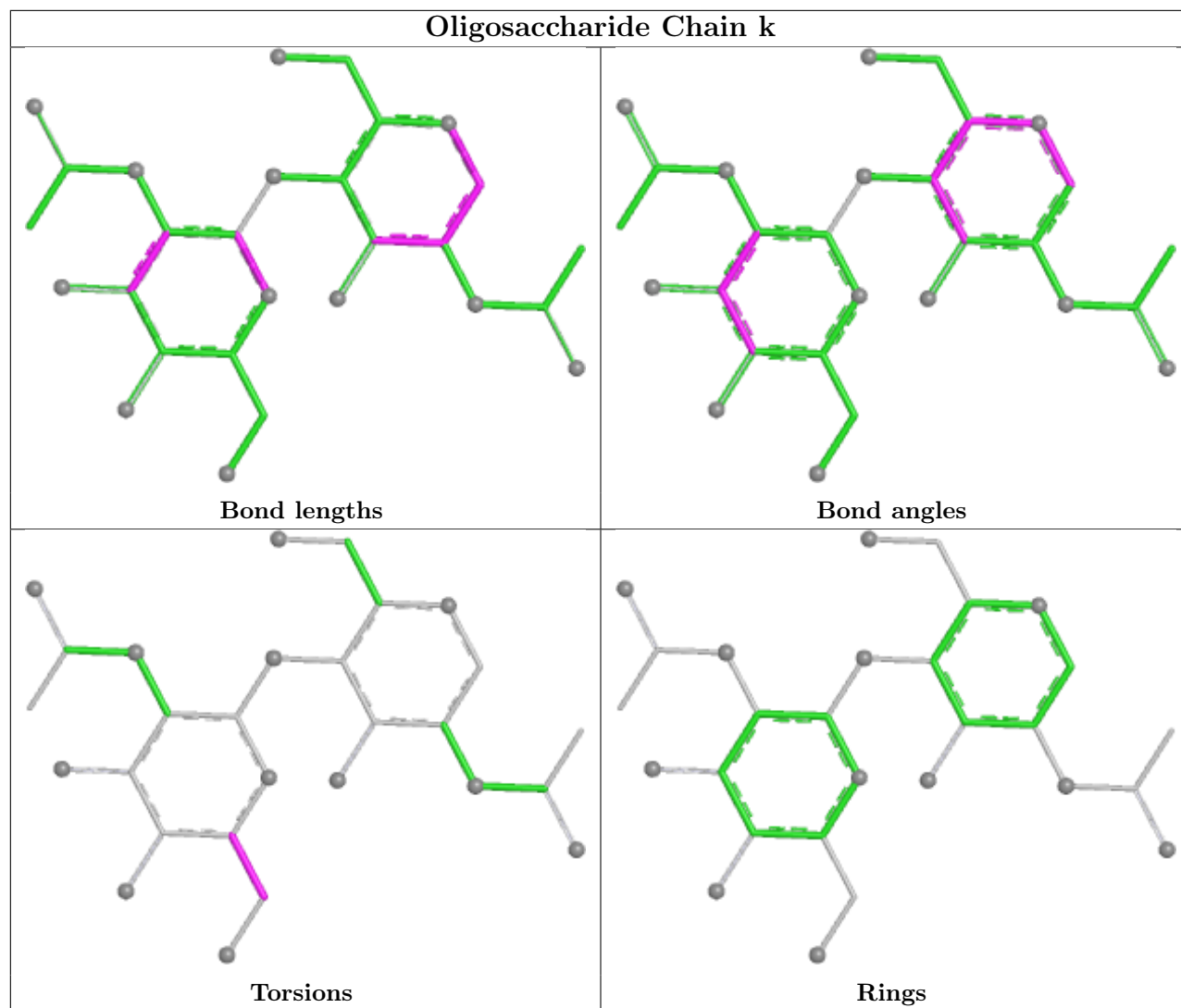


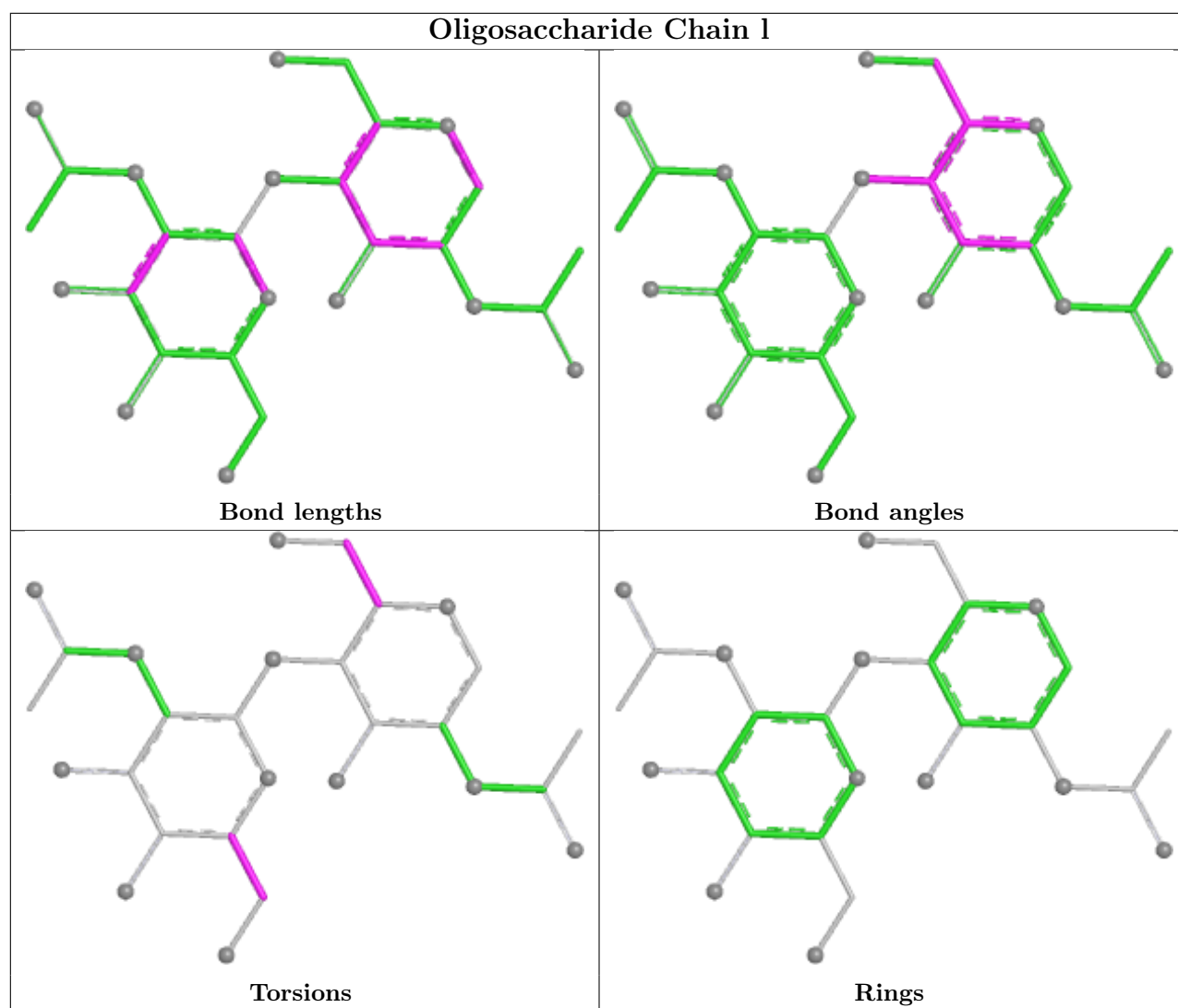


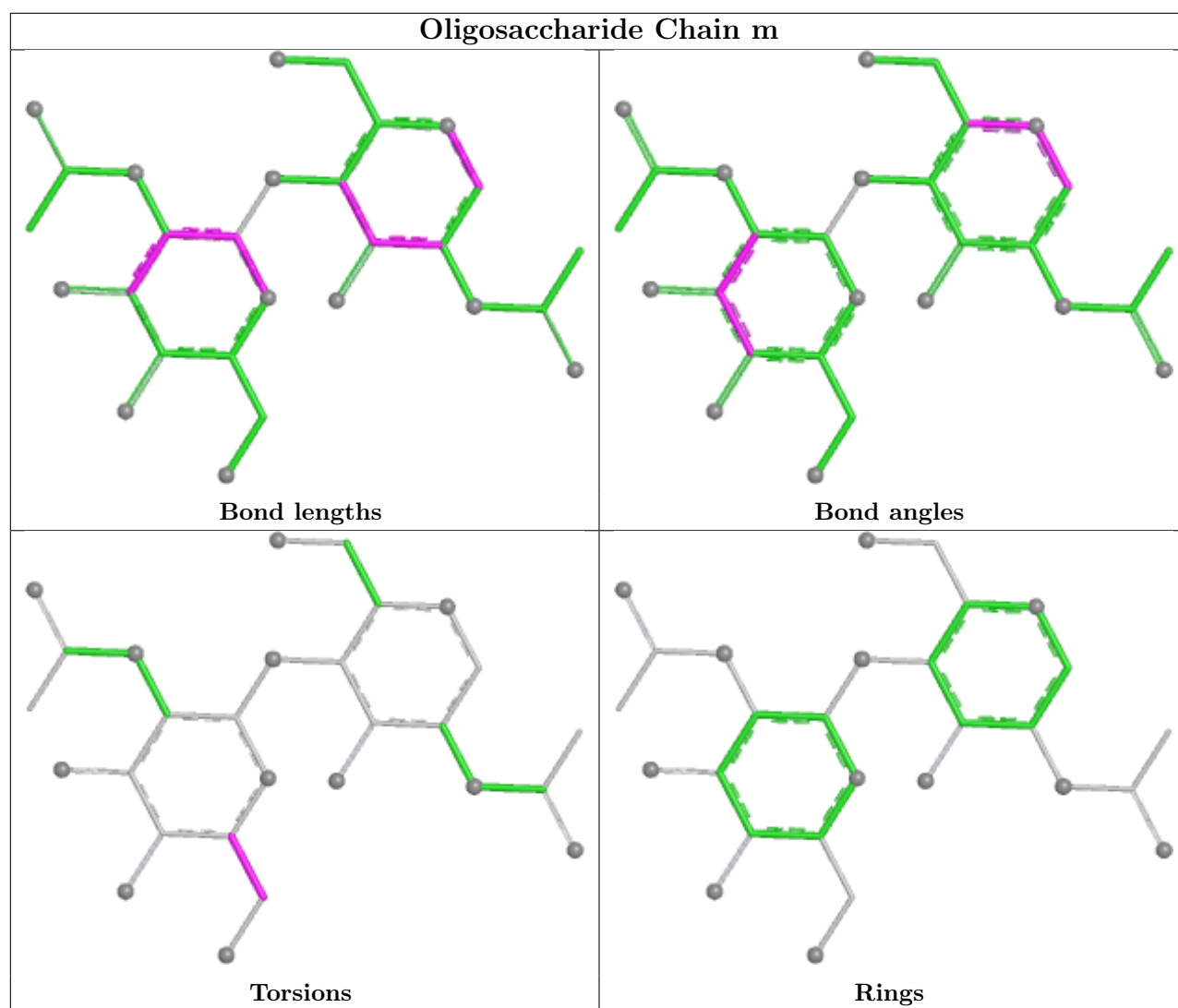


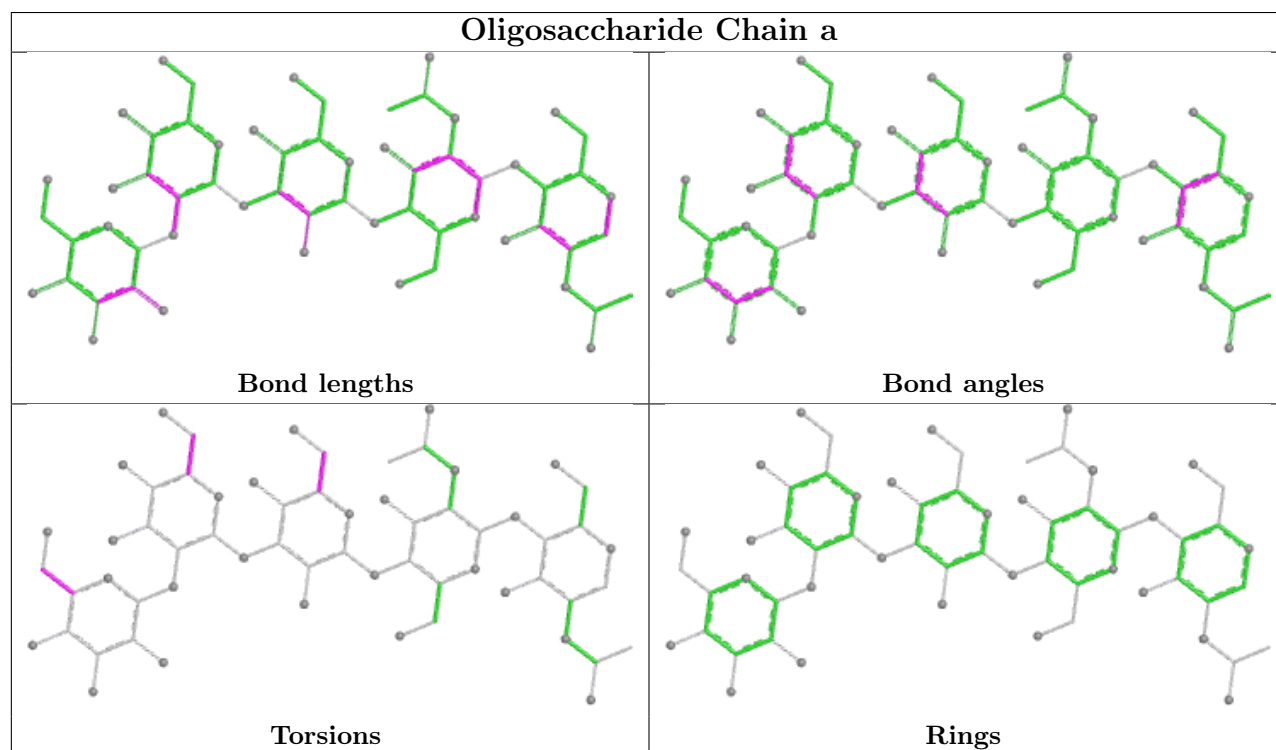
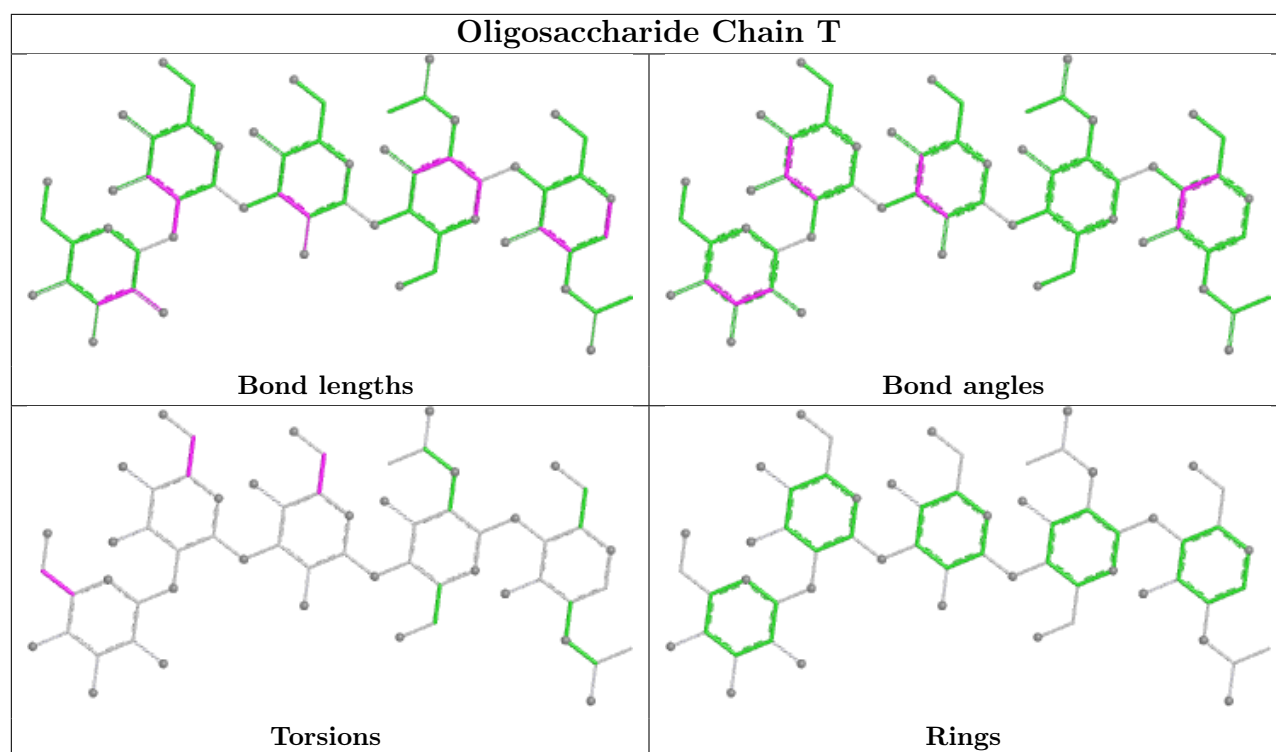


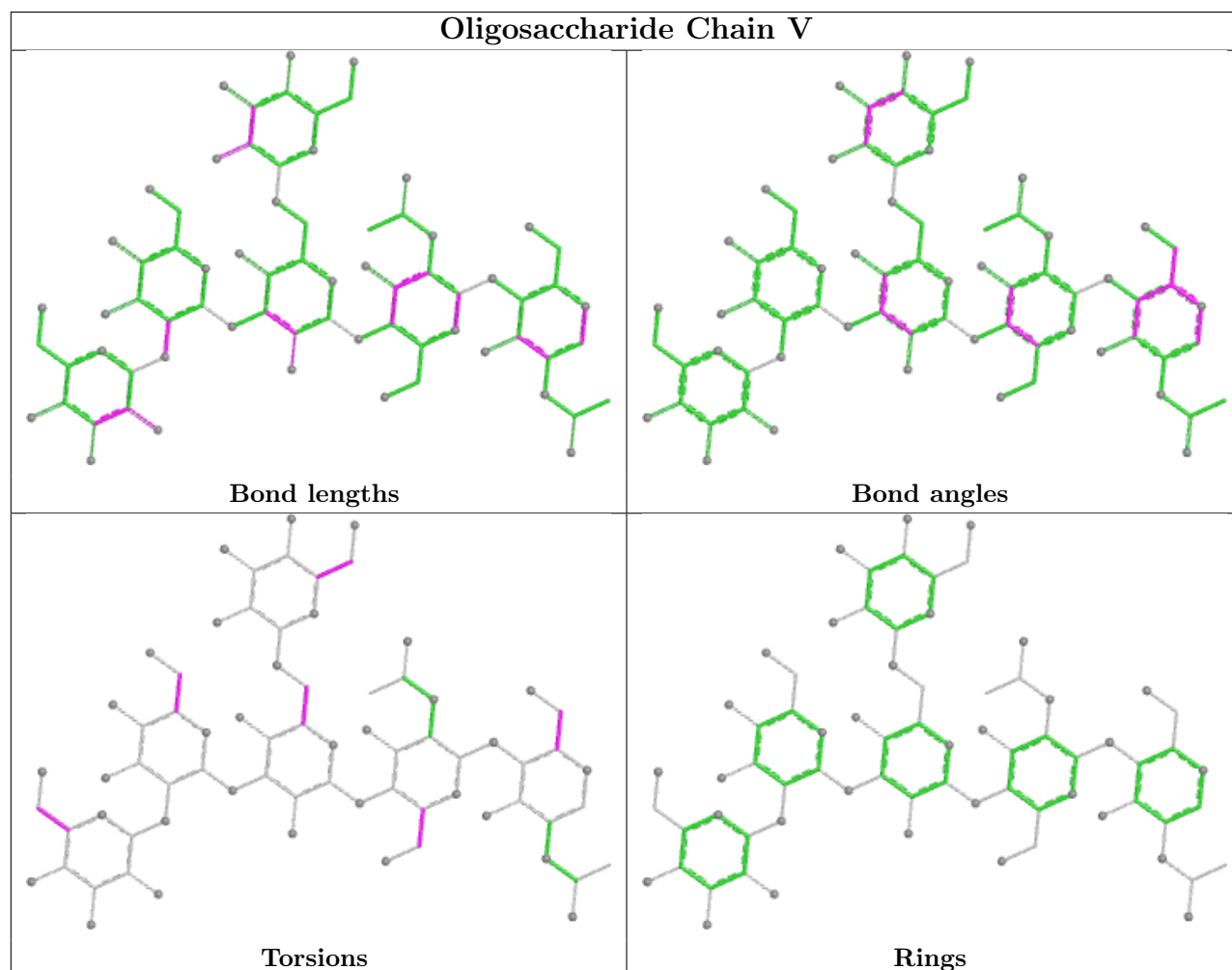
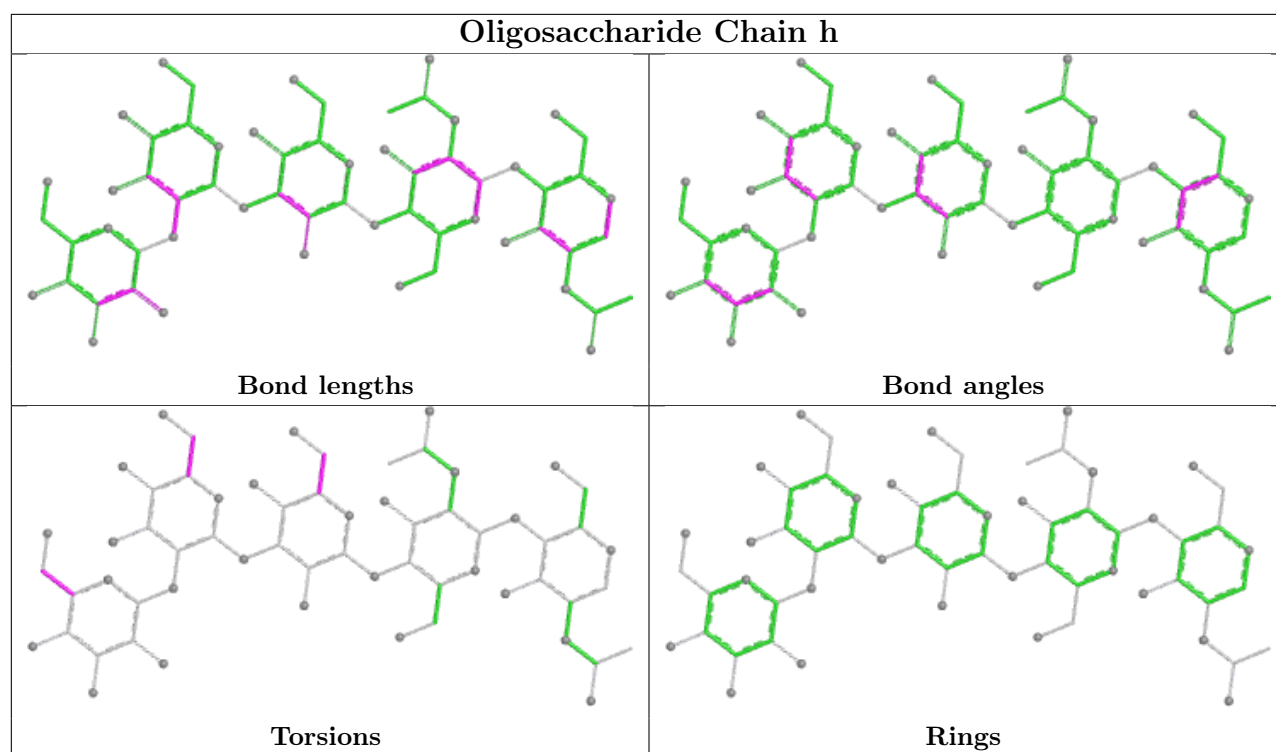


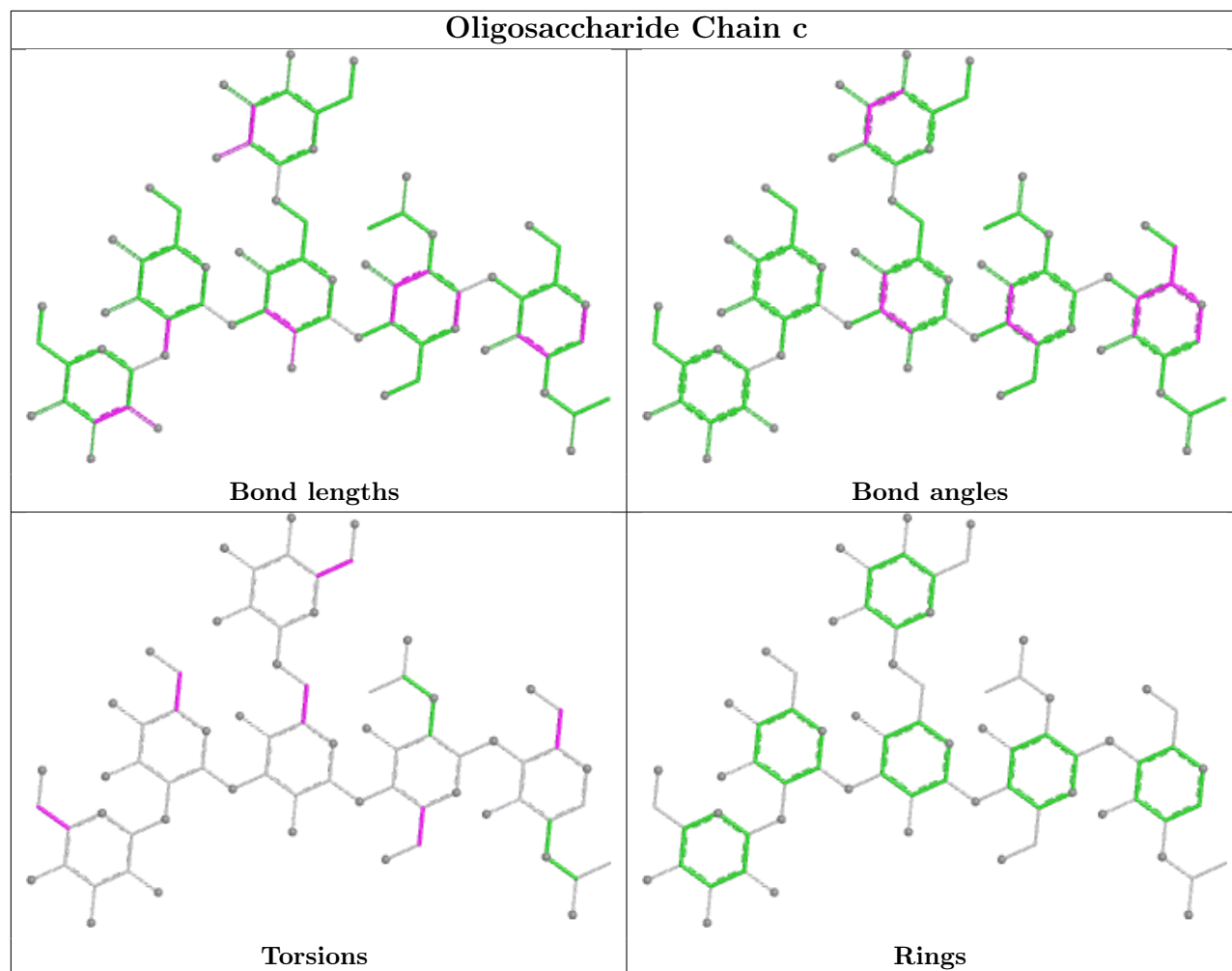


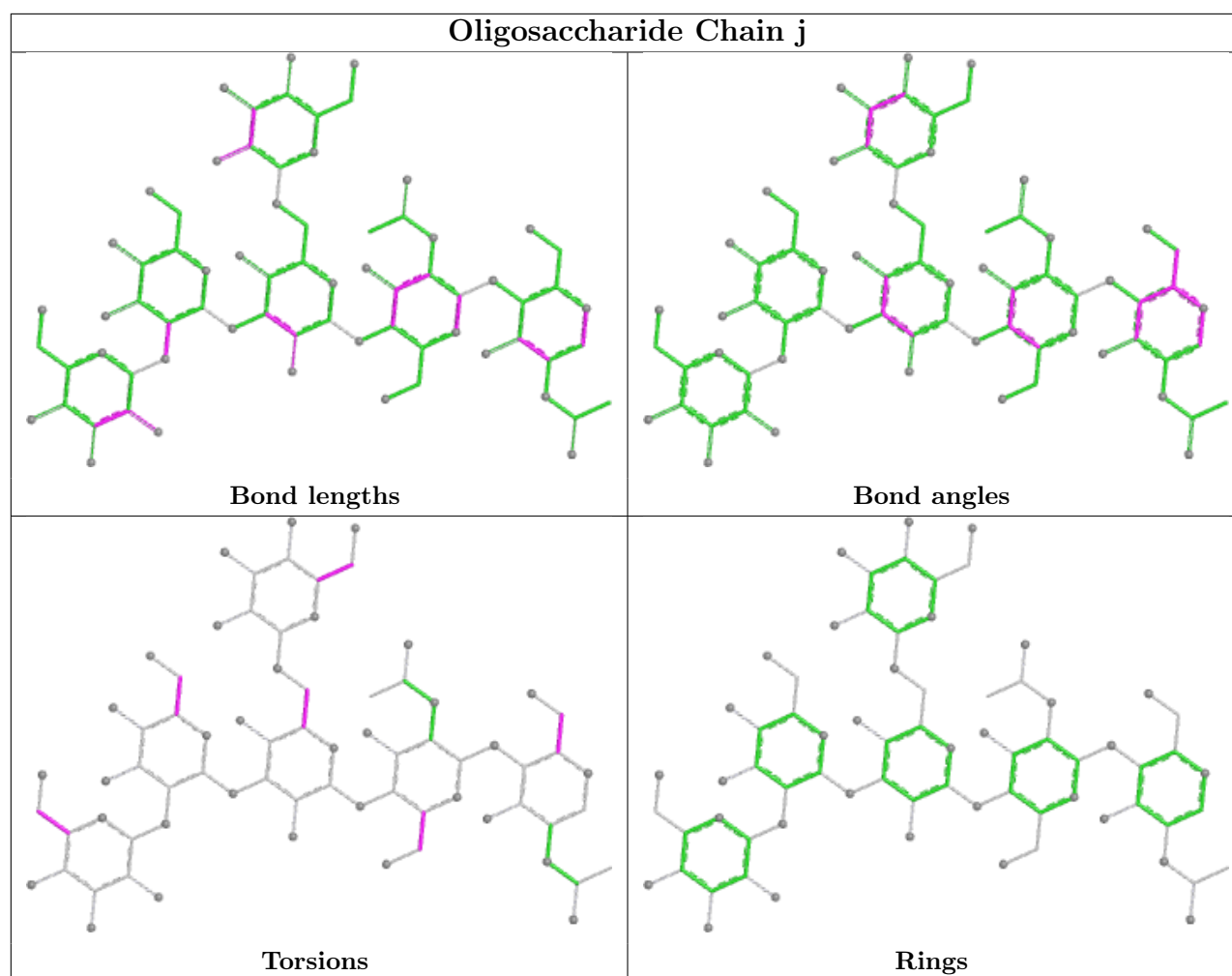












5.6 Ligand geometry [i](#)

33 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
10	NAG	D	703	2	14,14,15	2.06	2 (14%)	17,19,21	1.09	2 (11%)
10	NAG	C	603	1	14,14,15	2.08	2 (14%)	17,19,21	0.62	0
10	NAG	J	612	1	14,14,15	2.09	2 (14%)	17,19,21	0.76	0
10	NAG	J	619	1	14,14,15	2.02	2 (14%)	17,19,21	0.98	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	A	625	1	14,14,15	2.04	2 (14%)	17,19,21	0.87	1 (5%)
10	NAG	C	619	1	14,14,15	2.02	2 (14%)	17,19,21	0.98	2 (11%)
10	NAG	A	624	1	14,14,15	2.07	2 (14%)	17,19,21	0.87	0
10	NAG	J	603	1	14,14,15	2.07	2 (14%)	17,19,21	0.61	0
10	NAG	M	704	2	14,14,15	2.09	2 (14%)	17,19,21	0.89	1 (5%)
10	NAG	C	624	1	14,14,15	2.08	2 (14%)	17,19,21	0.88	0
10	NAG	M	703	2	14,14,15	2.06	2 (14%)	17,19,21	1.09	2 (11%)
10	NAG	C	623	1	14,14,15	2.12	2 (14%)	17,19,21	1.27	3 (17%)
10	NAG	C	604	1	14,14,15	2.06	2 (14%)	17,19,21	1.23	2 (11%)
10	NAG	A	619	1	14,14,15	2.03	2 (14%)	17,19,21	0.98	2 (11%)
10	NAG	A	628	1	14,14,15	2.03	2 (14%)	17,19,21	1.01	2 (11%)
10	NAG	A	623	1	14,14,15	2.13	2 (14%)	17,19,21	1.27	3 (17%)
10	NAG	J	625	1	14,14,15	2.04	2 (14%)	17,19,21	0.87	1 (5%)
10	NAG	C	628	1	14,14,15	2.03	2 (14%)	17,19,21	1.00	2 (11%)
10	NAG	A	622	1	14,14,15	2.06	2 (14%)	17,19,21	0.91	1 (5%)
10	NAG	C	622	1	14,14,15	2.05	2 (14%)	17,19,21	0.90	1 (5%)
10	NAG	A	612	1	14,14,15	2.08	2 (14%)	17,19,21	0.76	0
10	NAG	B	703	2	14,14,15	2.06	2 (14%)	17,19,21	1.09	2 (11%)
10	NAG	A	603	1	14,14,15	2.08	2 (14%)	17,19,21	0.61	0
10	NAG	D	704	2	14,14,15	2.08	2 (14%)	17,19,21	0.89	1 (5%)
10	NAG	J	628	1	14,14,15	2.03	2 (14%)	17,19,21	1.01	2 (11%)
10	NAG	C	612	1	14,14,15	2.09	2 (14%)	17,19,21	0.76	0
10	NAG	B	704	2	14,14,15	2.08	2 (14%)	17,19,21	0.90	1 (5%)
10	NAG	J	622	1	14,14,15	2.07	2 (14%)	17,19,21	0.90	1 (5%)
10	NAG	J	604	1	14,14,15	2.06	2 (14%)	17,19,21	1.22	2 (11%)
10	NAG	J	624	1	14,14,15	2.08	2 (14%)	17,19,21	0.87	0
10	NAG	C	625	1	14,14,15	2.04	2 (14%)	17,19,21	0.87	1 (5%)
10	NAG	A	604	1	14,14,15	2.06	2 (14%)	17,19,21	1.23	2 (11%)
10	NAG	J	623	1	14,14,15	2.12	2 (14%)	17,19,21	1.28	3 (17%)

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
10	NAG	D	703	2	-	2/6/23/26	0/1/1/1
10	NAG	C	603	1	-	1/6/23/26	0/1/1/1
10	NAG	J	612	1	-	2/6/23/26	0/1/1/1
10	NAG	J	619	1	-	1/6/23/26	0/1/1/1
10	NAG	A	625	1	-	2/6/23/26	0/1/1/1
10	NAG	C	619	1	-	1/6/23/26	0/1/1/1
10	NAG	A	624	1	-	2/6/23/26	0/1/1/1
10	NAG	J	603	1	-	1/6/23/26	0/1/1/1
10	NAG	M	704	2	-	2/6/23/26	0/1/1/1
10	NAG	C	624	1	-	2/6/23/26	0/1/1/1
10	NAG	M	703	2	-	2/6/23/26	0/1/1/1
10	NAG	C	623	1	-	2/6/23/26	0/1/1/1
10	NAG	C	604	1	-	2/6/23/26	0/1/1/1
10	NAG	A	619	1	-	1/6/23/26	0/1/1/1
10	NAG	A	628	1	-	1/6/23/26	0/1/1/1
10	NAG	A	623	1	-	2/6/23/26	0/1/1/1
10	NAG	J	625	1	-	2/6/23/26	0/1/1/1
10	NAG	C	628	1	-	1/6/23/26	0/1/1/1
10	NAG	A	622	1	-	2/6/23/26	0/1/1/1
10	NAG	C	622	1	-	2/6/23/26	0/1/1/1
10	NAG	A	612	1	-	2/6/23/26	0/1/1/1
10	NAG	B	703	2	-	2/6/23/26	0/1/1/1
10	NAG	A	603	1	-	1/6/23/26	0/1/1/1
10	NAG	D	704	2	-	2/6/23/26	0/1/1/1
10	NAG	J	628	1	-	1/6/23/26	0/1/1/1
10	NAG	C	612	1	-	2/6/23/26	0/1/1/1
10	NAG	B	704	2	-	2/6/23/26	0/1/1/1
10	NAG	J	622	1	-	2/6/23/26	0/1/1/1
10	NAG	J	604	1	-	2/6/23/26	0/1/1/1
10	NAG	J	624	1	-	2/6/23/26	0/1/1/1
10	NAG	C	625	1	-	2/6/23/26	0/1/1/1
10	NAG	A	604	1	-	2/6/23/26	0/1/1/1
10	NAG	J	623	1	-	2/6/23/26	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	622	NAG	O5-C1	6.79	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	623	NAG	O5-C1	6.77	1.55	1.43
10	J	623	NAG	O5-C1	6.75	1.55	1.43
10	C	623	NAG	O5-C1	6.75	1.55	1.43
10	C	612	NAG	O5-C1	6.75	1.55	1.43
10	A	622	NAG	O5-C1	6.74	1.55	1.43
10	J	612	NAG	O5-C1	6.74	1.55	1.43
10	A	612	NAG	O5-C1	6.72	1.55	1.43
10	C	604	NAG	O5-C1	6.72	1.55	1.43
10	C	622	NAG	O5-C1	6.71	1.55	1.43
10	J	604	NAG	O5-C1	6.71	1.55	1.43
10	A	604	NAG	O5-C1	6.70	1.54	1.43
10	C	603	NAG	O5-C1	6.66	1.54	1.43
10	A	603	NAG	O5-C1	6.66	1.54	1.43
10	J	603	NAG	O5-C1	6.63	1.54	1.43
10	J	624	NAG	O5-C1	6.63	1.54	1.43
10	C	624	NAG	O5-C1	6.63	1.54	1.43
10	M	704	NAG	O5-C1	6.61	1.54	1.43
10	A	624	NAG	O5-C1	6.59	1.54	1.43
10	B	704	NAG	O5-C1	6.59	1.54	1.43
10	D	704	NAG	O5-C1	6.58	1.54	1.43
10	A	619	NAG	O5-C1	6.51	1.54	1.43
10	C	619	NAG	O5-C1	6.49	1.54	1.43
10	A	628	NAG	O5-C1	6.49	1.54	1.43
10	C	628	NAG	O5-C1	6.48	1.54	1.43
10	J	619	NAG	O5-C1	6.46	1.54	1.43
10	J	628	NAG	O5-C1	6.45	1.54	1.43
10	J	625	NAG	O5-C1	6.36	1.54	1.43
10	A	625	NAG	O5-C1	6.31	1.54	1.43
10	C	625	NAG	O5-C1	6.30	1.54	1.43
10	D	703	NAG	O5-C1	6.30	1.54	1.43
10	B	703	NAG	O5-C1	6.29	1.54	1.43
10	M	703	NAG	O5-C1	6.28	1.54	1.43
10	D	703	NAG	C3-C2	-2.55	1.47	1.52
10	B	703	NAG	C3-C2	-2.55	1.47	1.52
10	C	624	NAG	C3-C2	-2.55	1.47	1.52
10	M	703	NAG	C3-C2	-2.54	1.47	1.52
10	A	623	NAG	C3-C2	-2.54	1.47	1.52
10	J	624	NAG	C3-C2	-2.54	1.47	1.52
10	A	624	NAG	C3-C2	-2.54	1.47	1.52
10	M	704	NAG	C3-C2	-2.53	1.47	1.52
10	B	704	NAG	C3-C2	-2.53	1.47	1.52
10	C	623	NAG	C3-C2	-2.52	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	704	NAG	C3-C2	-2.51	1.47	1.52
10	J	623	NAG	C3-C2	-2.49	1.47	1.52
10	J	625	NAG	C3-C2	-2.41	1.47	1.52
10	A	625	NAG	C3-C2	-2.41	1.47	1.52
10	A	603	NAG	C3-C2	-2.41	1.47	1.52
10	C	603	NAG	C3-C2	-2.40	1.47	1.52
10	J	603	NAG	C3-C2	-2.40	1.47	1.52
10	C	625	NAG	C3-C2	-2.38	1.47	1.52
10	C	612	NAG	C3-C2	-2.34	1.47	1.52
10	A	604	NAG	C3-C2	-2.34	1.47	1.52
10	C	604	NAG	C3-C2	-2.33	1.47	1.52
10	J	619	NAG	C3-C2	-2.33	1.47	1.52
10	J	612	NAG	C3-C2	-2.32	1.47	1.52
10	A	619	NAG	C3-C2	-2.30	1.47	1.52
10	C	622	NAG	C3-C2	-2.30	1.47	1.52
10	J	604	NAG	C3-C2	-2.30	1.47	1.52
10	A	612	NAG	C3-C2	-2.29	1.47	1.52
10	A	622	NAG	C3-C2	-2.28	1.47	1.52
10	C	619	NAG	C3-C2	-2.28	1.47	1.52
10	J	622	NAG	C3-C2	-2.28	1.47	1.52
10	J	628	NAG	C3-C2	-2.27	1.47	1.52
10	C	628	NAG	C3-C2	-2.25	1.47	1.52
10	A	628	NAG	C3-C2	-2.24	1.47	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	604	NAG	C4-C3-C2	-3.42	106.00	111.02
10	C	604	NAG	C4-C3-C2	-3.42	106.01	111.02
10	J	604	NAG	C4-C3-C2	-3.41	106.03	111.02
10	J	623	NAG	O5-C1-C2	-3.11	106.47	111.29
10	C	623	NAG	O5-C1-C2	-3.10	106.50	111.29
10	A	623	NAG	O5-C1-C2	-3.09	106.50	111.29
10	J	623	NAG	C4-C3-C2	-3.08	106.51	111.02
10	A	623	NAG	C4-C3-C2	-3.05	106.54	111.02
10	C	623	NAG	C4-C3-C2	-3.05	106.55	111.02
10	M	703	NAG	C4-C3-C2	-2.84	106.86	111.02
10	D	703	NAG	C4-C3-C2	-2.82	106.88	111.02
10	B	703	NAG	C4-C3-C2	-2.82	106.88	111.02
10	J	628	NAG	C1-O5-C5	-2.60	108.69	112.19
10	J	628	NAG	C4-C3-C2	-2.60	107.21	111.02
10	C	628	NAG	C4-C3-C2	-2.59	107.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	628	NAG	C1-O5-C5	-2.59	108.71	112.19
10	A	628	NAG	C4-C3-C2	-2.59	107.22	111.02
10	C	628	NAG	C1-O5-C5	-2.58	108.73	112.19
10	C	619	NAG	C4-C3-C2	-2.55	107.28	111.02
10	A	619	NAG	C4-C3-C2	-2.54	107.29	111.02
10	J	619	NAG	C4-C3-C2	-2.54	107.30	111.02
10	B	704	NAG	C4-C3-C2	-2.53	107.31	111.02
10	D	704	NAG	C4-C3-C2	-2.52	107.33	111.02
10	M	704	NAG	C4-C3-C2	-2.50	107.35	111.02
10	C	604	NAG	O5-C1-C2	-2.49	107.43	111.29
10	A	604	NAG	O5-C1-C2	-2.47	107.46	111.29
10	J	604	NAG	O5-C1-C2	-2.42	107.54	111.29
10	J	625	NAG	C1-O5-C5	-2.36	109.03	112.19
10	C	625	NAG	C1-O5-C5	-2.34	109.05	112.19
10	A	625	NAG	C1-O5-C5	-2.32	109.07	112.19
10	A	622	NAG	C4-C3-C2	-2.23	107.75	111.02
10	J	622	NAG	C4-C3-C2	-2.22	107.76	111.02
10	D	703	NAG	C1-O5-C5	-2.22	109.21	112.19
10	J	619	NAG	C1-O5-C5	-2.22	109.21	112.19
10	C	619	NAG	C1-O5-C5	-2.21	109.22	112.19
10	C	622	NAG	C4-C3-C2	-2.21	107.78	111.02
10	A	619	NAG	C1-O5-C5	-2.20	109.24	112.19
10	B	703	NAG	C1-O5-C5	-2.19	109.25	112.19
10	M	703	NAG	C1-O5-C5	-2.18	109.26	112.19
10	C	623	NAG	C2-N2-C7	-2.05	120.16	122.90
10	A	623	NAG	C2-N2-C7	-2.03	120.18	122.90
10	J	623	NAG	C2-N2-C7	-2.03	120.18	122.90

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	604	NAG	O5-C5-C6-O6
10	C	604	NAG	O5-C5-C6-O6
10	J	604	NAG	O5-C5-C6-O6
10	B	703	NAG	O5-C5-C6-O6
10	D	703	NAG	O5-C5-C6-O6
10	M	703	NAG	O5-C5-C6-O6
10	A	625	NAG	O5-C5-C6-O6
10	C	625	NAG	O5-C5-C6-O6
10	J	625	NAG	O5-C5-C6-O6
10	A	622	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	B	704	NAG	O5-C5-C6-O6
10	C	622	NAG	O5-C5-C6-O6
10	D	704	NAG	O5-C5-C6-O6
10	J	622	NAG	O5-C5-C6-O6
10	M	704	NAG	O5-C5-C6-O6
10	A	623	NAG	C4-C5-C6-O6
10	C	623	NAG	C4-C5-C6-O6
10	J	623	NAG	C4-C5-C6-O6
10	A	623	NAG	O5-C5-C6-O6
10	C	623	NAG	O5-C5-C6-O6
10	J	623	NAG	O5-C5-C6-O6
10	C	612	NAG	O5-C5-C6-O6
10	A	612	NAG	O5-C5-C6-O6
10	J	612	NAG	O5-C5-C6-O6
10	A	624	NAG	O5-C5-C6-O6
10	C	624	NAG	O5-C5-C6-O6
10	J	624	NAG	O5-C5-C6-O6
10	A	604	NAG	C4-C5-C6-O6
10	C	604	NAG	C4-C5-C6-O6
10	J	604	NAG	C4-C5-C6-O6
10	A	603	NAG	O5-C5-C6-O6
10	C	603	NAG	O5-C5-C6-O6
10	J	603	NAG	O5-C5-C6-O6
10	A	619	NAG	O5-C5-C6-O6
10	C	619	NAG	O5-C5-C6-O6
10	J	619	NAG	O5-C5-C6-O6
10	A	628	NAG	O5-C5-C6-O6
10	C	628	NAG	O5-C5-C6-O6
10	J	628	NAG	O5-C5-C6-O6
10	B	703	NAG	C4-C5-C6-O6
10	D	703	NAG	C4-C5-C6-O6
10	M	703	NAG	C4-C5-C6-O6
10	D	704	NAG	C4-C5-C6-O6
10	B	704	NAG	C4-C5-C6-O6
10	M	704	NAG	C4-C5-C6-O6
10	J	622	NAG	C4-C5-C6-O6
10	C	622	NAG	C4-C5-C6-O6
10	A	622	NAG	C4-C5-C6-O6
10	A	625	NAG	C4-C5-C6-O6
10	J	625	NAG	C4-C5-C6-O6
10	C	625	NAG	C4-C5-C6-O6
10	C	612	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	J	612	NAG	C4-C5-C6-O6
10	A	612	NAG	C4-C5-C6-O6
10	J	624	NAG	C4-C5-C6-O6
10	A	624	NAG	C4-C5-C6-O6
10	C	624	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	604	NAG	2	0
10	J	604	NAG	2	0
10	A	604	NAG	2	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.

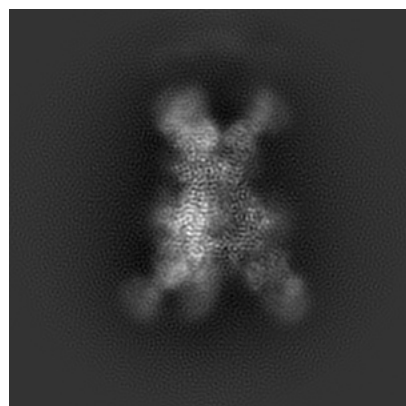
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7884. These allow visual inspection of the internal detail of the map and identification of artifacts.

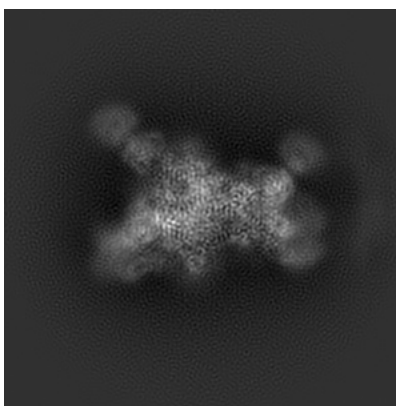
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

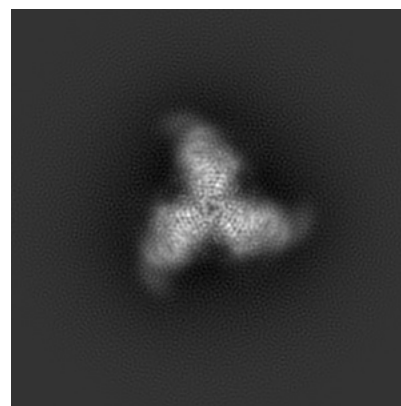
6.1.1 Primary map



X

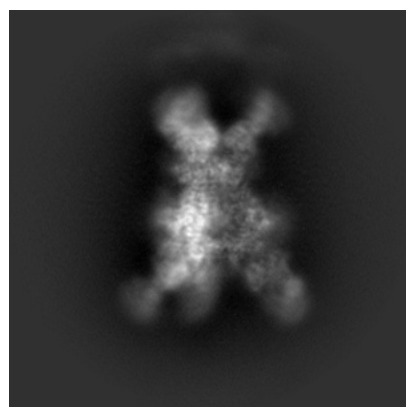


Y

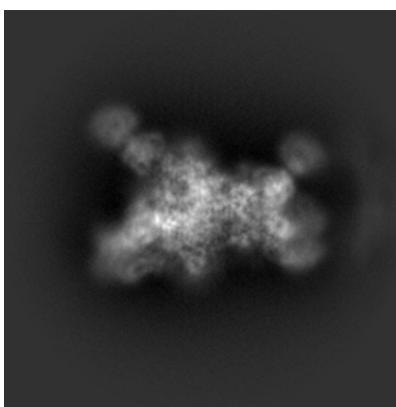


Z

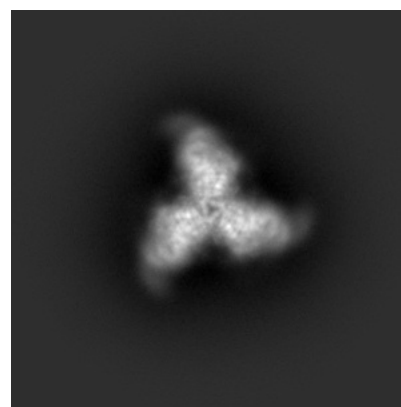
6.1.2 Raw map



X



Y

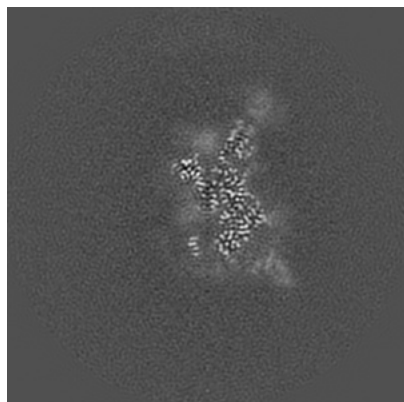


Z

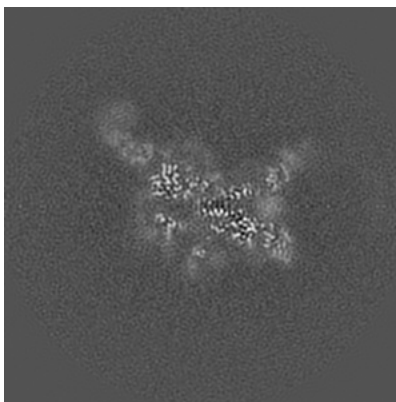
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

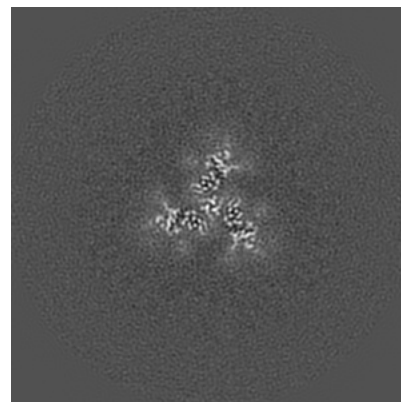
6.2.1 Primary map



X Index: 160

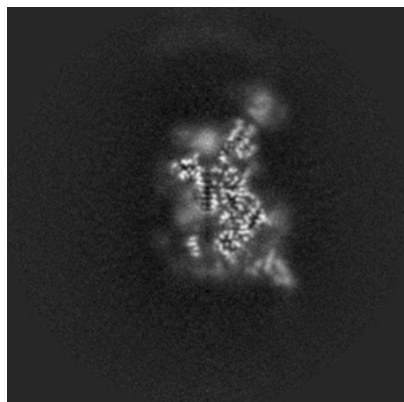


Y Index: 160

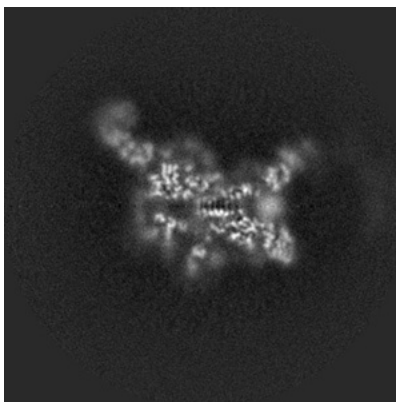


Z Index: 160

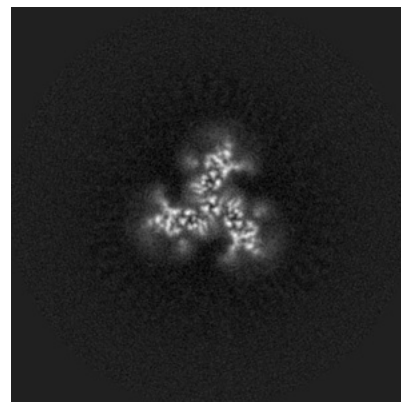
6.2.2 Raw map



X Index: 160



Y Index: 160

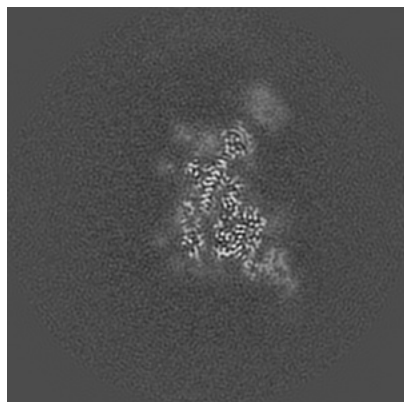


Z Index: 160

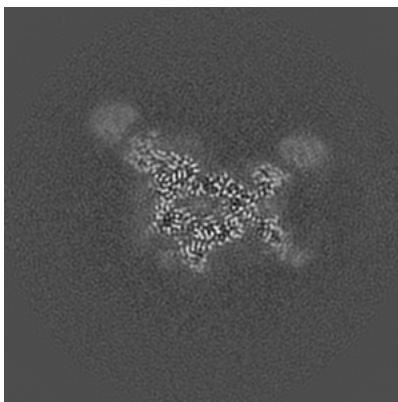
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

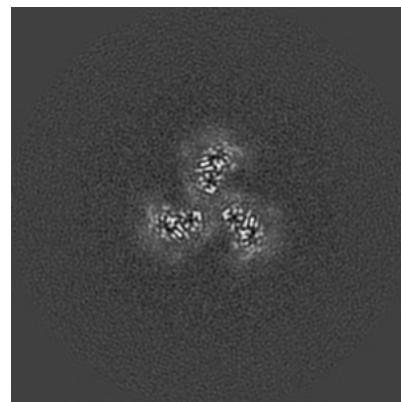
6.3.1 Primary map



X Index: 155

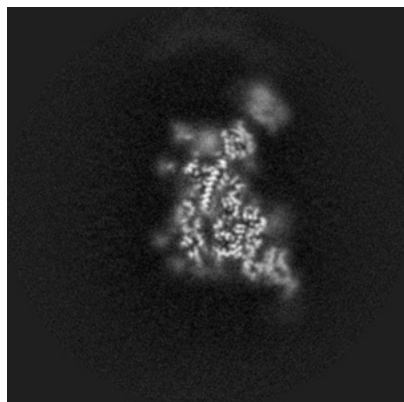


Y Index: 150

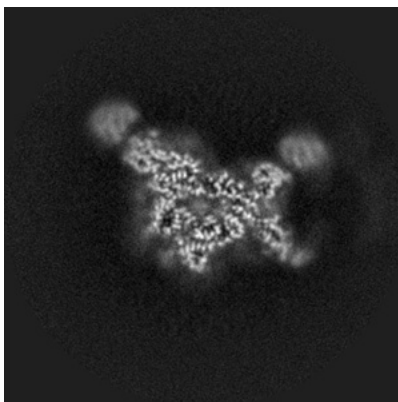


Z Index: 151

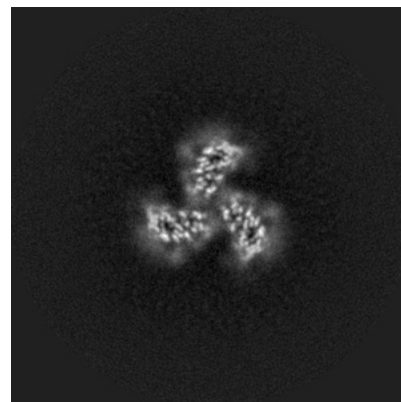
6.3.2 Raw map



X Index: 155



Y Index: 150

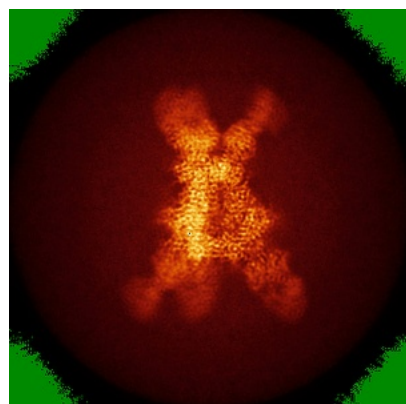


Z Index: 150

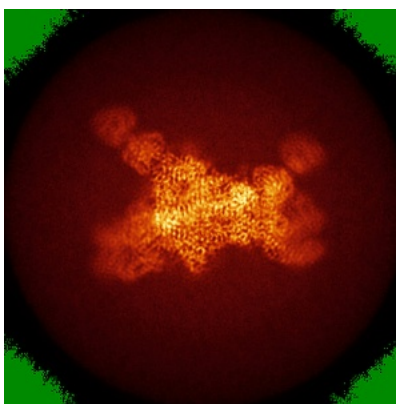
The images above show the largest variance slices of the map in three orthogonal directions.

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

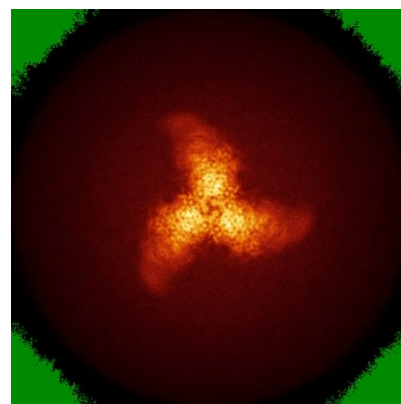
6.4.1 Primary map



X



Y

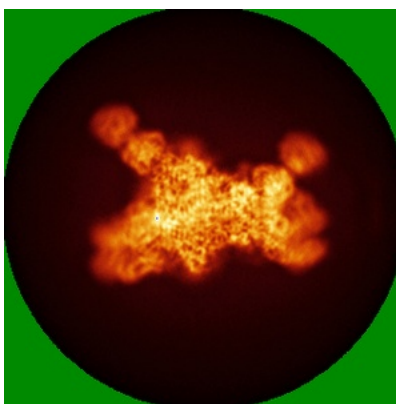


Z

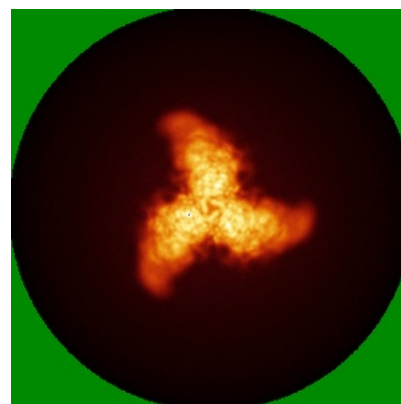
6.4.2 Raw map



X



Y

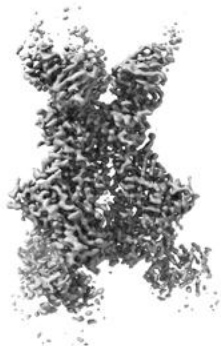


Z

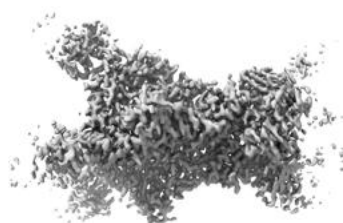
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

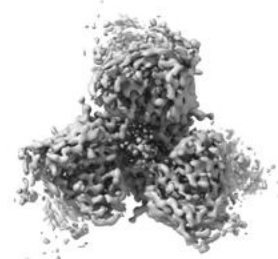
6.5.1 Primary map



X



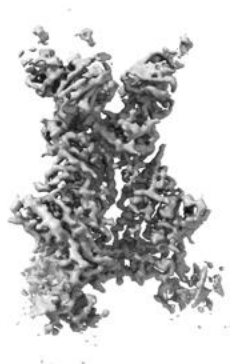
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

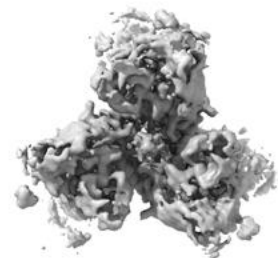
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

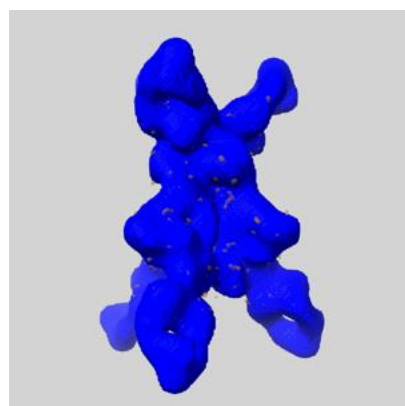
6.6 Mask visualisation [i](#)

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

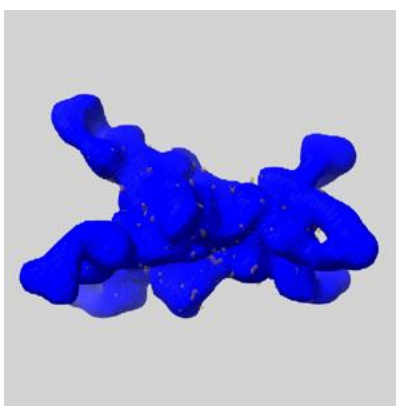
A mask typically either:

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

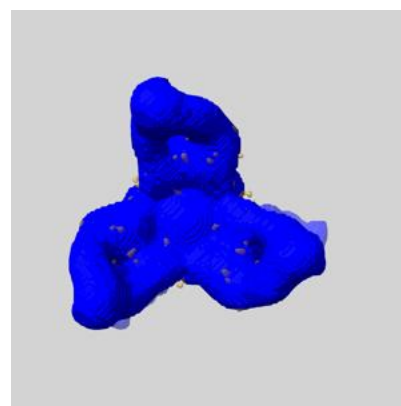
6.6.1 emd_7884_msk_1.map [i](#)



X



Y

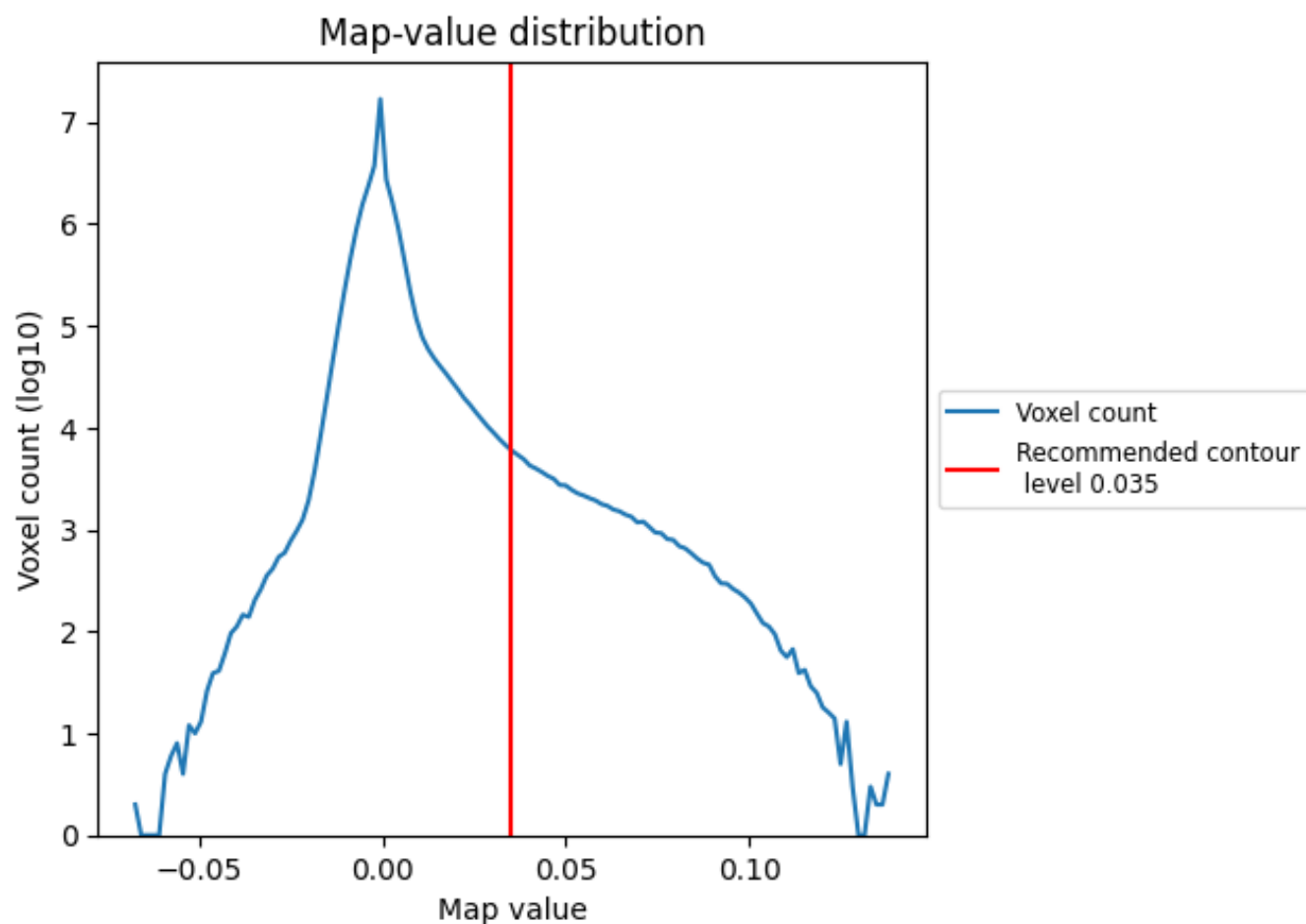


Z

7 Map analysis [i](#)

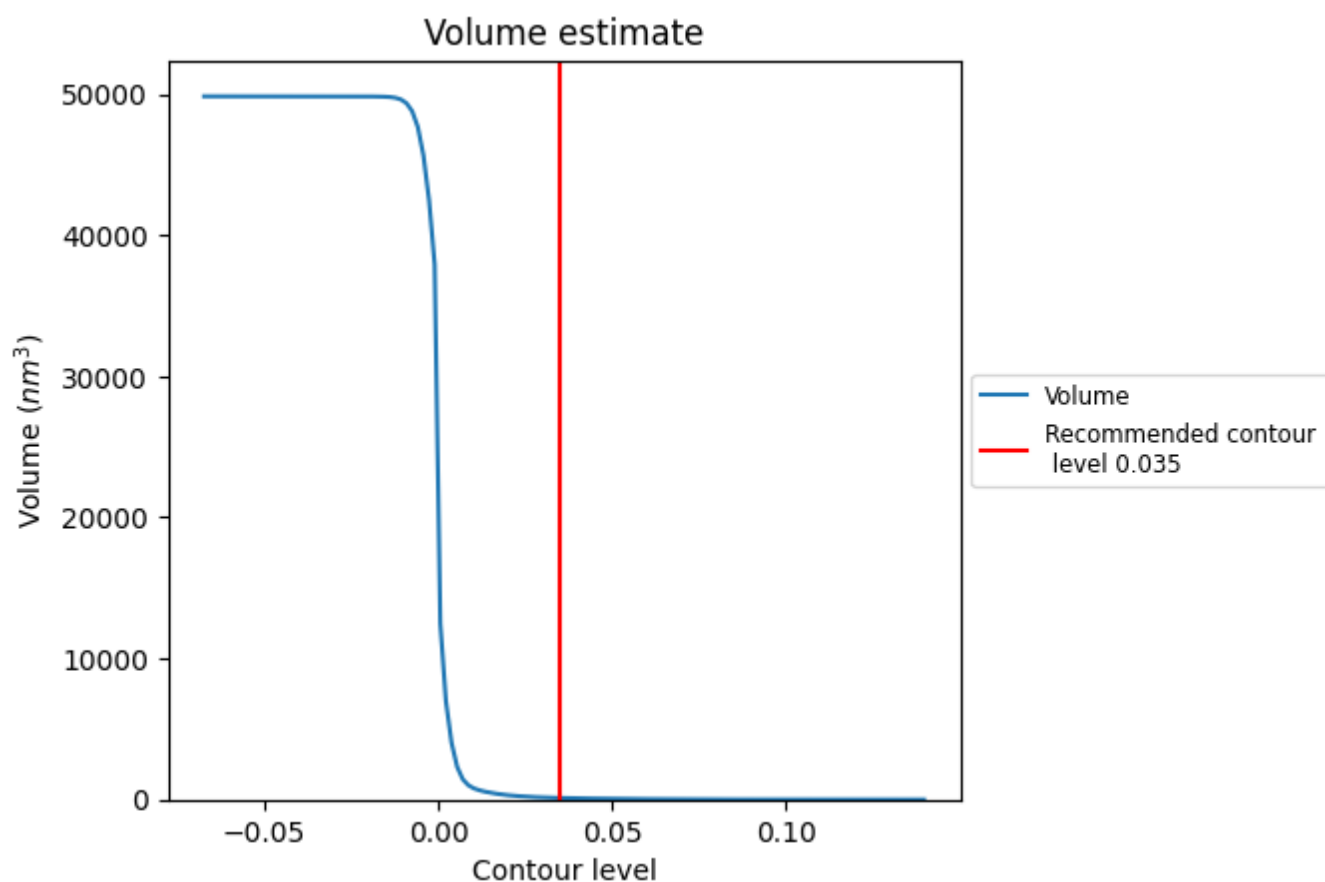
This section contains the results of statistical analysis of the map.

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.

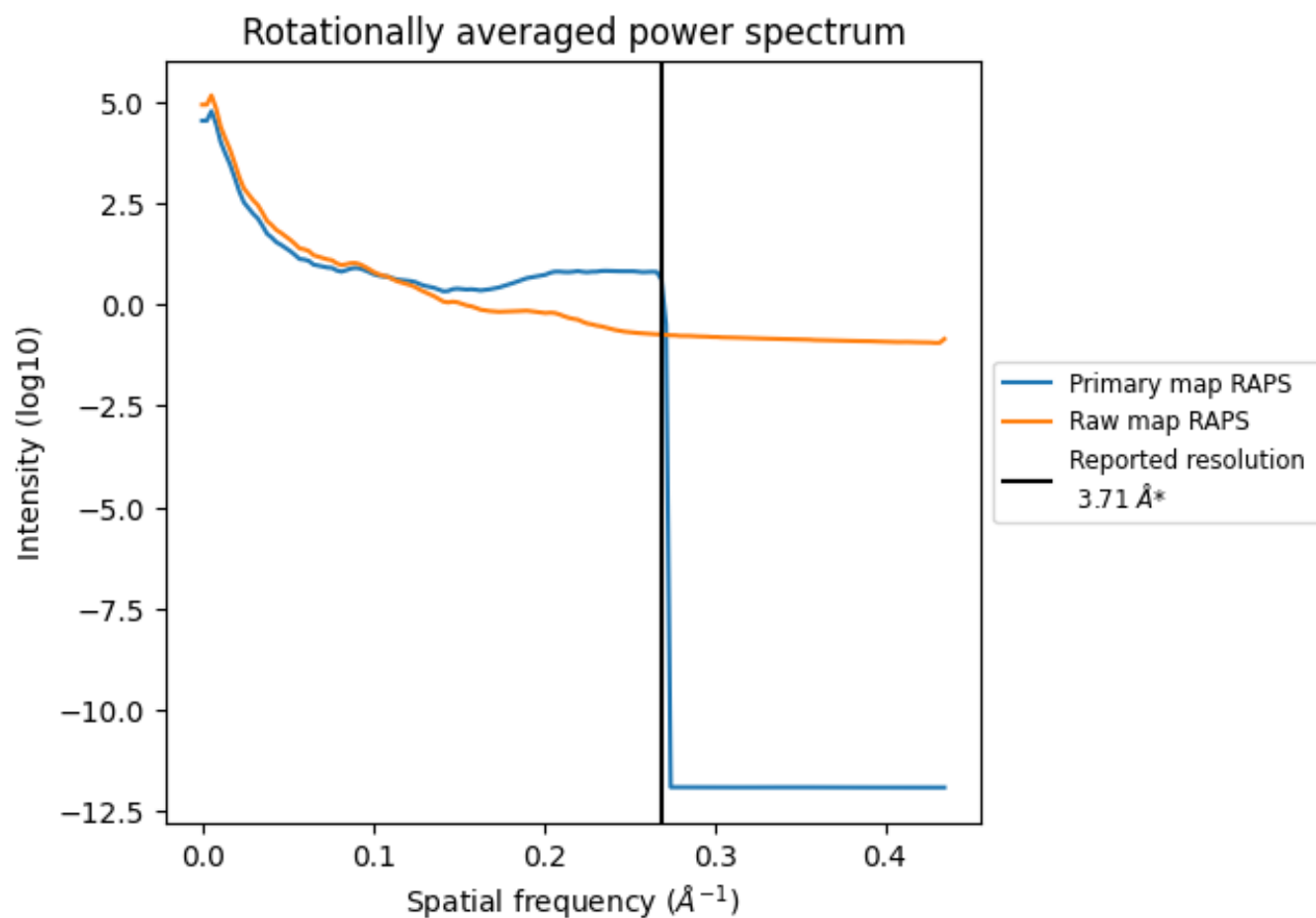
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 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 ⓘ

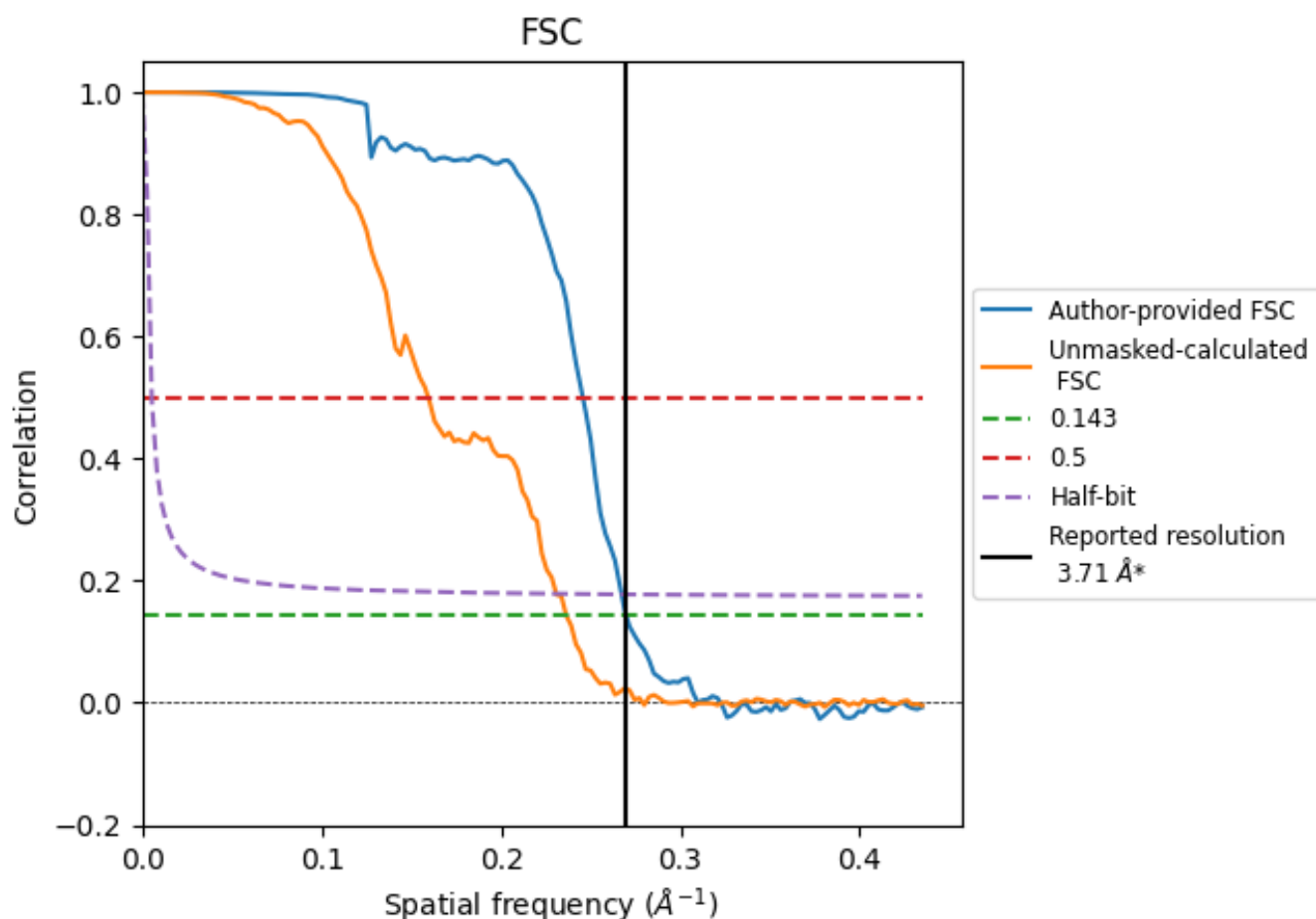


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

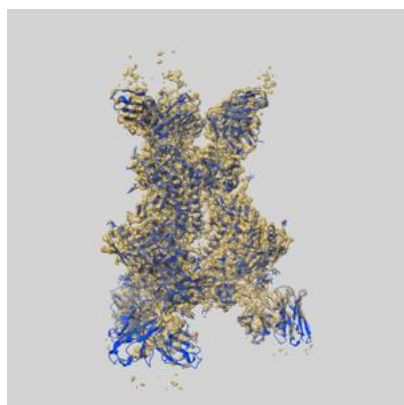
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	3.71	4.07	3.74
Unmasked-calculated*	4.23	6.27	4.33

*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 4.23 differs from the reported value 3.71 by more than 10 %

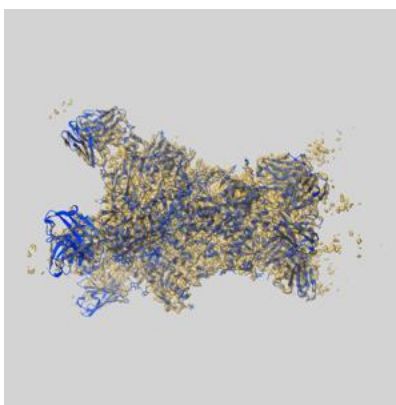
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7884 and PDB model 6NF5. Per-residue inclusion information can be found in section [3](#) on page [11](#).

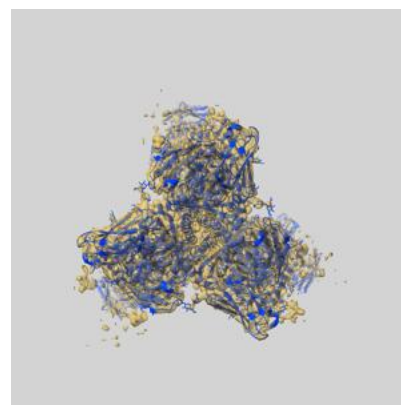
9.1 Map-model overlay [i](#)



X



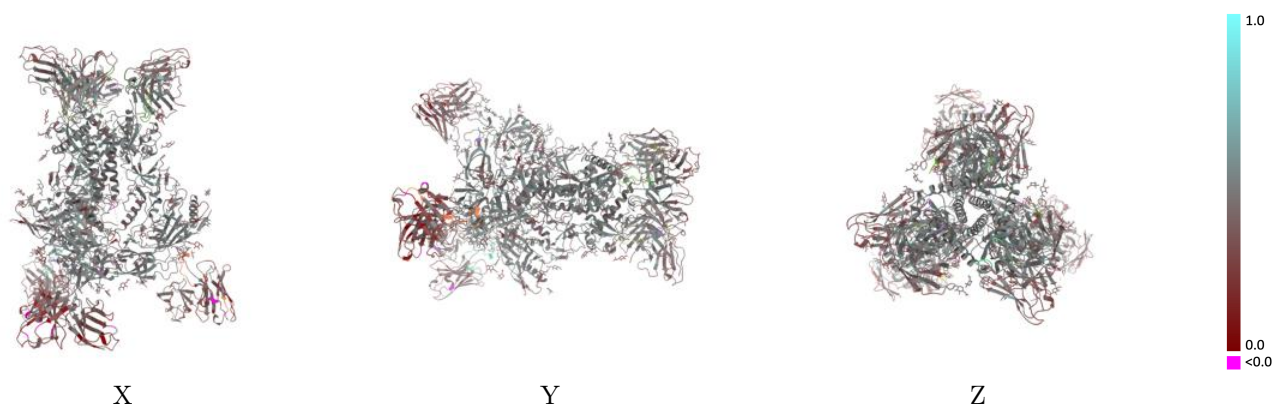
Y



Z

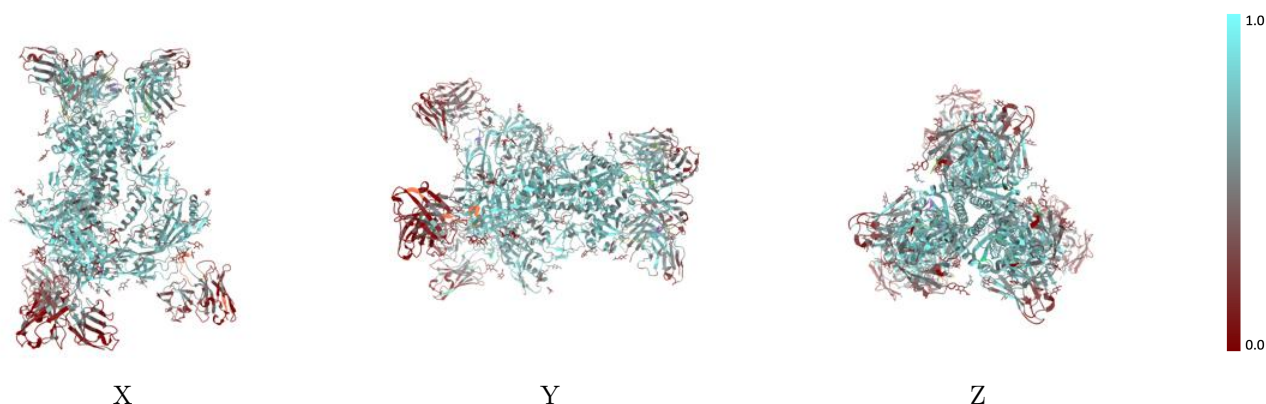
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



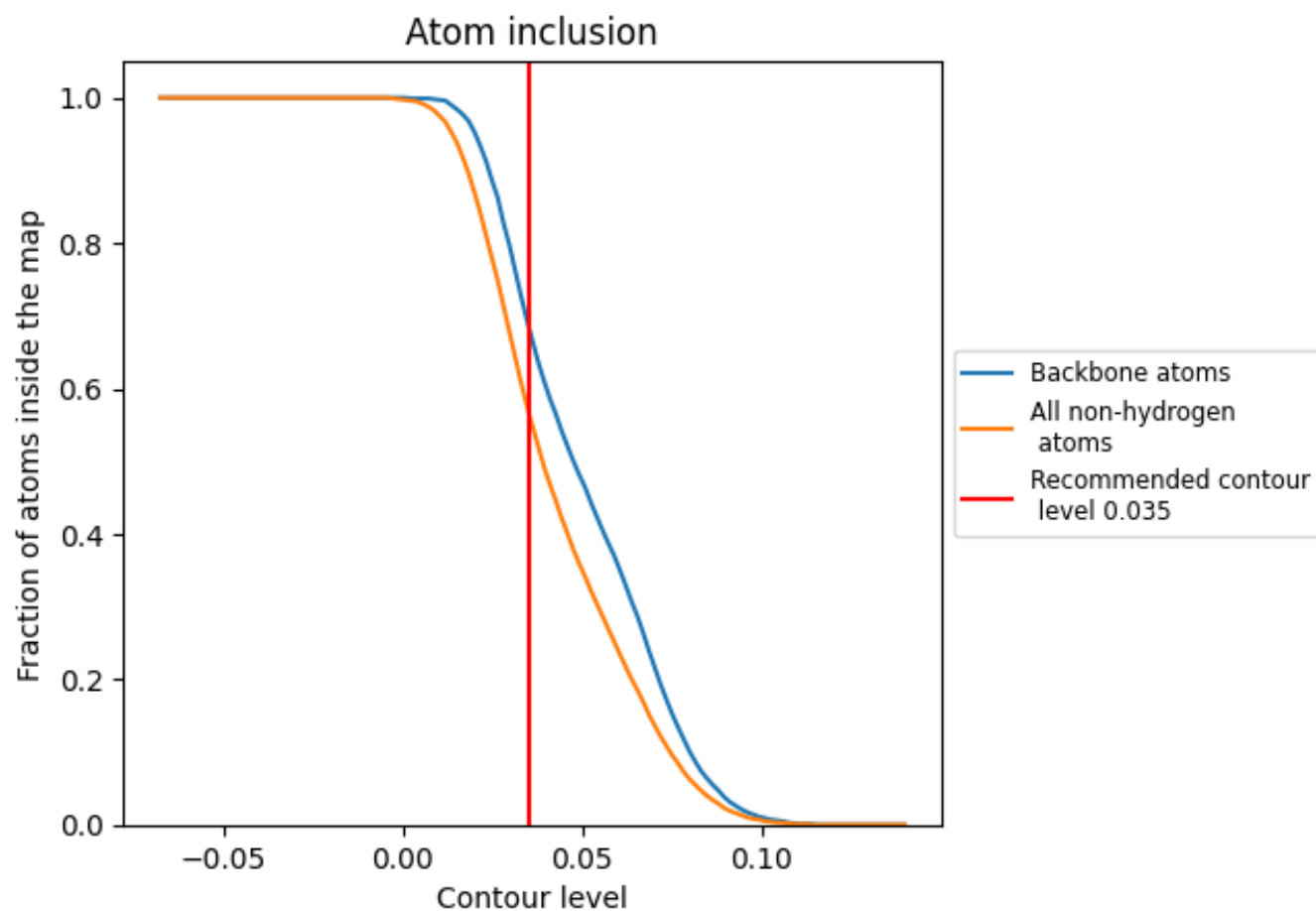
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 57% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5680	 0.4240
A	 0.6850	 0.4690
B	 0.6980	 0.4710
C	 0.6840	 0.4680
D	 0.7010	 0.4720
E	 0.2870	 0.3150
F	 0.2770	 0.3240
G	 0.5760	 0.4320
H	 0.2910	 0.3130
I	 0.5190	 0.3940
J	 0.6880	 0.4680
K	 0.5820	 0.4270
L	 0.2850	 0.3230
M	 0.6970	 0.4720
N	 0.5250	 0.3950
O	 0.2900	 0.3140
P	 0.2780	 0.3270
Q	 0.5810	 0.4310
R	 0.5220	 0.3930
S	 0.4640	 0.4190
T	 0.4100	 0.3910
U	 0.3570	 0.3910
V	 0.4580	 0.4650
W	 0.4290	 0.3550
X	 0.3210	 0.3120
Y	 0.3210	 0.4030
Z	 0.5000	 0.3920
a	 0.4100	 0.3920
b	 0.3570	 0.3930
c	 0.4580	 0.4630
d	 0.3930	 0.3600
e	 0.3570	 0.3090
f	 0.3930	 0.4080
g	 0.4640	 0.4140
h	 0.4430	 0.3940



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Chain	Atom inclusion	Q-score
i	 0.3570	 0.3930
j	 0.4580	 0.4740
k	 0.4290	 0.3610
l	 0.3570	 0.3060
m	 0.3570	 0.4190