



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:56 AM UTC

PDB ID : 7ZLK / pdb_00007zlk
EMDB ID : EMD-14783
Title : AMC009 SOSIPv5.2 in complex with Fabs ACS114 and ACS122
Authors : van Schooten, J.; Ozorowski, G.; Ward, A.
Deposited on : 2022-04-15
Resolution : 3.99 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:

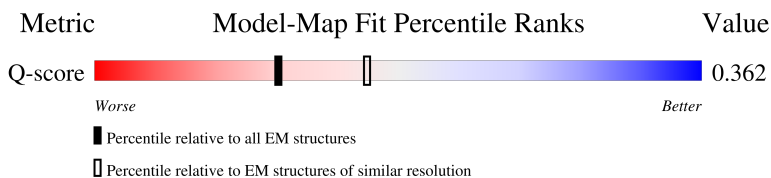
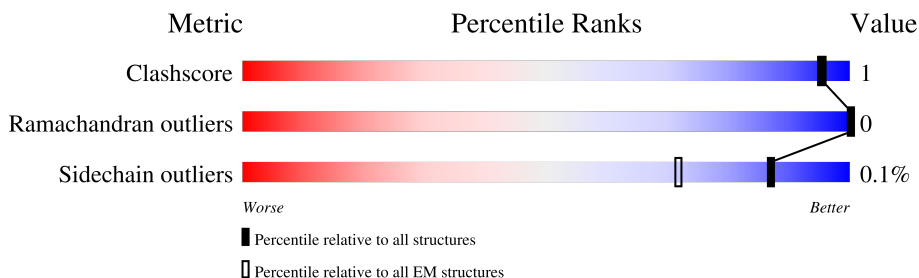
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.99 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	7463 (3.49 - 4.49)

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	482	
1	C	482	
1	D	482	
2	B	154	

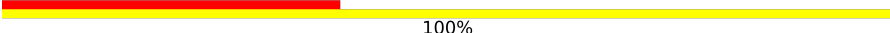
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Mol	Chain	Length	Quality of chain
2	E	154	
2	F	154	
3	H	120	
3	O	120	
3	Q	120	
4	L	112	
4	P	112	
4	R	112	
5	M	124	
5	S	124	
6	N	108	
6	T	108	
7	G	2	
7	V	2	
7	e	2	
8	I	5	
8	U	5	
8	W	5	
8	Y	5	
8	Z	5	
8	b	5	
8	f	5	
9	J	7	
9	X	7	
9	c	7	

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Mol	Chain	Length	Quality of chain
10	K	4	 25%75%
11	a	3	 67%100%
12	d	8	 38%100%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 23518 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 AMC009 SOSIPv5.2 envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	436	Total	C	N	O	S	0	0
			3460	2185	606	642	27		
1	C	436	Total	C	N	O	S	0	0
			3460	2185	606	642	27		
1	D	436	Total	C	N	O	S	0	0
			3460	2185	606	642	27		

- Molecule 2 is a protein called AMC009 SOSIPv5.2 envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			954	601	170	176	7		
2	E	123	Total	C	N	O	S	0	0
			982	616	176	183	7		
2	F	132	Total	C	N	O	S	0	0
			1058	662	187	202	7		

- Molecule 3 is a protein called ACS114 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	120	Total	C	N	O	S	0	0
			934	594	163	171	6		
3	O	120	Total	C	N	O	S	0	0
			934	594	163	171	6		
3	Q	120	Total	C	N	O	S	0	0
			934	594	163	171	6		

- Molecule 4 is a protein called ACS114 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	112	Total	C	N	O	S	0	0
			856	538	147	168	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	112	Total	C	N	O	S	0	0
			856	538	147	168	3		
4	R	112	Total	C	N	O	S	0	0
			856	538	147	168	3		

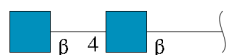
- Molecule 5 is a protein called ACS122 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	124	Total	C	N	O	S	0	0
			971	618	165	185	3		
5	S	119	Total	C	N	O	S	0	0
			938	598	160	177	3		

- Molecule 6 is a protein called ACS122 light chain.

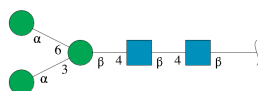
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	107	Total	C	N	O	S	0	0
			814	509	141	161	3		
6	T	107	Total	C	N	O	S	0	0
			814	509	141	161	3		

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



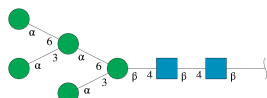
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	e	2	Total	C	N	O	0	0
			28	16	2	10		

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



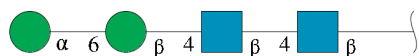
Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	5	Total	C	N	O	0	0
			61	34	2	25		
8	U	5	Total	C	N	O	0	0
			61	34	2	25		
8	W	5	Total	C	N	O	0	0
			61	34	2	25		
8	Y	5	Total	C	N	O	0	0
			61	34	2	25		
8	Z	5	Total	C	N	O	0	0
			61	34	2	25		
8	b	5	Total	C	N	O	0	0
			61	34	2	25		
8	f	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



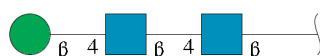
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	7	Total	C	N	O	0	0
			83	46	2	35		
9	X	7	Total	C	N	O	0	0
			83	46	2	35		
9	c	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 10 is an oligosaccharide called 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.



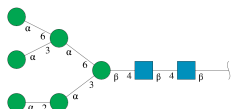
Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 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
11	a	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
12	d	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

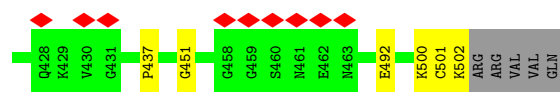


Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14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

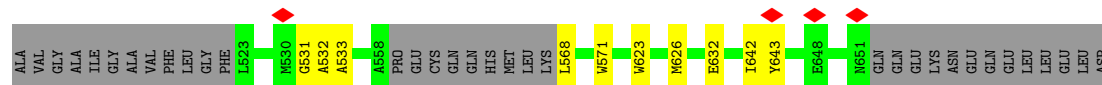
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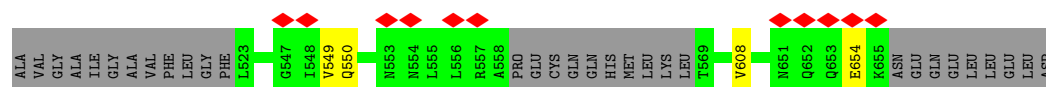
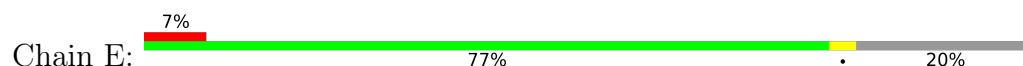
Mol	Chain	Residues	Atoms				AltConf
13	D	1	Total	C	N	O	0
			14	8	1	5	
13	D	1	Total	C	N	O	0
			14	8	1	5	
13	D	1	Total	C	N	O	0
			14	8	1	5	
13	D	1	Total	C	N	O	0
			14	8	1	5	
13	D	1	Total	C	N	O	0
			14	8	1	5	
13	D	1	Total	C	N	O	0
			14	8	1	5	



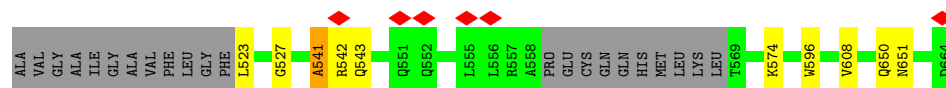
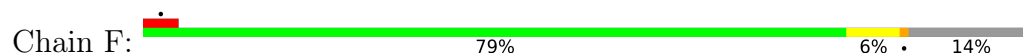
- Molecule 2: AMC009 SOSIPv5.2 envelope glycoprotein gp41



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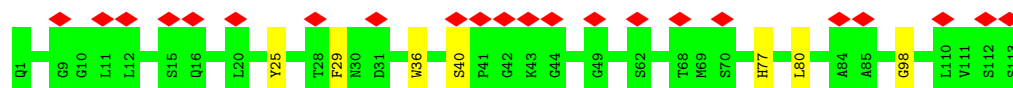
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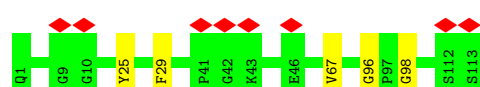
- Molecule 3: ACS114 heavy chain



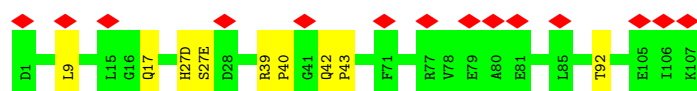
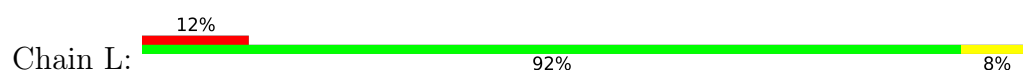
- Molecule 3: ACS114 heavy chain



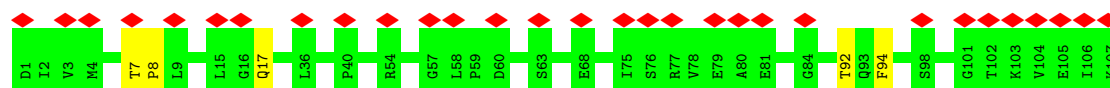
- Molecule 3: ACS114 heavy chain



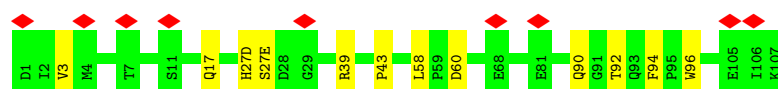
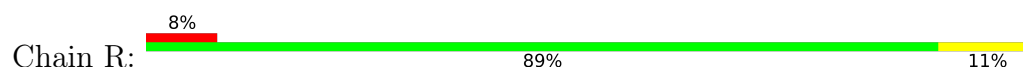
- Molecule 4: ACS114 light chain



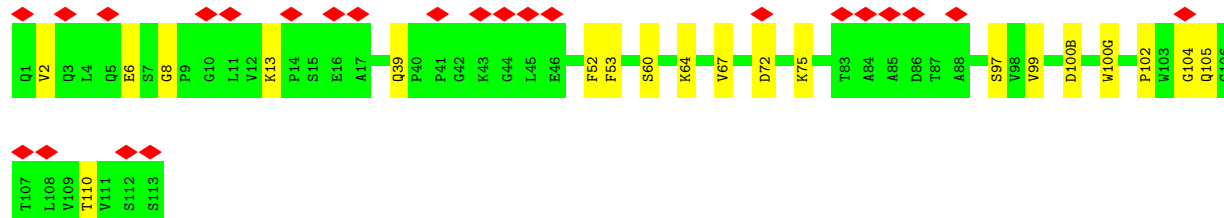
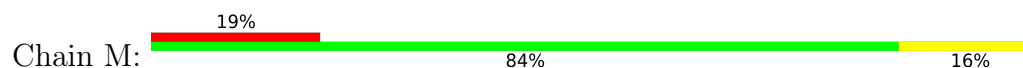
- Molecule 4: ACS114 light chain



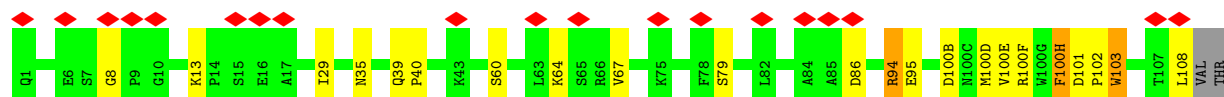
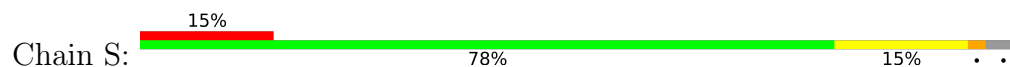
- Molecule 4: ACS114 light chain



- Molecule 5: ACS122 heavy chain

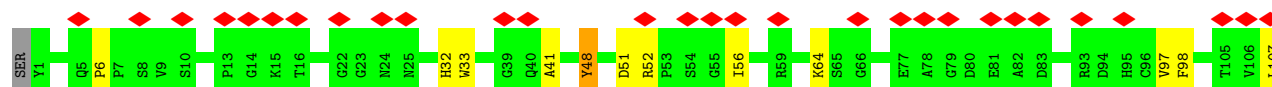
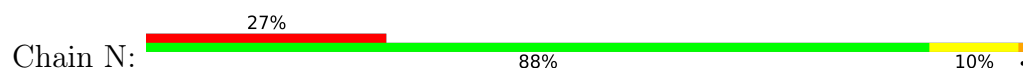


- Molecule 5: ACS122 heavy chain

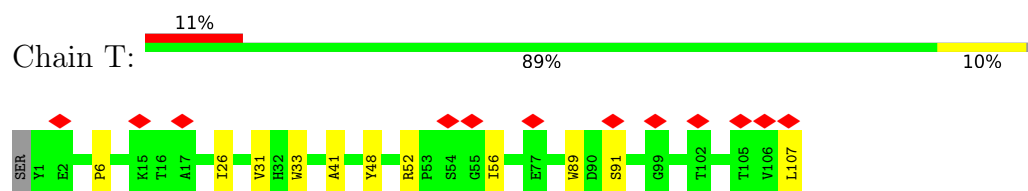


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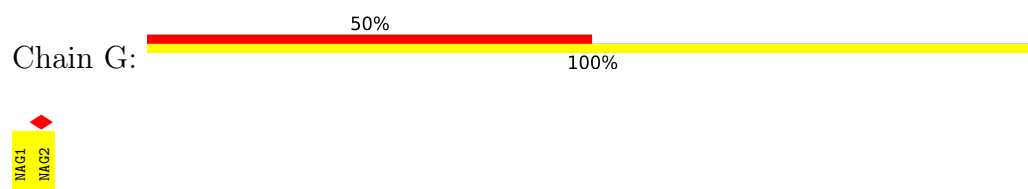
- Molecule 6: ACS122 light chain



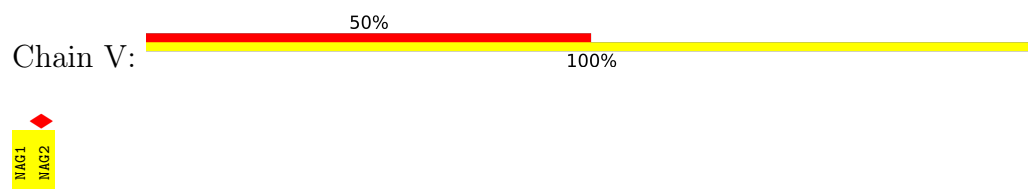
- Molecule 6: ACS122 light chain



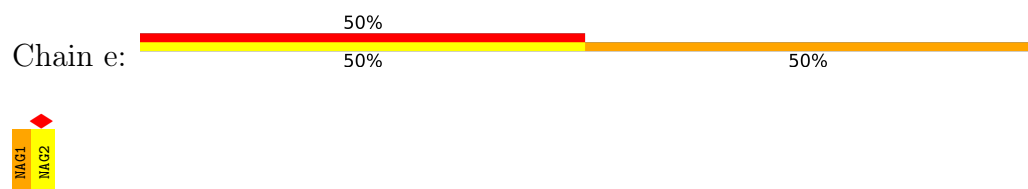
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



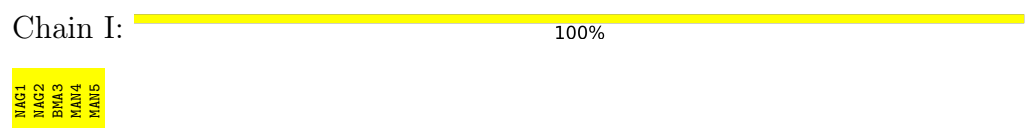
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





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

Chain W:  100%



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

Chain Y:  100%



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

Chain Z:  80% 20%



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

Chain b:  20% 100%



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

Chain f:  20% 100%



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

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



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



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- Molecule 10: 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 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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



NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	159597	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 ($e^-/\text{\AA}^2$)	49.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.164	Depositor
Minimum map value	-0.731	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	345.0, 345.0, 345.0	wwPDB
Map dimensions	300, 300, 300	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: 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	A	1.09	3/3535 (0.1%)	1.34	47/4800 (1.0%)
1	C	1.06	3/3535 (0.1%)	1.27	30/4800 (0.6%)
1	D	1.06	4/3535 (0.1%)	1.31	32/4800 (0.7%)
2	B	1.11	1/970 (0.1%)	1.28	5/1317 (0.4%)
2	E	1.08	0/998	1.18	4/1353 (0.3%)
2	F	1.13	2/1074 (0.2%)	1.16	5/1456 (0.3%)
3	H	0.97	0/963	1.29	7/1314 (0.5%)
3	O	0.98	0/963	1.24	7/1314 (0.5%)
3	Q	1.05	1/963 (0.1%)	1.30	7/1314 (0.5%)
4	L	0.99	0/875	1.42	10/1190 (0.8%)
4	P	1.02	0/875	1.38	4/1190 (0.3%)
4	R	1.00	1/875 (0.1%)	1.42	10/1190 (0.8%)
5	M	1.04	0/997	1.34	18/1361 (1.3%)
5	S	1.09	2/964 (0.2%)	1.50	21/1315 (1.6%)
6	N	1.05	2/834 (0.2%)	1.30	12/1136 (1.1%)
6	T	1.05	1/834 (0.1%)	1.35	9/1136 (0.8%)
All	All	1.06	20/22790 (0.1%)	1.31	228/30986 (0.7%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	102	PRO	N-CD	10.15	1.61	1.47
1	D	308	HIS	CB-CG	-7.27	1.40	1.50
6	N	107	LEU	CB-CG	6.73	1.67	1.53
6	T	107	LEU	CB-CG	6.34	1.66	1.53
3	Q	29	PHE	CB-CG	-5.97	1.36	1.50
2	B	568	LEU	CB-CG	5.96	1.65	1.53
1	C	35	TRP	CD2-CE3	5.95	1.49	1.40
1	D	35	TRP	CD2-CE3	5.93	1.49	1.40
1	A	35	TRP	CZ2-CH2	5.92	1.48	1.37
1	C	35	TRP	CZ2-CH2	5.92	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	32	HIS	CB-CG	-5.84	1.42	1.50
5	S	108	LEU	CB-CG	5.77	1.65	1.53
1	D	35	TRP	CZ2-CH2	5.75	1.48	1.37
1	C	184	ILE	CB-CG1	5.59	1.64	1.53
2	F	523	LEU	CB-CG	5.38	1.64	1.53
1	A	184	ILE	CB-CG1	5.30	1.64	1.53
1	D	184	ILE	CB-CG1	5.23	1.64	1.53
4	R	96	TRP	NE1-CE2	-5.21	1.31	1.37
2	F	651	ASN	CB-CG	-5.20	1.39	1.52
1	A	35	TRP	CD2-CE3	5.11	1.48	1.40

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	101	ASP	N-CA-C	13.80	140.32	109.81
3	Q	29	PHE	N-CA-C	12.18	127.64	113.02
3	H	29	PHE	N-CA-C	11.01	126.23	113.02
4	P	92	THR	N-CA-C	10.22	122.50	111.36
5	S	102	PRO	N-CA-C	-9.58	100.56	113.40
4	R	92	THR	N-CA-C	8.93	121.09	111.36
4	L	92	THR	N-CA-C	8.89	121.05	111.36
5	S	100(H)	PHE	N-CA-C	8.86	123.46	108.23
1	A	53	PHE	CA-CB-CG	8.78	122.58	113.80
1	D	194	ILE	N-CA-C	8.31	119.09	110.62
2	F	541	ALA	N-CA-C	-8.25	99.64	110.53
4	R	39	ARG	N-CA-C	-8.04	99.96	109.93
1	C	298	ARG	CA-C-N	8.02	127.66	119.56
1	C	298	ARG	C-N-CA	8.02	127.66	119.56
1	A	219	ALA	CA-C-N	7.98	127.93	120.03
1	A	219	ALA	C-N-CA	7.98	127.93	120.03
2	F	543	GLN	N-CA-C	-7.92	103.45	113.43
5	M	13	LYS	CA-C-N	7.92	127.58	119.82
5	M	13	LYS	C-N-CA	7.92	127.58	119.82
4	L	39	ARG	N-CA-C	-7.86	100.18	109.93
1	C	437	PRO	CA-C-N	7.86	127.87	119.78
1	C	437	PRO	C-N-CA	7.86	127.87	119.78
1	A	133	ASP	N-CA-C	7.78	122.11	111.54
1	D	205	CYS	CA-C-N	7.73	127.45	119.56
1	D	205	CYS	C-N-CA	7.73	127.45	119.56
1	C	194	ILE	N-CA-C	7.69	118.46	110.62
5	M	39	GLN	CA-C-N	7.65	125.25	119.66
5	M	39	GLN	C-N-CA	7.65	125.25	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	492	GLU	CA-C-N	7.60	127.31	119.56
1	D	492	GLU	C-N-CA	7.60	127.31	119.56
1	C	497	ALA	CA-C-N	7.51	127.50	119.76
1	C	497	ALA	C-N-CA	7.51	127.50	119.76
1	A	237	GLY	CA-C-N	7.47	127.39	119.85
1	A	237	GLY	C-N-CA	7.47	127.39	119.85
6	T	56	ILE	CA-C-N	7.31	127.31	119.78
6	T	56	ILE	C-N-CA	7.31	127.31	119.78
5	M	102	PRO	N-CA-C	-7.29	97.46	112.47
1	A	194	ILE	N-CA-C	7.24	118.87	110.62
5	S	13	LYS	CA-C-N	7.20	126.91	119.56
5	S	13	LYS	C-N-CA	7.20	126.91	119.56
4	R	43	PRO	N-CA-C	-7.19	101.93	110.70
3	H	98	GLY	CA-C-N	7.12	126.83	119.56
3	H	98	GLY	C-N-CA	7.12	126.83	119.56
1	A	437	PRO	N-CA-C	-7.01	103.08	110.58
5	S	103	TRP	N-CA-C	7.01	120.74	111.28
1	D	169	VAL	N-CA-C	6.98	118.58	109.58
1	D	181	ILE	N-CA-C	6.95	117.84	108.11
3	O	98	GLY	CA-C-N	6.94	126.64	119.56
3	O	98	GLY	C-N-CA	6.94	126.64	119.56
4	R	94	PHE	N-CA-C	6.91	122.24	113.25
3	Q	98	GLY	CA-C-N	6.90	126.59	119.56
3	Q	98	GLY	C-N-CA	6.90	126.59	119.56
1	D	162	THR	N-CA-C	-6.87	99.50	109.59
1	A	353	PHE	CA-CB-CG	6.83	120.62	113.80
1	A	492	GLU	CA-C-N	6.74	126.88	119.87
1	A	492	GLU	C-N-CA	6.74	126.88	119.87
5	M	8	GLY	CA-C-N	6.73	127.31	120.04
5	M	8	GLY	C-N-CA	6.73	127.31	120.04
1	C	237	GLY	CA-C-N	6.71	126.67	119.76
1	C	237	GLY	C-N-CA	6.71	126.67	119.76
3	Q	67	VAL	N-CA-C	6.69	117.54	108.17
2	E	608	VAL	CA-C-N	6.68	126.64	120.03
2	E	608	VAL	C-N-CA	6.68	126.64	120.03
4	P	17	GLN	CA-C-N	6.63	127.02	119.92
4	P	17	GLN	C-N-CA	6.63	127.02	119.92
2	B	626	MET	N-CA-C	6.61	120.26	109.76
2	B	632	GLU	N-CA-C	6.59	118.54	111.36
4	L	17	GLN	CA-C-N	6.57	126.95	119.92
4	L	17	GLN	C-N-CA	6.57	126.95	119.92
5	S	64	LYS	N-CA-C	6.56	118.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	ASP	CA-C-N	6.55	127.07	119.47
1	C	368	ASP	C-N-CA	6.55	127.07	119.47
1	A	205	CYS	CA-C-N	6.54	126.23	119.56
1	A	205	CYS	C-N-CA	6.54	126.23	119.56
1	D	437	PRO	N-CA-C	-6.50	102.77	110.70
1	D	424	ILE	N-CA-C	6.49	117.19	108.11
1	C	72	HIS	CA-CB-CG	-6.47	107.33	113.80
1	C	440	ARG	N-CA-C	6.44	120.43	112.58
1	A	334	SER	N-CA-C	6.36	119.33	108.02
2	F	608	VAL	CA-C-N	6.36	126.32	120.03
2	F	608	VAL	C-N-CA	6.36	126.32	120.03
4	R	90	GLN	N-CA-C	6.33	118.99	111.33
1	D	376	PHE	CA-CB-CG	6.32	120.12	113.80
3	H	96	GLY	CA-C-N	6.32	126.29	119.78
3	H	96	GLY	C-N-CA	6.32	126.29	119.78
5	S	8	GLY	CA-C-N	6.32	127.46	120.45
5	S	8	GLY	C-N-CA	6.32	127.46	120.45
1	A	333	ILE	CA-C-N	-6.32	113.89	122.86
1	A	333	ILE	C-N-CA	-6.32	113.89	122.86
5	S	100(H)	PHE	CB-CA-C	-6.28	100.44	111.05
1	D	368	ASP	CA-C-N	6.24	126.70	119.47
1	D	368	ASP	C-N-CA	6.24	126.70	119.47
1	D	451	GLY	N-CA-C	6.23	119.89	111.72
3	O	40	SER	CA-C-N	6.23	127.63	119.84
3	O	40	SER	C-N-CA	6.23	127.63	119.84
4	R	17	GLN	CA-C-N	6.22	126.19	120.03
4	R	17	GLN	C-N-CA	6.22	126.19	120.03
1	A	256	SER	N-CA-C	6.21	117.74	110.41
1	D	267	GLU	N-CA-C	6.17	117.81	111.14
1	D	80	ASN	CA-C-N	6.15	126.33	120.31
1	D	80	ASN	C-N-CA	6.15	126.33	120.31
1	D	437	PRO	CA-C-N	6.12	126.03	119.85
1	D	437	PRO	C-N-CA	6.12	126.03	119.85
5	M	104	GLY	N-CA-C	-6.12	102.75	112.66
1	A	71	THR	N-CA-C	-6.10	105.80	113.18
5	M	67	VAL	N-CA-C	6.06	117.48	108.46
1	A	417	PRO	N-CA-C	-6.04	101.78	111.38
1	A	80	ASN	CA-C-N	6.03	125.99	119.78
1	A	80	ASN	C-N-CA	6.03	125.99	119.78
3	H	67	VAL	N-CA-C	6.03	116.61	108.17
6	T	6	PRO	CA-C-N	6.02	125.90	119.28
6	T	6	PRO	C-N-CA	6.02	125.90	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	39	GLN	CA-C-N	6.01	124.05	119.66
5	S	39	GLN	C-N-CA	6.01	124.05	119.66
4	P	94	PHE	N-CA-C	6.00	121.05	113.25
5	S	60	SER	CA-C-N	6.00	126.16	119.32
5	S	60	SER	C-N-CA	6.00	126.16	119.32
1	D	89	VAL	N-CA-C	-5.99	99.07	108.23
5	S	86	ASP	CA-CB-CG	5.98	118.58	112.60
1	D	75	VAL	CA-C-N	5.97	125.93	119.78
1	D	75	VAL	C-N-CA	5.97	125.93	119.78
6	N	6	PRO	CA-C-N	5.96	125.83	119.28
6	N	6	PRO	C-N-CA	5.96	125.83	119.28
1	A	437	PRO	CA-C-N	5.95	125.86	119.85
1	A	437	PRO	C-N-CA	5.95	125.86	119.85
3	Q	25	TYR	N-CA-C	5.93	120.21	112.92
1	A	211	GLU	CA-C-N	5.92	125.83	119.85
1	A	211	GLU	C-N-CA	5.92	125.83	119.85
5	M	64	LYS	N-CA-C	5.90	118.49	111.71
1	A	262	ASN	CA-CB-CG	5.89	118.49	112.60
1	C	100	MET	N-CA-C	-5.87	104.83	112.23
1	A	273	ARG	N-CA-C	5.85	119.46	111.39
6	T	52	ARG	CA-C-N	5.84	126.03	120.31
6	T	52	ARG	C-N-CA	5.84	126.03	120.31
4	R	3	VAL	N-CA-C	5.79	116.22	108.11
6	N	41	ALA	CA-C-N	5.77	125.72	119.78
6	N	41	ALA	C-N-CA	5.77	125.72	119.78
1	D	182	VAL	CB-CA-C	-5.75	104.56	110.71
1	A	341	THR	N-CA-C	-5.68	105.17	111.36
1	A	353	PHE	CB-CA-C	-5.67	102.60	111.39
1	C	182	VAL	CA-C-N	5.66	125.61	119.78
1	C	182	VAL	C-N-CA	5.66	125.61	119.78
1	A	258	GLN	N-CA-C	5.66	118.22	111.71
4	L	43	PRO	N-CA-C	-5.65	103.81	110.70
6	N	98	PHE	CA-CB-CG	5.65	119.45	113.80
5	M	2	VAL	N-CA-C	5.64	115.98	107.75
1	D	374	HIS	CA-CB-CG	5.63	119.43	113.80
3	H	25	TYR	N-CA-C	5.60	119.81	112.92
1	A	436	ALA	CA-C-N	5.58	123.68	119.66
1	A	436	ALA	C-N-CA	5.58	123.68	119.66
1	D	123	THR	CA-C-N	5.58	125.28	119.82
1	D	123	THR	C-N-CA	5.58	125.28	119.82
3	O	29	PHE	CA-CB-CG	-5.57	108.23	113.80
5	S	79	SER	N-CA-C	5.55	118.14	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ILE	N-CA-C	-5.55	101.79	108.45
5	S	102	PRO	CA-N-CD	-5.51	104.28	112.00
6	T	41	ALA	CA-C-N	5.51	125.42	119.85
6	T	41	ALA	C-N-CA	5.51	125.42	119.85
1	A	182	VAL	CA-C-N	5.48	125.43	119.78
1	A	182	VAL	C-N-CA	5.48	125.43	119.78
1	D	237	GLY	CA-C-N	5.47	125.38	119.85
1	D	237	GLY	C-N-CA	5.47	125.38	119.85
5	S	67	VAL	N-CA-C	5.47	116.36	108.48
6	N	52	ARG	CA-C-N	5.47	125.67	120.31
6	N	52	ARG	C-N-CA	5.47	125.67	120.31
1	A	497	ALA	CA-C-N	5.46	125.36	119.85
1	A	497	ALA	C-N-CA	5.46	125.36	119.85
6	T	33	TRP	N-CA-C	5.43	118.08	109.50
1	C	267	GLU	N-CA-C	5.42	117.27	111.36
1	C	261	LEU	CA-C-N	5.39	129.79	122.19
1	C	261	LEU	C-N-CA	5.39	129.79	122.19
6	N	56	ILE	CA-C-N	5.36	125.30	119.78
6	N	56	ILE	C-N-CA	5.36	125.30	119.78
5	S	40	PRO	N-CA-C	-5.36	105.33	110.47
1	A	40	TYR	N-CA-C	5.35	119.37	112.41
1	A	261	LEU	CA-C-N	5.35	129.72	122.07
1	A	261	LEU	C-N-CA	5.35	129.72	122.07
4	L	42	GLN	CA-C-N	5.35	125.89	120.38
4	L	42	GLN	C-N-CA	5.35	125.89	120.38
5	M	60	SER	CA-C-N	5.34	125.66	119.47
5	M	60	SER	C-N-CA	5.34	125.66	119.47
1	C	424	ILE	N-CA-C	5.33	115.63	108.17
5	M	52	PHE	CA-CB-CG	5.30	119.10	113.80
5	M	110	THR	CA-C-N	-5.29	116.06	123.10
5	M	110	THR	C-N-CA	-5.29	116.06	123.10
4	L	40	PRO	N-CA-C	5.29	121.47	113.81
1	D	120	VAL	N-CA-C	5.28	116.39	109.58
1	A	89	VAL	N-CA-C	5.26	115.83	108.89
1	C	469	ARG	CA-C-N	5.26	125.17	119.76
1	C	469	ARG	C-N-CA	5.26	125.17	119.76
1	A	199	SER	N-CA-C	5.25	117.65	109.52
1	C	159	PHE	N-CA-C	5.24	116.81	108.79
5	S	101	ASP	CA-C-N	5.24	124.56	118.85
5	S	101	ASP	C-N-CA	5.24	124.56	118.85
4	L	39	ARG	CB-CA-C	5.23	116.95	109.26
1	C	436	ALA	CA-C-N	5.23	125.77	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	ALA	C-N-CA	5.23	125.77	120.38
1	D	156	ASN	CA-CB-CG	5.23	117.83	112.60
2	B	626	MET	CA-C-N	5.21	131.49	121.54
2	B	626	MET	C-N-CA	5.21	131.49	121.54
6	N	97	VAL	N-CA-C	5.16	115.34	108.11
3	O	77	HIS	N-CA-C	5.16	117.38	109.07
1	D	372	VAL	N-CA-C	5.15	115.92	110.72
5	M	97	SER	N-CA-C	5.15	116.67	108.79
1	A	383	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	272	ILE	N-CA-C	5.13	116.55	111.67
5	M	99	VAL	N-CA-C	5.12	115.23	107.80
6	N	48	TYR	N-CA-C	-5.11	100.43	108.00
1	C	123	THR	CA-C-N	5.11	124.83	119.82
1	C	123	THR	C-N-CA	5.11	124.83	119.82
4	R	58	LEU	CA-C-N	5.10	125.04	119.78
4	R	58	LEU	C-N-CA	5.10	125.04	119.78
1	C	205	CYS	CA-C-N	5.10	125.04	119.78
1	C	205	CYS	C-N-CA	5.10	125.04	119.78
4	L	9	LEU	N-CA-C	-5.10	107.19	113.41
2	E	654	GLU	CA-C-N	5.06	130.81	121.70
2	E	654	GLU	C-N-CA	5.06	130.81	121.70
1	D	359	ILE	N-CA-C	5.05	115.24	108.17
3	O	25	TYR	N-CA-C	5.04	119.39	112.88
1	A	208	VAL	N-CA-C	5.02	115.54	108.36
2	F	527	GLY	N-CA-C	-5.02	106.88	115.61
1	C	79	PRO	N-CA-C	-5.01	103.42	111.38
6	N	33	TRP	N-CA-C	5.01	117.56	109.40
1	A	368	ASP	CA-C-N	5.00	125.27	119.47
1	A	368	ASP	C-N-CA	5.00	125.27	119.47
2	B	571	TRP	N-CA-C	-5.00	107.83	114.04
3	Q	96	GLY	CA-C-N	5.00	124.91	119.76
3	Q	96	GLY	C-N-CA	5.00	124.91	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3460	0	3412	10	0
1	C	3460	0	3410	4	0
1	D	3460	0	3410	6	0
2	B	954	0	945	3	0
2	E	982	0	969	1	0
2	F	1058	0	1038	3	0
3	H	934	0	900	0	0
3	O	934	0	900	1	0
3	Q	934	0	900	0	0
4	L	856	0	848	1	0
4	P	856	0	848	1	0
4	R	856	0	848	2	0
5	M	971	0	948	6	0
5	S	938	0	913	7	0
6	N	814	0	785	4	0
6	T	814	0	785	4	0
7	G	28	0	25	0	0
7	V	28	0	25	0	0
7	e	28	0	25	2	0
8	I	61	0	52	0	0
8	U	61	0	52	0	0
8	W	61	0	52	0	0
8	Y	61	0	52	0	0
8	Z	61	0	52	1	0
8	b	61	0	52	0	0
8	f	61	0	52	0	0
9	J	83	0	70	0	0
9	X	83	0	70	0	0
9	c	83	0	70	0	0
10	K	50	0	43	0	0
11	a	39	0	34	0	0
12	d	94	0	79	0	0
13	A	70	0	65	1	0
13	C	112	0	104	0	0
13	D	112	0	104	0	0
All	All	23518	0	22937	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:ARG:HH12	8:Z:1:NAG:H81	1.65	0.62
5:M:100(G):TRP:HE1	6:N:48:TYR:H	1.48	0.62
5:S:100(D):MET:HE2	6:T:91:SER:HA	1.82	0.60
5:S:100(H):PHE:O	5:S:103:TRP:NE1	2.35	0.60
5:S:35:ASN:ND2	5:S:95:GLU:HB2	2.20	0.57
1:A:113:ASP:OD1	1:A:429:LYS:NZ	2.38	0.56
1:D:501:CYS:O	1:D:502:LYS:C	2.47	0.56
1:D:265:LEU:HD11	7:e:1:NAG:H81	1.89	0.55
1:A:59:LYS:NZ	1:A:62:ASP:OD2	2.40	0.55
1:D:500:LYS:NZ	6:N:51:ASP:OD2	2.39	0.55
1:A:501:CYS:O	1:A:502:LYS:C	2.51	0.53
1:D:107:ASP:OD1	2:F:574:LYS:NZ	2.42	0.52
1:A:133:ASP:OD1	1:A:155:LYS:NZ	2.43	0.52
1:C:231:LYS:NZ	1:C:267:GLU:OE1	2.43	0.51
2:B:531:GLY:O	2:B:532:ALA:C	2.55	0.50
5:M:100(G):TRP:NE1	6:N:48:TYR:H	2.11	0.49
4:R:60:ASP:OD1	4:R:60:ASP:N	2.46	0.48
2:B:642:ILE:O	2:B:643:TYR:C	2.54	0.48
1:A:40:TYR:O	1:A:40:TYR:CG	2.65	0.48
1:C:72:HIS:ND1	1:C:72:HIS:N	2.57	0.47
5:S:100(B):ASP:OD1	5:S:100(B):ASP:N	2.45	0.47
1:A:490:LYS:NZ	1:A:492:GLU:OE2	2.49	0.46
1:A:363:GLN:HB2	13:A:605:NAG:H82	1.98	0.46
4:L:27(D):HIS:ND1	4:L:27(E):SER:N	2.64	0.46
6:T:26:ILE:HG23	6:T:31:VAL:HG21	1.97	0.46
1:C:123:THR:N	1:C:124:PRO:CD	2.78	0.46
1:A:123:THR:N	1:A:124:PRO:CD	2.79	0.46
4:R:27(D):HIS:ND1	4:R:27(E):SER:N	2.64	0.45
5:S:100(F):ARG:HD2	6:T:89:TRP:CE2	2.50	0.45
5:M:100(B):ASP:N	5:M:100(B):ASP:OD1	2.43	0.45
1:D:265:LEU:CD1	7:e:1:NAG:H81	2.46	0.44
1:A:63:THR:O	1:A:64:GLU:C	2.58	0.44
2:F:596:TRP:O	2:F:650:GLN:HG2	2.17	0.44
5:S:100(E):VAL:HG21	6:T:48:TYR:CE1	2.52	0.44
1:A:345:ILE:O	1:A:349:LEU:N	2.50	0.44
2:F:541:ALA:O	2:F:542:ARG:HB2	2.17	0.44
6:N:64:LYS:HE3	6:N:64:LYS:HB3	1.87	0.42
1:D:123:THR:N	1:D:124:PRO:CD	2.82	0.42
5:M:6:GLU:OE2	5:M:105:GLN:N	2.51	0.42
2:B:533:ALA:HB3	2:B:623:TRP:HA	2.00	0.42
5:S:29:ILE:HA	5:S:94:ARG:HH21	1.84	0.42
2:E:549:VAL:O	2:E:550:GLN:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:72:ASP:OD2	5:M:75:LYS:NZ	2.40	0.41
3:O:36:TRP:CE2	3:O:80:LEU:HB2	2.55	0.41
4:P:7:THR:HB	4:P:8:PRO:HD3	2.03	0.41
5:M:53:PHE:CD2	5:M:53:PHE:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/482 (89%)	413 (96%)	15 (4%)	0	100	100
1	C	428/482 (89%)	422 (99%)	6 (1%)	0	100	100
1	D	428/482 (89%)	414 (97%)	14 (3%)	0	100	100
2	B	116/154 (75%)	110 (95%)	6 (5%)	0	100	100
2	E	119/154 (77%)	116 (98%)	3 (2%)	0	100	100
2	F	128/154 (83%)	122 (95%)	6 (5%)	0	100	100
3	H	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
3	O	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
3	Q	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
4	L	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
4	P	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
4	R	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
5	M	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
5	S	117/124 (94%)	113 (97%)	4 (3%)	0	100	100
6	N	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
6	T	105/108 (97%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2780/3068 (91%)	2699 (97%)	81 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	393/429 (92%)	393 (100%)	0	100	100
1	C	393/429 (92%)	393 (100%)	0	100	100
1	D	393/429 (92%)	392 (100%)	1 (0%)	86	85
2	B	102/130 (78%)	102 (100%)	0	100	100
2	E	105/130 (81%)	105 (100%)	0	100	100
2	F	114/130 (88%)	114 (100%)	0	100	100
3	H	101/101 (100%)	101 (100%)	0	100	100
3	O	101/101 (100%)	101 (100%)	0	100	100
3	Q	101/101 (100%)	101 (100%)	0	100	100
4	L	98/98 (100%)	98 (100%)	0	100	100
4	P	98/98 (100%)	98 (100%)	0	100	100
4	R	98/98 (100%)	98 (100%)	0	100	100
5	M	109/109 (100%)	109 (100%)	0	100	100
5	S	104/109 (95%)	103 (99%)	1 (1%)	68	76
6	N	90/91 (99%)	90 (100%)	0	100	100
6	T	90/91 (99%)	90 (100%)	0	100	100
All	All	2490/2674 (93%)	2488 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	88	ASN

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Mol	Chain	Res	Type
5	S	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
2	B	575	GLN
2	B	650	GLN
1	C	82	GLN
1	C	92	ASN
1	C	344	GLN
1	C	413	HIS
1	C	442	GLN
1	D	344	GLN
1	D	352	GLN
1	D	413	HIS
2	F	575	GLN
3	H	100	HIS
5	M	39	GLN
6	N	36	GLN
4	P	37	GLN
3	Q	100	HIS
6	T	32	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

77 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	1	1,7	14,14,15	2.38	7 (50%)	17,19,21	1.09	2 (11%)
7	NAG	G	2	7	14,14,15	2.09	4 (28%)	17,19,21	0.94	1 (5%)
8	NAG	I	1	1,8	14,14,15	2.21	6 (42%)	17,19,21	1.56	3 (17%)
8	NAG	I	2	8	14,14,15	2.24	6 (42%)	17,19,21	1.33	4 (23%)
8	BMA	I	3	8	11,11,12	1.46	3 (27%)	15,15,17	0.66	0
8	MAN	I	4	8	11,11,12	1.96	5 (45%)	15,15,17	0.61	0
8	MAN	I	5	8	11,11,12	1.93	6 (54%)	15,15,17	0.70	0
9	NAG	J	1	1,9	14,14,15	1.95	4 (28%)	17,19,21	1.20	1 (5%)
9	NAG	J	2	9	14,14,15	2.13	6 (42%)	17,19,21	1.26	2 (11%)
9	BMA	J	3	9	11,11,12	1.41	3 (27%)	15,15,17	0.62	0
9	MAN	J	4	9	11,11,12	1.38	2 (18%)	15,15,17	0.60	0
9	MAN	J	5	9	11,11,12	1.89	5 (45%)	15,15,17	0.80	0
9	MAN	J	6	9	11,11,12	1.80	4 (36%)	15,15,17	0.77	0
9	MAN	J	7	9	11,11,12	1.91	5 (45%)	15,15,17	0.75	0
10	NAG	K	1	1,10	14,14,15	2.13	7 (50%)	17,19,21	2.63	5 (29%)
10	NAG	K	2	10	14,14,15	2.03	5 (35%)	17,19,21	1.29	3 (17%)
10	BMA	K	3	10	11,11,12	0.73	0	15,15,17	0.87	0
10	MAN	K	4	10	11,11,12	1.98	6 (54%)	15,15,17	0.72	0
8	NAG	U	1	1,8	14,14,15	2.09	7 (50%)	17,19,21	1.28	2 (11%)
8	NAG	U	2	8	14,14,15	2.13	4 (28%)	17,19,21	1.13	3 (17%)
8	BMA	U	3	8	11,11,12	1.43	2 (18%)	15,15,17	0.65	0
8	MAN	U	4	8	11,11,12	1.97	6 (54%)	15,15,17	0.91	1 (6%)
8	MAN	U	5	8	11,11,12	1.87	5 (45%)	15,15,17	0.75	0
7	NAG	V	1	1,7	14,14,15	2.31	7 (50%)	17,19,21	1.30	2 (11%)
7	NAG	V	2	7	14,14,15	2.06	6 (42%)	17,19,21	0.93	2 (11%)
8	NAG	W	1	1,8	14,14,15	1.81	2 (14%)	17,19,21	1.14	2 (11%)
8	NAG	W	2	8	14,14,15	1.80	5 (35%)	17,19,21	1.01	1 (5%)
8	BMA	W	3	8	11,11,12	1.39	2 (18%)	15,15,17	0.63	0
8	MAN	W	4	8	11,11,12	1.83	4 (36%)	15,15,17	0.73	0
8	MAN	W	5	8	11,11,12	1.96	5 (45%)	15,15,17	0.67	0
9	NAG	X	1	1,9	14,14,15	1.77	2 (14%)	17,19,21	1.18	2 (11%)
9	NAG	X	2	9	14,14,15	1.83	4 (28%)	17,19,21	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BMA	X	3	9	11,11,12	1.36	2 (18%)	15,15,17	0.59	0
9	MAN	X	4	9	11,11,12	1.35	1 (9%)	15,15,17	0.68	0
9	MAN	X	5	9	11,11,12	1.88	4 (36%)	15,15,17	0.75	0
9	MAN	X	6	9	11,11,12	1.74	4 (36%)	15,15,17	0.78	0
9	MAN	X	7	9	11,11,12	1.95	4 (36%)	15,15,17	0.66	0
8	NAG	Y	1	1,8	14,14,15	1.99	5 (35%)	17,19,21	1.08	1 (5%)
8	NAG	Y	2	8	14,14,15	1.86	5 (35%)	17,19,21	1.03	1 (5%)
8	BMA	Y	3	8	11,11,12	1.36	3 (27%)	15,15,17	0.60	0
8	MAN	Y	4	8	11,11,12	1.94	5 (45%)	15,15,17	0.71	0
8	MAN	Y	5	8	11,11,12	1.87	5 (45%)	15,15,17	0.69	0
8	NAG	Z	1	1,8	14,14,15	2.08	4 (28%)	17,19,21	1.17	3 (17%)
8	NAG	Z	2	8	14,14,15	1.98	4 (28%)	17,19,21	0.90	0
8	BMA	Z	3	8	11,11,12	1.53	3 (27%)	15,15,17	0.71	0
8	MAN	Z	4	8	11,11,12	2.04	5 (45%)	15,15,17	0.74	0
8	MAN	Z	5	8	11,11,12	1.89	5 (45%)	15,15,17	0.70	0
11	NAG	a	1	11,1	14,14,15	2.11	6 (42%)	17,19,21	1.03	0
11	NAG	a	2	11	14,14,15	2.07	6 (42%)	17,19,21	0.95	1 (5%)
11	BMA	a	3	11	11,11,12	1.99	6 (54%)	15,15,17	0.65	0
8	NAG	b	1	1,8	14,14,15	2.04	4 (28%)	17,19,21	1.00	1 (5%)
8	NAG	b	2	8	14,14,15	0.51	0	17,19,21	1.09	1 (5%)
8	BMA	b	3	8	11,11,12	1.42	3 (27%)	15,15,17	0.58	0
8	MAN	b	4	8	11,11,12	1.90	5 (45%)	15,15,17	0.74	0
8	MAN	b	5	8	11,11,12	1.98	5 (45%)	15,15,17	0.69	0
9	NAG	c	1	1,9	14,14,15	1.94	5 (35%)	17,19,21	1.18	1 (5%)
9	NAG	c	2	9	14,14,15	1.93	6 (42%)	17,19,21	1.03	1 (5%)
9	BMA	c	3	9	11,11,12	1.42	3 (27%)	15,15,17	0.63	0
9	MAN	c	4	9	11,11,12	1.52	2 (18%)	15,15,17	0.92	0
9	MAN	c	5	9	11,11,12	1.89	5 (45%)	15,15,17	0.71	0
9	MAN	c	6	9	11,11,12	1.91	5 (45%)	15,15,17	0.83	0
9	MAN	c	7	9	11,11,12	1.97	6 (54%)	15,15,17	0.70	0
12	NAG	d	1	1,12	14,14,15	1.97	7 (50%)	17,19,21	1.34	2 (11%)
12	NAG	d	2	12	14,14,15	2.00	5 (35%)	17,19,21	0.93	1 (5%)
12	BMA	d	3	12	11,11,12	1.39	2 (18%)	15,15,17	0.69	0
12	MAN	d	4	12	11,11,12	1.01	2 (18%)	15,15,17	1.57	2 (13%)
12	MAN	d	5	12	11,11,12	1.96	5 (45%)	15,15,17	0.79	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	d	6	12	11,11,12	1.42	2 (18%)	15,15,17	0.70	0
12	MAN	d	7	12	11,11,12	1.98	6 (54%)	15,15,17	0.60	0
12	MAN	d	8	12	11,11,12	1.95	6 (54%)	15,15,17	0.68	0
7	NAG	e	1	1,7	14,14,15	2.06	5 (35%)	17,19,21	1.00	1 (5%)
7	NAG	e	2	7	14,14,15	2.02	6 (42%)	17,19,21	1.01	1 (5%)
8	NAG	f	1	1,8	14,14,15	2.11	6 (42%)	17,19,21	1.10	2 (11%)
8	NAG	f	2	8	14,14,15	1.90	5 (35%)	17,19,21	0.94	1 (5%)
8	BMA	f	3	8	11,11,12	1.43	3 (27%)	15,15,17	0.58	0
8	MAN	f	4	8	11,11,12	1.99	5 (45%)	15,15,17	0.64	0
8	MAN	f	5	8	11,11,12	1.88	5 (45%)	15,15,17	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
8	NAG	I	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	BMA	I	3	8	-	0/2/19/22	0/1/1/1
8	MAN	I	4	8	-	2/2/19/22	0/1/1/1
8	MAN	I	5	8	-	1/2/19/22	0/1/1/1
9	NAG	J	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
9	BMA	J	3	9	-	0/2/19/22	0/1/1/1
9	MAN	J	4	9	-	0/2/19/22	0/1/1/1
9	MAN	J	5	9	-	1/2/19/22	0/1/1/1
9	MAN	J	6	9	-	1/2/19/22	0/1/1/1
9	MAN	J	7	9	-	1/2/19/22	0/1/1/1
10	NAG	K	1	1,10	-	3/6/23/26	0/1/1/1
10	NAG	K	2	10	-	1/6/23/26	0/1/1/1
10	BMA	K	3	10	-	2/2/19/22	0/1/1/1
10	MAN	K	4	10	-	0/2/19/22	0/1/1/1
8	NAG	U	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	U	2	8	-	0/6/23/26	0/1/1/1
8	BMA	U	3	8	-	2/2/19/22	0/1/1/1
8	MAN	U	4	8	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	U	5	8	-	0/2/19/22	0/1/1/1
7	NAG	V	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
8	NAG	W	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
8	BMA	W	3	8	-	0/2/19/22	0/1/1/1
8	MAN	W	4	8	-	1/2/19/22	0/1/1/1
8	MAN	W	5	8	-	1/2/19/22	0/1/1/1
9	NAG	X	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	0/6/23/26	0/1/1/1
9	BMA	X	3	9	-	0/2/19/22	0/1/1/1
9	MAN	X	4	9	-	2/2/19/22	0/1/1/1
9	MAN	X	5	9	-	0/2/19/22	0/1/1/1
9	MAN	X	6	9	-	0/2/19/22	0/1/1/1
9	MAN	X	7	9	-	0/2/19/22	0/1/1/1
8	NAG	Y	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	1/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	5	8	-	0/2/19/22	0/1/1/1
8	NAG	Z	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Z	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Z	4	8	-	1/2/19/22	0/1/1/1
8	MAN	Z	5	8	-	1/2/19/22	0/1/1/1
11	NAG	a	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	a	2	11	-	0/6/23/26	0/1/1/1
11	BMA	a	3	11	-	0/2/19/22	0/1/1/1
8	NAG	b	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	BMA	b	3	8	-	0/2/19/22	0/1/1/1
8	MAN	b	4	8	-	1/2/19/22	0/1/1/1
8	MAN	b	5	8	-	1/2/19/22	0/1/1/1
9	NAG	c	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	c	2	9	-	0/6/23/26	0/1/1/1
9	BMA	c	3	9	-	0/2/19/22	0/1/1/1
9	MAN	c	4	9	-	1/2/19/22	0/1/1/1
9	MAN	c	5	9	-	1/2/19/22	0/1/1/1
9	MAN	c	6	9	-	0/2/19/22	0/1/1/1
9	MAN	c	7	9	-	1/2/19/22	0/1/1/1
12	NAG	d	1	1,12	-	0/6/23/26	0/1/1/1
12	NAG	d	2	12	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BMA	d	3	12	-	1/2/19/22	0/1/1/1
12	MAN	d	4	12	-	2/2/19/22	0/1/1/1
12	MAN	d	5	12	-	0/2/19/22	0/1/1/1
12	MAN	d	6	12	-	2/2/19/22	0/1/1/1
12	MAN	d	7	12	-	0/2/19/22	0/1/1/1
12	MAN	d	8	12	-	0/2/19/22	0/1/1/1
7	NAG	e	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
8	NAG	f	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	BMA	f	3	8	-	0/2/19/22	0/1/1/1
8	MAN	f	4	8	-	0/2/19/22	0/1/1/1
8	MAN	f	5	8	-	0/2/19/22	0/1/1/1

All (341) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	NAG	C1-C2	6.19	1.60	1.52
11	a	1	NAG	C1-C2	5.47	1.59	1.52
7	V	1	NAG	C1-C2	5.46	1.59	1.52
8	Z	1	NAG	C1-C2	5.40	1.59	1.52
8	U	2	NAG	C1-C2	5.38	1.59	1.52
8	I	2	NAG	C1-C2	5.27	1.59	1.52
8	b	1	NAG	C1-C2	5.22	1.59	1.52
8	I	1	NAG	C1-C2	5.21	1.59	1.52
8	f	1	NAG	C1-C2	5.18	1.59	1.52
9	c	1	NAG	C1-C2	5.09	1.59	1.52
9	J	2	NAG	C1-C2	5.07	1.59	1.52
7	G	2	NAG	C1-C2	5.05	1.59	1.52
8	W	1	NAG	C1-C2	5.00	1.59	1.52
10	K	1	NAG	C1-C2	4.92	1.59	1.52
8	Y	1	NAG	C1-C2	4.91	1.59	1.52
7	e	1	NAG	C1-C2	4.86	1.59	1.52
7	e	2	NAG	C1-C2	4.80	1.58	1.52
7	V	2	NAG	C1-C2	4.77	1.58	1.52
12	d	2	NAG	C1-C2	4.74	1.58	1.52
8	U	1	NAG	C1-C2	4.73	1.58	1.52
12	d	1	NAG	C1-C2	4.69	1.58	1.52
11	a	2	NAG	C1-C2	4.68	1.58	1.52
9	J	1	NAG	C1-C2	4.60	1.58	1.52
9	X	1	NAG	C1-C2	4.54	1.58	1.52
8	Z	2	NAG	C1-C2	4.50	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	2	NAG	C1-C2	4.36	1.58	1.52
8	f	2	NAG	C1-C2	4.36	1.58	1.52
9	X	2	NAG	C1-C2	4.31	1.58	1.52
10	K	2	NAG	C1-C2	4.16	1.58	1.52
8	Y	2	NAG	C1-C2	4.03	1.57	1.52
8	W	2	NAG	C1-C2	3.88	1.57	1.52
7	e	1	NAG	O5-C5	3.54	1.50	1.43
8	Z	4	MAN	O5-C5	3.52	1.50	1.43
8	U	4	MAN	O5-C5	3.47	1.50	1.43
12	d	8	MAN	O5-C5	3.36	1.50	1.43
7	V	1	NAG	O5-C5	3.36	1.50	1.43
12	d	7	MAN	O5-C5	3.35	1.50	1.43
8	b	5	MAN	C2-C3	3.34	1.57	1.52
8	W	5	MAN	O5-C5	3.29	1.49	1.43
8	I	5	MAN	C2-C3	3.29	1.57	1.52
11	a	3	BMA	O5-C5	3.29	1.49	1.43
10	K	4	MAN	O5-C5	3.28	1.49	1.43
7	V	2	NAG	O5-C5	3.27	1.49	1.43
9	c	7	MAN	O5-C5	3.26	1.49	1.43
8	I	5	MAN	O5-C5	3.25	1.49	1.43
8	b	5	MAN	O5-C5	3.24	1.49	1.43
9	X	7	MAN	O5-C5	3.24	1.49	1.43
8	f	4	MAN	O5-C5	3.23	1.49	1.43
8	I	4	MAN	O5-C5	3.21	1.49	1.43
8	f	5	MAN	O5-C5	3.21	1.49	1.43
9	c	6	MAN	O5-C5	3.21	1.49	1.43
8	Y	4	MAN	C2-C3	3.21	1.57	1.52
8	W	5	MAN	C2-C3	3.20	1.57	1.52
8	Y	4	MAN	O5-C5	3.20	1.49	1.43
7	G	2	NAG	O5-C5	3.20	1.49	1.43
8	U	5	MAN	O5-C5	3.19	1.49	1.43
11	a	3	BMA	C2-C3	3.18	1.57	1.52
8	f	4	MAN	C2-C3	3.18	1.57	1.52
9	X	7	MAN	C2-C3	3.18	1.57	1.52
8	Y	5	MAN	O5-C5	3.17	1.49	1.43
11	a	2	NAG	O5-C5	3.17	1.49	1.43
8	U	2	NAG	O5-C5	3.17	1.49	1.43
12	d	8	MAN	C2-C3	3.17	1.57	1.52
9	J	5	MAN	O5-C5	3.15	1.49	1.43
8	I	2	NAG	C3-C2	3.15	1.59	1.52
10	K	2	NAG	C4-C5	3.15	1.59	1.53
8	Z	2	NAG	O5-C5	3.14	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Z	4	MAN	C1-C2	3.14	1.59	1.52
10	K	2	NAG	O5-C5	3.14	1.49	1.43
12	d	5	MAN	C2-C3	3.14	1.57	1.52
8	Z	5	MAN	O5-C5	3.13	1.49	1.43
8	U	4	MAN	C2-C3	3.12	1.57	1.52
12	d	5	MAN	O5-C5	3.12	1.49	1.43
9	X	5	MAN	C2-C3	3.10	1.57	1.52
9	J	7	MAN	O5-C5	3.09	1.49	1.43
9	X	5	MAN	O5-C5	3.09	1.49	1.43
12	d	7	MAN	C2-C3	3.09	1.57	1.52
8	b	4	MAN	O5-C5	3.08	1.49	1.43
8	f	1	NAG	O5-C5	3.08	1.49	1.43
9	J	7	MAN	C2-C3	3.07	1.57	1.52
8	I	2	NAG	C2-N2	3.05	1.51	1.46
10	K	4	MAN	C2-C3	3.05	1.57	1.52
12	d	2	NAG	O5-C5	3.04	1.49	1.43
9	c	5	MAN	C2-C3	3.03	1.57	1.52
9	c	7	MAN	C2-C3	3.02	1.57	1.52
8	U	5	MAN	C2-C3	3.02	1.57	1.52
8	b	1	NAG	O5-C5	3.01	1.49	1.43
8	f	5	MAN	C2-C3	3.01	1.57	1.52
9	c	5	MAN	O5-C5	3.01	1.49	1.43
9	J	6	MAN	O5-C5	3.01	1.49	1.43
7	e	2	NAG	O5-C5	3.00	1.49	1.43
8	b	4	MAN	C2-C3	2.99	1.57	1.52
8	W	4	MAN	O5-C5	2.98	1.49	1.43
8	I	1	NAG	O5-C5	2.98	1.49	1.43
7	G	1	NAG	O5-C5	2.98	1.49	1.43
8	Z	5	MAN	C2-C3	2.97	1.57	1.52
10	K	1	NAG	O5-C5	2.97	1.49	1.43
11	a	1	NAG	O5-C5	2.97	1.49	1.43
8	f	4	MAN	C1-C2	2.97	1.59	1.52
8	I	4	MAN	C2-C3	2.96	1.57	1.52
9	J	6	MAN	C2-C3	2.95	1.57	1.52
8	I	4	MAN	C1-C2	2.94	1.59	1.52
9	J	2	NAG	C3-C2	2.93	1.58	1.52
8	Z	1	NAG	O5-C5	2.93	1.49	1.43
8	Y	5	MAN	C2-C3	2.92	1.57	1.52
12	d	5	MAN	C1-C2	2.92	1.59	1.52
8	Z	4	MAN	C2-C3	2.91	1.56	1.52
8	W	2	NAG	O5-C5	2.91	1.49	1.43
9	c	6	MAN	C2-C3	2.90	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	4	MAN	C2-C3	2.89	1.56	1.52
7	V	1	NAG	C4-C5	2.86	1.59	1.53
9	J	5	MAN	C1-C2	2.86	1.59	1.52
8	f	2	NAG	O5-C5	2.84	1.49	1.43
9	X	6	MAN	O5-C5	2.82	1.48	1.43
8	U	1	NAG	O5-C5	2.81	1.48	1.43
8	Y	2	NAG	O5-C5	2.78	1.48	1.43
7	G	2	NAG	C3-C2	2.76	1.58	1.52
11	a	3	BMA	C1-C2	2.73	1.58	1.52
12	d	7	MAN	C1-C2	2.72	1.58	1.52
9	c	2	NAG	O5-C5	2.71	1.48	1.43
9	X	6	MAN	C2-C3	2.70	1.56	1.52
12	d	1	NAG	O5-C5	2.69	1.48	1.43
9	J	2	NAG	C2-N2	2.69	1.50	1.46
9	J	5	MAN	C2-C3	2.69	1.56	1.52
8	Y	1	NAG	O5-C5	2.67	1.48	1.43
7	e	1	NAG	C4-C5	2.67	1.58	1.53
10	K	1	NAG	C3-C2	2.66	1.58	1.52
9	c	7	MAN	C1-C2	2.66	1.58	1.52
8	b	4	MAN	C1-C2	2.64	1.58	1.52
8	W	5	MAN	C1-C2	2.63	1.58	1.52
9	X	7	MAN	C1-C2	2.62	1.58	1.52
9	J	1	NAG	O5-C5	2.62	1.48	1.43
8	Z	3	BMA	C2-C3	2.62	1.56	1.52
9	c	6	MAN	C1-C2	2.62	1.58	1.52
7	V	1	NAG	C2-N2	2.61	1.50	1.46
8	I	1	NAG	C4-C3	2.61	1.59	1.52
9	J	2	NAG	O5-C5	2.59	1.48	1.43
10	K	4	MAN	C4-C5	2.58	1.58	1.53
8	b	4	MAN	C4-C5	2.58	1.58	1.53
8	Z	5	MAN	C1-C2	2.57	1.58	1.52
9	c	7	MAN	C4-C5	2.57	1.58	1.53
8	I	2	NAG	O5-C5	2.57	1.48	1.43
8	I	1	NAG	C3-C2	2.56	1.57	1.52
9	c	4	MAN	O5-C5	2.56	1.48	1.43
9	J	1	NAG	C4-C3	2.55	1.59	1.52
8	I	1	NAG	O4-C4	2.55	1.49	1.43
11	a	2	NAG	C4-C5	2.53	1.58	1.53
8	I	2	NAG	C4-C3	2.53	1.58	1.52
8	W	4	MAN	C1-C2	2.53	1.58	1.52
8	Y	4	MAN	C1-C2	2.53	1.58	1.52
8	b	5	MAN	C1-C2	2.53	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	1	NAG	C4-C5	2.53	1.58	1.53
8	U	2	NAG	C3-C2	2.52	1.57	1.52
9	c	5	MAN	C1-C2	2.52	1.58	1.52
8	f	3	BMA	O5-C5	2.51	1.48	1.43
12	d	6	MAN	O5-C5	2.50	1.48	1.43
7	V	2	NAG	C3-C2	2.50	1.57	1.52
8	Z	4	MAN	C4-C5	2.50	1.58	1.53
8	f	2	NAG	C3-C2	2.50	1.57	1.52
9	J	7	MAN	C1-C2	2.50	1.58	1.52
11	a	2	NAG	C3-C2	2.49	1.57	1.52
9	J	6	MAN	C1-C2	2.49	1.58	1.52
8	Z	2	NAG	C4-C5	2.49	1.58	1.53
7	G	1	NAG	O5-C1	2.49	1.47	1.43
9	J	7	MAN	C4-C5	2.49	1.58	1.53
10	K	2	NAG	C4-C3	2.49	1.58	1.52
9	c	6	MAN	C4-C5	2.48	1.58	1.53
8	f	1	NAG	O5-C1	2.48	1.47	1.43
9	J	5	MAN	C4-C5	2.48	1.58	1.53
9	X	7	MAN	C4-C5	2.47	1.58	1.53
8	I	4	MAN	C4-C5	2.46	1.58	1.53
8	W	3	BMA	O5-C5	2.45	1.48	1.43
9	X	5	MAN	C1-C2	2.45	1.58	1.52
8	b	3	BMA	O5-C5	2.45	1.48	1.43
9	X	2	NAG	O5-C5	2.44	1.48	1.43
10	K	4	MAN	C1-C2	2.44	1.58	1.52
8	Z	5	MAN	C4-C5	2.44	1.58	1.53
7	e	2	NAG	C3-C2	2.44	1.57	1.52
8	I	3	BMA	O5-C5	2.44	1.48	1.43
8	b	5	MAN	C4-C5	2.44	1.58	1.53
9	c	5	MAN	C4-C5	2.43	1.58	1.53
8	U	4	MAN	C4-C5	2.43	1.58	1.53
8	U	3	BMA	O5-C5	2.43	1.48	1.43
9	J	4	MAN	O5-C5	2.42	1.48	1.43
7	V	1	NAG	C3-C2	2.42	1.57	1.52
9	X	3	BMA	O5-C5	2.41	1.48	1.43
7	V	2	NAG	C4-C5	2.41	1.58	1.53
8	f	5	MAN	C4-C5	2.41	1.58	1.53
8	U	4	MAN	C1-C2	2.41	1.57	1.52
7	G	1	NAG	C4-C3	2.40	1.58	1.52
9	c	3	BMA	C2-C3	2.40	1.56	1.52
9	c	4	MAN	C2-C3	2.40	1.56	1.52
8	U	5	MAN	C4-C5	2.40	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	2	NAG	O5-C1	2.40	1.47	1.43
9	X	1	NAG	C4-C3	2.40	1.58	1.52
8	Y	2	NAG	C3-C2	2.40	1.57	1.52
8	Y	5	MAN	C4-C5	2.40	1.58	1.53
9	X	4	MAN	O5-C5	2.39	1.48	1.43
12	d	7	MAN	C4-C5	2.38	1.58	1.53
12	d	1	NAG	C2-N2	2.38	1.50	1.46
9	c	2	NAG	C4-C3	2.38	1.58	1.52
11	a	3	BMA	C4-C5	2.38	1.58	1.53
8	Z	2	NAG	C3-C2	2.38	1.57	1.52
8	I	3	BMA	C2-C3	2.37	1.56	1.52
9	J	6	MAN	C4-C5	2.37	1.58	1.53
9	c	1	NAG	C4-C3	2.36	1.58	1.52
9	J	3	BMA	O5-C5	2.36	1.48	1.43
12	d	8	MAN	C1-C2	2.36	1.57	1.52
8	I	5	MAN	C4-C5	2.35	1.58	1.53
12	d	2	NAG	C4-C5	2.35	1.58	1.53
8	Y	5	MAN	C1-C2	2.35	1.57	1.52
10	K	1	NAG	C4-C3	2.34	1.58	1.52
7	e	1	NAG	O5-C1	2.33	1.47	1.43
12	d	2	NAG	C3-C2	2.33	1.57	1.52
12	d	8	MAN	C4-C5	2.33	1.58	1.53
7	G	1	NAG	C4-C5	2.33	1.58	1.53
8	W	5	MAN	C4-C5	2.33	1.58	1.53
7	G	1	NAG	C3-C2	2.33	1.57	1.52
10	K	2	NAG	C3-C2	2.32	1.57	1.52
8	W	4	MAN	C4-C5	2.32	1.58	1.53
12	d	6	MAN	C2-C3	2.32	1.56	1.52
8	Z	3	BMA	O5-C5	2.32	1.47	1.43
8	f	4	MAN	C4-C5	2.31	1.58	1.53
8	Y	4	MAN	C4-C5	2.31	1.57	1.53
8	Y	1	NAG	C4-C5	2.30	1.57	1.53
7	V	1	NAG	O5-C1	2.30	1.47	1.43
10	K	1	NAG	C4-C5	2.30	1.57	1.53
9	X	2	NAG	C3-C2	2.30	1.57	1.52
8	b	1	NAG	O5-C1	2.29	1.47	1.43
8	Z	3	BMA	C1-C2	2.29	1.57	1.52
8	b	3	BMA	C2-C3	2.29	1.56	1.52
8	U	1	NAG	C3-C2	2.29	1.57	1.52
7	e	2	NAG	C2-N2	2.29	1.50	1.46
8	U	1	NAG	C2-N2	2.29	1.50	1.46
8	f	5	MAN	C1-C2	2.28	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	2	NAG	C4-C3	2.28	1.58	1.52
8	Y	2	NAG	C4-C5	2.28	1.57	1.53
8	Z	1	NAG	O5-C1	2.27	1.47	1.43
8	U	1	NAG	C4-C3	2.27	1.58	1.52
10	K	1	NAG	C2-N2	2.26	1.50	1.46
12	d	4	MAN	C1-C2	2.25	1.57	1.52
9	J	1	NAG	C4-C5	2.25	1.57	1.53
9	X	5	MAN	C4-C5	2.25	1.57	1.53
8	Y	2	NAG	C4-C3	2.25	1.58	1.52
7	e	2	NAG	C4-C5	2.25	1.57	1.53
8	Y	3	BMA	O5-C5	2.25	1.47	1.43
9	c	3	BMA	O5-C5	2.24	1.47	1.43
11	a	1	NAG	C4-C5	2.24	1.57	1.53
12	d	3	BMA	O5-C5	2.24	1.47	1.43
8	I	3	BMA	C1-C2	2.23	1.57	1.52
10	K	4	MAN	O5-C1	2.23	1.47	1.43
8	I	1	NAG	C4-C5	2.23	1.57	1.53
8	W	3	BMA	C2-C3	2.21	1.55	1.52
8	U	5	MAN	C1-C2	2.21	1.57	1.52
8	f	3	BMA	C2-C3	2.20	1.55	1.52
7	G	2	NAG	C4-C5	2.19	1.57	1.53
9	c	2	NAG	C4-C5	2.19	1.57	1.53
11	a	1	NAG	O5-C1	2.19	1.47	1.43
9	J	4	MAN	C2-C3	2.19	1.55	1.52
12	d	5	MAN	C4-C5	2.18	1.57	1.53
8	W	1	NAG	O5-C5	2.18	1.47	1.43
9	X	6	MAN	C1-C2	2.18	1.57	1.52
7	e	2	NAG	C4-C3	2.18	1.58	1.52
8	W	2	NAG	C3-C2	2.17	1.57	1.52
8	W	2	NAG	C4-C5	2.17	1.57	1.53
9	c	1	NAG	O5-C5	2.17	1.47	1.43
8	f	1	NAG	C4-C3	2.17	1.58	1.52
9	J	3	BMA	C2-C3	2.16	1.55	1.52
8	I	5	MAN	C1-C2	2.16	1.57	1.52
9	J	3	BMA	C1-C2	2.16	1.57	1.52
9	X	6	MAN	C4-C3	2.16	1.57	1.52
7	V	1	NAG	C4-C3	2.16	1.57	1.52
12	d	3	BMA	C1-C2	2.15	1.57	1.52
11	a	2	NAG	C4-C3	2.15	1.57	1.52
8	f	3	BMA	C1-C2	2.14	1.57	1.52
8	U	1	NAG	O4-C4	2.14	1.48	1.43
9	c	6	MAN	C4-C3	2.13	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	3	BMA	C1-C2	2.13	1.57	1.52
11	a	3	BMA	O5-C1	2.13	1.47	1.43
12	d	5	MAN	C4-C3	2.12	1.57	1.52
8	Z	4	MAN	O5-C1	2.12	1.47	1.43
8	W	5	MAN	C4-C3	2.11	1.57	1.52
9	c	2	NAG	C3-C2	2.11	1.56	1.52
8	Y	1	NAG	O5-C1	2.11	1.47	1.43
11	a	1	NAG	C4-C3	2.11	1.57	1.52
8	f	2	NAG	C4-C3	2.10	1.57	1.52
8	U	3	BMA	C1-C2	2.10	1.57	1.52
8	I	2	NAG	C4-C5	2.10	1.57	1.53
11	a	1	NAG	C3-C2	2.10	1.56	1.52
12	d	2	NAG	C4-C3	2.10	1.57	1.52
8	Y	3	BMA	C1-C2	2.10	1.57	1.52
12	d	8	MAN	C4-C3	2.09	1.57	1.52
9	c	1	NAG	C3-C2	2.09	1.56	1.52
8	b	3	BMA	C1-C2	2.09	1.57	1.52
8	Y	5	MAN	C4-C3	2.09	1.57	1.52
8	f	1	NAG	C4-C5	2.09	1.57	1.53
9	c	7	MAN	O5-C1	2.09	1.47	1.43
8	f	2	NAG	C4-C5	2.09	1.57	1.53
12	d	7	MAN	C4-C3	2.08	1.57	1.52
12	d	1	NAG	C3-C2	2.08	1.56	1.52
9	c	1	NAG	C4-C5	2.08	1.57	1.53
8	Y	4	MAN	O5-C1	2.07	1.47	1.43
12	d	1	NAG	O5-C1	2.07	1.47	1.43
9	X	3	BMA	C2-C3	2.07	1.55	1.52
8	f	5	MAN	C4-C3	2.07	1.57	1.52
9	J	2	NAG	C4-C5	2.07	1.57	1.53
8	U	4	MAN	C4-C3	2.07	1.57	1.52
8	f	4	MAN	C4-C3	2.07	1.57	1.52
12	d	1	NAG	C4-C5	2.07	1.57	1.53
8	W	2	NAG	C4-C3	2.06	1.57	1.52
7	V	2	NAG	C4-C3	2.06	1.57	1.52
9	c	5	MAN	O5-C1	2.06	1.47	1.43
8	b	5	MAN	C4-C3	2.06	1.57	1.52
8	Y	3	BMA	C2-C3	2.06	1.55	1.52
9	J	5	MAN	C4-C3	2.05	1.57	1.52
9	J	7	MAN	C4-C3	2.05	1.57	1.52
12	d	8	MAN	O5-C1	2.05	1.47	1.43
11	a	2	NAG	C2-N2	2.05	1.49	1.46
12	d	4	MAN	O2-C2	2.04	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	1	NAG	C3-C2	2.04	1.56	1.52
8	f	1	NAG	C3-C2	2.04	1.56	1.52
8	I	5	MAN	C4-C3	2.04	1.57	1.52
12	d	7	MAN	O5-C1	2.04	1.47	1.43
8	U	5	MAN	C4-C3	2.04	1.57	1.52
8	Z	1	NAG	C4-C5	2.04	1.57	1.53
8	U	4	MAN	O5-C1	2.04	1.47	1.43
10	K	4	MAN	C4-C3	2.03	1.57	1.52
8	b	4	MAN	C4-C3	2.03	1.57	1.52
9	X	2	NAG	C2-N2	2.03	1.49	1.46
7	V	2	NAG	C2-N2	2.03	1.49	1.46
10	K	1	NAG	O5-C1	2.03	1.47	1.43
9	c	7	MAN	C4-C3	2.03	1.57	1.52
9	c	2	NAG	C2-N2	2.03	1.49	1.46
8	Z	5	MAN	C4-C3	2.02	1.57	1.52
8	I	4	MAN	O5-C1	2.02	1.47	1.43
12	d	1	NAG	C4-C3	2.01	1.57	1.52
7	e	1	NAG	C4-C3	2.01	1.57	1.52
8	b	1	NAG	C3-C2	2.01	1.56	1.52
7	G	1	NAG	O4-C4	2.01	1.47	1.43
8	I	5	MAN	O5-C1	2.00	1.47	1.43
11	a	3	BMA	C4-C3	2.00	1.57	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	1	NAG	C8-C7-N2	7.61	128.75	116.12
10	K	1	NAG	O7-C7-N2	-4.74	113.60	121.98
12	d	4	MAN	O2-C2-C1	4.64	119.84	109.22
10	K	1	NAG	C2-N2-C7	4.39	128.79	122.90
8	I	1	NAG	O4-C4-C3	4.16	120.18	110.38
8	b	2	NAG	C1-O5-C5	3.70	117.14	112.19
12	d	1	NAG	C8-C7-N2	3.42	121.79	116.12
8	I	1	NAG	C8-C7-N2	3.00	121.10	116.12
10	K	2	NAG	O4-C4-C3	-2.95	103.42	110.38
12	d	4	MAN	O2-C2-C3	-2.92	104.10	110.15
8	I	1	NAG	O7-C7-C8	-2.90	116.89	122.05
8	U	1	NAG	C8-C7-N2	2.87	120.87	116.12
7	V	1	NAG	O4-C4-C3	-2.83	103.69	110.38
8	W	2	NAG	C8-C7-N2	2.78	120.73	116.12
9	c	1	NAG	O4-C4-C5	-2.72	102.63	109.32
8	I	2	NAG	C8-C7-N2	2.69	120.59	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Z	1	NAG	C8-C7-N2	2.63	120.47	116.12
9	X	1	NAG	O4-C4-C5	-2.62	102.87	109.32
8	f	1	NAG	C8-C7-N2	2.61	120.45	116.12
12	d	1	NAG	O7-C7-C8	-2.58	117.46	122.05
10	K	2	NAG	O5-C5-C6	-2.57	102.66	107.66
9	J	2	NAG	C8-C7-N2	2.56	120.36	116.12
10	K	1	NAG	C4-C3-C2	-2.54	107.30	111.02
10	K	1	NAG	O7-C7-C8	-2.47	117.65	122.05
8	U	2	NAG	C8-C7-N2	2.46	120.19	116.12
8	I	2	NAG	C1-O5-C5	2.45	115.47	112.19
8	Y	1	NAG	C8-C7-N2	2.45	120.18	116.12
8	U	1	NAG	O7-C7-C8	-2.44	117.72	122.05
7	V	2	NAG	C8-C7-N2	2.41	120.12	116.12
9	J	1	NAG	C8-C7-N2	2.34	120.00	116.12
9	J	2	NAG	C1-O5-C5	2.34	115.32	112.19
7	G	2	NAG	C8-C7-N2	2.28	119.91	116.12
8	Z	1	NAG	O7-C7-C8	-2.28	117.99	122.05
11	a	2	NAG	C8-C7-N2	2.25	119.84	116.12
9	X	1	NAG	C8-C7-N2	2.23	119.82	116.12
7	e	2	NAG	C8-C7-N2	2.20	119.77	116.12
7	G	1	NAG	C8-C7-N2	2.19	119.74	116.12
8	W	1	NAG	C1-O5-C5	2.16	115.08	112.19
7	V	1	NAG	C8-C7-N2	2.15	119.68	116.12
8	b	1	NAG	C8-C7-N2	2.15	119.68	116.12
9	X	2	NAG	C8-C7-N2	2.13	119.65	116.12
8	U	2	NAG	O7-C7-C8	-2.13	118.26	122.05
9	c	2	NAG	C1-O5-C5	2.13	115.04	112.19
8	Y	2	NAG	C8-C7-N2	2.12	119.64	116.12
8	W	1	NAG	C1-C2-N2	-2.08	107.15	110.43
8	U	2	NAG	O4-C4-C5	-2.08	104.21	109.32
8	f	1	NAG	O7-C7-C8	-2.07	118.37	122.05
8	I	2	NAG	O7-C7-C8	-2.06	118.39	122.05
8	f	2	NAG	C8-C7-N2	2.05	119.52	116.12
8	Z	1	NAG	C1-O5-C5	2.05	114.93	112.19
7	G	1	NAG	O4-C4-C3	2.04	115.19	110.38
12	d	5	MAN	C1-O5-C5	2.04	114.92	112.19
8	I	2	NAG	O4-C4-C3	2.04	115.19	110.38
8	U	4	MAN	C1-O5-C5	2.04	114.92	112.19
7	e	1	NAG	C8-C7-N2	2.03	119.48	116.12
7	V	2	NAG	O7-C7-C8	-2.02	118.45	122.05
12	d	2	NAG	C8-C7-N2	2.01	119.45	116.12
10	K	2	NAG	C8-C7-N2	2.01	119.45	116.12

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	b	2	NAG	C8-C7-N2-C2
8	b	2	NAG	O7-C7-N2-C2
9	X	4	MAN	C4-C5-C6-O6
9	X	4	MAN	O5-C5-C6-O6
8	U	3	BMA	C4-C5-C6-O6
8	U	3	BMA	O5-C5-C6-O6
12	d	6	MAN	O5-C5-C6-O6
12	d	4	MAN	O5-C5-C6-O6
10	K	1	NAG	C8-C7-N2-C2
10	K	1	NAG	O7-C7-N2-C2
8	I	4	MAN	O5-C5-C6-O6
8	U	4	MAN	O5-C5-C6-O6
8	f	2	NAG	C4-C5-C6-O6
12	d	6	MAN	C4-C5-C6-O6
12	d	4	MAN	C4-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6
8	W	5	MAN	O5-C5-C6-O6
8	Z	5	MAN	O5-C5-C6-O6
8	b	5	MAN	O5-C5-C6-O6
9	J	5	MAN	O5-C5-C6-O6
9	J	7	MAN	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
10	K	3	BMA	C4-C5-C6-O6
8	I	5	MAN	O5-C5-C6-O6
12	d	3	BMA	O5-C5-C6-O6
9	c	4	MAN	O5-C5-C6-O6
8	b	4	MAN	O5-C5-C6-O6
9	J	6	MAN	O5-C5-C6-O6
8	W	4	MAN	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
9	c	7	MAN	O5-C5-C6-O6
9	c	5	MAN	O5-C5-C6-O6
8	Z	4	MAN	O5-C5-C6-O6
8	I	4	MAN	C4-C5-C6-O6
10	K	3	BMA	O5-C5-C6-O6
7	V	1	NAG	C3-C2-N2-C7
9	J	2	NAG	C3-C2-N2-C7
10	K	1	NAG	C3-C2-N2-C7
7	e	1	NAG	C4-C5-C6-O6
7	V	1	NAG	C1-C2-N2-C7

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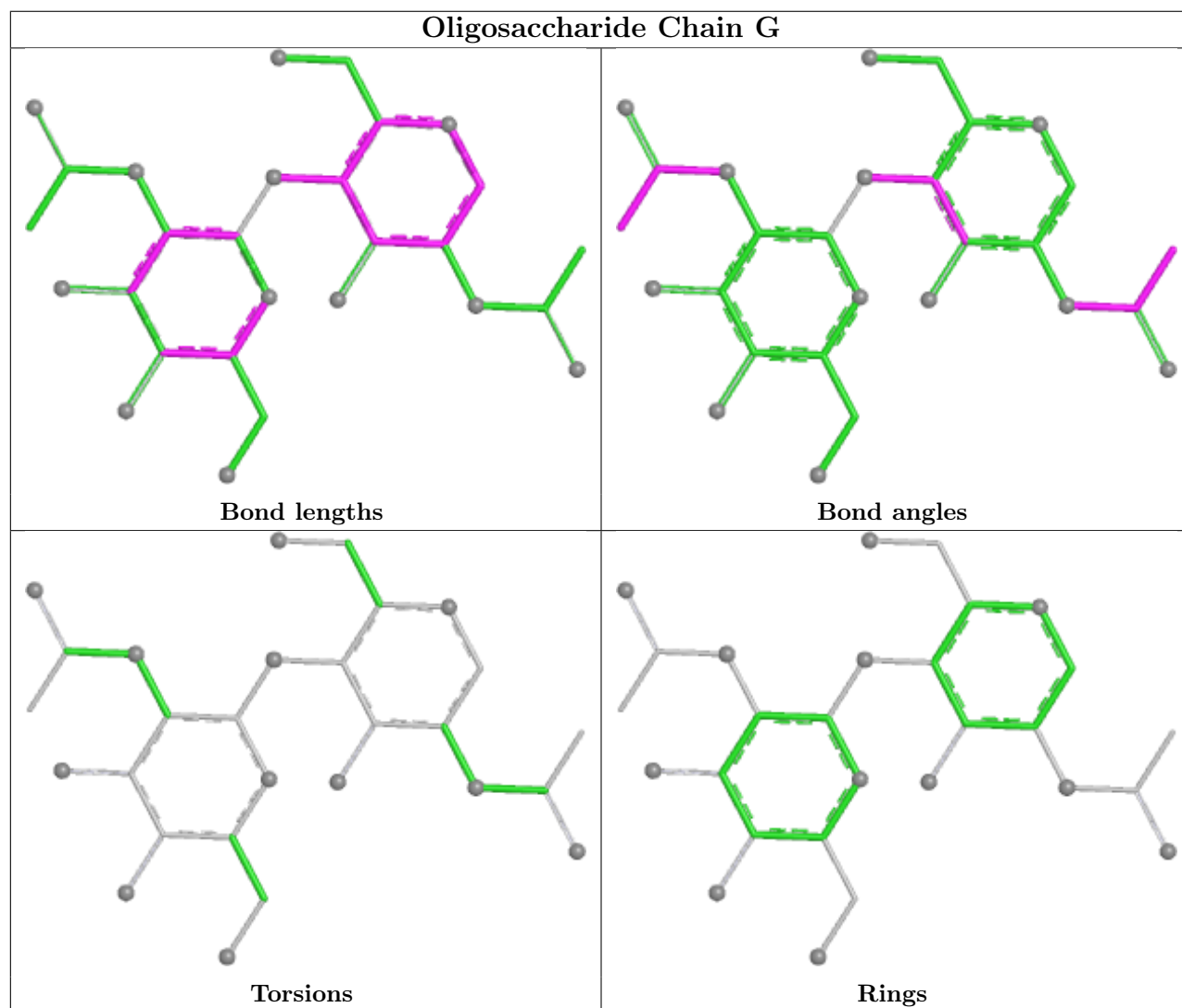
Mol	Chain	Res	Type	Atoms
9	J	1	NAG	C1-C2-N2-C7
9	J	2	NAG	C1-C2-N2-C7

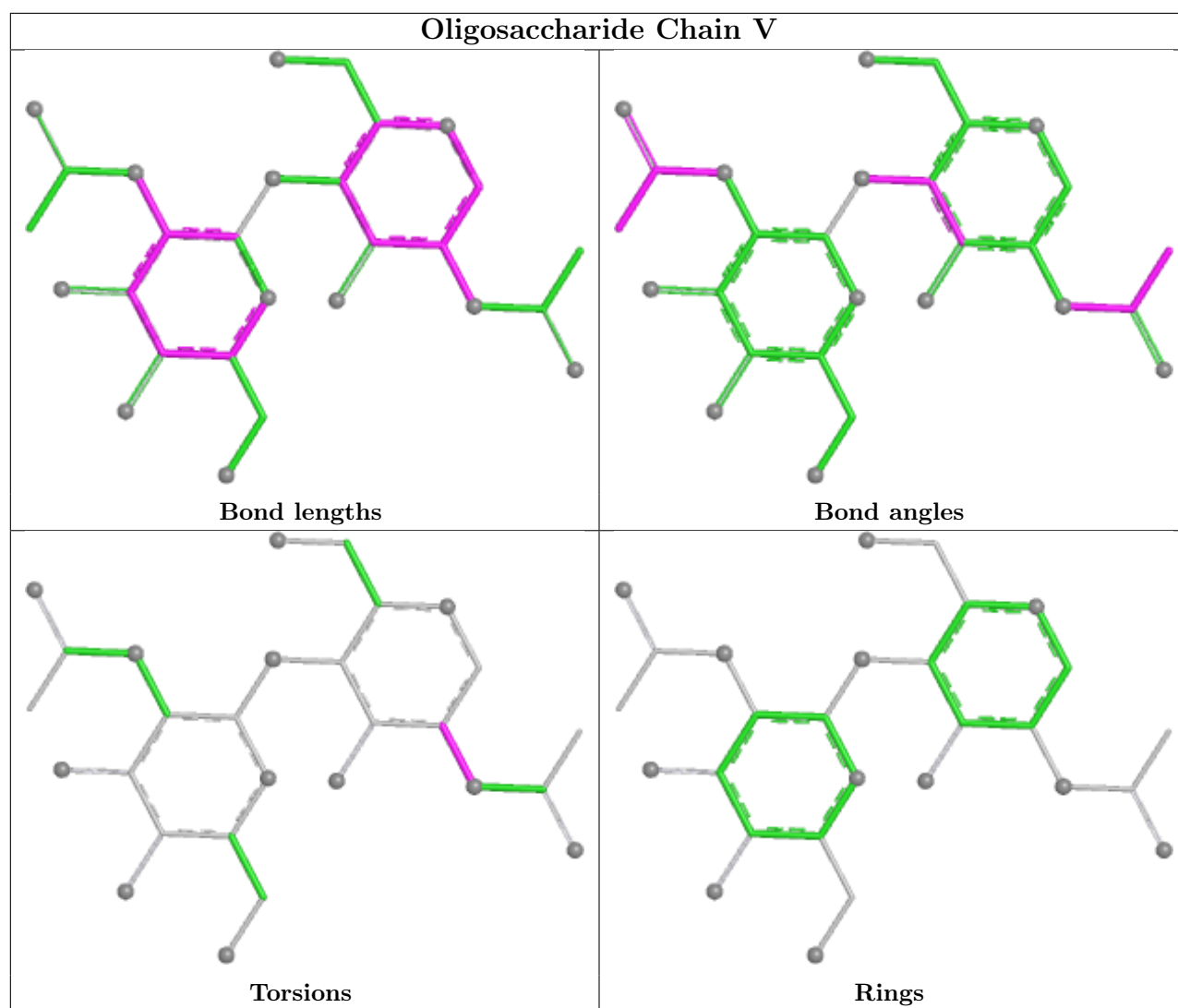
There are no ring outliers.

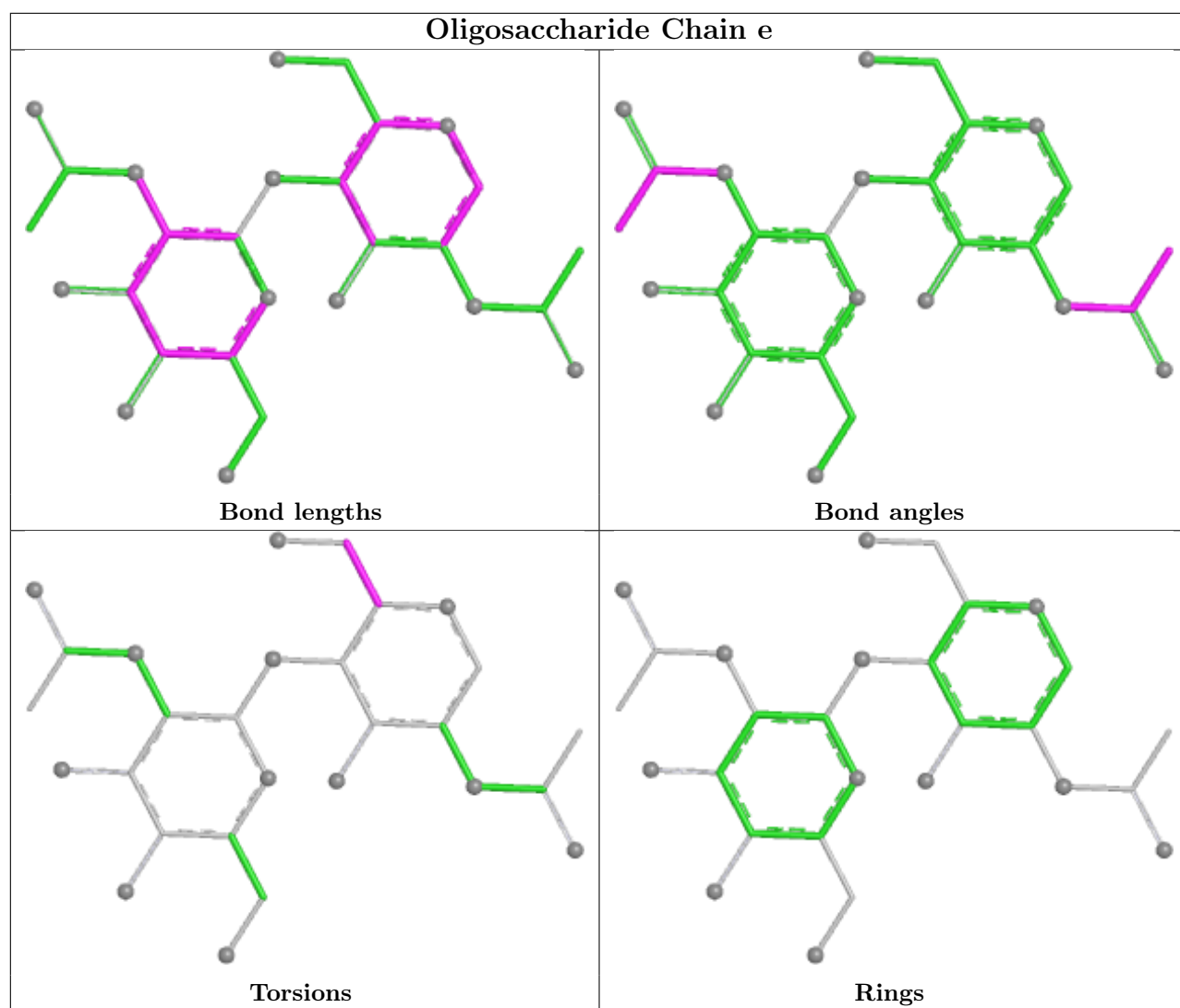
2 monomers are involved in 3 short contacts:

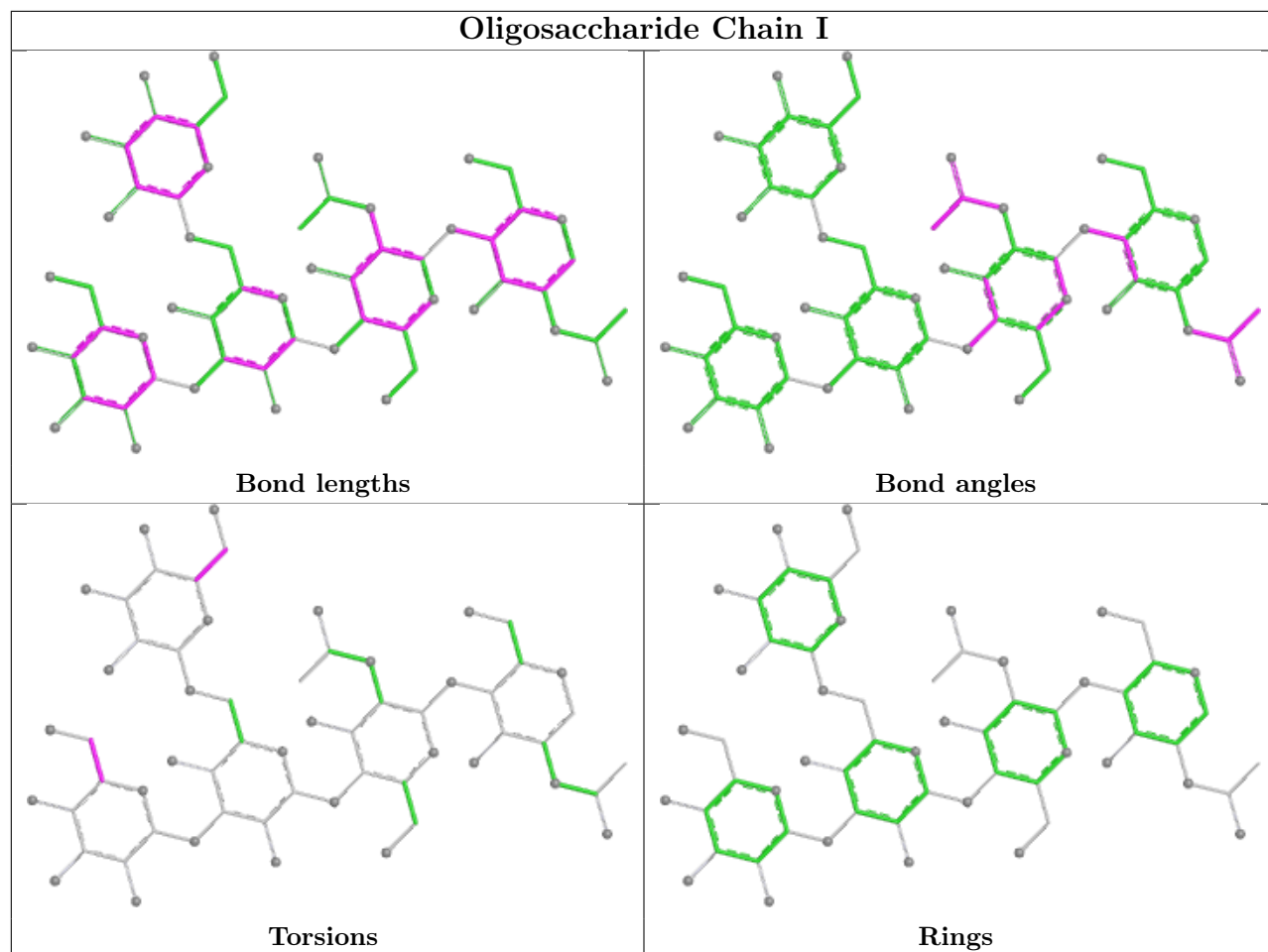
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	e	1	NAG	2	0
8	Z	1	NAG	1	0

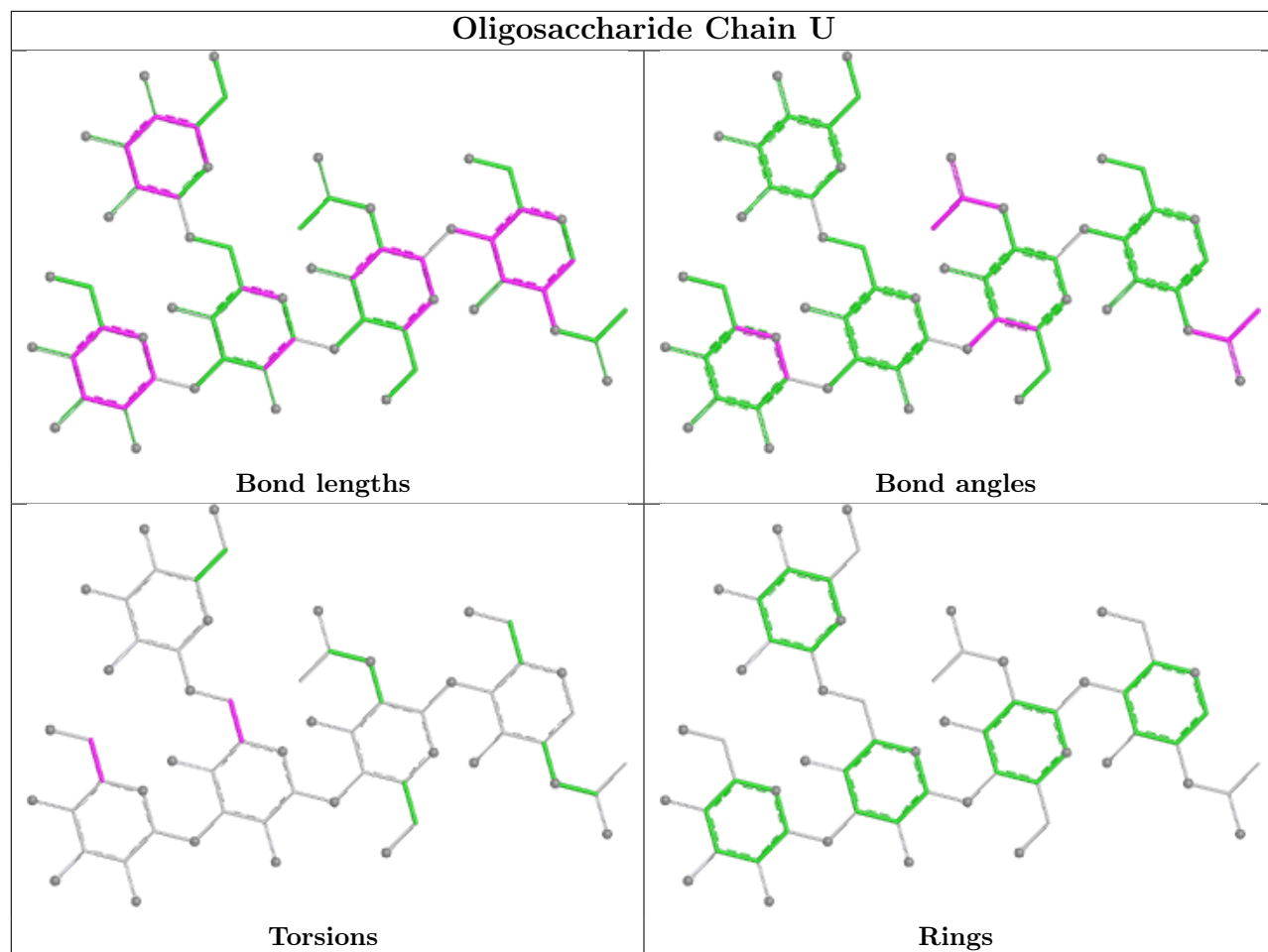
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

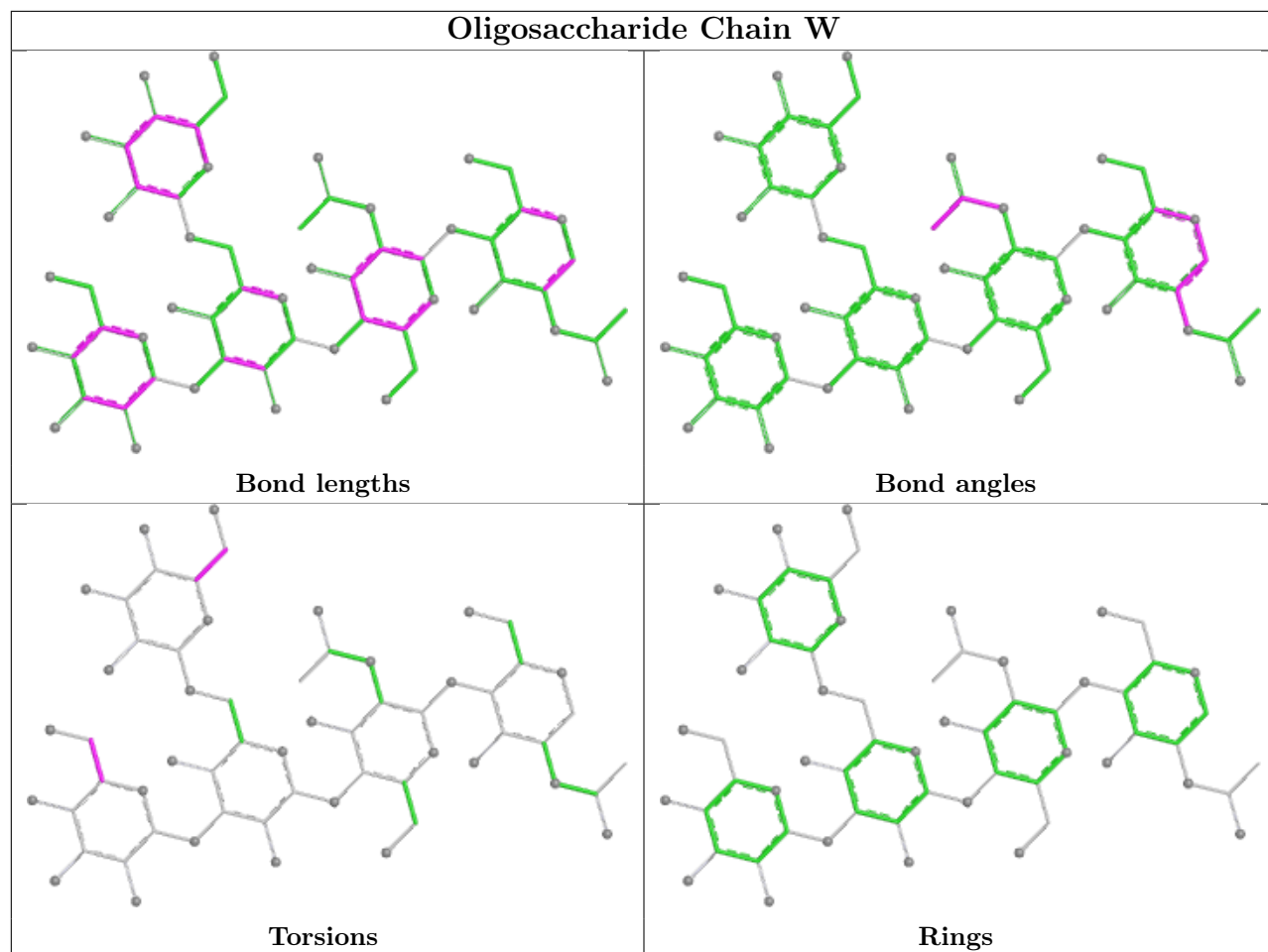


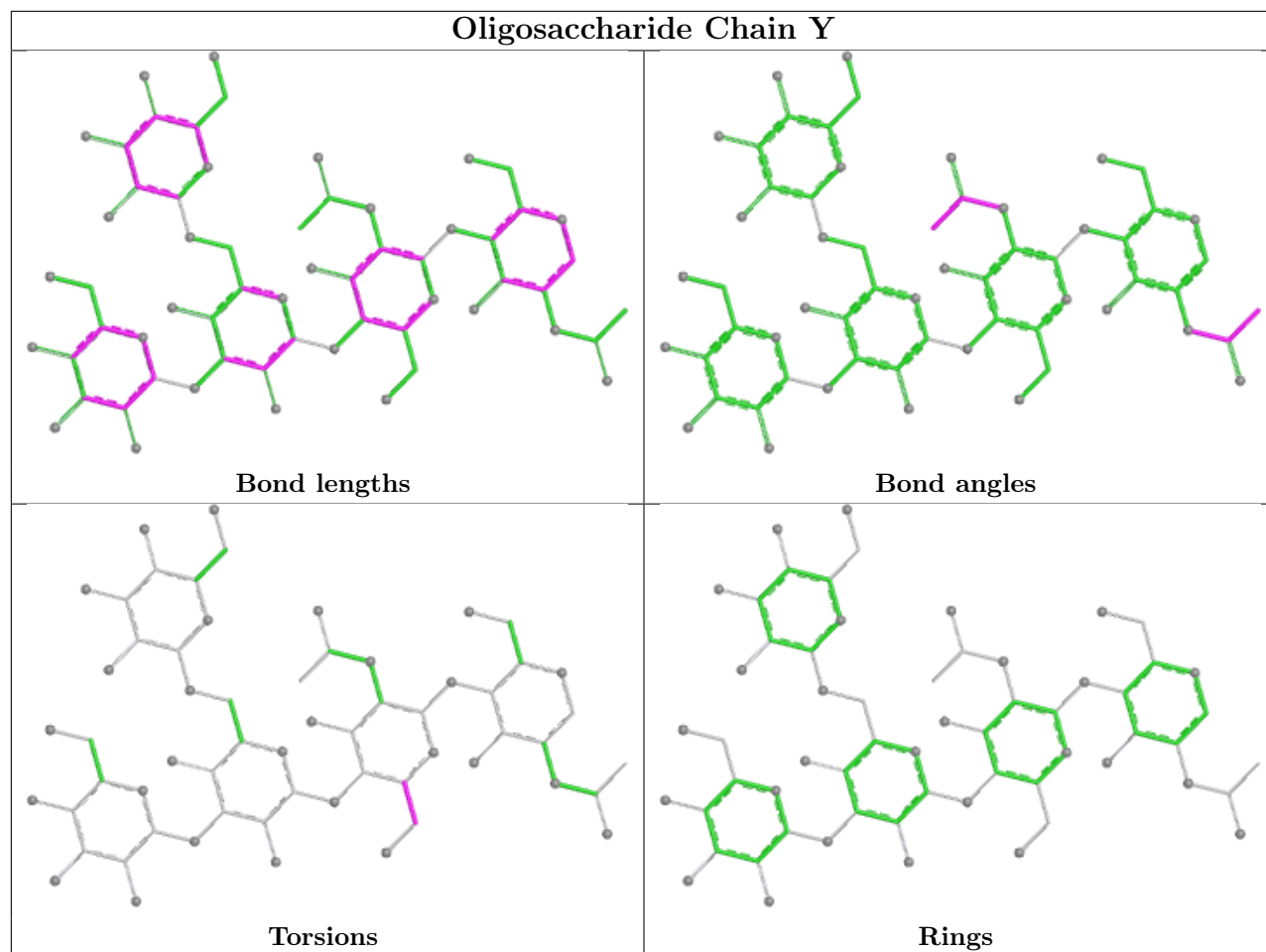


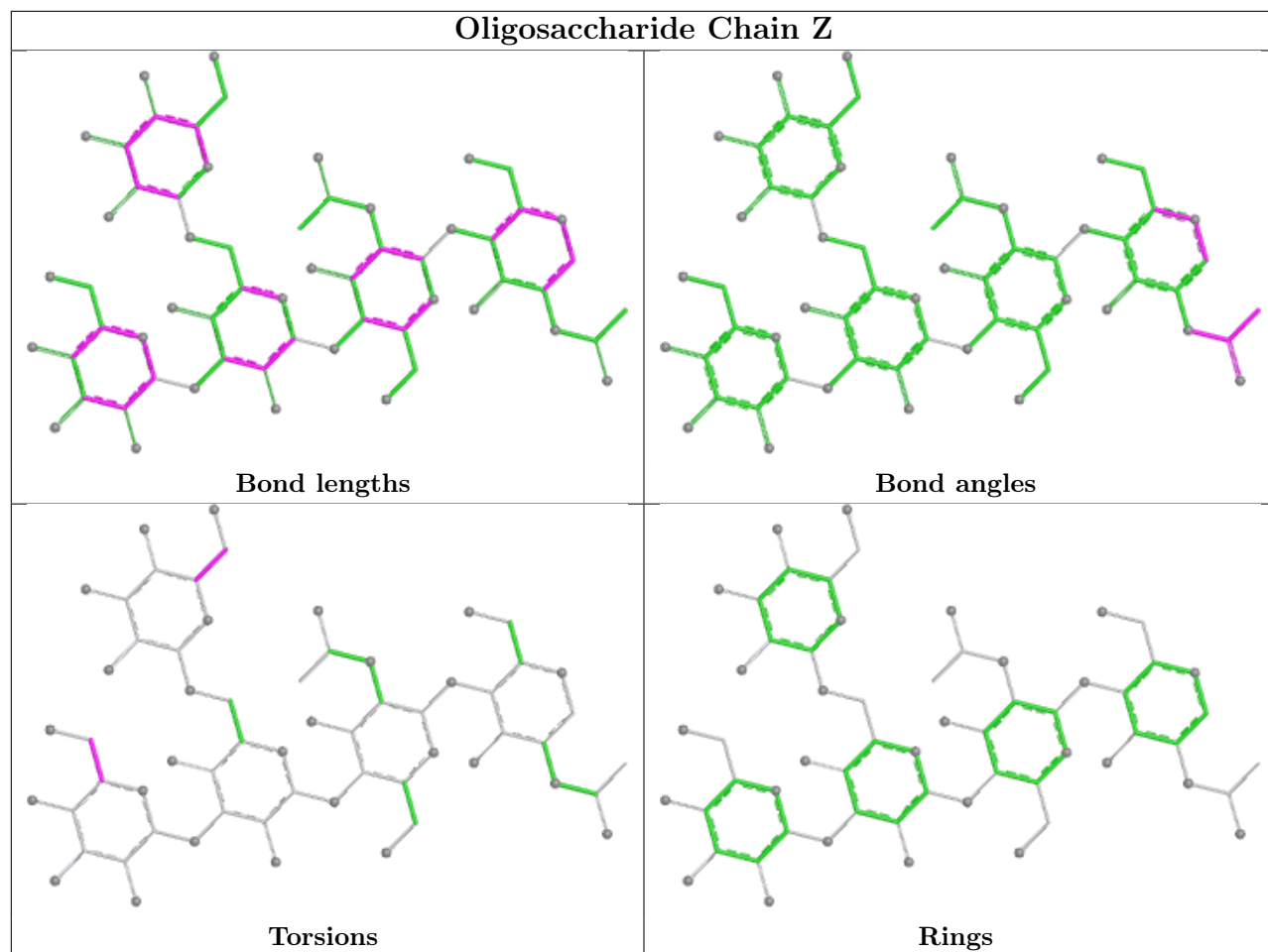


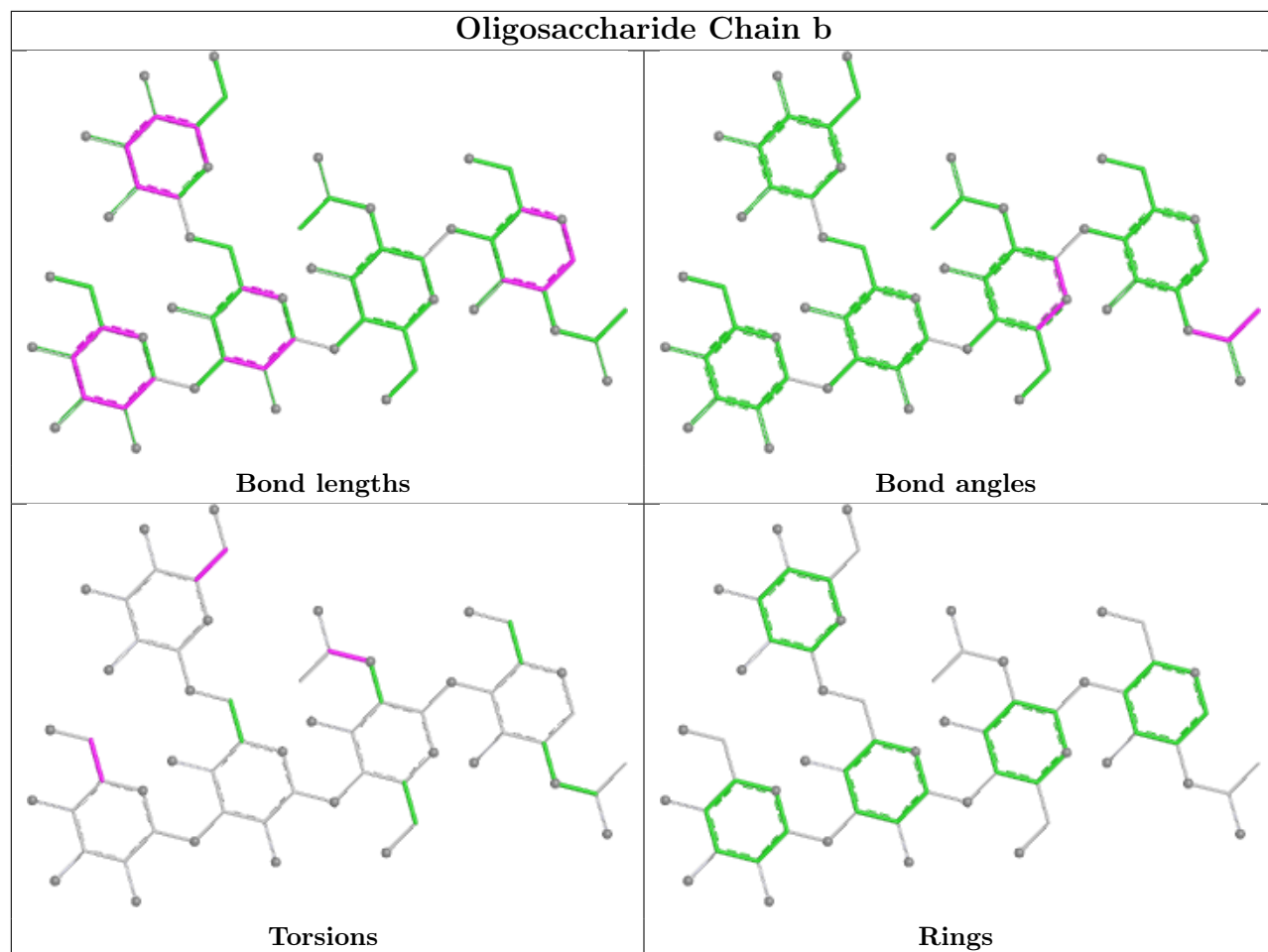


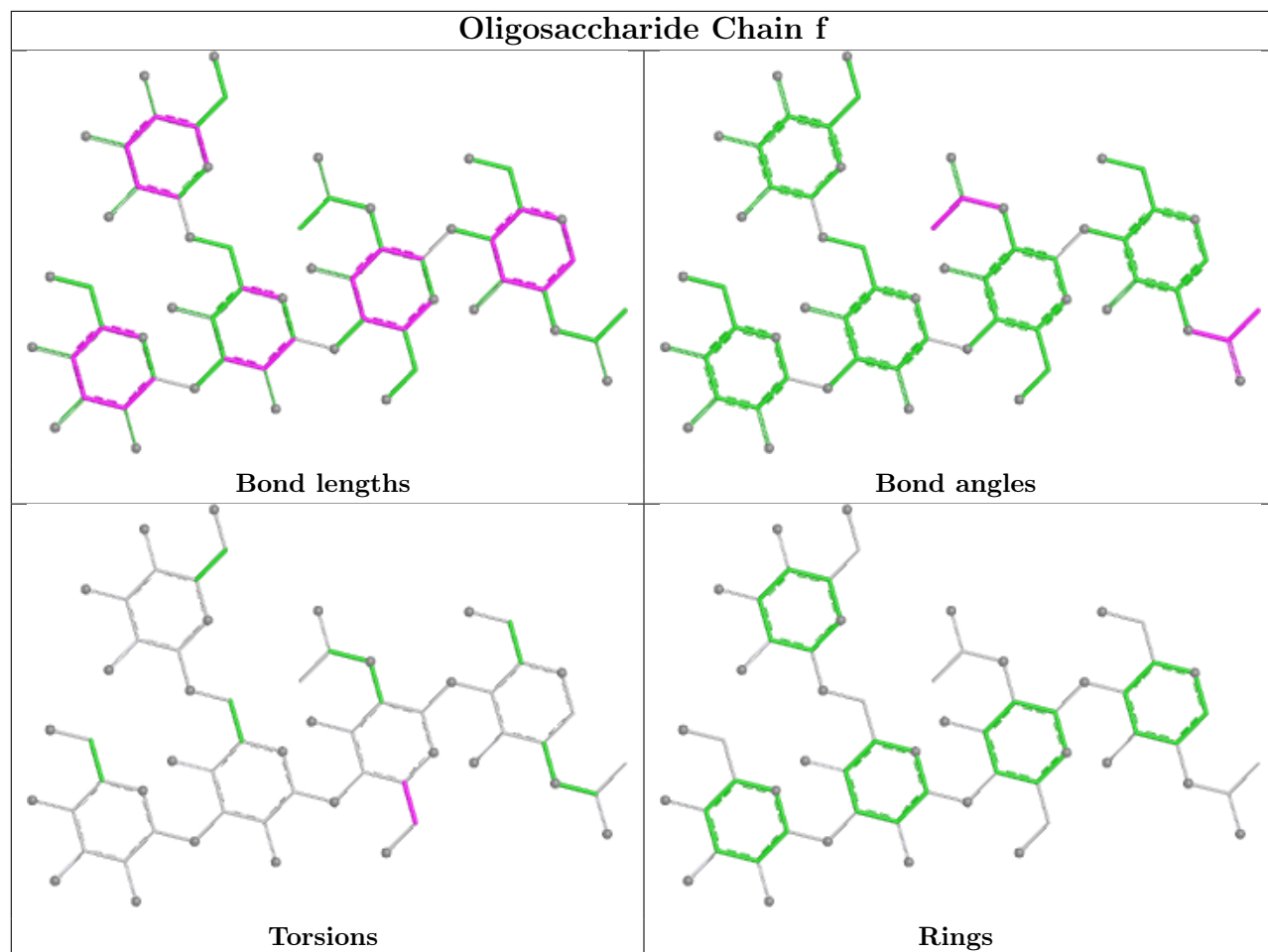


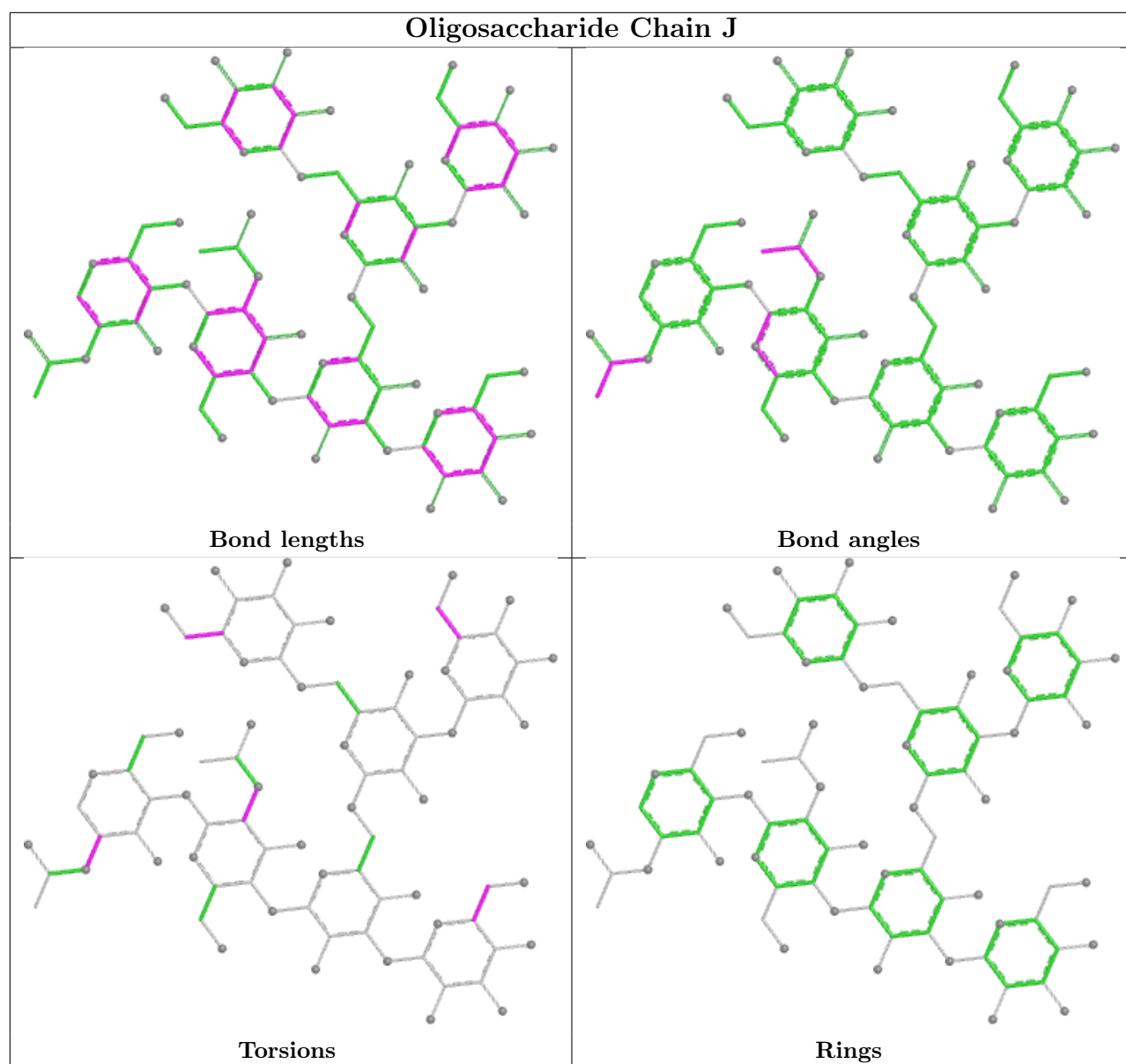


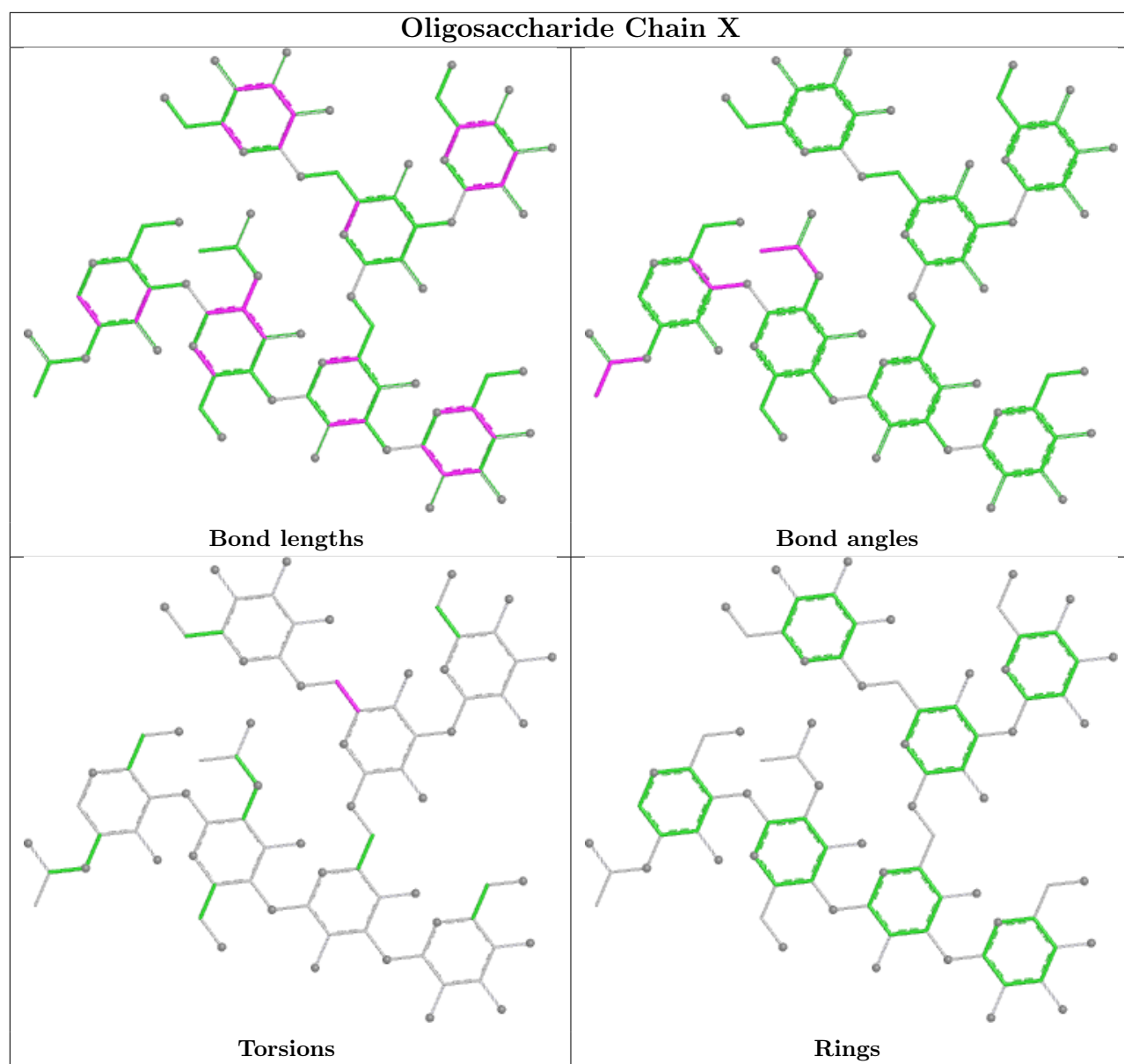


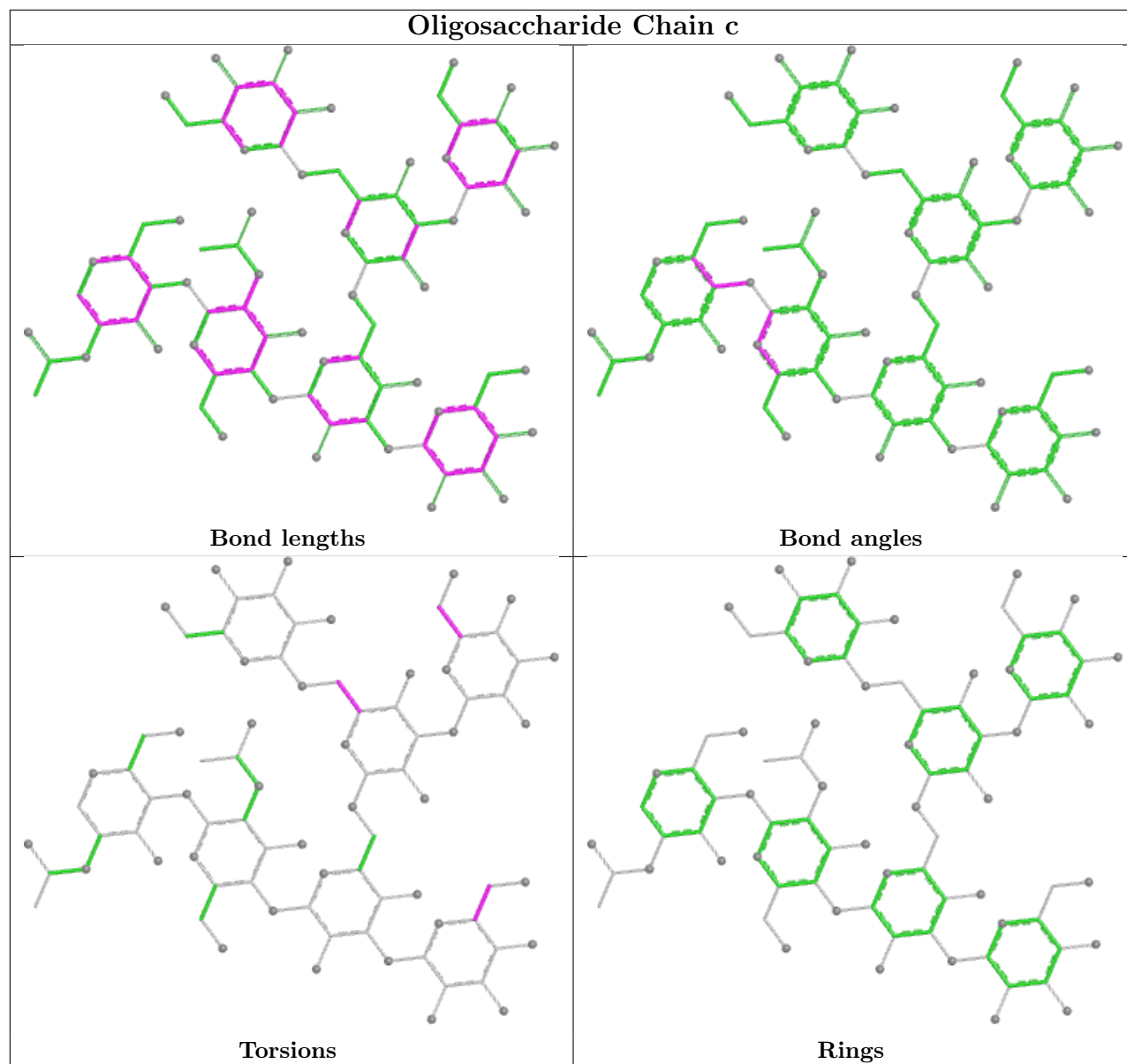


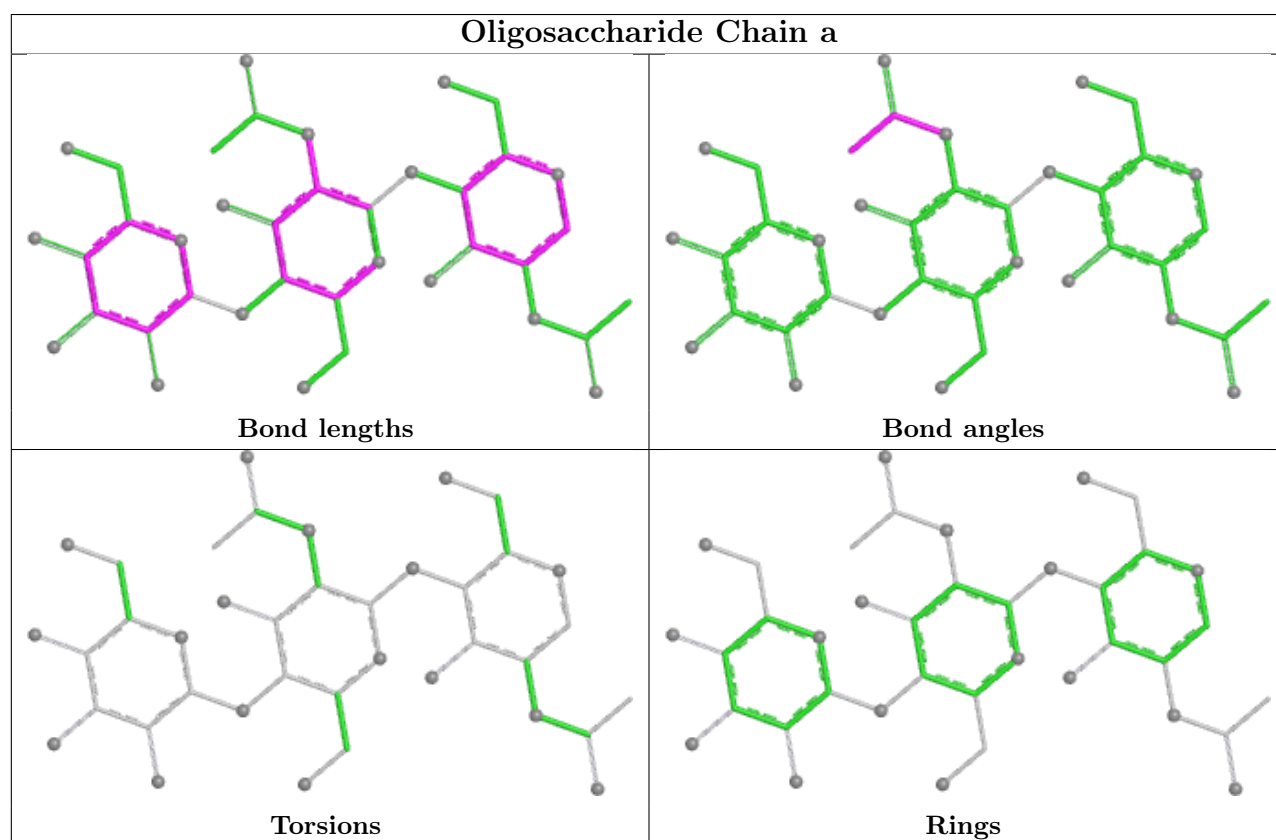
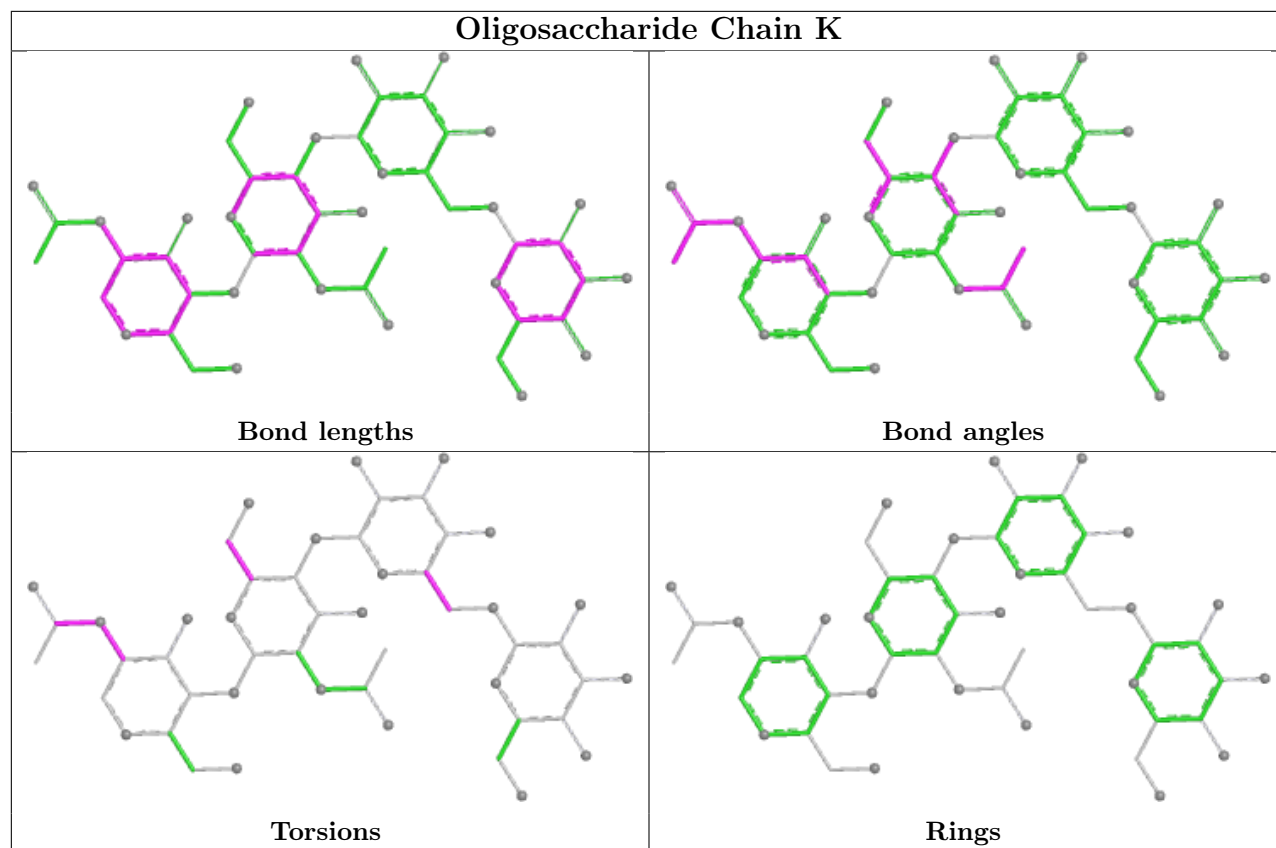


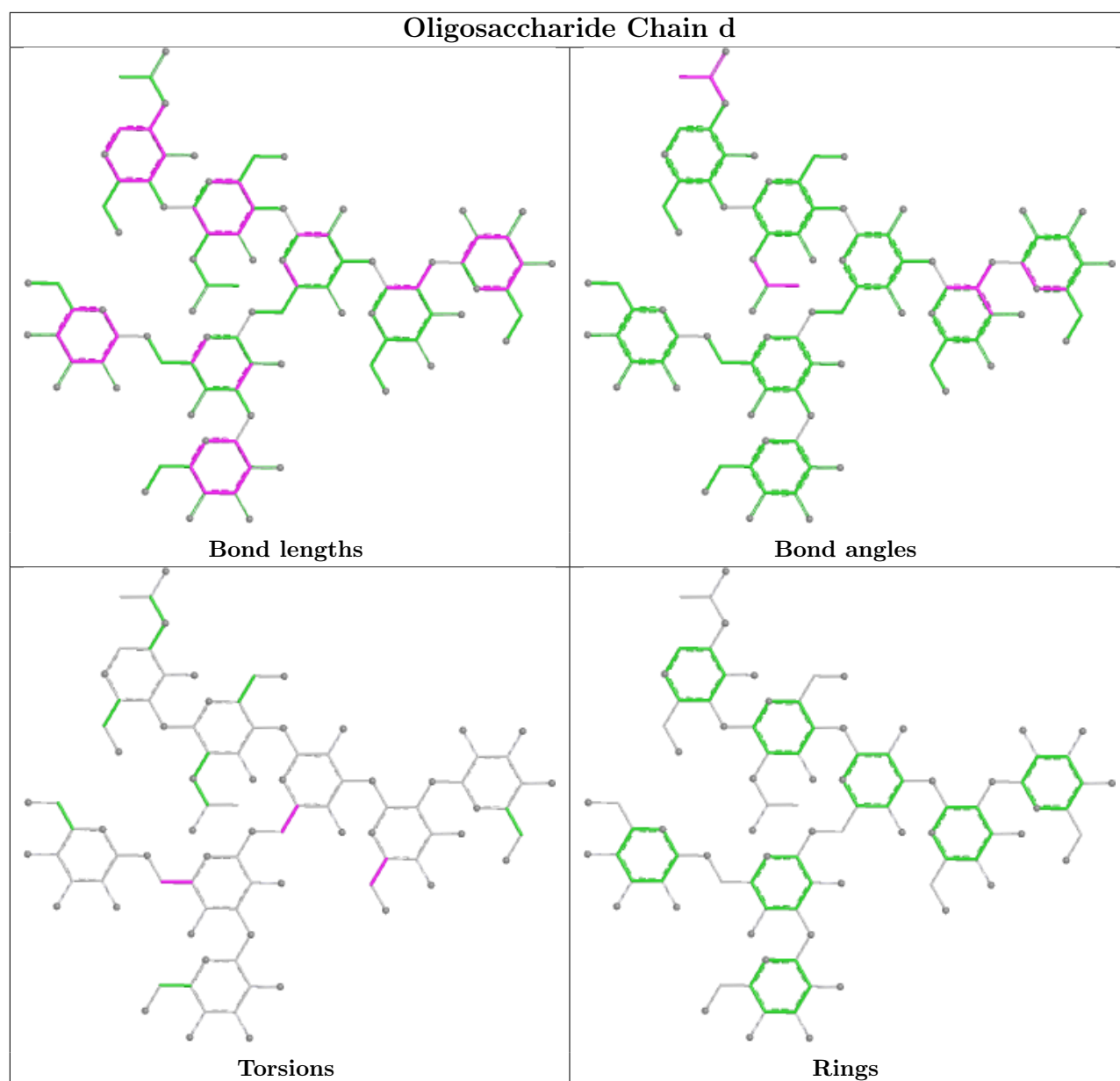












5.6 Ligand geometry [i](#)

21 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
13	NAG	C	605	1	14,14,15	2.15	6 (42%)	17,19,21	1.00	2 (11%)
13	NAG	D	602	1	14,14,15	2.19	5 (35%)	17,19,21	1.01	1 (5%)
13	NAG	A	602	1	14,14,15	2.18	5 (35%)	17,19,21	0.95	0
13	NAG	C	601	1	14,14,15	2.19	5 (35%)	17,19,21	0.98	1 (5%)
13	NAG	C	608	1	14,14,15	2.23	5 (35%)	17,19,21	1.00	1 (5%)
13	NAG	C	602	1	14,14,15	2.13	4 (28%)	17,19,21	0.93	0
13	NAG	C	604	1	14,14,15	2.26	6 (42%)	17,19,21	1.05	1 (5%)
13	NAG	D	606	1	14,14,15	2.17	7 (50%)	17,19,21	0.94	1 (5%)
13	NAG	D	603	1	14,14,15	0.46	0	17,19,21	0.76	0
13	NAG	C	603	1	14,14,15	2.17	5 (35%)	17,19,21	1.02	1 (5%)
13	NAG	A	601	1	14,14,15	2.22	5 (35%)	17,19,21	0.98	1 (5%)
13	NAG	A	605	1	14,14,15	2.18	6 (42%)	17,19,21	1.15	2 (11%)
13	NAG	A	604	1	14,14,15	2.28	6 (42%)	17,19,21	0.97	1 (5%)
13	NAG	D	608	1	14,14,15	0.40	0	17,19,21	0.83	1 (5%)
13	NAG	A	603	1	14,14,15	2.15	4 (28%)	17,19,21	1.07	2 (11%)
13	NAG	D	607	1	14,14,15	2.10	6 (42%)	17,19,21	1.06	1 (5%)
13	NAG	C	606	1	14,14,15	2.11	5 (35%)	17,19,21	0.94	1 (5%)
13	NAG	D	604	1	14,14,15	2.08	5 (35%)	17,19,21	1.13	1 (5%)
13	NAG	C	607	1	14,14,15	2.07	5 (35%)	17,19,21	1.08	1 (5%)
13	NAG	D	601	1	14,14,15	2.11	5 (35%)	17,19,21	0.96	1 (5%)
13	NAG	D	605	1	14,14,15	2.40	7 (50%)	17,19,21	1.17	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
13	NAG	C	605	1	-	1/6/23/26	0/1/1/1
13	NAG	D	602	1	-	0/6/23/26	0/1/1/1
13	NAG	A	602	1	-	0/6/23/26	0/1/1/1
13	NAG	C	601	1	-	0/6/23/26	0/1/1/1
13	NAG	C	608	1	-	0/6/23/26	0/1/1/1
13	NAG	C	602	1	-	0/6/23/26	0/1/1/1
13	NAG	C	604	1	-	0/6/23/26	0/1/1/1
13	NAG	D	606	1	-	0/6/23/26	0/1/1/1
13	NAG	D	603	1	-	2/6/23/26	0/1/1/1
13	NAG	C	603	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	601	1	-	1/6/23/26	0/1/1/1
13	NAG	A	605	1	-	0/6/23/26	0/1/1/1
13	NAG	A	604	1	-	0/6/23/26	0/1/1/1
13	NAG	D	608	1	-	3/6/23/26	0/1/1/1
13	NAG	A	603	1	-	0/6/23/26	0/1/1/1
13	NAG	D	607	1	-	1/6/23/26	0/1/1/1
13	NAG	C	606	1	-	1/6/23/26	0/1/1/1
13	NAG	D	604	1	-	1/6/23/26	0/1/1/1
13	NAG	C	607	1	-	0/6/23/26	0/1/1/1
13	NAG	D	601	1	-	0/6/23/26	0/1/1/1
13	NAG	D	605	1	-	0/6/23/26	0/1/1/1

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	605	NAG	C1-C2	6.09	1.60	1.52
13	A	604	NAG	C1-C2	5.88	1.60	1.52
13	A	601	NAG	C1-C2	5.87	1.60	1.52
13	A	602	NAG	C1-C2	5.86	1.60	1.52
13	C	601	NAG	C1-C2	5.81	1.60	1.52
13	C	608	NAG	C1-C2	5.74	1.60	1.52
13	C	603	NAG	C1-C2	5.63	1.60	1.52
13	C	604	NAG	C1-C2	5.60	1.60	1.52
13	A	605	NAG	C1-C2	5.54	1.59	1.52
13	C	602	NAG	C1-C2	5.53	1.59	1.52
13	A	603	NAG	C1-C2	5.50	1.59	1.52
13	D	602	NAG	C1-C2	5.44	1.59	1.52
13	D	601	NAG	C1-C2	5.41	1.59	1.52
13	C	606	NAG	C1-C2	5.37	1.59	1.52
13	D	607	NAG	C1-C2	5.35	1.59	1.52
13	D	604	NAG	C1-C2	5.27	1.59	1.52
13	C	605	NAG	C1-C2	5.26	1.59	1.52
13	C	607	NAG	C1-C2	5.04	1.59	1.52
13	D	606	NAG	C1-C2	4.94	1.59	1.52
13	C	604	NAG	O5-C5	3.45	1.50	1.43
13	D	601	NAG	O5-C5	3.43	1.50	1.43
13	C	607	NAG	O5-C5	3.43	1.50	1.43
13	C	608	NAG	O5-C5	3.40	1.50	1.43
13	D	605	NAG	O5-C5	3.38	1.50	1.43
13	D	606	NAG	O5-C5	3.38	1.50	1.43
13	A	604	NAG	O5-C5	3.36	1.50	1.43
13	A	603	NAG	O5-C5	3.28	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	606	NAG	O5-C5	3.26	1.49	1.43
13	A	602	NAG	O5-C5	3.22	1.49	1.43
13	D	602	NAG	O5-C5	3.21	1.49	1.43
13	C	605	NAG	O5-C5	3.21	1.49	1.43
13	A	605	NAG	O5-C5	3.19	1.49	1.43
13	C	603	NAG	O5-C5	3.19	1.49	1.43
13	A	601	NAG	O5-C5	3.18	1.49	1.43
13	C	602	NAG	O5-C5	3.16	1.49	1.43
13	D	607	NAG	O5-C5	3.14	1.49	1.43
13	C	601	NAG	O5-C5	3.13	1.49	1.43
13	D	605	NAG	C3-C2	3.11	1.59	1.52
13	D	604	NAG	O5-C5	3.04	1.49	1.43
13	D	606	NAG	O5-C1	2.83	1.48	1.43
13	C	607	NAG	O5-C1	2.77	1.48	1.43
13	C	604	NAG	C3-C2	2.75	1.58	1.52
13	C	605	NAG	O5-C1	2.74	1.48	1.43
13	A	604	NAG	O5-C1	2.72	1.48	1.43
13	D	602	NAG	C3-C2	2.71	1.58	1.52
13	A	601	NAG	O5-C1	2.69	1.48	1.43
13	C	604	NAG	O5-C1	2.67	1.48	1.43
13	C	608	NAG	O5-C1	2.65	1.48	1.43
13	D	605	NAG	O5-C1	2.62	1.48	1.43
13	A	605	NAG	O5-C1	2.61	1.48	1.43
13	A	603	NAG	O5-C1	2.57	1.48	1.43
13	D	606	NAG	C2-N2	2.56	1.50	1.46
13	C	602	NAG	C3-C2	2.53	1.57	1.52
13	D	602	NAG	O5-C1	2.52	1.47	1.43
13	C	601	NAG	O5-C1	2.49	1.47	1.43
13	C	606	NAG	O5-C1	2.48	1.47	1.43
13	C	603	NAG	O5-C1	2.47	1.47	1.43
13	D	604	NAG	O5-C1	2.43	1.47	1.43
13	C	602	NAG	O5-C1	2.38	1.47	1.43
13	C	603	NAG	C3-C2	2.37	1.57	1.52
13	D	601	NAG	O5-C1	2.35	1.47	1.43
13	A	604	NAG	C3-C2	2.32	1.57	1.52
13	D	606	NAG	C4-C5	2.32	1.58	1.53
13	A	605	NAG	C3-C2	2.30	1.57	1.52
13	D	604	NAG	C4-C5	2.27	1.57	1.53
13	D	607	NAG	C4-C5	2.27	1.57	1.53
13	C	605	NAG	C4-C5	2.26	1.57	1.53
13	A	603	NAG	C3-C2	2.26	1.57	1.52
13	A	602	NAG	C3-C2	2.25	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	608	NAG	C3-C2	2.25	1.57	1.52
13	D	604	NAG	C3-C2	2.25	1.57	1.52
13	A	602	NAG	O5-C1	2.25	1.47	1.43
13	C	601	NAG	C3-C2	2.25	1.57	1.52
13	D	601	NAG	C3-C2	2.23	1.57	1.52
13	C	605	NAG	C3-C2	2.22	1.57	1.52
13	D	605	NAG	C4-C3	2.22	1.58	1.52
13	C	604	NAG	C4-C5	2.21	1.57	1.53
13	D	601	NAG	C4-C5	2.21	1.57	1.53
13	A	602	NAG	C4-C5	2.20	1.57	1.53
13	A	601	NAG	C3-C2	2.20	1.57	1.52
13	A	601	NAG	C4-C5	2.18	1.57	1.53
13	A	604	NAG	C4-C5	2.17	1.57	1.53
13	C	606	NAG	C4-C5	2.16	1.57	1.53
13	C	607	NAG	C3-C2	2.16	1.57	1.52
13	D	605	NAG	C4-C5	2.15	1.57	1.53
13	D	607	NAG	O5-C1	2.15	1.47	1.43
13	A	605	NAG	C4-C5	2.15	1.57	1.53
13	D	607	NAG	C3-C2	2.14	1.57	1.52
13	C	608	NAG	C4-C5	2.14	1.57	1.53
13	C	603	NAG	C4-C5	2.13	1.57	1.53
13	A	605	NAG	C2-N2	2.13	1.49	1.46
13	C	601	NAG	C4-C5	2.12	1.57	1.53
13	D	605	NAG	C2-N2	2.11	1.49	1.46
13	C	606	NAG	C3-C2	2.11	1.56	1.52
13	D	606	NAG	C4-C3	2.11	1.57	1.52
13	C	604	NAG	C4-C3	2.09	1.57	1.52
13	D	606	NAG	C3-C2	2.08	1.56	1.52
13	D	602	NAG	C4-C5	2.07	1.57	1.53
13	C	605	NAG	C2-N2	2.06	1.49	1.46
13	A	604	NAG	C2-N2	2.05	1.49	1.46
13	D	607	NAG	C2-N2	2.05	1.49	1.46
13	C	607	NAG	C4-C5	2.01	1.57	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	605	NAG	C8-C7-N2	2.84	120.83	116.12
13	C	607	NAG	C1-C2-N2	-2.63	106.30	110.43
13	D	602	NAG	C8-C7-N2	2.61	120.45	116.12
13	A	605	NAG	O7-C7-C8	-2.55	117.52	122.05
13	D	604	NAG	C1-C2-N2	-2.54	106.42	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	605	NAG	C1-C2-N2	-2.50	106.49	110.43
13	C	605	NAG	C8-C7-N2	2.50	120.26	116.12
13	C	604	NAG	C8-C7-N2	2.46	120.19	116.12
13	C	608	NAG	C8-C7-N2	2.33	119.98	116.12
13	C	606	NAG	C8-C7-N2	2.28	119.91	116.12
13	D	607	NAG	C8-C7-N2	2.23	119.82	116.12
13	D	606	NAG	C8-C7-N2	2.20	119.76	116.12
13	D	608	NAG	C2-N2-C7	-2.16	120.01	122.90
13	C	603	NAG	C8-C7-N2	2.15	119.69	116.12
13	A	604	NAG	C8-C7-N2	2.08	119.57	116.12
13	D	601	NAG	C8-C7-N2	2.06	119.54	116.12
13	C	601	NAG	C8-C7-N2	2.06	119.53	116.12
13	D	605	NAG	O7-C7-C8	-2.05	118.41	122.05
13	C	605	NAG	O7-C7-C8	-2.04	118.42	122.05
13	D	605	NAG	C8-C7-N2	2.03	119.48	116.12
13	A	603	NAG	C8-C7-N2	2.00	119.44	116.12
13	A	603	NAG	C1-O5-C5	2.00	114.87	112.19
13	A	601	NAG	C8-C7-N2	2.00	119.44	116.12

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	603	NAG	C8-C7-N2-C2
13	D	603	NAG	O7-C7-N2-C2
13	D	608	NAG	C8-C7-N2-C2
13	D	608	NAG	O7-C7-N2-C2
13	C	605	NAG	O5-C5-C6-O6
13	D	604	NAG	O5-C5-C6-O6
13	A	601	NAG	O5-C5-C6-O6
13	D	607	NAG	O5-C5-C6-O6
13	C	606	NAG	O5-C5-C6-O6
13	D	608	NAG	O5-C5-C6-O6
13	C	603	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	605	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.

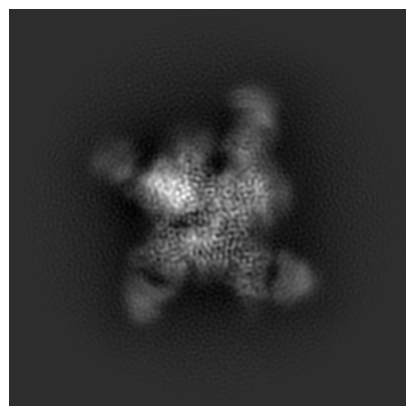
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14783. These allow visual inspection of the internal detail of the map and identification of artifacts.

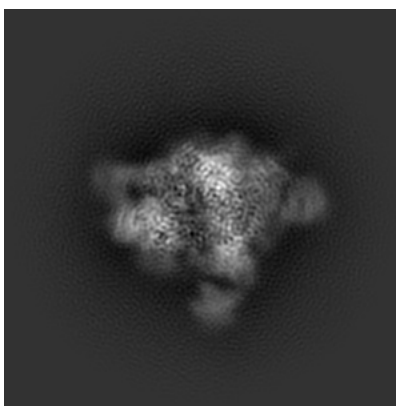
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

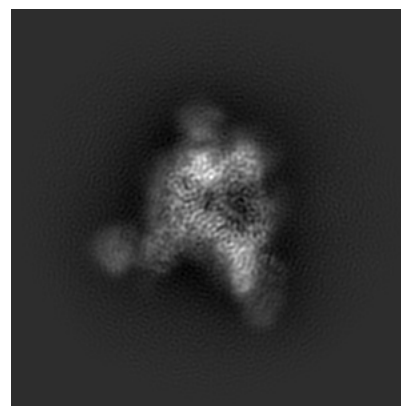
6.1.1 Primary map



X

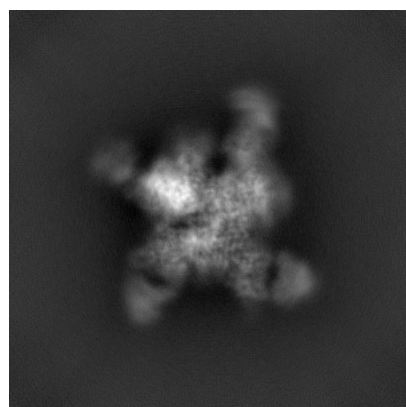


Y

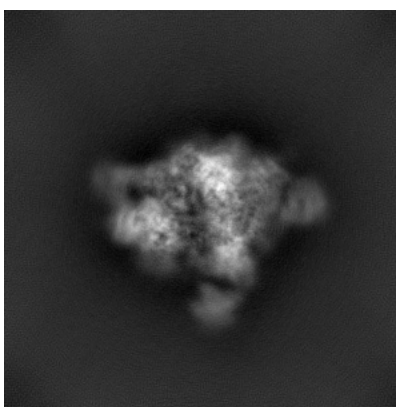


Z

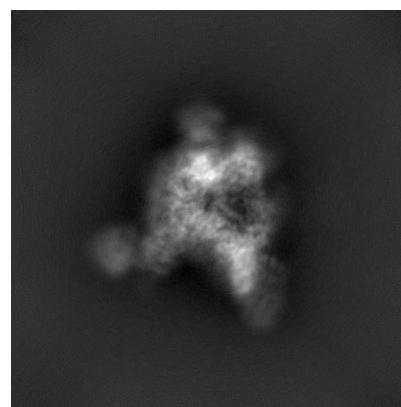
6.1.2 Raw map



X



Y

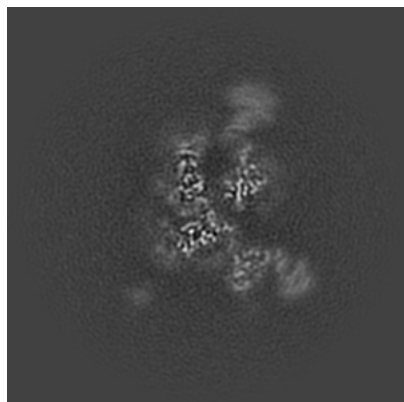


Z

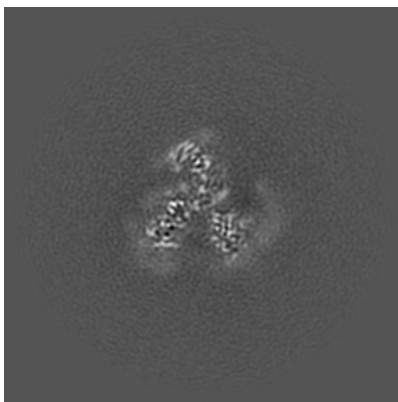
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

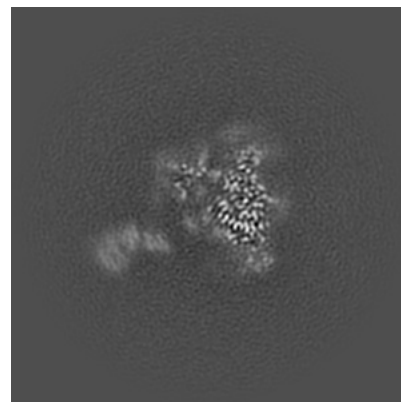
6.2.1 Primary map



X Index: 150

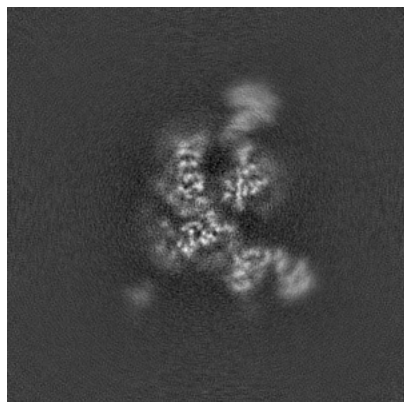


Y Index: 150

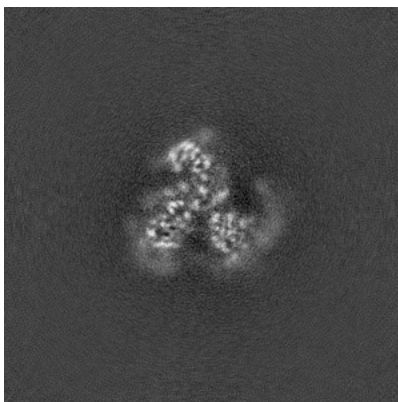


Z Index: 150

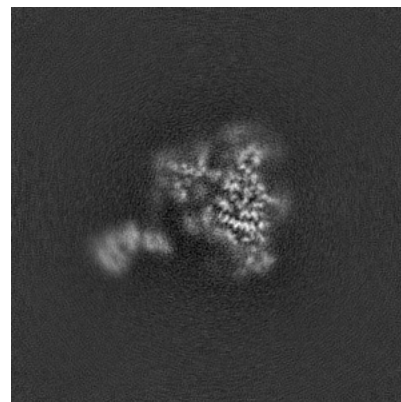
6.2.2 Raw map



X Index: 150



Y Index: 150

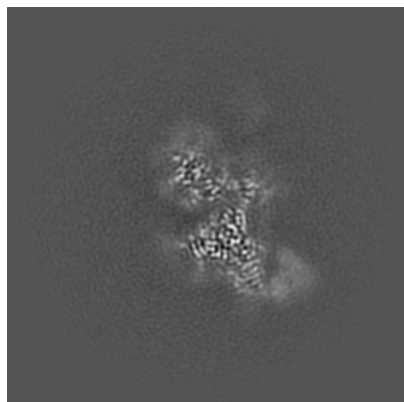


Z Index: 150

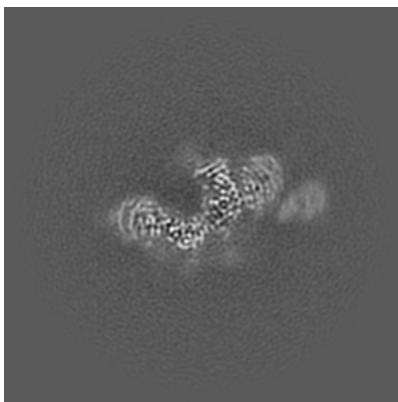
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

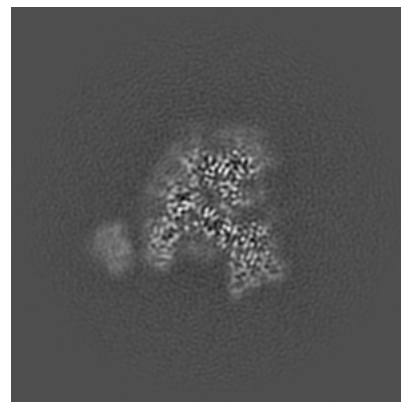
6.3.1 Primary map



X Index: 136

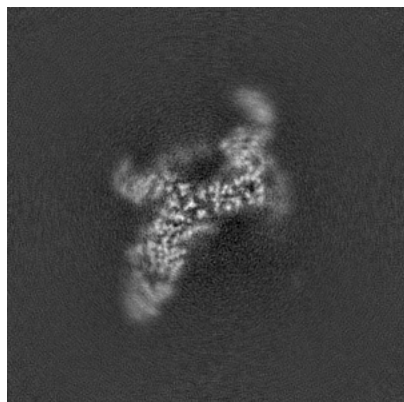


Y Index: 176

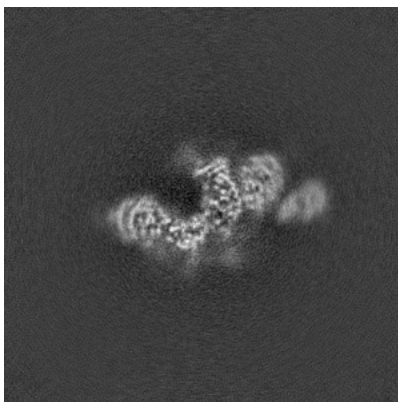


Z Index: 164

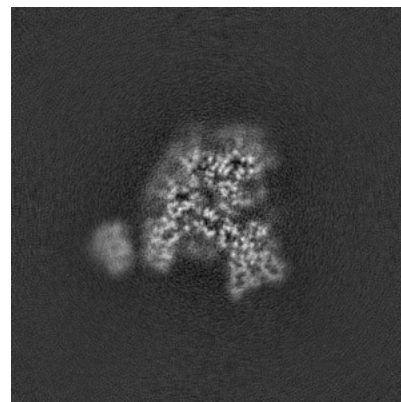
6.3.2 Raw map



X Index: 167



Y Index: 176

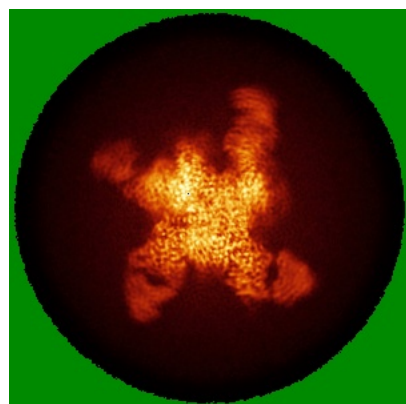


Z Index: 164

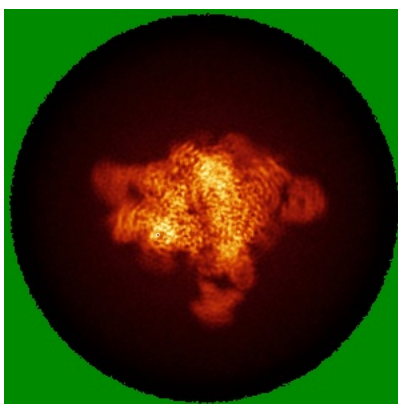
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

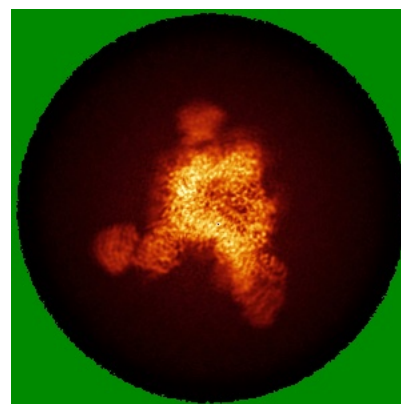
6.4.1 Primary map



X

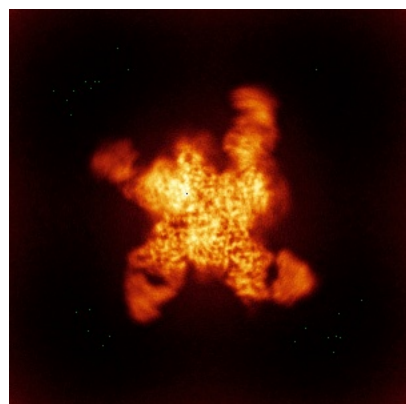


Y

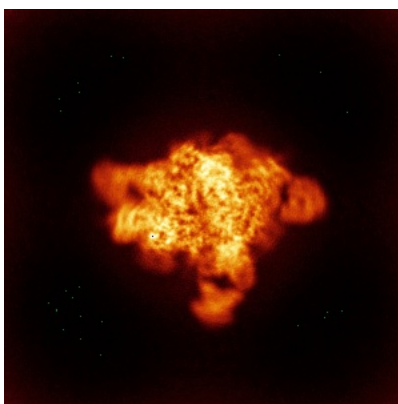


Z

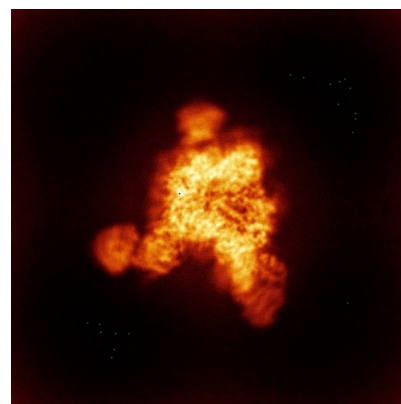
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

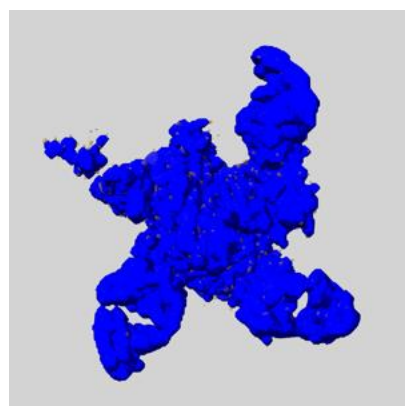
6.6 Mask visualisation [i](#)

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

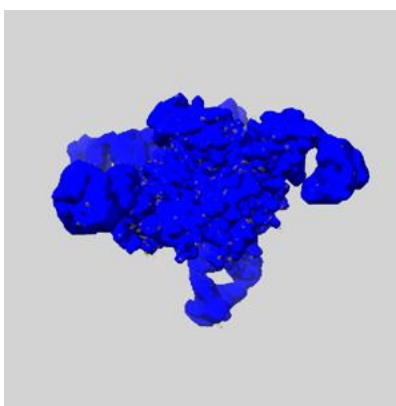
A mask typically either:

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

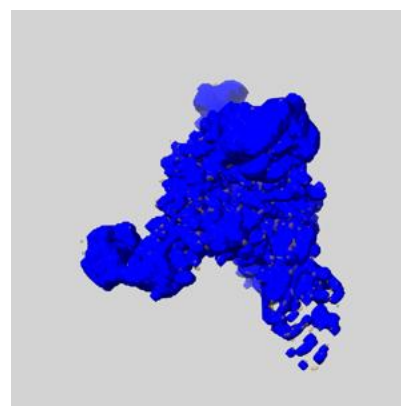
6.6.1 emd_14783_msk_1.map [i](#)



X



Y

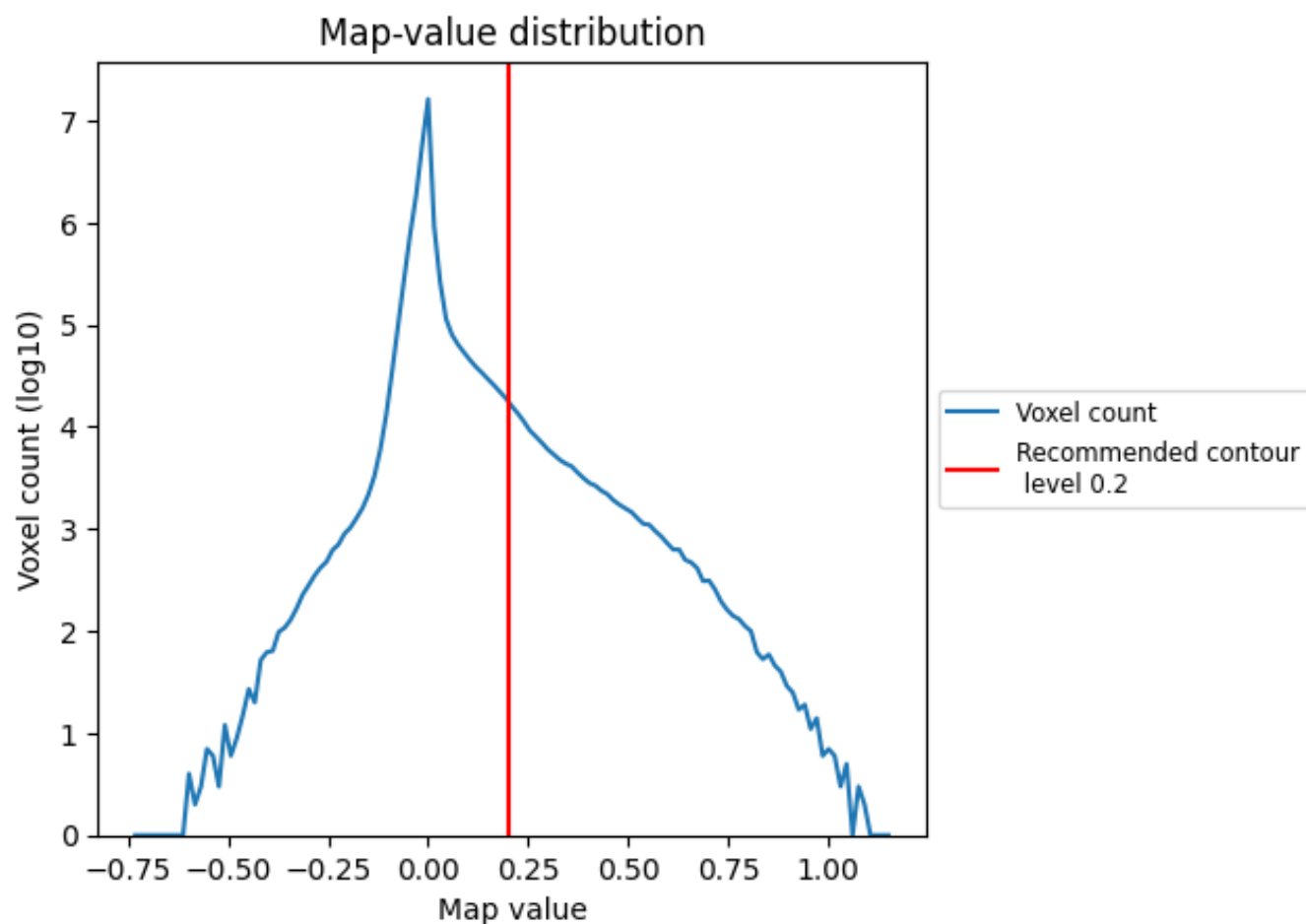


Z

7 Map analysis [i](#)

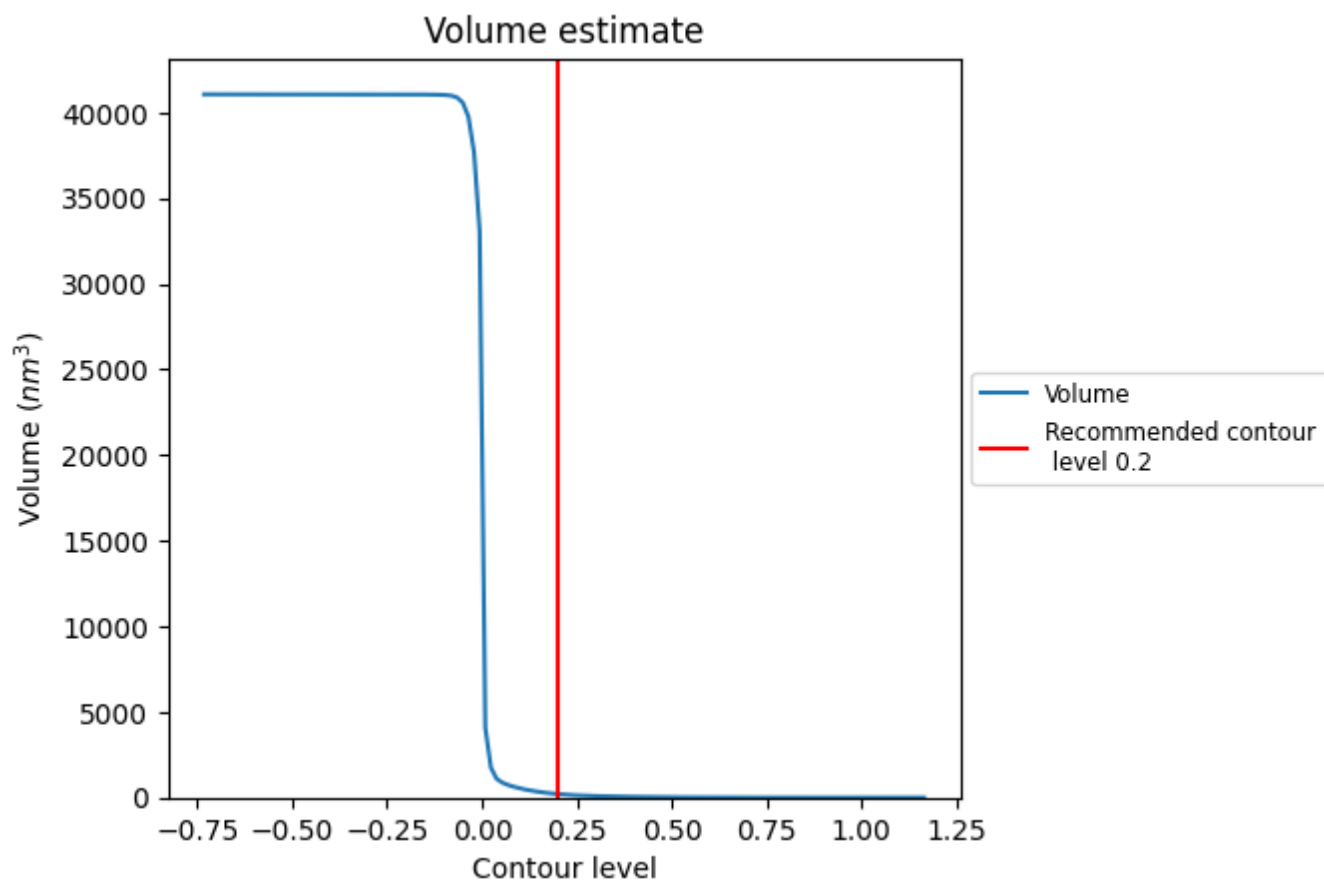
This section contains the results of statistical analysis of the map.

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.

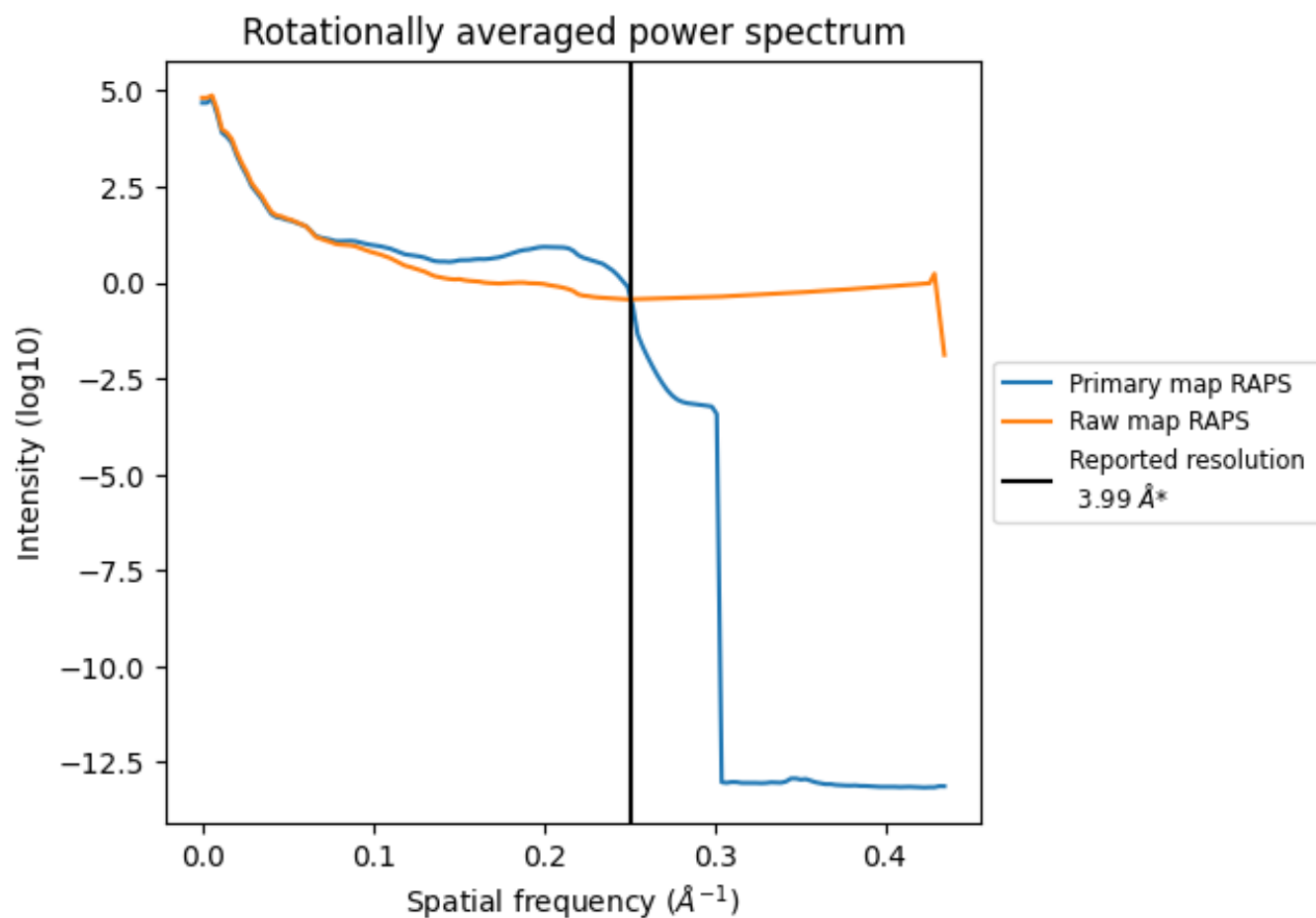
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm³; this corresponds to an approximate mass of 186 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 ⓘ

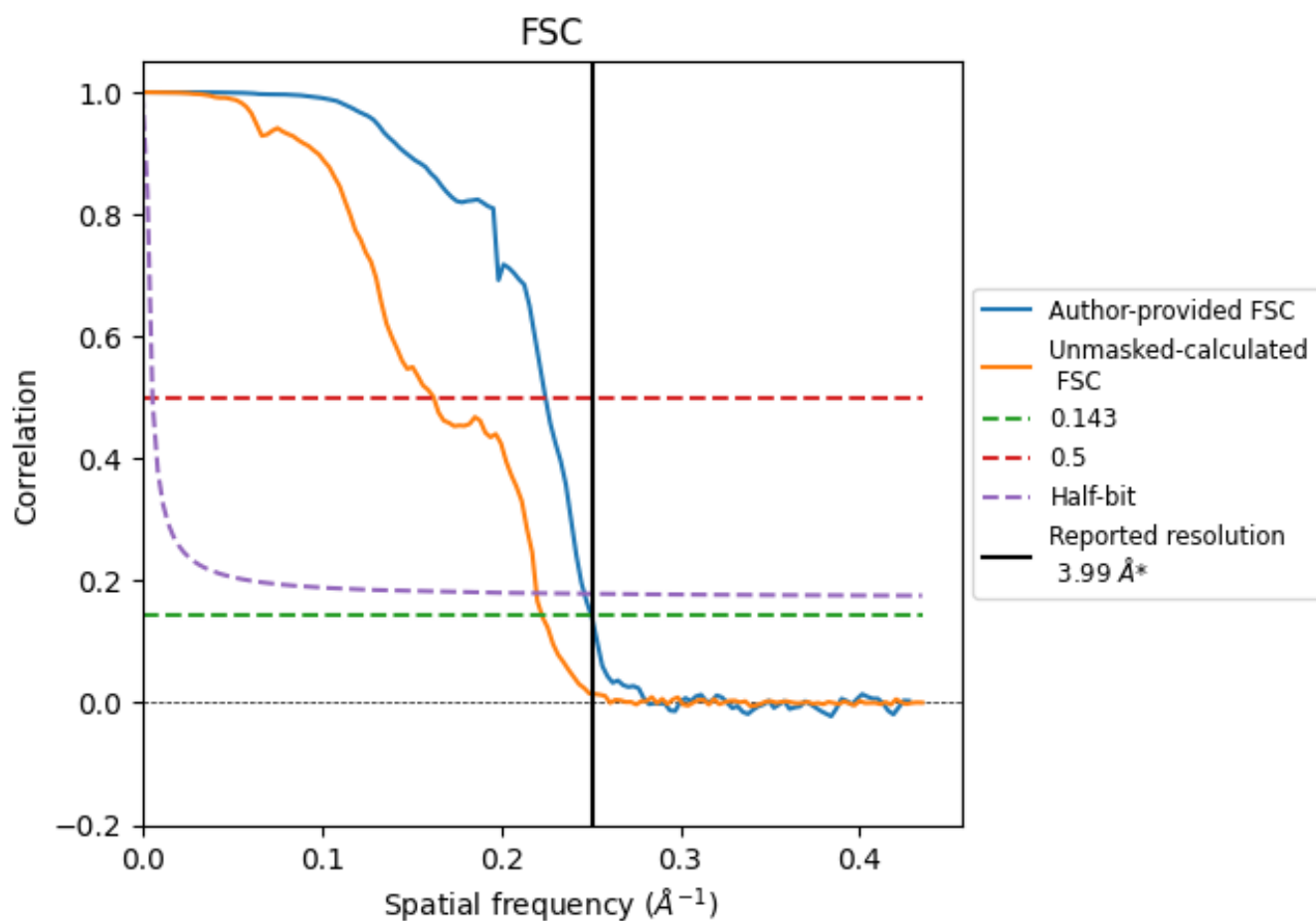


*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

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 0.251 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

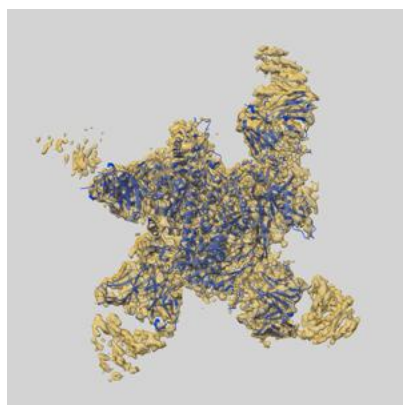
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.99	-	-
Author-provided FSC curve	3.99	4.45	4.06
Unmasked-calculated*	4.49	6.15	4.55

*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 4.49 differs from the reported value 3.99 by more than 10 %

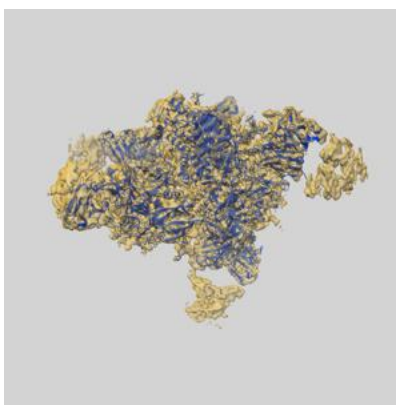
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14783 and PDB model 7ZLK. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

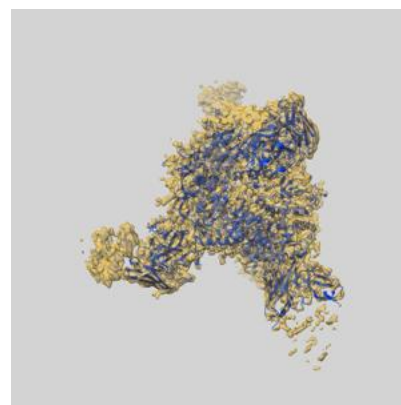
9.1 Map-model overlay [i](#)



X



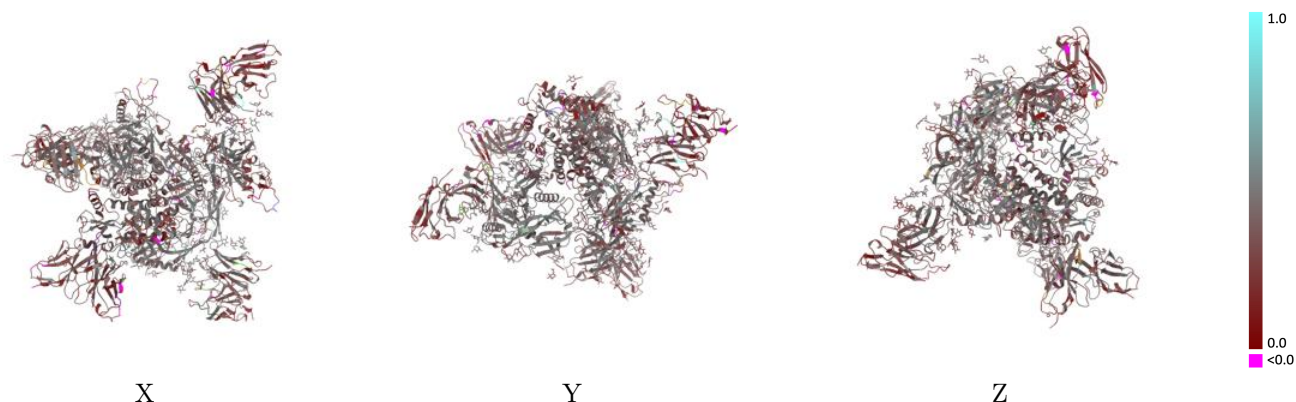
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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](#)

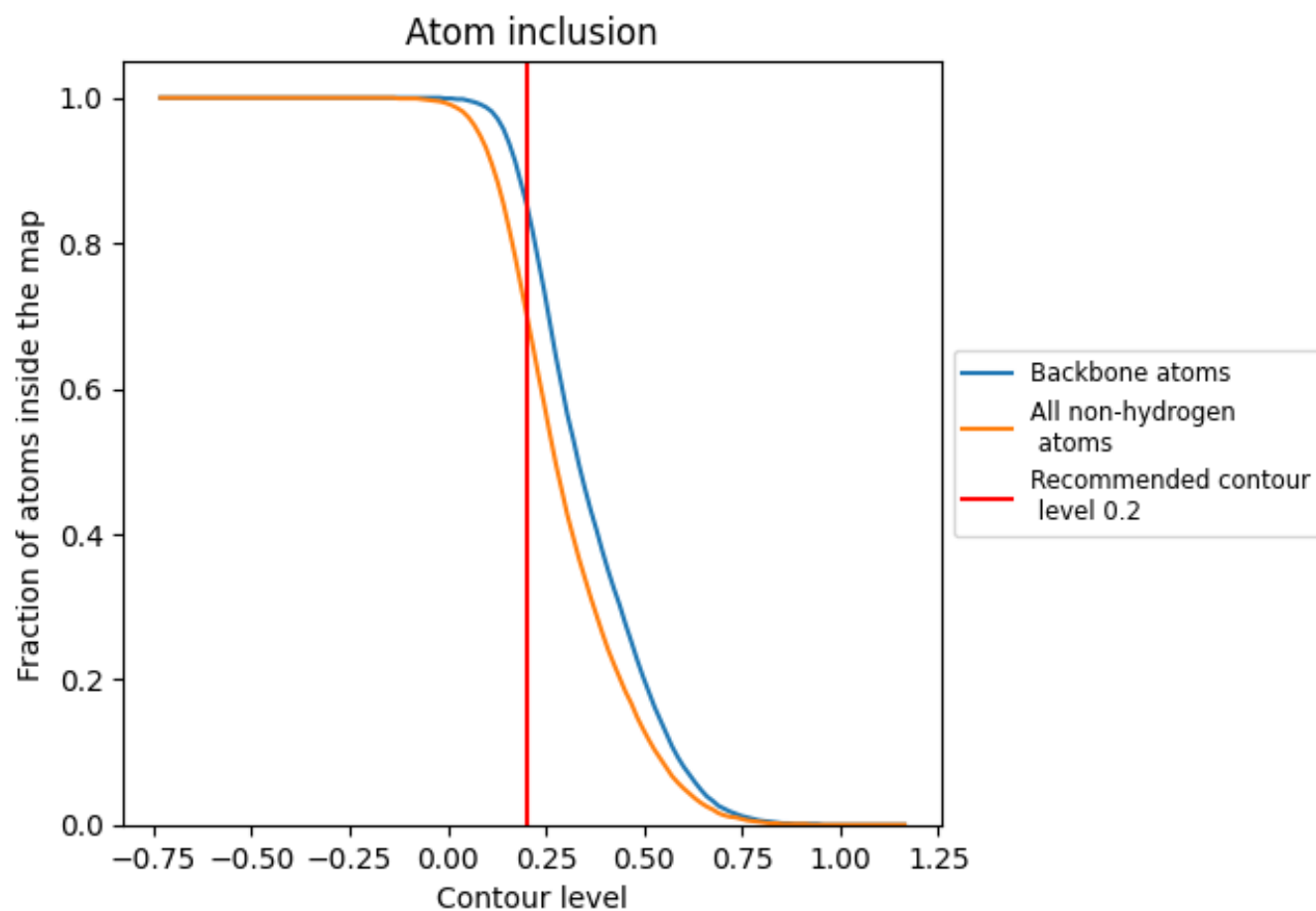


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7060	 0.3620
A	 0.7360	 0.3790
B	 0.7200	 0.3160
C	 0.7820	 0.4190
D	 0.7380	 0.3960
E	 0.7000	 0.3360
F	 0.7640	 0.3810
G	 0.4640	 0.2640
H	 0.7290	 0.3550
I	 0.6230	 0.2870
J	 0.7350	 0.3800
K	 0.7400	 0.3500
L	 0.6610	 0.2940
M	 0.6040	 0.3710
N	 0.5210	 0.3630
O	 0.6370	 0.2890
P	 0.5480	 0.2510
Q	 0.7540	 0.3650
R	 0.6870	 0.2940
S	 0.6460	 0.3140
T	 0.6530	 0.3190
U	 0.6890	 0.4000
V	 0.3570	 0.2970
W	 0.7700	 0.4240
X	 0.7590	 0.4040
Y	 0.7870	 0.4140
Z	 0.8530	 0.4550
a	 0.4360	 0.3680
b	 0.6720	 0.4090
c	 0.7350	 0.3550
d	 0.5850	 0.3400
e	 0.3930	 0.2400
f	 0.7050	 0.4040

