



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 04:00 AM UTC

PDB ID : 7MEP / pdb_00007mep
EMDB ID : EMD-23801
Title : BG505 SOSIP.v5.2(7S) in complex with the monoclonal antibodies Rh.33172 mAb.1 and RM19R
Authors : Antanasijevic, A.; Ward, A.B.
Deposited on : 2021-04-07
Resolution : 3.50 Å(reported)
Based on initial model : 6VFL

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

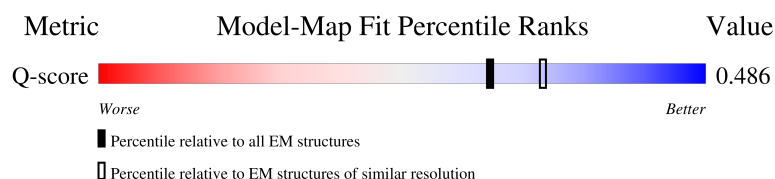
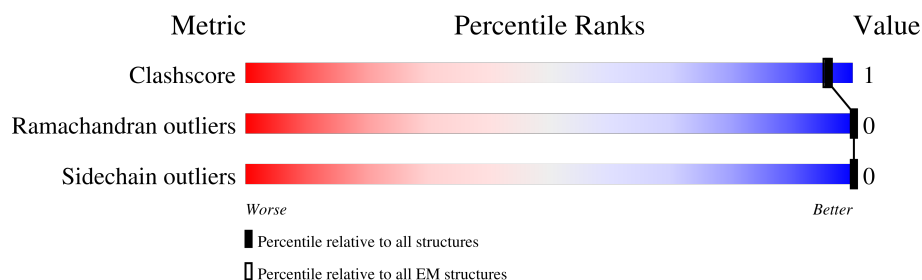
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	G	107	18% 91% 7% ..
1	J	107	21% 88% 8% ..
1	K	107	21% 87% 11% .
2	I	121	19% 88% 10% .

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Mol	Chain	Length	Quality of chain
2	M	121	
2	N	121	
3	A	666	
3	B	666	
3	C	666	
3	D	666	
3	E	666	
3	F	666	
4	H	129	
5	L	107	
6	O	5	
6	U	5	
6	Y	5	
7	P	2	
7	Q	2	
7	R	2	
7	S	2	
7	T	2	
7	V	2	
7	W	2	
7	X	2	
7	Z	2	
7	a	2	
7	b	2	
7	c	2	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21636 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 RM19R mAb Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	105	Total	C	N	O	S	0	0
			817	511	142	161	3		
1	J	104	Total	C	N	O	S	0	0
			808	505	140	160	3		
1	K	105	Total	C	N	O	S	0	0
			817	511	142	161	3		

- Molecule 2 is a protein called RM19R mAb Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	118	Total	C	N	O	S	0	0
			915	579	158	176	2		
2	M	118	Total	C	N	O	S	0	0
			915	579	158	176	2		
2	N	118	Total	C	N	O	S	0	0
			915	579	158	176	2		

- Molecule 3 is a protein called BG505 SOSIPv5.2(7S) - gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	440	Total	C	N	O	S	0	0
			3477	2186	612	651	28		
3	B	123	Total	C	N	O	S	0	0
			985	618	170	191	6		
3	C	441	Total	C	N	O	S	0	0
			3487	2191	615	653	28		
3	E	123	Total	C	N	O	S	0	0
			985	618	170	191	6		
3	D	443	Total	C	N	O	S	0	0
			3499	2199	617	655	28		
3	F	123	Total	C	N	O	S	0	0
			985	618	170	191	6		

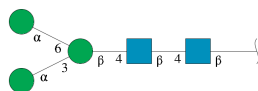
- Molecule 4 is a protein called Rh.33172 mAb.1 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	128	Total	C	N	O	S	0	0
			995	619	170	200	6		

- Molecule 5 is a protein called Rh.33172 mAb.1 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	107	Total	C	N	O	S	0	0
			803	503	132	163	5		

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



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

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



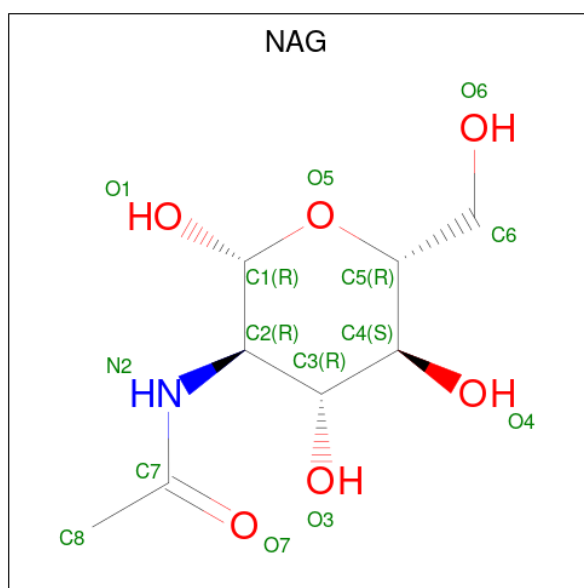
Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	2	Total	C	N	O	0	0
			28	16	2	10		
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	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	c	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

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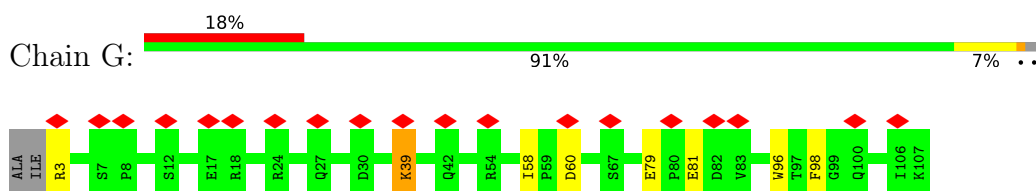
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Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	

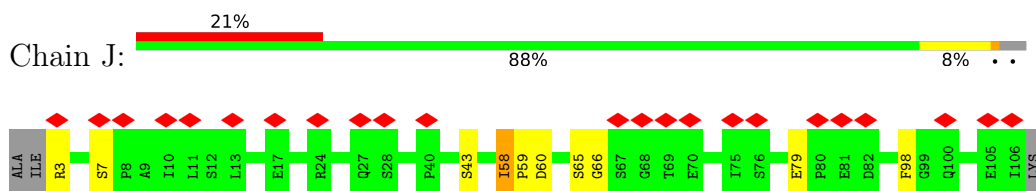
3 Residue-property plots [i](#)

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

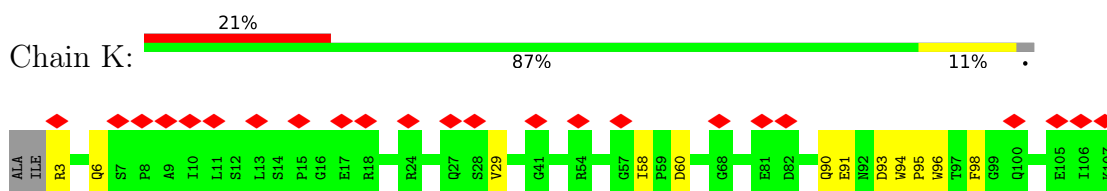
- Molecule 1: RM19R mAb Light chain



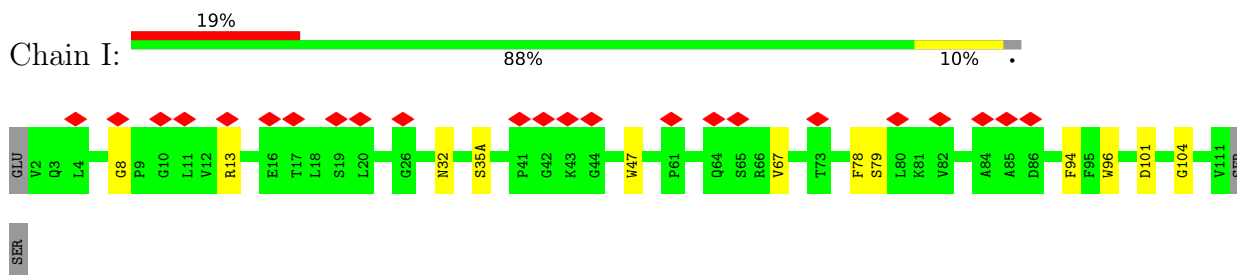
- Molecule 1: RM19R mAb Light chain



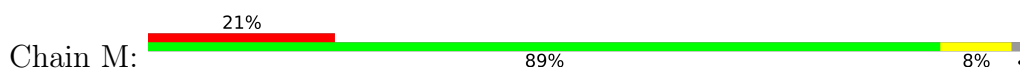
- Molecule 1: RM19R mAb Light chain

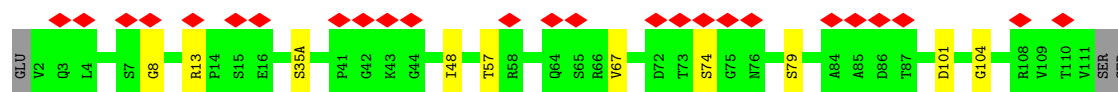


- Molecule 2: RM19R mAb Heavy chain

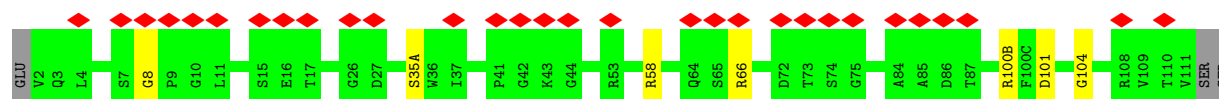


- Molecule 2: RM19R mAb Heavy chain

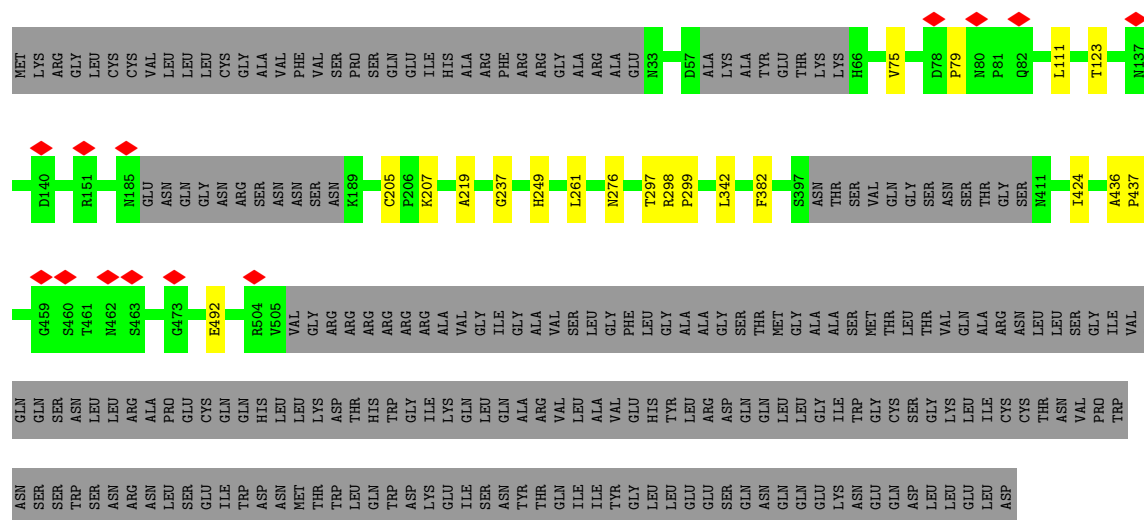




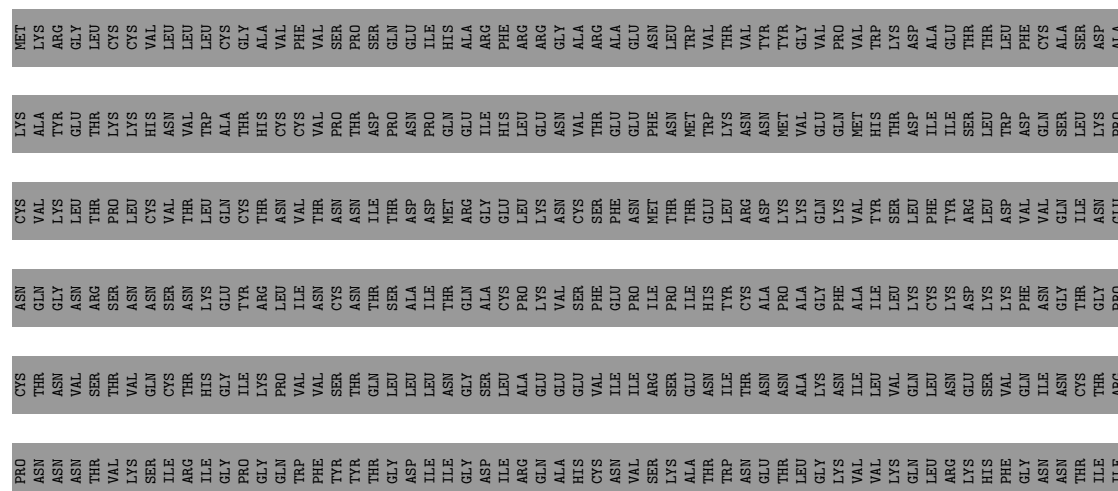
• Molecule 2: RM19R mAb Heavy chain

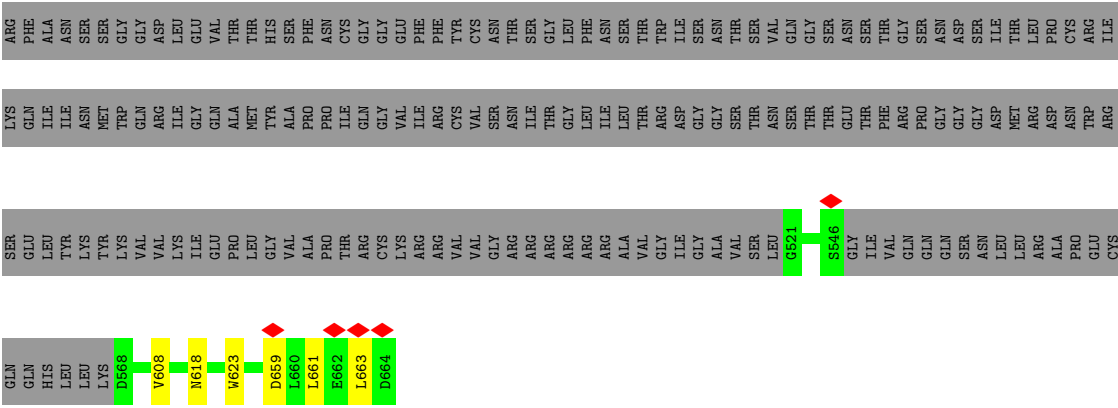


• Molecule 3: BG505 SOSIPv5.2(7S) - gp120

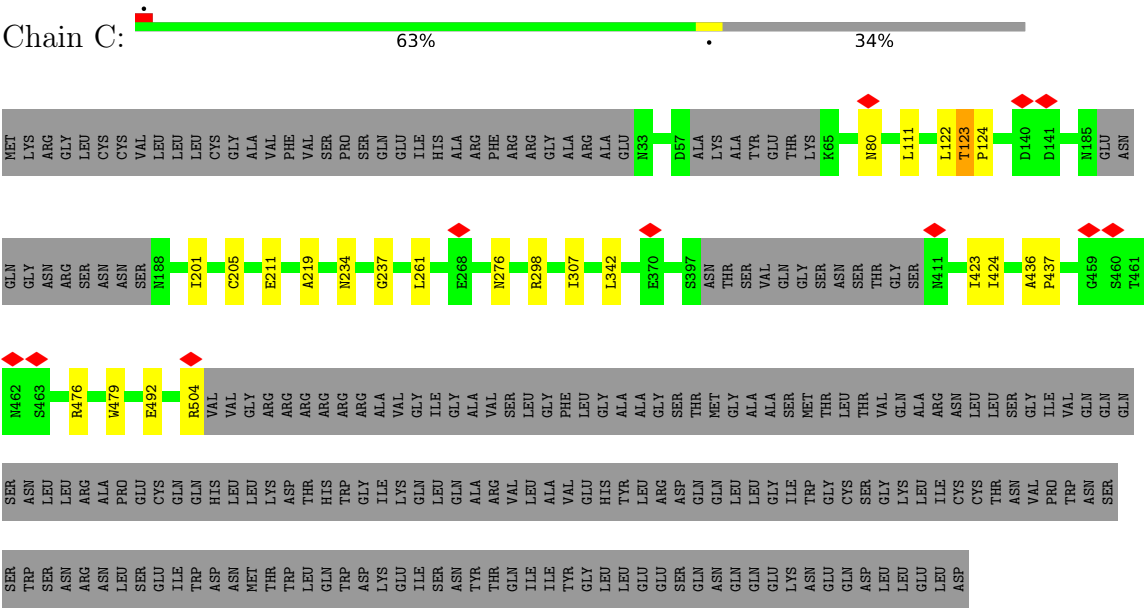


• Molecule 3: BG505 SOSIPv5.2(7S) - gp120

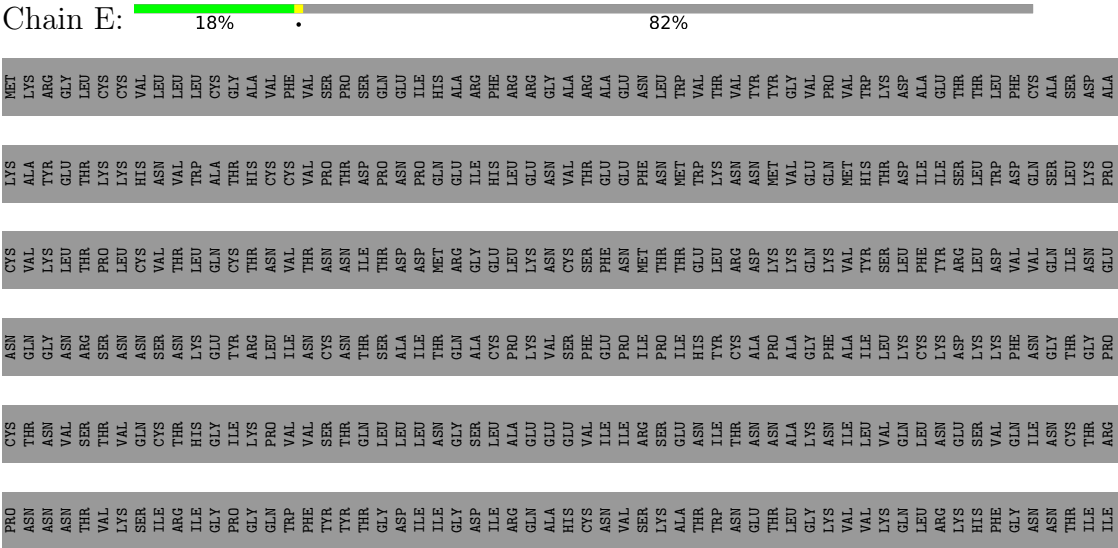




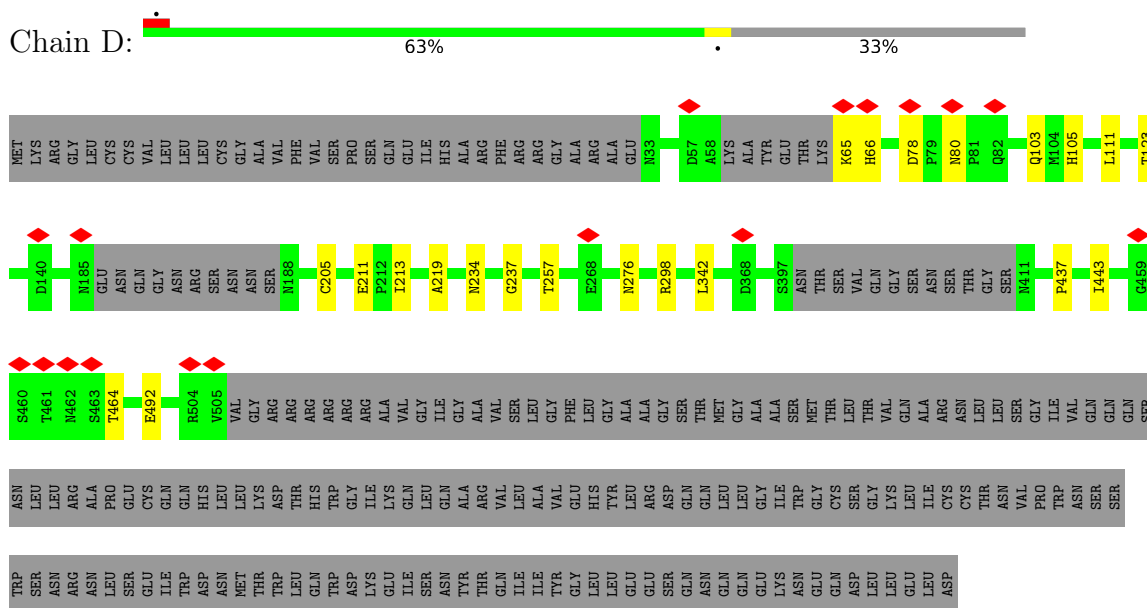
● Molecule 3: BG505 SOSIPv5.2(7S) - gp120



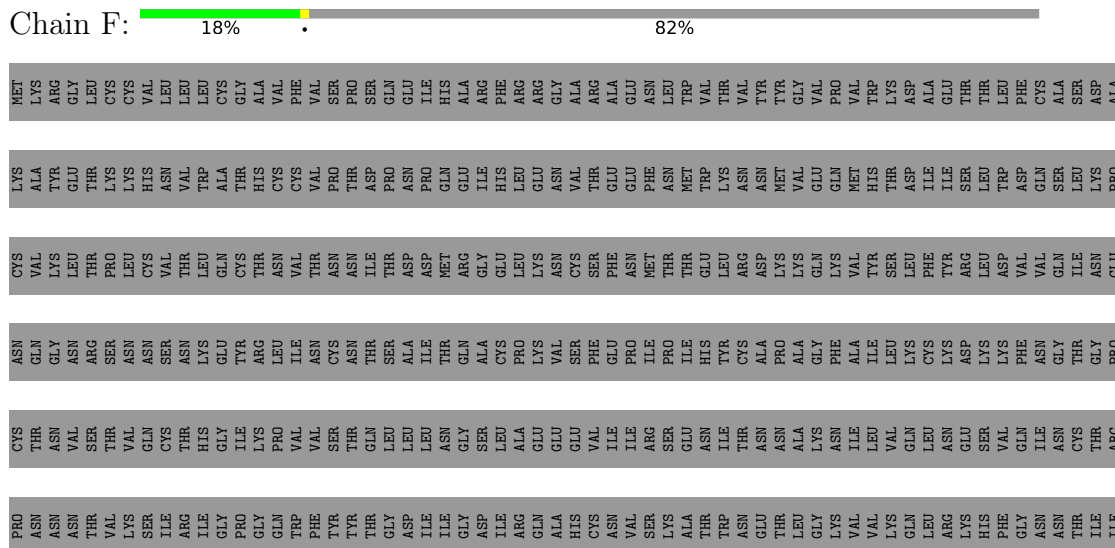
● Molecule 3: BG505 SOSIPv5.2(7S) - gp120

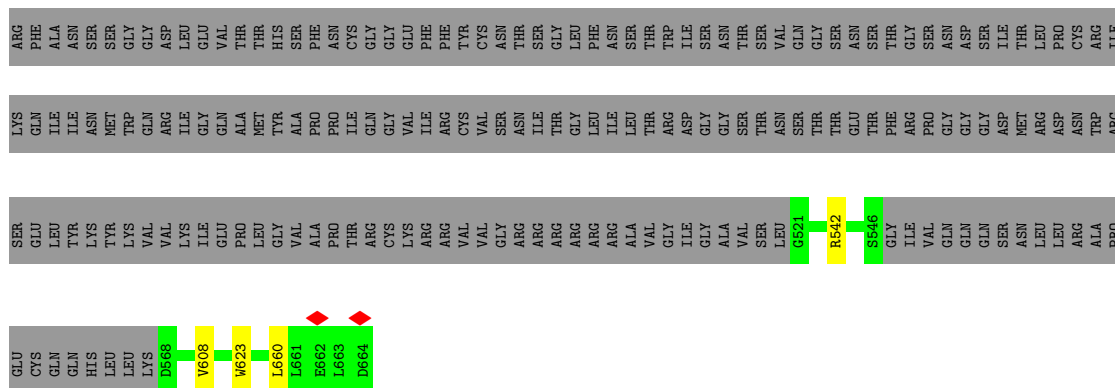


- Molecule 3: BG505 SOSIP_{v5.2}(7S) - gp120

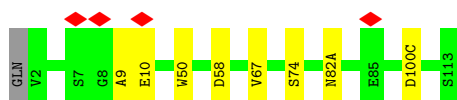


- Molecule 3: BG505 SOSIP_{v5.2}(7S) - gp120

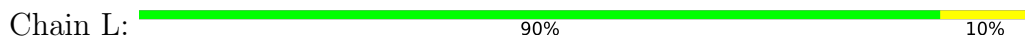




- Molecule 4: Rh.33172 mAb.1 Heavy chain



- Molecule 5: Rh.33172 mAb.1 Light chain



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



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



- Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



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



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



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



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



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



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



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



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



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



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



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



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

Chain c:

100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.7	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.044	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	370.8, 370.8, 370.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	1.14	1/837 (0.1%)	1.27	5/1137 (0.4%)
1	J	1.17	1/828 (0.1%)	1.31	8/1126 (0.7%)
1	K	1.12	2/837 (0.2%)	1.26	4/1137 (0.4%)
2	I	1.09	1/939 (0.1%)	1.34	13/1281 (1.0%)
2	M	1.08	0/939	1.35	13/1281 (1.0%)
2	N	1.12	1/939 (0.1%)	1.26	8/1281 (0.6%)
3	A	1.19	1/3549 (0.0%)	1.26	29/4820 (0.6%)
3	B	1.22	1/1004 (0.1%)	1.15	6/1362 (0.4%)
3	C	1.17	2/3559 (0.1%)	1.23	26/4832 (0.5%)
3	D	1.19	2/3571 (0.1%)	1.27	29/4849 (0.6%)
3	E	1.24	1/1004 (0.1%)	1.06	5/1362 (0.4%)
3	F	1.25	1/1004 (0.1%)	1.06	3/1362 (0.2%)
4	H	1.16	0/1018	1.19	3/1385 (0.2%)
5	L	1.12	0/819	1.27	6/1113 (0.5%)
All	All	1.17	14/20847 (0.1%)	1.24	158/28328 (0.6%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	504	ARG	NE-CZ	7.98	1.41	1.33
1	K	3	ARG	NE-CZ	7.15	1.41	1.33
1	K	6	GLN	CG-CD	-6.50	1.35	1.52
1	J	3	ARG	NE-CZ	6.38	1.40	1.33
2	I	96	TRP	NE1-CE2	-6.09	1.30	1.37
3	B	623	TRP	NE1-CE2	-6.03	1.30	1.37
3	F	623	TRP	NE1-CE2	-5.79	1.31	1.37
3	A	111	LEU	CB-CG	-5.51	1.42	1.53
1	G	3	ARG	NE-CZ	5.49	1.39	1.33
3	D	105	HIS	CB-CG	-5.45	1.42	1.50
2	N	100(B)	ARG	CG-CD	-5.35	1.36	1.52
3	C	111	LEU	CB-CG	-5.22	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	111	LEU	CB-CG	-5.19	1.43	1.53
3	E	631	TRP	NE1-CE2	-5.12	1.31	1.37

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	659	ASP	N-CA-C	8.91	120.99	111.28
3	A	492	GLU	CA-C-N	8.81	128.55	119.56
3	A	492	GLU	C-N-CA	8.81	128.55	119.56
3	C	492	GLU	CA-C-N	8.80	128.53	119.56
3	C	492	GLU	C-N-CA	8.80	128.53	119.56
3	A	298	ARG	CA-C-N	8.29	127.94	119.56
3	A	298	ARG	C-N-CA	8.29	127.94	119.56
3	D	492	GLU	CA-C-N	8.23	127.96	119.56
3	D	492	GLU	C-N-CA	8.23	127.96	119.56
3	C	298	ARG	CA-C-N	8.21	127.93	119.56
3	C	298	ARG	C-N-CA	8.21	127.93	119.56
3	D	464	THR	N-CA-C	-7.56	104.58	113.88
2	M	101	ASP	CA-CB-CG	7.39	119.99	112.60
3	D	257	THR	N-CA-C	7.38	122.58	113.50
3	A	436	ALA	CA-C-N	7.36	125.04	119.66
3	A	436	ALA	C-N-CA	7.36	125.04	119.66
3	D	342	LEU	N-CA-C	-7.35	103.93	113.12
3	D	298	ARG	CA-C-N	7.29	126.92	119.56
3	D	298	ARG	C-N-CA	7.29	126.92	119.56
2	I	101	ASP	CA-CB-CG	7.24	119.84	112.60
2	M	67	VAL	N-CA-C	7.18	118.16	108.11
3	C	219	ALA	CA-C-N	7.14	127.10	120.03
3	C	219	ALA	C-N-CA	7.14	127.10	120.03
3	A	276	ASN	CA-CB-CG	7.01	119.61	112.60
2	I	13	ARG	CA-C-N	6.96	126.66	119.56
2	I	13	ARG	C-N-CA	6.96	126.66	119.56
4	H	82(A)	ASN	N-CA-C	6.89	119.81	111.82
3	D	219	ALA	CA-C-N	6.81	126.78	120.03
3	D	219	ALA	C-N-CA	6.81	126.78	120.03
3	D	437	PRO	CA-C-N	6.81	126.77	120.03
3	D	437	PRO	C-N-CA	6.81	126.77	120.03
3	D	205	CYS	CA-C-N	6.77	126.46	119.56
3	D	205	CYS	C-N-CA	6.77	126.46	119.56
1	G	58	ILE	CA-C-N	6.69	126.67	119.78
1	G	58	ILE	C-N-CA	6.69	126.67	119.78
3	A	437	PRO	CA-C-N	6.56	126.53	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	437	PRO	C-N-CA	6.56	126.53	120.03
3	A	237	GLY	CA-C-N	6.55	126.52	119.78
3	A	237	GLY	C-N-CA	6.55	126.52	119.78
3	A	342	LEU	N-CA-C	-6.55	103.35	112.45
1	J	79	GLU	CA-C-N	6.52	127.03	119.47
1	J	79	GLU	C-N-CA	6.52	127.03	119.47
3	B	618	ASN	CA-CB-CG	6.50	119.10	112.60
3	A	219	ALA	CA-C-N	6.49	126.46	120.03
3	A	219	ALA	C-N-CA	6.49	126.46	120.03
3	D	437	PRO	N-CA-C	-6.48	103.64	110.58
2	N	104	GLY	CA-C-N	6.46	126.69	119.32
2	N	104	GLY	C-N-CA	6.46	126.69	119.32
3	D	276	ASN	CA-CB-CG	6.46	119.06	112.60
3	C	276	ASN	CA-CB-CG	6.41	119.01	112.60
2	M	48	ILE	N-CA-C	-6.35	105.64	111.67
2	I	78	PHE	CA-CB-CG	6.35	120.15	113.80
3	C	80	ASN	CA-C-N	6.33	126.24	119.85
3	C	80	ASN	C-N-CA	6.33	126.24	119.85
5	L	99	GLY	CA-C-N	6.19	126.16	119.78
5	L	99	GLY	C-N-CA	6.19	126.16	119.78
3	A	75	VAL	CA-C-N	6.18	126.15	120.03
3	A	75	VAL	C-N-CA	6.18	126.15	120.03
3	C	437	PRO	CA-C-N	6.16	126.13	120.03
3	C	437	PRO	C-N-CA	6.16	126.13	120.03
5	L	50	GLY	N-CA-C	-6.11	98.97	112.17
3	C	237	GLY	CA-C-N	6.11	126.07	119.78
3	C	237	GLY	C-N-CA	6.11	126.07	119.78
2	I	94	PHE	CA-CB-CG	6.00	119.80	113.80
2	I	104	GLY	CA-C-N	5.98	125.60	119.56
2	I	104	GLY	C-N-CA	5.98	125.60	119.56
3	D	80	ASN	CA-C-N	5.96	125.87	119.85
3	D	80	ASN	C-N-CA	5.96	125.87	119.85
3	C	205	CYS	CA-C-N	5.94	126.05	119.87
3	C	205	CYS	C-N-CA	5.94	126.05	119.87
3	C	261	LEU	CA-C-N	5.93	130.56	122.19
3	C	261	LEU	C-N-CA	5.93	130.56	122.19
2	M	35(A)	SER	N-CA-C	5.92	118.18	109.24
2	I	35(A)	SER	N-CA-C	5.90	117.93	109.14
3	D	237	GLY	CA-C-N	5.89	125.85	119.78
3	D	237	GLY	C-N-CA	5.89	125.85	119.78
1	G	79	GLU	CA-C-N	5.83	127.12	119.84
1	G	79	GLU	C-N-CA	5.83	127.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	661	LEU	N-CA-C	-5.83	105.48	112.59
3	F	608	VAL	CA-C-N	5.80	125.76	119.78
3	F	608	VAL	C-N-CA	5.80	125.76	119.78
2	I	67	VAL	N-CA-C	5.79	117.08	108.46
3	A	424	ILE	N-CA-C	5.78	116.20	108.11
1	J	58	ILE	CA-C-N	5.77	125.73	119.78
1	J	58	ILE	C-N-CA	5.77	125.73	119.78
1	K	58	ILE	CA-C-N	5.70	125.65	119.78
1	K	58	ILE	C-N-CA	5.70	125.65	119.78
2	M	79	SER	N-CA-C	5.69	117.72	109.07
1	K	91	GLU	N-CA-C	5.68	119.40	111.56
2	N	35(A)	SER	N-CA-C	5.67	117.59	109.14
2	N	8	GLY	CA-C-N	5.67	125.60	119.76
2	N	8	GLY	C-N-CA	5.67	125.60	119.76
3	A	299	PRO	N-CA-C	5.66	120.94	113.86
3	A	79	PRO	N-CA-C	-5.66	102.38	111.38
3	A	205	CYS	CA-C-N	5.64	125.74	119.87
3	A	205	CYS	C-N-CA	5.64	125.74	119.87
3	C	424	ILE	N-CA-C	5.64	116.06	108.17
5	L	79	GLN	CA-C-N	5.63	125.31	119.56
5	L	79	GLN	C-N-CA	5.63	125.31	119.56
3	B	608	VAL	CA-C-N	5.62	125.53	119.85
3	B	608	VAL	C-N-CA	5.62	125.53	119.85
2	N	101	ASP	CA-CB-CG	5.62	118.22	112.60
3	C	342	LEU	N-CA-C	-5.57	104.71	112.45
2	I	79	SER	N-CA-C	5.57	117.53	109.07
2	I	32	ASN	N-CA-C	5.55	116.69	108.86
3	E	608	VAL	CA-C-N	5.54	125.49	119.78
3	E	608	VAL	C-N-CA	5.54	125.49	119.78
2	M	104	GLY	CA-C-N	5.54	125.15	119.56
2	M	104	GLY	C-N-CA	5.54	125.15	119.56
2	I	8	GLY	CA-C-N	5.54	125.30	119.76
2	I	8	GLY	C-N-CA	5.54	125.30	119.76
1	K	98	PHE	CA-CB-CG	5.53	119.33	113.80
3	B	663	LEU	N-CA-C	5.51	119.00	111.39
1	J	43	SER	CA-C-N	5.51	125.45	119.78
1	J	43	SER	C-N-CA	5.51	125.45	119.78
5	L	17	ASP	CA-CB-CG	5.47	118.07	112.60
3	C	123	THR	CA-C-N	5.44	125.11	119.56
3	C	123	THR	C-N-CA	5.44	125.11	119.56
3	D	213	ILE	N-CA-C	-5.44	101.92	108.45
3	A	123	THR	CA-C-N	5.38	125.05	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	123	THR	C-N-CA	5.38	125.05	119.56
2	M	13	ARG	CA-C-N	5.33	125.65	119.47
2	M	13	ARG	C-N-CA	5.33	125.65	119.47
3	D	78	ASP	CA-C-N	5.32	124.93	119.56
3	D	78	ASP	C-N-CA	5.32	124.93	119.56
4	H	67	VAL	N-CA-C	5.31	115.54	108.11
1	G	39	LYS	N-CA-C	-5.28	103.13	109.83
3	E	660	LEU	N-CA-C	-5.28	106.68	113.23
3	C	436	ALA	CA-C-N	5.28	123.51	119.66
3	C	436	ALA	C-N-CA	5.28	123.51	119.66
3	E	636	SER	CA-C-N	5.27	127.87	120.28
3	E	636	SER	C-N-CA	5.27	127.87	120.28
3	D	443	ILE	N-CA-C	5.25	115.53	108.17
3	D	211	GLU	CA-C-N	5.25	125.17	119.76
3	D	211	GLU	C-N-CA	5.25	125.17	119.76
3	D	123	THR	CA-C-N	5.24	124.90	119.56
3	D	123	THR	C-N-CA	5.24	124.90	119.56
3	A	249	HIS	CA-C-N	-5.21	114.99	120.31
3	A	249	HIS	C-N-CA	-5.21	114.99	120.31
1	J	7	SER	N-CA-C	5.21	119.83	112.75
2	M	74	SER	N-CA-C	-5.20	106.08	112.90
3	A	297	THR	N-CA-C	5.20	116.97	109.07
3	D	103	GLN	CA-C-N	-5.18	113.33	120.28
3	D	103	GLN	C-N-CA	-5.18	113.33	120.28
3	A	261	LEU	CA-C-N	5.18	129.47	122.07
3	A	261	LEU	C-N-CA	5.18	129.47	122.07
2	M	57	THR	N-CA-C	5.11	117.44	109.52
3	C	211	GLU	CA-C-N	5.11	125.02	119.76
3	C	211	GLU	C-N-CA	5.11	125.02	119.76
1	J	98	PHE	CA-CB-CG	5.10	118.90	113.80
3	C	307	ILE	N-CA-C	5.09	116.05	108.46
4	H	74	SER	N-CA-C	-5.08	104.72	112.04
2	M	8	GLY	CA-C-N	5.07	125.30	119.83
2	M	8	GLY	C-N-CA	5.07	125.30	119.83
2	N	66	ARG	CA-C-N	-5.05	115.93	122.94
2	N	66	ARG	C-N-CA	-5.05	115.93	122.94
3	F	660	LEU	N-CA-C	5.04	119.28	113.38
3	A	382	PHE	N-CA-C	5.03	116.90	107.99

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	G	817	0	786	5	0
1	J	808	0	773	3	0
1	K	817	0	786	9	0
2	I	915	0	883	3	0
2	M	915	0	883	0	0
2	N	915	0	883	1	0
3	A	3477	0	3408	1	0
3	B	985	0	940	0	0
3	C	3487	0	3418	8	0
3	D	3499	0	3432	2	0
3	E	985	0	940	0	0
3	F	985	0	940	1	0
4	H	995	0	930	7	0
5	L	803	0	789	4	0
6	O	61	0	52	0	0
6	U	61	0	52	0	0
6	Y	61	0	52	0	0
7	P	28	0	25	0	0
7	Q	28	0	25	0	0
7	R	28	0	25	0	0
7	S	28	0	25	1	0
7	T	28	0	25	0	0
7	V	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0
7	Z	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
8	A	182	0	169	0	0
8	B	42	0	39	0	0
8	C	210	0	195	0	0
8	D	196	0	182	0	0
8	E	42	0	39	1	0
8	F	42	0	39	0	0
All	All	21636	0	20910	40	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 (40) 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)
5:L:52:SER:HB3	7:S:2:NAG:H5	1.78	0.65
1:K:94:TRP:O	1:K:94:TRP:CE3	2.50	0.64
4:H:50:TRP:CD1	4:H:58:ASP:HB3	2.34	0.62
1:G:96:TRP:O	2:I:47:TRP:CD1	2.53	0.61
5:L:90:GLN:HE21	5:L:97:THR:HB	1.64	0.61
4:H:9:ALA:O	4:H:10:GLU:HG3	2.05	0.56
1:G:96:TRP:O	2:I:47:TRP:HD1	1.89	0.55
3:D:234:ASN:OD1	3:D:234:ASN:C	2.49	0.54
4:H:50:TRP:NE1	4:H:58:ASP:HB3	2.22	0.54
3:C:201:ILE:HD11	3:C:423:ILE:HG12	1.90	0.53
3:D:65:LYS:HG2	3:D:66:HIS:H	1.72	0.53
3:A:207:LYS:NZ	4:H:100(C):ASP:OD2	2.41	0.53
1:K:94:TRP:N	1:K:95:PRO:HD2	2.24	0.53
1:K:94:TRP:C	1:K:94:TRP:CD2	2.86	0.52
5:L:18:ARG:NH2	5:L:74:THR:HG21	2.25	0.51
1:K:29:VAL:HG23	1:K:90:GLN:HG3	1.92	0.51
1:G:39:LYS:NZ	1:G:81:GLU:OE2	2.44	0.51
4:H:50:TRP:HE1	4:H:58:ASP:HB3	1.77	0.49
1:J:60:ASP:OD1	1:J:60:ASP:N	2.46	0.48
3:F:542:ARG:HG2	3:F:542:ARG:O	2.13	0.48
1:K:60:ASP:OD1	1:K:60:ASP:N	2.46	0.48
3:C:201:ILE:CD1	3:C:423:ILE:HG23	2.44	0.48
1:G:60:ASP:OD1	1:G:60:ASP:N	2.47	0.47
1:K:93:ASP:O	1:K:96:TRP:HD1	1.96	0.47
5:L:103:LYS:NZ	5:L:105:ASP:OD1	2.49	0.46
8:E:702:NAG:O7	8:E:702:NAG:O3	2.29	0.45
1:K:94:TRP:O	1:K:96:TRP:N	2.50	0.44
3:C:234:ASN:OD1	3:C:234:ASN:C	2.61	0.43
3:C:122:LEU:HB2	3:C:201:ILE:O	2.19	0.43
3:C:201:ILE:HD11	3:C:423:ILE:HG23	2.00	0.42
4:H:9:ALA:O	4:H:10:GLU:CG	2.67	0.42
3:C:123:THR:N	3:C:124:PRO:CD	2.83	0.41
3:C:476:ARG:HA	3:C:479:TRP:CD1	2.55	0.41
1:K:94:TRP:CG	2:N:58:ARG:HD3	2.55	0.41
3:C:201:ILE:O	3:C:201:ILE:HG23	2.20	0.41
1:K:93:ASP:O	1:K:96:TRP:CD1	2.73	0.41
1:J:58:ILE:HA	1:J:59:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:65:SER:OG	1:J:66:GLY:N	2.54	0.40
1:G:98:PHE:CE1	2:I:47:TRP:CD1	3.09	0.40
4:H:9:ALA:C	4:H:10:GLU:HG3	2.46	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	G	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
1	J	102/107 (95%)	97 (95%)	5 (5%)	0	100	100
1	K	103/107 (96%)	101 (98%)	2 (2%)	0	100	100
2	I	116/121 (96%)	116 (100%)	0	0	100	100
2	M	116/121 (96%)	116 (100%)	0	0	100	100
2	N	116/121 (96%)	116 (100%)	0	0	100	100
3	A	432/666 (65%)	428 (99%)	4 (1%)	0	100	100
3	B	119/666 (18%)	117 (98%)	2 (2%)	0	100	100
3	C	433/666 (65%)	427 (99%)	6 (1%)	0	100	100
3	D	435/666 (65%)	430 (99%)	5 (1%)	0	100	100
3	E	119/666 (18%)	118 (99%)	1 (1%)	0	100	100
3	F	119/666 (18%)	116 (98%)	3 (2%)	0	100	100
4	H	126/129 (98%)	125 (99%)	1 (1%)	0	100	100
5	L	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
All	All	2544/4916 (52%)	2506 (98%)	38 (2%)	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	G	91/92 (99%)	91 (100%)	0	100	100
1	J	90/92 (98%)	90 (100%)	0	100	100
1	K	91/92 (99%)	91 (100%)	0	100	100
2	I	101/104 (97%)	101 (100%)	0	100	100
2	M	101/104 (97%)	101 (100%)	0	100	100
2	N	101/104 (97%)	101 (100%)	0	100	100
3	A	397/588 (68%)	397 (100%)	0	100	100
3	B	107/588 (18%)	107 (100%)	0	100	100
3	C	398/588 (68%)	398 (100%)	0	100	100
3	D	399/588 (68%)	399 (100%)	0	100	100
3	E	107/588 (18%)	107 (100%)	0	100	100
3	F	107/588 (18%)	107 (100%)	0	100	100
4	H	106/107 (99%)	106 (100%)	0	100	100
5	L	92/92 (100%)	92 (100%)	0	100	100
All	All	2288/4315 (53%)	2288 (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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	591	GLN
4	H	39	GLN
1	J	38	GLN
2	M	39	GLN
3	C	105	HIS
3	C	195	ASN
3	C	374	HIS
3	E	591	GLN
3	E	607	ASN

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Mol	Chain	Res	Type
3	E	658	GLN
1	K	38	GLN
2	N	39	GLN
3	D	33	ASN
3	D	99	ASN

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 ⓘ

39 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	O	1	3,6	14,14,15	1.96	3 (21%)	17,19,21	1.17	3 (17%)
6	NAG	O	2	6	14,14,15	1.79	5 (35%)	17,19,21	0.92	1 (5%)
6	BMA	O	3	6	11,11,12	1.37	2 (18%)	15,15,17	0.58	0
6	MAN	O	4	6	11,11,12	1.84	4 (36%)	15,15,17	0.73	0
6	MAN	O	5	6	11,11,12	1.92	5 (45%)	15,15,17	0.73	0
7	NAG	P	1	3,7	14,14,15	2.13	4 (28%)	17,19,21	1.04	1 (5%)
7	NAG	P	2	7	14,14,15	1.96	5 (35%)	17,19,21	0.90	1 (5%)
7	NAG	Q	1	3,7	14,14,15	2.02	3 (21%)	17,19,21	1.26	2 (11%)
7	NAG	Q	2	7	14,14,15	1.98	4 (28%)	17,19,21	0.88	1 (5%)
7	NAG	R	1	3,7	14,14,15	2.23	6 (42%)	17,19,21	1.17	2 (11%)
7	NAG	R	2	7	14,14,15	1.92	6 (42%)	17,19,21	1.04	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	S	1	3,7	14,14,15	0.38	0	17,19,21	0.73	0
7	NAG	S	2	7	14,14,15	0.37	0	17,19,21	0.56	0
7	NAG	T	1	3,7	14,14,15	1.96	5 (35%)	17,19,21	1.17	3 (17%)
7	NAG	T	2	7	14,14,15	1.88	4 (28%)	17,19,21	0.86	1 (5%)
6	NAG	U	1	3,6	14,14,15	1.92	3 (21%)	17,19,21	1.26	3 (17%)
6	NAG	U	2	6	14,14,15	1.94	4 (28%)	17,19,21	0.98	2 (11%)
6	BMA	U	3	6	11,11,12	1.45	3 (27%)	15,15,17	0.68	0
6	MAN	U	4	6	11,11,12	1.91	5 (45%)	15,15,17	0.83	0
6	MAN	U	5	6	11,11,12	1.88	4 (36%)	15,15,17	0.71	0
7	NAG	V	1	3,7	14,14,15	1.99	3 (21%)	17,19,21	1.22	2 (11%)
7	NAG	V	2	7	14,14,15	2.05	5 (35%)	17,19,21	0.86	1 (5%)
7	NAG	W	1	3,7	14,14,15	2.05	5 (35%)	17,19,21	1.03	1 (5%)
7	NAG	W	2	7	14,14,15	2.02	5 (35%)	17,19,21	0.89	0
7	NAG	X	1	3,7	14,14,15	2.00	4 (28%)	17,19,21	1.11	2 (11%)
7	NAG	X	2	7	14,14,15	1.93	5 (35%)	17,19,21	0.86	1 (5%)
6	NAG	Y	1	3,6	14,14,15	1.96	4 (28%)	17,19,21	1.14	2 (11%)
6	NAG	Y	2	6	14,14,15	1.93	5 (35%)	17,19,21	1.00	2 (11%)
6	BMA	Y	3	6	11,11,12	1.38	2 (18%)	15,15,17	0.62	0
6	MAN	Y	4	6	11,11,12	1.80	4 (36%)	15,15,17	0.69	0
6	MAN	Y	5	6	11,11,12	1.95	6 (54%)	15,15,17	0.71	0
7	NAG	Z	1	3,7	14,14,15	2.11	4 (28%)	17,19,21	1.02	0
7	NAG	Z	2	7	14,14,15	1.99	5 (35%)	17,19,21	0.86	1 (5%)
7	NAG	a	1	3,7	14,14,15	2.04	5 (35%)	17,19,21	1.14	2 (11%)
7	NAG	a	2	7	14,14,15	1.97	4 (28%)	17,19,21	0.88	1 (5%)
7	NAG	b	1	3,7	14,14,15	2.07	5 (35%)	17,19,21	0.96	1 (5%)
7	NAG	b	2	7	14,14,15	1.92	5 (35%)	17,19,21	0.92	1 (5%)
7	NAG	c	1	3,7	14,14,15	2.02	4 (28%)	17,19,21	1.15	2 (11%)
7	NAG	c	2	7	14,14,15	1.97	4 (28%)	17,19,21	0.89	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
6	NAG	O	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1

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

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	1	NAG	C1-C2	5.90	1.60	1.52
7	Z	1	NAG	C1-C2	5.56	1.59	1.52
6	O	1	NAG	C1-C2	5.55	1.59	1.52
7	P	1	NAG	C1-C2	5.49	1.59	1.52
7	V	1	NAG	C1-C2	5.43	1.59	1.52
7	Q	1	NAG	C1-C2	5.41	1.59	1.52
7	a	1	NAG	C1-C2	5.24	1.59	1.52
6	Y	1	NAG	C1-C2	5.23	1.59	1.52
6	U	1	NAG	C1-C2	5.23	1.59	1.52
7	X	1	NAG	C1-C2	5.18	1.59	1.52
7	b	1	NAG	C1-C2	5.12	1.59	1.52
7	c	1	NAG	C1-C2	5.11	1.59	1.52
7	T	1	NAG	C1-C2	4.92	1.59	1.52
7	V	2	NAG	C1-C2	4.83	1.58	1.52
7	W	2	NAG	C1-C2	4.80	1.58	1.52
7	W	1	NAG	C1-C2	4.78	1.58	1.52
7	a	2	NAG	C1-C2	4.74	1.58	1.52
7	X	2	NAG	C1-C2	4.69	1.58	1.52
7	c	2	NAG	C1-C2	4.65	1.58	1.52
7	Z	2	NAG	C1-C2	4.55	1.58	1.52
7	Q	2	NAG	C1-C2	4.55	1.58	1.52
7	T	2	NAG	C1-C2	4.55	1.58	1.52
7	P	2	NAG	C1-C2	4.52	1.58	1.52
7	b	2	NAG	C1-C2	4.51	1.58	1.52
6	U	2	NAG	C1-C2	4.48	1.58	1.52
7	R	2	NAG	C1-C2	4.42	1.58	1.52
6	Y	2	NAG	C1-C2	4.13	1.58	1.52
6	O	2	NAG	C1-C2	3.97	1.57	1.52
6	U	2	NAG	O5-C5	3.33	1.49	1.43
6	Y	5	MAN	O5-C5	3.29	1.49	1.43
7	P	1	NAG	O5-C5	3.28	1.49	1.43
6	O	5	MAN	O5-C5	3.28	1.49	1.43
6	Y	2	NAG	O5-C5	3.27	1.49	1.43
7	Q	2	NAG	O5-C5	3.24	1.49	1.43
6	U	5	MAN	O5-C5	3.22	1.49	1.43
7	Z	2	NAG	O5-C5	3.21	1.49	1.43
6	Y	5	MAN	C2-C3	3.18	1.57	1.52
7	V	2	NAG	O5-C5	3.18	1.49	1.43
7	W	2	NAG	O5-C5	3.17	1.49	1.43
7	P	2	NAG	O5-C5	3.14	1.49	1.43
7	c	2	NAG	O5-C5	3.14	1.49	1.43
7	W	1	NAG	O5-C5	3.10	1.49	1.43
7	a	2	NAG	O5-C5	3.09	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	5	MAN	C2-C3	3.09	1.57	1.52
6	U	5	MAN	C2-C3	3.08	1.57	1.52
6	U	4	MAN	C2-C3	3.08	1.57	1.52
7	Z	1	NAG	O5-C5	3.05	1.49	1.43
6	Y	4	MAN	O5-C5	3.03	1.49	1.43
7	T	2	NAG	O5-C5	2.99	1.49	1.43
6	O	4	MAN	C2-C3	2.97	1.57	1.52
7	b	1	NAG	O5-C5	2.94	1.49	1.43
6	U	4	MAN	O5-C5	2.93	1.49	1.43
7	X	2	NAG	O5-C5	2.92	1.49	1.43
6	O	4	MAN	O5-C5	2.88	1.49	1.43
6	O	2	NAG	O5-C5	2.83	1.49	1.43
7	b	2	NAG	O5-C5	2.80	1.48	1.43
6	Y	4	MAN	C2-C3	2.77	1.56	1.52
7	c	1	NAG	O5-C5	2.74	1.48	1.43
6	U	4	MAN	C1-C2	2.74	1.58	1.52
7	a	1	NAG	O5-C5	2.70	1.48	1.43
7	Q	1	NAG	O5-C5	2.69	1.48	1.43
7	X	1	NAG	O5-C5	2.69	1.48	1.43
7	V	1	NAG	O5-C5	2.63	1.48	1.43
6	U	3	BMA	O5-C5	2.60	1.48	1.43
7	R	2	NAG	C3-C2	2.58	1.57	1.52
6	U	4	MAN	C4-C5	2.58	1.58	1.53
7	T	1	NAG	O5-C5	2.57	1.48	1.43
6	O	5	MAN	C4-C5	2.56	1.58	1.53
6	Y	1	NAG	O5-C5	2.56	1.48	1.43
7	R	1	NAG	C2-N2	2.55	1.50	1.46
7	W	2	NAG	C3-C2	2.54	1.57	1.52
7	b	2	NAG	C3-C2	2.54	1.57	1.52
7	V	2	NAG	C3-C2	2.53	1.57	1.52
6	O	4	MAN	C1-C2	2.53	1.58	1.52
7	R	1	NAG	C4-C3	2.52	1.58	1.52
6	O	4	MAN	C4-C5	2.52	1.58	1.53
7	W	1	NAG	O5-C1	2.49	1.47	1.43
7	Z	2	NAG	C3-C2	2.48	1.57	1.52
6	O	3	BMA	O5-C5	2.48	1.48	1.43
7	R	2	NAG	O5-C5	2.48	1.48	1.43
6	Y	4	MAN	C1-C2	2.48	1.58	1.52
7	R	2	NAG	C4-C5	2.46	1.58	1.53
7	R	2	NAG	C2-N2	2.45	1.50	1.46
7	Q	2	NAG	C3-C2	2.43	1.57	1.52
7	Z	1	NAG	C4-C5	2.43	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	b	1	NAG	O5-C1	2.42	1.47	1.43
7	Q	2	NAG	C4-C5	2.40	1.58	1.53
6	Y	4	MAN	C4-C5	2.38	1.58	1.53
6	Y	3	BMA	O5-C5	2.38	1.48	1.43
6	Y	5	MAN	C1-C2	2.37	1.57	1.52
7	P	1	NAG	C4-C5	2.37	1.58	1.53
6	Y	5	MAN	C4-C5	2.36	1.58	1.53
6	U	1	NAG	O5-C5	2.34	1.48	1.43
7	R	1	NAG	C3-C2	2.34	1.57	1.52
7	V	2	NAG	C4-C5	2.33	1.58	1.53
6	U	5	MAN	C4-C5	2.33	1.58	1.53
6	O	5	MAN	C1-C2	2.32	1.57	1.52
7	c	2	NAG	C3-C2	2.32	1.57	1.52
7	P	2	NAG	C4-C5	2.32	1.58	1.53
7	a	2	NAG	C4-C5	2.32	1.58	1.53
6	Y	2	NAG	C3-C2	2.31	1.57	1.52
6	U	5	MAN	C1-C2	2.31	1.57	1.52
7	X	2	NAG	C4-C5	2.30	1.57	1.53
7	a	2	NAG	C3-C2	2.30	1.57	1.52
7	W	2	NAG	C4-C5	2.29	1.57	1.53
7	c	2	NAG	C4-C5	2.27	1.57	1.53
6	O	2	NAG	C3-C2	2.26	1.57	1.52
7	P	2	NAG	C3-C2	2.26	1.57	1.52
6	U	1	NAG	C3-C2	2.26	1.57	1.52
6	O	1	NAG	O5-C5	2.25	1.47	1.43
6	U	2	NAG	C4-C5	2.25	1.57	1.53
6	O	1	NAG	C3-C2	2.25	1.57	1.52
6	U	2	NAG	C3-C2	2.25	1.57	1.52
7	b	2	NAG	C4-C5	2.24	1.57	1.53
7	T	2	NAG	C3-C2	2.24	1.57	1.52
7	Z	2	NAG	C4-C5	2.24	1.57	1.53
7	c	1	NAG	O5-C1	2.23	1.47	1.43
7	X	2	NAG	C3-C2	2.23	1.57	1.52
7	c	1	NAG	C4-C5	2.23	1.57	1.53
7	W	1	NAG	C3-C2	2.22	1.57	1.52
7	a	1	NAG	C4-C5	2.22	1.57	1.53
7	P	2	NAG	C2-N2	2.21	1.49	1.46
6	O	2	NAG	C4-C5	2.20	1.57	1.53
7	T	2	NAG	C4-C5	2.20	1.57	1.53
7	b	2	NAG	C4-C3	2.20	1.58	1.52
7	V	1	NAG	C4-C5	2.19	1.57	1.53
7	a	1	NAG	C3-C2	2.19	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	1	NAG	O5-C1	2.19	1.47	1.43
7	P	1	NAG	O5-C1	2.18	1.47	1.43
7	b	1	NAG	C4-C5	2.17	1.57	1.53
7	b	1	NAG	C3-C2	2.16	1.57	1.52
7	W	1	NAG	C4-C5	2.16	1.57	1.53
6	Y	5	MAN	O5-C1	2.16	1.47	1.43
6	Y	3	BMA	C2-C3	2.16	1.55	1.52
6	Y	2	NAG	C4-C3	2.16	1.57	1.52
7	V	2	NAG	C2-N2	2.15	1.49	1.46
7	X	1	NAG	C4-C5	2.15	1.57	1.53
7	R	1	NAG	O5-C5	2.15	1.47	1.43
6	Y	1	NAG	C3-C2	2.14	1.57	1.52
7	T	1	NAG	C2-N2	2.14	1.49	1.46
6	O	3	BMA	C2-C3	2.12	1.55	1.52
7	T	1	NAG	C4-C5	2.12	1.57	1.53
6	O	2	NAG	C4-C3	2.11	1.57	1.52
7	W	2	NAG	C2-N2	2.11	1.49	1.46
6	U	3	BMA	C2-C3	2.09	1.55	1.52
7	R	2	NAG	C4-C3	2.09	1.57	1.52
7	X	1	NAG	O5-C1	2.09	1.47	1.43
6	Y	1	NAG	C4-C5	2.09	1.57	1.53
7	Q	1	NAG	C4-C5	2.08	1.57	1.53
6	O	5	MAN	C4-C3	2.08	1.57	1.52
7	R	1	NAG	C4-C5	2.07	1.57	1.53
7	Z	2	NAG	C2-N2	2.06	1.49	1.46
7	T	1	NAG	O5-C1	2.06	1.47	1.43
6	Y	2	NAG	C4-C5	2.06	1.57	1.53
6	Y	5	MAN	C4-C3	2.05	1.57	1.52
7	a	1	NAG	O5-C1	2.05	1.47	1.43
6	U	4	MAN	C4-C3	2.04	1.57	1.52
7	X	2	NAG	C4-C3	2.03	1.57	1.52
6	U	3	BMA	C1-C2	2.02	1.57	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	1	NAG	C8-C7-N2	2.81	120.77	116.12
7	a	1	NAG	C8-C7-N2	2.76	120.70	116.12
7	V	1	NAG	C8-C7-N2	2.75	120.68	116.12
7	T	1	NAG	C8-C7-N2	2.70	120.59	116.12
7	R	1	NAG	C8-C7-N2	2.66	120.53	116.12
7	R	2	NAG	C8-C7-N2	2.62	120.46	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	c	1	NAG	C8-C7-N2	2.57	120.37	116.12
6	Y	2	NAG	C8-C7-N2	2.55	120.34	116.12
7	X	1	NAG	C8-C7-N2	2.47	120.22	116.12
7	W	1	NAG	C8-C7-N2	2.47	120.22	116.12
6	U	1	NAG	C1-O5-C5	2.44	115.45	112.19
7	Q	1	NAG	C1-C2-N2	-2.44	106.59	110.43
6	U	1	NAG	C8-C7-N2	2.43	120.16	116.12
6	Y	1	NAG	C8-C7-N2	2.36	120.03	116.12
6	U	2	NAG	C8-C7-N2	2.34	119.99	116.12
7	b	2	NAG	C8-C7-N2	2.27	119.88	116.12
7	a	1	NAG	O7-C7-C8	-2.26	118.03	122.05
7	P	1	NAG	C8-C7-N2	2.26	119.86	116.12
6	U	1	NAG	O7-C7-C8	-2.24	118.06	122.05
6	O	1	NAG	C8-C7-N2	2.23	119.82	116.12
7	R	1	NAG	O7-C7-C8	-2.17	118.19	122.05
6	Y	2	NAG	O7-C7-C8	-2.17	118.20	122.05
6	O	1	NAG	C1-C2-N2	-2.15	107.04	110.43
7	b	1	NAG	C8-C7-N2	2.15	119.68	116.12
7	c	2	NAG	C8-C7-N2	2.14	119.66	116.12
7	X	2	NAG	C8-C7-N2	2.12	119.64	116.12
6	O	1	NAG	C1-O5-C5	2.12	115.03	112.19
6	O	2	NAG	C8-C7-N2	2.12	119.63	116.12
7	V	1	NAG	O7-C7-C8	-2.12	118.28	122.05
7	V	2	NAG	C8-C7-N2	2.09	119.59	116.12
7	T	1	NAG	C1-C2-N2	-2.09	107.14	110.43
7	P	2	NAG	C8-C7-N2	2.07	119.55	116.12
6	Y	1	NAG	O7-C7-C8	-2.06	118.38	122.05
7	Z	2	NAG	C8-C7-N2	2.06	119.53	116.12
7	R	2	NAG	C1-O5-C5	2.06	114.94	112.19
7	a	2	NAG	C8-C7-N2	2.05	119.52	116.12
6	U	2	NAG	O7-C7-C8	-2.05	118.41	122.05
7	Q	2	NAG	C8-C7-N2	2.03	119.49	116.12
7	T	1	NAG	O7-C7-C8	-2.02	118.46	122.05
7	c	1	NAG	O7-C7-C8	-2.01	118.48	122.05
7	T	2	NAG	C8-C7-N2	2.01	119.44	116.12
7	X	1	NAG	C1-C2-N2	-2.00	107.28	110.43

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	3	BMA	O5-C5-C6-O6

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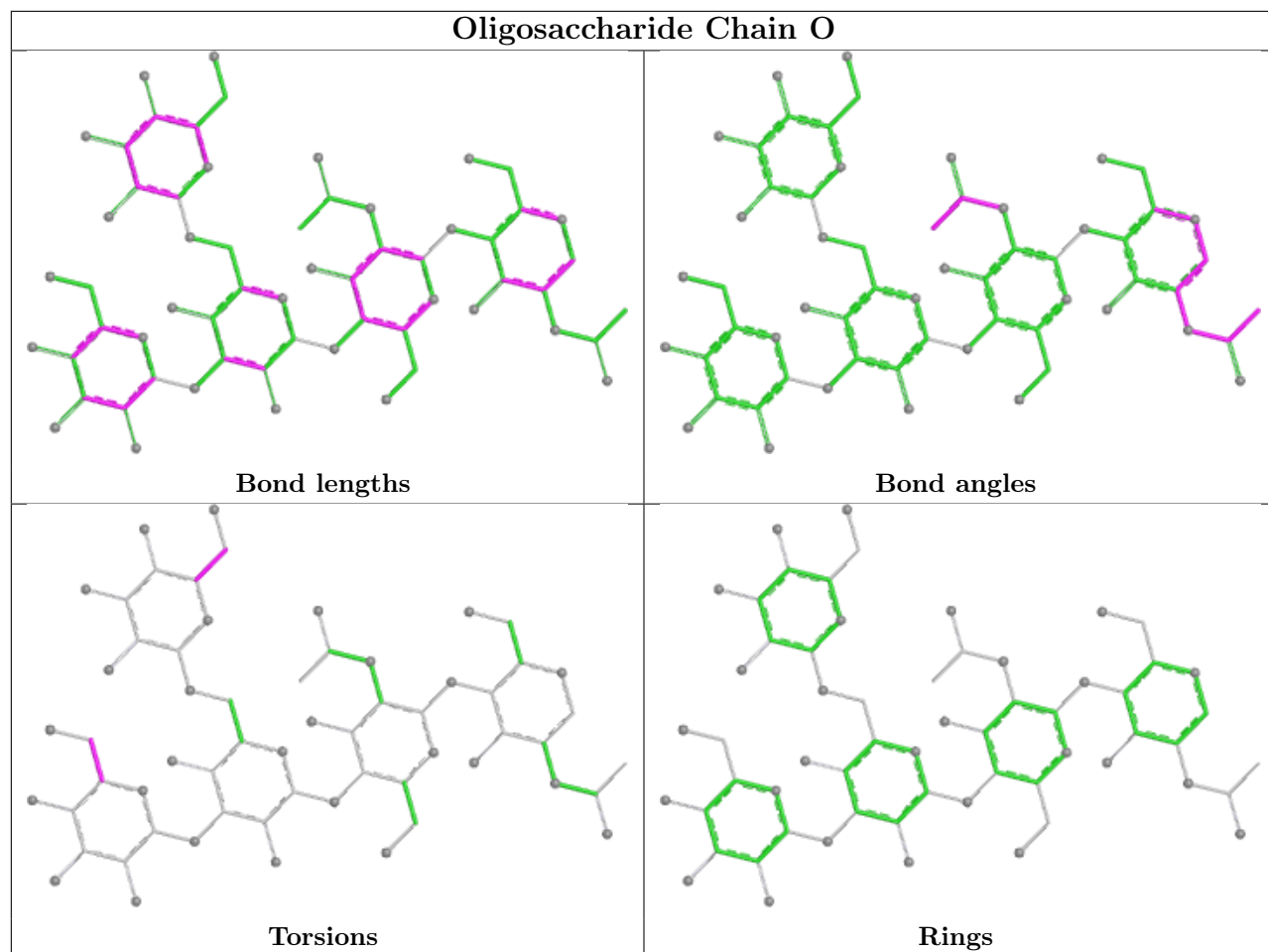
Mol	Chain	Res	Type	Atoms
6	U	3	BMA	C4-C5-C6-O6
7	S	2	NAG	C8-C7-N2-C2
6	Y	3	BMA	O5-C5-C6-O6
6	Y	4	MAN	O5-C5-C6-O6
7	S	2	NAG	O7-C7-N2-C2
6	O	4	MAN	O5-C5-C6-O6
6	O	5	MAN	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
6	U	4	MAN	O5-C5-C6-O6
6	Y	3	BMA	C4-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
6	Y	4	MAN	C4-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	S	1	NAG	C8-C7-N2-C2
7	S	1	NAG	O7-C7-N2-C2
6	O	4	MAN	C4-C5-C6-O6

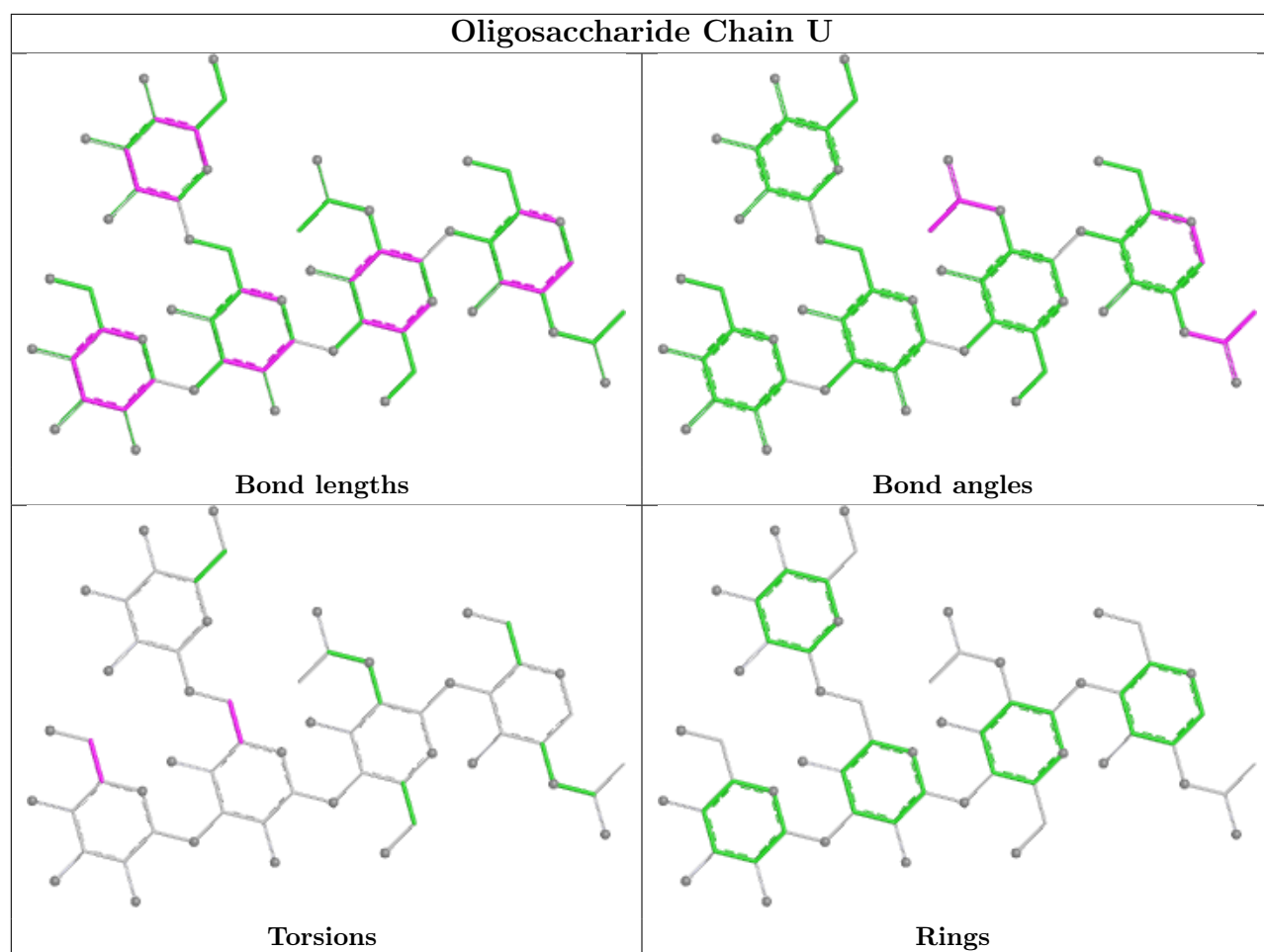
There are no ring outliers.

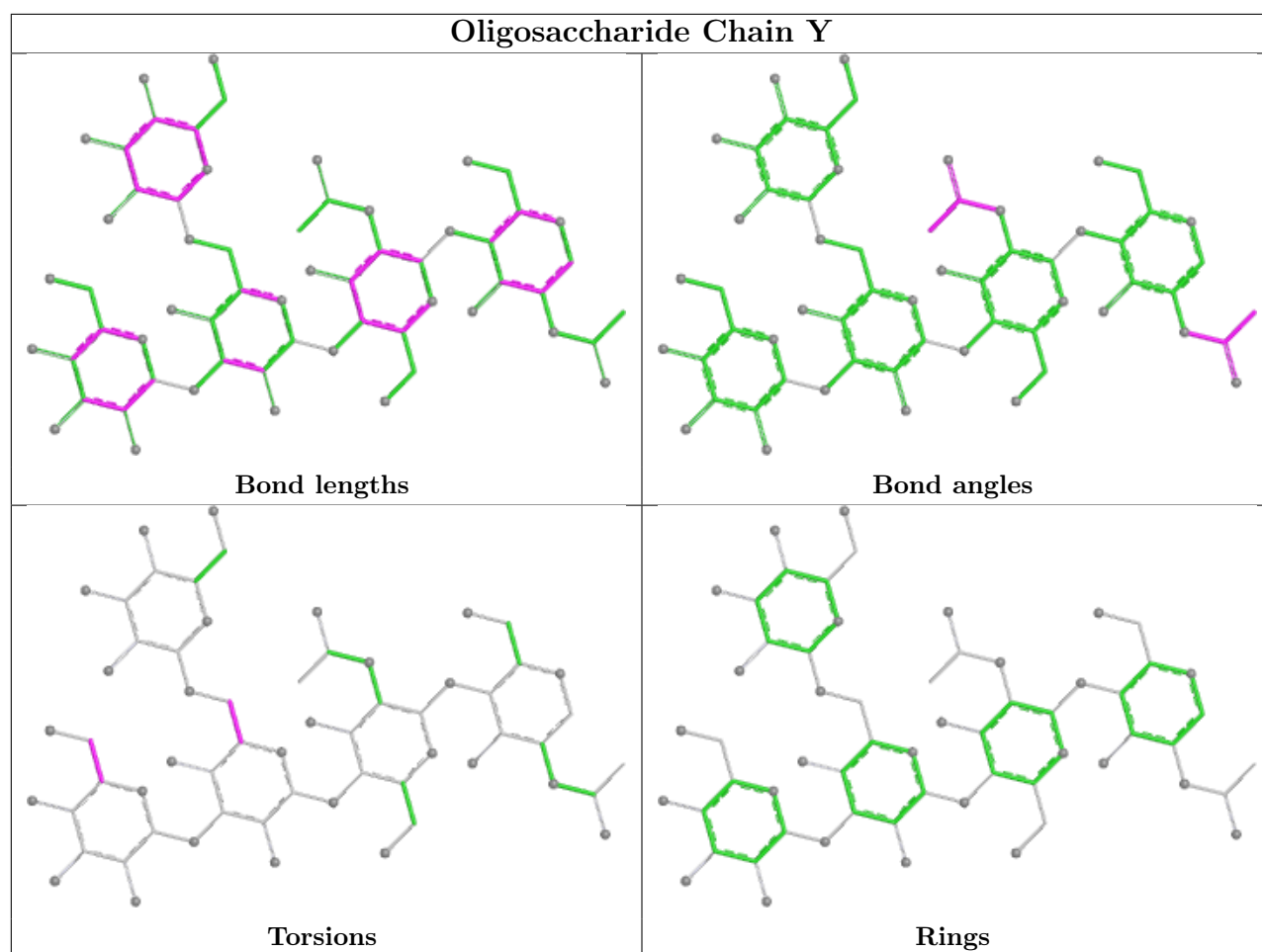
1 monomer is involved in 1 short contact:

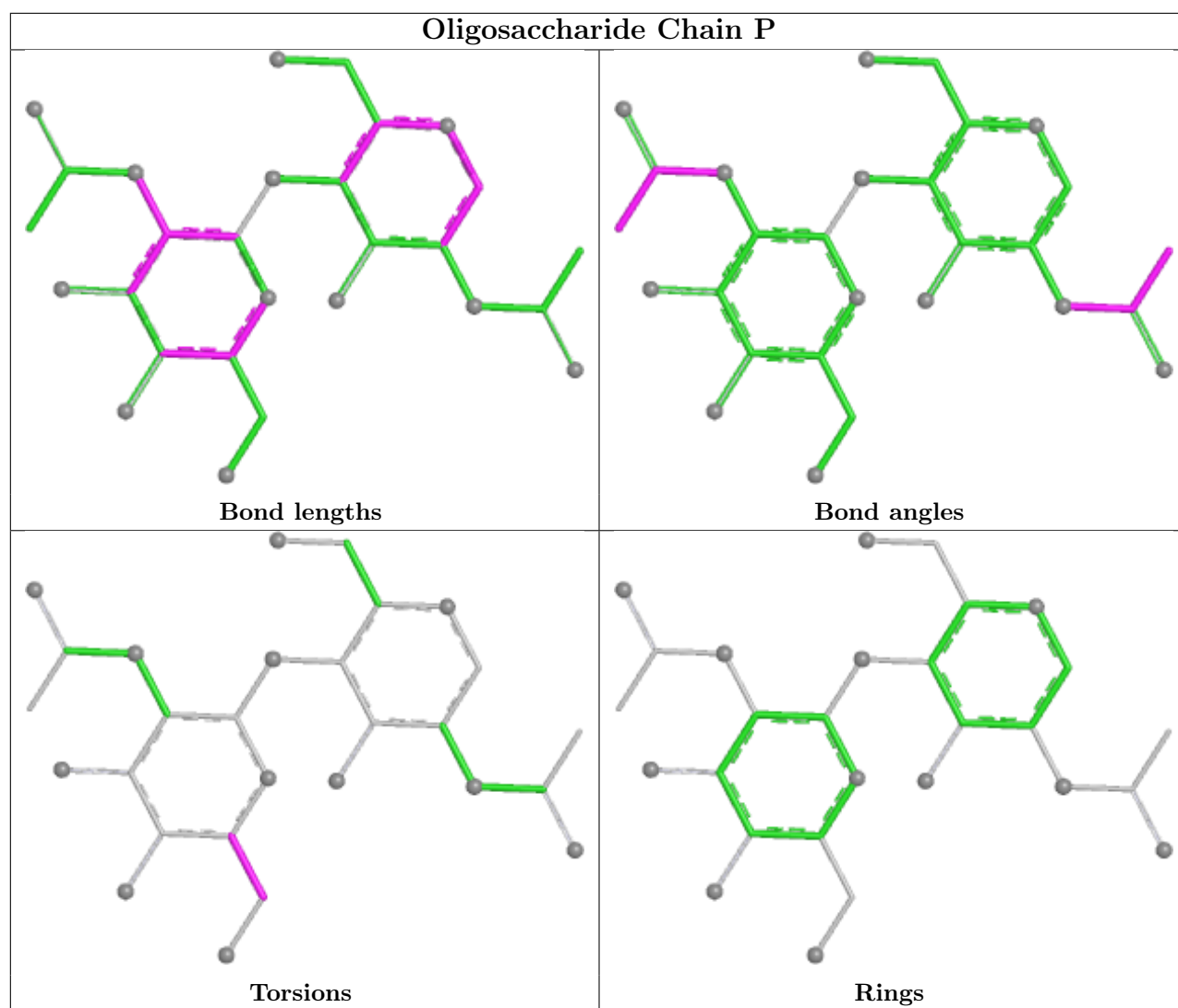
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	S	2	NAG	1	0

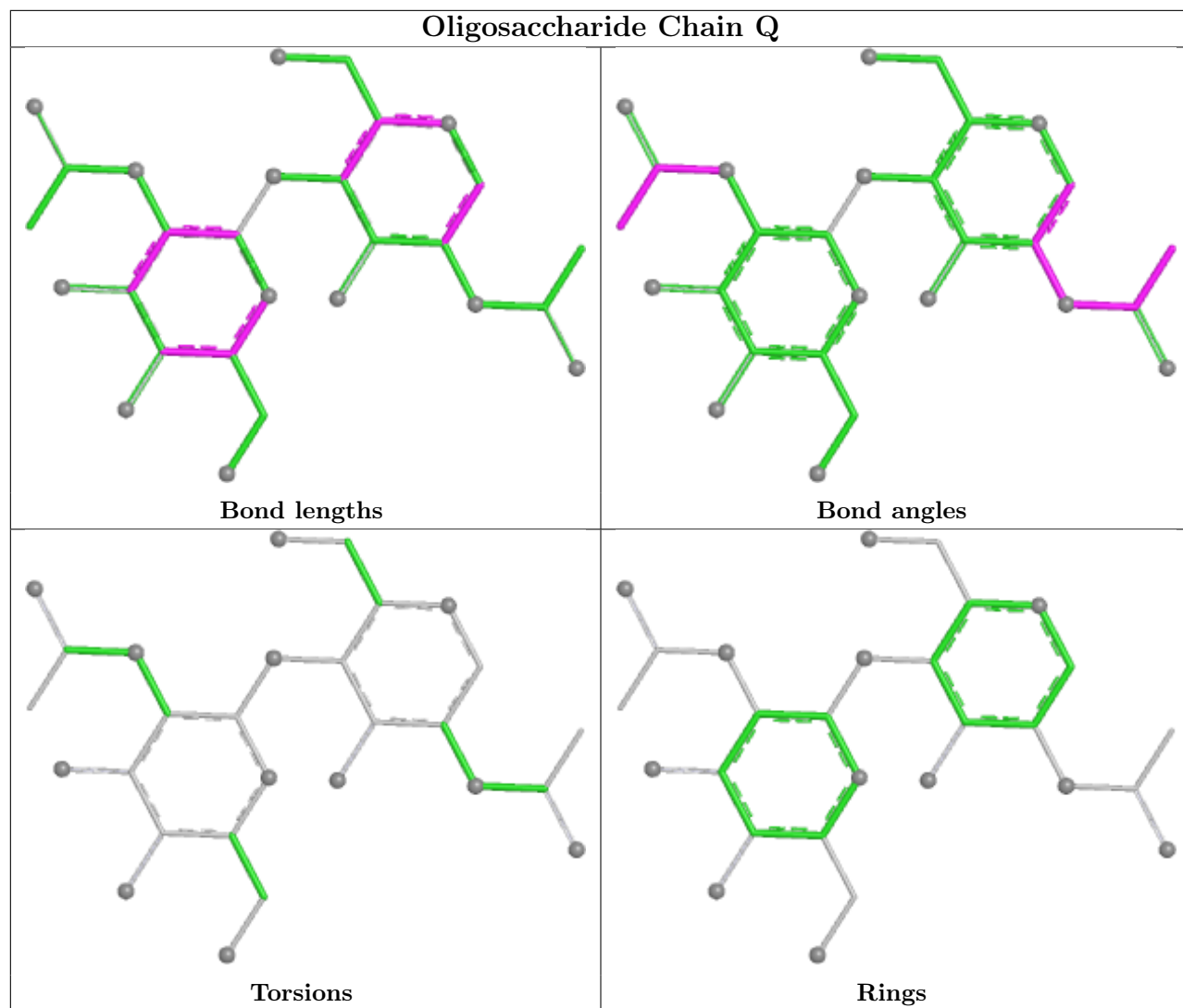
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

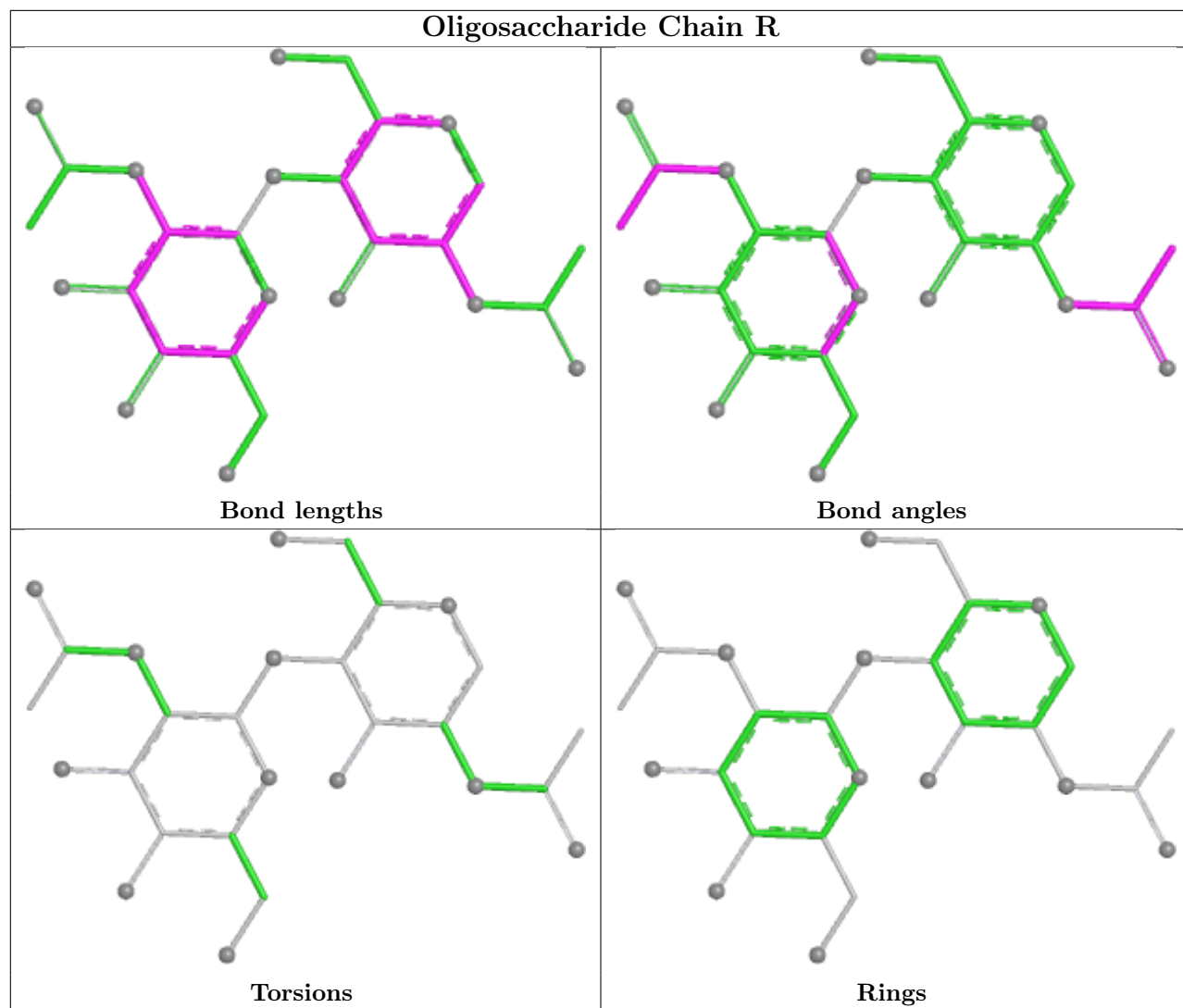


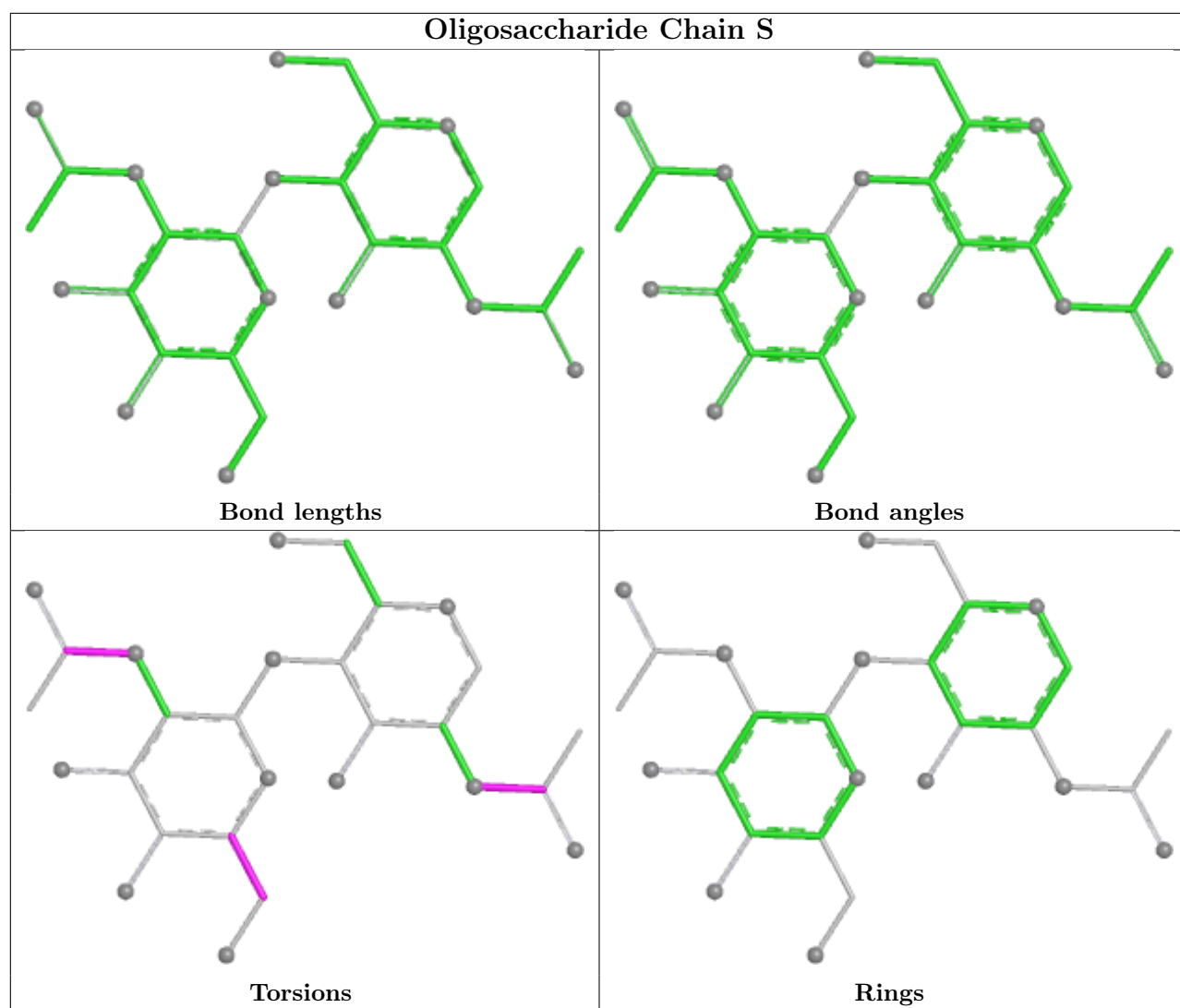


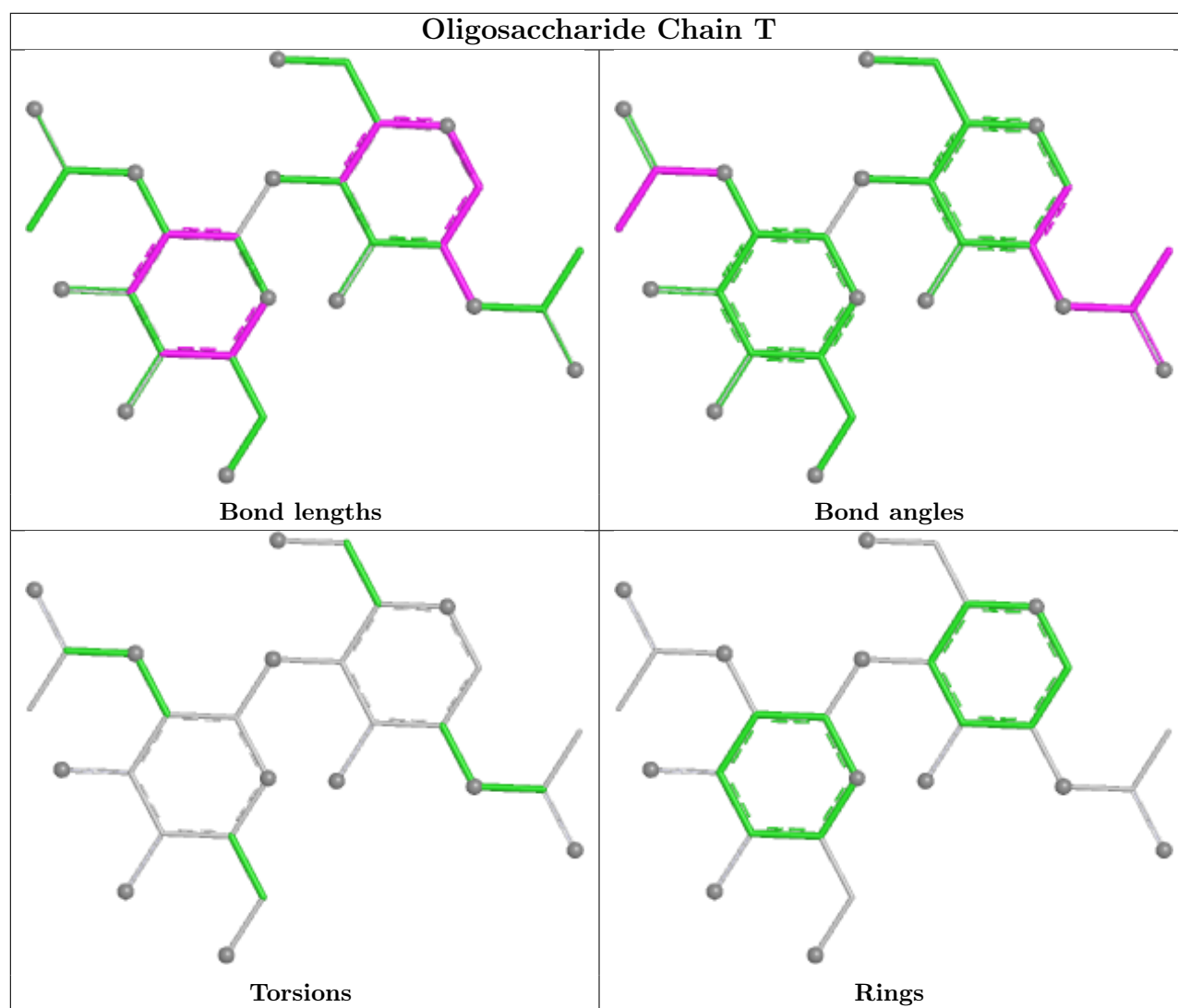


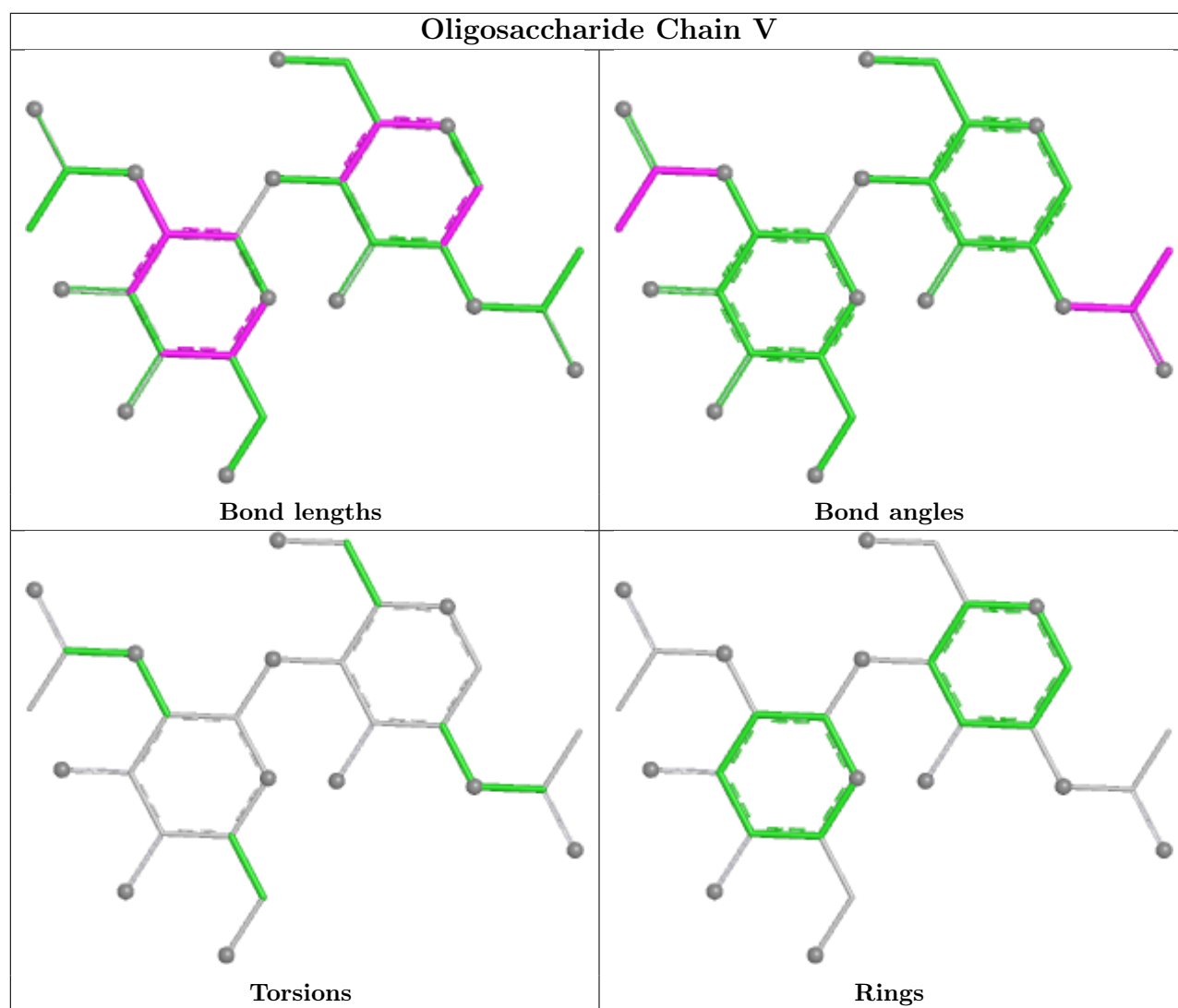


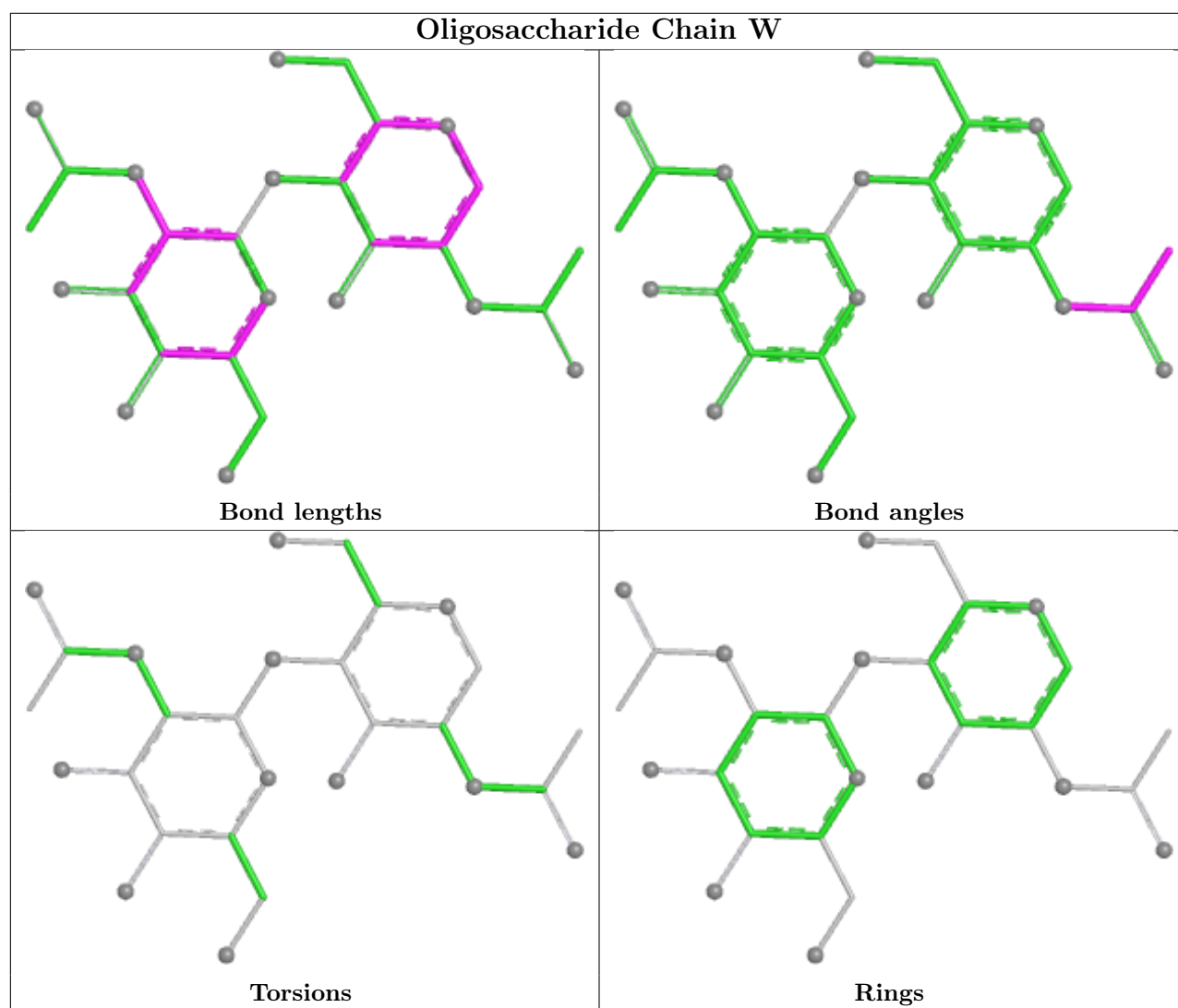


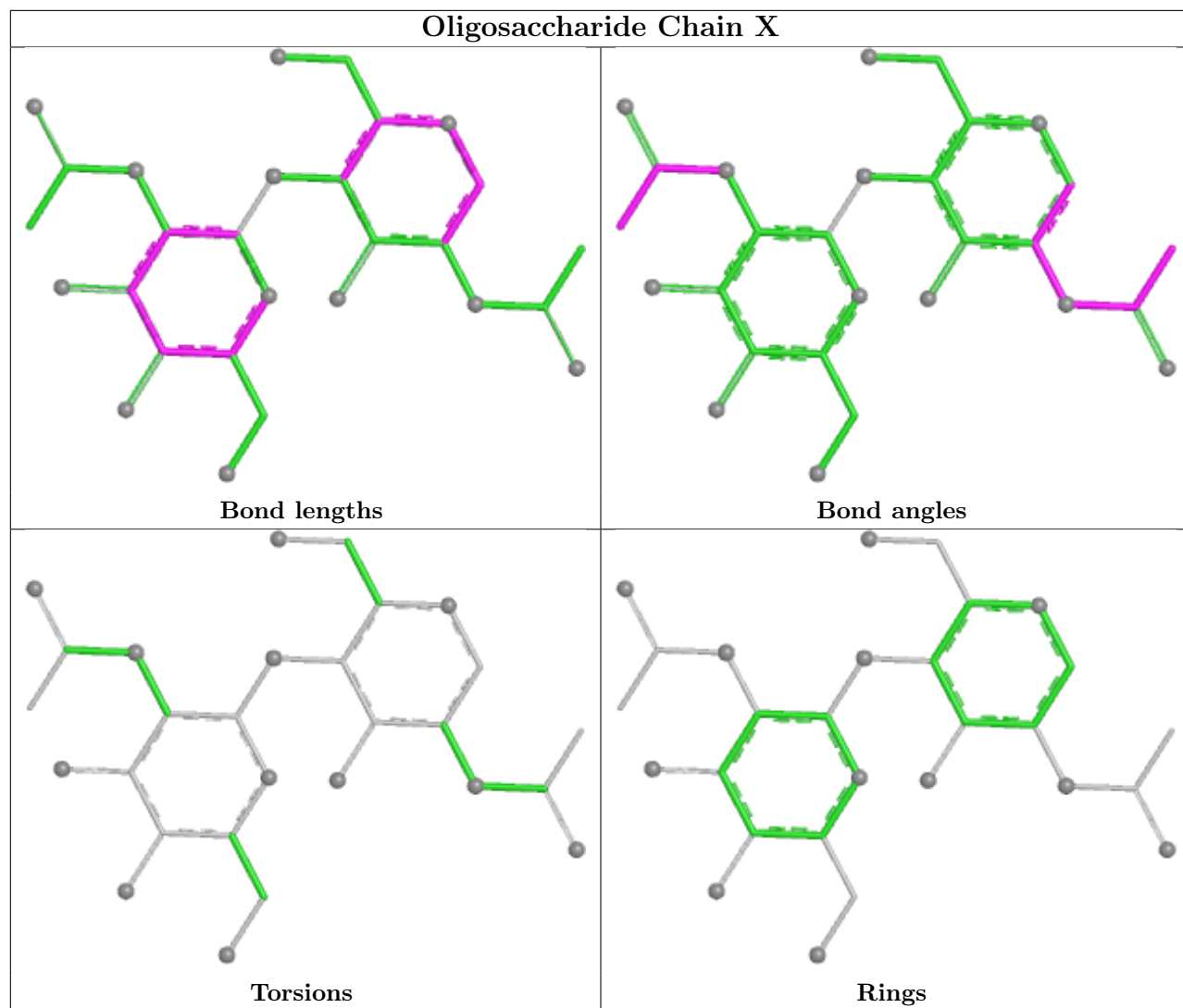


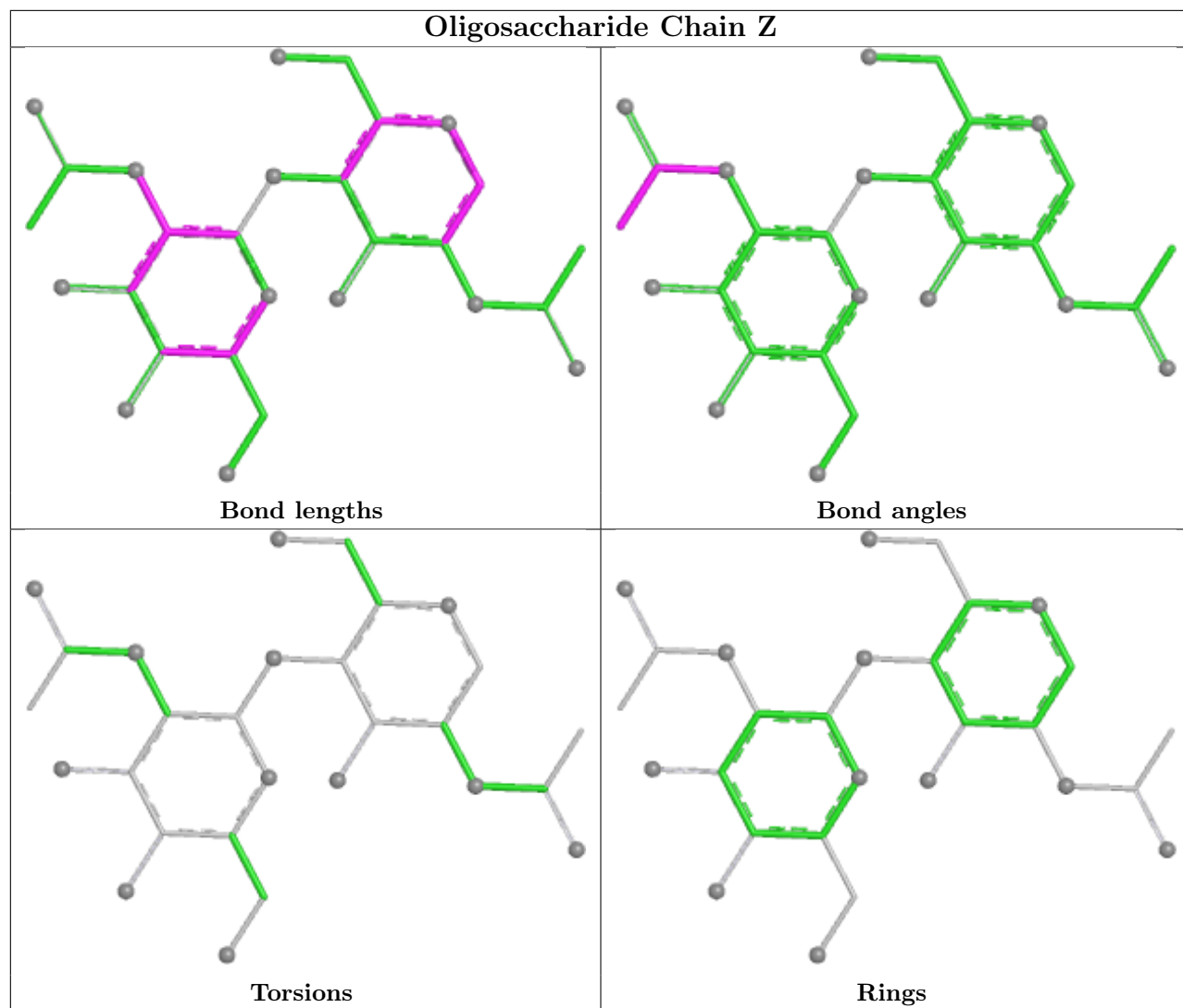


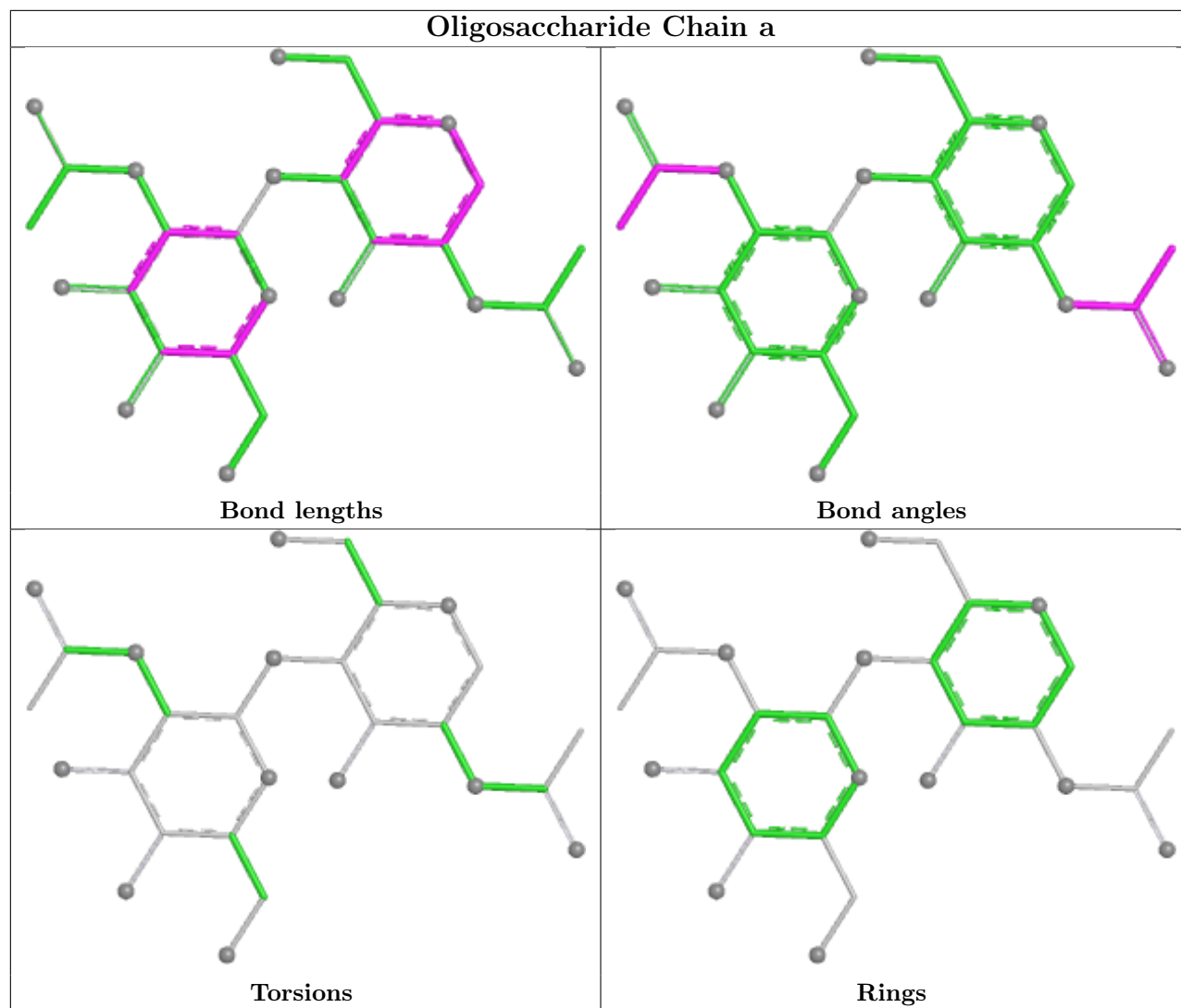


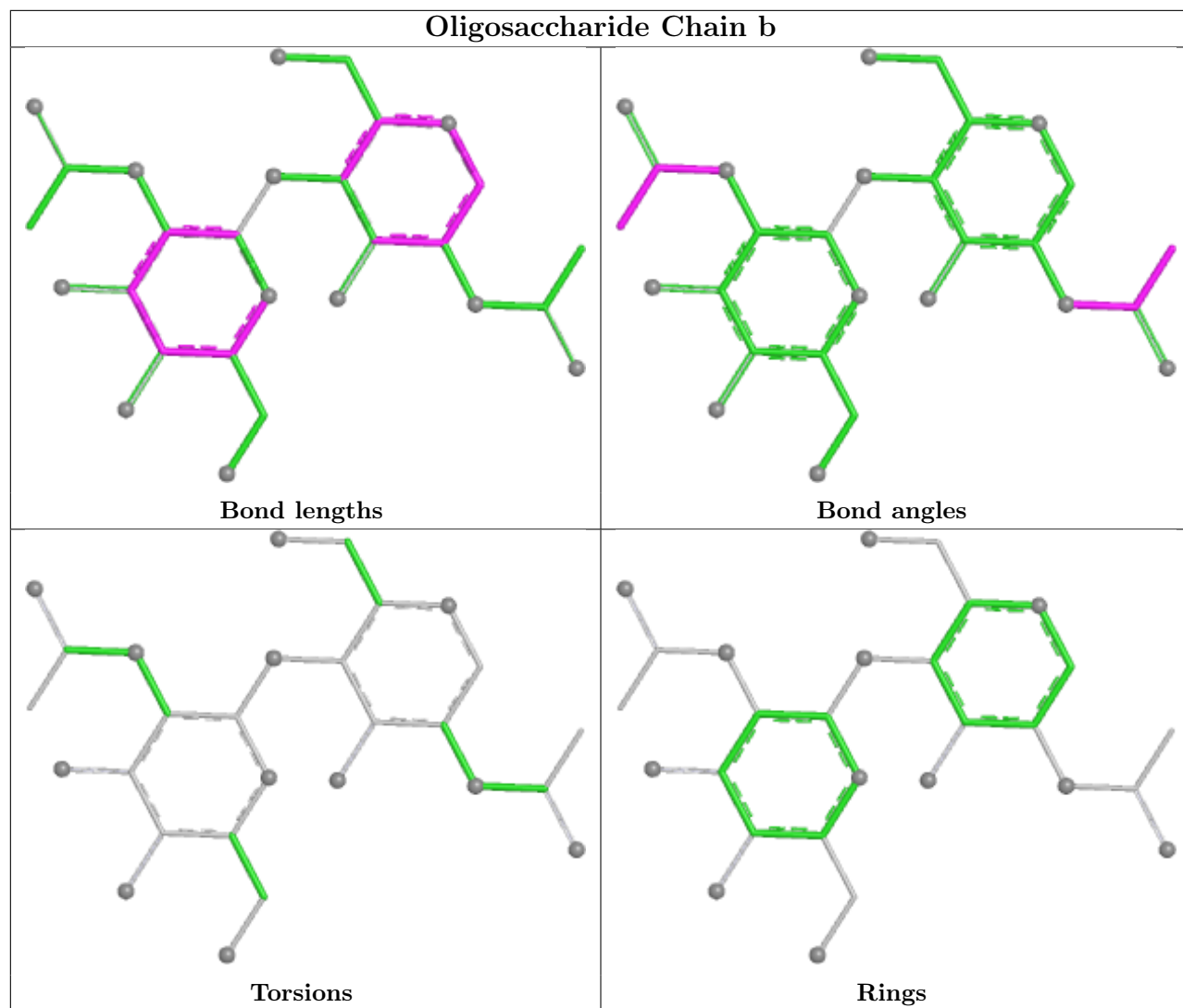


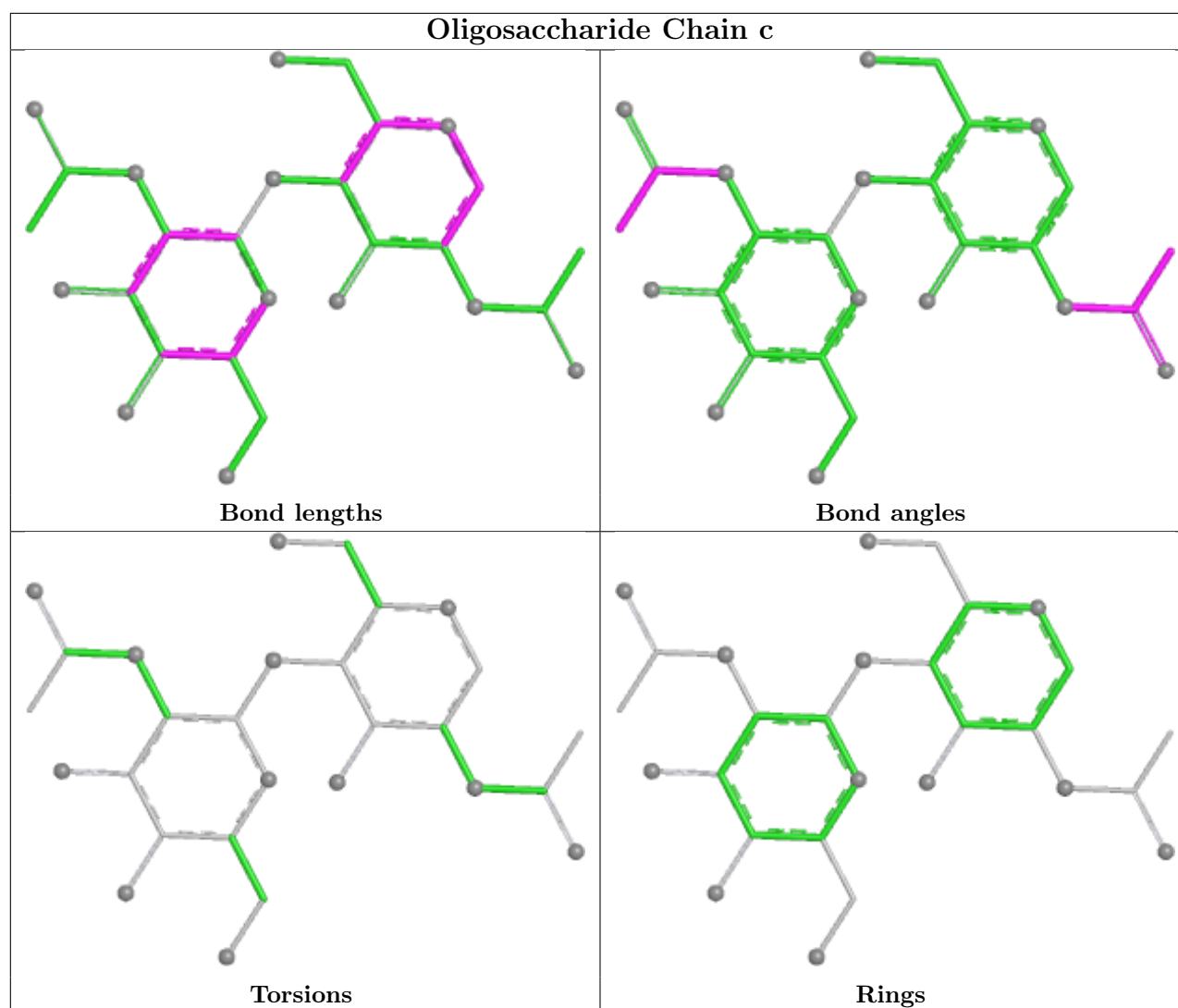












5.6 Ligand geometry [i](#)

51 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	B	701	3	14,14,15	2.17	6 (42%)	17,19,21	1.07	1 (5%)
8	NAG	A	711	3	14,14,15	2.41	4 (28%)	17,19,21	1.21	2 (11%)
8	NAG	D	701	3	14,14,15	2.17	5 (35%)	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	715	3	14,14,15	2.11	6 (42%)	17,19,21	1.31	4 (23%)
8	NAG	F	702	3	14,14,15	2.16	6 (42%)	17,19,21	1.09	2 (11%)
8	NAG	D	711	3	14,14,15	2.12	5 (35%)	17,19,21	1.10	2 (11%)
8	NAG	C	714	3	14,14,15	2.23	6 (42%)	17,19,21	0.96	0
8	NAG	D	702	3	14,14,15	2.13	5 (35%)	17,19,21	1.14	1 (5%)
8	NAG	A	703	3	14,14,15	1.97	3 (21%)	17,19,21	1.03	0
8	NAG	A	712	3	14,14,15	2.20	6 (42%)	17,19,21	1.03	1 (5%)
8	NAG	C	703	3	14,14,15	2.11	4 (28%)	17,19,21	1.17	2 (11%)
8	NAG	D	714	3	14,14,15	2.19	6 (42%)	17,19,21	1.01	1 (5%)
8	NAG	D	703	3	14,14,15	2.06	5 (35%)	17,19,21	1.17	3 (17%)
8	NAG	A	713	3	14,14,15	2.06	5 (35%)	17,19,21	1.03	1 (5%)
8	NAG	C	708	3	14,14,15	2.29	6 (42%)	17,19,21	0.95	1 (5%)
8	NAG	C	712	3	14,14,15	2.13	5 (35%)	17,19,21	1.21	2 (11%)
8	NAG	C	709	3	14,14,15	2.15	5 (35%)	17,19,21	0.96	1 (5%)
8	NAG	D	713	3	14,14,15	2.22	6 (42%)	17,19,21	0.99	1 (5%)
8	NAG	A	710	3	14,14,15	2.03	5 (35%)	17,19,21	1.27	2 (11%)
8	NAG	C	705	3	14,14,15	2.06	4 (28%)	17,19,21	1.15	2 (11%)
8	NAG	A	705	3	14,14,15	2.21	6 (42%)	17,19,21	1.18	1 (5%)
8	NAG	A	708	3	14,14,15	1.98	5 (35%)	17,19,21	1.20	2 (11%)
8	NAG	A	709	3	14,14,15	2.21	5 (35%)	17,19,21	1.11	1 (5%)
8	NAG	E	702	3	14,14,15	0.38	0	17,19,21	0.51	0
8	NAG	D	708	3	14,14,15	2.20	6 (42%)	17,19,21	1.00	1 (5%)
8	NAG	B	702	3	14,14,15	2.15	7 (50%)	17,19,21	1.11	2 (11%)
8	NAG	E	701	3	14,14,15	2.17	6 (42%)	17,19,21	1.04	2 (11%)
8	NAG	D	712	3	14,14,15	2.22	5 (35%)	17,19,21	0.98	1 (5%)
8	NAG	A	706	3	14,14,15	2.07	5 (35%)	17,19,21	1.08	1 (5%)
8	NAG	C	706	3	14,14,15	0.37	0	17,19,21	0.52	0
8	NAG	F	701	3	14,14,15	2.20	5 (35%)	17,19,21	0.97	1 (5%)
8	NAG	F	703	3	14,14,15	2.27	5 (35%)	17,19,21	1.11	2 (11%)
8	NAG	A	702	3	14,14,15	2.15	4 (28%)	17,19,21	1.13	1 (5%)
8	NAG	D	706	3	14,14,15	0.37	0	17,19,21	0.57	0
8	NAG	E	703	3	14,14,15	2.32	6 (42%)	17,19,21	1.35	2 (11%)
8	NAG	C	704	3	14,14,15	2.09	5 (35%)	17,19,21	1.13	2 (11%)
8	NAG	C	707	3	14,14,15	2.14	5 (35%)	17,19,21	1.01	1 (5%)
8	NAG	D	709	3	14,14,15	1.94	5 (35%)	17,19,21	1.29	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	710	3	14,14,15	1.94	5 (35%)	17,19,21	1.08	1 (5%)
8	NAG	A	707	3	14,14,15	2.16	6 (42%)	17,19,21	1.01	1 (5%)
8	NAG	B	703	3	14,14,15	2.36	6 (42%)	17,19,21	1.31	3 (17%)
8	NAG	D	705	3	14,14,15	2.05	5 (35%)	17,19,21	1.14	3 (17%)
8	NAG	A	704	3	14,14,15	1.97	5 (35%)	17,19,21	1.16	2 (11%)
8	NAG	C	711	3	14,14,15	2.27	6 (42%)	17,19,21	0.99	0
8	NAG	D	707	3	14,14,15	1.94	4 (28%)	17,19,21	1.08	1 (5%)
8	NAG	C	702	3	14,14,15	2.11	4 (28%)	17,19,21	1.09	2 (11%)
8	NAG	C	713	3	14,14,15	2.38	5 (35%)	17,19,21	0.84	0
8	NAG	D	704	3	14,14,15	2.07	4 (28%)	17,19,21	0.96	1 (5%)
8	NAG	C	701	3	14,14,15	2.10	4 (28%)	17,19,21	1.05	1 (5%)
8	NAG	A	701	3	14,14,15	2.22	4 (28%)	17,19,21	1.00	2 (11%)
8	NAG	D	710	3	14,14,15	2.28	6 (42%)	17,19,21	1.02	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	701	3	-	0/6/23/26	0/1/1/1
8	NAG	A	711	3	-	0/6/23/26	0/1/1/1
8	NAG	D	701	3	-	1/6/23/26	0/1/1/1
8	NAG	C	715	3	-	1/6/23/26	0/1/1/1
8	NAG	F	702	3	-	0/6/23/26	0/1/1/1
8	NAG	D	711	3	-	0/6/23/26	0/1/1/1
8	NAG	C	714	3	-	1/6/23/26	0/1/1/1
8	NAG	D	702	3	-	1/6/23/26	0/1/1/1
8	NAG	A	703	3	-	1/6/23/26	0/1/1/1
8	NAG	A	712	3	-	2/6/23/26	0/1/1/1
8	NAG	C	703	3	-	0/6/23/26	0/1/1/1
8	NAG	D	714	3	-	0/6/23/26	0/1/1/1
8	NAG	D	703	3	-	0/6/23/26	0/1/1/1
8	NAG	A	713	3	-	0/6/23/26	0/1/1/1
8	NAG	C	708	3	-	1/6/23/26	0/1/1/1
8	NAG	C	712	3	-	1/6/23/26	0/1/1/1
8	NAG	C	709	3	-	0/6/23/26	0/1/1/1
8	NAG	D	713	3	-	0/6/23/26	0/1/1/1
8	NAG	A	710	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	705	3	-	0/6/23/26	0/1/1/1
8	NAG	A	705	3	-	1/6/23/26	0/1/1/1
8	NAG	A	708	3	-	1/6/23/26	0/1/1/1
8	NAG	A	709	3	-	0/6/23/26	0/1/1/1
8	NAG	E	702	3	-	1/6/23/26	0/1/1/1
8	NAG	D	708	3	-	2/6/23/26	0/1/1/1
8	NAG	B	702	3	-	0/6/23/26	0/1/1/1
8	NAG	E	701	3	-	0/6/23/26	0/1/1/1
8	NAG	D	712	3	-	2/6/23/26	0/1/1/1
8	NAG	A	706	3	-	0/6/23/26	0/1/1/1
8	NAG	C	706	3	-	2/6/23/26	0/1/1/1
8	NAG	F	701	3	-	0/6/23/26	0/1/1/1
8	NAG	F	703	3	-	0/6/23/26	0/1/1/1
8	NAG	A	702	3	-	2/6/23/26	0/1/1/1
8	NAG	D	706	3	-	2/6/23/26	0/1/1/1
8	NAG	E	703	3	-	1/6/23/26	0/1/1/1
8	NAG	C	704	3	-	1/6/23/26	0/1/1/1
8	NAG	C	707	3	-	1/6/23/26	0/1/1/1
8	NAG	D	709	3	-	1/6/23/26	0/1/1/1
8	NAG	C	710	3	-	1/6/23/26	0/1/1/1
8	NAG	A	707	3	-	1/6/23/26	0/1/1/1
8	NAG	B	703	3	-	1/6/23/26	0/1/1/1
8	NAG	D	705	3	-	0/6/23/26	0/1/1/1
8	NAG	A	704	3	-	0/6/23/26	0/1/1/1
8	NAG	C	711	3	-	1/6/23/26	0/1/1/1
8	NAG	D	707	3	-	2/6/23/26	0/1/1/1
8	NAG	C	702	3	-	0/6/23/26	0/1/1/1
8	NAG	C	713	3	-	0/6/23/26	0/1/1/1
8	NAG	D	704	3	-	1/6/23/26	0/1/1/1
8	NAG	C	701	3	-	1/6/23/26	0/1/1/1
8	NAG	A	701	3	-	0/6/23/26	0/1/1/1
8	NAG	D	710	3	-	0/6/23/26	0/1/1/1

All (247) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	711	NAG	C1-C2	6.86	1.61	1.52
8	C	713	NAG	C1-C2	6.64	1.61	1.52
8	B	703	NAG	C1-C2	6.30	1.60	1.52
8	A	701	NAG	C1-C2	6.11	1.60	1.52
8	F	703	NAG	C1-C2	6.11	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	701	NAG	C1-C2	6.07	1.60	1.52
8	D	710	NAG	C1-C2	6.04	1.60	1.52
8	C	711	NAG	C1-C2	5.98	1.60	1.52
8	E	703	NAG	C1-C2	5.97	1.60	1.52
8	D	701	NAG	C1-C2	5.95	1.60	1.52
8	C	708	NAG	C1-C2	5.92	1.60	1.52
8	A	702	NAG	C1-C2	5.88	1.60	1.52
8	C	714	NAG	C1-C2	5.83	1.60	1.52
8	C	703	NAG	C1-C2	5.81	1.60	1.52
8	C	702	NAG	C1-C2	5.78	1.60	1.52
8	D	702	NAG	C1-C2	5.76	1.60	1.52
8	A	709	NAG	C1-C2	5.76	1.60	1.52
8	D	713	NAG	C1-C2	5.64	1.60	1.52
8	B	701	NAG	C1-C2	5.60	1.60	1.52
8	D	708	NAG	C1-C2	5.59	1.60	1.52
8	A	705	NAG	C1-C2	5.58	1.59	1.52
8	D	714	NAG	C1-C2	5.56	1.59	1.52
8	E	701	NAG	C1-C2	5.56	1.59	1.52
8	C	704	NAG	C1-C2	5.55	1.59	1.52
8	C	709	NAG	C1-C2	5.52	1.59	1.52
8	D	704	NAG	C1-C2	5.44	1.59	1.52
8	D	711	NAG	C1-C2	5.43	1.59	1.52
8	A	707	NAG	C1-C2	5.43	1.59	1.52
8	C	707	NAG	C1-C2	5.40	1.59	1.52
8	D	703	NAG	C1-C2	5.37	1.59	1.52
8	A	712	NAG	C1-C2	5.35	1.59	1.52
8	C	715	NAG	C1-C2	5.33	1.59	1.52
8	B	702	NAG	C1-C2	5.32	1.59	1.52
8	C	701	NAG	C1-C2	5.32	1.59	1.52
8	A	706	NAG	C1-C2	5.28	1.59	1.52
8	C	712	NAG	C1-C2	5.27	1.59	1.52
8	D	712	NAG	C1-C2	5.24	1.59	1.52
8	C	705	NAG	C1-C2	5.17	1.59	1.52
8	A	710	NAG	C1-C2	5.15	1.59	1.52
8	A	703	NAG	C1-C2	5.14	1.59	1.52
8	F	702	NAG	C1-C2	5.10	1.59	1.52
8	A	713	NAG	C1-C2	5.09	1.59	1.52
8	D	705	NAG	C1-C2	5.04	1.59	1.52
8	D	707	NAG	C1-C2	5.00	1.59	1.52
8	A	704	NAG	C1-C2	4.80	1.58	1.52
8	A	708	NAG	C1-C2	4.53	1.58	1.52
8	D	709	NAG	C1-C2	4.51	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	710	NAG	C1-C2	4.49	1.58	1.52
8	D	712	NAG	O5-C5	3.67	1.50	1.43
8	F	702	NAG	O5-C5	3.58	1.50	1.43
8	C	701	NAG	O5-C5	3.44	1.50	1.43
8	A	705	NAG	O5-C5	3.43	1.50	1.43
8	C	707	NAG	O5-C5	3.39	1.50	1.43
8	A	712	NAG	O5-C5	3.31	1.49	1.43
8	A	708	NAG	O5-C5	3.30	1.49	1.43
8	A	707	NAG	O5-C5	3.30	1.49	1.43
8	D	713	NAG	O5-C5	3.29	1.49	1.43
8	D	708	NAG	O5-C5	3.27	1.49	1.43
8	A	709	NAG	O5-C5	3.26	1.49	1.43
8	C	708	NAG	O5-C5	3.24	1.49	1.43
8	D	714	NAG	O5-C5	3.23	1.49	1.43
8	A	706	NAG	O5-C5	3.23	1.49	1.43
8	C	712	NAG	O5-C5	3.21	1.49	1.43
8	C	714	NAG	O5-C5	3.21	1.49	1.43
8	C	711	NAG	O5-C5	3.20	1.49	1.43
8	B	703	NAG	O5-C5	3.19	1.49	1.43
8	C	710	NAG	O5-C5	3.18	1.49	1.43
8	E	701	NAG	O5-C5	3.16	1.49	1.43
8	D	710	NAG	O5-C5	3.15	1.49	1.43
8	B	701	NAG	O5-C5	3.14	1.49	1.43
8	B	702	NAG	O5-C5	3.14	1.49	1.43
8	A	702	NAG	O5-C5	3.12	1.49	1.43
8	D	709	NAG	O5-C5	3.12	1.49	1.43
8	C	713	NAG	O5-C5	3.11	1.49	1.43
8	C	709	NAG	O5-C5	3.11	1.49	1.43
8	A	713	NAG	O5-C5	3.11	1.49	1.43
8	D	705	NAG	O5-C5	3.10	1.49	1.43
8	C	705	NAG	O5-C5	3.08	1.49	1.43
8	F	703	NAG	O5-C5	3.07	1.49	1.43
8	A	704	NAG	O5-C5	3.05	1.49	1.43
8	C	715	NAG	O5-C5	3.01	1.49	1.43
8	D	703	NAG	O5-C5	3.01	1.49	1.43
8	E	703	NAG	O5-C5	3.00	1.49	1.43
8	E	703	NAG	C3-C2	2.99	1.58	1.52
8	D	711	NAG	O5-C5	2.99	1.49	1.43
8	D	712	NAG	O5-C1	2.96	1.48	1.43
8	A	711	NAG	C3-C2	2.94	1.58	1.52
8	D	707	NAG	O5-C5	2.91	1.49	1.43
8	A	701	NAG	O5-C5	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	711	NAG	O5-C5	2.88	1.49	1.43
8	B	703	NAG	C3-C2	2.88	1.58	1.52
8	E	703	NAG	C2-N2	2.84	1.51	1.46
8	A	710	NAG	O5-C5	2.84	1.49	1.43
8	D	701	NAG	O5-C5	2.81	1.48	1.43
8	C	704	NAG	O5-C5	2.79	1.48	1.43
8	F	703	NAG	C3-C2	2.79	1.58	1.52
8	F	701	NAG	O5-C5	2.78	1.48	1.43
8	D	704	NAG	O5-C5	2.77	1.48	1.43
8	C	712	NAG	O5-C1	2.77	1.48	1.43
8	A	703	NAG	O5-C5	2.75	1.48	1.43
8	C	703	NAG	O5-C5	2.75	1.48	1.43
8	C	702	NAG	O5-C5	2.74	1.48	1.43
8	F	702	NAG	O5-C1	2.72	1.48	1.43
8	D	702	NAG	O5-C5	2.68	1.48	1.43
8	A	708	NAG	O5-C1	2.65	1.48	1.43
8	C	708	NAG	O5-C1	2.65	1.48	1.43
8	C	701	NAG	O5-C1	2.65	1.48	1.43
8	D	713	NAG	O5-C1	2.64	1.48	1.43
8	A	713	NAG	O5-C1	2.64	1.48	1.43
8	A	712	NAG	O5-C1	2.62	1.48	1.43
8	C	711	NAG	O5-C1	2.60	1.48	1.43
8	D	714	NAG	O5-C1	2.60	1.48	1.43
8	F	701	NAG	C3-C2	2.59	1.57	1.52
8	C	705	NAG	O5-C1	2.58	1.48	1.43
8	D	708	NAG	O5-C1	2.58	1.48	1.43
8	D	709	NAG	O5-C1	2.58	1.48	1.43
8	D	710	NAG	O5-C1	2.55	1.48	1.43
8	C	707	NAG	O5-C1	2.54	1.48	1.43
8	C	710	NAG	O5-C1	2.54	1.48	1.43
8	A	710	NAG	O5-C1	2.52	1.47	1.43
8	C	703	NAG	C3-C2	2.51	1.57	1.52
8	A	709	NAG	O5-C1	2.51	1.47	1.43
8	D	711	NAG	O5-C1	2.51	1.47	1.43
8	C	714	NAG	O5-C1	2.50	1.47	1.43
8	C	713	NAG	C3-C2	2.50	1.57	1.52
8	A	707	NAG	O5-C1	2.50	1.47	1.43
8	C	715	NAG	O5-C1	2.50	1.47	1.43
8	C	709	NAG	O5-C1	2.48	1.47	1.43
8	D	705	NAG	O5-C1	2.47	1.47	1.43
8	A	704	NAG	O5-C1	2.47	1.47	1.43
8	D	702	NAG	O5-C1	2.47	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	704	NAG	O5-C1	2.45	1.47	1.43
8	A	703	NAG	O5-C1	2.44	1.47	1.43
8	B	702	NAG	C3-C2	2.44	1.57	1.52
8	D	713	NAG	C4-C5	2.43	1.58	1.53
8	B	703	NAG	C2-N2	2.43	1.50	1.46
8	A	705	NAG	C4-C5	2.41	1.58	1.53
8	E	701	NAG	O5-C1	2.41	1.47	1.43
8	D	701	NAG	O5-C1	2.41	1.47	1.43
8	D	710	NAG	C4-C5	2.41	1.58	1.53
8	C	713	NAG	O5-C1	2.41	1.47	1.43
8	C	714	NAG	C3-C2	2.40	1.57	1.52
8	A	712	NAG	C2-N2	2.40	1.50	1.46
8	C	705	NAG	C3-C2	2.40	1.57	1.52
8	D	703	NAG	O5-C1	2.40	1.47	1.43
8	D	701	NAG	C3-C2	2.39	1.57	1.52
8	A	701	NAG	C3-C2	2.39	1.57	1.52
8	C	712	NAG	C3-C2	2.37	1.57	1.52
8	A	705	NAG	C2-N2	2.37	1.50	1.46
8	A	701	NAG	O5-C1	2.36	1.47	1.43
8	C	709	NAG	C3-C2	2.36	1.57	1.52
8	D	705	NAG	C3-C2	2.36	1.57	1.52
8	C	711	NAG	C4-C5	2.35	1.58	1.53
8	B	701	NAG	C4-C5	2.34	1.58	1.53
8	D	714	NAG	C3-C2	2.34	1.57	1.52
8	C	704	NAG	O5-C1	2.34	1.47	1.43
8	C	708	NAG	C3-C2	2.33	1.57	1.52
8	D	708	NAG	C3-C2	2.33	1.57	1.52
8	A	712	NAG	C3-C2	2.33	1.57	1.52
8	C	714	NAG	C4-C5	2.32	1.58	1.53
8	C	702	NAG	C3-C2	2.32	1.57	1.52
8	A	704	NAG	C3-C2	2.31	1.57	1.52
8	A	706	NAG	O5-C1	2.31	1.47	1.43
8	D	712	NAG	C3-C2	2.31	1.57	1.52
8	C	708	NAG	C4-C5	2.30	1.57	1.53
8	A	702	NAG	O5-C1	2.29	1.47	1.43
8	A	705	NAG	O5-C1	2.28	1.47	1.43
8	A	711	NAG	O5-C1	2.28	1.47	1.43
8	A	710	NAG	C3-C2	2.28	1.57	1.52
8	E	701	NAG	C3-C2	2.27	1.57	1.52
8	B	702	NAG	C4-C5	2.27	1.57	1.53
8	A	712	NAG	C4-C5	2.26	1.57	1.53
8	B	703	NAG	C4-C5	2.26	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	702	NAG	C3-C2	2.26	1.57	1.52
8	F	702	NAG	C3-C2	2.26	1.57	1.52
8	B	702	NAG	O5-C1	2.25	1.47	1.43
8	A	707	NAG	C4-C5	2.25	1.57	1.53
8	C	702	NAG	O5-C1	2.24	1.47	1.43
8	D	712	NAG	C4-C5	2.23	1.57	1.53
8	A	709	NAG	C4-C5	2.23	1.57	1.53
8	A	707	NAG	C3-C2	2.23	1.57	1.52
8	F	703	NAG	C4-C5	2.22	1.57	1.53
8	B	701	NAG	O5-C1	2.22	1.47	1.43
8	F	702	NAG	C4-C5	2.22	1.57	1.53
8	C	708	NAG	C2-N2	2.22	1.49	1.46
8	D	702	NAG	C3-C2	2.22	1.57	1.52
8	C	713	NAG	C4-C5	2.22	1.57	1.53
8	C	715	NAG	C2-N2	2.21	1.49	1.46
8	E	701	NAG	C4-C5	2.21	1.57	1.53
8	A	708	NAG	C3-C2	2.20	1.57	1.52
8	C	707	NAG	C3-C2	2.19	1.57	1.52
8	D	704	NAG	C2-N2	2.19	1.49	1.46
8	B	701	NAG	C3-C2	2.18	1.57	1.52
8	D	708	NAG	C2-N2	2.18	1.49	1.46
8	D	711	NAG	C3-C2	2.18	1.57	1.52
8	B	701	NAG	C4-C3	2.18	1.58	1.52
8	A	713	NAG	C3-C2	2.18	1.57	1.52
8	A	706	NAG	C4-C5	2.16	1.57	1.53
8	A	706	NAG	C3-C2	2.16	1.57	1.52
8	D	713	NAG	C4-C3	2.16	1.57	1.52
8	C	710	NAG	C3-C2	2.16	1.57	1.52
8	D	710	NAG	C3-C2	2.15	1.57	1.52
8	A	707	NAG	C2-N2	2.15	1.49	1.46
8	D	711	NAG	C4-C5	2.15	1.57	1.53
8	C	703	NAG	O5-C1	2.15	1.47	1.43
8	C	701	NAG	C4-C5	2.15	1.57	1.53
8	F	701	NAG	O5-C1	2.15	1.47	1.43
8	C	704	NAG	C4-C5	2.14	1.57	1.53
8	B	702	NAG	C2-N2	2.14	1.49	1.46
8	B	703	NAG	O5-C1	2.14	1.47	1.43
8	F	703	NAG	C2-N2	2.14	1.49	1.46
8	F	701	NAG	C4-C5	2.14	1.57	1.53
8	D	707	NAG	O5-C1	2.13	1.47	1.43
8	A	705	NAG	C4-C3	2.13	1.57	1.52
8	D	703	NAG	C4-C5	2.13	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	715	NAG	C3-C2	2.13	1.57	1.52
8	C	712	NAG	C4-C5	2.13	1.57	1.53
8	E	703	NAG	C4-C5	2.13	1.57	1.53
8	D	713	NAG	C3-C2	2.12	1.57	1.52
8	A	708	NAG	C4-C5	2.12	1.57	1.53
8	E	703	NAG	O5-C1	2.11	1.47	1.43
8	C	711	NAG	C3-C2	2.11	1.56	1.52
8	D	702	NAG	C4-C5	2.11	1.57	1.53
8	A	709	NAG	C3-C2	2.11	1.56	1.52
8	D	714	NAG	C4-C5	2.11	1.57	1.53
8	B	702	NAG	C4-C3	2.11	1.57	1.52
8	E	701	NAG	C4-C3	2.10	1.57	1.52
8	D	709	NAG	C4-C5	2.10	1.57	1.53
8	C	704	NAG	C2-N2	2.10	1.49	1.46
8	D	708	NAG	C4-C5	2.09	1.57	1.53
8	C	707	NAG	C4-C5	2.08	1.57	1.53
8	D	709	NAG	C3-C2	2.08	1.56	1.52
8	A	704	NAG	C4-C5	2.08	1.57	1.53
8	C	715	NAG	C4-C5	2.08	1.57	1.53
8	D	707	NAG	C4-C5	2.07	1.57	1.53
8	C	710	NAG	C4-C5	2.07	1.57	1.53
8	D	701	NAG	C4-C5	2.07	1.57	1.53
8	A	710	NAG	C4-C5	2.06	1.57	1.53
8	A	713	NAG	C4-C5	2.05	1.57	1.53
8	C	709	NAG	C4-C5	2.05	1.57	1.53
8	D	705	NAG	C4-C5	2.04	1.57	1.53
8	D	710	NAG	C2-N2	2.04	1.49	1.46
8	F	702	NAG	C4-C3	2.03	1.57	1.52
8	C	714	NAG	C4-C3	2.02	1.57	1.52
8	D	703	NAG	C3-C2	2.00	1.56	1.52
8	C	711	NAG	C2-N2	2.00	1.49	1.46
8	D	714	NAG	C2-N2	2.00	1.49	1.46

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	703	NAG	C2-N2-C7	3.93	128.16	122.90
8	D	709	NAG	C8-C7-N2	3.22	121.46	116.12
8	B	703	NAG	C2-N2-C7	3.14	127.11	122.90
8	A	708	NAG	C8-C7-N2	3.00	121.09	116.12
8	A	710	NAG	C8-C7-N2	2.99	121.08	116.12
8	C	715	NAG	C8-C7-N2	2.95	121.02	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	702	NAG	C8-C7-N2	2.93	120.98	116.12
8	C	712	NAG	C8-C7-N2	2.75	120.68	116.12
8	D	703	NAG	C8-C7-N2	2.74	120.66	116.12
8	A	709	NAG	C8-C7-N2	2.74	120.65	116.12
8	F	703	NAG	C8-C7-N2	2.73	120.65	116.12
8	A	704	NAG	C8-C7-N2	2.69	120.58	116.12
8	F	702	NAG	C8-C7-N2	2.61	120.44	116.12
8	A	705	NAG	C2-N2-C7	2.60	126.38	122.90
8	C	705	NAG	C8-C7-N2	2.55	120.35	116.12
8	A	710	NAG	O7-C7-C8	-2.54	117.53	122.05
8	C	712	NAG	O7-C7-C8	-2.54	117.54	122.05
8	B	703	NAG	C8-C7-N2	2.53	120.31	116.12
8	D	707	NAG	C1-C2-N2	-2.51	106.48	110.43
8	B	701	NAG	C8-C7-N2	2.47	120.22	116.12
8	D	711	NAG	C1-C2-N2	-2.47	106.54	110.43
8	C	715	NAG	C1-O5-C5	2.46	115.48	112.19
8	C	703	NAG	C1-O5-C5	2.43	115.45	112.19
8	F	703	NAG	O7-C7-C8	-2.41	117.76	122.05
8	E	701	NAG	C8-C7-N2	2.40	120.10	116.12
8	C	710	NAG	C8-C7-N2	2.38	120.07	116.12
8	D	708	NAG	C8-C7-N2	2.36	120.03	116.12
8	D	705	NAG	C8-C7-N2	2.36	120.03	116.12
8	F	702	NAG	O7-C7-C8	-2.35	117.87	122.05
8	B	703	NAG	O7-C7-C8	-2.34	117.88	122.05
8	A	706	NAG	C1-C2-N2	-2.34	106.74	110.43
8	A	702	NAG	C1-O5-C5	2.34	115.33	112.19
8	C	702	NAG	C1-O5-C5	2.33	115.31	112.19
8	A	711	NAG	C1-C2-N2	-2.32	106.78	110.43
8	A	704	NAG	O7-C7-C8	-2.31	117.94	122.05
8	C	705	NAG	O7-C7-C8	-2.30	117.96	122.05
8	D	709	NAG	O7-C7-C8	-2.29	117.98	122.05
8	D	710	NAG	C8-C7-N2	2.28	119.91	116.12
8	D	714	NAG	C8-C7-N2	2.28	119.89	116.12
8	C	704	NAG	C1-O5-C5	2.28	115.24	112.19
8	C	701	NAG	C1-C2-N2	-2.26	106.87	110.43
8	C	703	NAG	C8-C7-N2	2.24	119.84	116.12
8	D	702	NAG	C1-O5-C5	2.24	115.19	112.19
8	C	709	NAG	C8-C7-N2	2.22	119.79	116.12
8	C	704	NAG	C8-C7-N2	2.21	119.78	116.12
8	D	705	NAG	O7-C7-C8	-2.20	118.14	122.05
8	D	705	NAG	C1-O5-C5	2.20	115.13	112.19
8	B	702	NAG	O7-C7-C8	-2.19	118.16	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	713	NAG	C8-C7-N2	2.19	119.75	116.12
8	D	703	NAG	C1-C2-N2	-2.19	106.99	110.43
8	C	702	NAG	C8-C7-N2	2.17	119.71	116.12
8	C	707	NAG	C8-C7-N2	2.15	119.68	116.12
8	D	701	NAG	C1-O5-C5	2.15	115.06	112.19
8	D	712	NAG	C8-C7-N2	2.14	119.67	116.12
8	A	707	NAG	C8-C7-N2	2.14	119.67	116.12
8	C	708	NAG	C8-C7-N2	2.14	119.67	116.12
8	A	712	NAG	C8-C7-N2	2.12	119.63	116.12
8	A	708	NAG	O7-C7-C8	-2.11	118.29	122.05
8	C	715	NAG	O7-C7-C8	-2.10	118.31	122.05
8	F	701	NAG	C8-C7-N2	2.10	119.59	116.12
8	A	711	NAG	C8-C7-N2	2.09	119.59	116.12
8	E	703	NAG	O7-C7-C8	-2.09	118.33	122.05
8	A	701	NAG	C8-C7-N2	2.07	119.55	116.12
8	D	711	NAG	C8-C7-N2	2.06	119.54	116.12
8	D	713	NAG	C8-C7-N2	2.06	119.54	116.12
8	C	715	NAG	O5-C1-C2	-2.05	108.12	111.29
8	D	703	NAG	O7-C7-C8	-2.04	118.43	122.05
8	A	701	NAG	C1-O5-C5	2.03	114.90	112.19
8	D	704	NAG	C8-C7-N2	2.03	119.48	116.12
8	E	701	NAG	O7-C7-C8	-2.02	118.45	122.05

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	705	NAG	C1-C2-N2-C7
8	C	706	NAG	C8-C7-N2-C2
8	C	706	NAG	O7-C7-N2-C2
8	E	703	NAG	C3-C2-N2-C7
8	D	706	NAG	C8-C7-N2-C2
8	D	706	NAG	O7-C7-N2-C2
8	D	707	NAG	O5-C5-C6-O6
8	A	702	NAG	C4-C5-C6-O6
8	D	712	NAG	O5-C5-C6-O6
8	D	708	NAG	O5-C5-C6-O6
8	A	702	NAG	O5-C5-C6-O6
8	C	701	NAG	O5-C5-C6-O6
8	D	707	NAG	C4-C5-C6-O6
8	C	708	NAG	O5-C5-C6-O6
8	A	710	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	710	NAG	O5-C5-C6-O6
8	A	703	NAG	O5-C5-C6-O6
8	C	712	NAG	O5-C5-C6-O6
8	C	704	NAG	O5-C5-C6-O6
8	D	704	NAG	O5-C5-C6-O6
8	A	707	NAG	O5-C5-C6-O6
8	C	711	NAG	O5-C5-C6-O6
8	D	702	NAG	O5-C5-C6-O6
8	D	709	NAG	O5-C5-C6-O6
8	A	708	NAG	O5-C5-C6-O6
8	C	715	NAG	O5-C5-C6-O6
8	B	703	NAG	C3-C2-N2-C7
8	D	701	NAG	O5-C5-C6-O6
8	C	707	NAG	O5-C5-C6-O6
8	C	714	NAG	O5-C5-C6-O6
8	A	712	NAG	C1-C2-N2-C7
8	D	712	NAG	C4-C5-C6-O6
8	E	702	NAG	C3-C2-N2-C7
8	D	708	NAG	C4-C5-C6-O6
8	A	712	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	702	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.

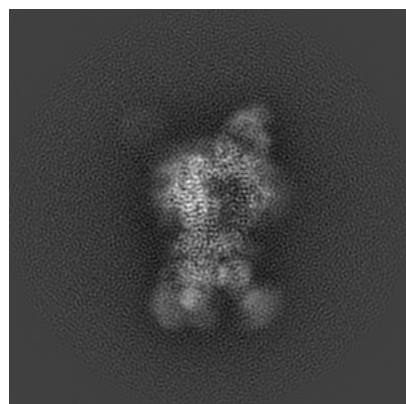
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23801. These allow visual inspection of the internal detail of the map and identification of artifacts.

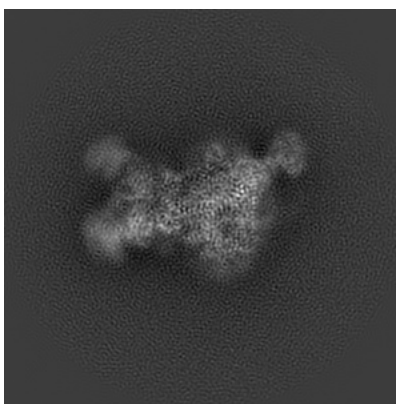
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

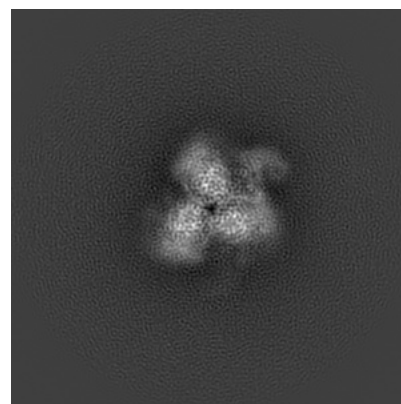
6.1.1 Primary map



X

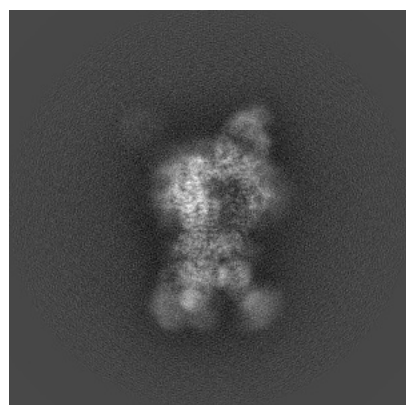


Y

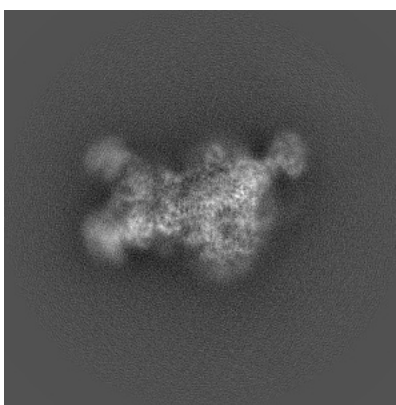


Z

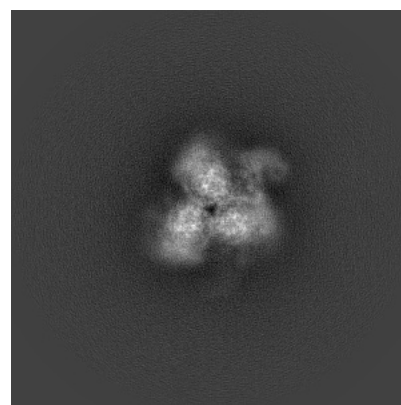
6.1.2 Raw map



X



Y

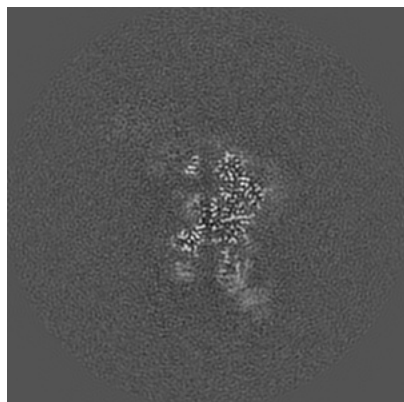


Z

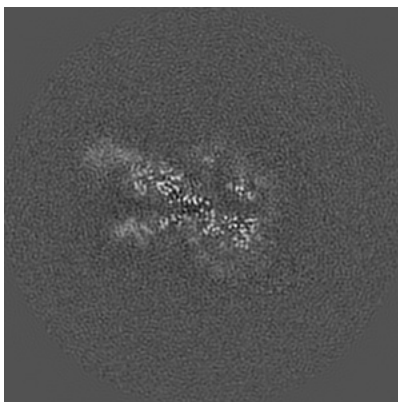
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

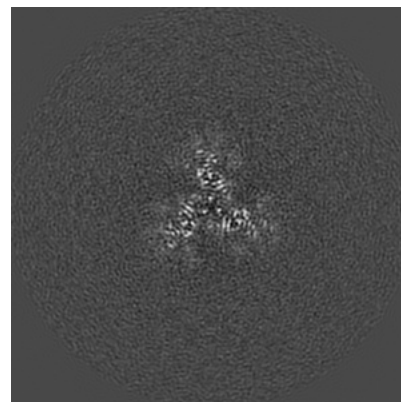
6.2.1 Primary map



X Index: 180

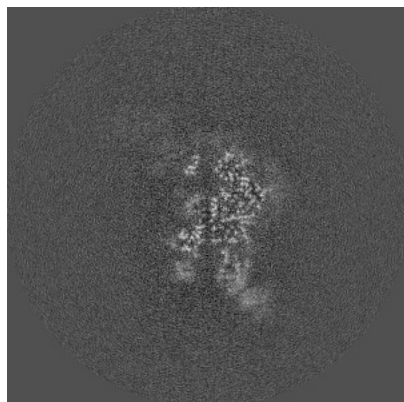


Y Index: 180

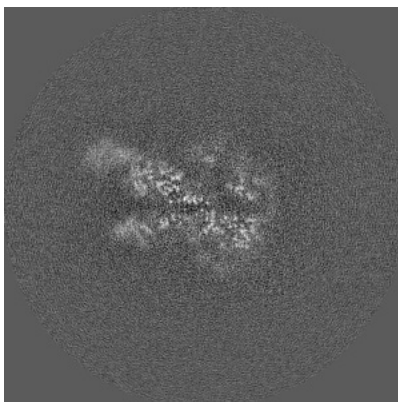


Z Index: 180

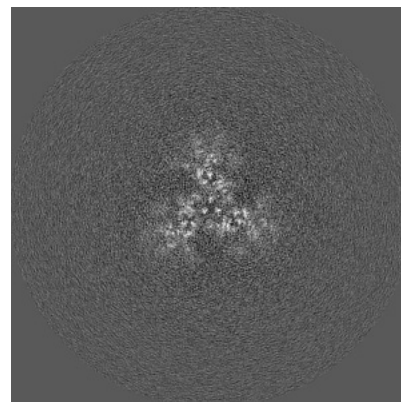
6.2.2 Raw map



X Index: 180



Y Index: 180

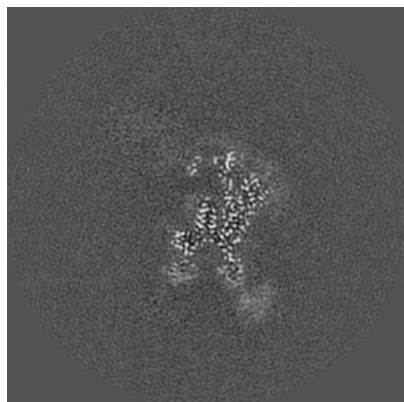


Z Index: 180

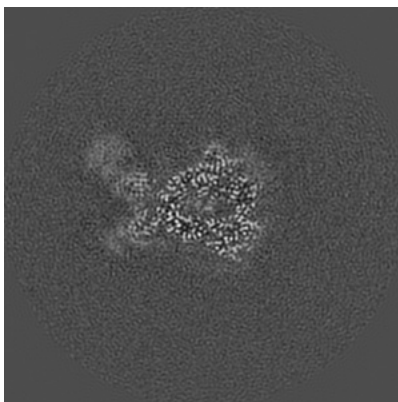
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

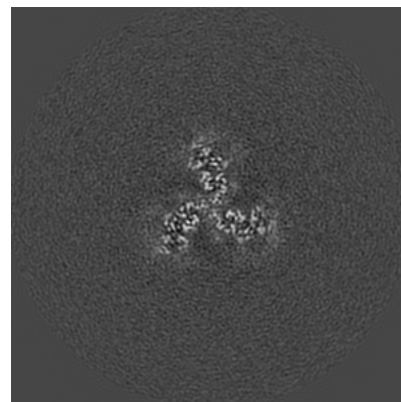
6.3.1 Primary map



X Index: 176

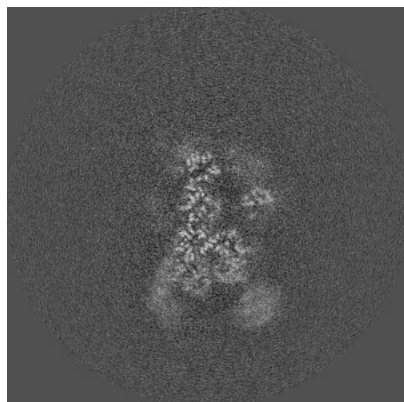


Y Index: 167

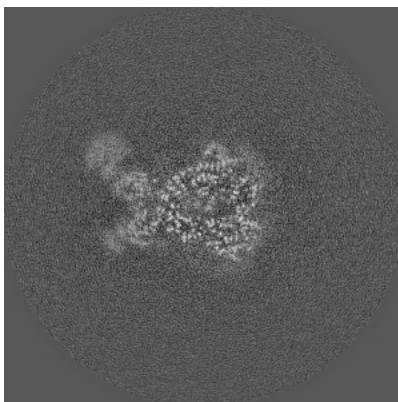


Z Index: 188

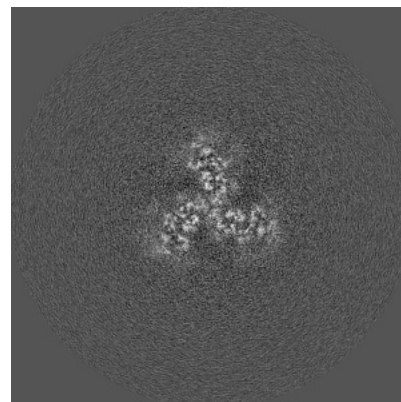
6.3.2 Raw map



X Index: 164



Y Index: 167

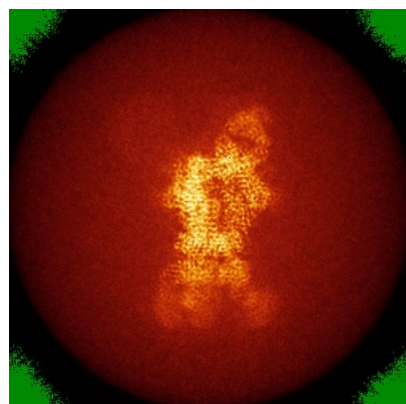


Z Index: 188

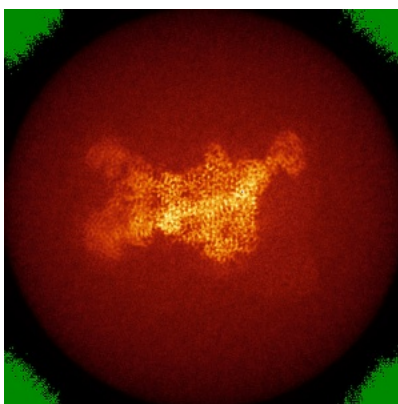
The images above show the largest variance slices of the map in three orthogonal directions.

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

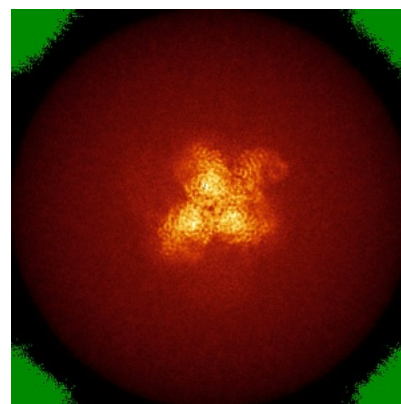
6.4.1 Primary map



X

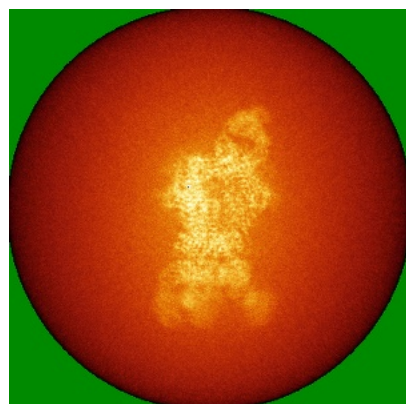


Y

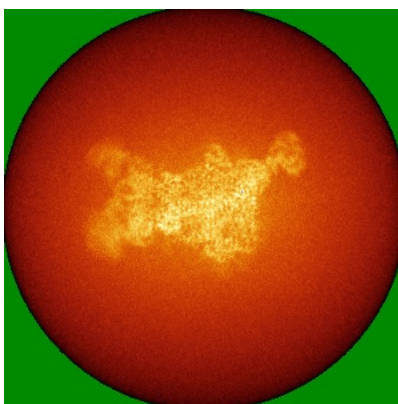


Z

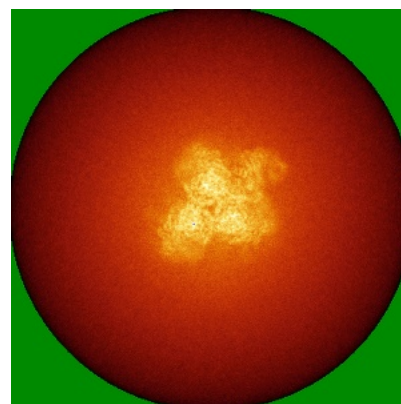
6.4.2 Raw map



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 0.009. 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.

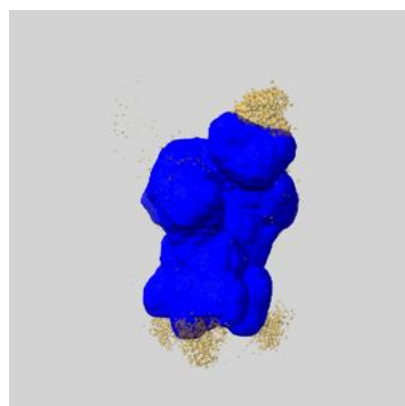
6.6 Mask visualisation [i](#)

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

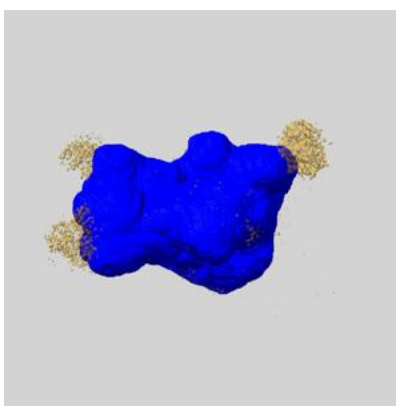
A mask typically either:

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

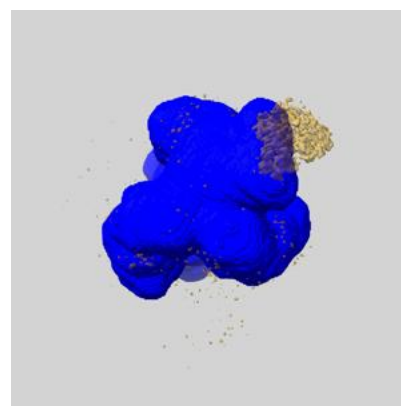
6.6.1 emd_23801_msk_1.map [i](#)



X



Y

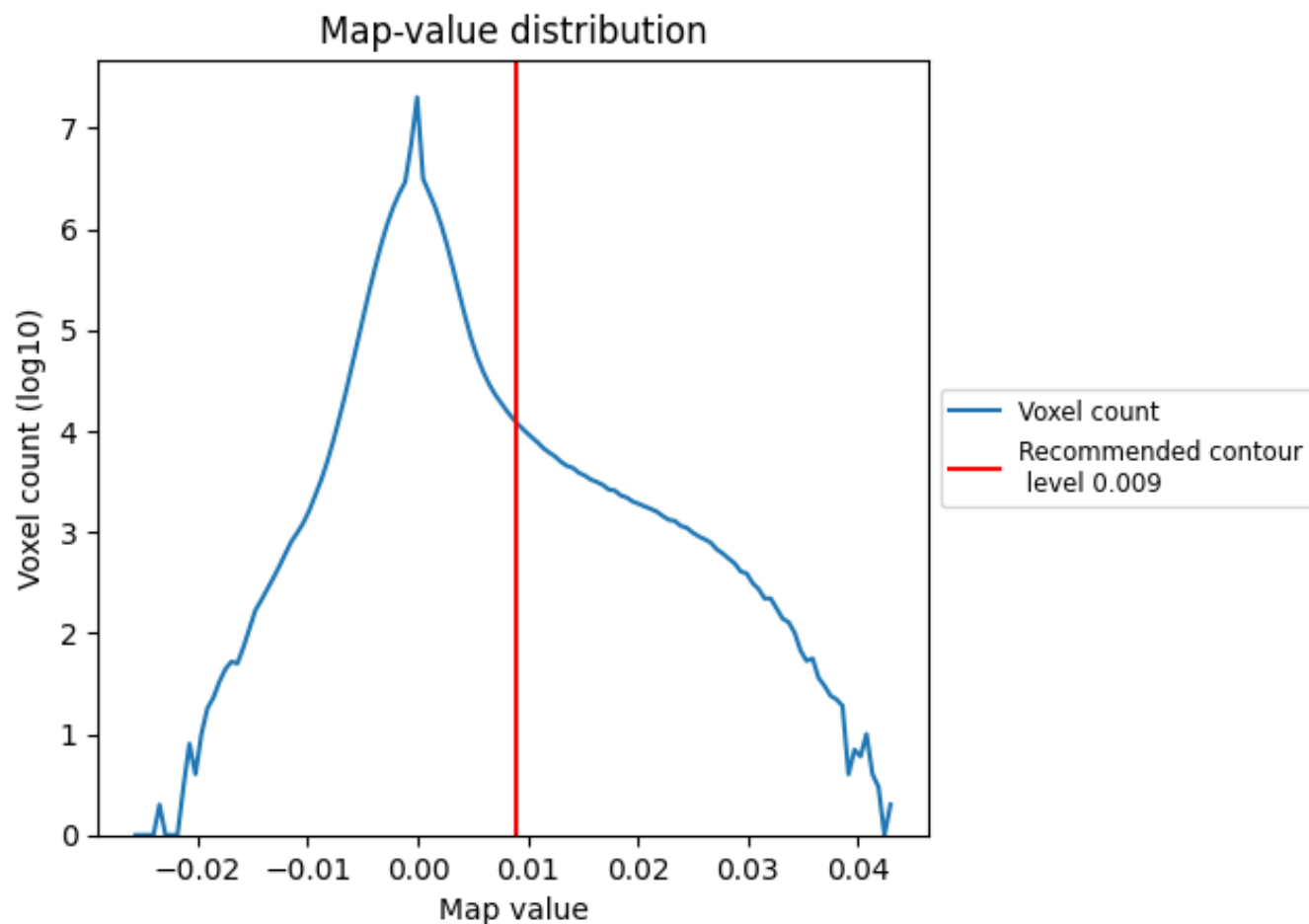


Z

7 Map analysis [i](#)

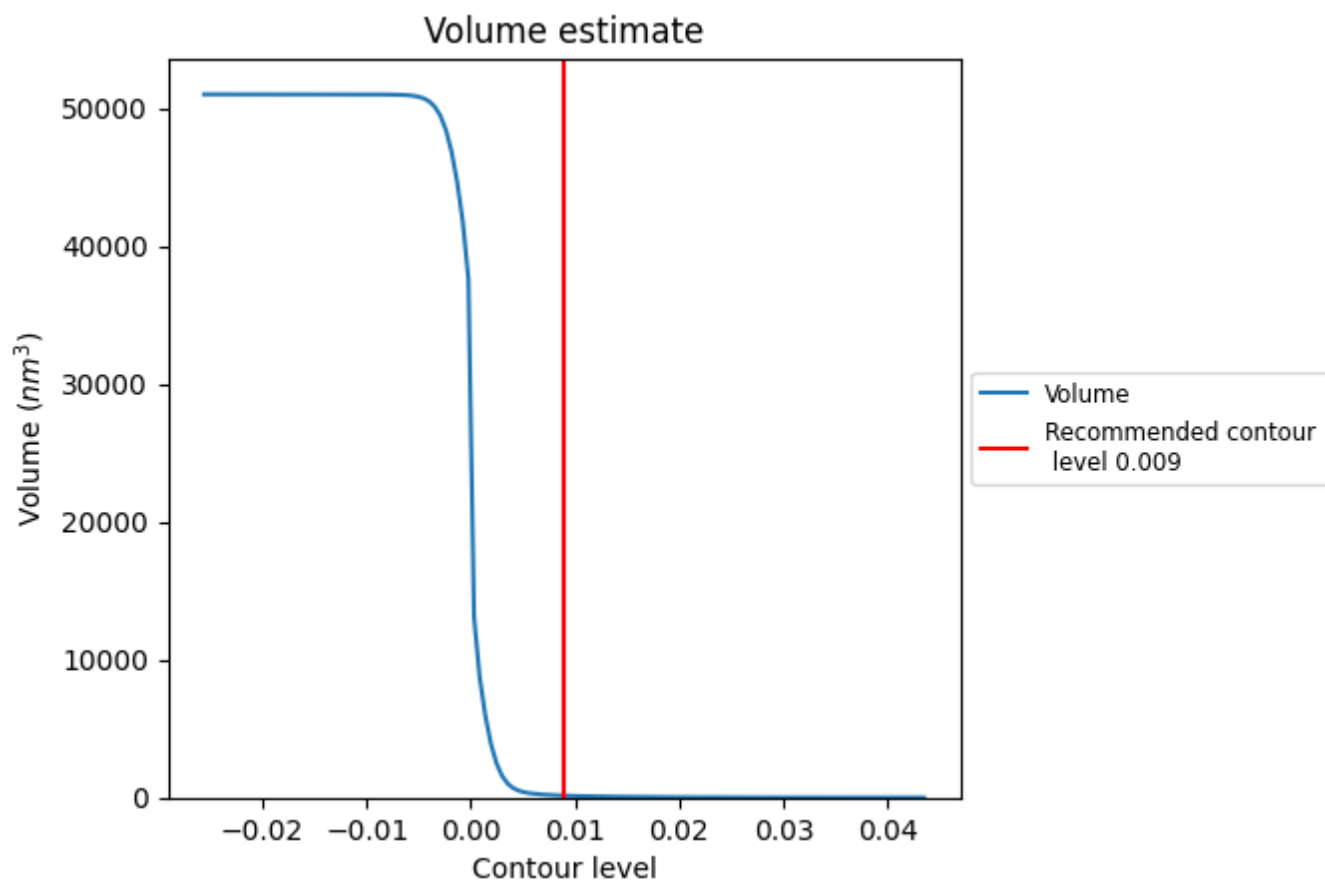
This section contains the results of statistical analysis of the map.

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.

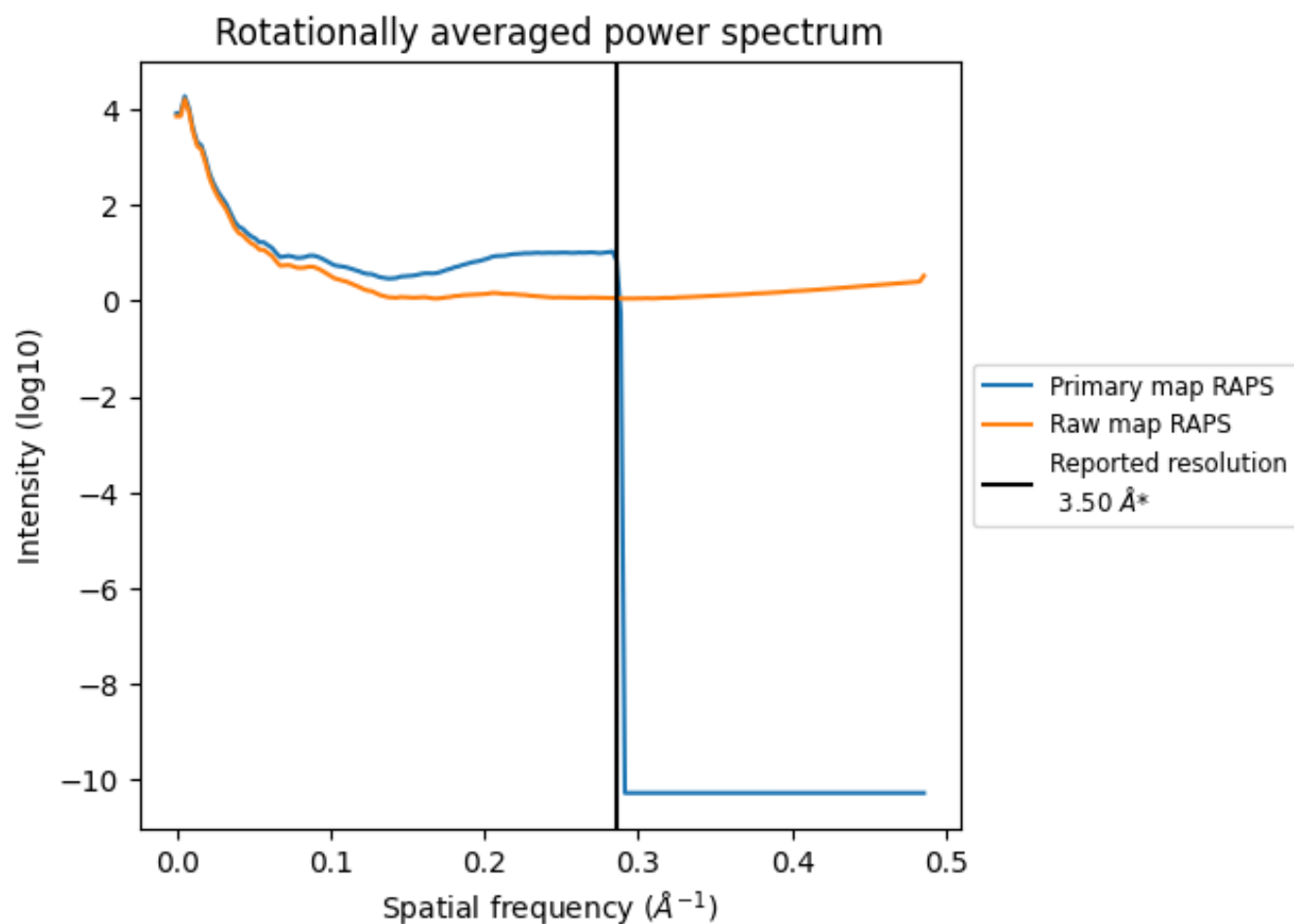
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 124 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 ⓘ

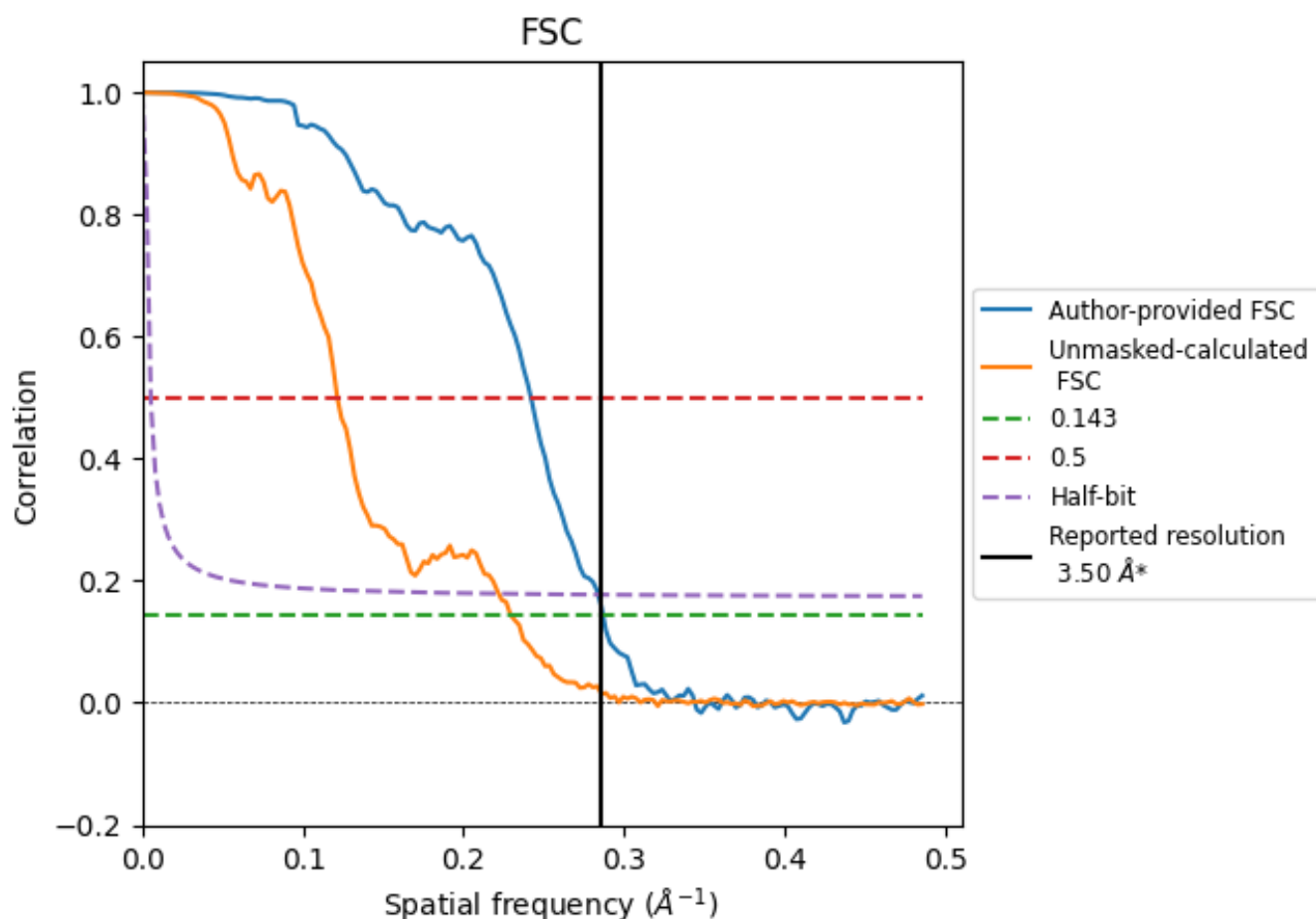


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

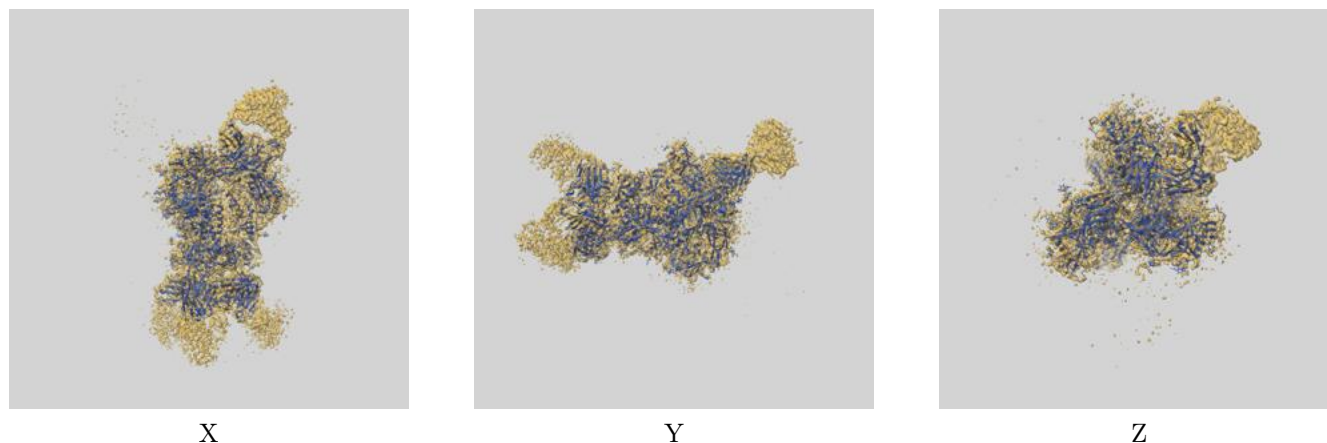
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.13	3.52
Unmasked-calculated*	4.36	8.24	4.51

*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 4.36 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

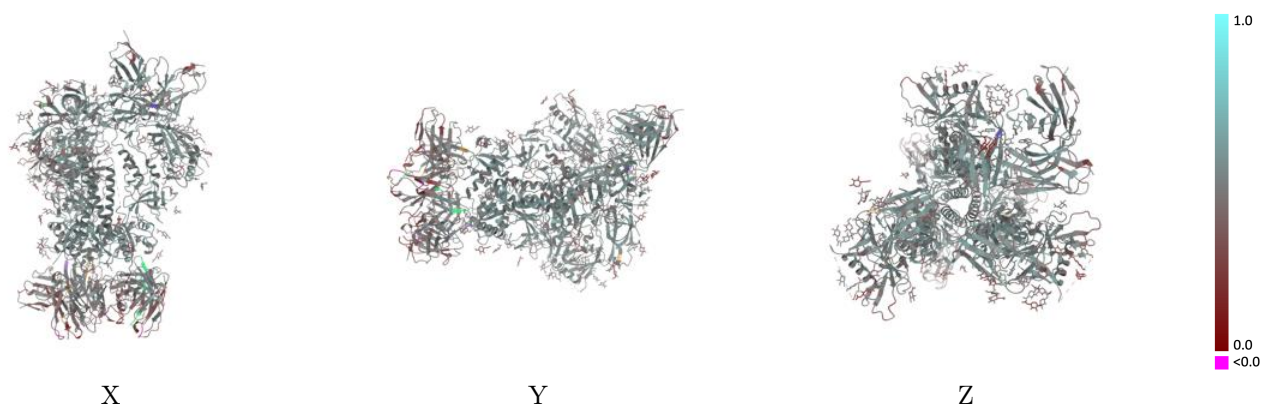
This section contains information regarding the fit between EMDB map EMD-23801 and PDB model 7MEP. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



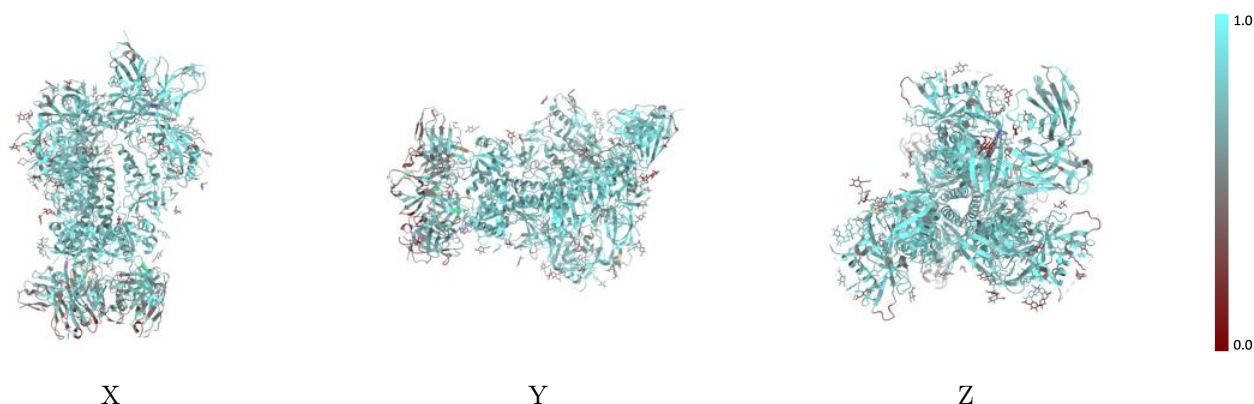
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



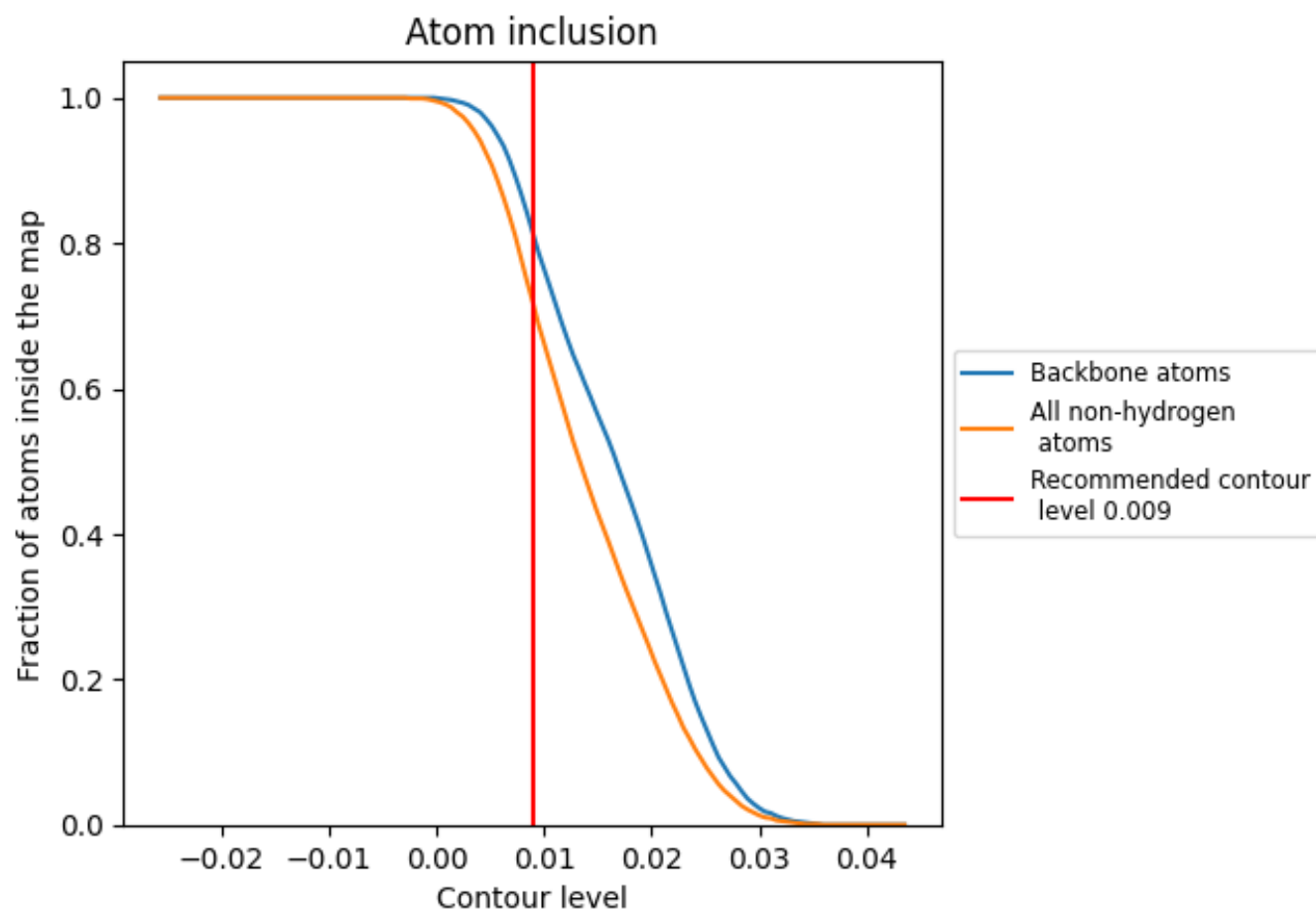
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7170	 0.4860
A	 0.7650	 0.5150
B	 0.7590	 0.5140
C	 0.7480	 0.5070
D	 0.7560	 0.5070
E	 0.7610	 0.5060
F	 0.7750	 0.5230
G	 0.6170	 0.4330
H	 0.7850	 0.5100
I	 0.6180	 0.4210
J	 0.6030	 0.4230
K	 0.5850	 0.4050
L	 0.7560	 0.4890
M	 0.6250	 0.4230
N	 0.5740	 0.4090
O	 0.5900	 0.4600
P	 0.4290	 0.3530
Q	 0.5000	 0.4480
R	 0.0360	 0.1160
S	 0.6790	 0.5550
T	 0.6070	 0.4380
U	 0.5900	 0.4340
V	 0.3930	 0.3300
W	 0.5000	 0.3790
X	 0.4640	 0.4200
Y	 0.5410	 0.4220
Z	 0.4640	 0.4640
a	 0.5000	 0.3990
b	 0.4290	 0.3290
c	 0.6790	 0.4590

