



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:05 AM UTC

PDB ID : 7WEC / pdb_00007wec
EMDB ID : EMD-32446
Title : SARS-CoV-2 Omicron variant spike protein with three XGv347 Fabs binding to three closed state RBDs
Authors : Wang, X.; Wang, L.
Deposited on : 2021-12-23
Resolution : 3.30 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

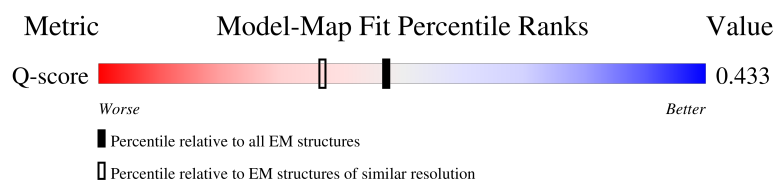
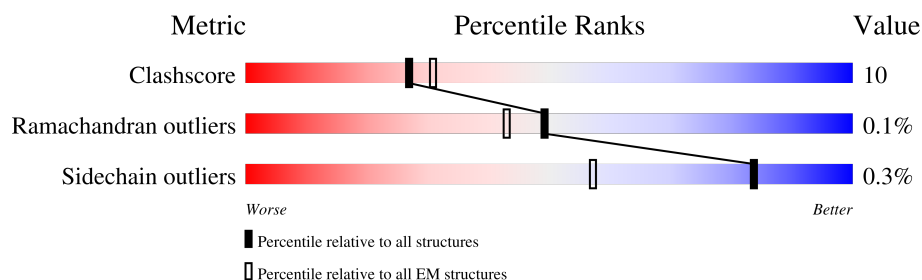
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	123	<div><div></div><div>68%</div><div>32%</div></div>
1	H	123	<div><div></div><div>59%</div><div>41%</div></div>
1	I	123	<div><div></div><div>67%</div><div>33%</div></div>
2	J	107	<div><div></div><div>74%</div><div>25%</div><div>.</div></div>


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	107	
2	L	107	
3	A	1270	
3	B	1270	
3	C	1270	
4	D	2	
4	E	2	
4	F	2	
4	M	2	
4	N	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
5	O	3	
5	V	3	
5	W	3	
5	c	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	d	3	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 32217 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 The heavy chain of Fab XGv347.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	123	Total	C	N	O	S	0	0
			941	588	158	189	6		
1	H	123	Total	C	N	O	S	0	0
			941	588	158	189	6		
1	I	123	Total	C	N	O	S	0	0
			941	588	158	189	6		

- Molecule 2 is a protein called The light chain of Fab XGv347.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	107	Total	C	N	O	S	0	0
			807	506	141	158	2		
2	K	107	Total	C	N	O	S	0	0
			807	506	141	158	2		
2	L	107	Total	C	N	O	S	0	0
			807	506	141	158	2		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		
3	B	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		
3	C	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ILE	THR	variant	UNP P0DTC2
A	140	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	209	GLU	-	insertion	UNP P0DTC2
A	210	PRO	-	insertion	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2
A	490	ARG	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	variant	UNP P0DTC2
B	140	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	GLU	-	insertion	UNP P0DTC2
B	210	PRO	-	insertion	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	336	ASP	GLY	variant	UNP P0DTC2
B	368	LEU	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	490	ARG	GLN	variant	UNP P0DTC2
B	493	SER	GLY	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	544	LYS	THR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	853	LYS	ASN	variant	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	978	PHE	LEU	variant	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	variant	UNP P0DTC2
C	140	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	209	GLU	-	insertion	UNP P0DTC2
C	210	PRO	-	insertion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	211	GLU	-	insertion	UNP P0DTC2
C	336	ASP	GLY	variant	UNP P0DTC2
C	368	LEU	SER	variant	UNP P0DTC2
C	370	PRO	SER	variant	UNP P0DTC2
C	372	PHE	SER	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	variant	UNP P0DTC2
C	443	SER	GLY	variant	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
C	481	ALA	GLU	variant	UNP P0DTC2
C	490	ARG	GLN	variant	UNP P0DTC2
C	493	SER	GLY	variant	UNP P0DTC2
C	495	ARG	GLN	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	variant	UNP P0DTC2
C	544	LYS	THR	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	variant	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	761	LYS	ASN	variant	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2
C	853	LYS	ASN	variant	UNP P0DTC2
C	951	HIS	GLN	variant	UNP P0DTC2
C	966	LYS	ASN	variant	UNP P0DTC2
C	978	PHE	LEU	variant	UNP P0DTC2

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



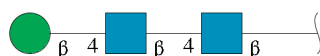
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



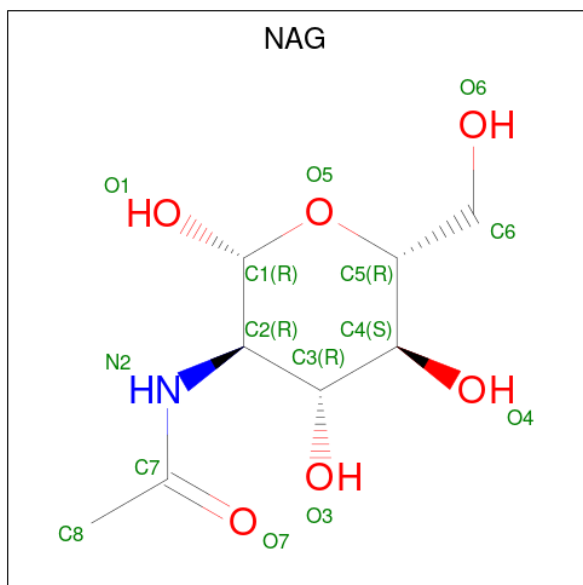
Mol	Chain	Residues	Atoms				AltConf	Trace
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	V	3	Total	C	N	O	0	0
			39	22	2	15		
5	W	3	Total	C	N	O	0	0
			39	22	2	15		
5	c	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

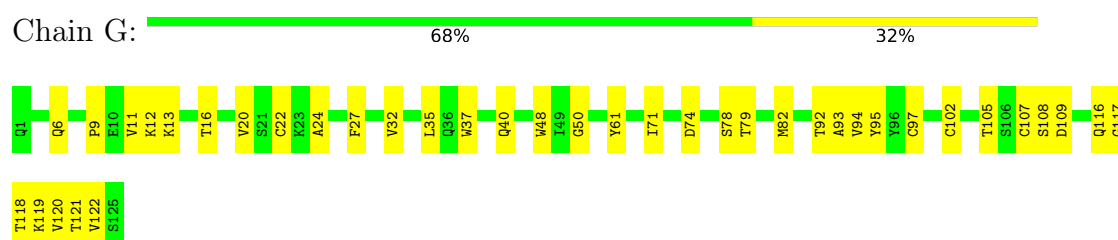
Continued from previous page...

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

3 Residue-property plots

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.

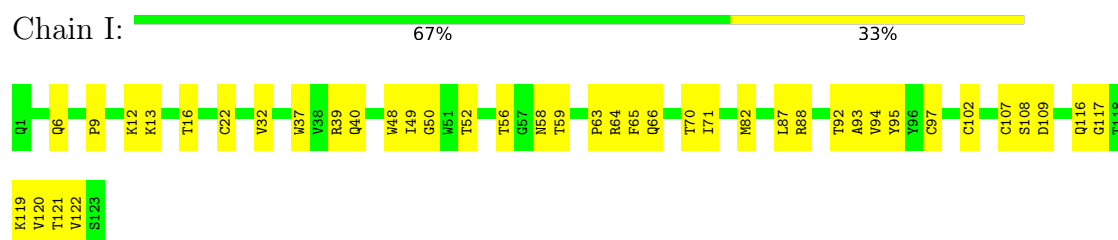
- Molecule 1: The heavy chain of Fab XGv347



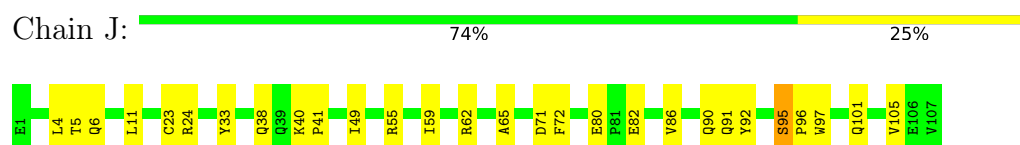
- Molecule 1: The heavy chain of Fab XGv347



- Molecule 1: The heavy chain of Fab XGv347



- Molecule 2: The light chain of Fab XGv347



- Molecule 2: The light chain of Fab XGv347

E1	L4	T5	P8	L11	L21	S22	C23	R24	L34	Y37	Q38	Q39	K40	P41	L47	L48	A56	P60	D61	R62	F63	T70	D71	F72	T73	L74	E80	P81	E82	Y87	Q90	Q91	Y92	P96	W97	Q101	V105	E106	L109
----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------

- Chain L:  72% 28%

E1	L4	T5	P8	L11	L21	S22	G23	C24	L34	Q38	Q39	K40	P41	R46	L47	L48	L49	A65	D71	E80	P81	E82	D83	F84	Y87	Q90	Q91	Y92	S95	P96	Y97	Q101	V105	E106	V107
----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------

- Chain A:  69% 17% 14%

[illegible]

- 





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

Chain N:  100%



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

Chain P:  100%



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

Chain Q:  50% 50%



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

Chain R:  50% 50%



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

Chain S:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  100%

NAG1
NAG2

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

Chain X:  50%

NAG1
NAG2

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

Chain Y:  50%


NAG1
NAG2

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

Chain Z:  100%

NAG1
NAG2

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

Chain a:  50%

NAG1
NAG2

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

Chain b:  100%

NAG1
NAG2

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

Chain O:  67% 33%

HA01
HA02
BM03

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

Chain V:  67% 33%

HA01
HA02
BM03

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

Chain W:  100%

HA01
HA02
BM03

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

Chain c:  67% 33%

HA01
HA02
BM03

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

Chain d:  100%

HA01
HA02
BM03

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.177	Depositor
Minimum map value	-2.513	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.219	Depositor
Map size (\AA)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.11	0/961	0.32	0/1306
1	H	0.12	0/961	0.34	0/1306
1	I	0.13	0/961	0.35	0/1306
2	J	0.12	0/826	0.38	0/1125
2	K	0.12	0/826	0.35	0/1125
2	L	0.15	0/826	0.41	0/1125
3	A	0.21	0/8837	0.36	0/12019
3	B	0.23	0/8837	0.40	3/12019 (0.0%)
3	C	0.24	0/8837	0.44	5/12019 (0.0%)
All	All	0.22	0/31872	0.40	8/43350 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	1
3	A	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	139	LEU	N-CA-C	-10.88	99.54	112.92
3	B	211	GLU	CB-CA-C	-5.50	110.21	116.54
3	C	140	ASP	N-CA-C	5.28	116.72	111.07
3	B	139	LEU	N-CA-C	-5.22	106.59	113.17
3	B	577	GLN	N-CA-C	-5.21	106.87	113.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	328	ASN	CB-CA-C	-5.06	101.89	110.19
3	C	140	ASP	CA-C-N	-5.02	116.02	123.05
3	C	140	ASP	C-N-CA	-5.02	116.02	123.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	161	CYS	Peptide
2	J	95	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	941	0	903	29	0
1	H	941	0	903	35	0
1	I	941	0	903	33	0
2	J	807	0	779	19	0
2	K	807	0	779	26	0
2	L	807	0	779	21	0
3	A	8632	0	8448	155	0
3	B	8632	0	8448	159	0
3	C	8632	0	8447	177	0
4	D	28	0	25	1	0
4	E	28	0	24	4	0
4	F	28	0	25	0	0
4	M	28	0	25	1	0
4	N	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	18	7	0
4	R	28	0	25	1	0
4	S	28	0	25	1	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	X	28	0	25	4	0
4	Y	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Z	28	0	25	0	0
4	a	28	0	25	2	0
4	b	28	0	25	0	0
5	O	39	0	34	1	0
5	V	39	0	34	1	0
5	W	39	0	34	0	0
5	c	39	0	34	1	0
5	d	39	0	34	0	0
6	A	140	0	128	2	0
6	B	154	0	143	8	0
6	C	140	0	124	1	0
All	All	32217	0	31346	628	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 10.

All (628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:184:LEU:CB	3:A:206:LEU:HD11	1.46	1.42
3:A:184:LEU:HB2	3:A:206:LEU:CD1	1.63	1.28
3:B:87:GLY:HA2	3:B:189:PHE:O	1.26	1.24
3:C:184:LEU:HB2	3:C:206:LEU:CD1	1.76	1.15
3:A:184:LEU:CB	3:A:206:LEU:CD1	2.20	1.12
3:B:93:ILE:HG23	3:B:206:LEU:CD1	1.84	1.07
3:C:184:LEU:HB2	3:C:206:LEU:HD12	1.37	1.04
3:C:184:LEU:CB	3:C:206:LEU:HD11	1.86	1.04
3:A:184:LEU:HB3	3:A:206:LEU:HD11	1.06	1.02
3:C:184:LEU:CB	3:C:206:LEU:CD1	2.36	1.02
3:C:184:LEU:HB3	3:C:206:LEU:HD11	1.44	1.00
1:H:95:TYR:O	1:H:117:GLY:HA2	1.66	0.93
1:I:95:TYR:O	1:I:117:GLY:HA2	1.71	0.91
3:A:184:LEU:HB2	3:A:206:LEU:HD13	1.56	0.86
3:C:463:ARG:HG3	4:Q:1:NAG:H2	1.60	0.84
1:G:95:TYR:O	1:G:117:GLY:HA2	1.76	0.84
2:J:4:LEU:HA	2:J:24:ARG:O	1.78	0.83
3:B:87:GLY:CA	3:B:189:PHE:O	2.21	0.82
3:B:100:ARG:HH21	3:B:120:ASN:HB3	1.46	0.80
3:B:735:CYS:SG	3:B:761:LYS:HE3	2.21	0.80
3:B:93:ILE:CG2	3:B:206:LEU:CD1	2.59	0.80
3:C:639:VAL:HG12	3:C:648:ILE:HG12	1.62	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1139:GLN:O	3:A:1143:ASP:N	2.14	0.79
3:B:122:THR:HA	3:B:169:PRO:HG3	1.65	0.79
1:I:6:GLN:HB3	1:I:116:GLN:HE22	1.47	0.79
3:A:376:CYS:HA	3:A:429:CYS:HB3	1.66	0.78
3:B:623:ALA:HA	3:B:631:ARG:HH22	1.49	0.78
3:C:376:CYS:HA	3:C:429:CYS:HB3	1.66	0.78
3:B:227:PRO:O	3:C:354:ARG:NH2	2.17	0.78
3:B:115:LEU:HD12	3:B:117:ILE:HD11	1.66	0.77
3:B:639:VAL:HG12	3:B:648:ILE:HG12	1.67	0.76
3:A:1142:LEU:O	3:A:1146:LYS:N	2.16	0.76
3:B:461:PHE:HB3	6:B:1301:NAG:H83	1.68	0.76
3:A:451:ARG:NH2	3:A:466:SER:O	2.19	0.75
3:A:601:THR:HG22	3:A:602:SER:H	1.51	0.75
3:C:100:ARG:NH1	3:C:119:ASN:OD1	2.19	0.75
3:A:1145:PHE:O	3:A:1149:LEU:N	2.17	0.75
1:H:102:CYS:HA	1:H:107:CYS:HB3	1.69	0.74
1:G:102:CYS:HA	1:G:107:CYS:HB3	1.69	0.74
3:B:93:ILE:HG23	3:B:206:LEU:HD11	1.70	0.74
3:C:184:LEU:CB	3:C:206:LEU:HD12	2.13	0.73
3:C:100:ARG:HH12	3:C:119:ASN:H	1.33	0.73
3:B:95:LYS:HB2	3:B:181:PHE:HA	1.71	0.73
3:B:376:CYS:HA	3:B:429:CYS:HB3	1.69	0.73
3:A:906:ILE:HD12	3:A:1044:TYR:HB3	1.72	0.72
3:A:808:LYS:HD3	3:A:810:SER:H	1.56	0.71
3:A:866:MET:HE3	3:B:696:LEU:HD21	1.73	0.71
3:B:906:ILE:HD12	3:B:1044:TYR:HB3	1.73	0.71
3:C:142:LYS:HB2	3:C:150:SER:HB2	1.73	0.70
3:B:100:ARG:HE	3:B:120:ASN:HA	1.56	0.70
3:C:906:ILE:HD12	3:C:1044:TYR:HB3	1.73	0.70
3:B:320:THR:OG1	3:B:534:LYS:NZ	2.24	0.70
1:G:9:PRO:HB3	1:G:119:LYS:HB3	1.73	0.70
3:C:735:CYS:SG	3:C:761:LYS:HE3	2.31	0.69
3:A:194:GLY:HA3	6:B:1301:NAG:H82	1.73	0.69
1:I:102:CYS:HA	1:I:107:CYS:HB3	1.76	0.68
3:B:113:GLN:H	3:C:463:ARG:HH21	1.41	0.68
1:I:63:PRO:HA	1:I:66:GLN:HE22	1.58	0.67
2:L:5:THR:HA	2:L:101:GLN:HE22	1.60	0.67
3:B:622:HIS:O	3:B:631:ARG:NH1	2.28	0.67
3:B:93:ILE:HG23	3:B:206:LEU:HD12	1.73	0.67
3:C:759:GLN:OE1	3:C:762:ARG:NH2	2.28	0.67
3:C:451:ARG:HG2	4:Q:2:NAG:O4	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:SER:HB3	3:C:132:GLN:HB2	1.77	0.66
3:A:95:LYS:HB2	3:A:181:PHE:HA	1.77	0.66
3:A:639:VAL:HG12	3:A:648:ILE:HG12	1.76	0.66
2:K:90:GLN:NE2	2:K:91:GLN:O	2.25	0.66
3:C:475:LYS:HZ2	3:C:477:CYS:HB2	1.61	0.65
3:A:454:ARG:HE	4:X:2:NAG:H3	1.61	0.65
3:C:375:LYS:NZ	3:C:377:TYR:OH	2.30	0.65
2:J:33:TYR:HB3	2:J:92:TYR:HB2	1.79	0.65
2:L:95:SER:HB2	2:L:96:PRO:HD3	1.79	0.64
1:H:32:VAL:HG21	1:H:105:THR:HG22	1.78	0.64
3:A:159:ASN:HD22	3:A:160:ASN:HD22	1.43	0.64
3:B:354:ARG:HG2	3:B:393:TYR:HE1	1.62	0.64
3:B:460:PRO:O	6:B:1301:NAG:O3	2.16	0.64
3:C:465:ILE:HD11	4:Q:1:NAG:H83	1.79	0.64
1:H:92:THR:HA	1:H:120:VAL:O	1.98	0.64
2:J:92:TYR:O	2:J:97:TRP:NE1	2.31	0.64
3:B:552:SER:HB3	3:B:583:ASP:HB2	1.78	0.64
2:L:40:LYS:HE2	2:L:41:PRO:HD2	1.80	0.63
3:B:877:GLY:O	3:B:881:SER:OG	2.17	0.63
3:C:552:SER:HB3	3:C:583:ASP:HB2	1.81	0.63
3:C:184:LEU:HB3	3:C:206:LEU:CD1	2.17	0.63
3:C:1142:LEU:O	3:C:1146:LYS:N	2.31	0.63
2:J:40:LYS:HE2	2:J:41:PRO:HD2	1.79	0.63
3:A:789:PRO:HG3	3:B:704:TYR:HB3	1.81	0.63
3:B:93:ILE:CG2	3:B:206:LEU:HD13	2.28	0.63
3:B:442:VAL:O	3:B:495:ARG:NH2	2.32	0.62
3:C:192:ILE:HG22	3:C:197:LYS:HZ1	1.63	0.62
3:C:1050:PRO:O	3:C:1051:GLN:NE2	2.28	0.62
2:L:4:LEU:HA	2:L:24:ARG:O	2.00	0.62
3:C:99:ILE:HD12	3:C:99:ILE:H	1.63	0.62
3:A:622:HIS:O	3:A:631:ARG:NH1	2.33	0.61
3:A:100:ARG:HD2	3:A:120:ASN:HA	1.82	0.61
3:A:375:LYS:NZ	3:A:377:TYR:OH	2.32	0.61
3:B:1142:LEU:O	3:B:1146:LYS:N	2.29	0.61
3:C:449:LEU:HB3	3:C:489:LEU:HD12	1.81	0.61
1:H:95:TYR:O	1:H:117:GLY:CA	2.47	0.61
3:A:94:GLU:OE2	3:A:99:ILE:N	2.28	0.61
3:B:1138:LEU:HA	3:B:1141:GLU:HB2	1.82	0.61
3:C:300:LEU:HD12	3:C:305:VAL:HG12	1.83	0.61
3:C:877:GLY:O	3:C:881:SER:OG	2.18	0.60
3:A:271:THR:HG23	3:A:288:CYS:HB2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:6:GLN:H	2:J:101:GLN:NE2	2.00	0.60
2:K:38:GLN:HE21	2:K:48:LEU:HD21	1.66	0.60
3:A:19:THR:O	3:A:21:ARG:NH1	2.35	0.60
3:C:108:LEU:HG	3:C:133:PHE:HD2	1.66	0.60
3:C:656:SER:HB2	3:C:695:SER:HB3	1.82	0.60
3:A:658:GLU:O	3:A:692:TYR:OH	2.18	0.59
3:B:112:THR:HG22	3:C:465:ILE:HB	1.83	0.59
1:I:92:THR:HA	1:I:120:VAL:O	2.02	0.59
3:A:314:ASN:OD1	3:A:315:PHE:N	2.33	0.59
3:B:883:TRP:HH2	3:B:901:TYR:HD2	1.50	0.59
3:A:296:THR:HA	3:A:299:THR:HG22	1.84	0.59
2:J:6:GLN:H	2:J:101:GLN:HE22	1.49	0.59
3:A:442:VAL:O	3:A:495:ARG:NH2	2.36	0.59
3:A:577:GLN:HB3	4:E:1:NAG:C1	2.27	0.59
3:C:127:LYS:NZ	3:C:161:CYS:SG	2.74	0.59
2:K:38:GLN:HG3	2:K:48:LEU:HD11	1.85	0.59
3:A:27:ALA:HB3	3:A:64:TRP:HB3	1.84	0.59
3:A:368:LEU:HG	3:A:370:PRO:HD2	1.85	0.58
3:A:773:LYS:NZ	3:A:777:GLU:OE2	2.35	0.58
3:C:1147:GLU:O	3:C:1151:LYS:N	2.31	0.58
2:J:24:ARG:HH22	2:J:71:ASP:HB2	1.68	0.58
1:H:29:PHE:H	1:H:78:SER:HB2	1.67	0.58
3:B:656:SER:HB2	3:B:695:SER:HB3	1.84	0.58
3:A:1140:PRO:HA	3:A:1143:ASP:HB2	1.85	0.58
3:C:124:VAL:O	3:C:167:SER:N	2.31	0.58
3:B:1123:CYS:HB2	3:B:1129:ILE:HD13	1.86	0.58
3:C:863:THR:HG22	3:C:866:MET:HE3	1.86	0.58
1:H:6:GLN:H	1:H:116:GLN:HE22	1.50	0.58
3:A:463:ARG:NH2	3:C:113:GLN:OE1	2.36	0.57
3:C:119:ASN:HB3	3:C:124:VAL:HG22	1.85	0.57
3:B:658:GLU:O	3:B:692:TYR:OH	2.20	0.57
3:B:714:ASN:HB3	3:B:1067:ALA:HB3	1.85	0.57
2:L:24:ARG:HA	2:L:24:ARG:NH1	2.18	0.57
3:A:97:ASN:ND2	3:A:100:ARG:HH21	2.01	0.57
3:C:64:TRP:CZ2	3:C:211:GLU:HG2	2.39	0.57
3:C:430:VAL:HG12	3:C:509:VAL:HG22	1.87	0.57
3:A:471:GLN:HA	3:A:485:CYS:HB3	1.85	0.57
3:B:368:LEU:HG	3:B:370:PRO:HD2	1.85	0.57
2:J:90:GLN:NE2	2:J:97:TRP:HB3	2.19	0.57
1:H:9:PRO:HB3	1:H:119:LYS:HB3	1.86	0.57
2:K:24:ARG:HA	2:K:24:ARG:NH1	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:633:TYR:OH	3:B:648:ILE:O	2.12	0.57
3:C:658:GLU:O	3:C:692:TYR:OH	2.19	0.57
3:B:119:ASN:HA	3:B:123:ASN:O	2.04	0.56
3:C:307:LYS:HG3	3:C:597:PRO:HA	1.87	0.56
3:C:349:ALA:HA	4:Q:1:NAG:H82	1.86	0.56
4:T:1:NAG:H3	4:T:1:NAG:H83	1.86	0.56
3:A:877:GLY:O	3:A:881:SER:OG	2.21	0.56
3:A:94:GLU:OE2	3:A:98:ILE:N	2.38	0.56
3:A:324:VAL:HG12	3:A:539:ASN:HB3	1.88	0.56
1:I:95:TYR:O	1:I:117:GLY:CA	2.50	0.56
3:B:458:LEU:HA	4:D:1:NAG:H81	1.86	0.56
1:H:29:PHE:HB3	1:H:54:VAL:HG11	1.87	0.56
3:C:188:VAL:HG12	3:C:199:TYR:HB2	1.87	0.56
2:K:62:ARG:HH22	2:K:80:GLU:HB2	1.71	0.55
3:A:1122:ASN:OD1	3:A:1123:CYS:N	2.39	0.55
1:G:92:THR:HA	1:G:120:VAL:O	2.05	0.55
3:B:64:TRP:HE1	3:B:261:ALA:HB1	1.72	0.55
3:A:115:LEU:HD21	3:A:228:ILE:HG21	1.88	0.55
3:C:620:ALA:HB1	3:C:626:LEU:HD21	1.88	0.55
1:G:92:THR:HG22	1:G:122:VAL:H	1.72	0.55
3:A:96:SER:HB2	3:A:176:GLY:HA2	1.88	0.55
3:B:108:LEU:HD22	3:B:133:PHE:HD2	1.71	0.55
3:B:315:PHE:O	3:B:589:PHE:HA	2.07	0.55
3:A:376:CYS:HA	3:A:429:CYS:CB	2.35	0.55
4:M:1:NAG:H62	4:M:2:NAG:H62	1.88	0.55
3:A:41:LYS:HG3	3:B:559:PHE:HD2	1.70	0.55
1:H:86:SER:HB2	1:H:88:ARG:HH12	1.72	0.55
1:I:71:ILE:HG12	1:I:82:MET:HG2	1.89	0.55
3:A:883:TRP:HH2	3:A:901:TYR:HD2	1.54	0.55
3:B:81:VAL:HG21	3:B:234:ARG:HG2	1.88	0.55
3:B:471:GLN:HA	3:B:485:CYS:HB3	1.88	0.55
4:a:1:NAG:H83	4:a:1:NAG:H3	1.89	0.54
1:H:92:THR:HG22	1:H:122:VAL:H	1.71	0.54
1:I:87:LEU:HB3	1:I:122:VAL:HG21	1.89	0.54
3:B:375:LYS:NZ	3:B:377:TYR:OH	2.37	0.54
1:H:52:THR:HG22	1:H:59:THR:HG22	1.89	0.54
1:I:9:PRO:HB3	1:I:119:LYS:HB3	1.89	0.54
3:A:14:GLN:HG2	3:A:151:GLU:HG3	1.87	0.54
3:C:1136:ASP:HB3	3:C:1139:GLN:HB2	1.88	0.54
2:L:84:PHE:HA	2:L:105:VAL:HG23	1.89	0.54
3:B:430:VAL:HG12	3:B:509:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:THR:O	3:C:61:ASN:HA	2.06	0.54
2:K:11:LEU:HD13	2:K:105:VAL:HG12	1.88	0.54
3:C:21:ARG:HH12	3:C:79:ASN:H	1.54	0.54
3:C:899:MET:HE3	3:C:1046:LEU:HD13	1.90	0.54
1:I:108:SER:OG	1:I:109:ASP:N	2.41	0.54
3:A:1050:PRO:O	3:A:1051:GLN:NE2	2.35	0.54
3:B:209:GLU:HG2	3:B:211:GLU:HB2	1.89	0.54
3:C:883:TRP:HH2	3:C:901:TYR:HD2	1.55	0.54
1:G:92:THR:HB	1:G:121:THR:HG22	1.90	0.54
3:C:637:SER:OG	3:C:638:ASN:N	2.41	0.53
3:C:95:LYS:HB2	3:C:181:PHE:HA	1.90	0.53
3:B:300:LEU:HD12	3:B:305:VAL:HG12	1.90	0.53
2:L:22:SER:OG	2:L:71:ASP:OD1	2.26	0.53
3:B:1145:PHE:O	3:B:1149:LEU:N	2.35	0.53
1:G:108:SER:OG	1:G:109:ASP:N	2.41	0.53
3:B:195:TYR:HE1	3:B:227:PRO:HB3	1.74	0.53
3:B:287:ASP:OD1	3:B:287:ASP:N	2.42	0.53
3:B:1146:LYS:HE2	3:B:1149:LEU:HD12	1.91	0.53
3:C:354:ARG:NH2	3:C:393:TYR:OH	2.38	0.53
1:G:20:VAL:HB	1:G:82:MET:HE3	1.91	0.53
3:B:637:SER:HB3	3:B:649:GLY:HA2	1.90	0.53
3:C:376:CYS:HA	3:C:429:CYS:CB	2.37	0.53
2:J:90:GLN:NE2	2:J:91:GLN:O	2.32	0.53
3:C:139:LEU:HD23	3:C:139:LEU:H	1.73	0.53
3:A:1123:CYS:HB2	3:A:1129:ILE:HD13	1.91	0.53
3:B:799:PHE:HB3	3:B:803:LEU:HD23	1.91	0.53
3:C:174:LEU:HG	3:C:175:GLU:OE1	2.09	0.53
1:H:20:VAL:HB	1:H:82:MET:HE3	1.90	0.52
1:H:94:VAL:HA	1:H:118:THR:O	2.10	0.52
2:J:95:SER:OG	2:J:96:PRO:HD3	2.08	0.52
3:A:131:PHE:HB2	3:A:133:PHE:CE1	2.45	0.52
3:A:623:ALA:HA	3:A:631:ARG:HH12	1.74	0.52
3:B:104:PHE:HB2	3:B:115:LEU:HD23	1.91	0.52
2:J:62:ARG:NH2	2:J:80:GLU:H	2.07	0.52
3:A:363:SER:O	3:A:367:ASN:ND2	2.42	0.52
1:H:39:ARG:HB2	1:H:49:ILE:HD11	1.90	0.52
2:K:4:LEU:HA	2:K:24:ARG:O	2.09	0.52
3:B:227:PRO:HB2	3:C:354:ARG:HH22	1.74	0.52
3:B:773:LYS:NZ	3:B:777:GLU:OE2	2.39	0.52
3:C:102:TRP:HB2	3:C:117:ILE:HB	1.91	0.52
1:G:48:TRP:CZ3	2:J:96:PRO:HB3	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:970:ILE:HD12	3:A:981:LEU:HD11	1.92	0.52
3:C:125:VAL:HA	3:C:166:VAL:HA	1.92	0.52
3:A:594:VAL:HG12	3:A:607:VAL:HG12	1.92	0.52
2:K:22:SER:OG	2:K:71:ASP:OD2	2.27	0.52
3:A:123:ASN:HA	3:A:169:PRO:HG3	1.91	0.52
3:A:799:PHE:HB3	3:A:803:LEU:HD23	1.91	0.52
3:A:641:GLN:NE2	3:A:642:THR:O	2.40	0.52
3:B:376:CYS:HA	3:B:429:CYS:CB	2.37	0.52
1:G:24:ALA:HB1	1:G:27:PHE:HB3	1.91	0.52
3:A:200:SER:HB3	3:A:223:LEU:HD13	1.91	0.51
3:B:1050:PRO:O	3:B:1051:GLN:NE2	2.34	0.51
3:C:442:VAL:O	3:C:495:ARG:NH2	2.39	0.51
3:C:714:ASN:HB3	3:C:1067:ALA:HB3	1.93	0.51
3:C:331:ASN:HB2	3:C:358:CYS:HA	1.91	0.51
3:B:147:TRP:CE2	3:B:255:TRP:HZ2	2.28	0.51
3:B:401:GLY:HA2	3:B:505:TYR:HD1	1.75	0.51
3:C:368:LEU:HG	3:C:370:PRO:HD2	1.93	0.51
3:B:753:TYR:OH	3:B:991:ASP:OD1	2.28	0.51
3:A:601:THR:HG22	3:A:602:SER:N	2.24	0.51
3:B:354:ARG:HG2	3:B:393:TYR:CE1	2.45	0.51
3:C:626:LEU:HD12	3:C:631:ARG:HG2	1.92	0.51
3:A:129:CYS:HA	3:A:161:CYS:HB2	1.93	0.51
3:A:704:TYR:HB3	3:C:789:PRO:HG3	1.93	0.51
3:A:140:ASP:HB2	3:A:240:ALA:HA	1.93	0.51
3:B:101:GLY:C	3:B:238:LEU:HB2	2.36	0.51
3:B:115:LEU:HD13	3:B:128:VAL:HG22	1.91	0.51
3:B:454:ARG:NH1	3:B:456:SER:O	2.42	0.51
3:B:902:ARG:NH1	3:B:1046:LEU:O	2.44	0.51
3:B:607:VAL:HB	3:B:633:TYR:CE2	2.46	0.51
3:B:723:ILE:HG13	3:B:1058:VAL:HG22	1.93	0.51
3:C:647:LEU:H	3:C:647:LEU:HD23	1.75	0.51
3:C:195:TYR:CD1	3:C:227:PRO:HB3	2.46	0.51
3:C:911:ASN:O	3:C:915:GLU:HG2	2.11	0.51
3:A:1145:PHE:CE2	3:B:1146:LYS:HD2	2.46	0.51
3:C:799:PHE:HB3	3:C:803:LEU:HD23	1.93	0.51
3:C:1136:ASP:OD1	3:C:1137:PRO:HD2	2.11	0.51
3:B:117:ILE:HD12	3:B:126:ILE:HG23	1.93	0.50
3:A:982:ASP:OD1	3:A:982:ASP:N	2.44	0.50
3:B:53:ASP:OD1	3:B:54:LEU:N	2.38	0.50
1:H:13:LYS:O	1:H:16:THR:OG1	2.29	0.50
1:I:12:LYS:HB2	1:I:122:VAL:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1123:CYS:HB2	3:C:1129:ILE:HD13	1.93	0.50
1:H:92:THR:HB	1:H:121:THR:HG22	1.93	0.50
3:B:113:GLN:N	3:C:463:ARG:HH21	2.09	0.50
1:I:13:LYS:O	1:I:16:THR:OG1	2.24	0.50
3:A:100:ARG:HH22	3:A:147:TRP:HH2	1.58	0.50
2:L:92:TYR:HA	2:L:97:TRP:NE1	2.27	0.50
3:A:292:PRO:HG2	3:A:605:VAL:HG21	1.94	0.50
1:I:22:CYS:HB2	1:I:37:TRP:CH2	2.47	0.50
3:B:108:LEU:HD22	3:B:133:PHE:CD2	2.46	0.50
3:B:189:PHE:HD1	3:B:198:ILE:HG23	1.76	0.50
1:G:32:VAL:HG11	1:G:105:THR:HA	1.94	0.49
3:A:942:LEU:HD12	3:A:945:LEU:HD12	1.94	0.49
3:C:119:ASN:HA	3:C:123:ASN:O	2.12	0.49
3:A:346:SER:OG	3:A:449:LEU:O	2.30	0.49
3:A:452:LEU:HD11	3:A:490:ARG:HB2	1.94	0.49
3:B:93:ILE:HG21	3:B:206:LEU:HD13	1.92	0.49
1:H:24:ALA:HB1	1:H:27:PHE:HB3	1.95	0.49
3:A:159:ASN:ND2	3:A:160:ASN:HD22	2.09	0.49
3:A:97:ASN:HB2	3:A:173:ASP:HB2	1.95	0.49
3:B:81:VAL:HG23	3:B:235:PHE:H	1.77	0.49
3:B:789:PRO:HG3	3:C:704:TYR:HB3	1.95	0.49
3:C:129:CYS:HB3	3:C:131:PHE:CE2	2.47	0.49
1:G:95:TYR:O	1:G:117:GLY:CA	2.54	0.49
1:I:37:TRP:CH2	1:I:97:CYS:HB3	2.48	0.49
3:A:307:LYS:HG3	3:A:597:PRO:HA	1.94	0.49
3:A:430:VAL:HG12	3:A:509:VAL:HG22	1.93	0.49
3:C:374:PHE:HD1	3:C:431:ILE:HG12	1.77	0.49
3:A:451:ARG:NE	4:X:2:NAG:O3	2.46	0.49
3:B:191:ASN:HD21	3:B:231:ASN:HA	1.77	0.49
3:C:108:LEU:HD23	3:C:133:PHE:HB2	1.94	0.49
2:K:21:LEU:HD12	2:K:87:TYR:CD2	2.48	0.49
3:B:102:TRP:HB2	3:B:117:ILE:HB	1.94	0.49
3:B:595:ILE:HB	3:B:606:ALA:HB3	1.95	0.49
3:C:1139:GLN:HA	3:C:1142:LEU:HG	1.93	0.49
2:L:8:PRO:HD2	2:L:21:LEU:HD22	1.95	0.49
3:A:208:ARG:HG3	3:A:214:PRO:HB3	1.95	0.49
3:B:626:LEU:HB2	3:B:631:ARG:HD2	1.93	0.49
3:B:200:SER:HB3	3:B:223:LEU:HB2	1.95	0.48
3:C:723:ILE:HG13	3:C:1058:VAL:HG22	1.94	0.48
3:B:401:GLY:HA2	3:B:505:TYR:CD1	2.49	0.48
3:B:1098:HIS:CE1	5:V:1:NAG:H5	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:47:LEU:HD23	2:K:48:LEU:N	2.28	0.48
3:A:464:ASP:CG	3:A:465:ILE:H	2.21	0.48
3:A:945:LEU:HD21	3:A:1056:GLY:HA3	1.94	0.48
3:B:188:VAL:HG12	3:B:199:TYR:HB2	1.95	0.48
3:C:178:GLN:HG2	3:C:258:GLY:HA2	1.95	0.48
3:C:463:ARG:O	3:C:464:ASP:HB3	2.13	0.48
1:G:12:LYS:HB2	1:G:122:VAL:HG22	1.94	0.48
1:H:37:TRP:CH2	1:H:97:CYS:HB3	2.47	0.48
2:K:63:PHE:HB3	2:K:74:LEU:HD11	1.96	0.48
3:A:714:ASN:HB3	3:A:1067:ALA:HB3	1.96	0.48
3:C:1145:PHE:HA	3:C:1148:GLU:HB3	1.95	0.48
1:G:37:TRP:CH2	1:G:97:CYS:HB3	2.49	0.48
2:J:38:GLN:HA	2:J:86:VAL:O	2.14	0.48
3:B:543:LEU:HD21	3:B:570:THR:HG21	1.95	0.48
3:C:454:ARG:NH2	3:C:464:ASP:OD2	2.37	0.48
1:G:13:LYS:O	1:G:16:THR:OG1	2.32	0.48
3:A:552:SER:HB2	3:A:583:ASP:HB2	1.95	0.48
3:C:560:GLN:O	3:C:574:ARG:NH1	2.47	0.48
1:G:35:LEU:HD11	1:G:97:CYS:HB2	1.95	0.48
3:C:1138:LEU:HA	3:C:1141:GLU:HB2	1.96	0.48
1:H:48:TRP:CZ2	1:H:50:GLY:HA2	2.49	0.47
2:K:80:GLU:OE1	2:K:82:GLU:HG2	2.14	0.47
3:C:172:MET:HG3	3:C:185:ARG:HH22	1.79	0.47
1:I:64:ARG:HG3	1:I:65:PHE:CE1	2.49	0.47
1:H:108:SER:OG	1:H:109:ASP:N	2.47	0.47
3:C:226:LEU:HB2	3:C:228:ILE:HG12	1.97	0.47
1:G:61:TYR:OH	1:G:71:ILE:N	2.39	0.47
3:B:627:THR:HB	3:B:628:PRO:HD3	1.96	0.47
3:B:978:PHE:O	3:B:983:LYS:NZ	2.47	0.47
3:C:373:THR:HB	3:C:432:ALA:HB3	1.96	0.47
1:I:63:PRO:HD3	2:K:96:PRO:HG2	1.95	0.47
2:L:49:ILE:HG21	2:L:65:ALA:HB2	1.96	0.47
3:A:64:TRP:CD1	3:A:263:TYR:CE1	3.03	0.47
3:C:575:ASP:HB3	3:C:578:THR:O	2.14	0.47
3:C:577:GLN:H	3:C:577:GLN:HG2	1.48	0.47
3:A:808:LYS:HG2	3:A:809:PRO:HD2	1.97	0.47
1:G:94:VAL:HG22	1:G:119:LYS:HD3	1.96	0.47
2:K:60:PRO:HG2	2:K:62:ARG:HG2	1.97	0.47
3:A:143:ASN:HA	3:A:144:ASN:HA	1.52	0.47
3:A:818:LEU:HD23	3:A:936:SER:HB3	1.97	0.47
3:A:902:ARG:NH1	3:A:1046:LEU:O	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:407:ILE:O	3:B:422:LEU:HD12	2.15	0.47
3:C:169:PRO:HB2	3:C:172:MET:HE1	1.96	0.47
3:C:200:SER:HB3	3:C:223:LEU:HB2	1.96	0.47
1:G:94:VAL:HA	1:G:118:THR:O	2.14	0.47
1:I:48:TRP:CZ3	2:K:96:PRO:HB3	2.50	0.47
2:J:11:LEU:HD13	2:J:105:VAL:HG12	1.97	0.47
3:B:700:ASN:OD1	3:B:701:SER:N	2.48	0.47
2:K:8:PRO:HD2	2:K:21:LEU:HD22	1.95	0.47
2:L:80:GLU:HG2	2:L:81:PRO:HD2	1.97	0.47
3:B:942:LEU:HD12	3:B:945:LEU:HD12	1.97	0.47
3:C:740:CYS:HB3	3:C:746:CYS:HB3	1.69	0.47
1:H:61:TYR:OH	1:H:71:ILE:N	2.37	0.47
3:C:641:GLN:NE2	3:C:642:THR:O	2.45	0.47
3:B:52:GLN:HB2	3:B:271:THR:HG22	1.97	0.46
3:C:62:VAL:HG12	3:C:265:GLY:HA3	1.97	0.46
3:C:102:TRP:CE3	3:C:237:THR:HB	2.50	0.46
1:H:74:ASP:HB3	1:H:79:THR:HG22	1.97	0.46
2:L:24:ARG:HA	2:L:24:ARG:HH11	1.80	0.46
3:C:141:HIS:ND1	3:C:255:TRP:HB3	2.31	0.46
3:C:822:LYS:HE2	3:C:936:SER:HA	1.97	0.46
3:A:127:LYS:HB3	3:A:131:PHE:HZ	1.79	0.46
3:B:982:ASP:OD1	3:B:982:ASP:N	2.49	0.46
3:B:1139:GLN:HA	3:B:1142:LEU:HG	1.97	0.46
1:I:32:VAL:HG22	3:C:453:PHE:HE2	1.79	0.46
2:J:55:ARG:NH1	2:J:59:ILE:O	2.48	0.46
3:A:128:VAL:O	3:A:161:CYS:HB2	2.15	0.46
3:A:1126:VAL:HG23	3:C:914:TYR:HB3	1.96	0.46
3:C:894:PRO:HB2	3:C:897:MET:HG2	1.98	0.46
3:A:637:SER:OG	3:A:638:ASN:N	2.48	0.46
3:C:945:LEU:HD21	3:C:1056:GLY:HA3	1.96	0.46
1:G:35:LEU:HD21	1:G:97:CYS:HB2	1.96	0.46
1:I:92:THR:HG22	1:I:122:VAL:H	1.81	0.46
3:A:229:GLY:HA2	6:B:1301:NAG:H81	1.97	0.46
2:J:5:THR:O	2:J:23:CYS:HA	2.16	0.46
2:L:80:GLU:OE1	2:L:82:GLU:HG2	2.16	0.46
3:A:368:LEU:HD22	6:A:1305:NAG:H83	1.97	0.46
3:C:79:ASN:HB3	3:C:239:LEU:HD22	1.97	0.46
3:C:942:LEU:HD12	3:C:945:LEU:HD12	1.98	0.46
3:A:723:ILE:HG13	3:A:1058:VAL:HG22	1.97	0.46
3:B:42:VAL:HG11	3:C:564:ARG:HG3	1.97	0.46
3:B:224:VAL:HG13	3:B:224:VAL:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1098:HIS:CE1	5:c:1:NAG:H5	2.50	0.46
3:C:1150:ASP:OD1	3:C:1154:LYS:NZ	2.38	0.46
1:H:92:THR:HB	1:H:121:THR:HA	1.98	0.45
3:A:576:PRO:C	4:E:1:NAG:H83	2.41	0.45
3:B:1138:LEU:O	3:B:1142:LEU:N	2.49	0.45
3:C:451:ARG:NH2	3:C:466:SER:O	2.49	0.45
2:K:40:LYS:HE2	2:K:41:PRO:HD2	1.96	0.45
3:A:740:CYS:HB3	3:A:746:CYS:HB3	1.72	0.45
3:A:901:TYR:CE2	3:B:1104:ARG:HD2	2.52	0.45
3:B:191:ASN:HB3	3:B:196:PHE:HA	1.97	0.45
3:B:734:ASP:OD1	3:C:314:ASN:ND2	2.48	0.45
3:B:740:CYS:HB3	3:B:746:CYS:HB3	1.82	0.45
3:B:767:ILE:HD11	3:B:1009:LEU:HD22	1.99	0.45
3:A:229:GLY:HA2	6:B:1301:NAG:C8	2.46	0.45
2:K:24:ARG:HH12	2:K:70:THR:HG22	1.81	0.45
3:B:600:ASN:HD21	6:B:1308:NAG:H83	1.81	0.45
3:C:142:LYS:O	3:C:143:ASN:HB2	2.15	0.45
3:A:532:LYS:NZ	3:A:551:GLU:HB2	2.32	0.45
3:A:620:ALA:HB1	3:A:626:LEU:HD21	1.99	0.45
3:A:696:LEU:HD22	3:C:870:TYR:CE1	2.52	0.45
3:B:195:TYR:CE1	3:B:227:PRO:HB3	2.51	0.45
3:C:306:GLU:O	3:C:310:TYR:OH	2.27	0.45
3:C:348:TYR:CE1	3:C:449:LEU:HB2	2.52	0.45
1:I:70:THR:O	1:I:82:MET:HA	2.16	0.45
3:B:207:VAL:O	3:B:207:VAL:HG23	2.17	0.45
3:B:609:TYR:HE2	3:B:648:ILE:HD12	1.81	0.45
1:G:74:ASP:O	1:G:78:SER:N	2.50	0.45
1:H:102:CYS:CA	1:H:107:CYS:HB3	2.36	0.45
1:I:32:VAL:HG22	3:C:453:PHE:CE2	2.52	0.45
3:B:188:VAL:CG1	3:B:199:TYR:HB2	2.47	0.45
3:A:577:GLN:N	4:E:1:NAG:C8	2.77	0.45
3:C:127:LYS:HA	3:C:163:PHE:O	2.17	0.45
3:C:339:PHE:CE2	3:C:508:VAL:HG11	2.52	0.45
3:A:399:ILE:HD11	3:A:404:VAL:HA	1.98	0.45
3:C:600:ASN:HD21	6:C:1307:NAG:H83	1.82	0.45
3:A:68:ILE:HB	3:A:76:ARG:HB3	1.99	0.44
3:A:98:ILE:HG22	3:A:239:LEU:HB2	1.98	0.44
3:A:466:SER:HB3	4:X:2:NAG:H2	1.98	0.44
3:B:368:LEU:HD23	3:B:371:PHE:CE1	2.52	0.44
3:B:434:ASN:HA	3:B:505:TYR:HD2	1.82	0.44
3:C:184:LEU:CD2	3:C:206:LEU:HD11	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:23:CYS:SG	2:K:72:PHE:HB2	2.57	0.44
3:B:714:ASN:C	3:B:1067:ALA:HB3	2.42	0.44
3:B:1047:MET:HE2	3:B:1049:PHE:CZ	2.52	0.44
3:C:464:ASP:O	4:Q:1:NAG:O4	2.36	0.44
3:C:1146:LYS:HE2	3:C:1149:LEU:HD12	1.99	0.44
1:I:39:ARG:HB2	1:I:49:ILE:HD11	1.99	0.44
1:I:88:ARG:HD3	1:I:88:ARG:N	2.32	0.44
3:A:560:GLN:O	3:A:574:ARG:NH1	2.50	0.44
3:A:700:ASN:OD1	3:A:701:SER:N	2.50	0.44
3:B:606:ALA:HA	3:B:633:TYR:OH	2.17	0.44
3:C:118:VAL:O	3:C:124:VAL:HA	2.18	0.44
3:C:212:ASP:O	3:C:213:LEU:C	2.60	0.44
1:H:12:LYS:HB2	1:H:122:VAL:HG22	1.99	0.44
3:A:95:LYS:HD3	3:A:182:LYS:H	1.83	0.44
3:B:134:CYS:HB3	6:B:1305:NAG:H83	1.98	0.44
3:B:622:HIS:HB3	3:B:625:GLN:OE1	2.17	0.44
3:C:108:LEU:HG	3:C:133:PHE:CD2	2.49	0.44
3:C:138:PHE:HD2	3:C:141:HIS:H	1.65	0.44
1:H:3:GLN:OE1	1:H:5:VAL:HG13	2.17	0.44
3:A:129:CYS:HB3	3:A:131:PHE:CZ	2.52	0.44
3:A:566:ILE:H	3:A:566:ILE:HD12	1.83	0.44
3:A:575:ASP:HB3	3:A:578:THR:O	2.17	0.44
1:G:102:CYS:HA	1:G:107:CYS:CB	2.45	0.44
1:I:37:TRP:CZ2	1:I:97:CYS:HB3	2.53	0.44
3:C:530:LEU:HD11	3:C:582:LEU:HD11	1.99	0.44
2:K:24:ARG:HA	2:K:24:ARG:HH11	1.82	0.44
2:L:34:LEU:HA	2:L:90:GLN:O	2.18	0.44
3:A:64:TRP:CZ3	3:A:66:HIS:HB2	2.52	0.44
4:X:1:NAG:O6	4:X:2:NAG:N2	2.49	0.44
2:L:11:LEU:HD13	2:L:105:VAL:HG12	2.00	0.44
3:A:1142:LEU:O	3:A:1146:LYS:HG2	2.17	0.44
3:B:284:ASP:OD1	3:B:285:ALA:N	2.51	0.44
3:C:198:ILE:HB	3:C:224:VAL:HG12	2.00	0.44
3:A:103:ILE:HD11	3:A:238:LEU:HD21	1.99	0.44
3:A:188:VAL:HG12	3:A:199:TYR:HB2	1.98	0.44
3:A:347:VAL:HG11	3:A:415:ILE:HD11	2.00	0.44
3:A:1100:PHE:HE1	3:A:1111:ILE:HD13	1.83	0.44
3:B:273:LEU:HB3	3:B:286:VAL:HG12	2.00	0.44
1:G:6:GLN:HG3	1:G:22:CYS:HB3	2.00	0.43
2:K:90:GLN:NE2	2:K:97:TRP:HB3	2.33	0.43
3:A:341:ALA:HB3	3:A:344:PHE:HE1	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:ASP:HA	3:C:240:ALA:HA	2.00	0.43
3:B:458:LEU:HD13	3:B:462:GLU:HB2	1.98	0.43
3:A:366:TYR:HD1	3:A:374:PHE:HE2	1.66	0.43
3:B:621:ILE:HG23	3:B:631:ARG:HB3	2.01	0.43
3:C:26:PRO:HB3	3:C:65:PHE:CE1	2.53	0.43
1:G:11:VAL:HA	1:G:121:THR:O	2.19	0.43
2:J:23:CYS:SG	2:J:72:PHE:HB2	2.58	0.43
2:L:47:LEU:HD23	2:L:48:LEU:N	2.34	0.43
3:A:97:ASN:ND2	3:A:172:MET:SD	2.85	0.43
3:A:274:LEU:HD23	3:A:282:ILE:HD12	1.99	0.43
3:B:1130:VAL:HG22	3:B:1131:ASN:H	1.84	0.43
3:C:458:LEU:HD22	4:Q:1:NAG:H61	1.99	0.43
3:B:95:LYS:HG2	3:B:177:LYS:HD3	2.00	0.43
3:B:189:PHE:CD1	3:B:198:ILE:HG23	2.52	0.43
3:C:719:VAL:HG22	3:C:1062:VAL:HG22	1.99	0.43
2:K:92:TYR:O	2:K:97:TRP:NE1	2.51	0.43
3:A:368:LEU:HD23	3:A:371:PHE:CE1	2.53	0.43
3:A:637:SER:HB3	3:A:649:GLY:HA2	2.01	0.43
3:B:192:ILE:O	3:B:195:TYR:HB2	2.18	0.43
3:C:1138:LEU:O	3:C:1142:LEU:N	2.51	0.43
2:K:47:LEU:HD22	2:K:56:ALA:HB2	2.00	0.43
2:L:38:GLN:O	2:L:46:ARG:HG2	2.19	0.43
3:B:641:GLN:OE1	3:B:646:CYS:HB3	2.18	0.43
3:C:756:PHE:CE2	3:C:757:CYS:HB3	2.53	0.43
1:G:48:TRP:CZ2	1:G:50:GLY:HA2	2.54	0.43
3:A:320:THR:OG1	3:A:534:LYS:NZ	2.35	0.43
3:C:184:LEU:HB3	3:C:203:THR:OG1	2.19	0.43
3:A:642:THR:OG1	3:A:645:GLY:O	2.35	0.43
3:A:1095:ASN:HD22	5:O:1:NAG:H83	1.84	0.43
3:B:317:VAL:HA	3:B:625:GLN:O	2.19	0.43
1:H:19:LYS:HA	1:H:82:MET:O	2.19	0.43
3:A:159:ASN:HD22	3:A:160:ASN:ND2	2.12	0.43
1:H:19:LYS:HD2	1:H:81:TYR:HB3	2.01	0.42
1:H:35:LEU:HB3	1:H:99:ALA:HB2	2.01	0.42
3:B:127:LYS:HA	3:B:163:PHE:O	2.18	0.42
3:C:374:PHE:CD1	3:C:431:ILE:HG12	2.53	0.42
3:A:109:ASP:N	3:A:109:ASP:OD1	2.51	0.42
3:A:129:CYS:HA	3:A:161:CYS:CB	2.49	0.42
3:B:191:ASN:ND2	3:B:232:ILE:HG13	2.33	0.42
3:B:226:LEU:HG	3:B:227:PRO:HD2	2.01	0.42
3:C:368:LEU:HD23	3:C:371:PHE:CE1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:52:THR:HG22	1:I:59:THR:HA	2.01	0.42
3:A:472:ALA:N	3:A:484:ASN:O	2.49	0.42
3:B:783:LYS:HA	3:B:783:LYS:HD2	1.77	0.42
3:C:543:LEU:HD23	3:C:570:THR:HG21	2.01	0.42
2:K:34:LEU:HA	2:K:90:GLN:O	2.19	0.42
3:A:104:PHE:HB2	3:A:115:LEU:HB2	2.01	0.42
3:A:578:THR:HG23	3:A:580:GLU:OE1	2.19	0.42
3:B:89:TYR:OH	3:B:186:GLU:OE2	2.36	0.42
3:C:100:ARG:HG3	3:C:139:LEU:HD13	2.01	0.42
3:C:565:ASP:OD1	3:C:565:ASP:N	2.51	0.42
2:J:49:ILE:HG21	2:J:65:ALA:HB2	2.01	0.42
3:B:79:ASN:N	3:B:80:PRO:HD3	2.34	0.42
3:B:434:ASN:HA	3:B:505:TYR:CD2	2.54	0.42
3:C:348:TYR:O	4:Q:2:NAG:H2	2.20	0.42
1:H:30:THR:HG23	1:H:31:ASP:N	2.34	0.42
2:K:37:TYR:O	2:K:87:TYR:HA	2.19	0.42
3:B:659:CYS:HB2	3:B:694:MET:HG2	2.02	0.42
3:B:746:CYS:SG	3:B:994:ILE:HD11	2.59	0.42
3:B:1149:LEU:HD11	3:C:1146:LYS:NZ	2.35	0.42
3:C:182:LYS:HD2	3:C:205:ILE:HA	2.02	0.42
1:I:48:TRP:CZ2	1:I:50:GLY:HA2	2.55	0.42
3:A:1149:LEU:HD21	3:B:1149:LEU:HD13	2.02	0.42
3:B:863:THR:HG23	3:B:866:MET:H	1.85	0.42
3:C:368:LEU:HD12	3:C:368:LEU:HA	1.84	0.42
3:C:1139:GLN:OE1	3:C:1142:LEU:HD11	2.20	0.42
3:A:131:PHE:HB3	3:A:155:TYR:HB2	2.01	0.42
3:A:641:GLN:HG2	6:A:1309:NAG:H83	1.78	0.42
3:A:767:ILE:O	3:A:771:GLN:HG2	2.19	0.42
3:C:347:VAL:HG22	3:C:399:ILE:HG22	2.01	0.42
3:A:866:MET:HE1	3:B:694:MET:HE2	2.01	0.42
3:B:400:ARG:HH21	3:B:402:ASP:HB2	1.84	0.42
3:C:68:ILE:HD11	3:C:76:ARG:HH21	1.85	0.42
3:C:144:ASN:HA	3:C:255:TRP:HA	2.02	0.42
1:H:74:ASP:O	1:H:78:SER:N	2.53	0.42
2:J:80:GLU:OE1	2:J:82:GLU:HG2	2.19	0.42
3:A:755:SER:O	3:A:759:GLN:HG2	2.20	0.42
3:A:106:THR:HA	3:A:233:THR:HG22	2.01	0.41
3:A:210:PRO:O	3:A:211:GLU:HB2	2.19	0.41
3:B:239:LEU:HD23	3:B:239:LEU:H	1.85	0.41
3:C:53:ASP:HB2	3:C:55:PHE:CE2	2.54	0.41
3:C:85:ASN:HD22	3:C:266:TYR:HE1	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:ILE:HG23	3:C:240:ALA:H	1.84	0.41
1:I:49:ILE:HG23	1:I:65:PHE:CD2	2.55	0.41
3:A:307:LYS:HG2	3:A:661:ILE:HD11	2.01	0.41
3:A:577:GLN:O	4:E:1:NAG:O3	2.32	0.41
3:B:93:ILE:HG12	3:B:184:LEU:HD13	2.01	0.41
3:B:919:LEU:HD11	4:S:1:NAG:H3	2.02	0.41
2:K:5:THR:HG23	2:K:101:GLN:HE22	1.84	0.41
3:A:139:LEU:HB2	3:A:240:ALA:HB2	2.01	0.41
3:C:109:ASP:N	3:C:109:ASP:OD1	2.51	0.41
3:C:196:PHE:HD2	3:C:226:LEU:HD12	1.86	0.41
3:C:710:ALA:HA	3:C:1071:ASN:HA	2.03	0.41
3:A:1078:ILE:HD12	3:A:1130:VAL:O	2.21	0.41
3:B:324:VAL:O	3:B:527:SER:HA	2.21	0.41
3:C:399:ILE:HD11	3:C:404:VAL:HA	2.01	0.41
1:I:92:THR:HB	1:I:121:THR:HA	2.02	0.41
1:I:94:VAL:HG22	1:I:119:LYS:HD3	2.01	0.41
3:B:37:TYR:OH	3:B:54:LEU:O	2.25	0.41
3:B:579:LEU:HD21	4:R:2:NAG:H83	2.01	0.41
3:B:710:ALA:HA	3:B:1071:ASN:HA	2.02	0.41
3:C:301:LYS:HD3	3:C:301:LYS:HA	1.80	0.41
3:C:1078:ILE:HD11	3:C:1132:ASN:CB	2.50	0.41
1:I:49:ILE:HG23	1:I:65:PHE:HD2	1.85	0.41
3:A:1079:CYS:HB2	3:A:1123:CYS:HB2	1.89	0.41
3:B:354:ARG:HH11	3:B:393:TYR:HE1	1.69	0.41
3:B:641:GLN:NE2	3:B:642:THR:O	2.53	0.41
3:C:902:ARG:NH1	3:C:1046:LEU:O	2.53	0.41
1:H:37:TRP:CZ3	1:H:97:CYS:HB3	2.56	0.41
2:L:91:GLN:NE2	2:L:97:TRP:CD1	2.89	0.41
3:A:330:THR:O	3:A:359:VAL:HB	2.21	0.41
3:B:451:ARG:NE	3:B:464:ASP:OD2	2.54	0.41
3:B:797:PHE:HD2	3:B:924:PHE:CD2	2.39	0.41
3:C:33:THR:O	3:C:33:THR:HG22	2.21	0.41
3:C:615:THR:C	3:C:618:PRO:HD2	2.46	0.41
3:A:655:ASN:OD1	3:A:655:ASN:N	2.53	0.41
3:B:14:GLN:NE2	3:B:15:CYS:O	2.54	0.41
3:B:866:MET:HG2	3:C:696:LEU:HD21	2.03	0.41
3:C:797:PHE:HD2	3:C:924:PHE:CD2	2.39	0.41
3:C:930:LYS:HE2	3:C:930:LYS:HB2	1.87	0.41
1:G:6:GLN:H	1:G:116:GLN:NE2	2.18	0.41
1:G:37:TRP:CZ2	1:G:82:MET:HE2	2.55	0.41
1:H:6:GLN:H	1:H:116:GLN:NE2	2.15	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:92:TYR:C	2:L:97:TRP:HE1	2.28	0.41
3:A:26:PRO:HB3	3:A:65:PHE:CE1	2.56	0.41
3:A:559:PHE:CD2	3:C:41:LYS:HE3	2.56	0.41
3:B:227:PRO:HB2	3:C:354:ARG:NH2	2.36	0.41
3:B:461:PHE:CB	6:B:1301:NAG:H83	2.46	0.41
3:B:733:VAL:HG11	3:B:1001:LEU:HD21	2.03	0.41
3:C:141:HIS:HB2	3:C:252:SER:O	2.21	0.41
3:C:191:ASN:OD1	3:C:191:ASN:N	2.54	0.41
1:G:40:GLN:O	1:G:93:ALA:HB1	2.21	0.40
1:I:109:ASP:OD2	3:C:475:LYS:HG2	2.20	0.40
3:A:330:THR:O	3:A:331:ASN:C	2.64	0.40
3:C:292:PRO:HG2	3:C:605:VAL:HG21	2.01	0.40
3:C:514:LEU:O	3:C:516:HIS:ND1	2.54	0.40
1:I:40:GLN:O	1:I:93:ALA:HB1	2.21	0.40
3:A:357:ASN:H	3:A:520:THR:HB	1.85	0.40
3:A:1130:VAL:HG22	3:A:1131:ASN:H	1.86	0.40
3:A:1138:LEU:HD23	3:A:1142:LEU:HD23	2.03	0.40
3:B:113:GLN:H	3:C:463:ARG:NH2	2.14	0.40
3:C:1071:ASN:HD21	4:a:1:NAG:H4	1.86	0.40
1:G:74:ASP:HB3	1:G:79:THR:HG22	2.03	0.40
1:H:23:LYS:HA	1:H:23:LYS:HE2	2.04	0.40
1:I:56:THR:HG23	1:I:58:ASN:H	1.86	0.40
3:A:366:TYR:HD1	3:A:374:PHE:CE2	2.39	0.40
3:C:178:GLN:NE2	3:C:257:ALA:O	2.54	0.40
2:L:21:LEU:HD12	2:L:87:TYR:HD2	1.86	0.40
3:A:565:ASP:OD1	3:A:565:ASP:N	2.54	0.40
3:C:637:SER:HB3	3:C:649:GLY:HA2	2.02	0.40
3:C:1047:MET:HE2	3:C:1049:PHE:CZ	2.55	0.40
2:L:95:SER:O	2:L:96:PRO:C	2.64	0.40
3:A:142:LYS:HD3	3:A:150:SER:HB2	2.04	0.40
3:C:191:ASN:HB2	3:C:196:PHE:HD1	1.87	0.40
3:C:324:VAL:H	3:C:528:THR:HG22	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
1	H	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
1	I	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
2	J	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	K	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	L	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
3	A	1088/1270 (86%)	1015 (93%)	72 (7%)	1 (0%)	48	75
3	B	1088/1270 (86%)	1013 (93%)	74 (7%)	1 (0%)	48	75
3	C	1088/1270 (86%)	1005 (92%)	80 (7%)	3 (0%)	36	65
All	All	3942/4500 (88%)	3675 (93%)	262 (7%)	5 (0%)	49	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	211	GLU
3	C	143	ASN
3	C	329	ILE
3	B	142	LYS
3	C	576	PRO

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	105/106 (99%)	105 (100%)	0	100	100
1	H	105/106 (99%)	105 (100%)	0	100	100
1	I	105/106 (99%)	105 (100%)	0	100	100
2	J	87/90 (97%)	87 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	87/90 (97%)	86 (99%)	1 (1%)	65	76
2	L	87/90 (97%)	87 (100%)	0	100	100
3	A	964/1112 (87%)	962 (100%)	2 (0%)	87	88
3	B	964/1112 (87%)	963 (100%)	1 (0%)	88	90
3	C	964/1112 (87%)	959 (100%)	5 (0%)	81	83
All	All	3468/3924 (88%)	3459 (100%)	9 (0%)	84	86

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

Mol	Chain	Res	Type
2	K	39	GLN
3	A	305	VAL
3	A	329	ILE
3	B	386	ASP
3	C	255	TRP
3	C	324	VAL
3	C	328	ASN
3	C	329	ILE
3	C	576	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	36	GLN
1	H	66	GLN
1	I	36	GLN
2	J	39	GLN
2	K	38	GLN
3	A	30	ASN
3	A	159	ASN
3	A	411	GLN
3	A	916	ASN
3	A	962	GLN
3	A	1098	HIS
3	A	1156	HIS
3	B	183	ASN
3	B	351	ASN
3	B	541	ASN
3	B	916	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	962	GLN
3	C	23	GLN
3	C	49	HIS
3	C	85	ASN
3	C	419	ASN
3	C	916	ASN
3	C	1116	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 ⓘ

47 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	$\# Z > 2$
4	NAG	D	1	4,3	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	E	1	4	14,14,15	0.91	1 (7%)	17,19,21	2.10	1 (5%)
4	NAG	E	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	F	1	4,3	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	M	1	4,3	14,14,15	0.25	0	17,19,21	0.35	0
4	NAG	M	2	4	14,14,15	0.93	1 (7%)	17,19,21	1.25	1 (5%)
4	NAG	N	1	4,3	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	N	2	4	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	O	1	3,5	14,14,15	0.29	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	O	2	5	14,14,15	0.27	0	17,19,21	0.45	0
5	BMA	O	3	5	11,11,12	0.55	0	15,15,17	0.70	0
4	NAG	P	1	4,3	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	P	2	4	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	Q	1	4	14,14,15	0.72	0	17,19,21	0.61	0
4	NAG	Q	2	4	14,14,15	0.47	0	17,19,21	1.31	2 (11%)
4	NAG	R	1	4	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	R	2	4	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	S	1	4,3	14,14,15	0.29	0	17,19,21	0.95	1 (5%)
4	NAG	S	2	4	14,14,15	0.64	0	17,19,21	0.62	0
4	NAG	T	1	4	14,14,15	0.44	0	17,19,21	1.34	2 (11%)
4	NAG	T	2	4	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	U	1	4,3	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	U	2	4	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	V	1	3,5	14,14,15	0.39	0	17,19,21	0.44	0
5	NAG	V	2	5	14,14,15	0.24	0	17,19,21	0.42	0
5	BMA	V	3	5	11,11,12	0.52	0	15,15,17	0.70	0
5	NAG	W	1	3,5	14,14,15	0.22	0	17,19,21	0.46	0
5	NAG	W	2	5	14,14,15	0.21	0	17,19,21	0.46	0
5	BMA	W	3	5	11,11,12	0.54	0	15,15,17	0.68	0
4	NAG	X	1	4,3	14,14,15	0.24	0	17,19,21	0.75	1 (5%)
4	NAG	X	2	4	14,14,15	0.26	0	17,19,21	0.62	0
4	NAG	Y	1	4	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	Y	2	4	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	Z	1	4,3	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	Z	2	4	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	a	1	4	14,14,15	0.43	0	17,19,21	1.37	2 (11%)
4	NAG	a	2	4	14,14,15	0.32	0	17,19,21	0.42	0
4	NAG	b	1	4,3	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	b	2	4	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	c	1	3,5	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	c	2	5	14,14,15	0.23	0	17,19,21	0.41	0
5	BMA	c	3	5	11,11,12	0.53	0	15,15,17	0.71	0
5	NAG	d	1	3,5	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	d	2	5	14,14,15	0.22	0	17,19,21	0.45	0
5	BMA	d	3	5	11,11,12	0.55	0	15,15,17	0.67	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
4	NAG	D	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
5	NAG	O	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
4	NAG	P	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	R	1	4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	4	-	6/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
5	NAG	V	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	BMA	V	3	5	-	1/2/19/22	0/1/1/1
5	NAG	W	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
4	NAG	X	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Z	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	0/6/23/26	0/1/1/1
4	NAG	a	1	4	-	6/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	b	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
5	NAG	c	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	BMA	c	3	5	-	1/2/19/22	0/1/1/1
5	NAG	d	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
5	BMA	d	3	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	2	NAG	O5-C1	3.32	1.49	1.43
4	E	1	NAG	C1-C2	2.22	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C2-N2-C7	-7.91	112.30	122.90
4	M	2	NAG	C1-O5-C5	4.90	118.75	112.19
4	a	1	NAG	C2-N2-C7	4.65	129.13	122.90
4	T	1	NAG	C2-N2-C7	4.58	129.04	122.90
4	Q	2	NAG	C1-O5-C5	4.38	118.06	112.19
4	S	1	NAG	C1-O5-C5	2.85	116.00	112.19
4	X	1	NAG	C1-O5-C5	2.29	115.25	112.19
4	Q	2	NAG	C3-C4-C5	-2.29	106.09	110.23
4	a	1	NAG	C1-C2-N2	2.23	113.95	110.43
4	T	1	NAG	C1-C2-N2	2.19	113.88	110.43

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	T	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	a	1	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	a	1	NAG	C8-C7-N2-C2
4	a	1	NAG	O7-C7-N2-C2
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	c	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

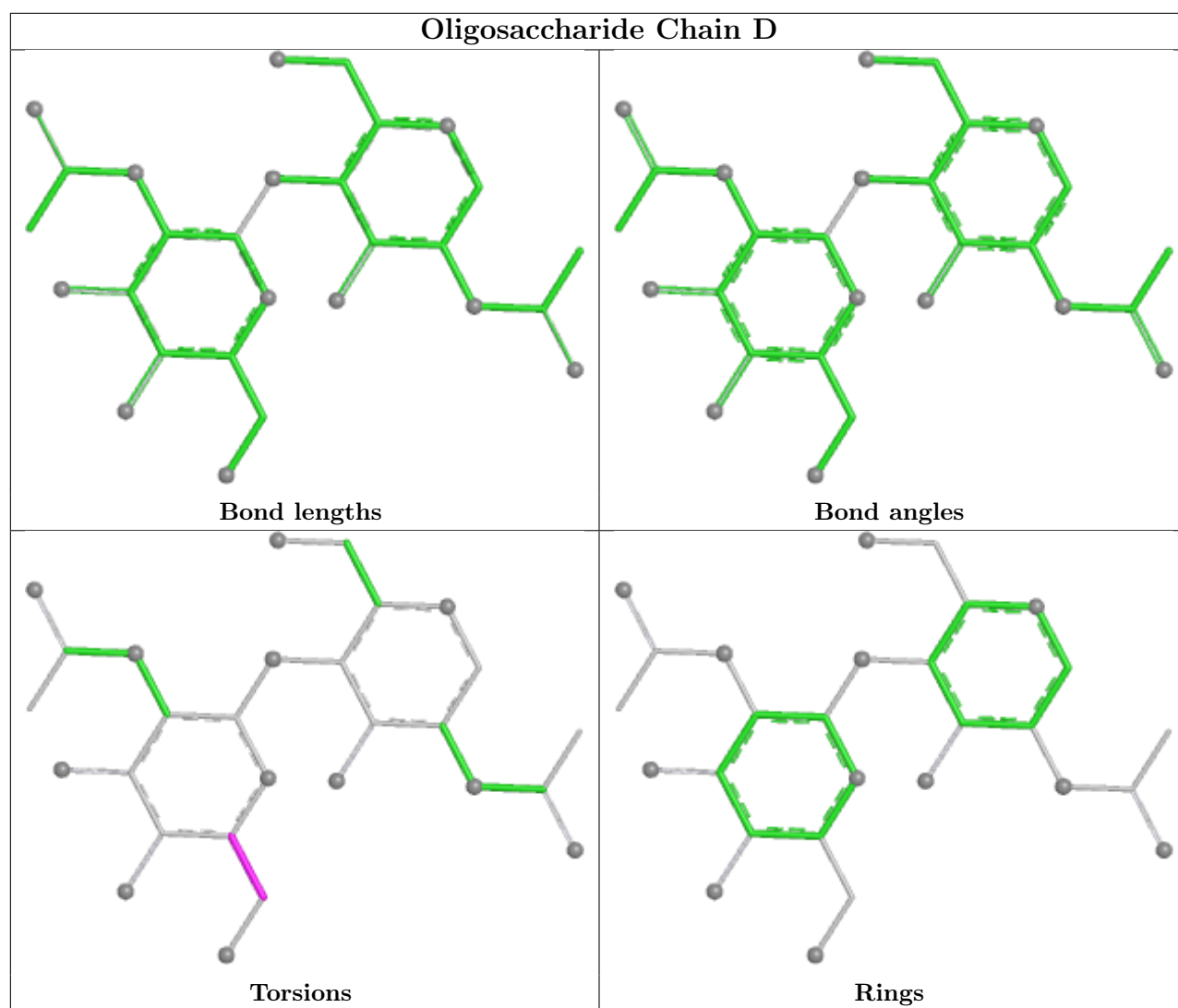
Mol	Chain	Res	Type	Atoms
4	U	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
4	T	1	NAG	C1-C2-N2-C7
4	a	1	NAG	C1-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	a	1	NAG	C3-C2-N2-C7
5	V	2	NAG	O5-C5-C6-O6
5	O	3	BMA	C4-C5-C6-O6

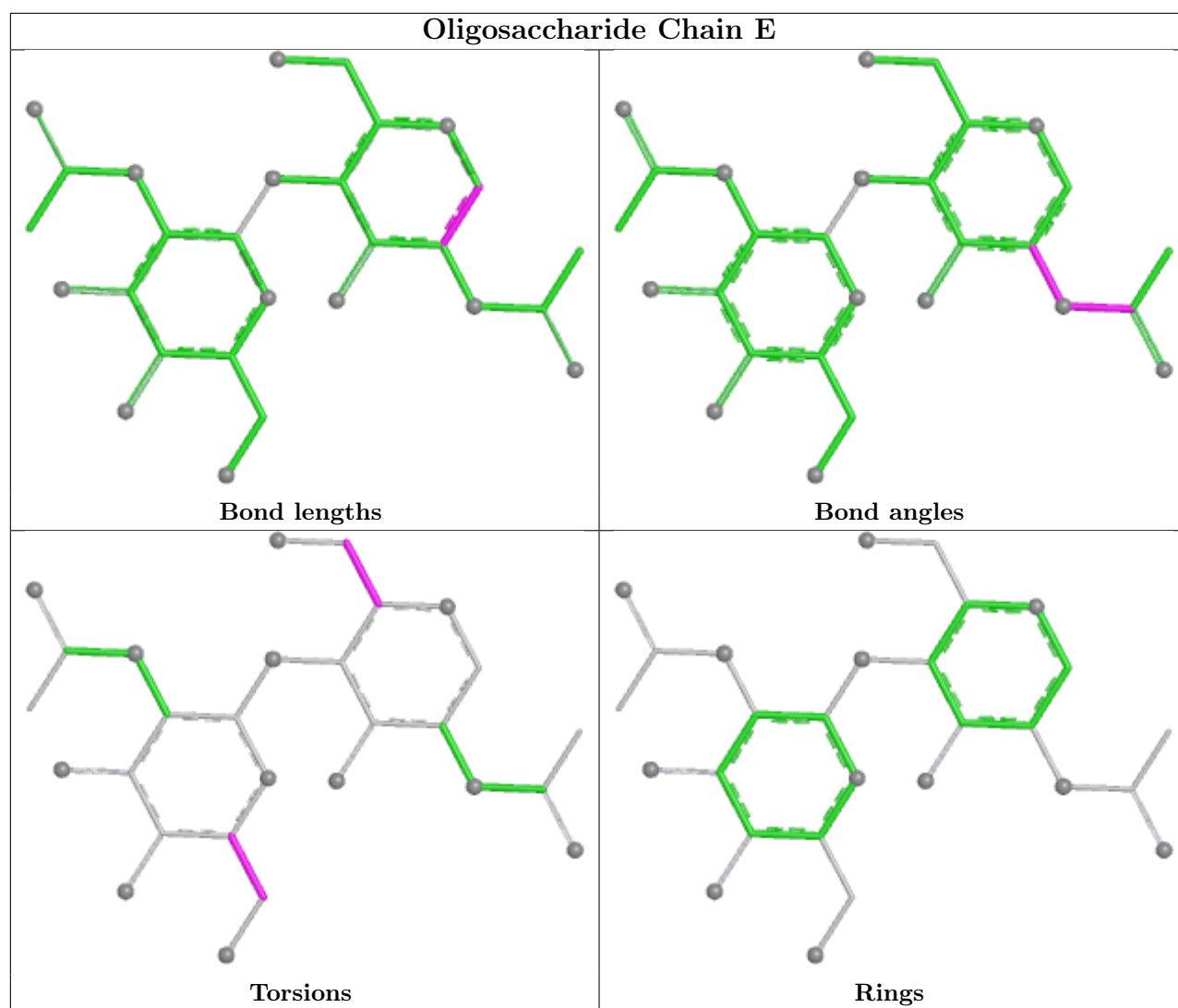
There are no ring outliers.

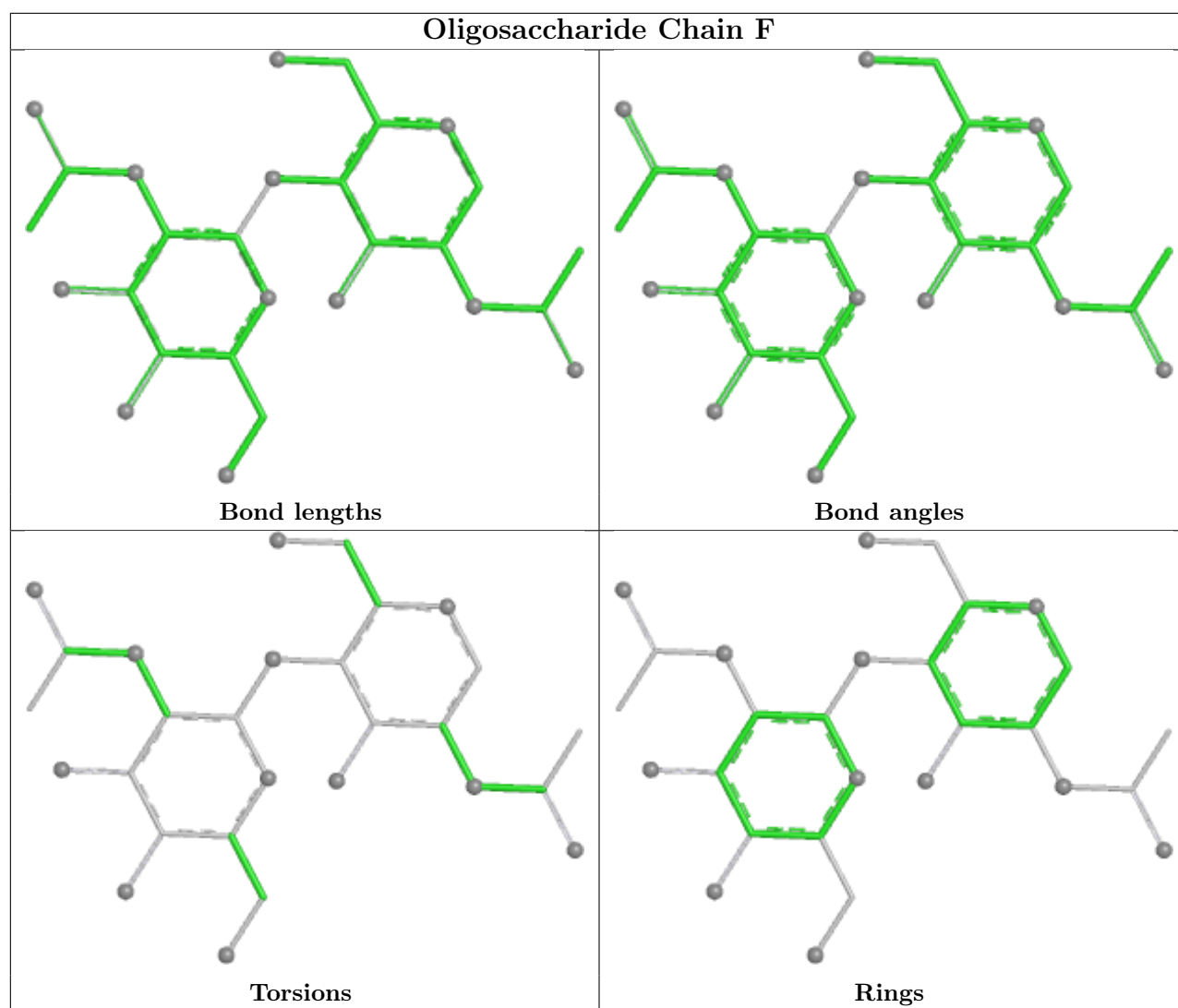
15 monomers are involved in 25 short contacts:

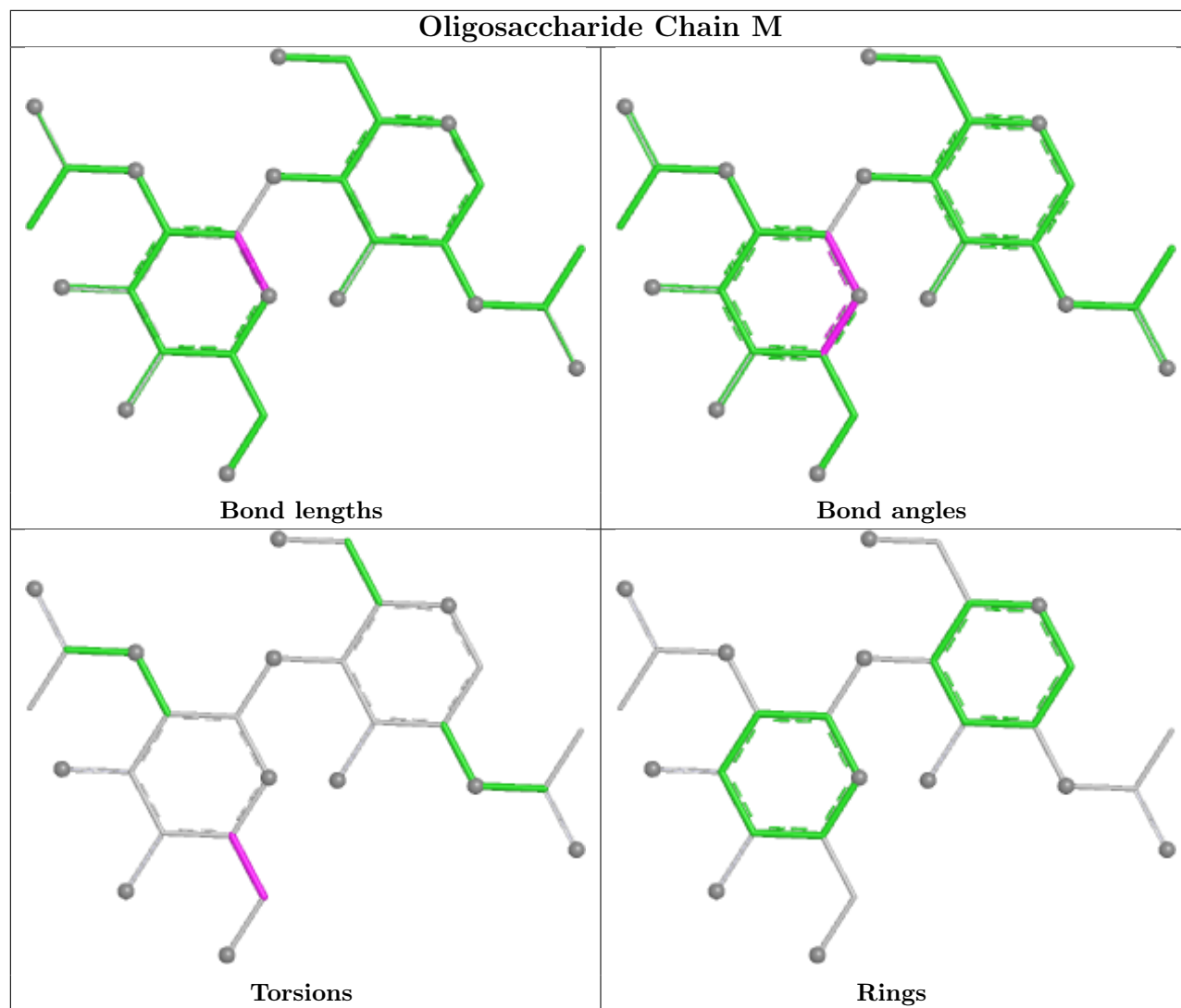
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
4	X	1	NAG	1	0
4	Q	1	NAG	5	0
4	T	1	NAG	1	0
4	M	2	NAG	1	0
5	V	1	NAG	1	0
4	X	2	NAG	4	0
4	E	1	NAG	4	0
4	R	2	NAG	1	0
4	S	1	NAG	1	0
5	c	1	NAG	1	0
4	M	1	NAG	1	0
4	Q	2	NAG	2	0
5	O	1	NAG	1	0
4	a	1	NAG	2	0

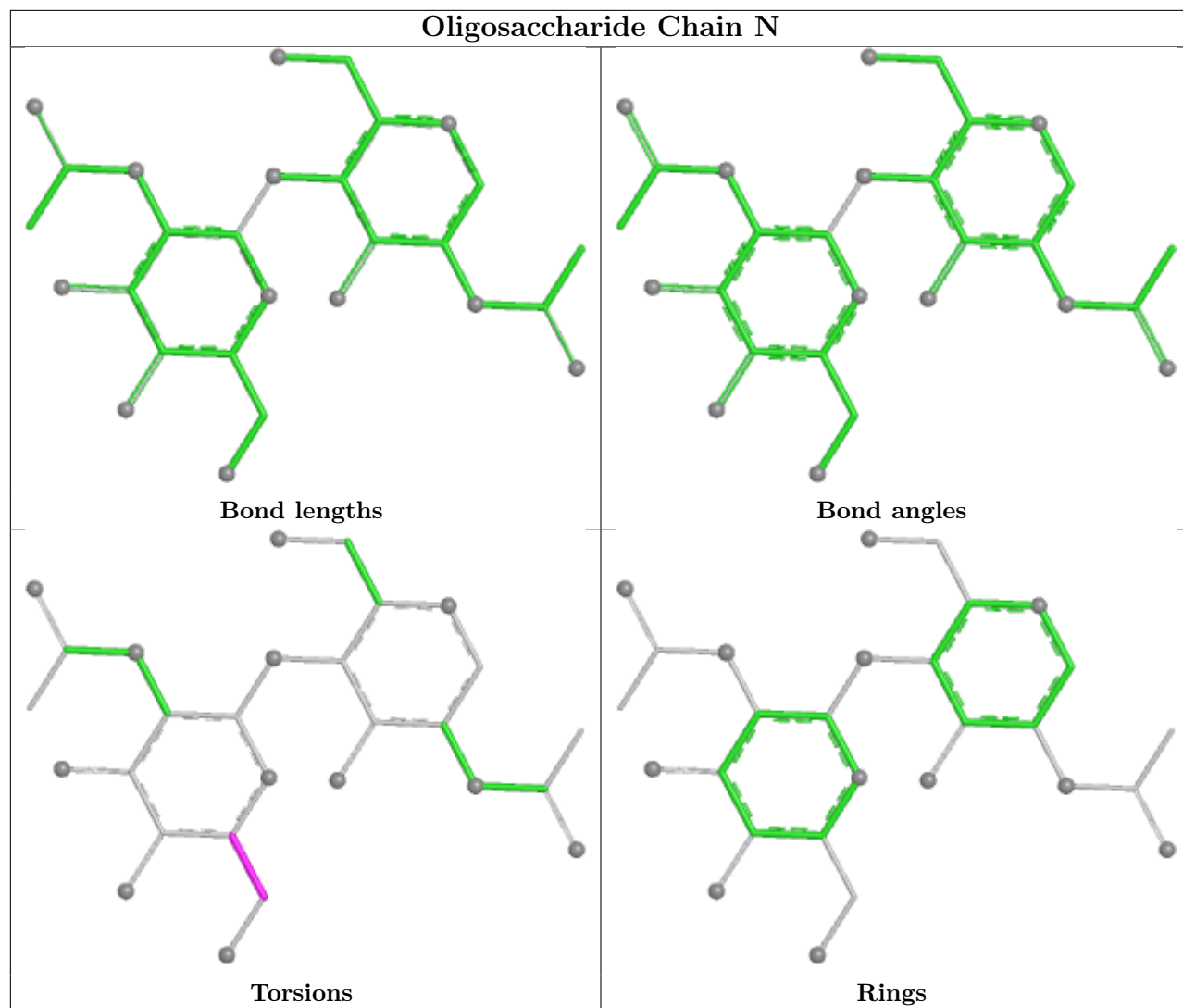
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

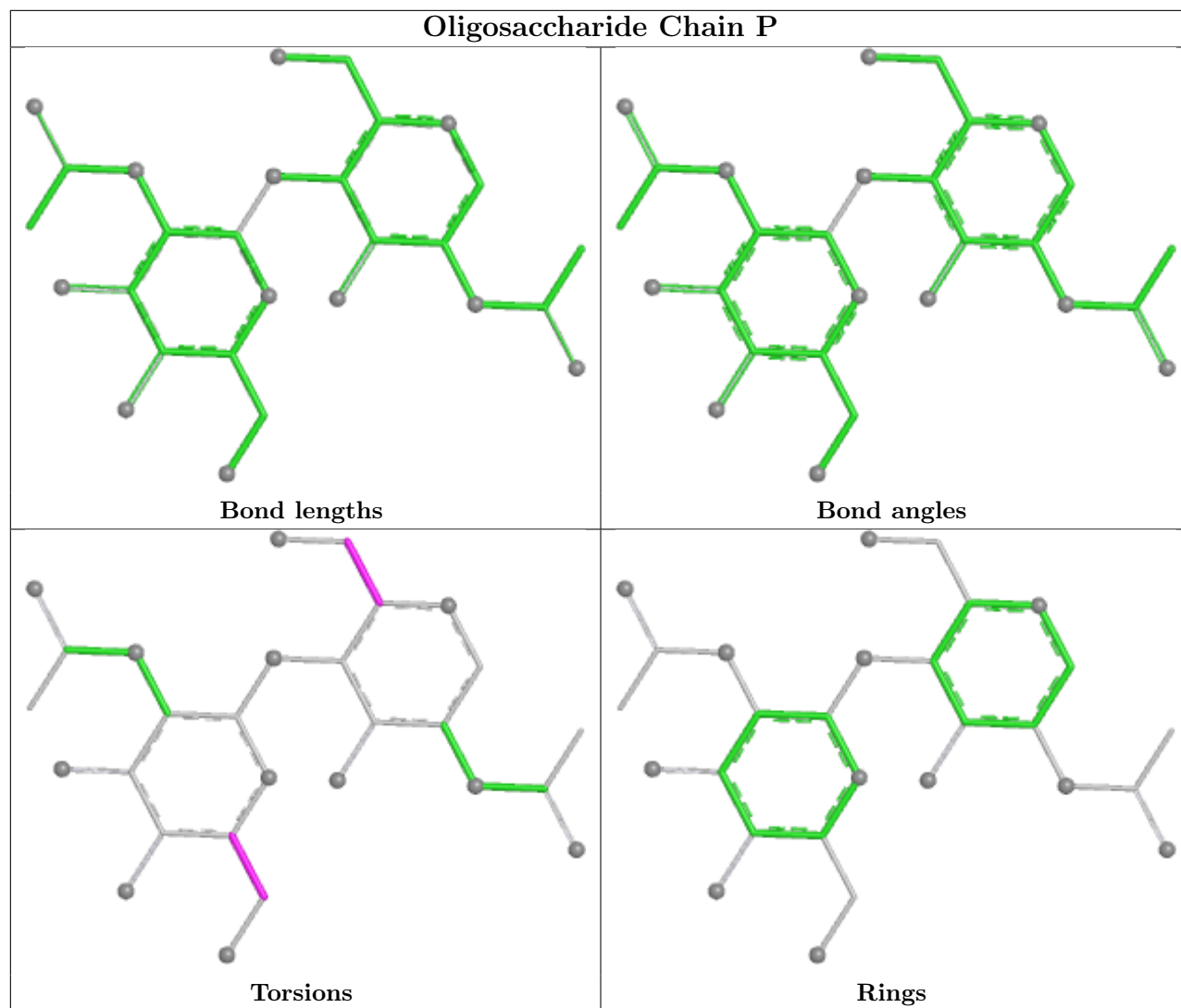


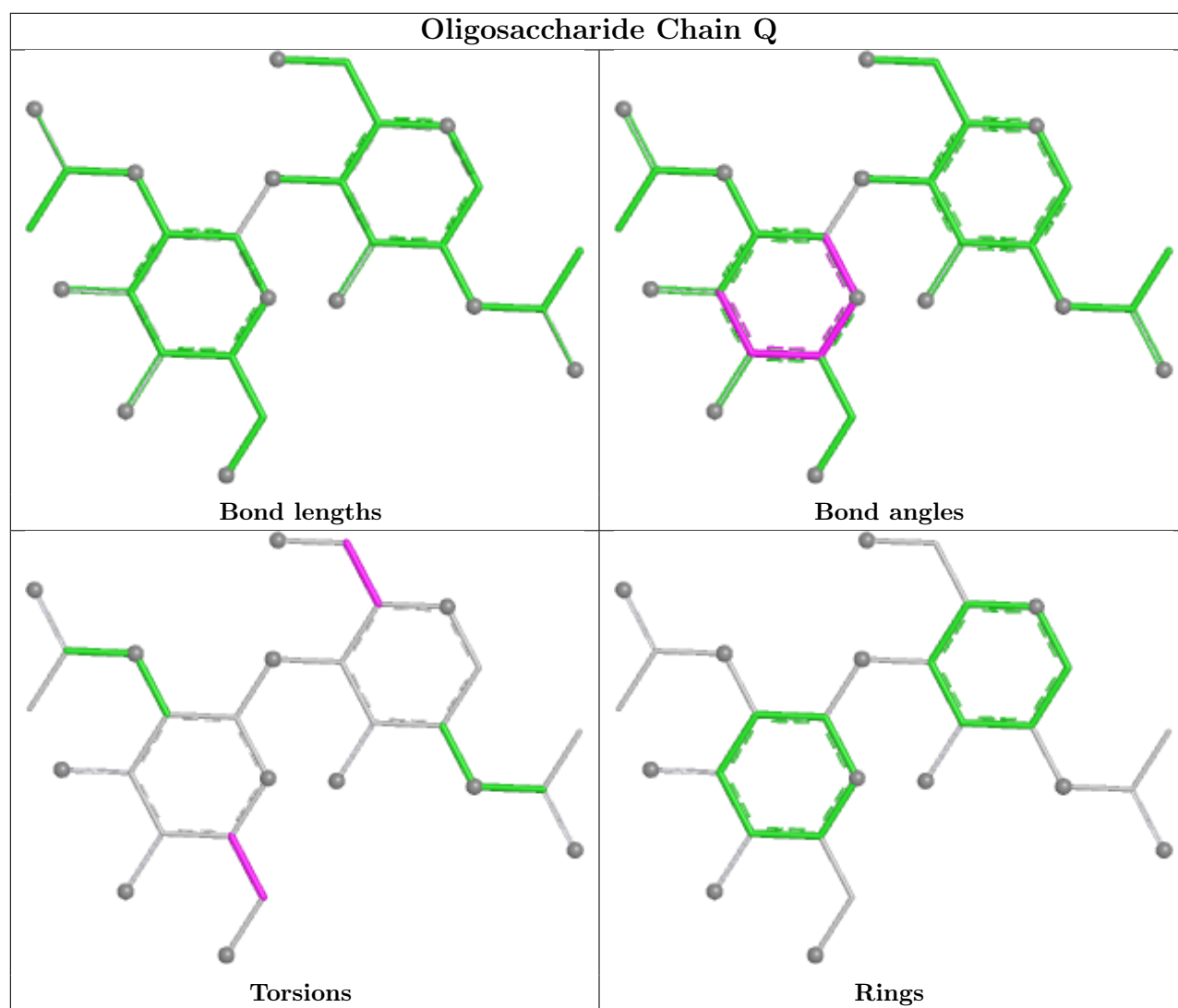


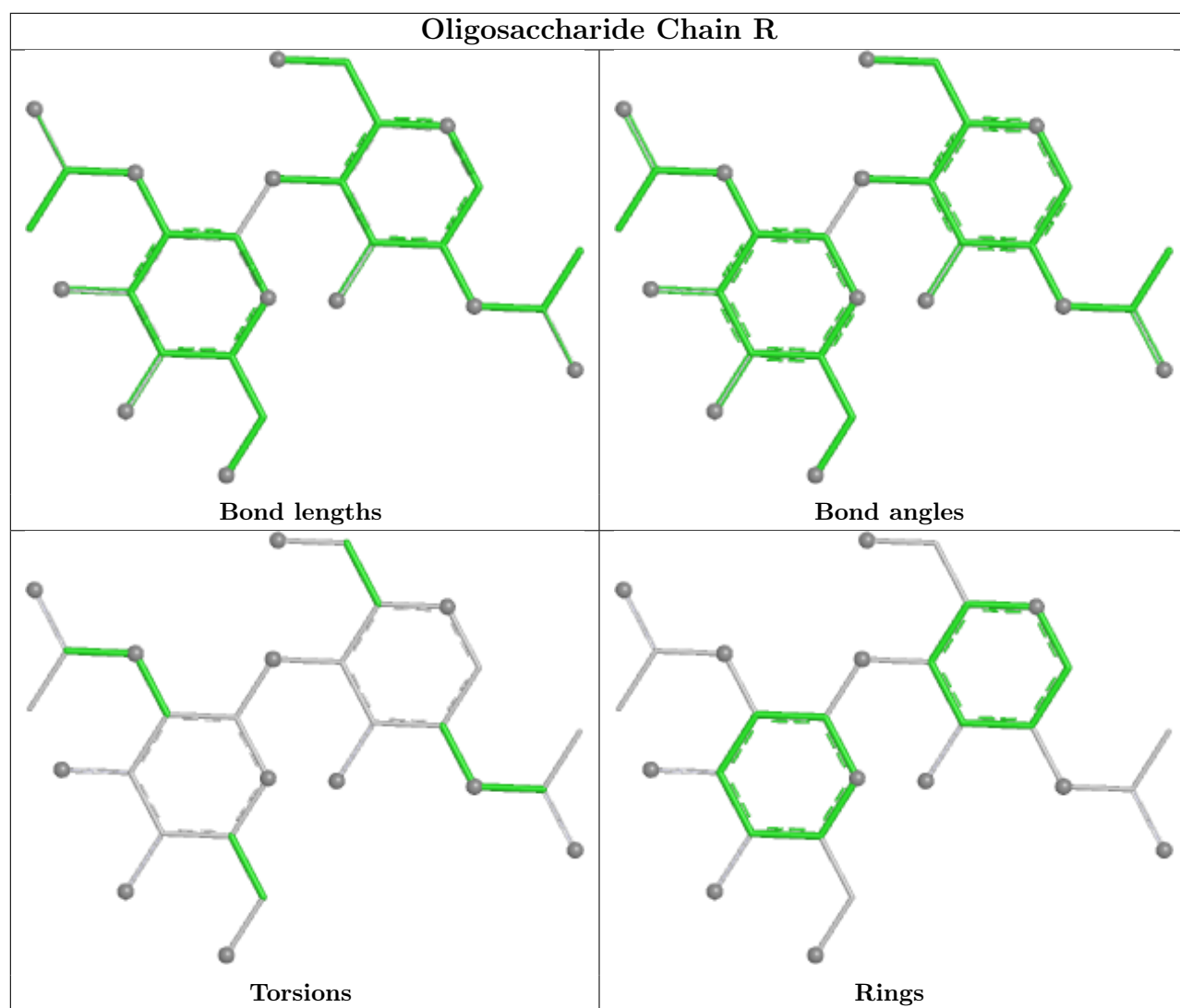


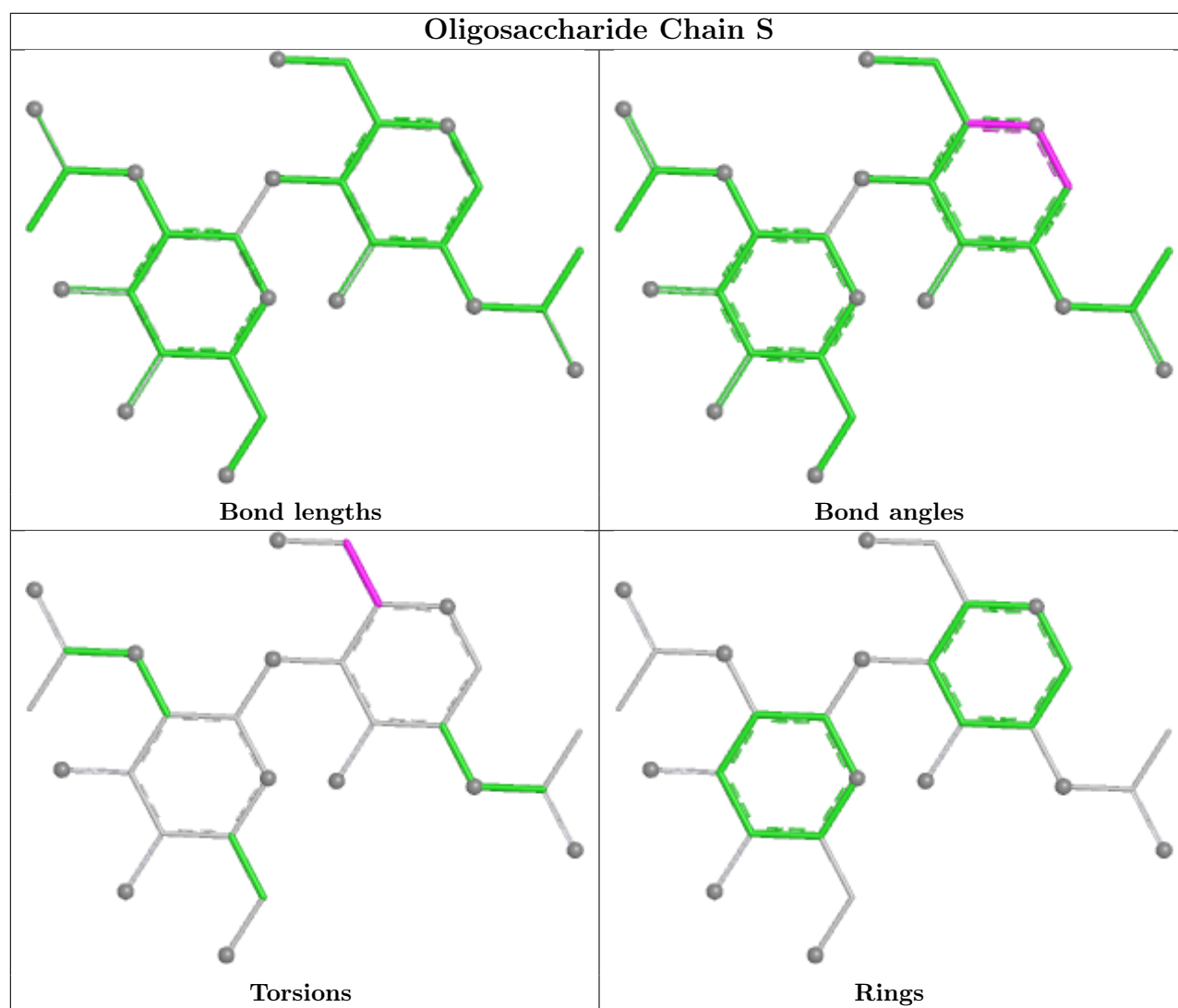


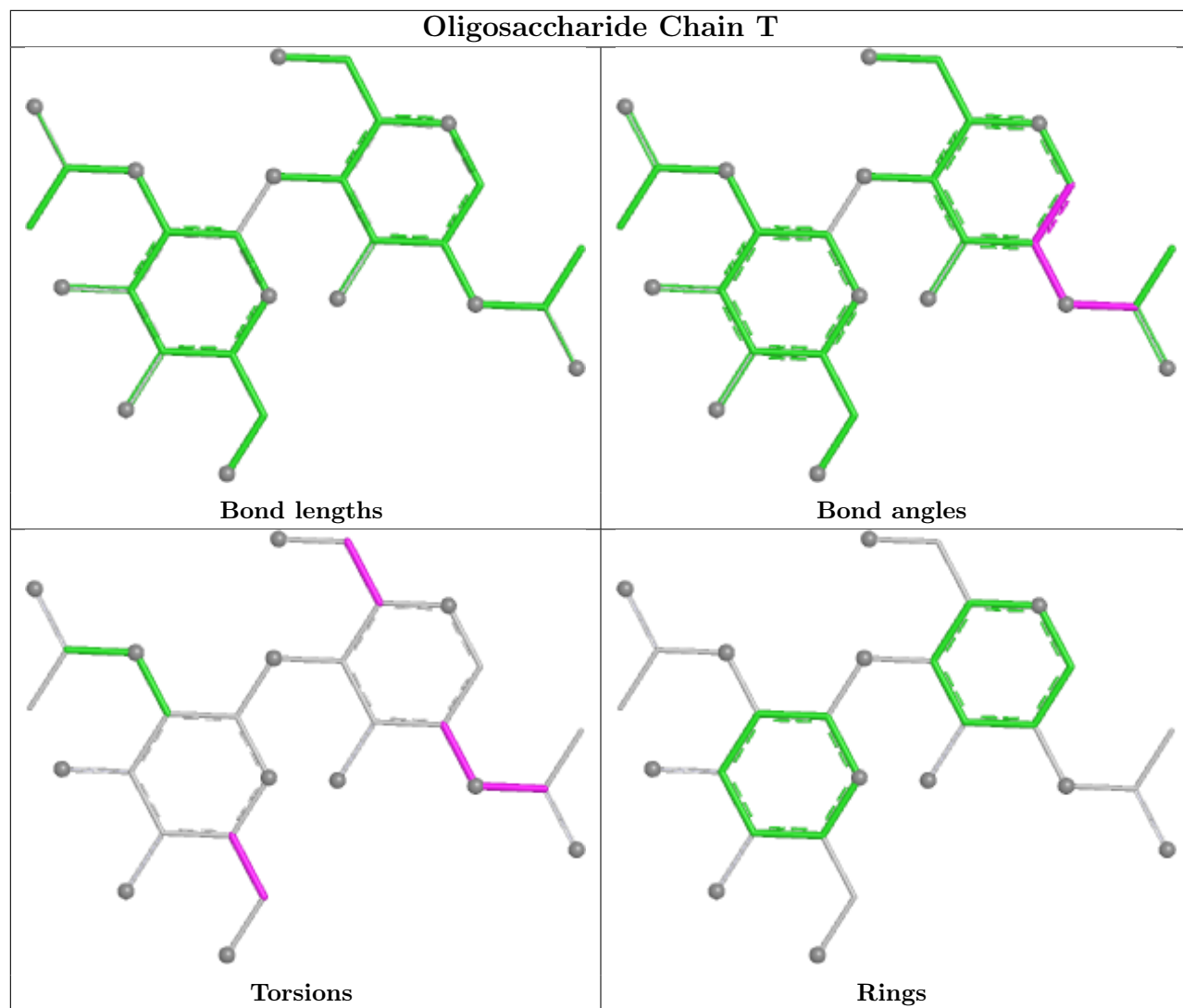


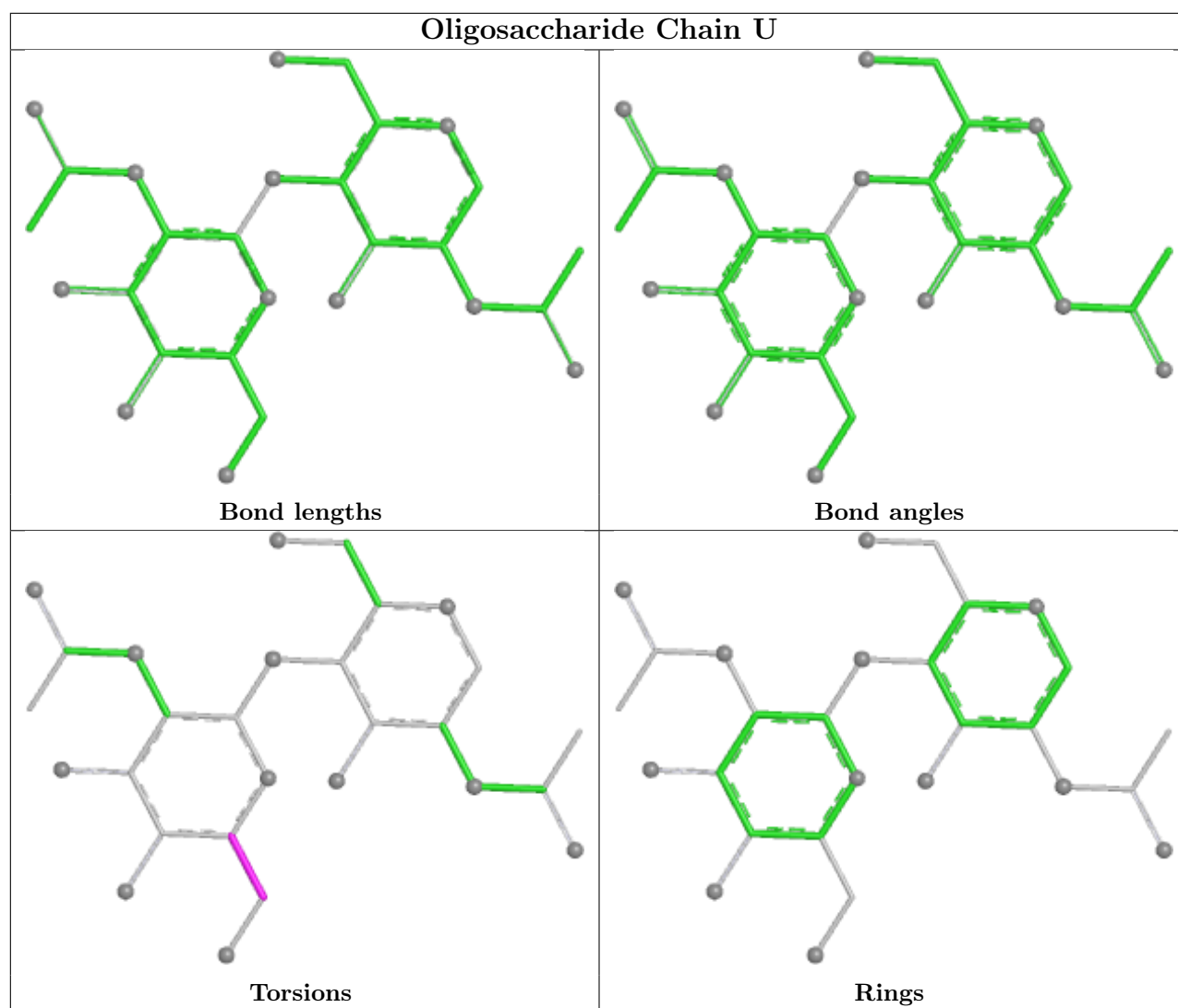


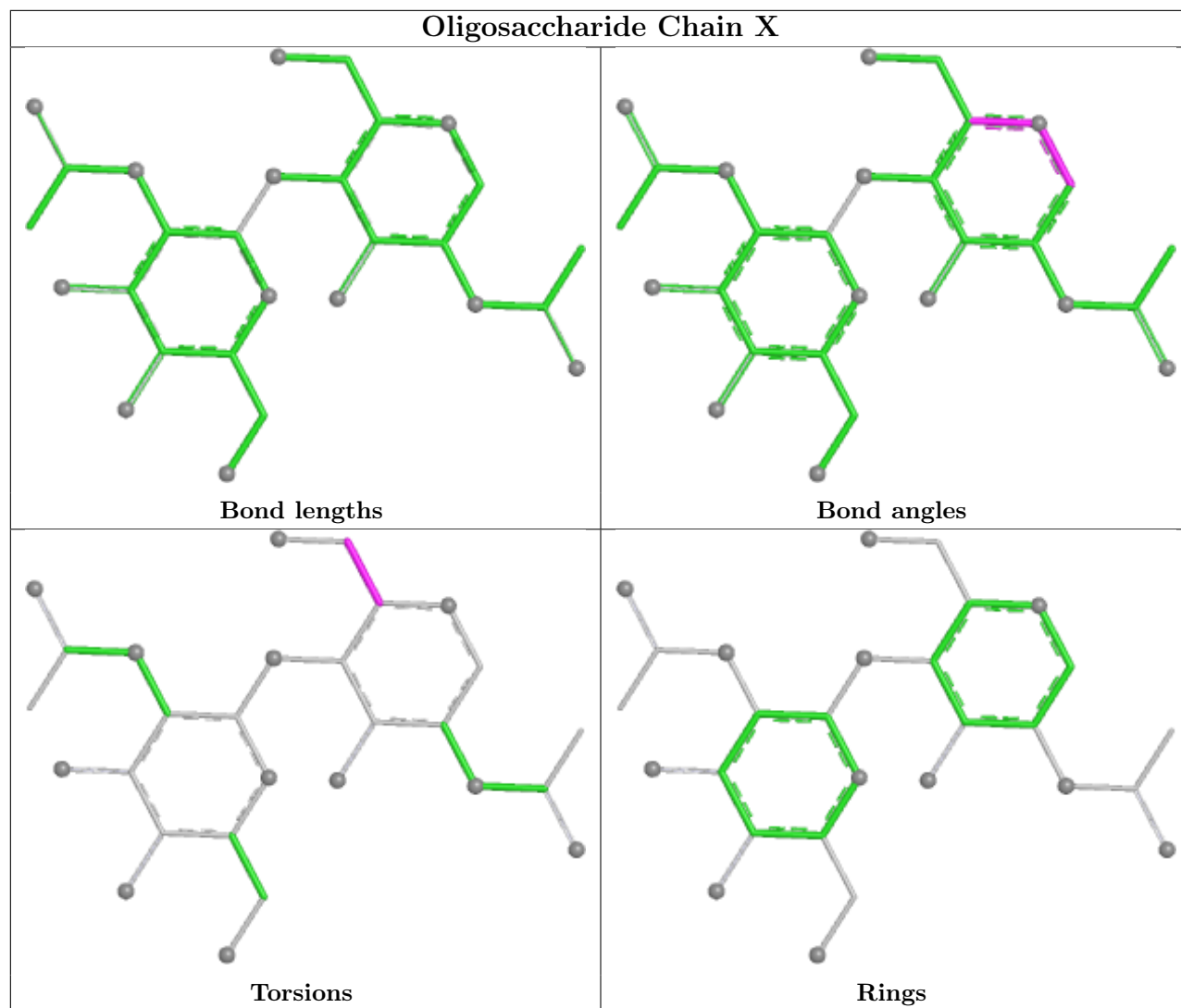


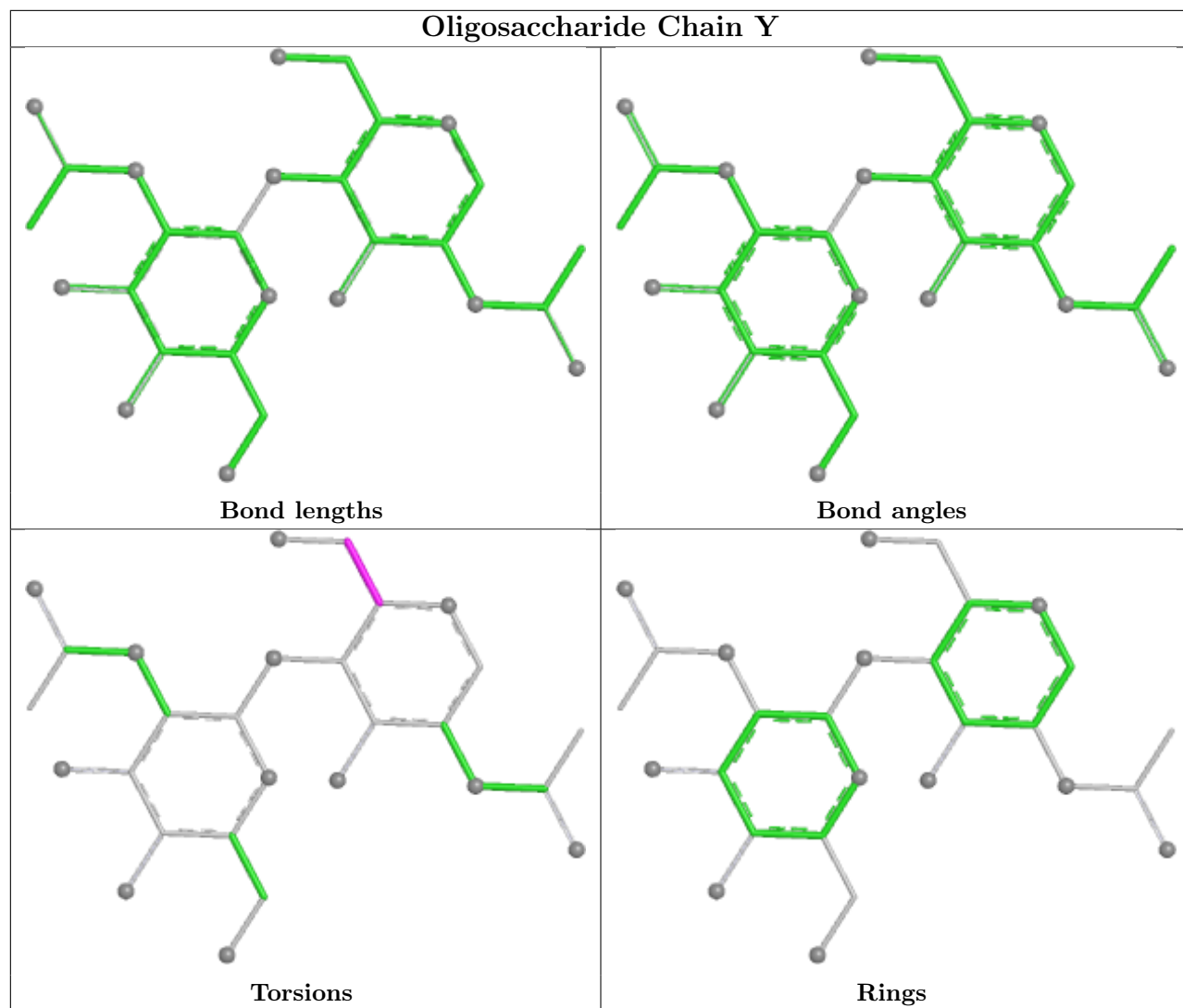


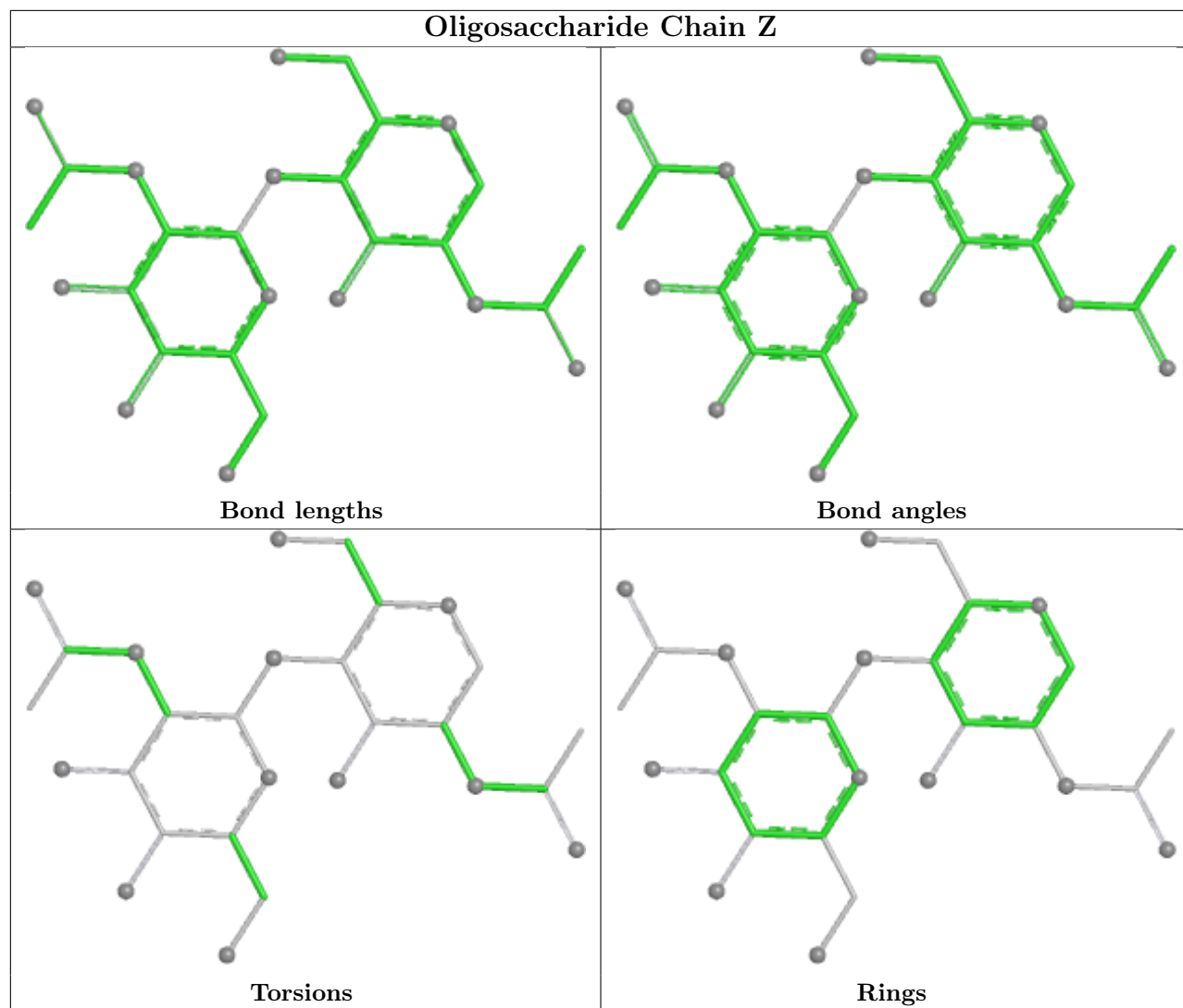


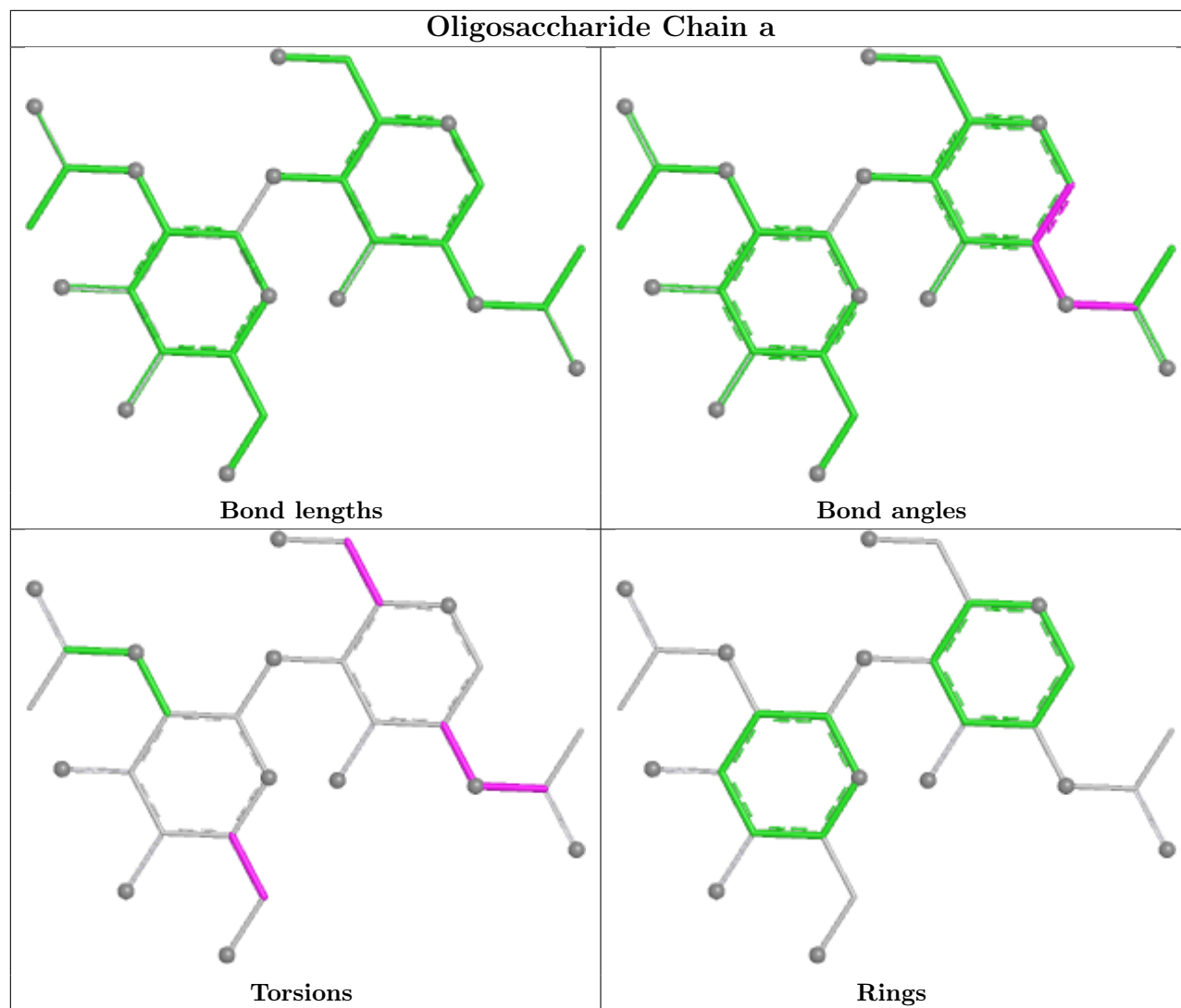


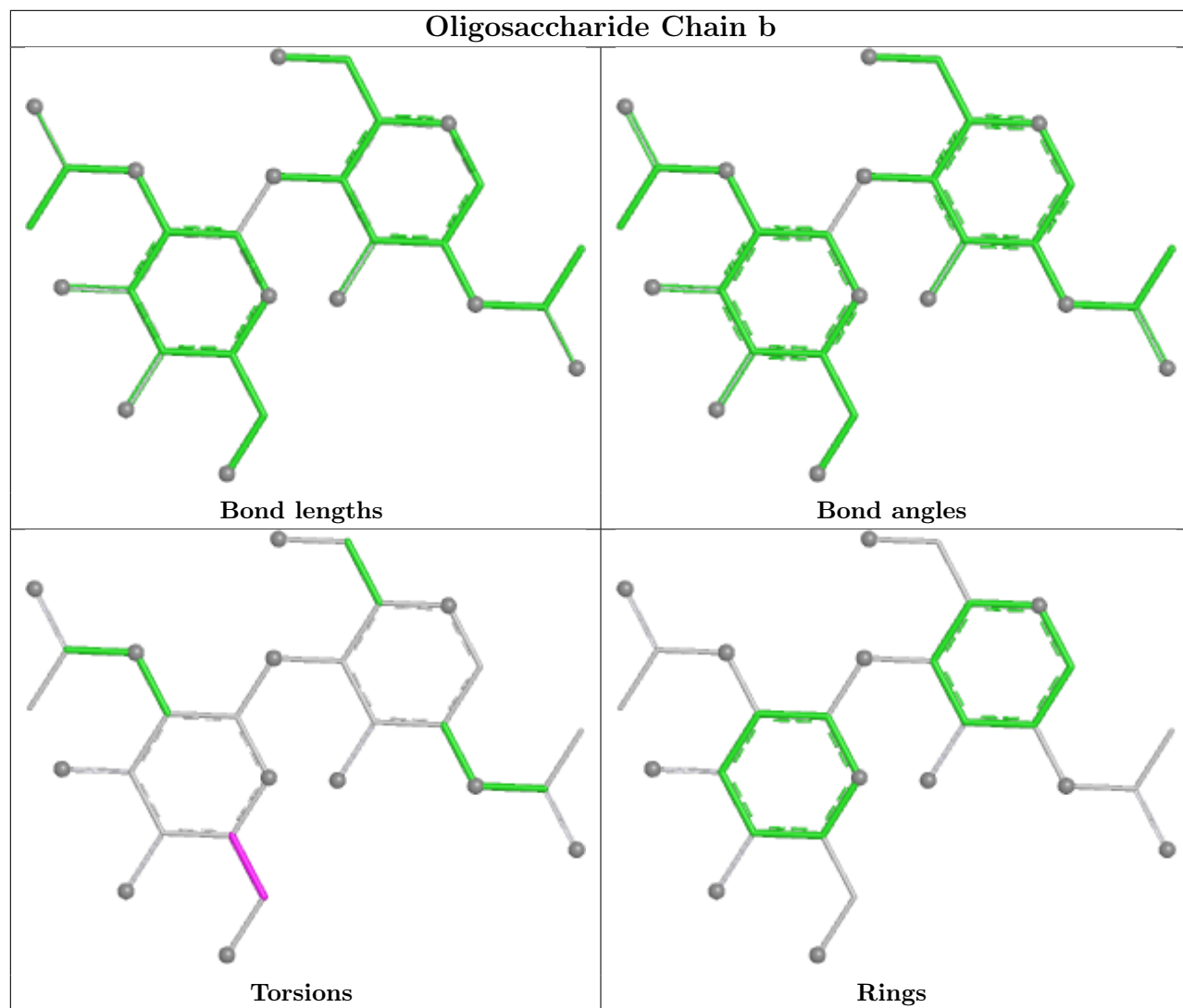


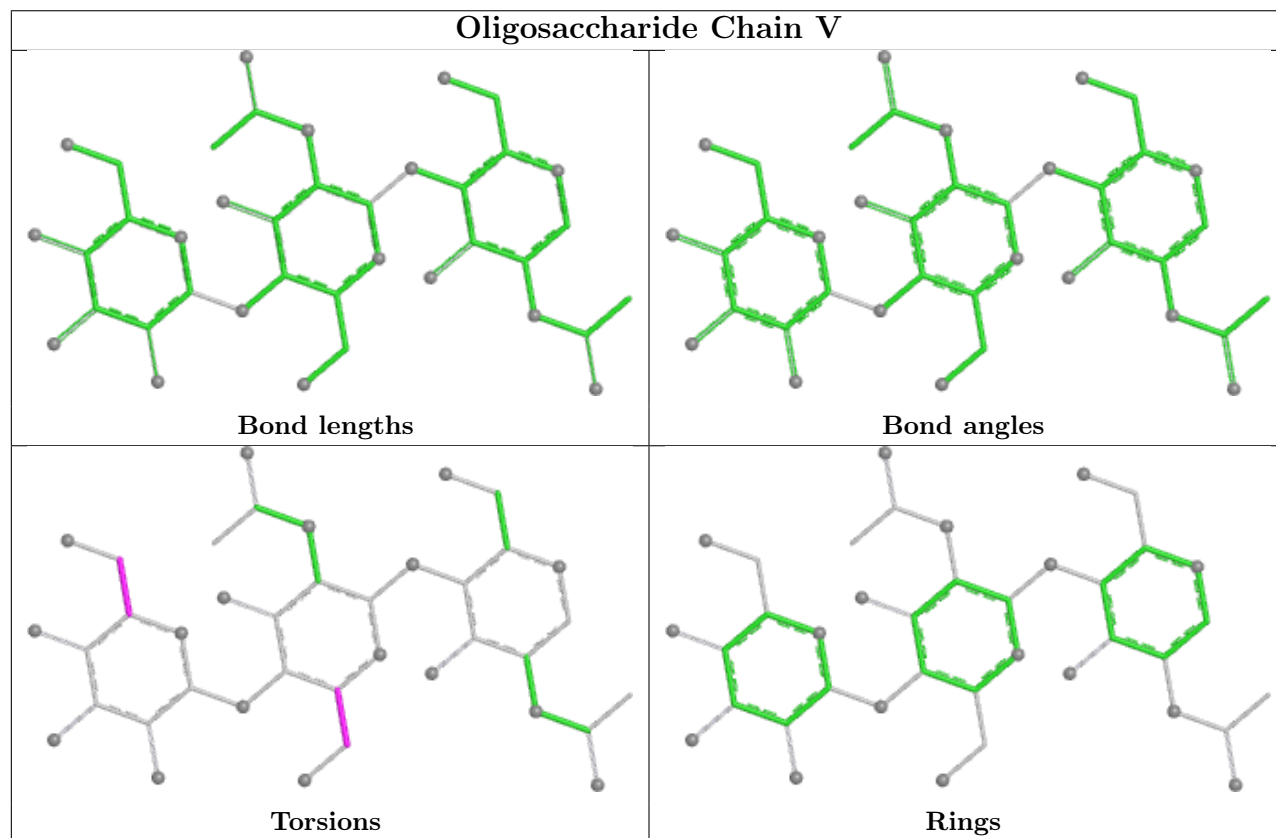
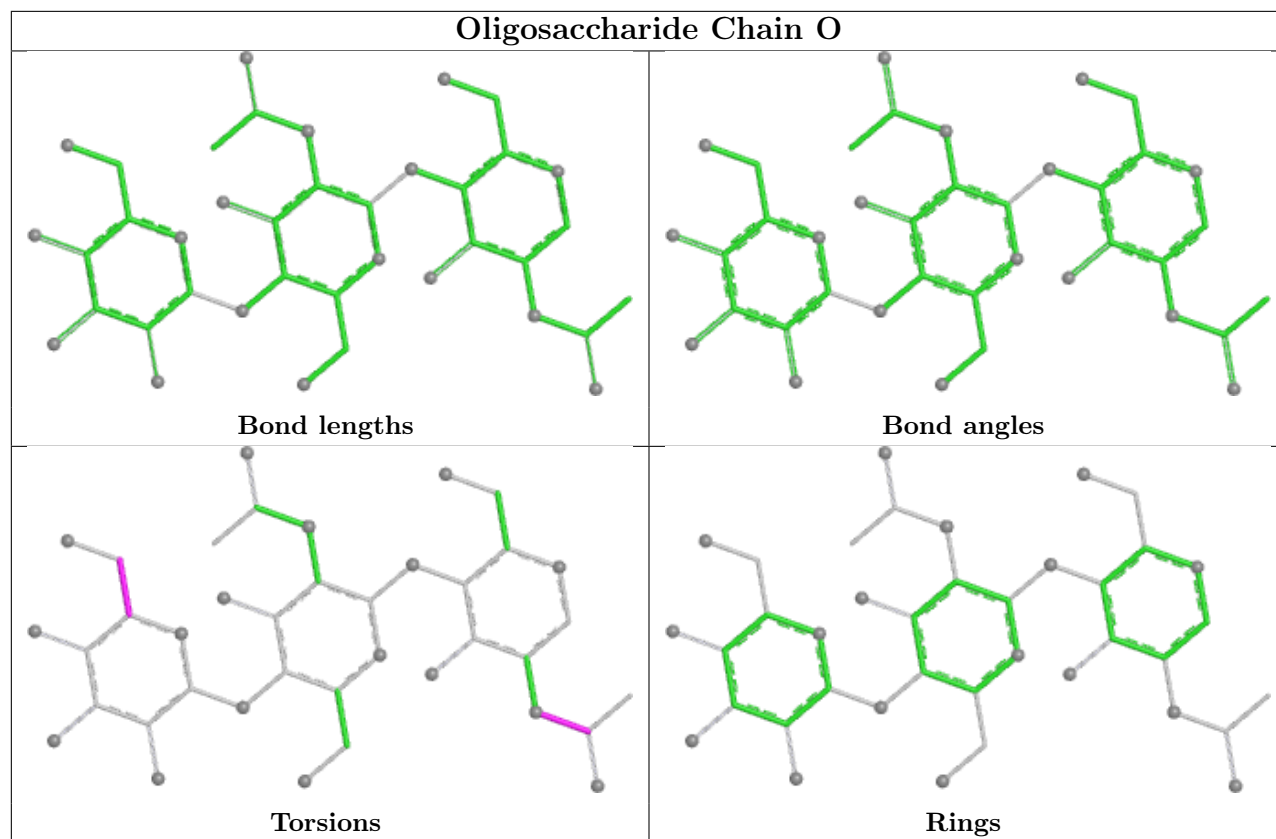


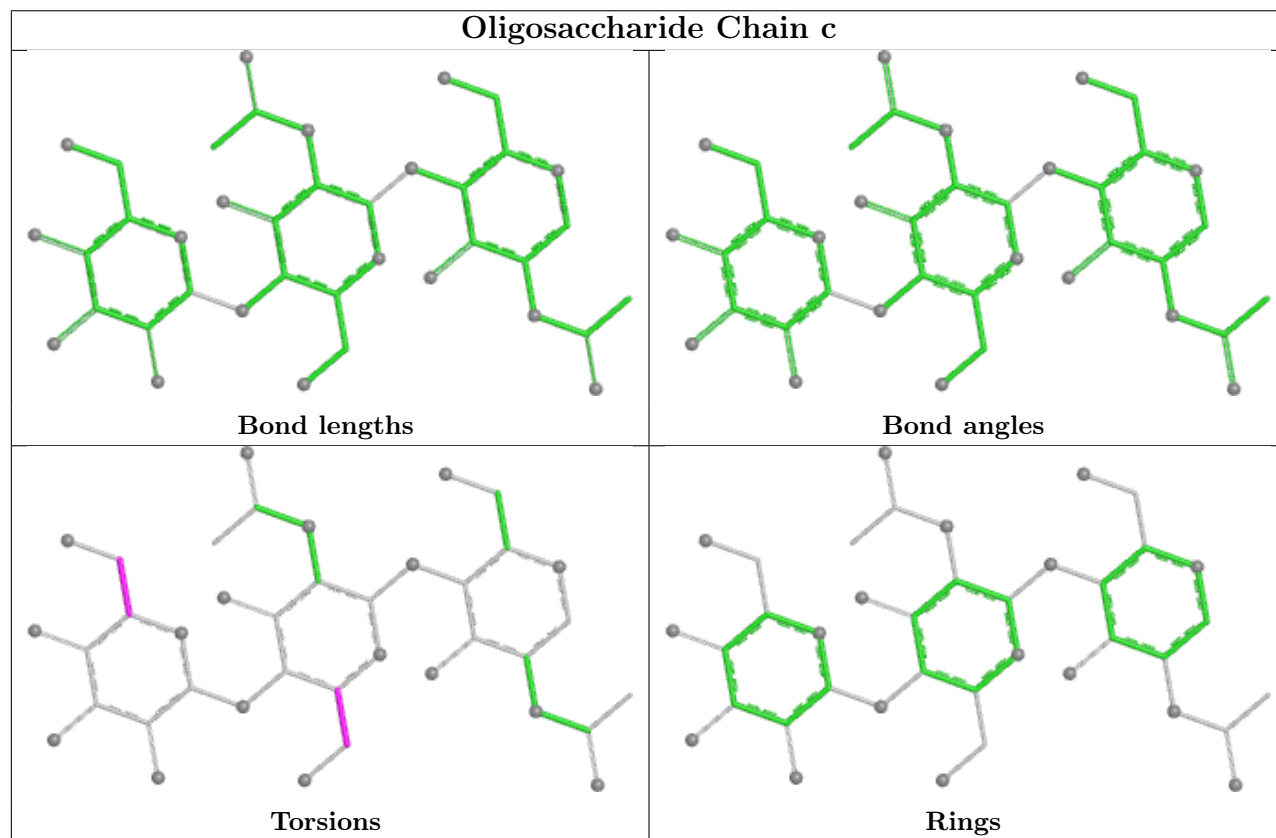
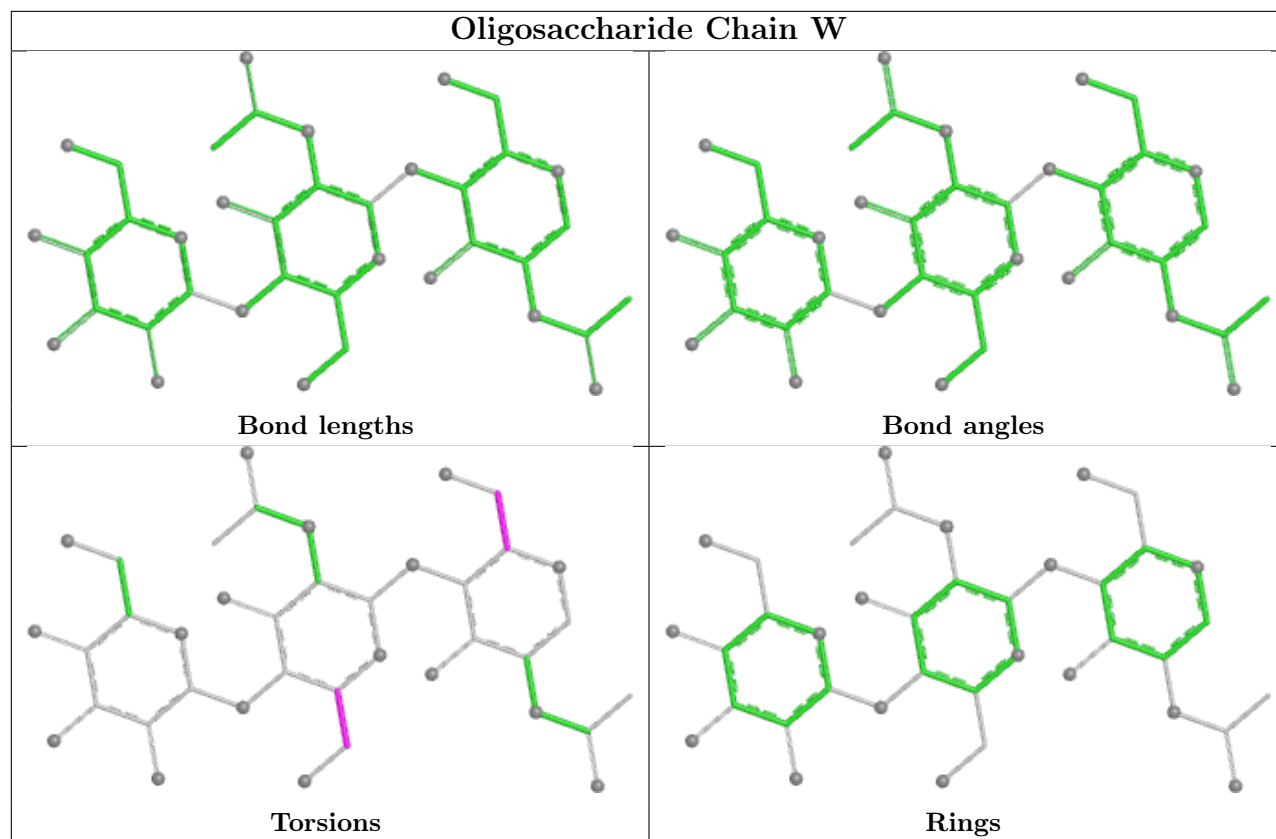


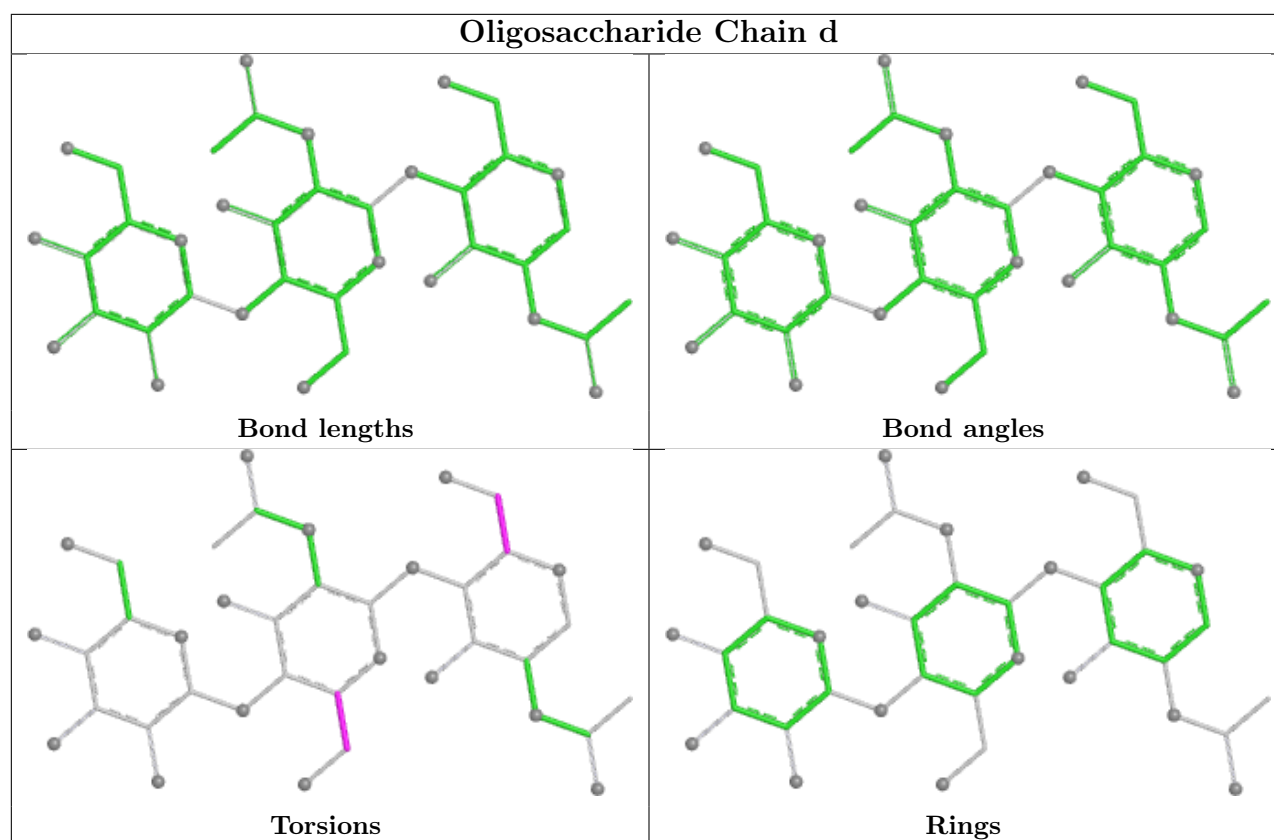












5.6 Ligand geometry [i](#)

31 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	$\# Z > 2$
6	NAG	B	1303	3	14,14,15	0.41	0	17,19,21	0.63	0
6	NAG	C	1305	-	14,14,15	0.19	0	17,19,21	0.45	0
6	NAG	B	1311	3	14,14,15	0.27	0	17,19,21	0.50	0
6	NAG	A	1303	3	14,14,15	0.27	0	17,19,21	0.41	0
6	NAG	B	1308	3	14,14,15	0.23	0	17,19,21	0.40	0
6	NAG	C	1306	3	14,14,15	0.39	0	17,19,21	0.66	1 (5%)
6	NAG	A	1301	-	14,14,15	0.25	0	17,19,21	0.42	0
6	NAG	C	1307	3	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	B	1310	3	14,14,15	0.37	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	1304	3	14,14,15	0.29	0	17,19,21	0.45	0
6	NAG	B	1305	3	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	C	1303	3	14,14,15	0.27	0	17,19,21	0.42	0
6	NAG	B	1306	-	14,14,15	0.24	0	17,19,21	0.58	0
6	NAG	A	1304	3	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	A	1309	3	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	B	1304	3	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	B	1309	3	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	B	1302	3	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	C	1310	3	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	B	1307	3	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	A	1308	3	14,14,15	0.20	0	17,19,21	0.40	0
6	NAG	A	1307	3	14,14,15	0.25	0	17,19,21	0.44	0
6	NAG	C	1302	3	14,14,15	0.22	0	17,19,21	0.51	0
6	NAG	A	1310	3	14,14,15	0.20	0	17,19,21	0.46	0
6	NAG	B	1301	-	14,14,15	0.17	0	17,19,21	0.54	0
6	NAG	C	1309	3	14,14,15	0.21	0	17,19,21	0.40	0
6	NAG	C	1308	3	14,14,15	0.20	0	17,19,21	0.40	0
6	NAG	A	1305	-	14,14,15	0.19	0	17,19,21	0.45	0
6	NAG	A	1302	3	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	A	1306	3	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	C	1301	3	14,14,15	0.22	0	17,19,21	0.45	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
6	NAG	B	1303	3	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1311	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1303	3	-	0/6/23/26	0/1/1/1
6	NAG	B	1308	3	-	3/6/23/26	0/1/1/1
6	NAG	C	1306	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	-	-	2/6/23/26	0/1/1/1
6	NAG	C	1307	3	-	3/6/23/26	0/1/1/1
6	NAG	B	1310	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1304	3	-	2/6/23/26	0/1/1/1
6	NAG	B	1305	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1303	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1309	3	-	2/6/23/26	0/1/1/1
6	NAG	B	1304	3	-	2/6/23/26	0/1/1/1
6	NAG	B	1309	3	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	3	-	0/6/23/26	0/1/1/1
6	NAG	C	1310	3	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1308	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1307	3	-	3/6/23/26	0/1/1/1
6	NAG	C	1302	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1310	3	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	-	-	1/6/23/26	0/1/1/1
6	NAG	C	1309	3	-	2/6/23/26	0/1/1/1
6	NAG	C	1308	3	-	2/6/23/26	0/1/1/1
6	NAG	A	1305	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	3	-	0/6/23/26	0/1/1/1
6	NAG	A	1306	3	-	2/6/23/26	0/1/1/1
6	NAG	C	1301	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1306	NAG	C1-O5-C5	2.21	115.14	112.19

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1304	NAG	C4-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	A	1309	NAG	C4-C5-C6-O6
6	B	1306	NAG	C4-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	A	1304	NAG	O5-C5-C6-O6
6	A	1310	NAG	O5-C5-C6-O6
6	A	1307	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	1302	NAG	O5-C5-C6-O6
6	C	1304	NAG	C4-C5-C6-O6
6	C	1310	NAG	O5-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	A	1309	NAG	O5-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	C	1309	NAG	O5-C5-C6-O6
6	A	1308	NAG	C4-C5-C6-O6
6	C	1310	NAG	C4-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	C	1302	NAG	C4-C5-C6-O6
6	A	1310	NAG	C4-C5-C6-O6
6	B	1311	NAG	O5-C5-C6-O6
6	A	1308	NAG	O5-C5-C6-O6
6	B	1309	NAG	O5-C5-C6-O6
6	B	1307	NAG	C4-C5-C6-O6
6	B	1311	NAG	C4-C5-C6-O6
6	B	1303	NAG	C8-C7-N2-C2
6	B	1303	NAG	O7-C7-N2-C2
6	B	1308	NAG	C8-C7-N2-C2
6	B	1308	NAG	O7-C7-N2-C2
6	C	1307	NAG	C8-C7-N2-C2
6	C	1307	NAG	O7-C7-N2-C2
6	C	1308	NAG	O5-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	B	1307	NAG	O5-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6
6	B	1309	NAG	C4-C5-C6-O6
6	C	1308	NAG	C4-C5-C6-O6
6	C	1306	NAG	C4-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	A	1306	NAG	O5-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	A	1307	NAG	C1-C2-N2-C7
6	B	1301	NAG	C1-C2-N2-C7
6	C	1305	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1308	NAG	1	0
6	C	1307	NAG	1	0
6	B	1305	NAG	1	0
6	A	1309	NAG	1	0
6	B	1301	NAG	6	0
6	A	1305	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.

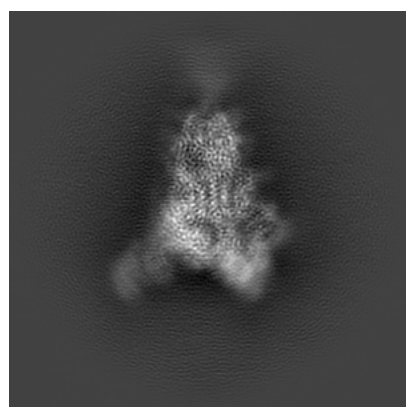
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32446. These allow visual inspection of the internal detail of the map and identification of artifacts.

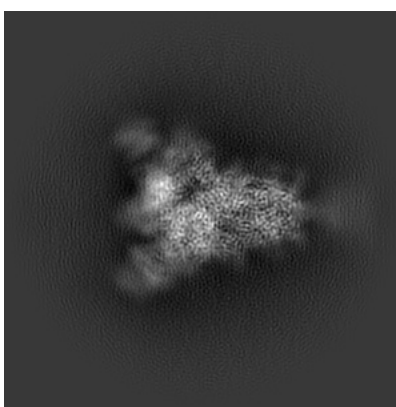
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

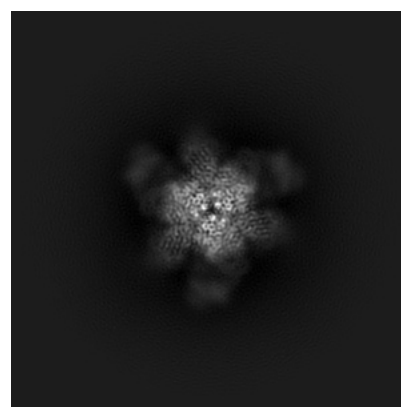
6.1.1 Primary map



X



Y

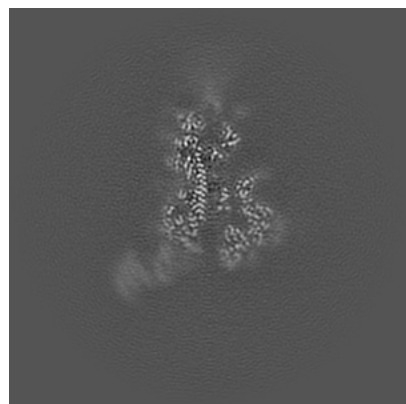


Z

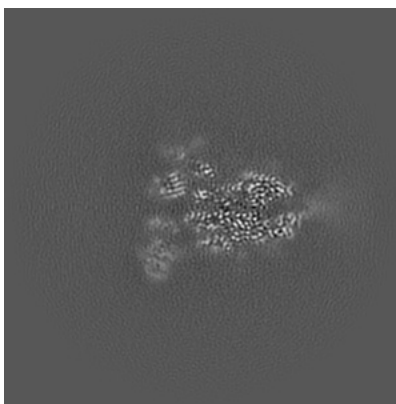
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

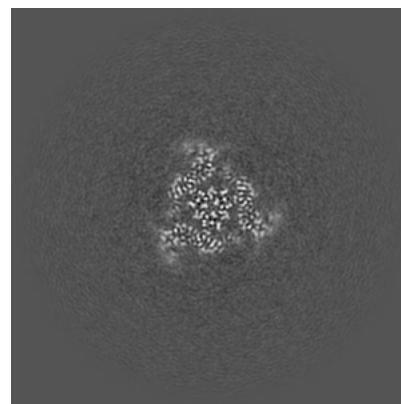
6.2.1 Primary map



X Index: 180



Y Index: 180

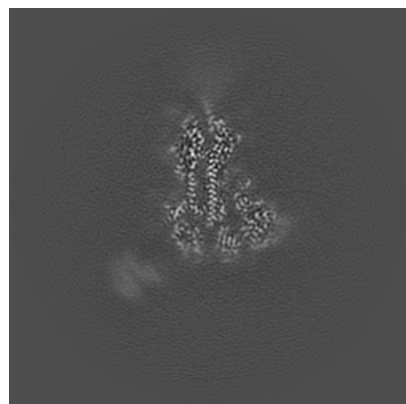


Z Index: 180

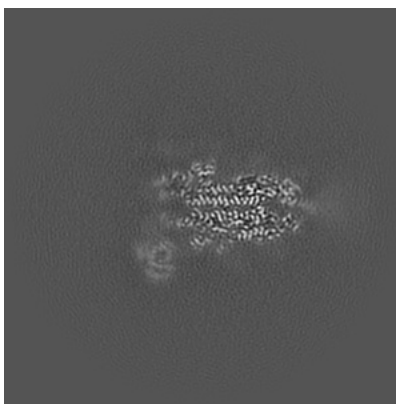
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

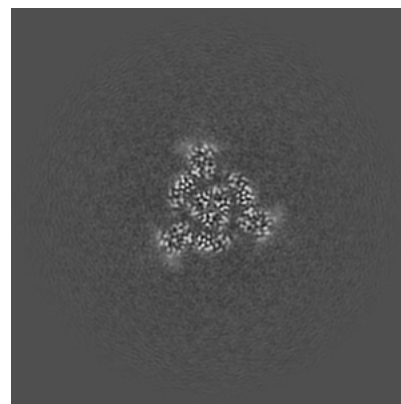
6.3.1 Primary map



X Index: 173



Y Index: 185

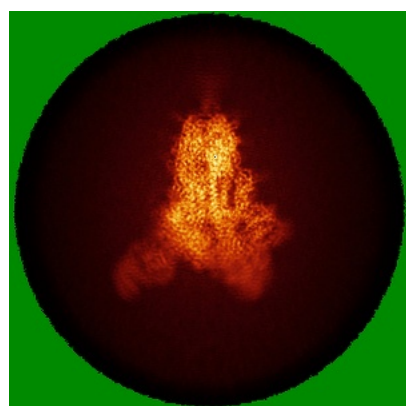


Z Index: 176

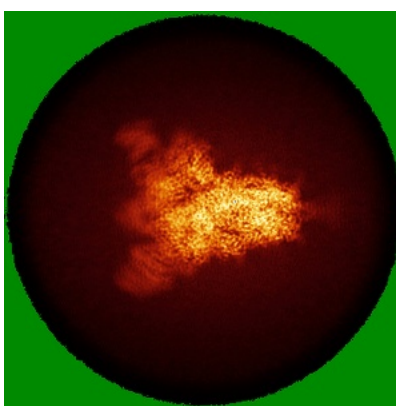
The images above show the largest variance slices of the map in three orthogonal directions.

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

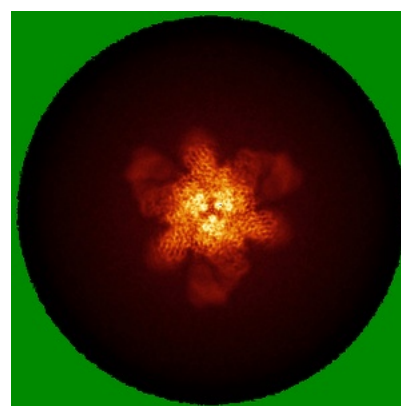
6.4.1 Primary map



X



Y

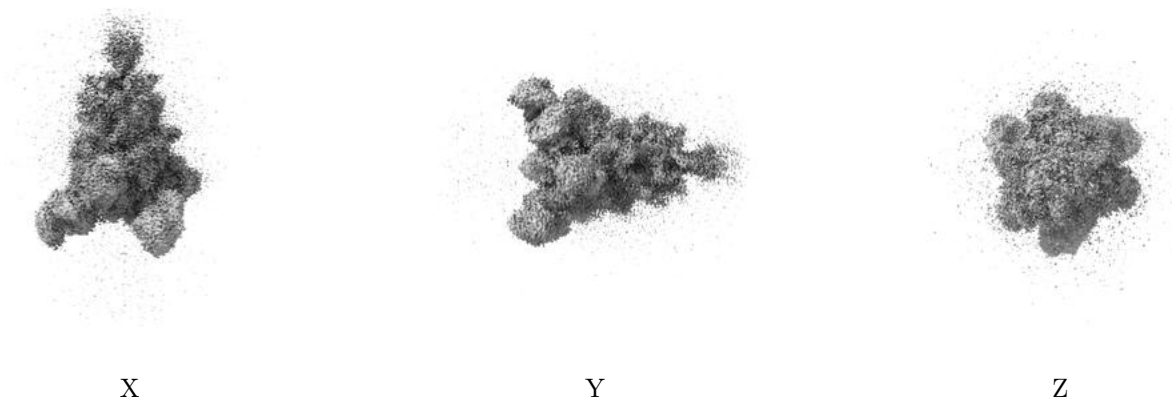


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.219. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

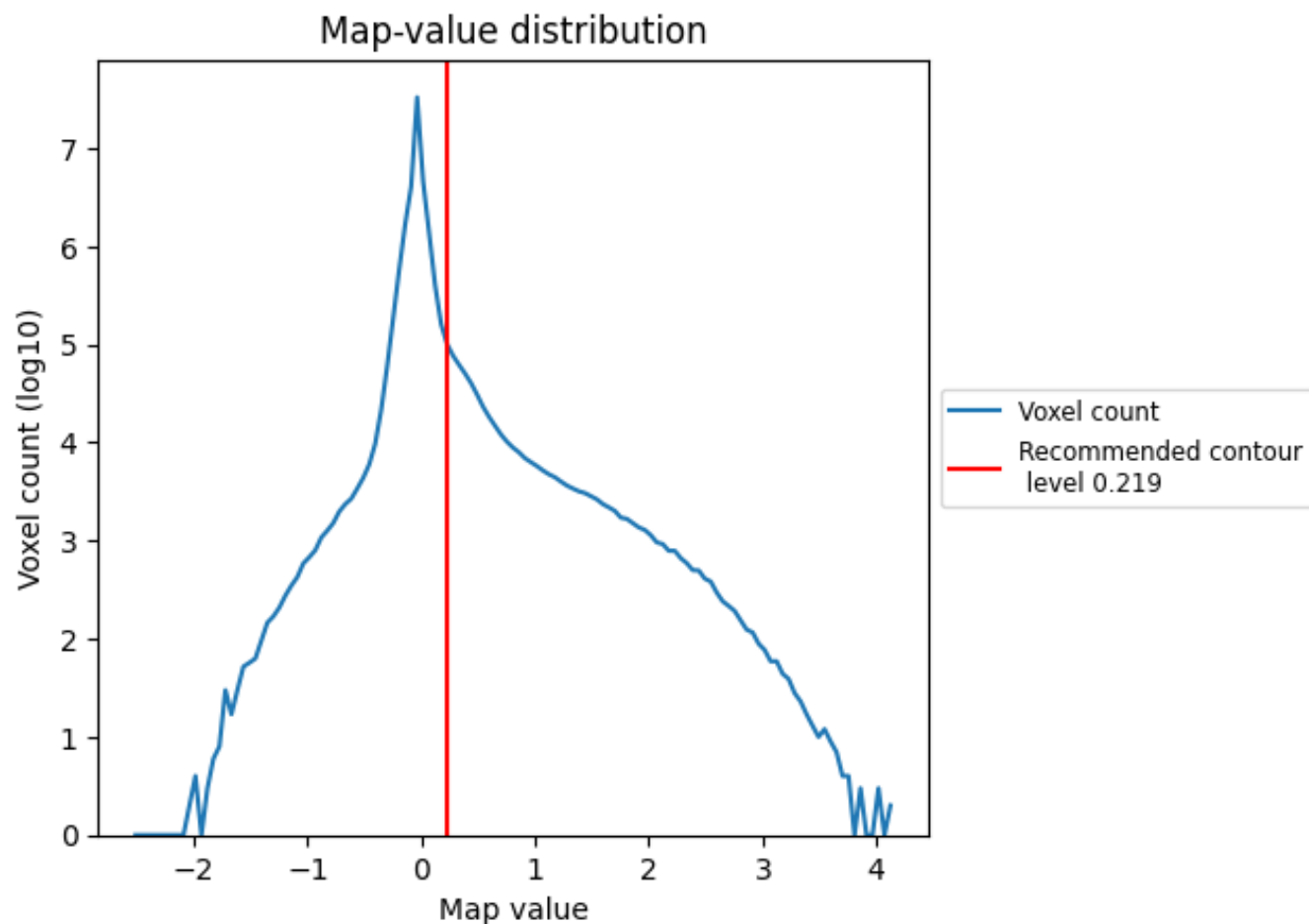
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

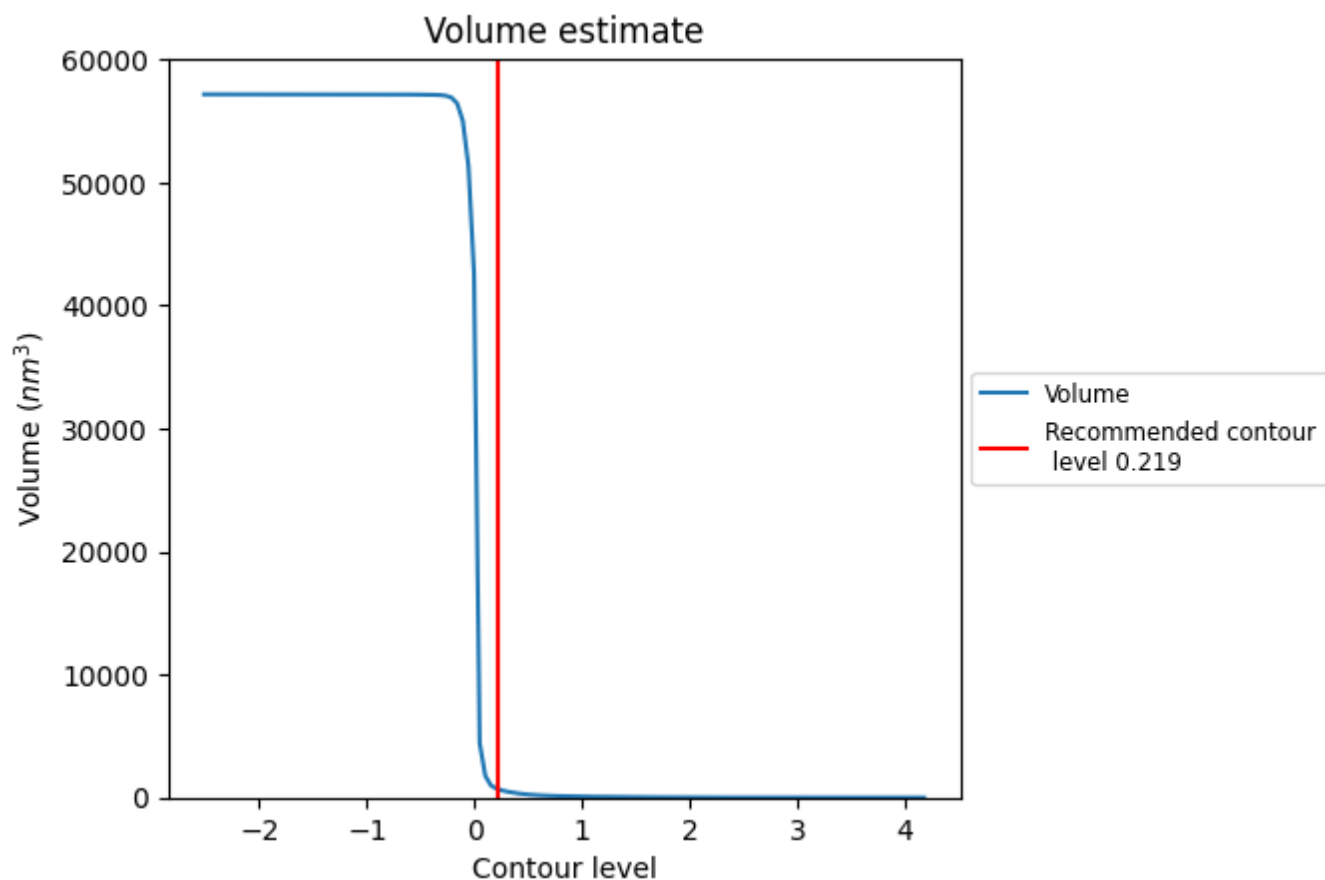
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

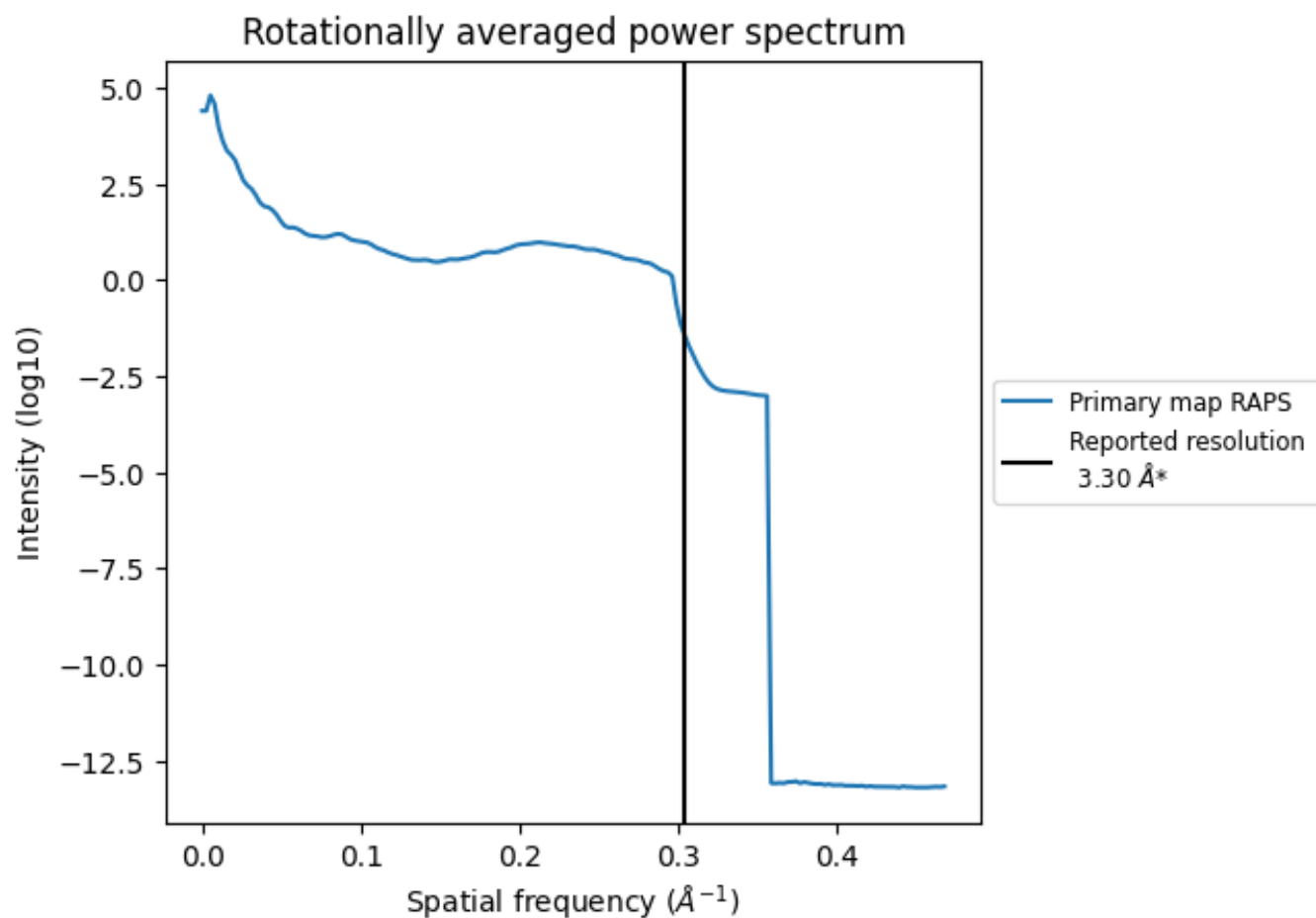
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 683 nm³; this corresponds to an approximate mass of 617 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 0.303 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

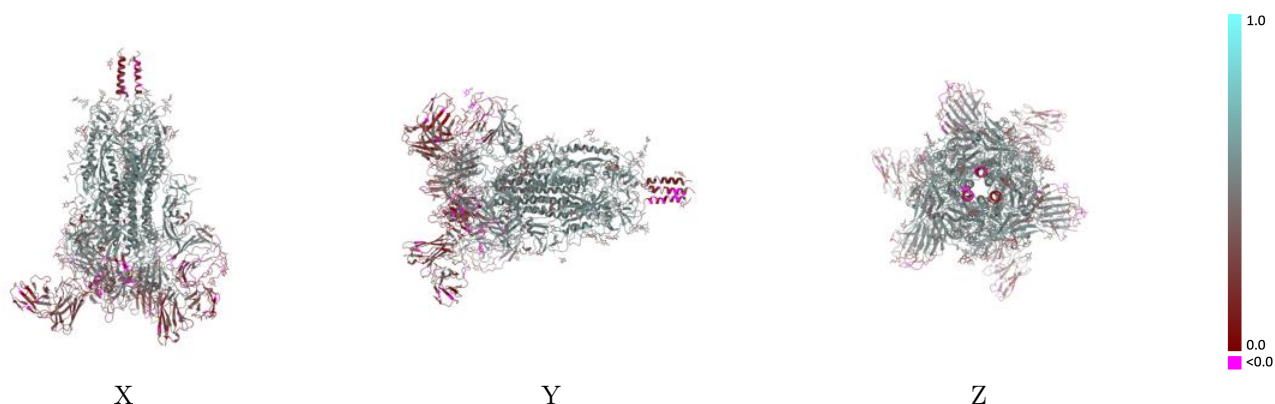
This section contains information regarding the fit between EMDB map EMD-32446 and PDB model 7WEC. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



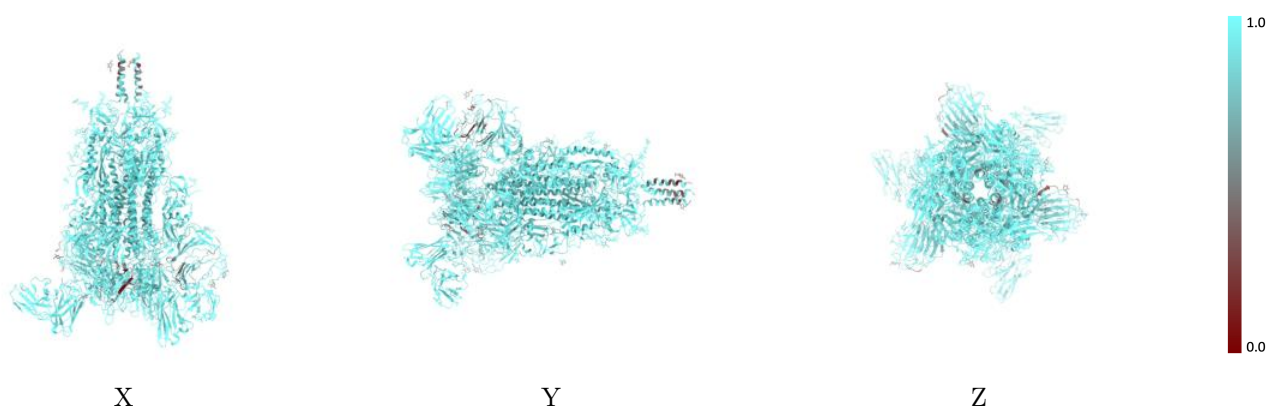
The images above show the 3D surface view of the map at the recommended contour level 0.219 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



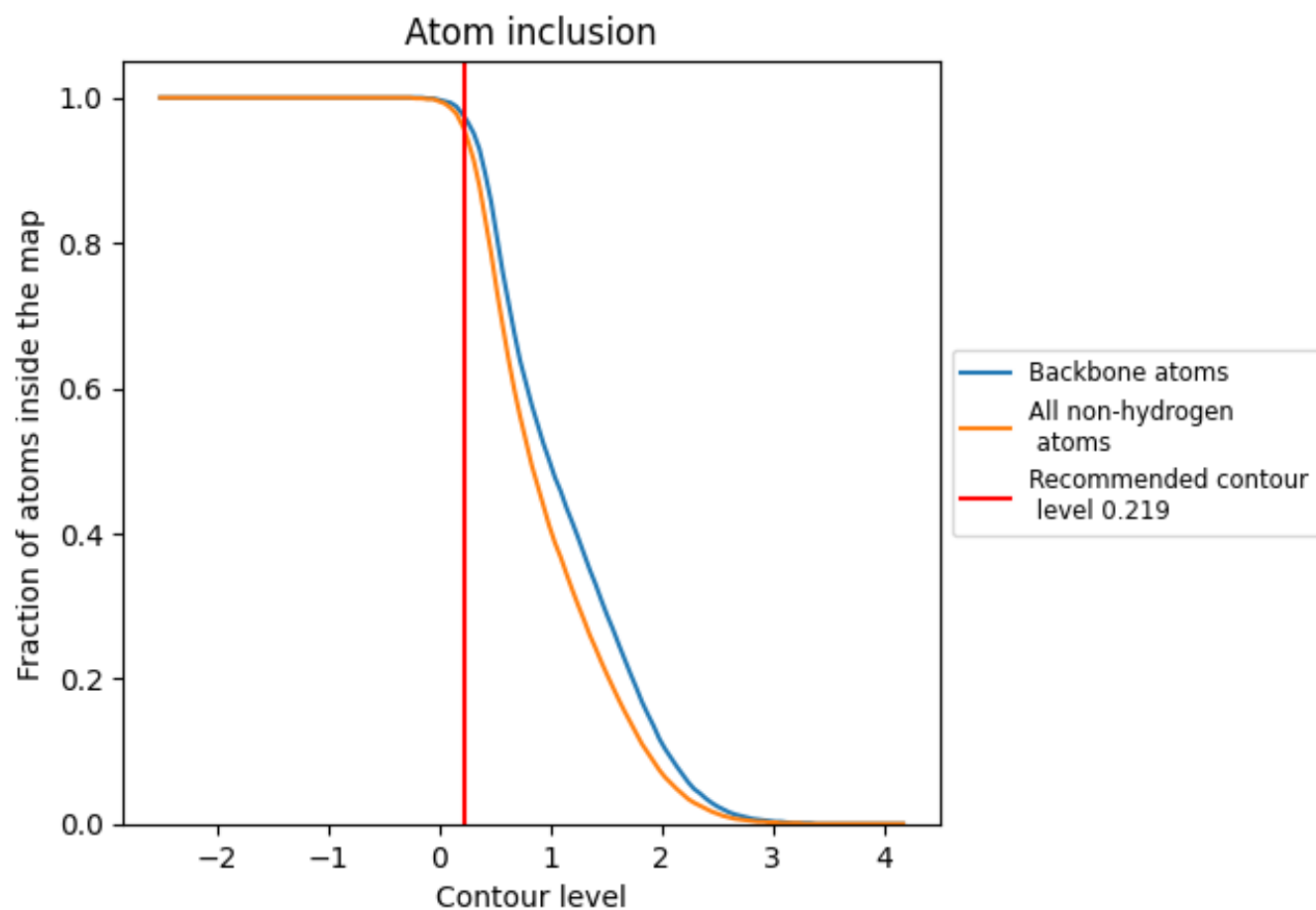
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.219).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.219) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.4330
A	 0.9740	 0.4810
B	 0.9470	 0.4570
C	 0.9560	 0.4560
D	 0.8570	 0.3460
E	 0.7140	 0.1970
F	 1.0000	 0.5010
G	 0.9600	 0.2780
H	 0.9560	 0.2770
I	 0.9570	 0.2840
J	 0.9700	 0.2870
K	 0.9680	 0.2870
L	 0.9660	 0.2640
M	 1.0000	 0.3480
N	 1.0000	 0.3780
O	 0.9490	 0.3830
P	 1.0000	 0.4900
Q	 0.8210	 0.2520
R	 0.6790	 0.3830
S	 0.8570	 0.3840
T	 0.8210	 0.2150
U	 1.0000	 0.3760
V	 1.0000	 0.3990
W	 0.9490	 0.4410
X	 0.6430	 0.1560
Y	 0.6790	 0.3690
Z	 1.0000	 0.4930
a	 0.8930	 0.2430
b	 1.0000	 0.3710
c	 0.9740	 0.3910
d	 0.9490	 0.4380

