



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:28 PM UTC

PDB ID : 9MSY / pdb_00009msy
EMDB ID : EMD-48591
Title : G002-480-0546 Fab in complex with V703-0537_T278M_L14 SOSIP and BG18 Fab
Authors : Phulera, S.; Ozorowski, G.; Ward, A.B.
Deposited on : 2025-01-10
Resolution : 3.40 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:

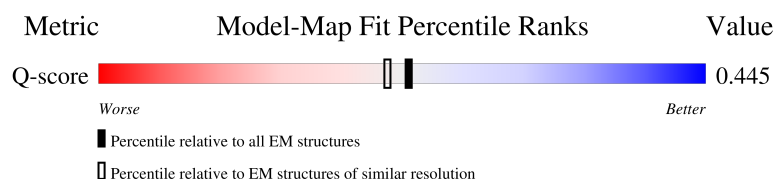
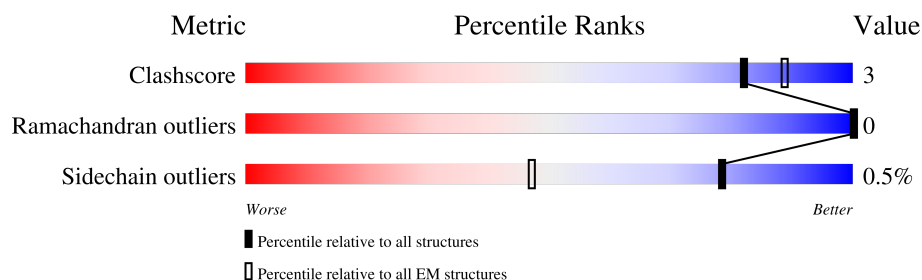
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.40 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	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	654	
1	B	654	
1	C	654	
2	G	233	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	233	
2	O	233	
3	I	214	
3	M	214	
3	Q	214	
4	L	211	
4	N	211	
4	R	211	
5	H	226	
5	K	226	
5	P	226	
6	D	2	
6	F	2	
6	S	2	
6	V	2	
6	W	2	
6	Y	2	
6	Z	2	
6	c	2	
6	d	2	
6	f	2	
6	g	2	
6	j	2	
7	E	3	
7	X	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	e	3	33% 100%
8	T	5	20% 80%
8	a	5	20% 80%
8	h	5	20% 80%
9	U	6	83% 17%
9	b	6	83% 17%
9	i	6	83% 17%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 24315 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 V703-0537_T278M_L14 SOSIP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	531	Total	C	N	O	S	0	0
			4189	2655	717	783	34		
1	B	531	Total	C	N	O	S	0	0
			4189	2655	717	783	34		
1	C	531	Total	C	N	O	S	0	0
			4189	2655	717	783	34		

- Molecule 2 is a protein called BG18 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	126	Total	C	N	O	S	0	0
			988	621	175	186	6		
2	J	126	Total	C	N	O	S	0	0
			988	621	175	186	6		
2	O	126	Total	C	N	O	S	0	0
			988	621	175	186	6		

- Molecule 3 is a protein called BG18 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	106	Total	C	N	O	S	0	0
			806	501	140	162	3		
3	M	106	Total	C	N	O	S	0	0
			806	501	140	162	3		
3	Q	106	Total	C	N	O	S	0	0
			806	501	140	162	3		

- Molecule 4 is a protein called G002-480-0546 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	102	Total	C	N	O	S	0	0
			771	486	128	155	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	102	Total	C	N	O	S	0	0
			771	486	128	155	2		
4	R	102	Total	C	N	O	S	0	0
			771	486	128	155	2		

- Molecule 5 is a protein called G002-480-0546 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	119	Total	C	N	O	S	0	0
			955	605	168	176	6		
5	K	119	Total	C	N	O	S	0	0
			955	605	168	176	6		
5	P	119	Total	C	N	O	S	0	0
			955	605	168	176	6		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



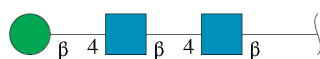
Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	2	Total	C	N	O	0	0
			28	16	2	10		
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	W	2	Total	C	N	O	0	0
			28	16	2	10		
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	c	2	Total	C	N	O	0	0
			28	16	2	10		
6	d	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

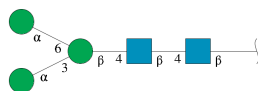
Mol	Chain	Residues	Atoms				AltConf	Trace
6	f	2	Total	C	N	O	0	0
			28	16	2	10		
6	g	2	Total	C	N	O	0	0
			28	16	2	10		
6	j	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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.



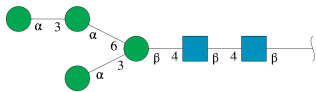
Mol	Chain	Residues	Atoms				AltConf	Trace
7	E	3	Total	C	N	O	0	0
			39	22	2	15		
7	X	3	Total	C	N	O	0	0
			39	22	2	15		
7	e	3	Total	C	N	O	0	0
			39	22	2	15		

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



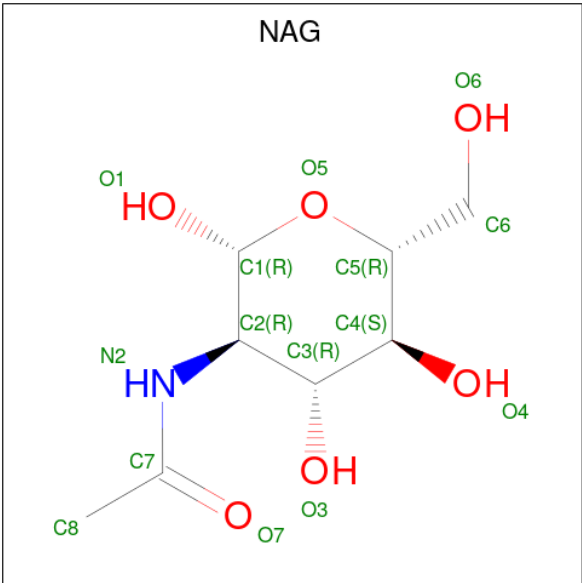
Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	5	Total	C	N	O	0	0
			61	34	2	25		
8	a	5	Total	C	N	O	0	0
			61	34	2	25		
8	h	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	6	Total	C	N	O	0	0
			72	40	2	30		
9	b	6	Total	C	N	O	0	0
			72	40	2	30		
9	i	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

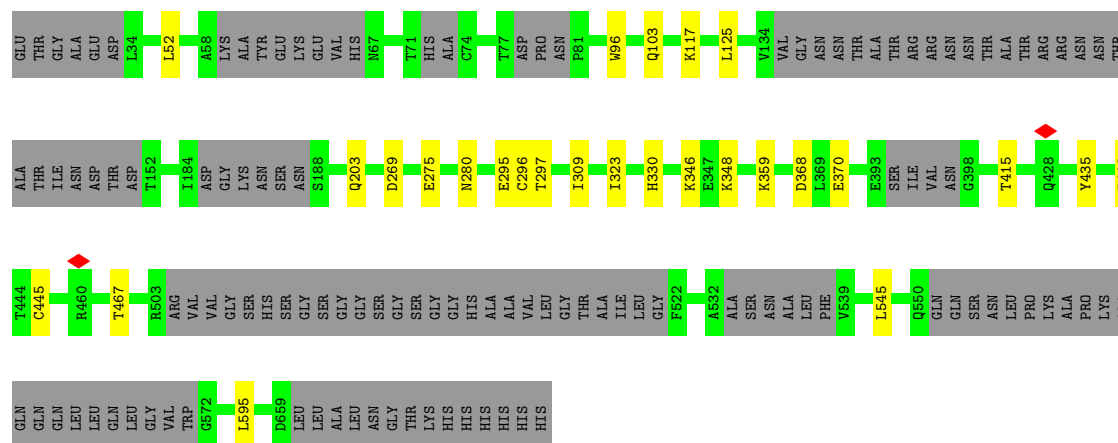


Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	

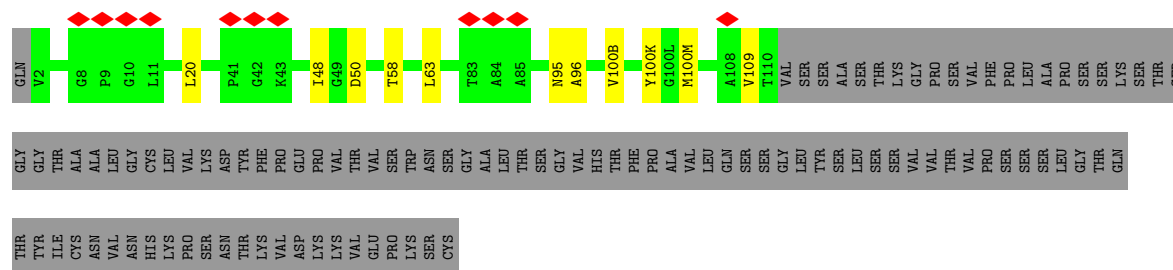
Continued on next page...

Continued from previous page...

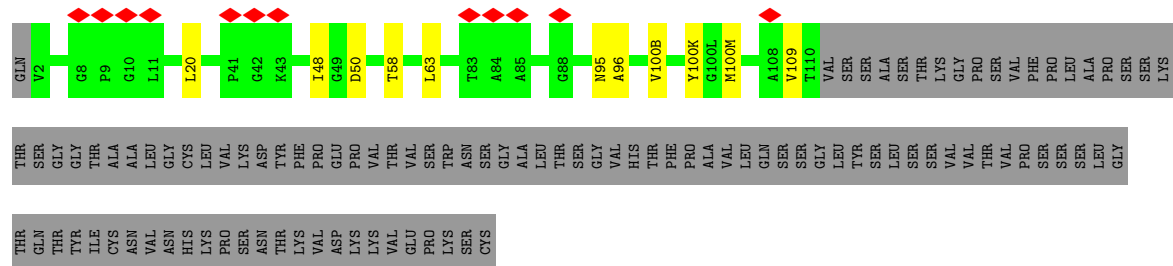
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	G	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14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



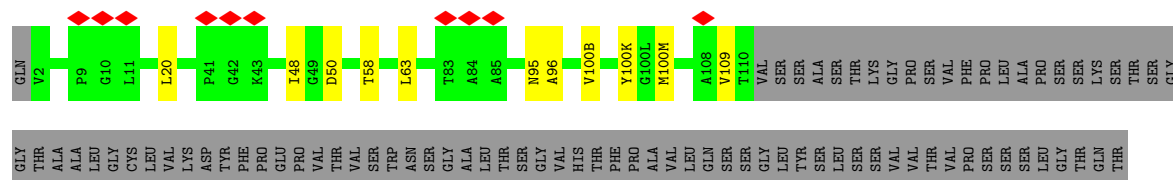
• Molecule 2: BG18 Fab heavy chain



• Molecule 2: BG18 Fab heavy chain



• Molecule 2: BG18 Fab heavy chain



TYR
ILE
CYS
ASN
VAL
ASN
HIS
LYS
PRO
SER
ASN
THR
LYS
VAL
ASP
LYS
LYS
VAL
GLU
PRO
LYS
SER
CYS

• Molecule 3: BG18 Fab light chain



SER
SER
E3
S12
V13
Q17
T18
G41
R54
S59
G60
R61
R76
G77
A80
D81
D82
T105
V106
L106A
GLY
GLN
PRO
LYS
ALA
ALA
SER
PRO
TYR
VAL
THR
LEU
PHE
THR
PRO
GLU
SER
GLN
LYS
GLU
SER
LEU
GLN
ALA
SER
ASN
LYS
ALA
CYS
THR
VAL
VAL
CYS
HIS
LEU
ILE
SER
ASP

PHE
TYR
PRO
GLY
VAL
VAL
THR
VAL
ALA
TRP
LYS
ASP
SER
SER
PRO
VAL
LYS
ALA
GLY
VAL
GLU
THR
THR
PRO
SER
LYS
GLN
SER
ASN
ASN
TYR
LYS
ALA
ALA
SER
SER
TYR
LEU
THR
LEU
PHE
THR
PRO
GLU
SER
SER
TRP
LYS
SER
HIS
ARG
ALA
SER
TYR
LYS
CYS
THR
GLN
VAL
THR
HIS
GLU

GLY
SER
THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

• Molecule 3: BG18 Fab light chain



SER
SER
E3
S12
V13
Q17
T18
G41
R54
S59
G60
R61
R76
G77
A80
D81
D82
T105
V106
L106A
GLY
GLN
PRO
LYS
ALA
ALA
SER
PRO
TYR
VAL
THR
LEU
PHE
THR
PRO
GLU
SER
SER
TRP
LYS
SER
HIS
ARG
ALA
SER
ASN
LYS
ALA
CYS
THR
VAL
VAL
CYS
HIS
LEU
ILE
SER
ASP

PHE
TYR
PRO
GLY
VAL
VAL
THR
VAL
ALA
TRP
LYS
ASP
SER
SER
PRO
VAL
LYS
ALA
GLY
VAL
GLU
THR
THR
PRO
SER
LYS
GLN
SER
ASN
ASN
TYR
LYS
ALA
ALA
SER
SER
TYR
LEU
THR
LEU
PHE
THR
PRO
GLU
SER
SER
TRP
LYS
SER
HIS
ARG
ALA
SER
TYR
LYS
CYS
THR
GLN
VAL
THR
HIS
GLU

GLY
SER
THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

• Molecule 3: BG18 Fab light chain

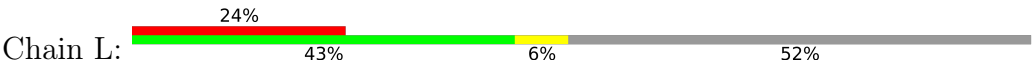


SER
SER
E3
S12
V13
Q17
T18
G41
R54
S59
G60
R61
R76
G77
A80
D81
D82
T105
V106
L106A
GLY
GLN
PRO
LYS
ALA
ALA
SER
PRO
TYR
VAL
THR
LEU
PHE
THR
PRO
GLU
SER
SER
TRP
LYS
SER
HIS
ARG
ALA
SER
ASN
LYS
ALA
CYS
THR
VAL
VAL
CYS
HIS
LEU
ILE
SER
ASP

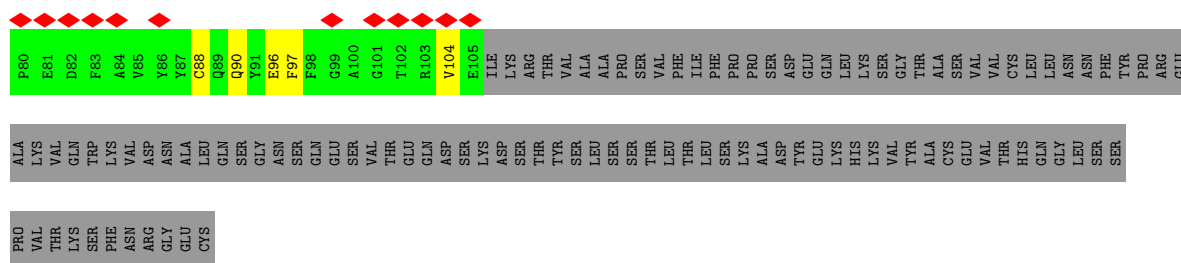
PHE
TYR
PRO
GLY
VAL
VAL
THR
VAL
ALA
TRP
LYS
ASP
SER
SER
PRO
VAL
LYS
ALA
GLY
VAL
GLU
THR
THR
PRO
SER
LYS
GLN
SER
ASN
ASN
TYR
LYS
ALA
ALA
SER
SER
TYR
LEU
THR
LEU
PHE
THR
PRO
GLU
SER
SER
TRP
LYS
SER
HIS
ARG
ALA
SER
TYR
LYS
CYS
THR
GLN
VAL
THR
HIS
GLU

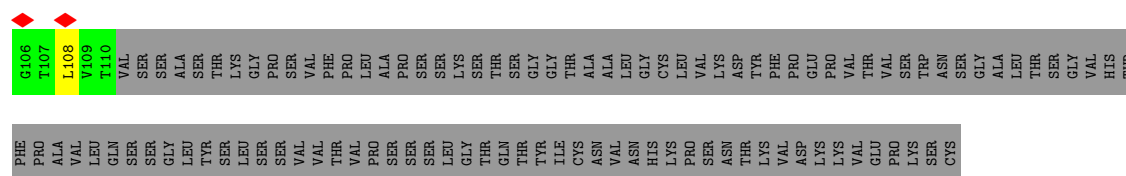
GLY
SER
THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

• Molecule 4: G002-480-0546 Fab light chain

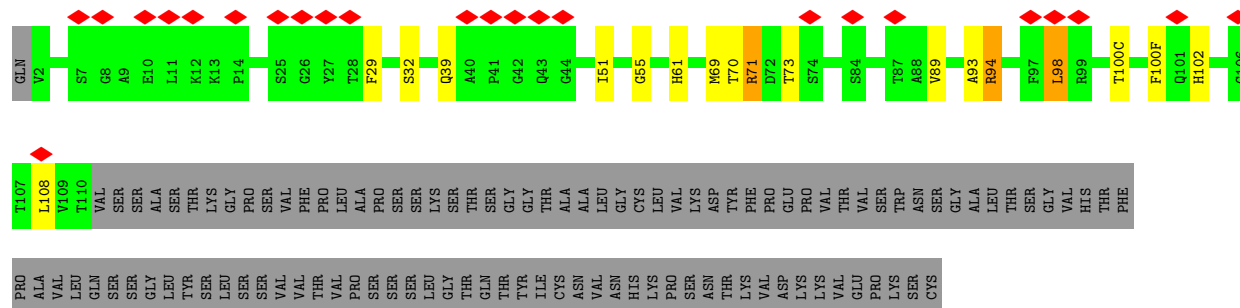


E1
I2
V3
L4
S7
P8
G9
T10
L11
S12
L13
S14
P15
G16
E17
G18
A19
T20
L21
C22
C23
R24
L28
S29
S30
S31
S32
L33
Q38
G41
L42
Y49
G50
A51
S52
I53
R54
A55
T56
G57
I58
P59
D60
R61
F62
S63
D70
T74
I75
S76
R77
L78
E79

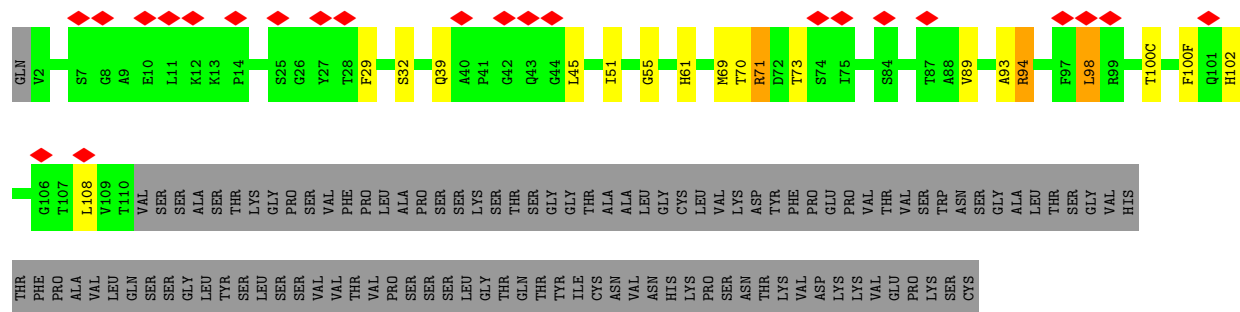
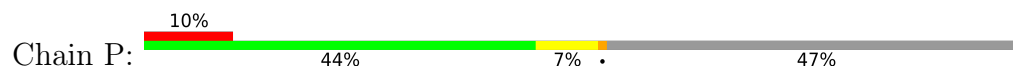




• Molecule 5: G002-480-0546 Fab heavy chain



• Molecule 5: G002-480-0546 Fab heavy chain



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



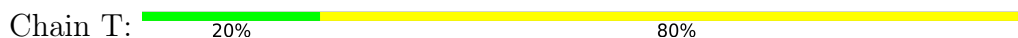
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



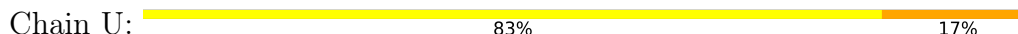
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



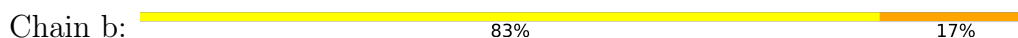
- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

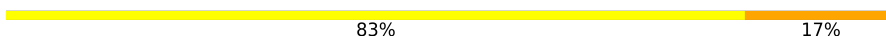


- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain i:



NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	51495	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	190000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.054	Depositor
Minimum map value	-0.587	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	413.56, 413.56, 413.56	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0339, 1.0339, 1.0339	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	A	0.24	0/4273	0.56	0/5793
1	B	0.24	0/4273	0.56	0/5793
1	C	0.24	0/4273	0.56	0/5793
2	G	0.21	0/1014	0.55	0/1380
2	J	0.22	0/1014	0.55	0/1380
2	O	0.22	0/1014	0.55	0/1380
3	I	0.22	0/825	0.48	0/1122
3	M	0.22	0/825	0.48	0/1122
3	Q	0.22	0/825	0.48	0/1122
4	L	0.22	0/788	0.54	0/1070
4	N	0.22	0/788	0.54	0/1070
4	R	0.22	0/788	0.54	0/1070
5	H	0.34	0/982	0.71	1/1334 (0.1%)
5	K	0.34	0/982	0.71	1/1334 (0.1%)
5	P	0.34	0/982	0.71	1/1334 (0.1%)
All	All	0.25	0/23646	0.57	3/32097 (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
5	H	0	2
5	K	0	2
5	P	0	2
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	55	GLY	N-CA-C	-5.86	107.59	115.21
5	H	55	GLY	N-CA-C	-5.85	107.61	115.21
5	P	55	GLY	N-CA-C	-5.84	107.62	115.21

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	H	71	ARG	Sidechain
5	H	94	ARG	Sidechain
5	K	71	ARG	Sidechain
5	K	94	ARG	Sidechain
5	P	71	ARG	Sidechain
5	P	94	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4189	0	4115	17	0
1	B	4189	0	4115	18	0
1	C	4189	0	4115	20	0
2	G	988	0	952	6	0
2	J	988	0	952	6	0
2	O	988	0	952	6	0
3	I	806	0	776	3	0
3	M	806	0	776	3	0
3	Q	806	0	776	3	0
4	L	771	0	748	6	0
4	N	771	0	748	6	0
4	R	771	0	748	7	0
5	H	955	0	904	12	0
5	K	955	0	904	13	0
5	P	955	0	904	15	0
6	D	28	0	25	0	0
6	F	28	0	25	0	0
6	S	28	0	25	0	0
6	V	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	W	28	0	25	0	0
6	Y	28	0	25	0	0
6	Z	28	0	25	0	0
6	c	28	0	25	0	0
6	d	28	0	25	0	0
6	f	28	0	25	0	0
6	g	28	0	25	0	0
6	j	28	0	25	0	0
7	E	39	0	34	0	0
7	X	39	0	34	0	0
7	e	39	0	34	0	0
8	T	61	0	52	0	0
8	a	61	0	52	0	0
8	h	61	0	52	0	0
9	U	72	0	61	1	0
9	b	72	0	61	1	0
9	i	72	0	61	1	0
10	A	98	0	91	0	0
10	B	98	0	91	0	0
10	C	98	0	91	0	0
10	G	14	0	13	0	0
10	J	14	0	13	0	0
10	O	14	0	13	0	0
All	All	24315	0	23538	121	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 3.

All (121) 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)
4:N:4:LEU:HD11	4:N:90:GLN:HB2	1.74	0.69
4:R:4:LEU:HD11	4:R:90:GLN:HB2	1.74	0.69
4:L:4:LEU:HD11	4:L:90:GLN:HB2	1.74	0.69
3:M:18:THR:HG21	3:M:76:ARG:HH11	1.61	0.66
3:Q:18:THR:HG21	3:Q:76:ARG:HH11	1.61	0.66
3:I:18:THR:HG21	3:I:76:ARG:HH11	1.61	0.65
5:H:51:ILE:HD11	5:H:71:ARG:HB3	1.79	0.65
5:K:51:ILE:HD11	5:K:71:ARG:HB3	1.79	0.64
1:C:467:THR:HG1	5:P:61:HIS:HE2	1.45	0.64
5:P:51:ILE:HD11	5:P:71:ARG:HB3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:THR:HG1	5:K:61:HIS:HE2	1.46	0.63
1:B:415:THR:HG21	2:J:100(B):VAL:HG11	1.81	0.62
1:C:415:THR:HG21	2:O:100(B):VAL:HG11	1.81	0.61
1:B:269:ASP:OD1	1:B:348:LYS:NZ	2.33	0.61
1:A:415:THR:HG21	2:G:100(B):VAL:HG11	1.81	0.60
1:A:269:ASP:OD1	1:A:348:LYS:NZ	2.33	0.60
1:A:467:THR:HG1	5:H:61:HIS:HE2	1.45	0.59
1:B:368:ASP:C	1:B:370:GLU:N	2.59	0.59
1:C:269:ASP:OD1	1:C:348:LYS:NZ	2.33	0.59
1:C:368:ASP:C	1:C:370:GLU:N	2.59	0.58
1:C:52:LEU:H	1:C:103:GLN:HE22	1.52	0.58
1:A:52:LEU:H	1:A:103:GLN:HE22	1.52	0.57
1:B:52:LEU:H	1:B:103:GLN:HE22	1.52	0.56
1:A:368:ASP:C	1:A:370:GLU:N	2.59	0.55
4:N:11:LEU:HB2	4:N:104:VAL:HA	1.90	0.53
4:L:11:LEU:HB2	4:L:104:VAL:HA	1.90	0.53
5:H:32:SER:HA	5:H:98:LEU:HD21	1.91	0.52
4:R:11:LEU:HB2	4:R:104:VAL:HA	1.90	0.52
5:K:51:ILE:HD12	5:K:69:MET:O	2.10	0.52
5:P:51:ILE:HD12	5:P:69:MET:O	2.10	0.52
1:A:280:ASN:ND2	4:L:96:GLU:OE2	2.43	0.52
1:B:280:ASN:ND2	4:N:96:GLU:OE2	2.43	0.51
1:C:280:ASN:ND2	4:R:96:GLU:OE2	2.43	0.51
5:P:32:SER:HA	5:P:98:LEU:HD21	1.91	0.51
5:K:32:SER:HA	5:K:98:LEU:HD21	1.91	0.51
5:H:51:ILE:HD12	5:H:69:MET:O	2.10	0.51
1:B:368:ASP:C	1:B:370:GLU:H	2.19	0.51
1:C:368:ASP:C	1:C:370:GLU:H	2.19	0.51
5:K:51:ILE:CD1	5:K:71:ARG:HB3	2.41	0.50
5:P:89:VAL:HG13	5:P:108:LEU:HG	1.94	0.50
1:B:346:LYS:HE2	1:B:359:LYS:HA	1.94	0.50
5:K:89:VAL:HG13	5:K:108:LEU:HG	1.94	0.50
2:O:50:ASP:OD1	2:O:58:THR:OG1	2.29	0.50
2:G:50:ASP:OD1	2:G:58:THR:OG1	2.29	0.50
5:H:29:PHE:HD2	5:H:73:THR:HG23	1.77	0.50
2:O:20:LEU:HD11	2:O:109:VAL:HG11	1.94	0.50
2:J:50:ASP:OD1	2:J:58:THR:OG1	2.29	0.50
5:K:29:PHE:HD2	5:K:73:THR:HG23	1.77	0.49
2:G:20:LEU:HD11	2:G:109:VAL:HG11	1.94	0.49
4:L:32:SER:HA	5:H:100(C):THR:HG21	1.94	0.49
5:H:51:ILE:CD1	5:H:71:ARG:HB3	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASP:C	1:A:370:GLU:H	2.19	0.49
1:C:346:LYS:HE2	1:C:359:LYS:HA	1.94	0.49
5:P:29:PHE:HD2	5:P:73:THR:HG23	1.77	0.49
5:P:51:ILE:CD1	5:P:71:ARG:HB3	2.41	0.49
5:H:89:VAL:HG13	5:H:108:LEU:HG	1.94	0.49
4:N:32:SER:HA	5:K:100(C):THR:HG21	1.94	0.49
4:R:32:SER:HA	5:P:100(C):THR:HG21	1.94	0.49
2:J:20:LEU:HD11	2:J:109:VAL:HG11	1.94	0.49
1:A:346:LYS:HE2	1:A:359:LYS:HA	1.94	0.49
1:A:296:CYS:O	1:A:445:CYS:N	2.47	0.47
1:C:467:THR:OG1	5:P:61:HIS:NE2	2.36	0.47
5:H:94:ARG:HH21	5:H:102:HIS:CD2	2.33	0.47
1:B:296:CYS:O	1:B:445:CYS:N	2.47	0.47
1:C:296:CYS:O	1:C:445:CYS:N	2.47	0.46
1:C:368:ASP:O	1:C:370:GLU:N	2.48	0.46
5:P:70:THR:HG22	5:P:71:ARG:N	2.30	0.46
5:P:94:ARG:HH21	5:P:102:HIS:CD2	2.33	0.46
5:K:70:THR:HG22	5:K:71:ARG:N	2.30	0.46
5:K:94:ARG:HH21	5:K:102:HIS:CD2	2.33	0.46
1:A:368:ASP:O	1:A:370:GLU:N	2.48	0.46
5:H:70:THR:HG22	5:H:71:ARG:N	2.30	0.46
1:B:323:ILE:O	3:M:54:ARG:NH2	2.50	0.45
1:B:368:ASP:O	1:B:370:GLU:N	2.48	0.45
1:C:125:LEU:HD21	1:C:309:ILE:HG21	2.00	0.44
1:A:323:ILE:O	3:I:54:ARG:NH2	2.50	0.44
1:B:595:LEU:HD21	1:C:545:LEU:HD23	2.00	0.44
1:A:595:LEU:HD21	1:B:545:LEU:HD23	2.00	0.44
4:R:33:LEU:HD21	4:R:88:CYS:HB2	2.00	0.44
1:A:125:LEU:HD21	1:A:309:ILE:HG21	2.00	0.44
4:N:31:SER:HA	4:N:50:GLY:HA2	1.99	0.44
5:K:93:ALA:HB1	5:K:100(F):PHE:HB3	2.00	0.44
1:C:297:THR:OG1	1:C:443:ILE:O	2.31	0.44
4:L:31:SER:HA	4:L:50:GLY:HA2	2.00	0.43
1:B:96:TRP:CG	1:B:275:GLU:HG3	2.53	0.43
4:N:33:LEU:HD21	4:N:88:CYS:HB2	2.00	0.43
1:A:96:TRP:CG	1:A:275:GLU:HG3	2.53	0.43
5:K:39:GLN:HB3	5:K:89:VAL:HB	2.00	0.43
5:H:93:ALA:HB1	5:H:100(F):PHE:HB3	2.00	0.43
4:R:31:SER:HA	4:R:50:GLY:HA2	1.99	0.43
1:B:203:GLN:HG3	1:B:435:TYR:HD2	1.84	0.43
5:P:39:GLN:HB3	5:P:89:VAL:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:33:LEU:HD21	4:L:88:CYS:HB2	2.00	0.43
1:B:125:LEU:HD21	1:B:309:ILE:HG21	2.00	0.43
1:C:96:TRP:CG	1:C:275:GLU:HG3	2.53	0.43
1:C:203:GLN:HG3	1:C:435:TYR:HD2	1.84	0.43
1:A:545:LEU:HD23	1:C:595:LEU:HD21	2.00	0.42
2:G:95:ASN:HD21	2:G:100(M):MET:HE2	1.84	0.42
1:B:297:THR:OG1	1:B:443:ILE:O	2.31	0.42
2:O:95:ASN:HD21	2:O:100(M):MET:HE2	1.84	0.42
2:J:95:ASN:HD21	2:J:100(M):MET:HE2	1.84	0.42
5:P:98:LEU:HD13	5:P:98:LEU:HA	1.77	0.42
5:P:93:ALA:HB1	5:P:100(F):PHE:HB3	2.00	0.42
2:G:96:ALA:HB3	2:G:100(K):TYR:HB3	2.02	0.42
5:H:39:GLN:HB3	5:H:89:VAL:HB	2.00	0.42
2:J:96:ALA:HB3	2:J:100(K):TYR:HB3	2.02	0.42
3:M:61:ARG:NH1	3:M:77:GLY:O	2.53	0.41
1:A:203:GLN:HG3	1:A:435:TYR:HD2	1.84	0.41
5:K:98:LEU:HD13	5:K:98:LEU:HA	1.77	0.41
3:Q:61:ARG:NH1	3:Q:77:GLY:O	2.53	0.41
1:A:295:GLU:HG2	9:U:1:NAG:H81	2.03	0.41
1:C:295:GLU:HG2	9:i:1:NAG:H81	2.03	0.41
3:I:61:ARG:NH1	3:I:77:GLY:O	2.53	0.41
2:O:48:ILE:HA	2:O:63:LEU:HD23	2.03	0.41
2:G:48:ILE:HA	2:G:63:LEU:HD23	2.03	0.41
1:B:295:GLU:HG2	9:b:1:NAG:H81	2.03	0.40
2:O:96:ALA:HB3	2:O:100(K):TYR:HB3	2.02	0.40
2:J:48:ILE:HA	2:J:63:LEU:HD23	2.03	0.40
1:C:323:ILE:O	3:Q:54:ARG:NH2	2.50	0.40
1:C:117:LYS:HE2	1:C:117:LYS:HB2	1.93	0.40
4:R:87:TYR:CE2	5:P:45:LEU:HG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/654 (78%)	477 (93%)	34 (7%)	0	100	100
1	B	511/654 (78%)	477 (93%)	34 (7%)	0	100	100
1	C	511/654 (78%)	477 (93%)	34 (7%)	0	100	100
2	G	124/233 (53%)	119 (96%)	5 (4%)	0	100	100
2	J	124/233 (53%)	119 (96%)	5 (4%)	0	100	100
2	O	124/233 (53%)	119 (96%)	5 (4%)	0	100	100
3	I	104/214 (49%)	100 (96%)	4 (4%)	0	100	100
3	M	104/214 (49%)	100 (96%)	4 (4%)	0	100	100
3	Q	104/214 (49%)	100 (96%)	4 (4%)	0	100	100
4	L	100/211 (47%)	91 (91%)	9 (9%)	0	100	100
4	N	100/211 (47%)	91 (91%)	9 (9%)	0	100	100
4	R	100/211 (47%)	91 (91%)	9 (9%)	0	100	100
5	H	117/226 (52%)	104 (89%)	13 (11%)	0	100	100
5	K	117/226 (52%)	104 (89%)	13 (11%)	0	100	100
5	P	117/226 (52%)	104 (89%)	13 (11%)	0	100	100
All	All	2868/4614 (62%)	2673 (93%)	195 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	471/566 (83%)	470 (100%)	1 (0%)	87	85
1	B	471/566 (83%)	470 (100%)	1 (0%)	87	85
1	C	471/566 (83%)	470 (100%)	1 (0%)	87	85
2	G	107/200 (54%)	107 (100%)	0	100	100
2	J	107/200 (54%)	107 (100%)	0	100	100
2	O	107/200 (54%)	107 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	90/183 (49%)	90 (100%)	0	100	100
3	M	90/183 (49%)	90 (100%)	0	100	100
3	Q	90/183 (49%)	90 (100%)	0	100	100
4	L	84/182 (46%)	82 (98%)	2 (2%)	43	62
4	N	84/182 (46%)	82 (98%)	2 (2%)	43	62
4	R	84/182 (46%)	82 (98%)	2 (2%)	43	62
5	H	99/192 (52%)	98 (99%)	1 (1%)	68	75
5	K	99/192 (52%)	98 (99%)	1 (1%)	68	75
5	P	99/192 (52%)	98 (99%)	1 (1%)	68	75
All	All	2553/3969 (64%)	2541 (100%)	12 (0%)	78	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	HIS
4	L	49	TYR
4	L	97	PHE
5	H	98	LEU
1	B	330	HIS
4	N	49	TYR
4	N	97	PHE
5	K	98	LEU
1	C	330	HIS
4	R	49	TYR
4	R	97	PHE
5	P	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	276	ASN
1	A	422	GLN
1	A	620	GLN
2	G	39	GLN
2	G	95	ASN
3	I	38	GLN
4	L	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	H	39	GLN
5	H	53	ASN
1	B	103	GLN
1	B	276	ASN
1	B	422	GLN
1	B	543	GLN
1	B	620	GLN
2	J	39	GLN
2	J	95	ASN
3	M	38	GLN
4	N	38	GLN
5	K	39	GLN
5	K	53	ASN
1	C	103	GLN
1	C	276	ASN
1	C	422	GLN
1	C	620	GLN
2	O	39	GLN
2	O	95	ASN
3	Q	38	GLN
4	R	38	GLN
5	P	39	GLN
5	P	53	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 ⓘ

66 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	D	1	6,1	14,14,15	0.72	0	17,19,21	0.89	1 (5%)
6	NAG	D	2	6	14,14,15	0.74	0	17,19,21	0.89	0
7	NAG	E	1	1,7	14,14,15	0.81	1 (7%)	17,19,21	1.91	2 (11%)
7	NAG	E	2	7	14,14,15	0.71	0	17,19,21	1.82	3 (17%)
7	BMA	E	3	7	11,11,12	0.81	0	15,15,17	0.95	1 (6%)
6	NAG	F	1	6,1	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
6	NAG	F	2	6	14,14,15	0.68	0	17,19,21	0.94	0
6	NAG	S	1	6,1	14,14,15	0.70	0	17,19,21	1.11	0
6	NAG	S	2	6	14,14,15	0.72	0	17,19,21	0.90	0
8	NAG	T	1	1,8	14,14,15	0.75	0	17,19,21	1.10	2 (11%)
8	NAG	T	2	8	14,14,15	0.74	0	17,19,21	0.86	0
8	BMA	T	3	8	11,11,12	0.87	0	15,15,17	2.36	5 (33%)
8	MAN	T	4	8	11,11,12	0.69	0	15,15,17	1.33	1 (6%)
8	MAN	T	5	8	11,11,12	0.68	0	15,15,17	1.35	1 (6%)
9	NAG	U	1	9,1	14,14,15	0.73	0	17,19,21	1.73	4 (23%)
9	NAG	U	2	9	14,14,15	0.87	1 (7%)	17,19,21	1.75	4 (23%)
9	BMA	U	3	9	11,11,12	0.99	0	15,15,17	2.67	6 (40%)
9	MAN	U	4	9	11,11,12	0.62	0	15,15,17	2.15	5 (33%)
9	MAN	U	5	9	11,11,12	0.73	0	15,15,17	1.32	1 (6%)
9	MAN	U	6	9	11,11,12	0.52	0	15,15,17	2.89	1 (6%)
6	NAG	V	1	6,1	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
6	NAG	V	2	6	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
6	NAG	W	1	6,1	14,14,15	0.71	0	17,19,21	0.89	1 (5%)
6	NAG	W	2	6	14,14,15	0.73	0	17,19,21	0.88	0
7	NAG	X	1	1,7	14,14,15	0.81	1 (7%)	17,19,21	1.91	2 (11%)
7	NAG	X	2	7	14,14,15	0.71	0	17,19,21	1.82	3 (17%)
7	BMA	X	3	7	11,11,12	0.81	0	15,15,17	0.95	1 (6%)
6	NAG	Y	1	6,1	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
6	NAG	Y	2	6	14,14,15	0.68	0	17,19,21	0.93	0
6	NAG	Z	1	6,1	14,14,15	0.70	0	17,19,21	1.11	0
6	NAG	Z	2	6	14,14,15	0.74	0	17,19,21	0.90	0
8	NAG	a	1	1,8	14,14,15	0.75	0	17,19,21	1.10	1 (5%)
8	NAG	a	2	8	14,14,15	0.73	0	17,19,21	0.86	0
8	BMA	a	3	8	11,11,12	0.87	0	15,15,17	2.36	5 (33%)
8	MAN	a	4	8	11,11,12	0.70	0	15,15,17	1.34	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	a	5	8	11,11,12	0.67	0	15,15,17	1.35	1 (6%)
9	NAG	b	1	9,1	14,14,15	0.74	0	17,19,21	1.72	4 (23%)
9	NAG	b	2	9	14,14,15	0.87	1 (7%)	17,19,21	1.75	4 (23%)
9	BMA	b	3	9	11,11,12	0.99	0	15,15,17	2.66	6 (40%)
9	MAN	b	4	9	11,11,12	0.62	0	15,15,17	2.15	5 (33%)
9	MAN	b	5	9	11,11,12	0.74	0	15,15,17	1.32	1 (6%)
9	MAN	b	6	9	11,11,12	0.53	0	15,15,17	2.89	1 (6%)
6	NAG	c	1	6,1	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
6	NAG	c	2	6	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
6	NAG	d	1	6,1	14,14,15	0.72	0	17,19,21	0.89	1 (5%)
6	NAG	d	2	6	14,14,15	0.74	0	17,19,21	0.89	0
7	NAG	e	1	1,7	14,14,15	0.81	1 (7%)	17,19,21	1.91	2 (11%)
7	NAG	e	2	7	14,14,15	0.71	0	17,19,21	1.82	3 (17%)
7	BMA	e	3	7	11,11,12	0.80	0	15,15,17	0.95	1 (6%)
6	NAG	f	1	6,1	14,14,15	0.72	0	17,19,21	0.83	1 (5%)
6	NAG	f	2	6	14,14,15	0.67	0	17,19,21	0.94	0
6	NAG	g	1	6,1	14,14,15	0.69	0	17,19,21	1.11	0
6	NAG	g	2	6	14,14,15	0.73	0	17,19,21	0.90	0
8	NAG	h	1	1,8	14,14,15	0.74	0	17,19,21	1.10	2 (11%)
8	NAG	h	2	8	14,14,15	0.74	0	17,19,21	0.86	0
8	BMA	h	3	8	11,11,12	0.87	0	15,15,17	2.37	5 (33%)
8	MAN	h	4	8	11,11,12	0.69	0	15,15,17	1.33	1 (6%)
8	MAN	h	5	8	11,11,12	0.69	0	15,15,17	1.35	1 (6%)
9	NAG	i	1	9,1	14,14,15	0.74	0	17,19,21	1.73	4 (23%)
9	NAG	i	2	9	14,14,15	0.86	1 (7%)	17,19,21	1.74	4 (23%)
9	BMA	i	3	9	11,11,12	0.99	0	15,15,17	2.67	6 (40%)
9	MAN	i	4	9	11,11,12	0.63	0	15,15,17	2.15	5 (33%)
9	MAN	i	5	9	11,11,12	0.73	0	15,15,17	1.32	1 (6%)
9	MAN	i	6	9	11,11,12	0.53	0	15,15,17	2.89	1 (6%)
6	NAG	j	1	6,1	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
6	NAG	j	2	6	14,14,15	0.72	0	17,19,21	0.92	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	D	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
7	NAG	E	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	E	2	7	-	1/6/23/26	0/1/1/1
7	BMA	E	3	7	-	0/2/19/22	0/1/1/1
6	NAG	F	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	1/6/23/26	0/1/1/1
8	NAG	T	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	MAN	T	4	8	-	2/2/19/22	0/1/1/1
8	MAN	T	5	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	U	2	9	-	0/6/23/26	0/1/1/1
9	BMA	U	3	9	-	2/2/19/22	0/1/1/1
9	MAN	U	4	9	-	2/2/19/22	0/1/1/1
9	MAN	U	5	9	-	1/2/19/22	0/1/1/1
9	MAN	U	6	9	-	2/2/19/22	0/1/1/1
6	NAG	V	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	V	2	6	-	1/6/23/26	0/1/1/1
6	NAG	W	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	0/6/23/26	0/1/1/1
7	NAG	X	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	1/6/23/26	0/1/1/1
7	BMA	X	3	7	-	0/2/19/22	0/1/1/1
6	NAG	Y	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	1/6/23/26	0/1/1/1
8	NAG	a	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1
8	BMA	a	3	8	-	0/2/19/22	0/1/1/1
8	MAN	a	4	8	-	2/2/19/22	0/1/1/1
8	MAN	a	5	8	-	0/2/19/22	0/1/1/1
9	NAG	b	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	b	2	9	-	0/6/23/26	0/1/1/1
9	BMA	b	3	9	-	2/2/19/22	0/1/1/1
9	MAN	b	4	9	-	2/2/19/22	0/1/1/1
9	MAN	b	5	9	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	2	NAG	C1-C2	2.18	1.55	1.52
9	U	2	NAG	C1-C2	2.16	1.55	1.52
9	i	2	NAG	C1-C2	2.16	1.55	1.52
7	X	1	NAG	C1-C2	2.14	1.55	1.52
7	E	1	NAG	C1-C2	2.12	1.55	1.52
7	e	1	NAG	C1-C2	2.11	1.55	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	6	MAN	C1-O5-C5	10.52	126.29	112.19
9	U	6	MAN	C1-O5-C5	10.52	126.28	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	6	MAN	C1-O5-C5	10.51	126.27	112.19
9	i	3	BMA	C1-O5-C5	7.78	122.62	112.19
9	U	3	BMA	C1-O5-C5	7.76	122.58	112.19
9	b	3	BMA	C1-O5-C5	7.75	122.57	112.19
8	h	3	BMA	C1-O5-C5	7.03	121.60	112.19
8	a	3	BMA	C1-O5-C5	7.02	121.59	112.19
8	T	3	BMA	C1-O5-C5	7.01	121.58	112.19
7	X	1	NAG	C2-N2-C7	6.15	131.14	122.90
7	E	1	NAG	C2-N2-C7	6.14	131.13	122.90
7	e	1	NAG	C2-N2-C7	6.12	131.10	122.90
7	X	2	NAG	C2-N2-C7	5.88	130.78	122.90
7	E	2	NAG	C2-N2-C7	5.88	130.78	122.90
7	e	2	NAG	C2-N2-C7	5.88	130.78	122.90
9	b	4	MAN	C1-O5-C5	5.83	120.00	112.19
9	i	4	MAN	C1-O5-C5	5.81	119.97	112.19
9	U	4	MAN	C1-O5-C5	5.80	119.95	112.19
9	U	2	NAG	C1-O5-C5	4.78	118.59	112.19
9	b	2	NAG	C1-O5-C5	4.77	118.58	112.19
9	i	2	NAG	C1-O5-C5	4.76	118.56	112.19
8	a	5	MAN	C1-O5-C5	4.37	118.04	112.19
8	T	5	MAN	C1-O5-C5	4.35	118.02	112.19
8	h	5	MAN	C1-O5-C5	4.34	118.01	112.19
8	T	4	MAN	C1-O5-C5	4.04	117.61	112.19
8	a	4	MAN	C1-O5-C5	4.04	117.61	112.19
8	h	4	MAN	C1-O5-C5	4.03	117.59	112.19
9	U	5	MAN	C1-O5-C5	3.98	117.52	112.19
9	b	5	MAN	C1-O5-C5	3.98	117.51	112.19
9	i	5	MAN	C1-O5-C5	3.96	117.50	112.19
9	i	1	NAG	O4-C4-C5	3.78	118.63	109.32
9	b	1	NAG	O4-C4-C5	3.78	118.63	109.32
9	U	1	NAG	O4-C4-C5	3.78	118.62	109.32
9	b	1	NAG	C1-O5-C5	3.55	116.94	112.19
9	i	1	NAG	C1-O5-C5	3.54	116.93	112.19
9	U	1	NAG	C1-O5-C5	3.54	116.93	112.19
9	i	3	BMA	C2-C3-C4	3.34	116.74	110.86
9	U	3	BMA	C2-C3-C4	3.34	116.73	110.86
9	b	3	BMA	C2-C3-C4	3.34	116.73	110.86
9	U	3	BMA	C3-C4-C5	3.31	116.24	110.23
9	i	3	BMA	C3-C4-C5	3.31	116.24	110.23
9	b	3	BMA	C3-C4-C5	3.31	116.23	110.23
7	E	3	BMA	C1-O5-C5	3.14	116.40	112.19
7	X	3	BMA	C1-O5-C5	3.13	116.38	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	3	BMA	C1-O5-C5	3.11	116.35	112.19
9	i	4	MAN	O3-C3-C4	3.03	117.52	110.38
9	U	4	MAN	O3-C3-C4	3.02	117.49	110.38
9	b	4	MAN	O3-C3-C4	3.01	117.47	110.38
8	T	3	BMA	C3-C4-C5	2.97	115.62	110.23
8	a	3	BMA	C3-C4-C5	2.97	115.61	110.23
7	X	1	NAG	C1-C2-N2	2.97	115.11	110.43
7	e	1	NAG	C1-C2-N2	2.97	115.11	110.43
8	h	3	BMA	C3-C4-C5	2.96	115.61	110.23
7	E	1	NAG	C1-C2-N2	2.96	115.09	110.43
9	U	4	MAN	C1-C2-C3	-2.88	105.45	109.64
9	i	4	MAN	C1-C2-C3	-2.87	105.47	109.64
9	b	4	MAN	C1-C2-C3	-2.85	105.49	109.64
9	b	3	BMA	O3-C3-C2	-2.75	104.44	110.05
9	U	3	BMA	O3-C3-C2	-2.75	104.45	110.05
9	i	3	BMA	O3-C3-C2	-2.74	104.45	110.05
9	U	1	NAG	C4-C3-C2	-2.72	107.03	111.02
9	i	1	NAG	C4-C3-C2	-2.72	107.04	111.02
9	b	1	NAG	C4-C3-C2	-2.71	107.04	111.02
8	a	3	BMA	C2-C3-C4	2.65	115.53	110.86
8	h	3	BMA	C2-C3-C4	2.65	115.52	110.86
8	T	3	BMA	C2-C3-C4	2.65	115.52	110.86
9	i	2	NAG	C3-C4-C5	-2.62	105.47	110.23
9	b	2	NAG	C3-C4-C5	-2.61	105.50	110.23
8	h	3	BMA	O4-C4-C3	-2.61	104.23	110.38
9	U	2	NAG	C3-C4-C5	-2.60	105.51	110.23
8	T	3	BMA	O4-C4-C3	-2.60	104.24	110.38
8	a	3	BMA	O4-C4-C3	-2.60	104.25	110.38
7	e	2	NAG	O7-C7-N2	2.59	126.55	121.98
7	X	2	NAG	O7-C7-N2	2.58	126.55	121.98
9	U	4	MAN	O2-C2-C3	2.58	115.50	110.15
7	E	2	NAG	O7-C7-N2	2.58	126.55	121.98
9	b	4	MAN	O2-C2-C3	2.58	115.50	110.15
7	E	2	NAG	C1-O5-C5	2.57	115.63	112.19
9	i	4	MAN	O2-C2-C3	2.57	115.47	110.15
7	X	2	NAG	C1-O5-C5	2.56	115.62	112.19
8	h	1	NAG	C1-O5-C5	2.55	115.60	112.19
8	T	1	NAG	C1-O5-C5	2.55	115.60	112.19
7	e	2	NAG	C1-O5-C5	2.55	115.60	112.19
8	a	1	NAG	C1-O5-C5	2.53	115.57	112.19
9	b	2	NAG	O3-C3-C2	-2.48	104.25	109.40
9	i	2	NAG	O3-C3-C2	-2.48	104.25	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	2	NAG	O3-C3-C2	-2.47	104.27	109.40
9	b	3	BMA	O5-C5-C4	2.34	116.52	110.83
9	U	3	BMA	O5-C5-C4	2.33	116.49	110.83
9	U	2	NAG	C2-N2-C7	2.32	126.01	122.90
9	i	3	BMA	O5-C5-C4	2.32	116.47	110.83
9	b	2	NAG	C2-N2-C7	2.31	126.00	122.90
9	i	2	NAG	C2-N2-C7	2.30	125.98	122.90
6	j	1	NAG	O5-C1-C2	-2.29	107.75	111.29
6	V	1	NAG	O5-C1-C2	-2.28	107.76	111.29
6	d	1	NAG	O5-C1-C2	-2.28	107.77	111.29
6	W	1	NAG	O5-C1-C2	-2.27	107.78	111.29
6	D	1	NAG	O5-C1-C2	-2.26	107.79	111.29
6	c	1	NAG	O5-C1-C2	-2.26	107.80	111.29
9	b	3	BMA	O4-C4-C3	-2.24	105.10	110.38
9	U	3	BMA	O4-C4-C3	-2.23	105.12	110.38
9	i	3	BMA	O4-C4-C3	-2.23	105.12	110.38
6	Y	1	NAG	O5-C1-C2	-2.18	107.92	111.29
6	f	1	NAG	O5-C1-C2	-2.17	107.93	111.29
9	i	1	NAG	C2-N2-C7	-2.15	120.02	122.90
6	F	1	NAG	O5-C1-C2	-2.15	107.96	111.29
9	U	1	NAG	C2-N2-C7	-2.15	120.02	122.90
9	b	1	NAG	C2-N2-C7	-2.14	120.04	122.90
9	i	4	MAN	O2-C2-C1	-2.14	104.33	109.22
9	b	4	MAN	O2-C2-C1	-2.13	104.34	109.22
9	U	4	MAN	O2-C2-C1	-2.12	104.36	109.22
8	T	3	BMA	O5-C5-C4	2.10	115.94	110.83
8	a	3	BMA	O5-C5-C4	2.10	115.93	110.83
8	h	3	BMA	O5-C5-C4	2.09	115.92	110.83
6	j	2	NAG	O5-C1-C2	-2.06	108.10	111.29
6	c	2	NAG	O5-C1-C2	-2.06	108.10	111.29
6	V	2	NAG	O5-C1-C2	-2.06	108.11	111.29
8	h	1	NAG	C2-N2-C7	2.02	125.60	122.90
8	T	1	NAG	C2-N2-C7	2.02	125.60	122.90

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	U	6	MAN	O5-C5-C6-O6
9	b	6	MAN	O5-C5-C6-O6
9	i	6	MAN	O5-C5-C6-O6
8	T	4	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	a	4	MAN	O5-C5-C6-O6
8	h	4	MAN	O5-C5-C6-O6
9	U	3	BMA	O5-C5-C6-O6
9	U	4	MAN	O5-C5-C6-O6
9	b	3	BMA	O5-C5-C6-O6
9	b	4	MAN	O5-C5-C6-O6
9	i	4	MAN	O5-C5-C6-O6
9	i	3	BMA	O5-C5-C6-O6
8	T	4	MAN	C4-C5-C6-O6
8	a	4	MAN	C4-C5-C6-O6
8	h	4	MAN	C4-C5-C6-O6
9	U	6	MAN	C4-C5-C6-O6
9	b	6	MAN	C4-C5-C6-O6
9	i	6	MAN	C4-C5-C6-O6
9	U	5	MAN	O5-C5-C6-O6
9	b	5	MAN	O5-C5-C6-O6
9	i	5	MAN	O5-C5-C6-O6
9	U	4	MAN	C4-C5-C6-O6
9	b	4	MAN	C4-C5-C6-O6
9	i	4	MAN	C4-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
6	j	1	NAG	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	Y	2	NAG	O5-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
7	E	1	NAG	C3-C2-N2-C7
7	X	1	NAG	C3-C2-N2-C7
7	e	1	NAG	C3-C2-N2-C7
6	V	2	NAG	O5-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
7	E	1	NAG	C1-C2-N2-C7
7	X	1	NAG	C1-C2-N2-C7
7	e	1	NAG	C1-C2-N2-C7
7	E	2	NAG	C3-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
7	e	2	NAG	C3-C2-N2-C7
9	U	3	BMA	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

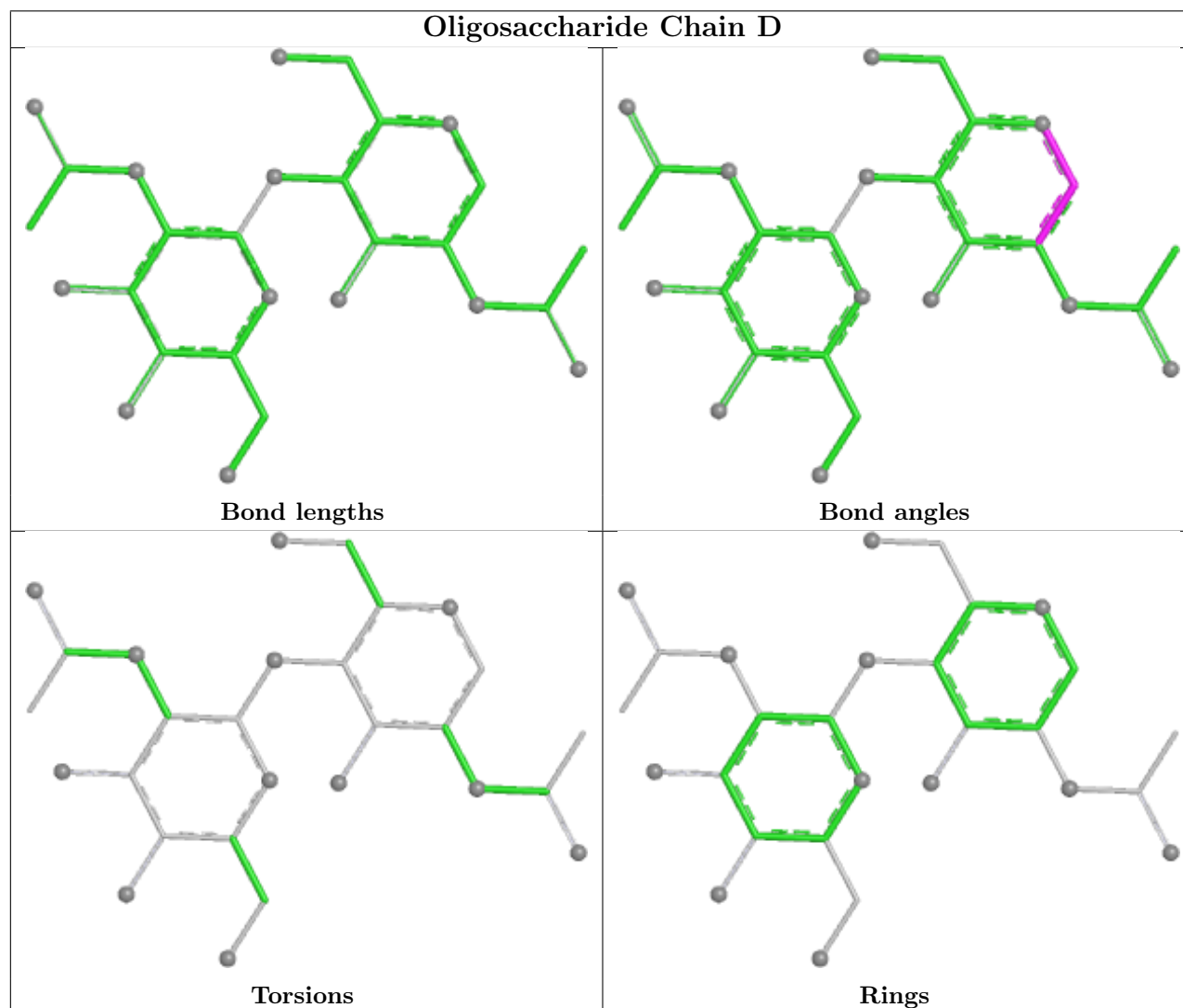
Mol	Chain	Res	Type	Atoms
9	b	3	BMA	C4-C5-C6-O6
9	i	3	BMA	C4-C5-C6-O6

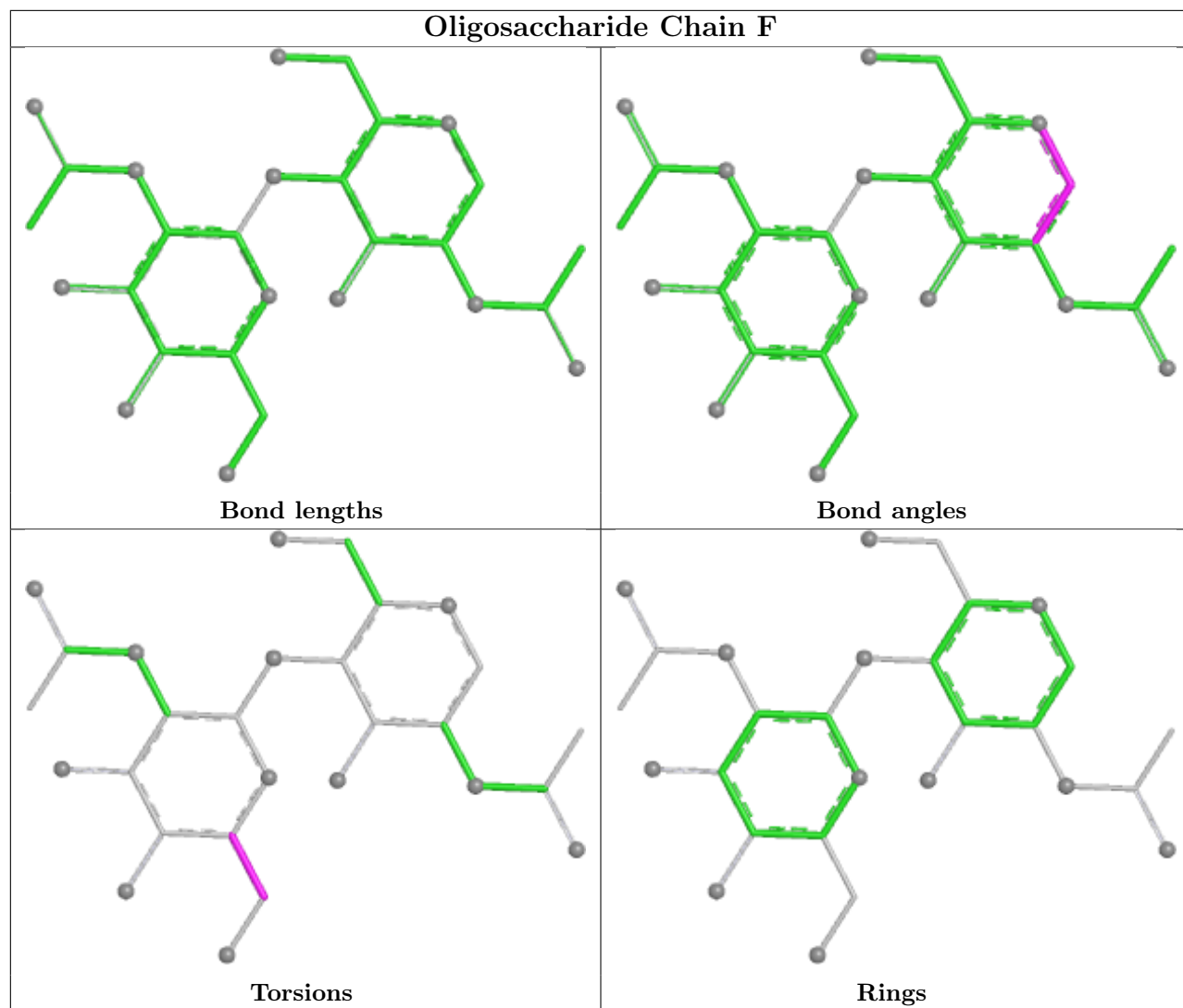
There are no ring outliers.

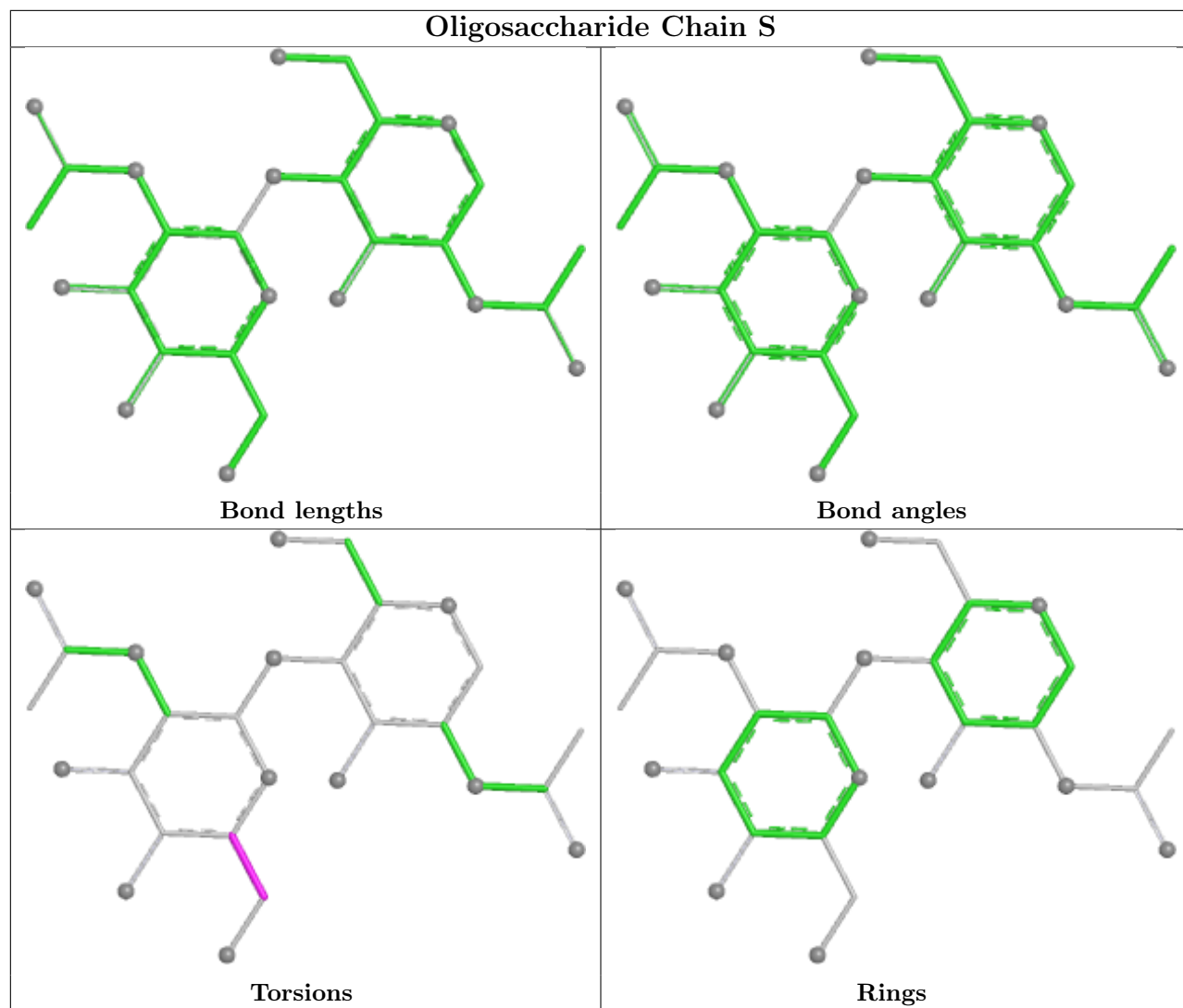
3 monomers are involved in 3 short contacts:

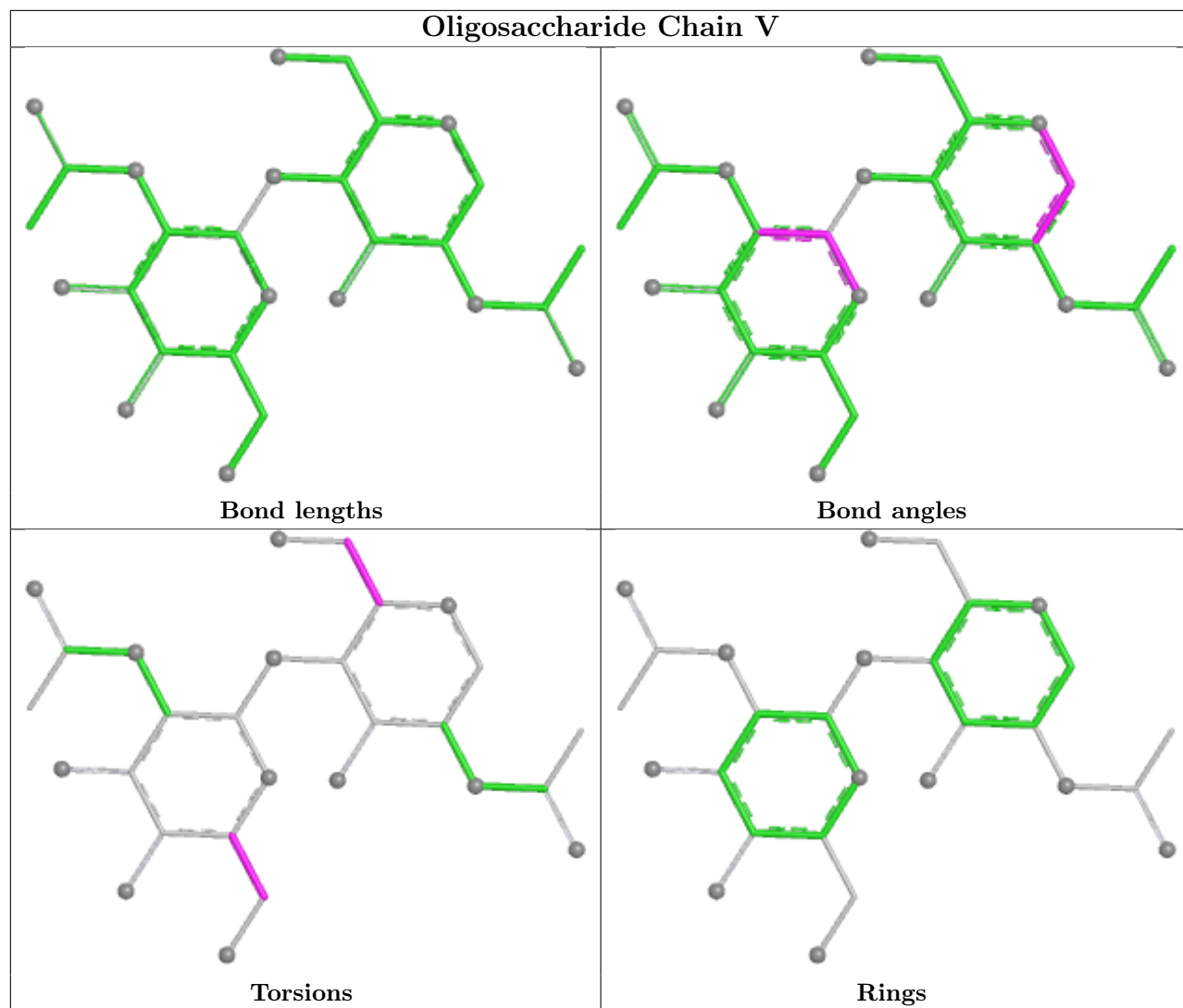
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	U	1	NAG	1	0
9	b	1	NAG	1	0
9	i	1	NAG	1	0

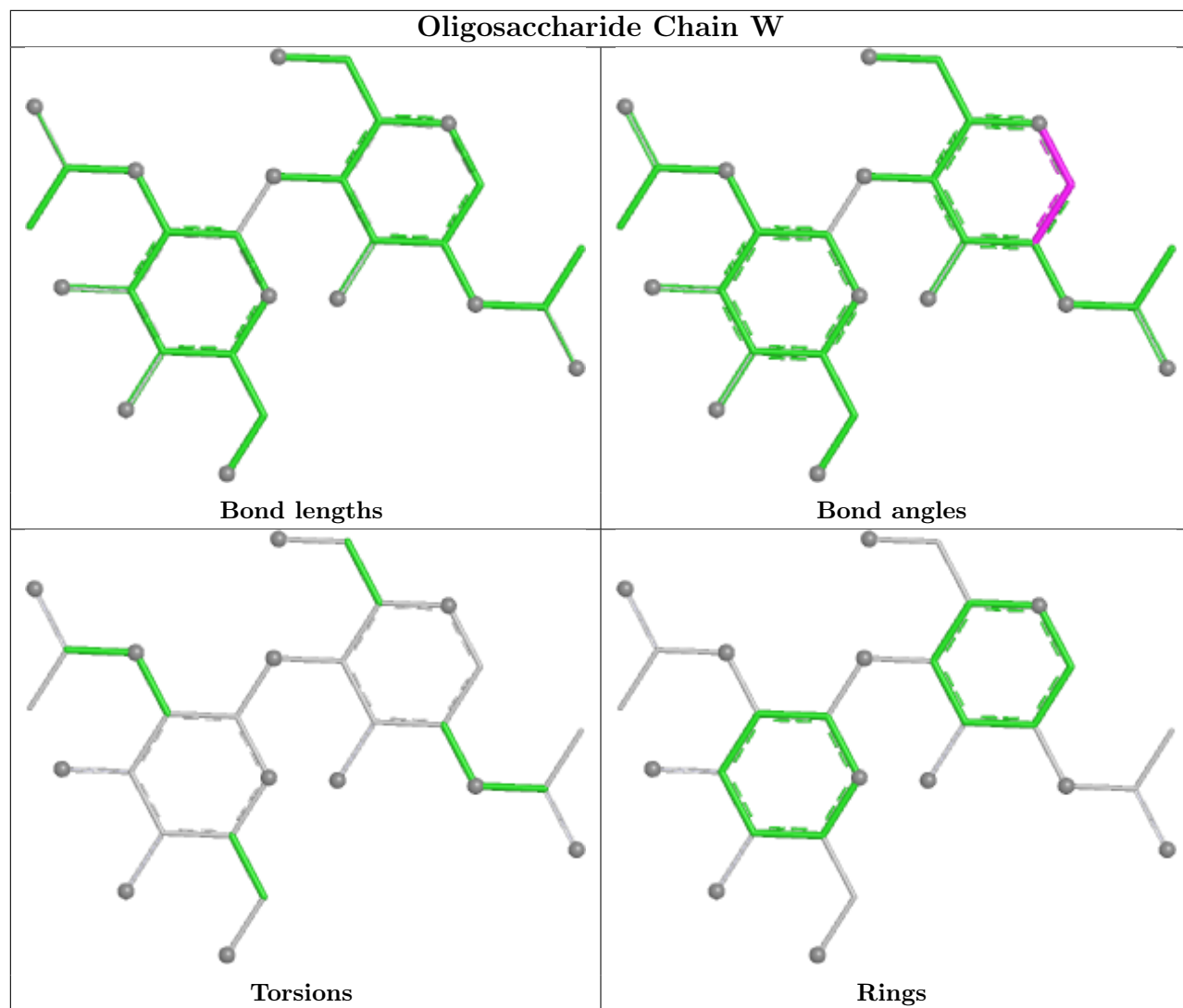
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

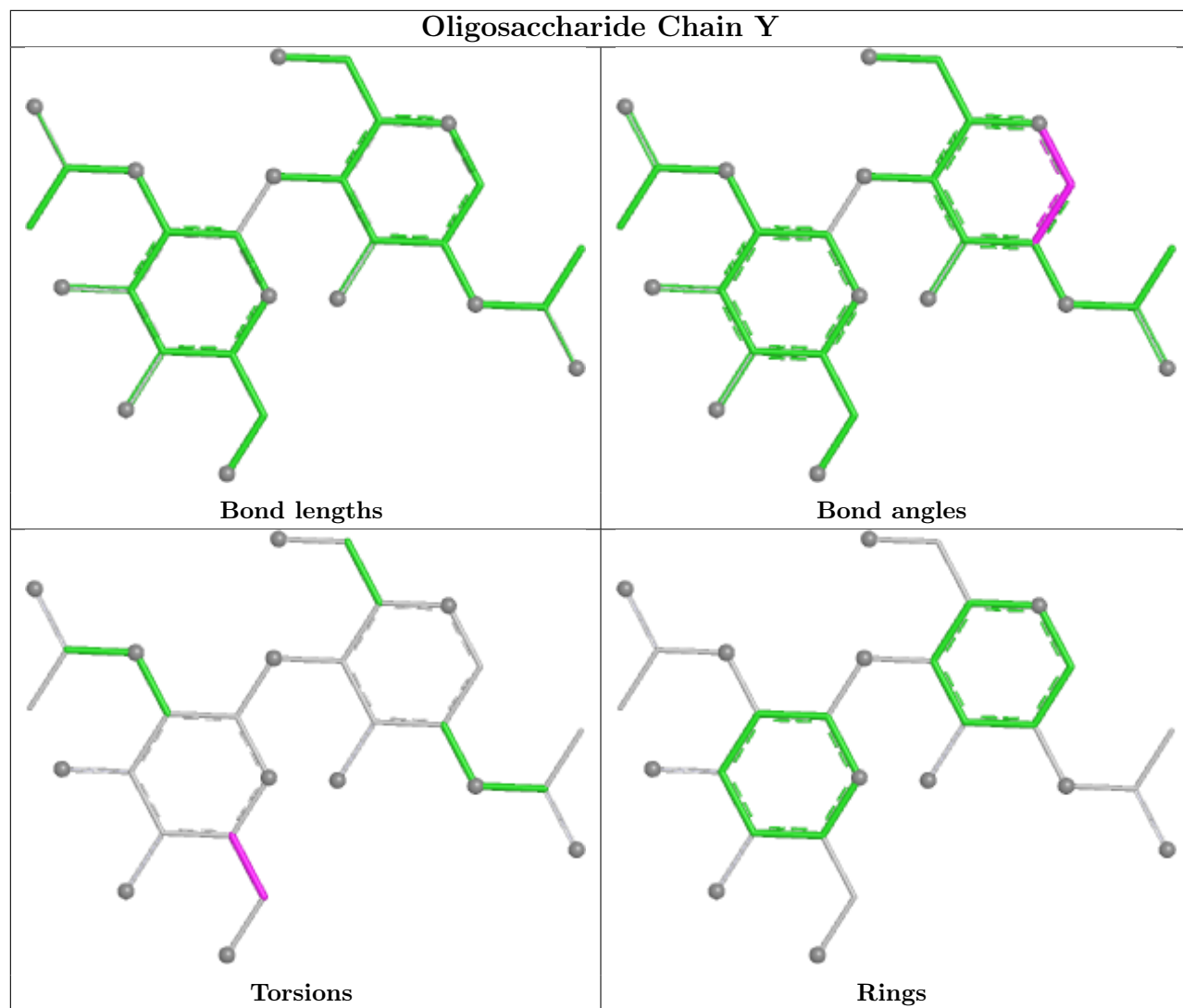


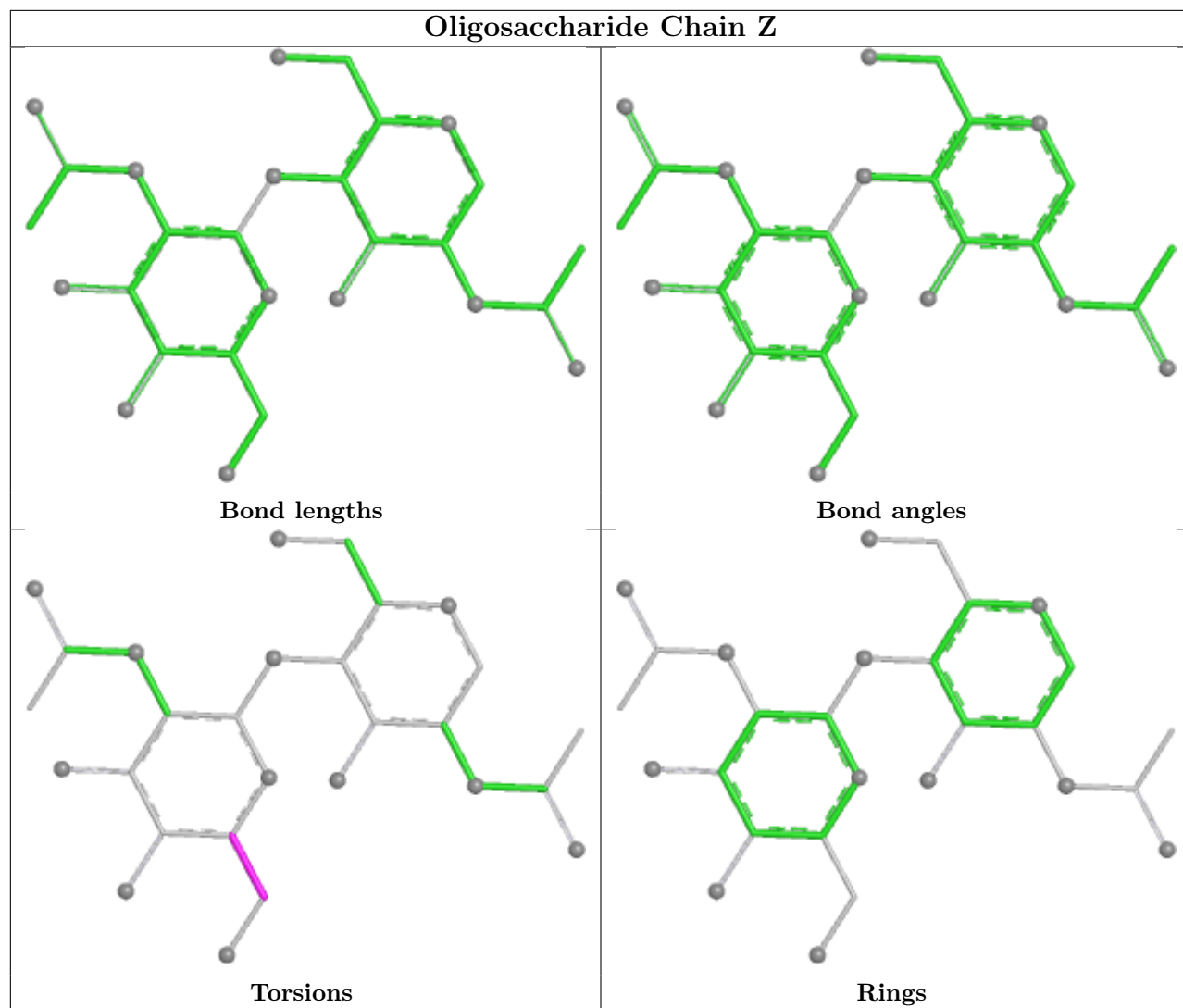


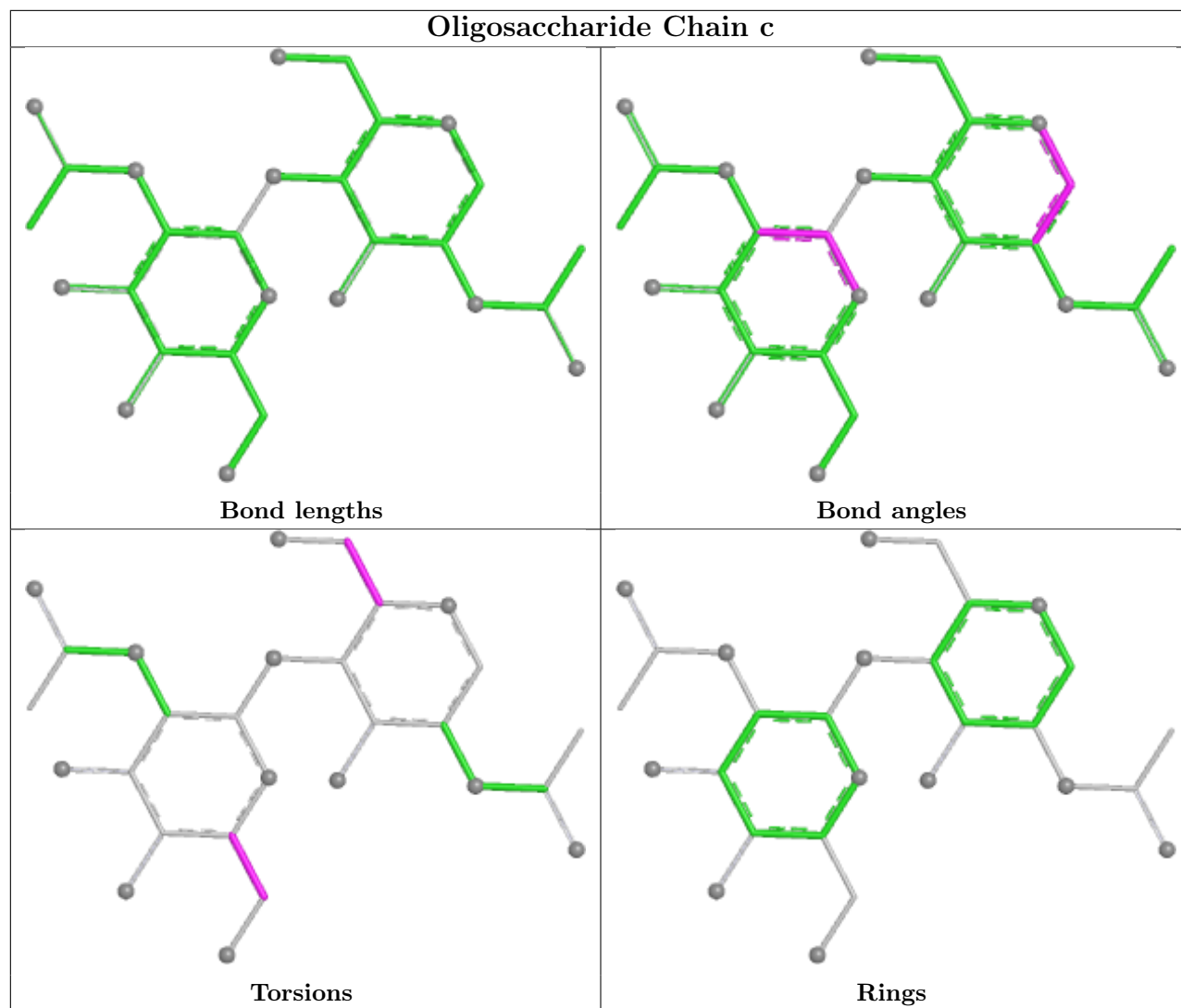


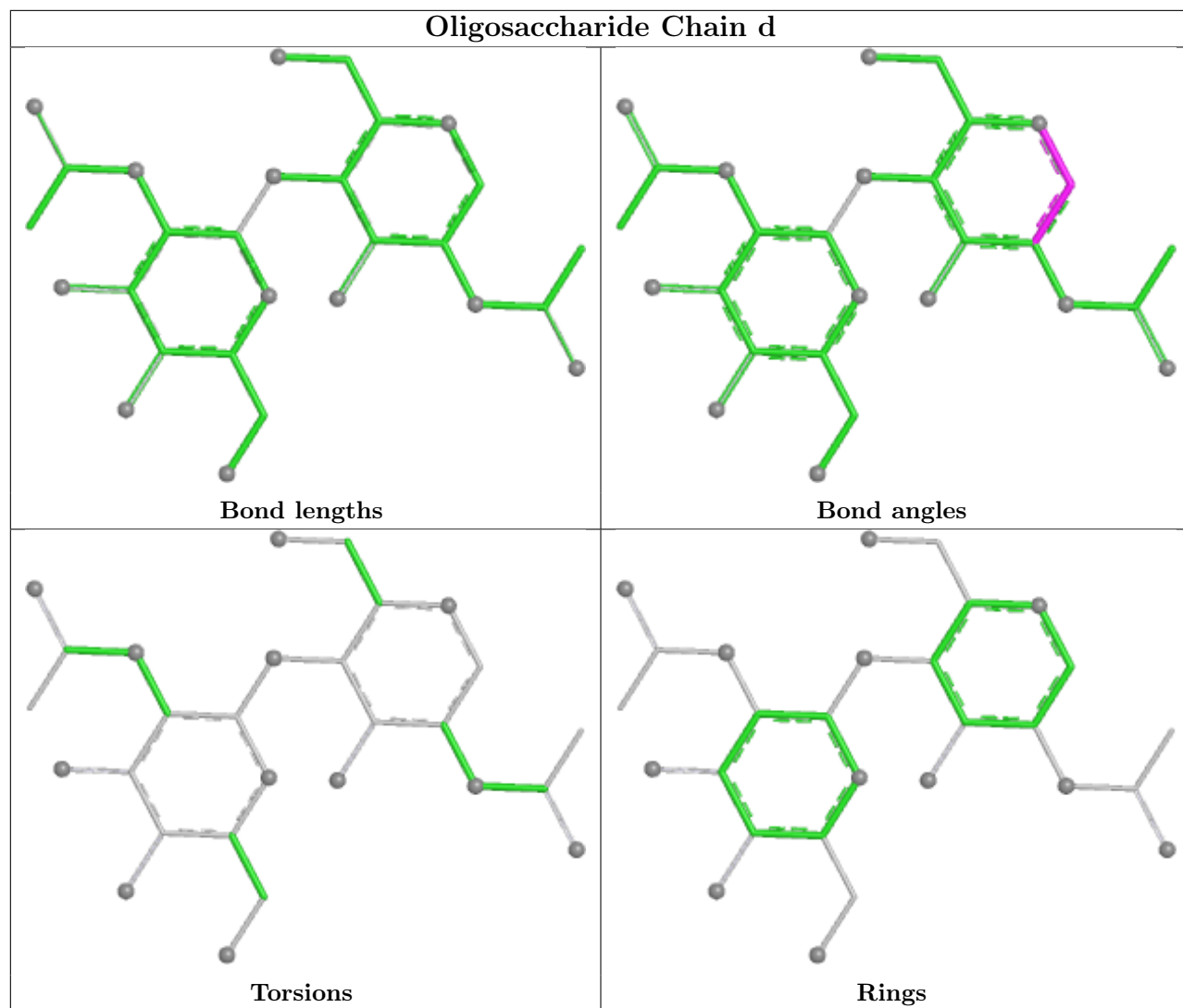


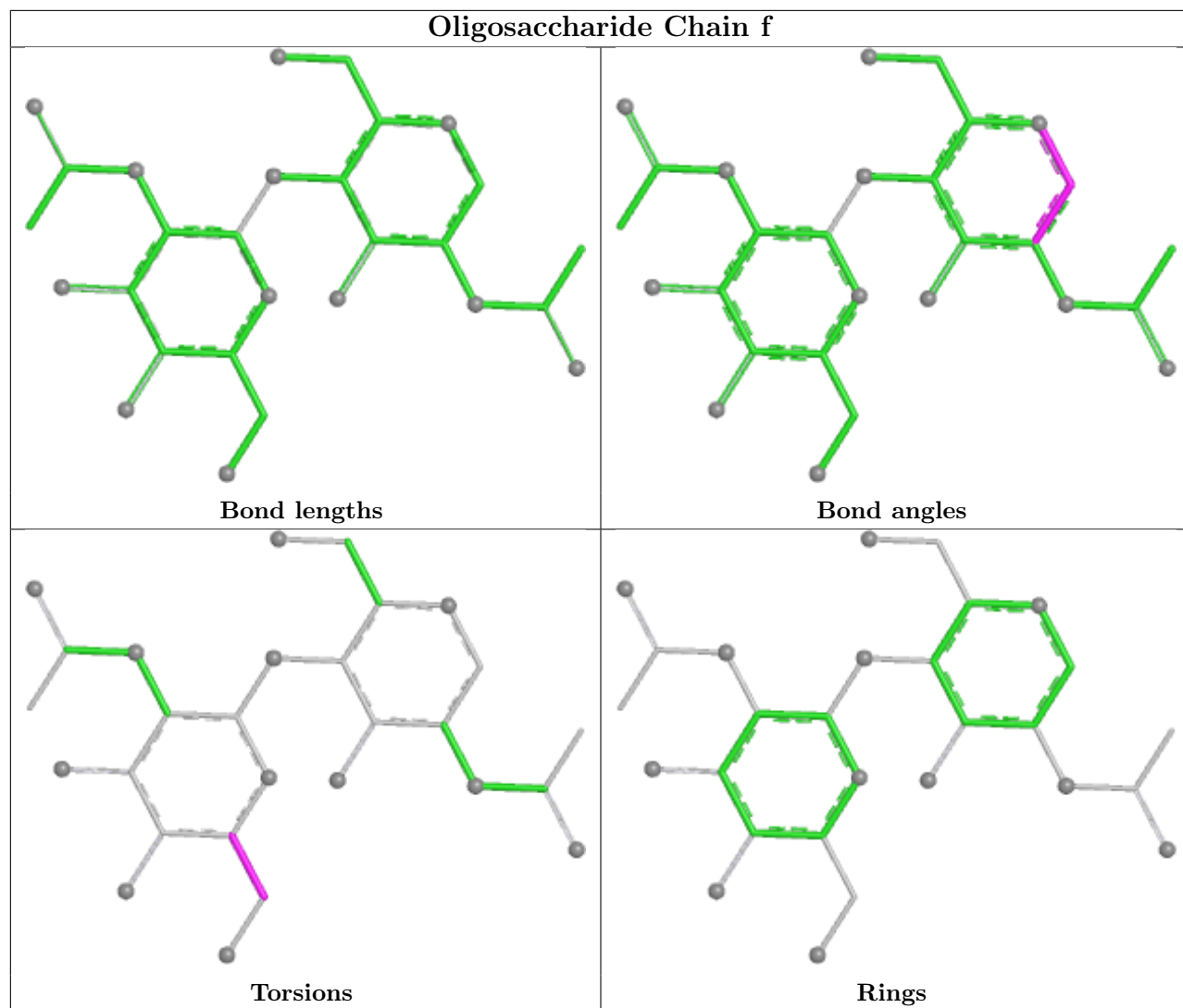


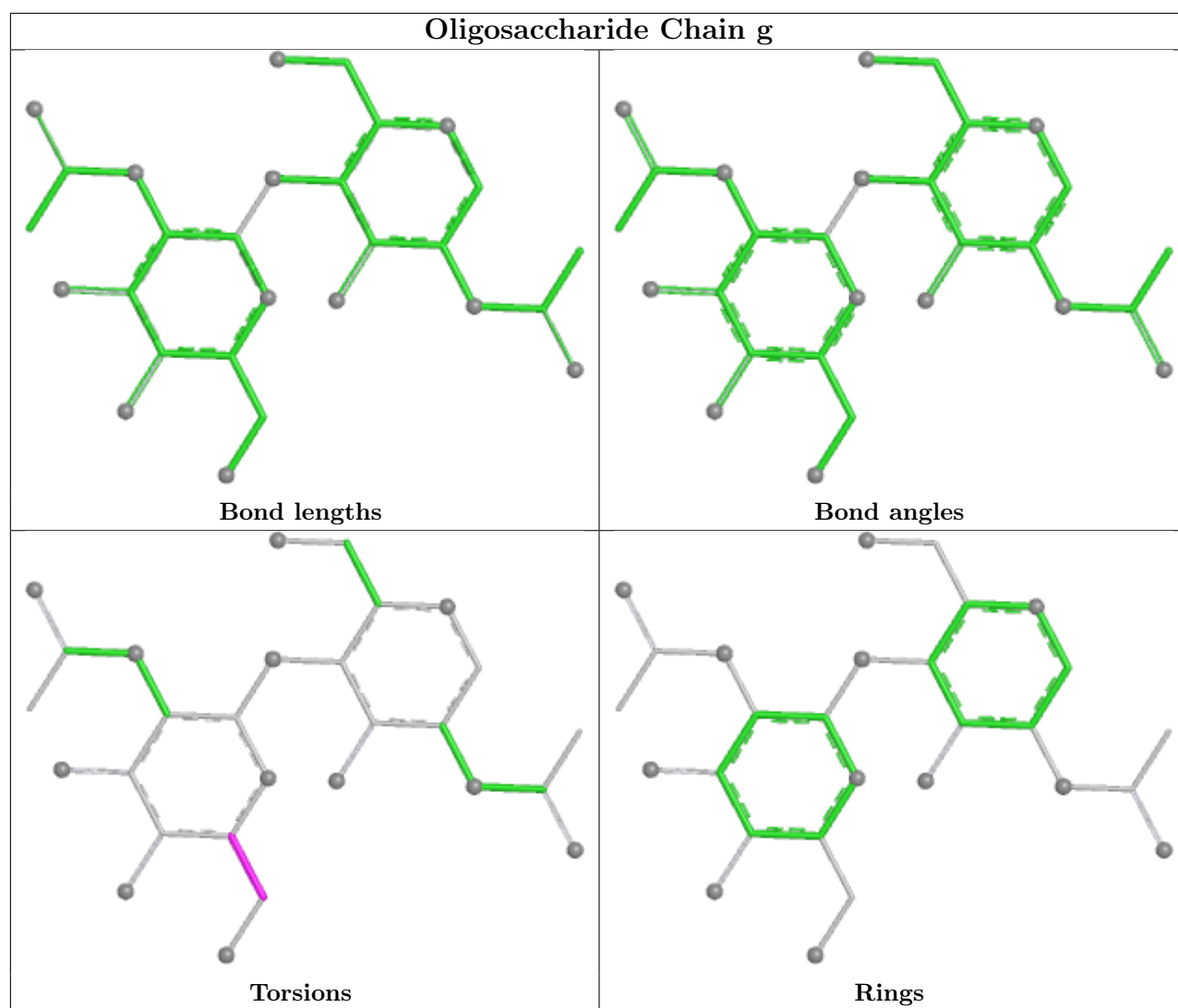


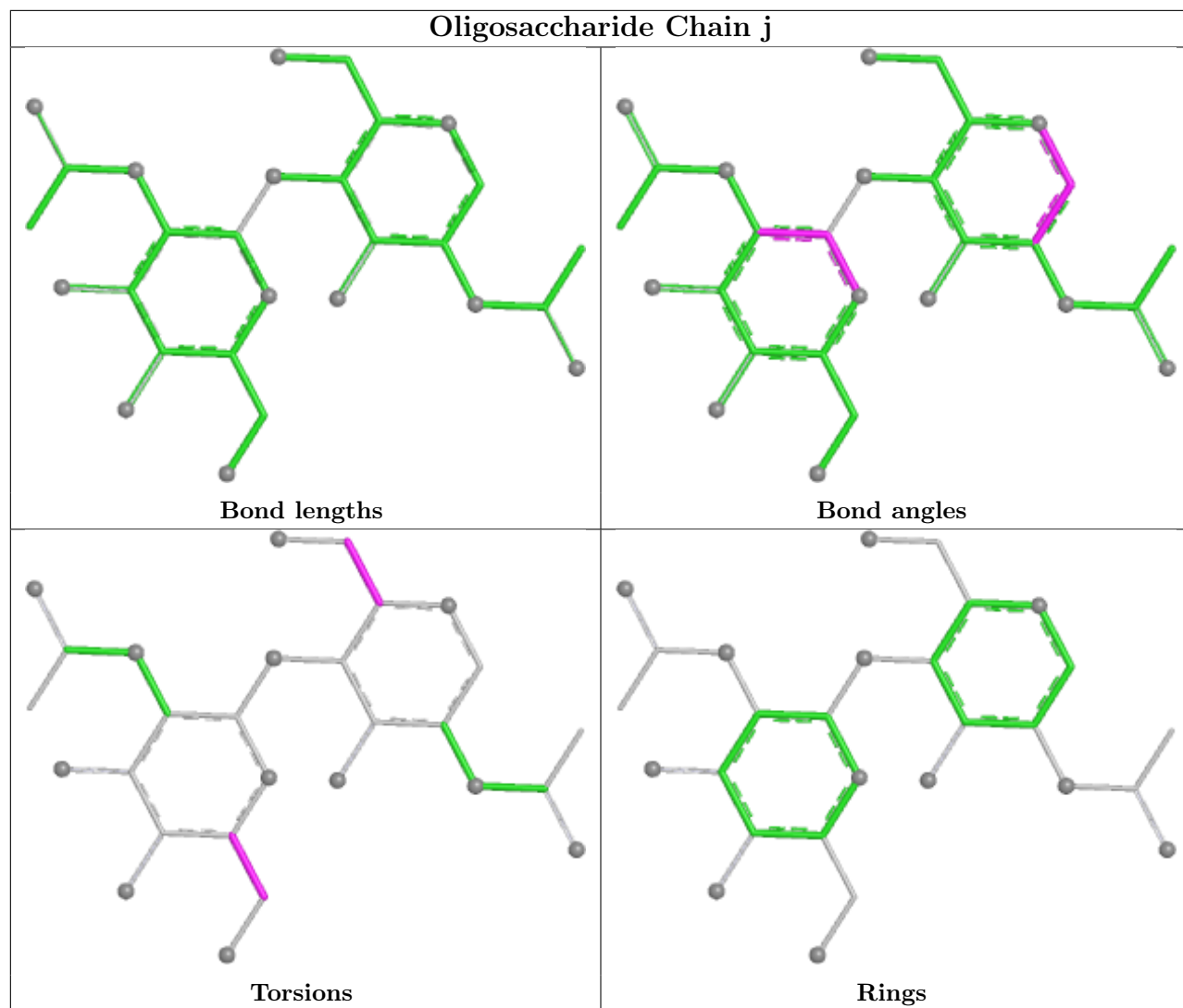


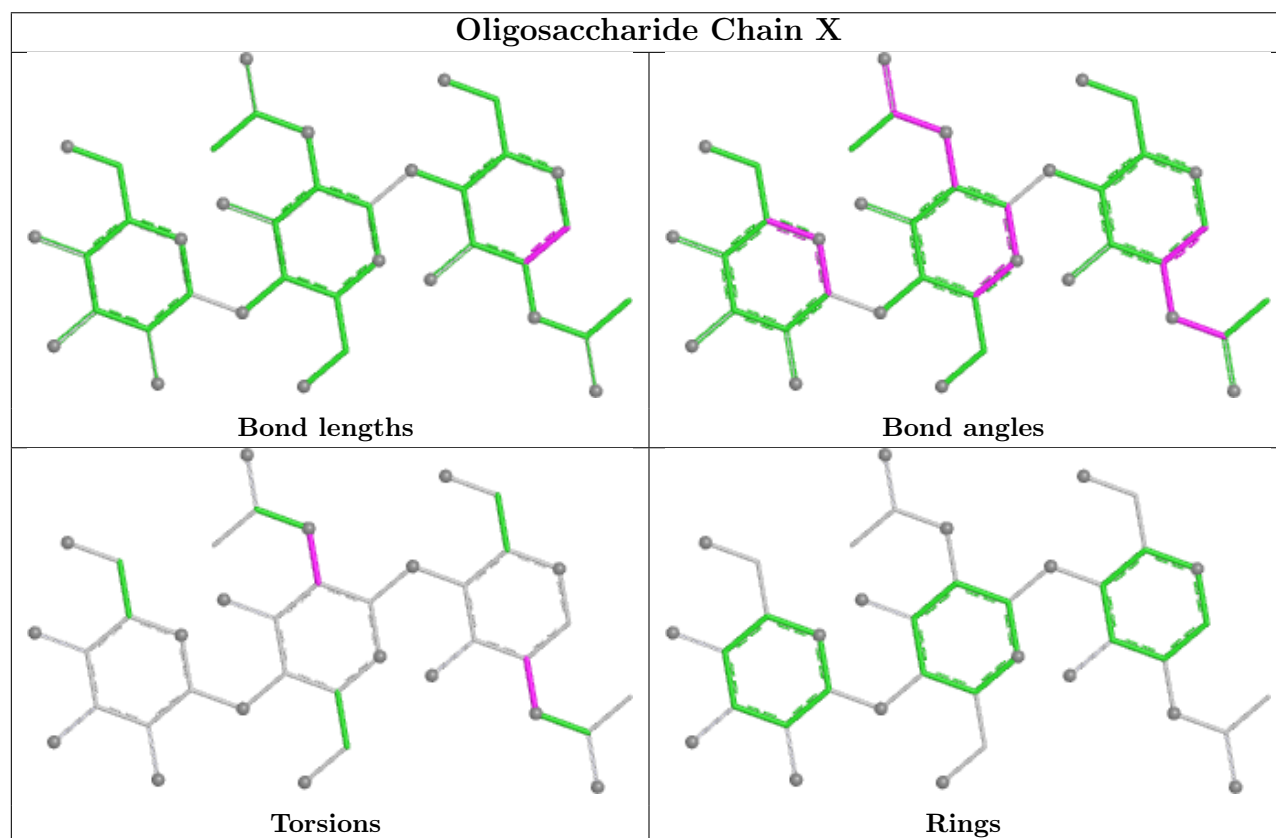
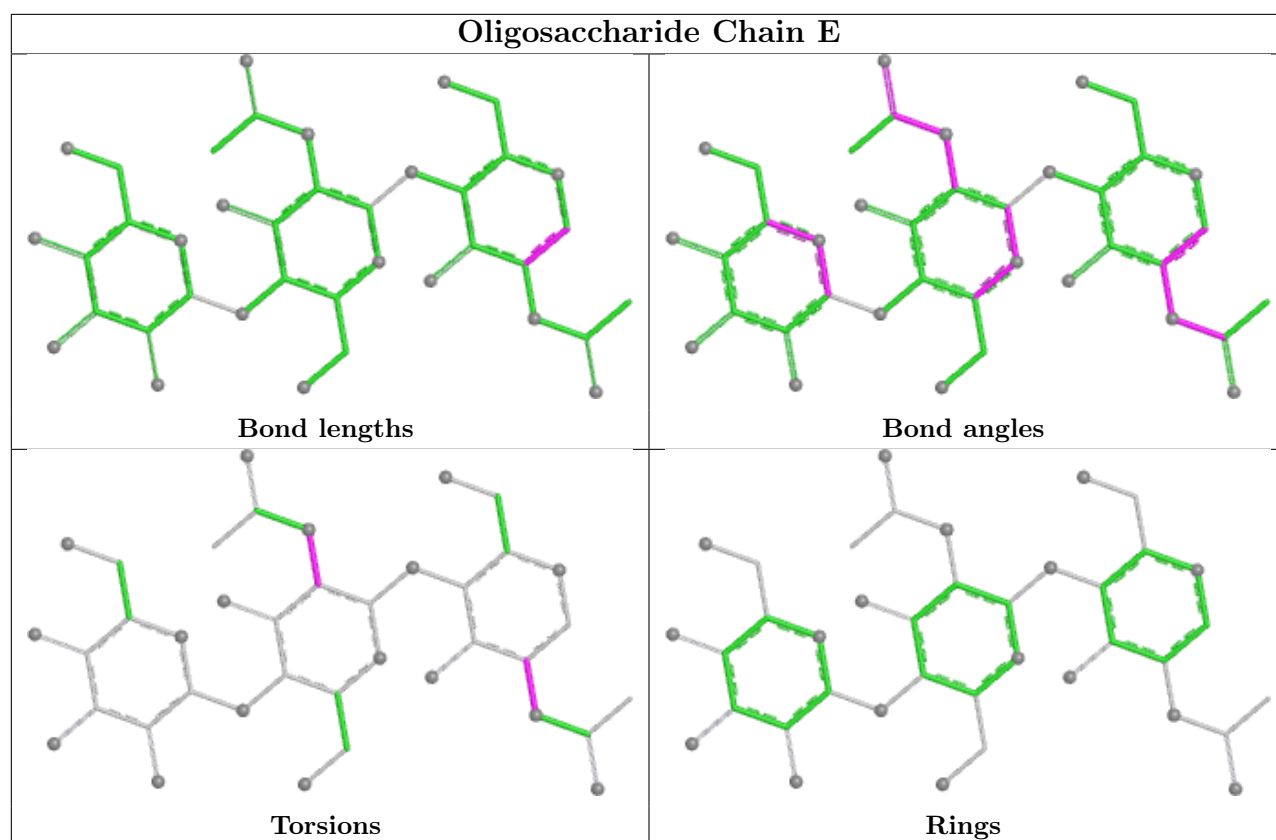


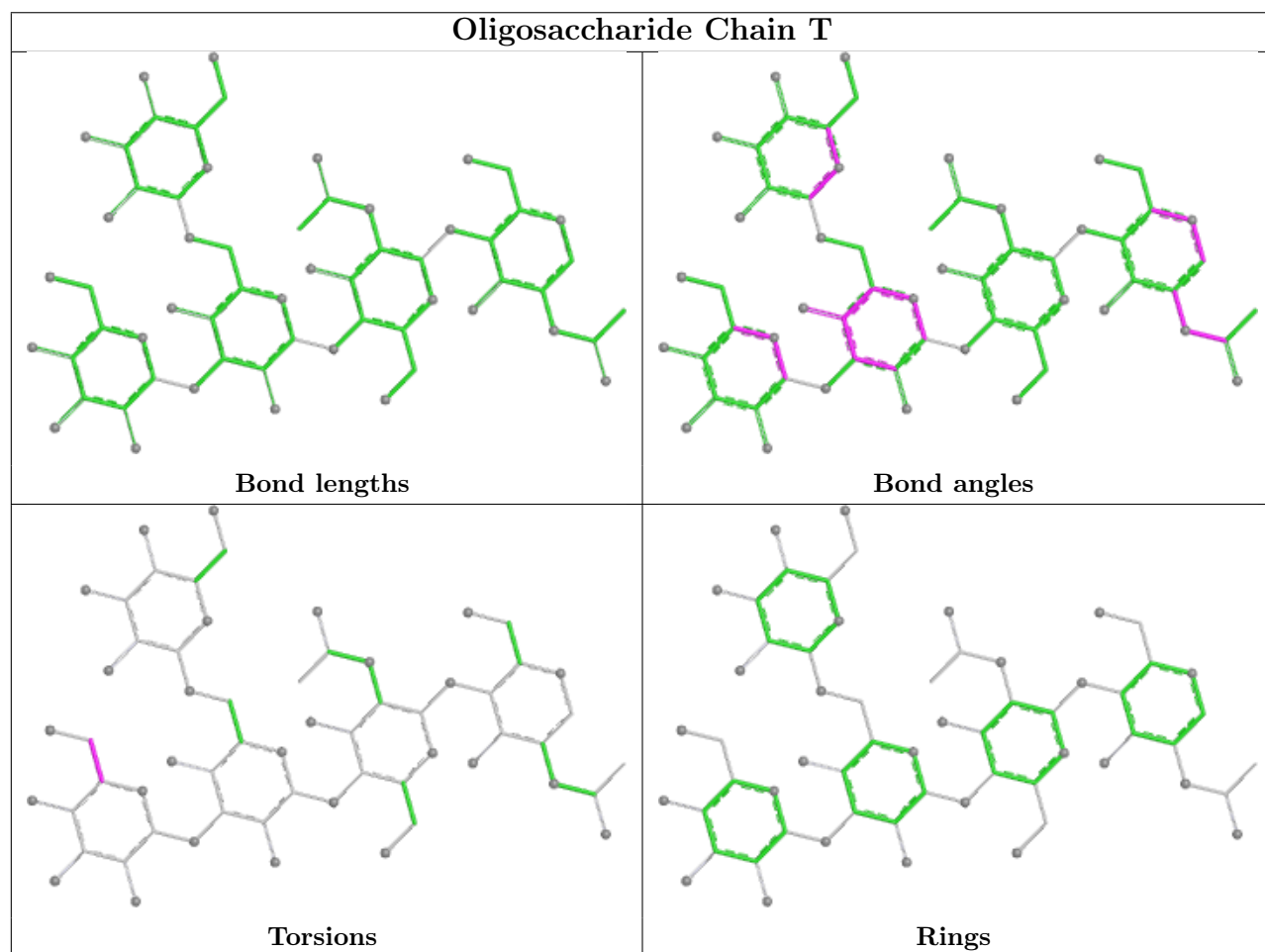
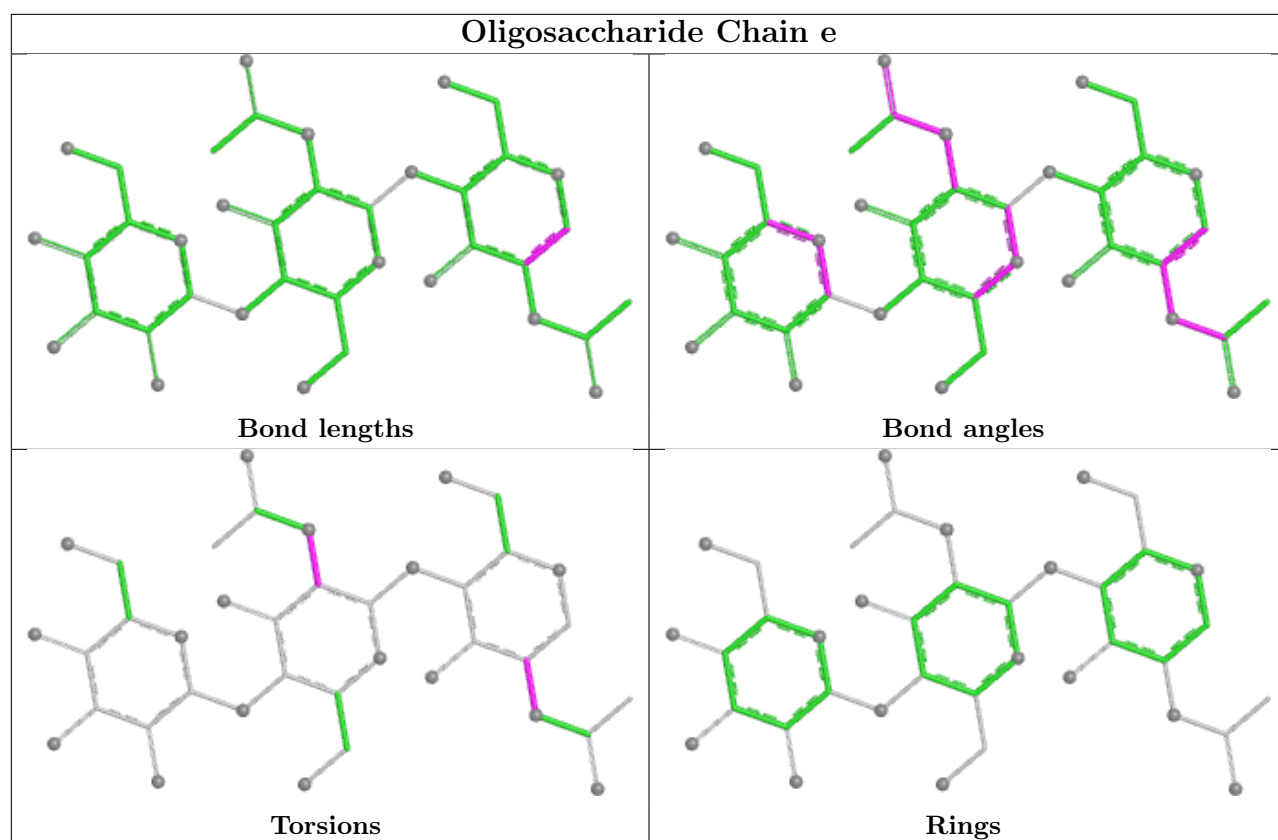


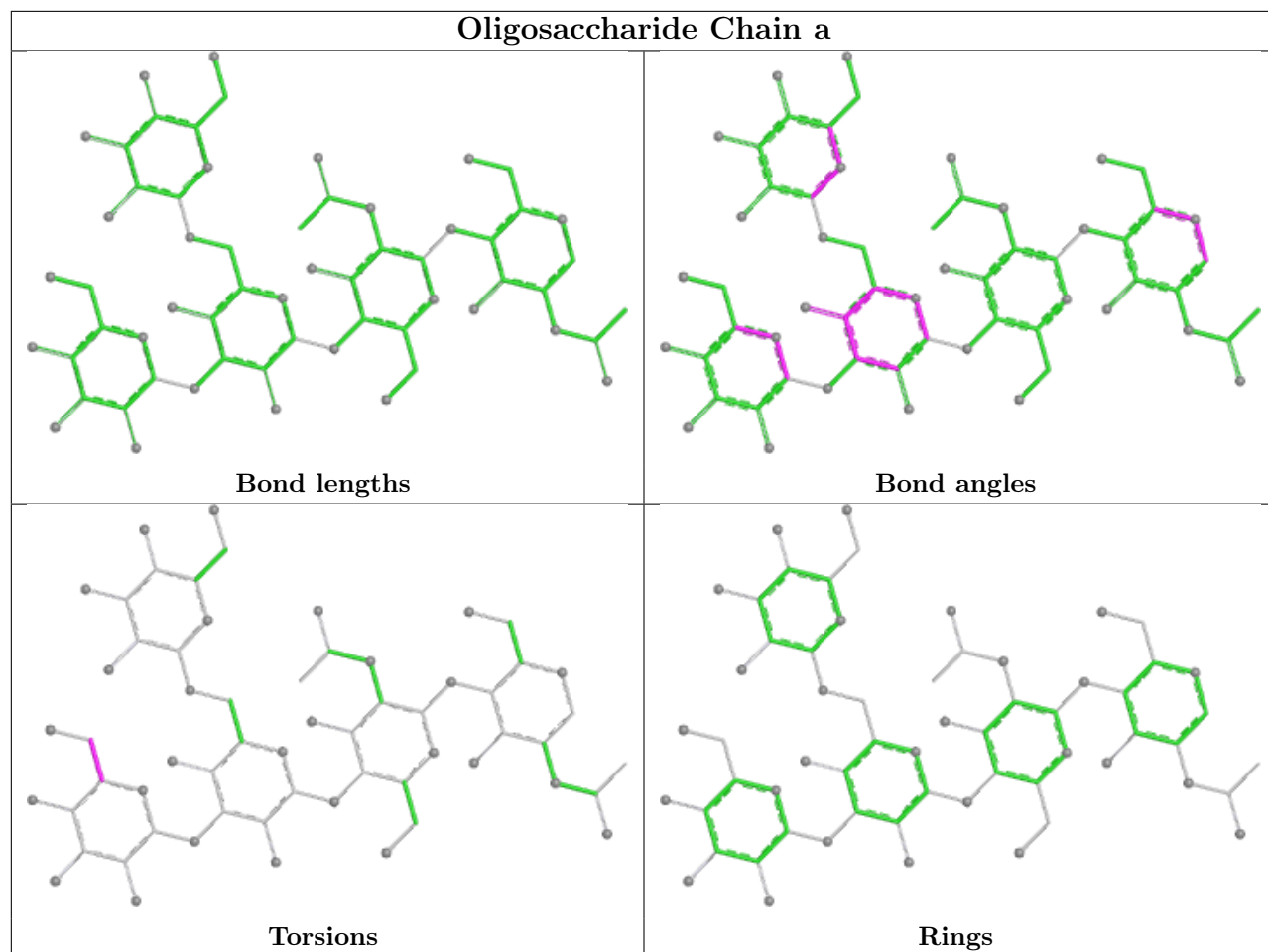


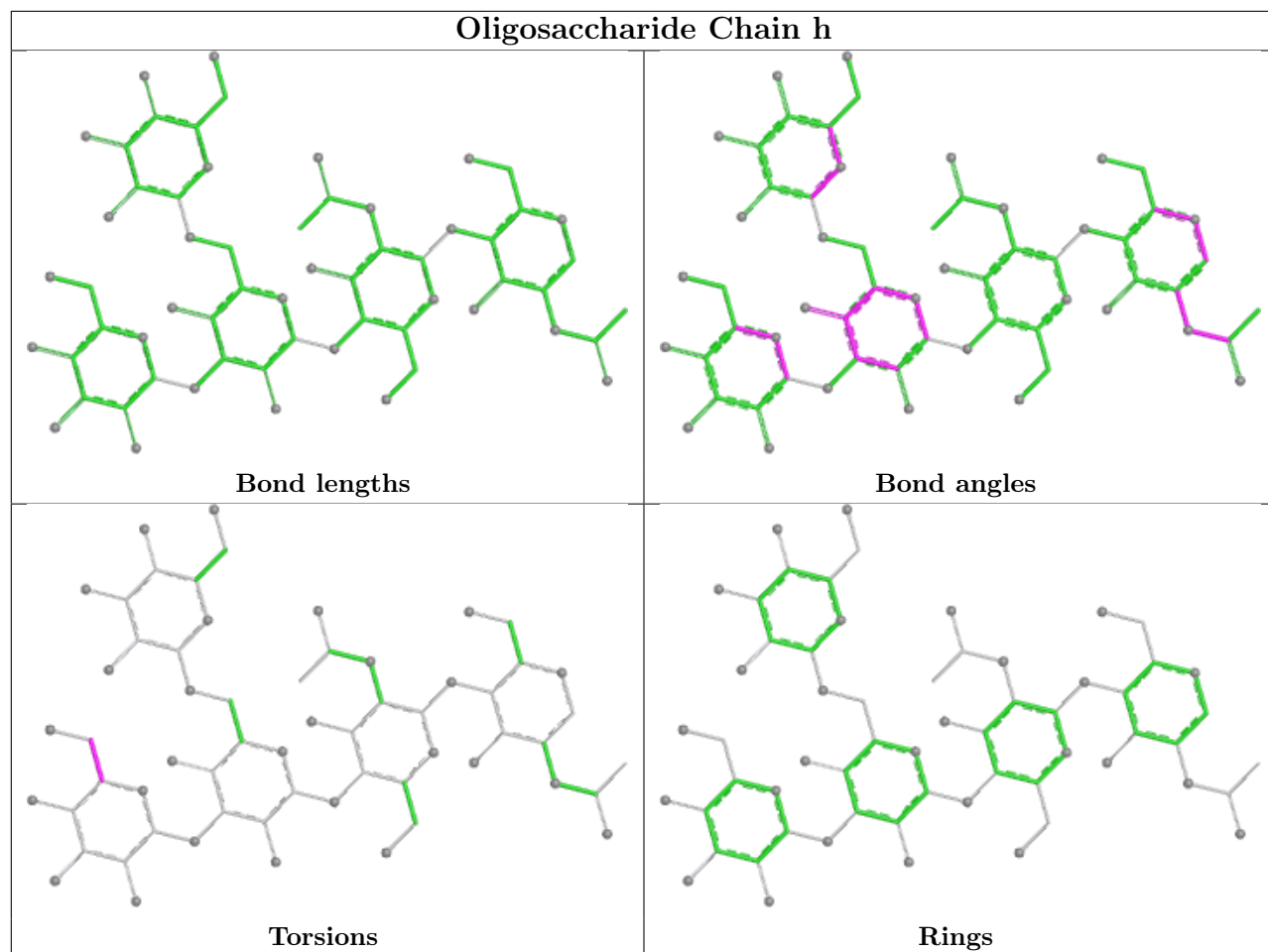


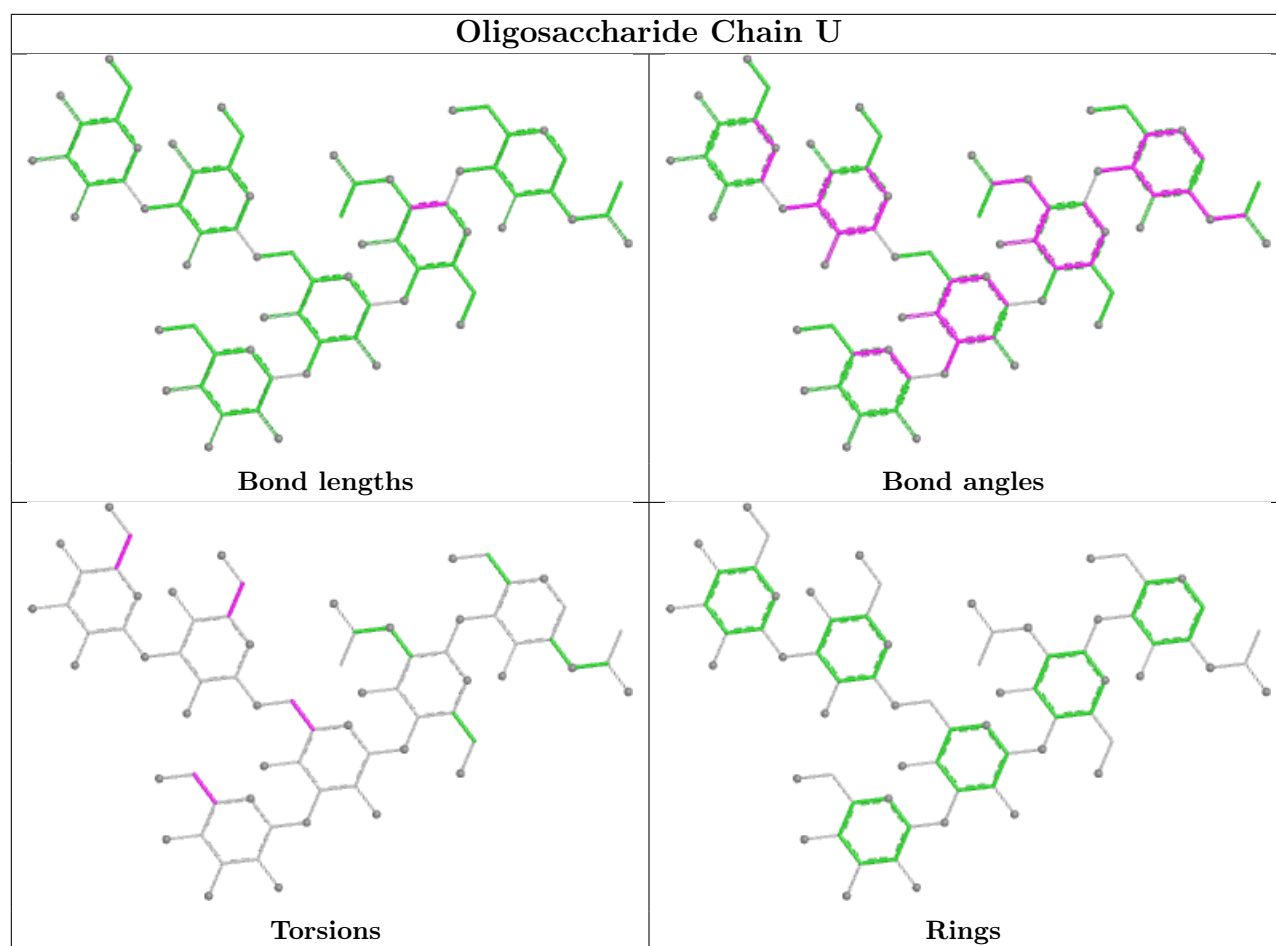


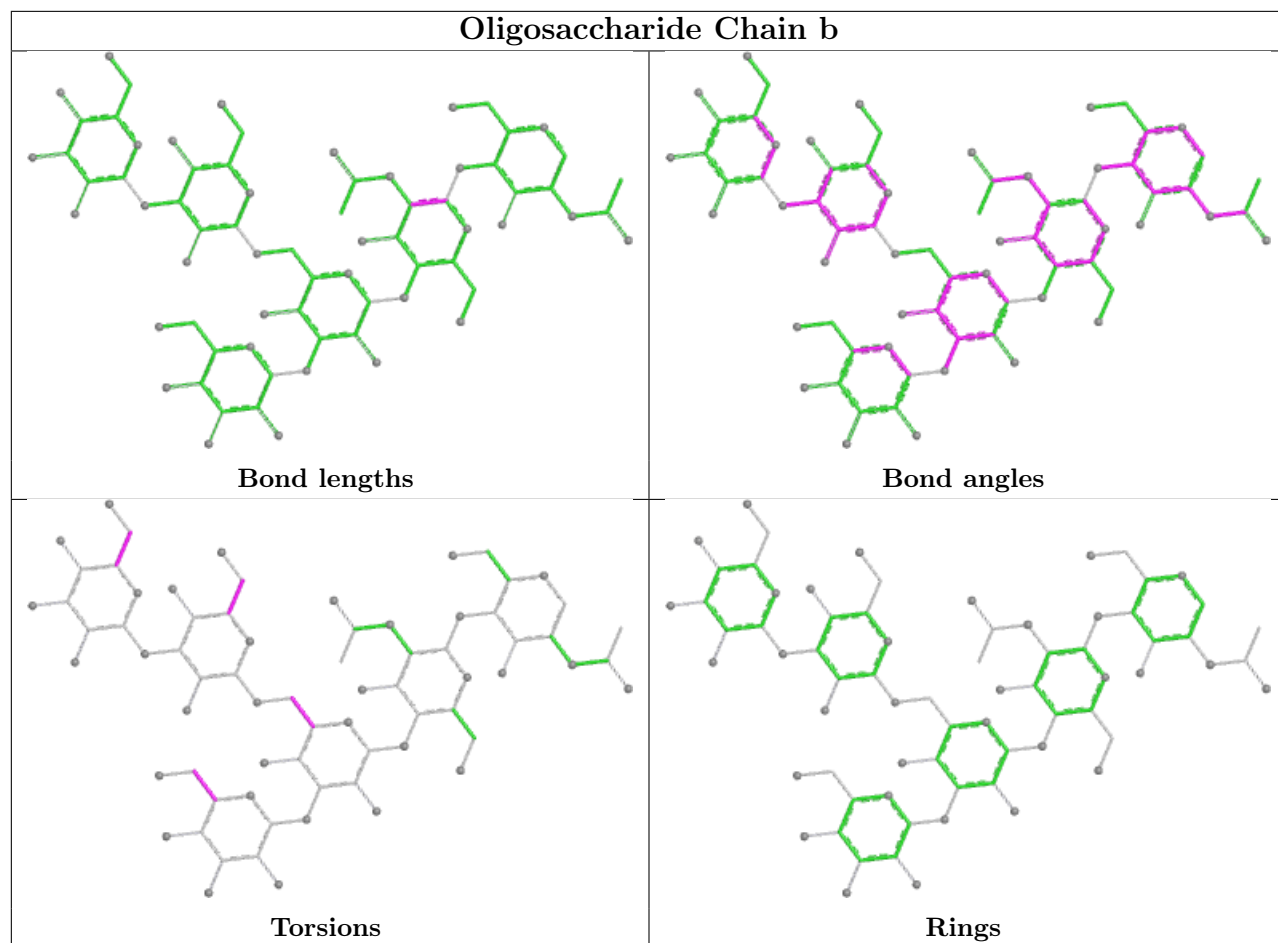


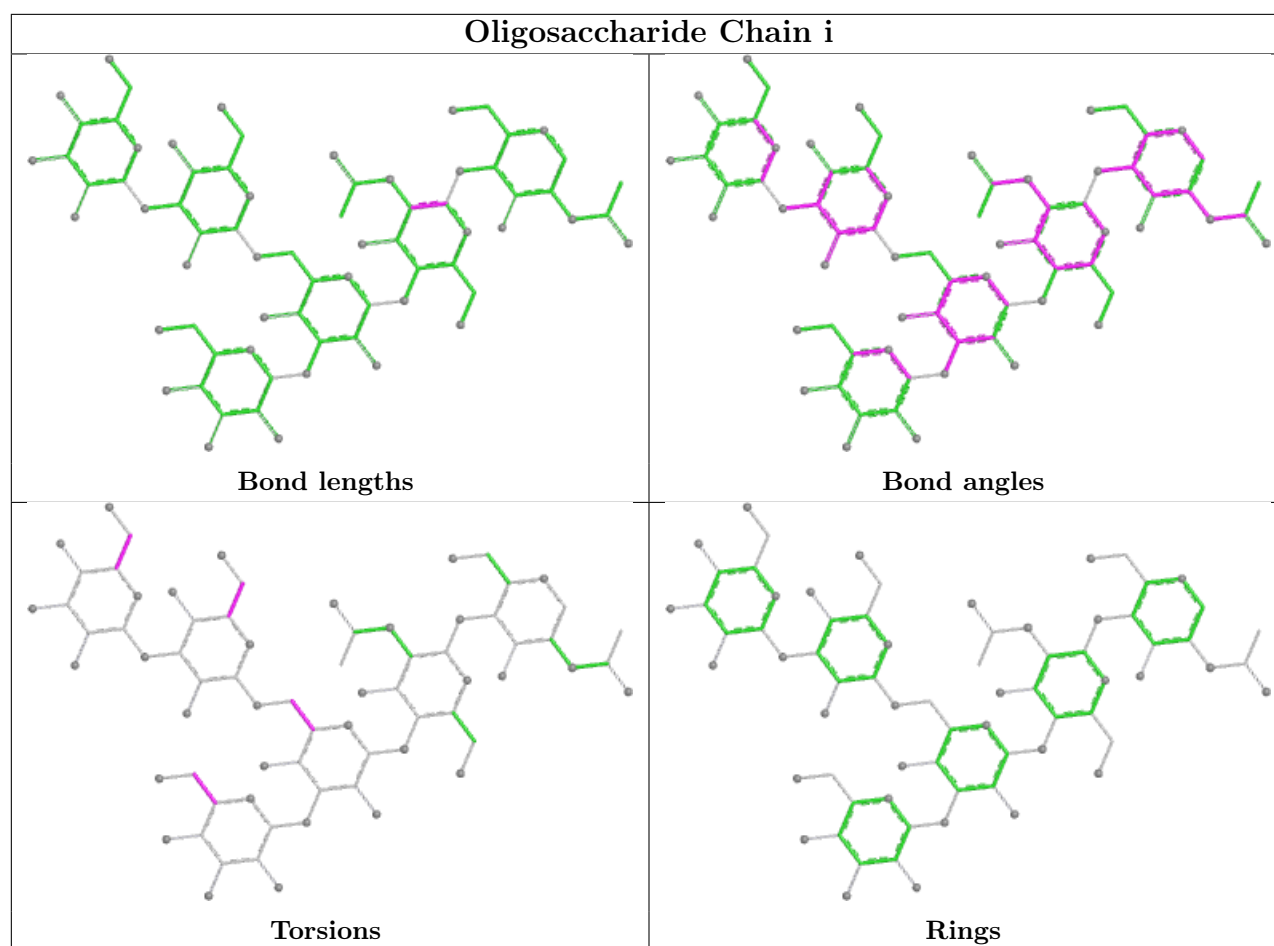












5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	NAG	B	706	1	14,14,15	0.73	0	17,19,21	1.00	0
10	NAG	C	704	1	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
10	NAG	A	705	1	14,14,15	0.77	0	17,19,21	0.88	1 (5%)
10	NAG	A	703	1	14,14,15	0.75	1 (7%)	17,19,21	2.11	3 (17%)
10	NAG	A	701	1	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
10	NAG	A	707	1	14,14,15	0.76	1 (7%)	17,19,21	1.37	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	B	703	1	14,14,15	0.74	0	17,19,21	2.12	3 (17%)
10	NAG	C	702	1	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
10	NAG	B	704	1	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
10	NAG	C	705	1	14,14,15	0.77	0	17,19,21	0.87	1 (5%)
10	NAG	B	701	1	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
10	NAG	B	702	1	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
10	NAG	C	703	1	14,14,15	0.75	1 (7%)	17,19,21	2.12	3 (17%)
10	NAG	A	704	1	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
10	NAG	B	705	1	14,14,15	0.77	0	17,19,21	0.88	1 (5%)
10	NAG	C	706	1	14,14,15	0.73	0	17,19,21	0.99	0
10	NAG	B	707	1	14,14,15	0.75	1 (7%)	17,19,21	1.37	1 (5%)
10	NAG	O	1301	2	14,14,15	0.73	0	17,19,21	0.85	0
10	NAG	J	1301	2	14,14,15	0.73	0	17,19,21	0.84	0
10	NAG	C	701	1	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
10	NAG	A	702	1	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
10	NAG	A	706	1	14,14,15	0.73	0	17,19,21	1.00	0
10	NAG	C	707	1	14,14,15	0.77	1 (7%)	17,19,21	1.37	1 (5%)
10	NAG	G	1301	2	14,14,15	0.74	0	17,19,21	0.85	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
10	NAG	B	706	1	-	1/6/23/26	0/1/1/1
10	NAG	C	704	1	-	1/6/23/26	0/1/1/1
10	NAG	A	705	1	-	0/6/23/26	0/1/1/1
10	NAG	A	703	1	-	2/6/23/26	0/1/1/1
10	NAG	A	701	1	-	1/6/23/26	0/1/1/1
10	NAG	A	707	1	-	2/6/23/26	0/1/1/1
10	NAG	B	703	1	-	2/6/23/26	0/1/1/1
10	NAG	C	702	1	-	1/6/23/26	0/1/1/1
10	NAG	B	704	1	-	1/6/23/26	0/1/1/1
10	NAG	C	705	1	-	0/6/23/26	0/1/1/1
10	NAG	B	701	1	-	1/6/23/26	0/1/1/1
10	NAG	B	702	1	-	1/6/23/26	0/1/1/1
10	NAG	C	703	1	-	2/6/23/26	0/1/1/1
10	NAG	A	704	1	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	705	1	-	0/6/23/26	0/1/1/1
10	NAG	C	706	1	-	1/6/23/26	0/1/1/1
10	NAG	B	707	1	-	2/6/23/26	0/1/1/1
10	NAG	O	1301	2	-	1/6/23/26	0/1/1/1
10	NAG	J	1301	2	-	1/6/23/26	0/1/1/1
10	NAG	C	701	1	-	1/6/23/26	0/1/1/1
10	NAG	A	702	1	-	1/6/23/26	0/1/1/1
10	NAG	A	706	1	-	1/6/23/26	0/1/1/1
10	NAG	C	707	1	-	2/6/23/26	0/1/1/1
10	NAG	G	1301	2	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	707	NAG	C1-C2	2.10	1.55	1.52
10	A	707	NAG	C1-C2	2.06	1.55	1.52
10	B	707	NAG	C1-C2	2.04	1.55	1.52
10	C	703	NAG	C1-C2	2.02	1.55	1.52
10	A	703	NAG	C1-C2	2.00	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	703	NAG	C2-N2-C7	7.77	133.31	122.90
10	C	703	NAG	C2-N2-C7	7.76	133.30	122.90
10	A	703	NAG	C2-N2-C7	7.75	133.29	122.90
10	A	707	NAG	C2-N2-C7	4.21	128.54	122.90
10	C	707	NAG	C2-N2-C7	4.19	128.51	122.90
10	B	707	NAG	C2-N2-C7	4.18	128.50	122.90
10	A	704	NAG	C1-O5-C5	2.67	115.76	112.19
10	B	704	NAG	C1-O5-C5	2.65	115.74	112.19
10	C	704	NAG	C1-O5-C5	2.64	115.72	112.19
10	B	703	NAG	C1-O5-C5	2.49	115.53	112.19
10	A	703	NAG	C1-O5-C5	2.47	115.50	112.19
10	C	703	NAG	C1-O5-C5	2.47	115.49	112.19
10	B	702	NAG	C2-N2-C7	2.39	126.10	122.90
10	C	702	NAG	C2-N2-C7	2.38	126.10	122.90
10	A	702	NAG	C2-N2-C7	2.37	126.08	122.90
10	C	701	NAG	O5-C1-C2	-2.19	107.90	111.29
10	A	701	NAG	O5-C1-C2	-2.19	107.91	111.29
10	B	701	NAG	O5-C1-C2	-2.18	107.92	111.29
10	A	705	NAG	C2-N2-C7	2.13	125.76	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	705	NAG	C2-N2-C7	2.13	125.75	122.90
10	B	705	NAG	C2-N2-C7	2.13	125.75	122.90
10	C	703	NAG	O7-C7-N2	2.06	125.63	121.98
10	A	703	NAG	O7-C7-N2	2.06	125.62	121.98
10	B	703	NAG	O7-C7-N2	2.04	125.58	121.98

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	703	NAG	C1-C2-N2-C7
10	B	703	NAG	C1-C2-N2-C7
10	C	703	NAG	C1-C2-N2-C7
10	A	707	NAG	C4-C5-C6-O6
10	B	707	NAG	C4-C5-C6-O6
10	C	707	NAG	C4-C5-C6-O6
10	A	707	NAG	O5-C5-C6-O6
10	B	707	NAG	O5-C5-C6-O6
10	C	707	NAG	O5-C5-C6-O6
10	A	701	NAG	O5-C5-C6-O6
10	B	701	NAG	O5-C5-C6-O6
10	C	701	NAG	O5-C5-C6-O6
10	A	703	NAG	O5-C5-C6-O6
10	B	703	NAG	O5-C5-C6-O6
10	C	703	NAG	O5-C5-C6-O6
10	A	704	NAG	O5-C5-C6-O6
10	B	704	NAG	O5-C5-C6-O6
10	C	704	NAG	O5-C5-C6-O6
10	A	706	NAG	O5-C5-C6-O6
10	B	706	NAG	O5-C5-C6-O6
10	C	706	NAG	O5-C5-C6-O6
10	A	702	NAG	O5-C5-C6-O6
10	B	702	NAG	O5-C5-C6-O6
10	C	702	NAG	O5-C5-C6-O6
10	G	1301	NAG	O5-C5-C6-O6
10	J	1301	NAG	O5-C5-C6-O6
10	O	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

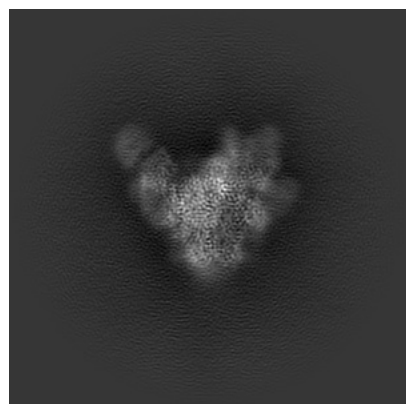
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48591. These allow visual inspection of the internal detail of the map and identification of artifacts.

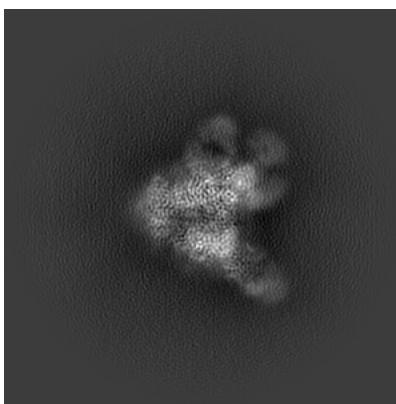
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

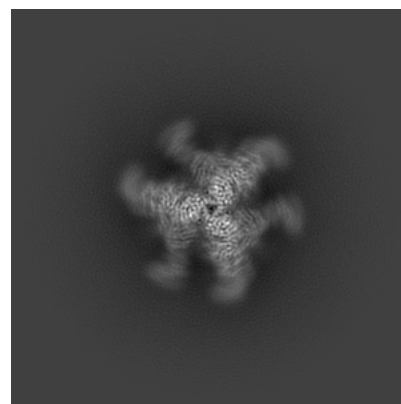
6.1.1 Primary map



X

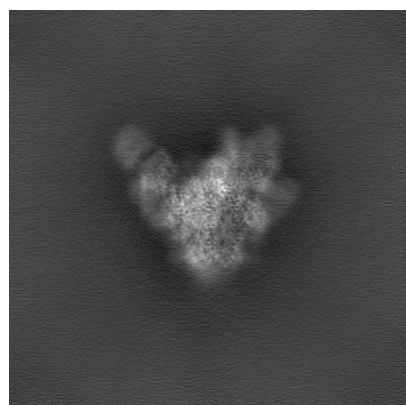


Y

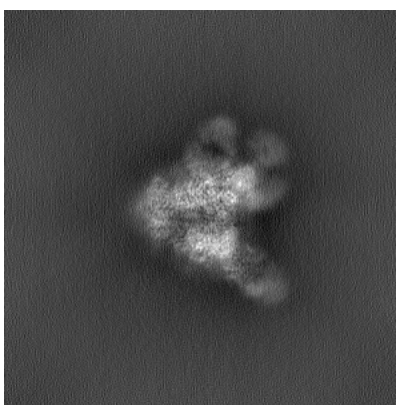


Z

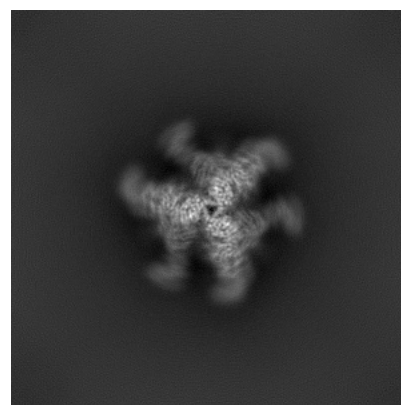
6.1.2 Raw map



X



Y

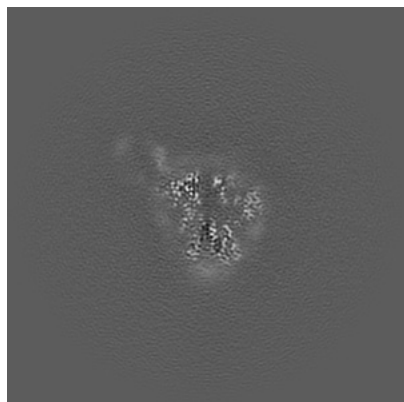


Z

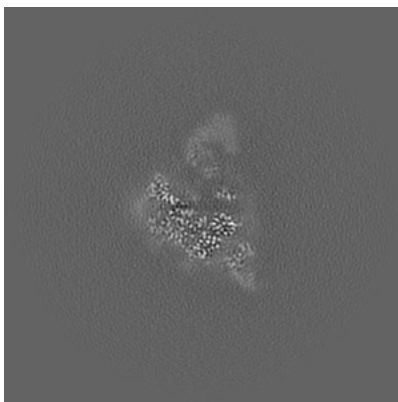
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

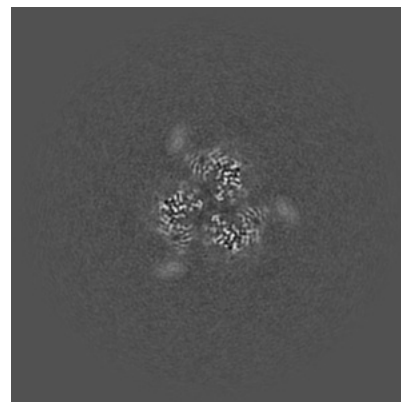
6.2.1 Primary map



X Index: 200

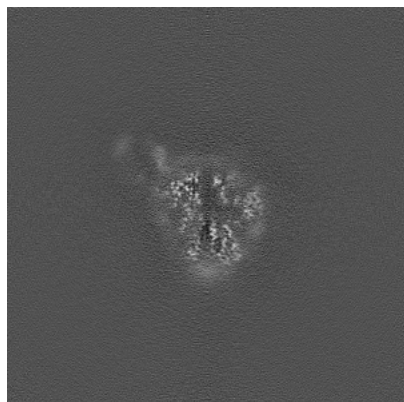


Y Index: 200

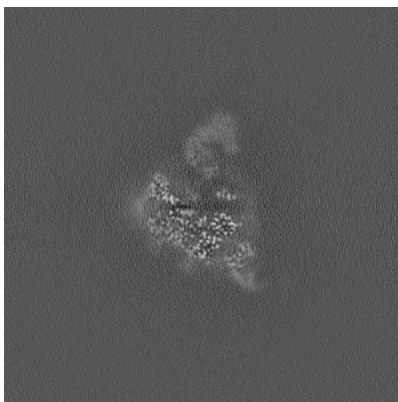


Z Index: 200

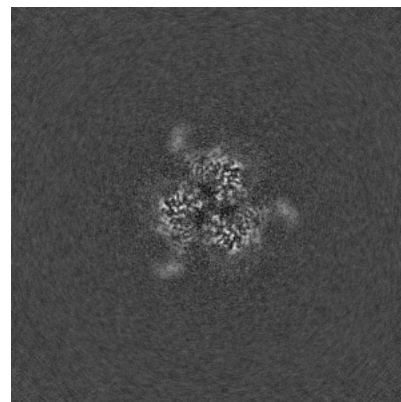
6.2.2 Raw map



X Index: 200



Y Index: 200

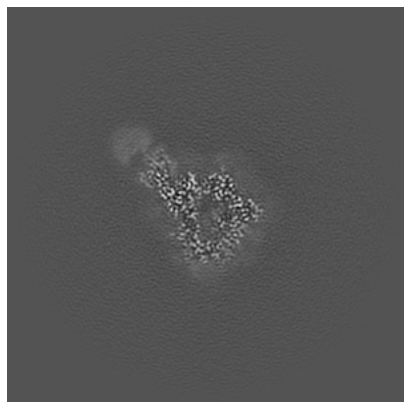


Z Index: 200

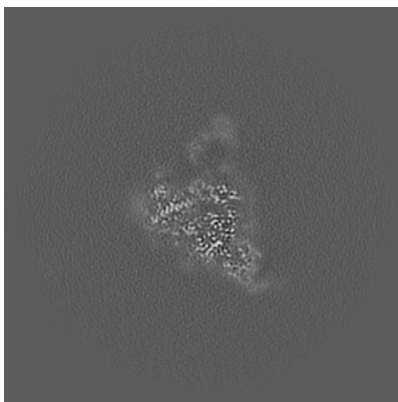
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

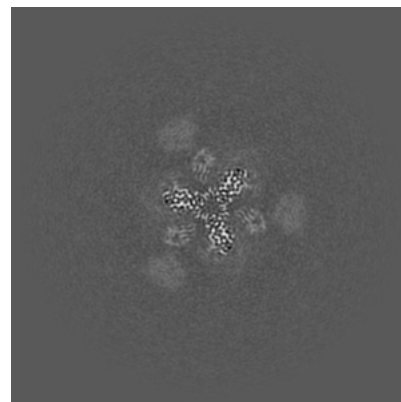
6.3.1 Primary map



X Index: 213

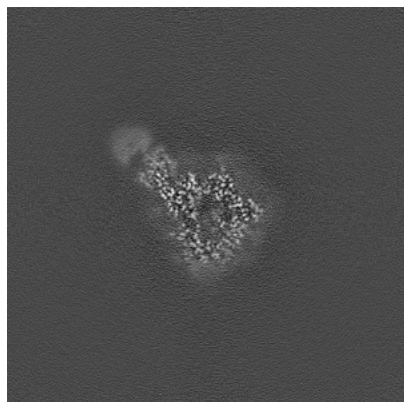


Y Index: 206

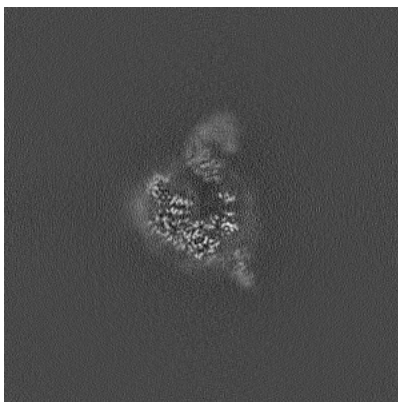


Z Index: 214

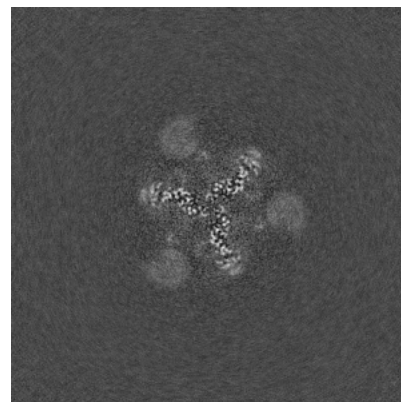
6.3.2 Raw map



X Index: 213



Y Index: 196

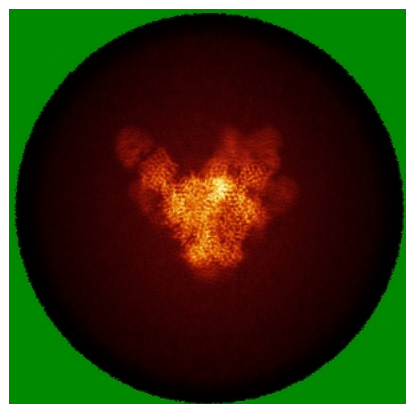


Z Index: 223

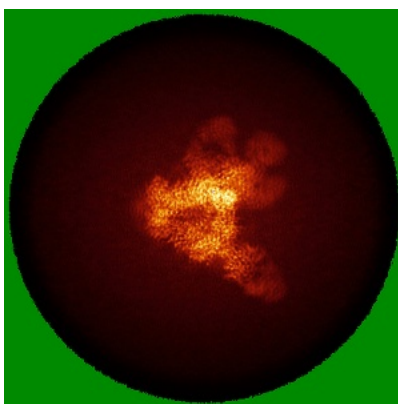
The images above show the largest variance slices of the map in three orthogonal directions.

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

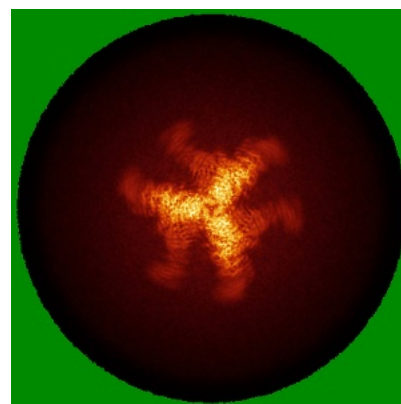
6.4.1 Primary map



X

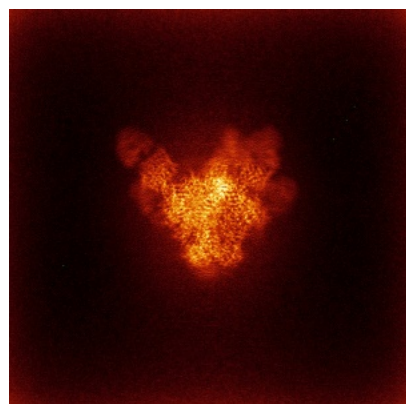


Y

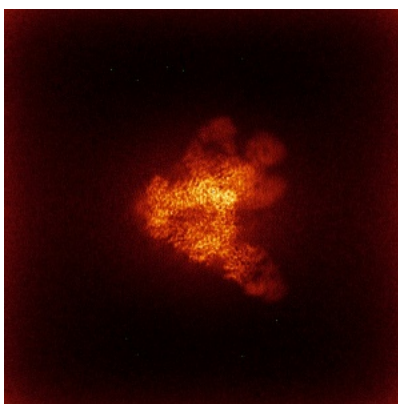


Z

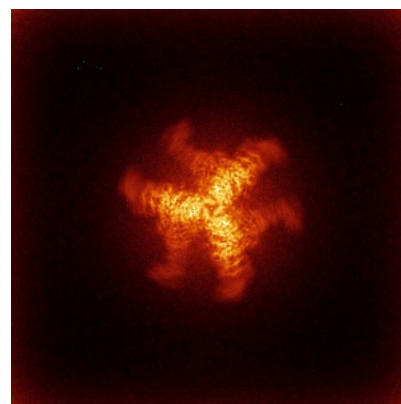
6.4.2 Raw map



X



Y

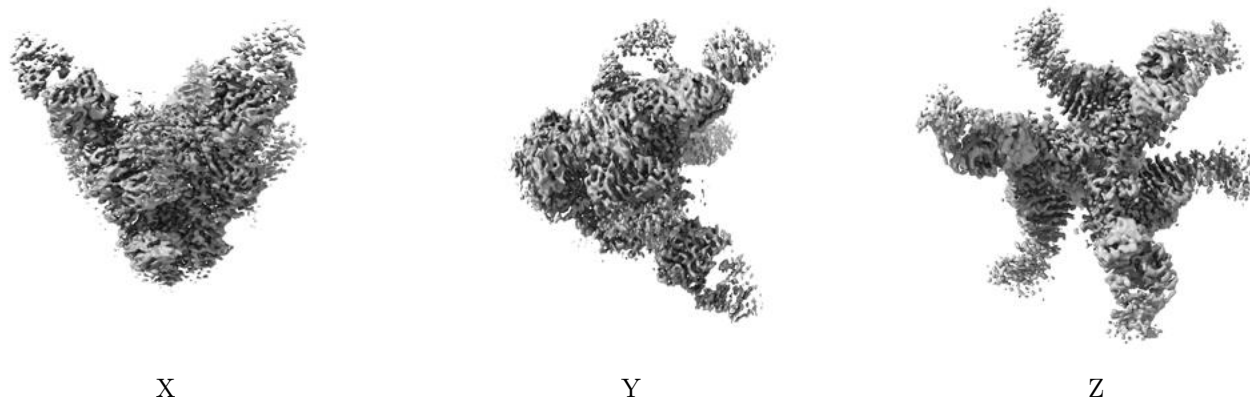


Z

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.

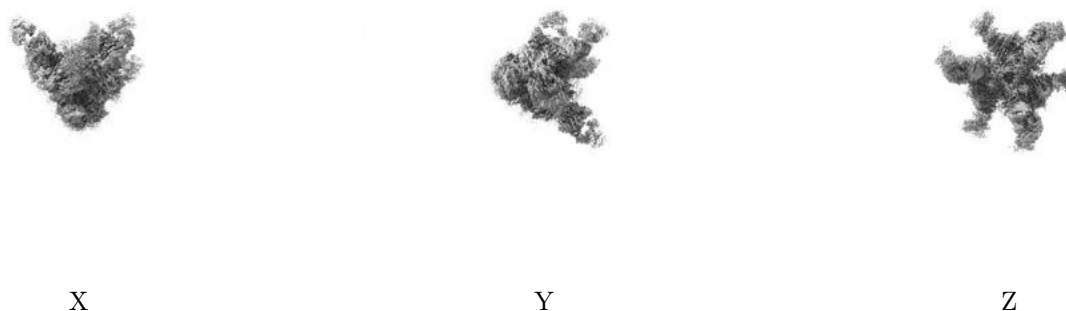
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

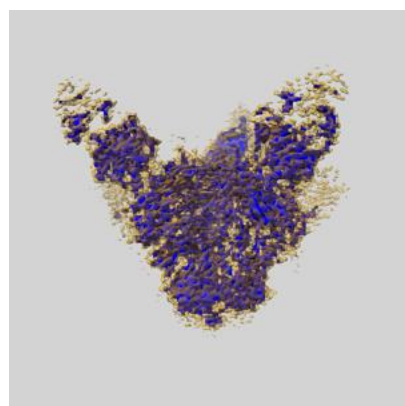
6.6 Mask visualisation [i](#)

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

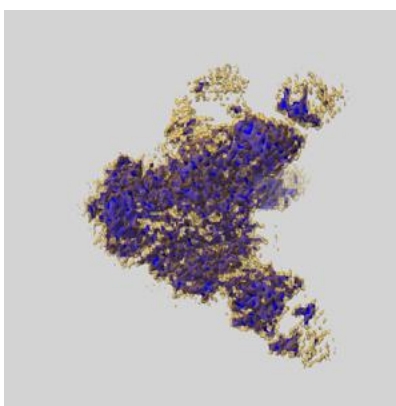
A mask typically either:

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

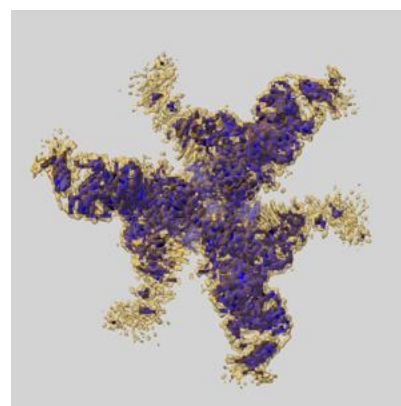
6.6.1 emd_48591_msk_1.map [i](#)



X



Y

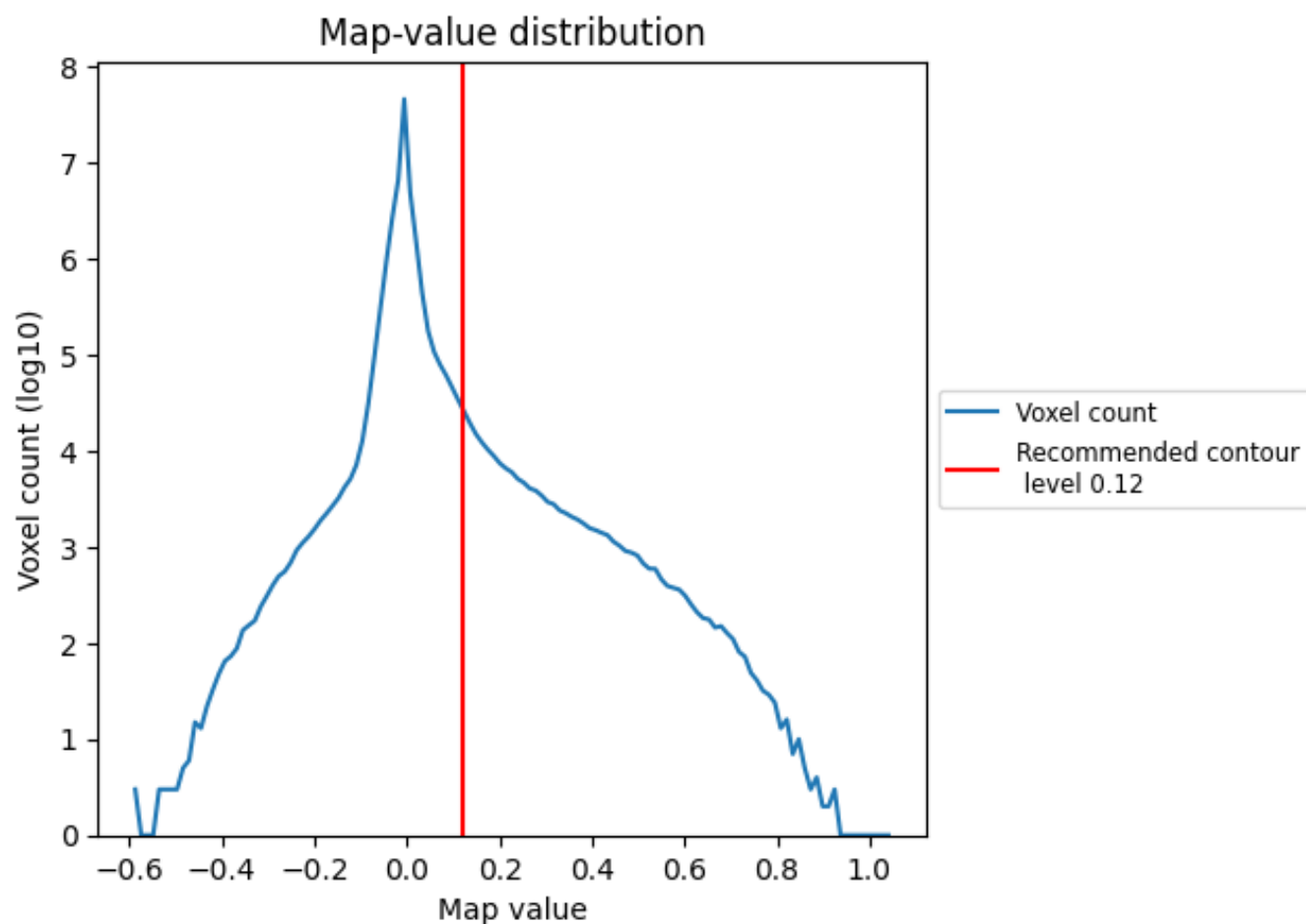


Z

7 Map analysis [i](#)

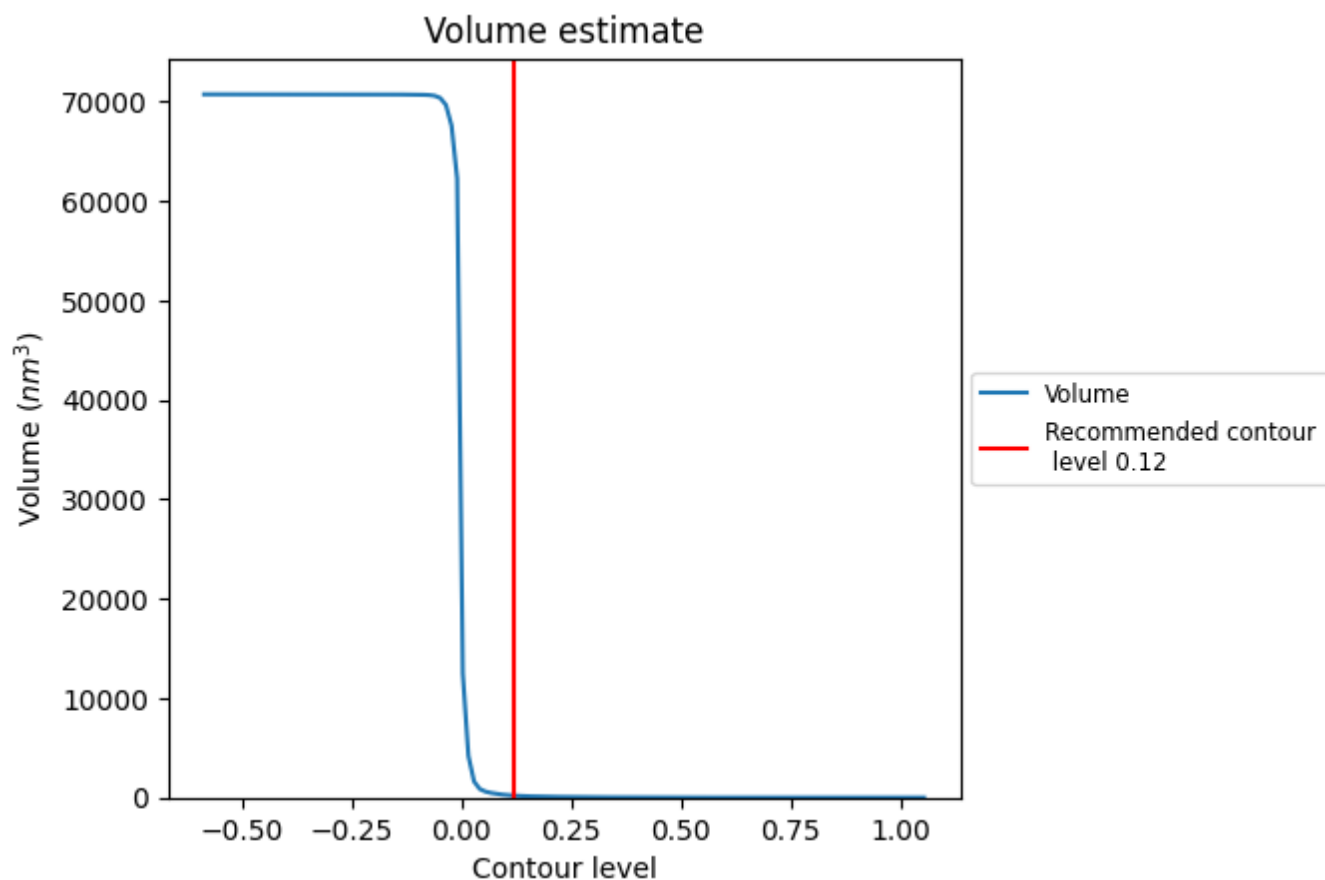
This section contains the results of statistical analysis of the map.

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.

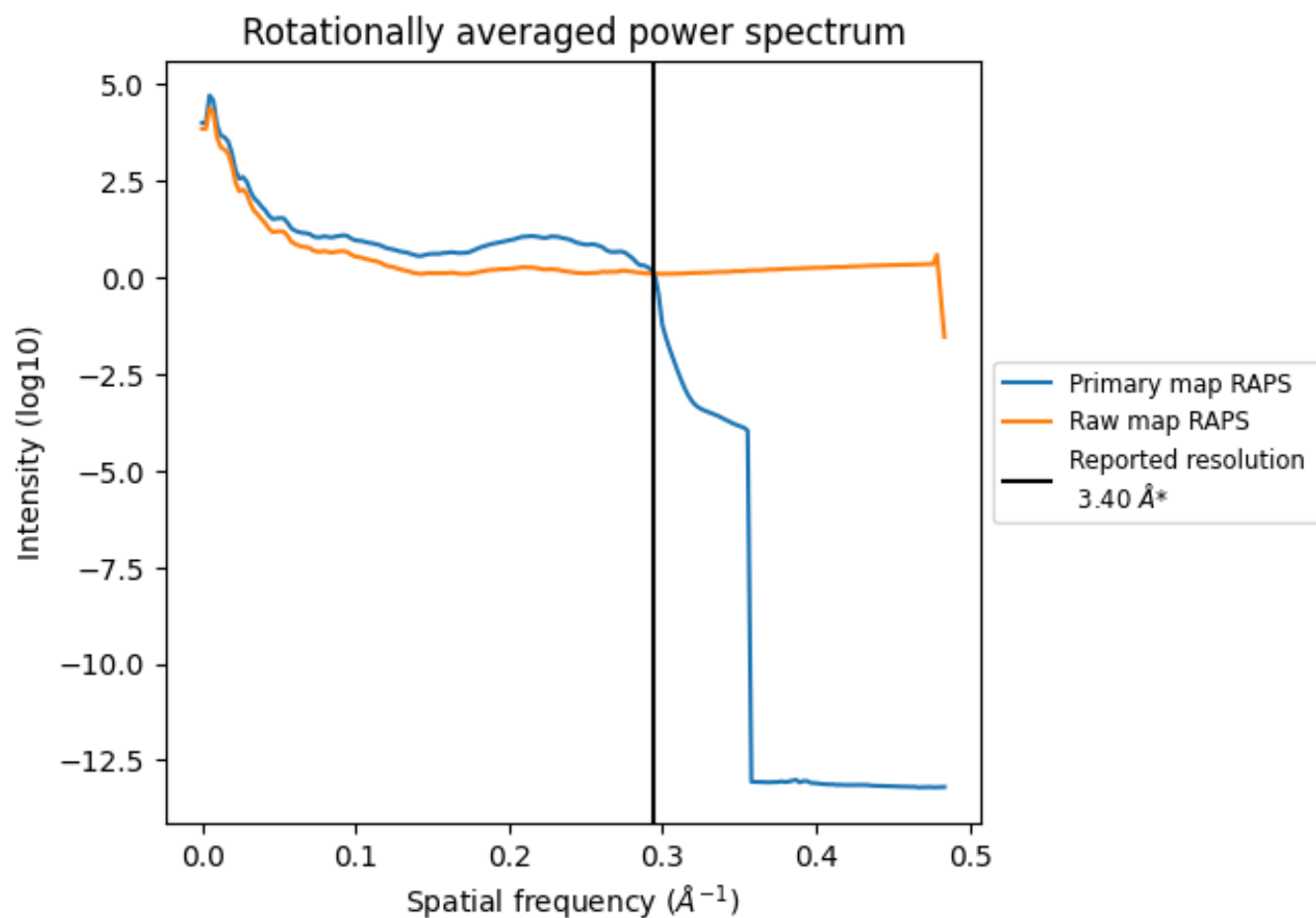
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 ⓘ

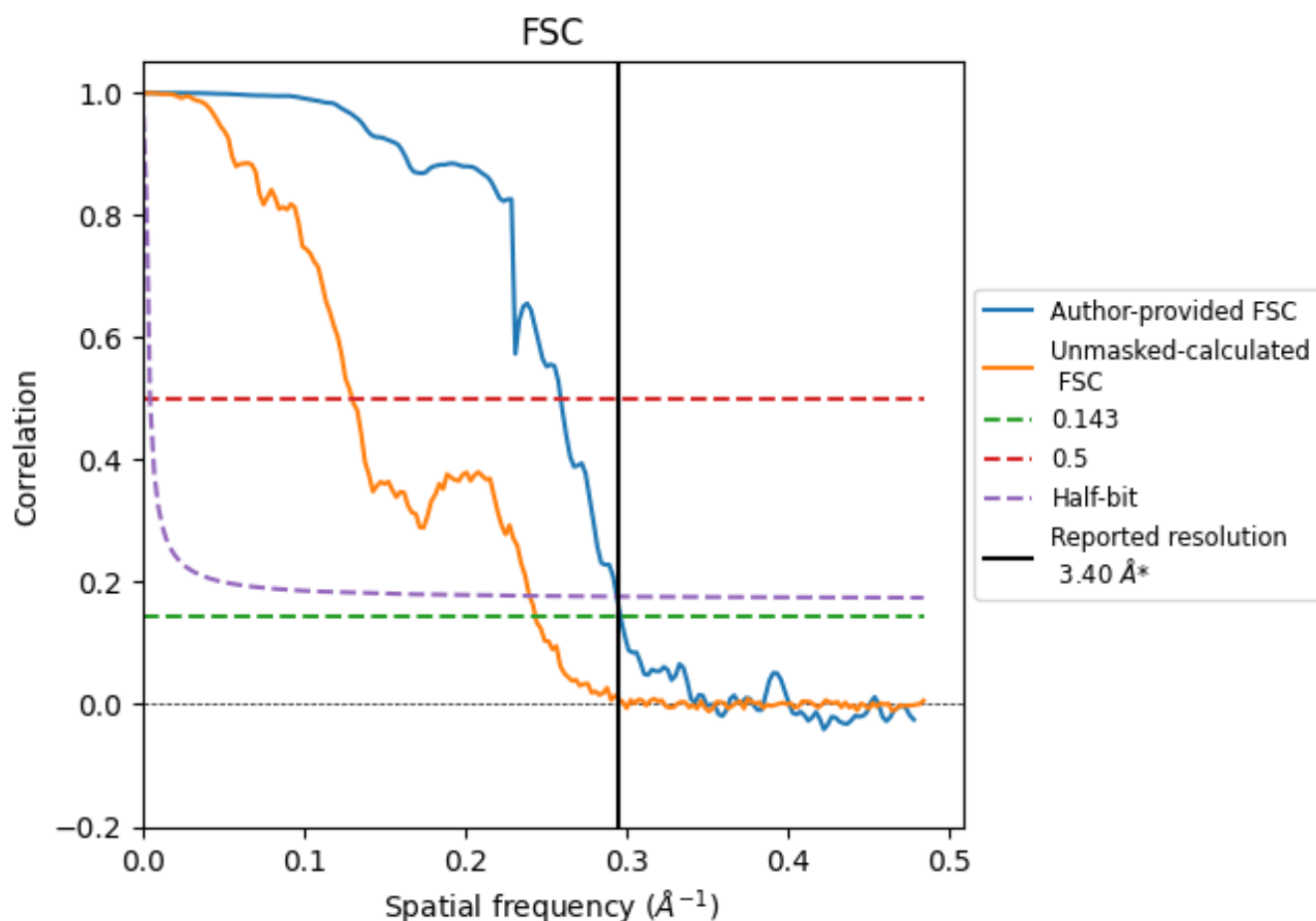


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

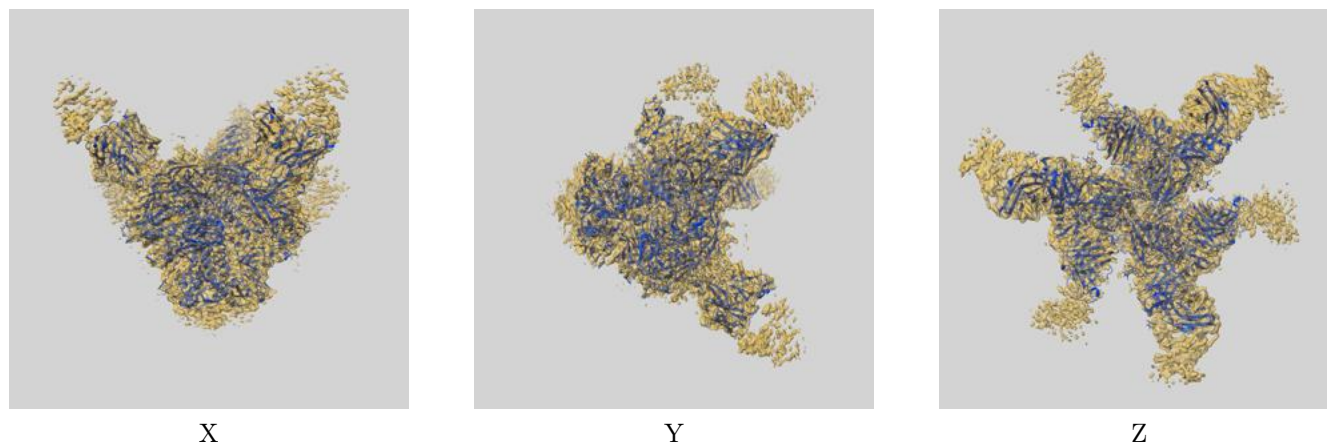
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.86	3.40
Unmasked-calculated*	4.11	7.70	4.17

*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 4.11 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

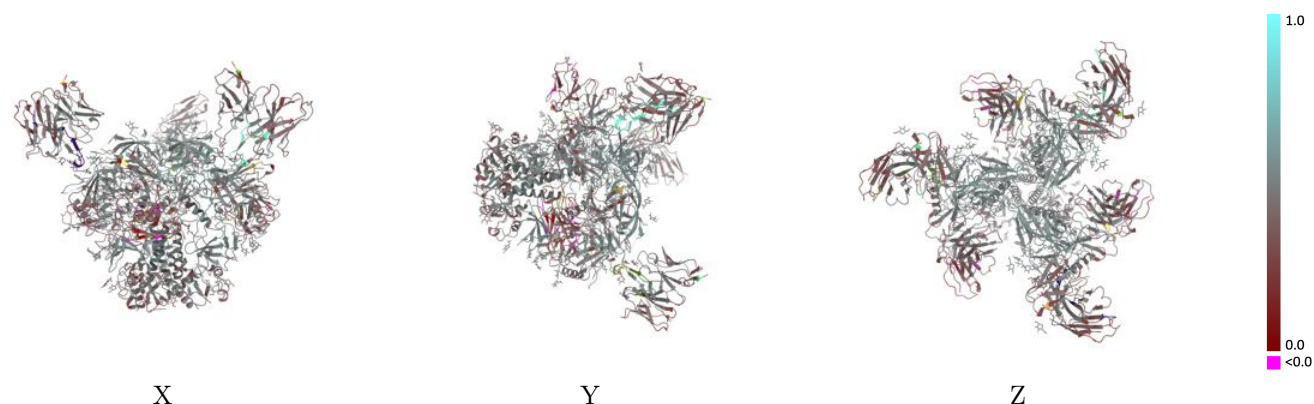
This section contains information regarding the fit between EMDB map EMD-48591 and PDB model 9MSY. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



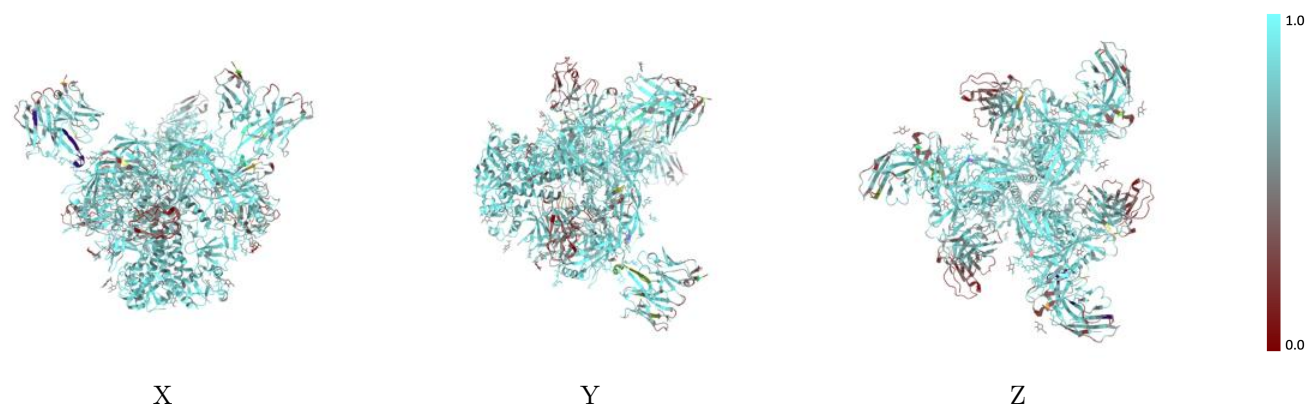
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



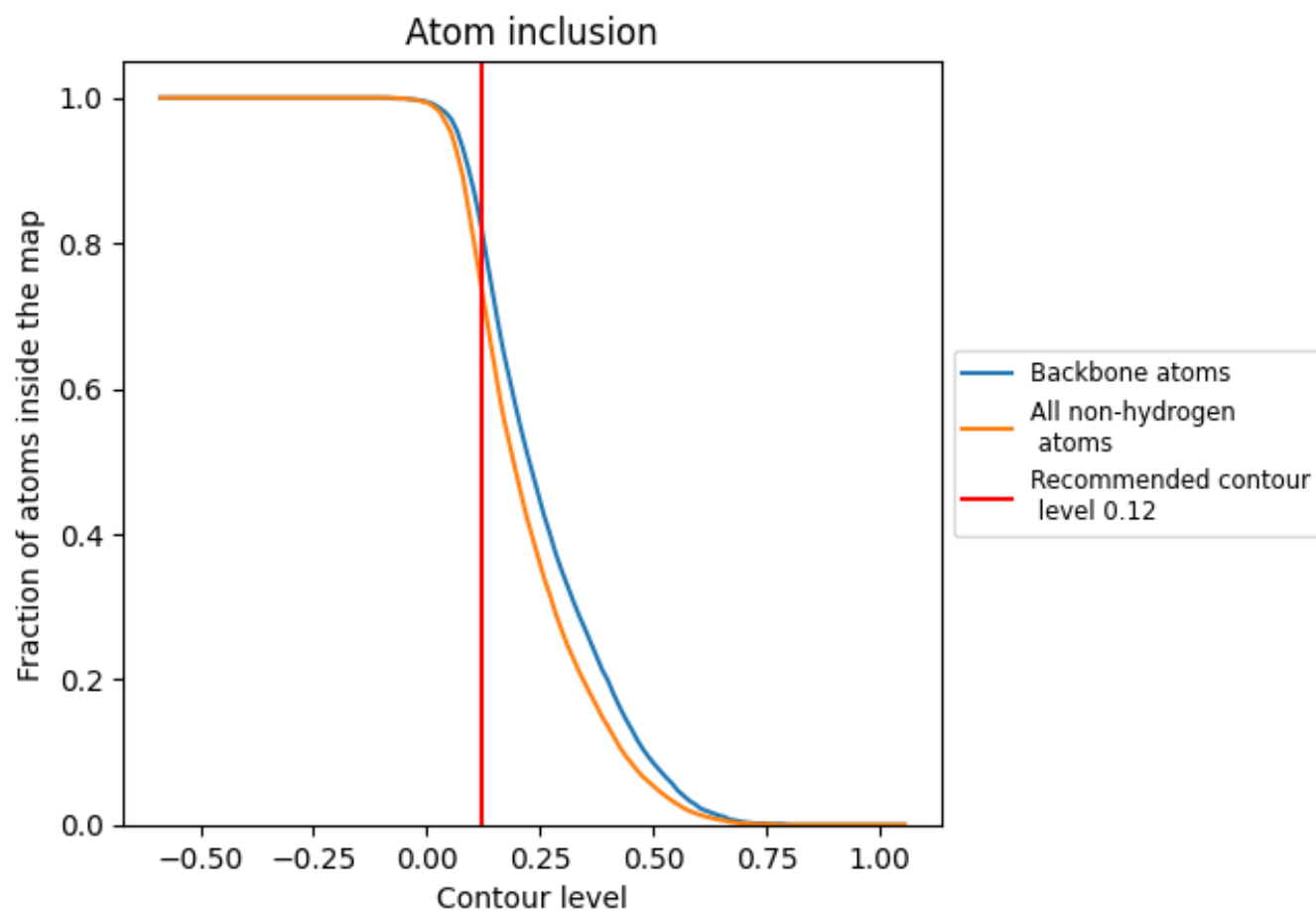
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.4450
A	 0.8330	 0.4860
B	 0.8340	 0.4860
C	 0.8300	 0.4870
D	 0.4290	 0.4860
E	 0.5640	 0.4440
F	 0.8210	 0.4640
G	 0.7370	 0.4140
H	 0.6300	 0.4130
I	 0.7050	 0.4260
J	 0.7320	 0.4150
K	 0.6280	 0.4160
L	 0.4170	 0.3050
M	 0.7070	 0.4230
N	 0.4140	 0.3060
O	 0.7370	 0.4170
P	 0.6260	 0.4170
Q	 0.7050	 0.4250
R	 0.4250	 0.3080
S	 0.6070	 0.4480
T	 0.8690	 0.5080
U	 0.8470	 0.4180
V	 0.6430	 0.4760
W	 0.4290	 0.4840
X	 0.5640	 0.4330
Y	 0.8210	 0.4960
Z	 0.6430	 0.4380
a	 0.8530	 0.5090
b	 0.8330	 0.4210
c	 0.6430	 0.5000
d	 0.4290	 0.4810
e	 0.5640	 0.4360
f	 0.8210	 0.4840
g	 0.6070	 0.4470
h	 0.8530	 0.5100



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.8470	 0.4100
j	 0.6430	 0.4610