



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 07:59 PM JST

PDB ID : 9XO0 / pdb_00009xo0
EMDB ID : EMD-67065
Title : PEDV HNXX spike trimer with three D0 down in complex with three N19 Fabs
Authors : Liu, J.; Wang, S.; Wang, J.; Su, M.; Li, Z.; Xiong, X.
Deposited on : 2025-11-13
Resolution : 2.13 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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) : 2.50

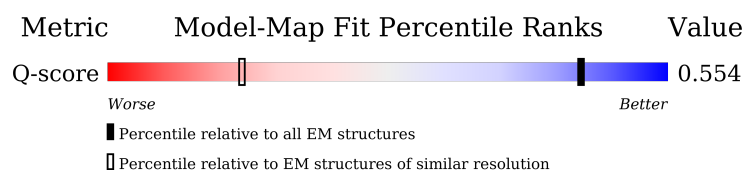
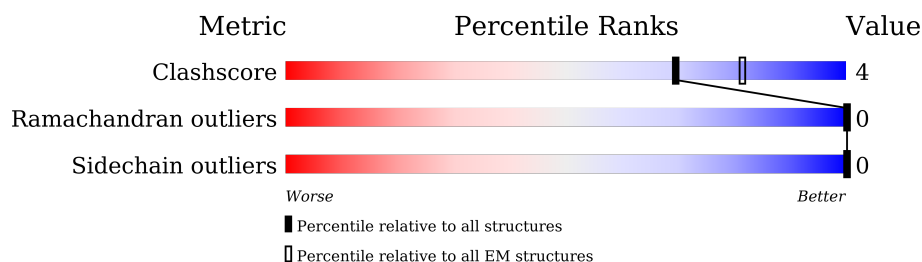
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.13 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.



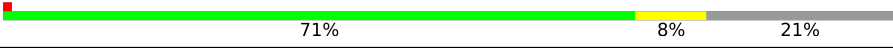
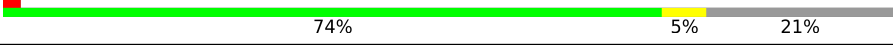
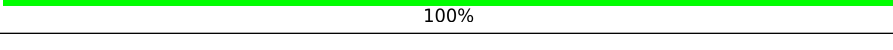
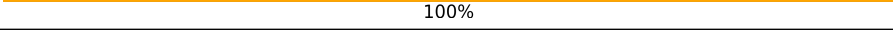
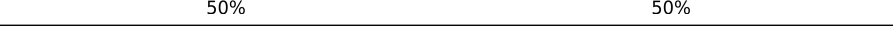
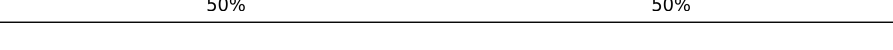
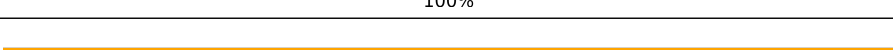
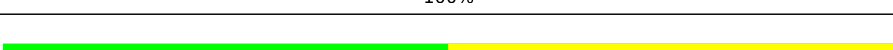
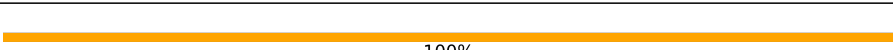
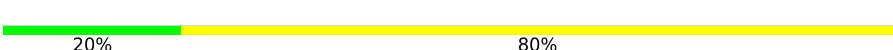
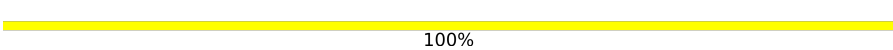
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2439 (1.64 - 2.63)

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	1327	
1	B	1327	
1	C	1327	
2	D	144	

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Mol	Chain	Length	Quality of chain
2	E	144	
2	F	144	
3	G	129	
3	H	129	
3	I	129	
4	J	2	
4	K	2	
4	L	2	
4	M	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
5	N	5	
5	S	5	
5	X	5	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 31377 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1102	Total	C	N	O	S	0	0
			8472	5409	1389	1630	44		
1	B	1102	Total	C	N	O	S	0	0
			8472	5409	1389	1630	44		
1	C	1102	Total	C	N	O	S	0	0
			8472	5409	1389	1630	44		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	SER	PHE	conflict	UNP A0A7G4RNN0
A	888	GLY	ARG	conflict	UNP A0A7G4RNN0
A	908	ASN	SER	conflict	UNP A0A7G4RNN0
A	1010	MET	ILE	conflict	UNP A0A7G4RNN0
B	10	SER	PHE	conflict	UNP A0A7G4RNN0
B	888	GLY	ARG	conflict	UNP A0A7G4RNN0
B	908	ASN	SER	conflict	UNP A0A7G4RNN0
B	1010	MET	ILE	conflict	UNP A0A7G4RNN0
C	10	SER	PHE	conflict	UNP A0A7G4RNN0
C	888	GLY	ARG	conflict	UNP A0A7G4RNN0
C	908	ASN	SER	conflict	UNP A0A7G4RNN0
C	1010	MET	ILE	conflict	UNP A0A7G4RNN0

- Molecule 2 is a protein called N19 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	117	Total	C	N	O	S	0	0
			881	548	153	176	4		
2	D	117	Total	C	N	O	S	0	0
			881	548	153	176	4		
2	E	117	Total	C	N	O	S	0	0
			881	548	153	176	4		

- Molecule 3 is a protein called N19 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	102	Total	C	N	O	S	0	0
			743	465	131	143	4		
3	H	102	Total	C	N	O	S	0	0
			743	465	131	143	4		
3	I	102	Total	C	N	O	S	0	0
			743	465	131	143	4		

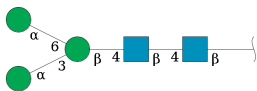
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	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	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	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		

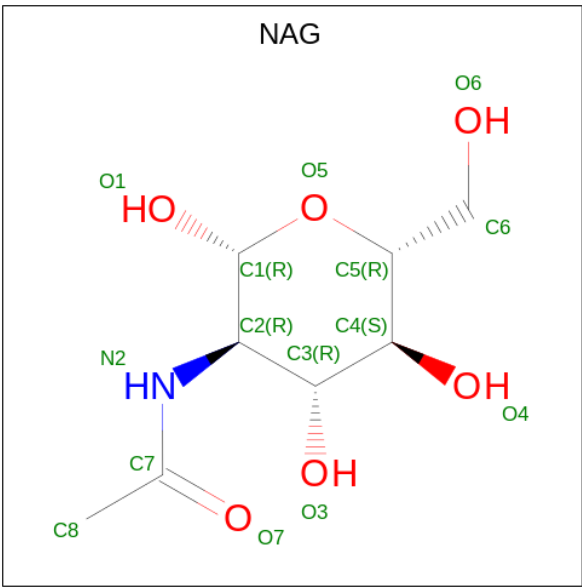
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	5	Total	C	N	O	0	0
			61	34	2	25		
5	S	5	Total	C	N	O	0	0
			61	34	2	25		
5	X	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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	

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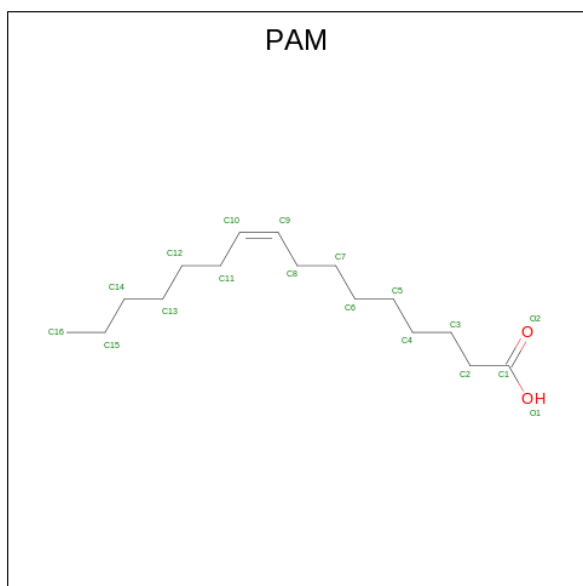
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B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

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

- Molecule 7 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $C_{16}H_{30}O_2$).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			18	16	2	
7	A	1	Total	C	O	0
			18	16	2	
7	B	1	Total	C	O	0
			18	16	2	
7	B	1	Total	C	O	0
			18	16	2	

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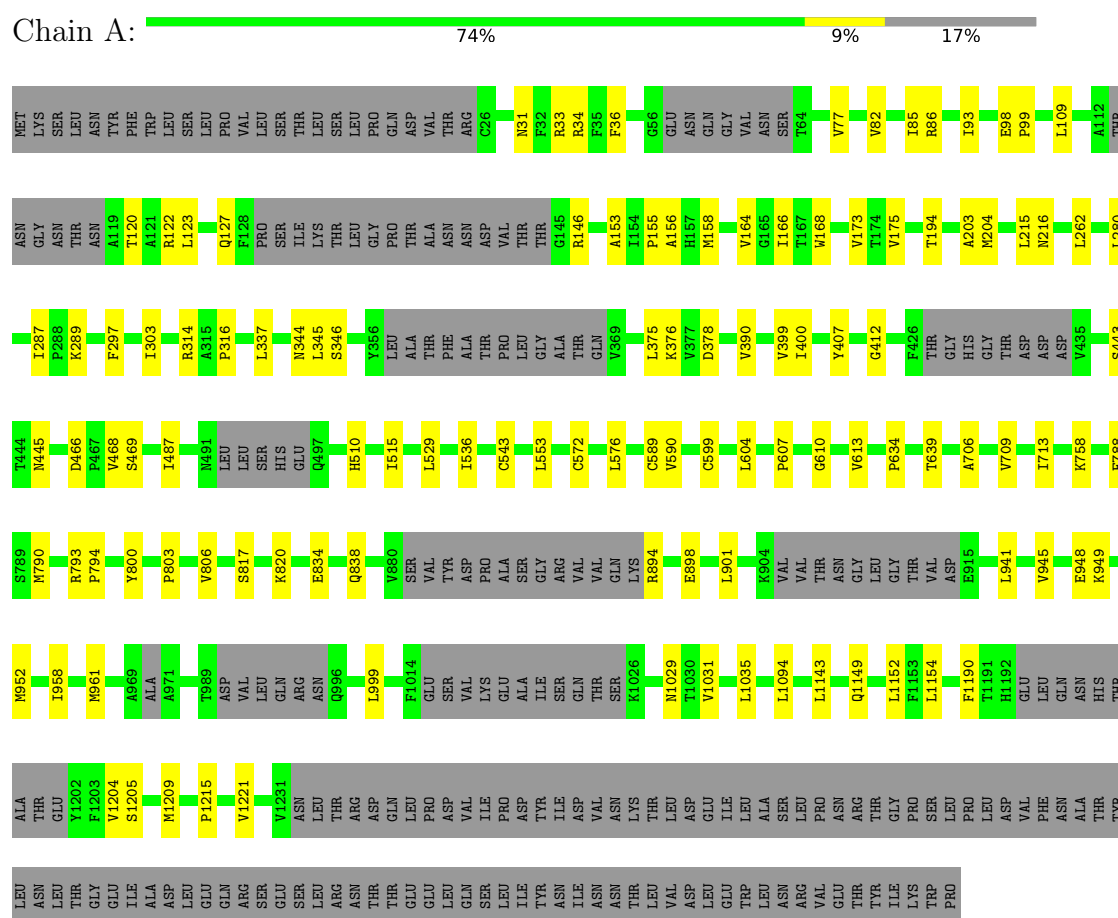
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Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	C	O	0
			18	16	2	
7	C	1	Total	C	O	0
			18	16	2	

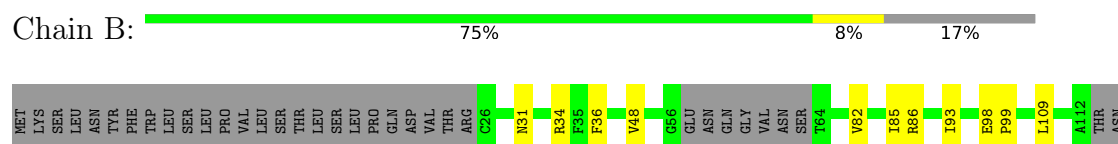
3 Residue-property plots

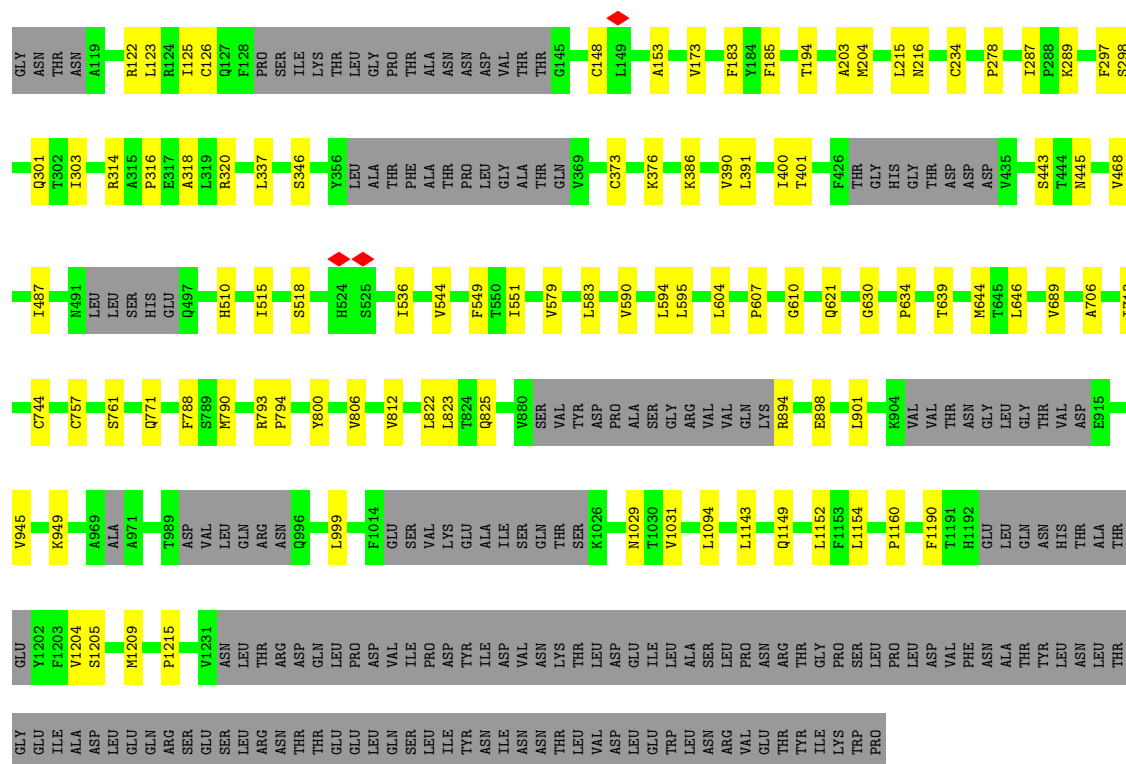
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

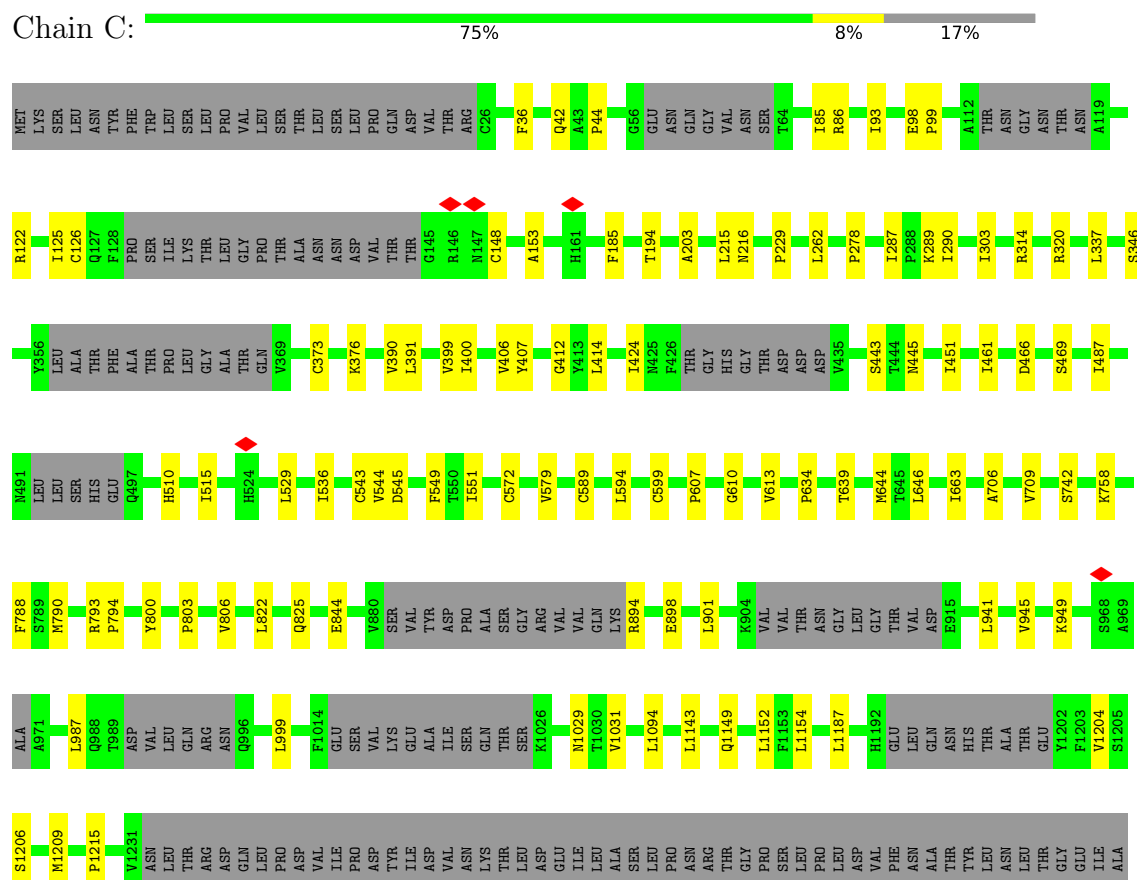


• Molecule 1: Spike glycoprotein





- Molecule 1: Spike glycoprotein



ASP
LEU
GLU
GLN
ARG
LEU
SER
GLU
SER
LEU
ARG
ASN
THR
THR
GLU
GLN
GLY
GLN
SER
GLY
ILE
TYR
ASN
ASN
THR
LEU
VAL
ASP
LEU
GLU
TRP
LEU
ASN
ARG
VAL
GLU
THR
TYR
ILE
LYS
TRP
PRO

● Molecule 2: N19 VH

Chain F:  71% 10% 19%

MET
GLU
PHE
ARG
LEU
ASN
TRP
VAL
VAL
LEU
PHE
ALA
LEU
LEU
GLN
GLY
VAL
GLN
GLY
E21
E25
G34
C41
V42
Y55
V56
A59
P60
G61
K62
T97
L100
Q101
M102
L105
D122
V123
W133
G136
V137
GLU
VAL
VAL
SER
SER
ALA

● Molecule 2: N19 VH

Chain D:  74% 7% 19%

MET
GLU
PHE
ARG
LEU
ASN
TRP
VAL
VAL
LEU
PHE
ALA
LEU
LEU
GLN
GLY
VAL
GLN
GLY
E21
E25
A59
K62
T77
R86
M89
R106
D109
D122
G136
V137
GLU
VAL
VAL
SER
SER
ALA

● Molecule 2: N19 VH

Chain E:  71% 10% 19%

MET
GLU
PHE
ARG
LEU
ASN
TRP
VAL
VAL
LEU
PHE
ALA
LEU
LEU
GLN
GLY
VAL
GLN
GLY
E21
V42
E52
V56
R57
Q58
A59
P60
G61
K62
L67
T88
T97
Q101
R106
T107
G108
D109
Y114
L126
W133
V137
GLU
VAL
VAL
SER
SER

ALA

● Molecule 3: N19 VL

Chain G:  71% 8% 21%

MET
ALA
TRP
THR
VAL
LEU
LEU
ILE
GLY
LEU
LEU
ALA
VAL
GLY
SER
GLY
VAL
ASP
SER
GLN
T21
L38
P53
P63
L66
Y69
R70
R74
F82
S83
G84
G85
I86
L93
G122
THR
HIS
LEU
THR
VAL
LEU
GLY

● Molecule 3: N19 VL

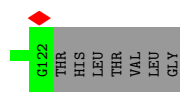
Chain H:  74% 5% 21%

MET
ALA
TRP
THR
VAL
LEU
LEU
ILE
GLY
LEU
LEU
ALA
VAL
GLY
SER
GLY
VAL
ASP
SER
GLN
T21
L38
P53
L66
Y69
R70
G77
G84
G85
I86
L93
G122
THR
HIS
LEU
THR
VAL
LEU
GLY

● Molecule 3: N19 VL

Chain I:  63% 16% 21%

MET
ALA
TRP
THR
VAL
LEU
LEU
ILE
GLY
LEU
LEU
ALA
VAL
GLY
SER
GLY
VAL
ASP
SER
GLN
T21
L38
T39
S50
P53
S54
W55
F56
Q57
Q62
P63
P64
R65
L66
L67
M68
Y69
N73
R74
V78
I86
K90
L93
Q99
A100
N101
T113
N116



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

Chain J:  50% 50%



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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  50% 50%



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

Chain O:  50% 50%



- 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:  100%

MAG1
MAG2

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

Chain R:  50%

MAG1
MAG2

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

Chain T:  50%

MAG1
MAG2

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

Chain U:  50%

MAG1
MAG2

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

Chain V:  100%

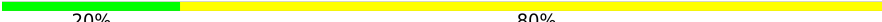
MAG1
MAG2

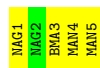
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50%

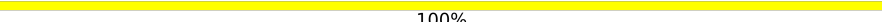
MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  20% 80%



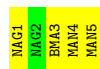
● Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



● Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  20% 80%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.612	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	418.5, 418.5, 418.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/8656	0.39	0/11768
1	B	0.19	0/8656	0.40	0/11768
1	C	0.19	0/8656	0.40	0/11768
2	D	0.13	0/902	0.32	0/1222
2	E	0.13	0/902	0.35	0/1222
2	F	0.15	0/902	0.30	0/1222
3	G	0.12	0/761	0.38	0/1035
3	H	0.12	0/761	0.37	0/1035
3	I	0.14	0/761	0.36	0/1035
All	All	0.19	0/30957	0.39	0/42075

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8472	0	8190	66	0
1	B	8472	0	8190	62	0
1	C	8472	0	8190	58	0
2	D	881	0	812	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	881	0	812	9	0
2	F	881	0	812	10	0
3	G	743	0	724	6	0
3	H	743	0	724	4	0
3	I	743	0	724	13	0
4	J	28	0	25	1	0
4	K	28	0	25	0	0
4	L	28	0	25	1	0
4	M	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	1	0
4	R	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	1	0
4	W	28	0	25	0	0
5	N	61	0	52	0	0
5	S	61	0	52	0	0
5	X	61	0	52	0	0
6	A	154	0	143	0	0
6	B	154	0	143	1	0
6	C	154	0	143	1	0
7	A	36	0	58	1	0
7	B	36	0	58	0	0
7	C	36	0	58	0	0
All	All	31377	0	30237	223	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 4.

All (223) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASN:HB2	1:A:378:ASP:HB2	1.76	0.68
3:G:66:LEU:HD21	3:G:69:TYR:HB3	1.77	0.66
1:C:709:VAL:HG11	1:C:758:LYS:HA	1.77	0.66
2:D:122:ASP:HB3	3:H:70:ARG:HH21	1.61	0.66
3:I:66:LEU:HD21	3:I:69:TYR:HB3	1.78	0.65
3:G:74:ARG:HH22	3:G:82:PHE:HB2	1.62	0.64
1:C:126:CYS:HB3	1:C:148:CYS:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HG11	1:B:234:CYS:HB3	1.80	0.63
3:G:38:LEU:HB2	3:G:93:LEU:HB3	1.80	0.63
1:B:346:SER:HB2	1:B:376:LYS:HB3	1.81	0.62
2:F:122:ASP:HB2	3:G:70:ARG:HH21	1.64	0.62
1:A:85:ILE:HG22	1:A:86:ARG:HG2	1.81	0.62
1:B:607:PRO:HG2	1:B:610:GLY:HA3	1.82	0.61
1:B:85:ILE:HG22	1:B:86:ARG:HG2	1.82	0.61
1:B:644:MET:HE3	1:B:646:LEU:HD21	1.81	0.61
1:C:85:ILE:HG22	1:C:86:ARG:HG2	1.82	0.61
1:A:709:VAL:HG11	1:A:758:LYS:HA	1.81	0.60
2:E:57:ARG:HB2	2:E:67:LEU:HD11	1.84	0.59
2:E:88:THR:HB	2:E:101:GLN:HB3	1.82	0.59
1:B:126:CYS:HB3	1:B:148:CYS:HA	1.84	0.59
1:B:551:ILE:HD12	1:B:579:VAL:HG21	1.83	0.59
1:A:127:GLN:HB2	1:A:146:ARG:HB2	1.85	0.58
1:C:346:SER:HB2	1:C:376:LYS:HB3	1.85	0.58
3:H:66:LEU:HD21	3:H:69:TYR:HB3	1.85	0.58
1:B:122:ARG:HD2	1:B:153:ALA:HB2	1.86	0.58
1:C:85:ILE:HD11	1:C:203:ALA:HB2	1.85	0.57
2:E:42:VAL:HG22	2:E:97:THR:HG22	1.86	0.57
1:A:790:MET:HE3	1:A:999:LEU:HB3	1.86	0.57
1:A:85:ILE:HD11	1:A:203:ALA:HB2	1.86	0.57
1:B:390:VAL:HG11	1:C:639:THR:HG23	1.86	0.57
2:F:59:ALA:HB3	2:F:62:LYS:HB2	1.86	0.57
1:B:790:MET:HE3	1:B:999:LEU:HB3	1.85	0.57
1:A:314:ARG:HH11	1:A:445:ASN:HD22	1.52	0.56
1:B:85:ILE:HD11	1:B:203:ALA:HB2	1.87	0.56
3:G:53:PRO:HG2	3:G:86:ILE:HD11	1.87	0.56
1:A:346:SER:HB2	1:A:376:LYS:HB3	1.89	0.55
1:B:518:SER:HB2	6:B:1411:NAG:H62	1.88	0.55
1:C:607:PRO:HG2	1:C:610:GLY:HA3	1.88	0.55
1:A:793:ARG:HB3	1:A:1029:ASN:HB3	1.88	0.55
1:A:36:PHE:HB3	1:A:215:LEU:HD21	1.88	0.55
2:D:59:ALA:HB3	2:D:62:LYS:HB2	1.88	0.54
3:H:53:PRO:HG2	3:H:86:ILE:HD11	1.88	0.54
1:B:297:PHE:HD1	1:B:303:ILE:HD12	1.71	0.54
1:B:1204:VAL:HG23	1:B:1215:PRO:HG3	1.88	0.54
1:C:1204:VAL:HG23	1:C:1215:PRO:HG3	1.88	0.54
1:B:793:ARG:HB3	1:B:1029:ASN:HB3	1.90	0.54
3:I:57:GLN:HG3	3:I:67:LEU:HD11	1.90	0.53
1:A:93:ILE:HA	1:A:194:THR:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:LEU:HD11	1:B:1152:LEU:HD22	1.91	0.53
1:C:551:ILE:HD12	1:C:579:VAL:HG21	1.90	0.53
3:I:53:PRO:HG2	3:I:86:ILE:HD11	1.89	0.53
1:A:1143:LEU:HB2	1:A:1154:LEU:HB2	1.91	0.53
1:A:639:THR:HG23	1:C:390:VAL:HG11	1.90	0.53
1:C:794:PRO:HG2	1:C:1031:VAL:HG22	1.91	0.53
2:F:102:MET:HE2	2:F:105:LEU:HD21	1.91	0.52
1:C:945:VAL:HG23	1:C:949:LYS:HD3	1.91	0.52
2:E:59:ALA:HB3	2:E:62:LYS:HB2	1.91	0.52
1:B:794:PRO:HG2	1:B:1031:VAL:HG22	1.91	0.52
1:A:345:LEU:HB3	1:A:375:LEU:HD11	1.92	0.52
1:B:806:VAL:HG11	1:B:1094:LEU:HD21	1.92	0.52
1:B:303:ILE:HG13	1:B:443:SER:HB2	1.91	0.52
2:D:106:ARG:HD3	2:D:109:ASP:HB2	1.91	0.52
1:B:487:ILE:HD13	1:B:706:ALA:HB2	1.92	0.52
1:B:337:LEU:HD21	1:B:400:ILE:HD13	1.91	0.51
1:B:93:ILE:HA	1:B:194:THR:HG22	1.91	0.51
1:A:120:THR:HG22	1:A:155:PRO:HA	1.93	0.51
1:C:793:ARG:HB3	1:C:1029:ASN:HB3	1.91	0.51
1:A:297:PHE:HD1	1:A:303:ILE:HD12	1.76	0.51
1:A:487:ILE:HD13	1:A:706:ALA:HB2	1.91	0.51
2:F:42:VAL:HG22	2:F:97:THR:HG22	1.92	0.51
1:A:337:LEU:HD21	1:A:400:ILE:HD13	1.91	0.51
1:A:806:VAL:HG11	1:A:1094:LEU:HD21	1.93	0.51
3:H:38:LEU:HB2	3:H:93:LEU:HB3	1.93	0.50
1:A:604:LEU:HD11	1:B:594:LEU:HD23	1.93	0.50
1:C:337:LEU:HD21	1:C:400:ILE:HD13	1.93	0.50
1:C:122:ARG:HD2	1:C:153:ALA:HB2	1.93	0.50
2:E:106:ARG:HD3	2:E:109:ASP:HB2	1.93	0.50
1:A:945:VAL:HG23	1:A:949:LYS:HD3	1.92	0.50
1:B:579:VAL:HA	1:B:583:LEU:HD12	1.92	0.50
1:C:894:ARG:HD2	1:C:898:GLU:HB3	1.94	0.50
7:A:1408:PAM:H51	1:B:689:VAL:HG11	1.93	0.50
1:A:158:MET:HE2	1:A:164:VAL:HG21	1.94	0.49
1:B:945:VAL:HG23	1:B:949:LYS:HD3	1.94	0.49
1:A:122:ARG:HD2	1:A:153:ALA:HB2	1.94	0.49
1:C:644:MET:HE2	1:C:646:LEU:HD21	1.94	0.49
3:I:38:LEU:HB2	3:I:93:LEU:HB3	1.94	0.49
1:A:156:ALA:HB1	1:A:158:MET:HE3	1.95	0.49
1:C:806:VAL:HG11	1:C:1094:LEU:HD21	1.94	0.49
1:C:487:ILE:HD13	1:C:706:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:HD11	1:A:1152:LEU:HD22	1.95	0.48
1:A:794:PRO:HG2	1:A:1031:VAL:HG22	1.95	0.48
3:I:74:ARG:HH11	3:I:78:VAL:HG13	1.78	0.48
2:E:52:GLU:HG3	2:E:126:LEU:HD12	1.96	0.48
1:A:98:GLU:HG3	1:A:99:PRO:HD3	1.96	0.48
1:A:77:VAL:HG23	1:A:168:TRP:HZ2	1.78	0.48
1:A:166:ILE:HG12	1:A:175:VAL:HG22	1.94	0.48
1:A:303:ILE:HG13	1:A:443:SER:HB2	1.96	0.48
3:I:39:THR:HG23	3:I:90:LYS:HD3	1.96	0.47
1:C:790:MET:HE3	1:C:999:LEU:HB3	1.96	0.47
3:I:99:GLN:HE22	3:I:101:ASN:HB3	1.79	0.47
1:A:800:TYR:CZ	1:A:1149:GLN:HA	2.49	0.47
1:C:98:GLU:HG3	1:C:99:PRO:HD3	1.95	0.47
1:C:901:LEU:HD11	1:C:1152:LEU:HD22	1.96	0.47
1:C:36:PHE:HB3	1:C:215:LEU:HD21	1.96	0.47
1:A:1204:VAL:HG23	1:A:1215:PRO:HG3	1.96	0.47
1:B:98:GLU:HG3	1:B:99:PRO:HD3	1.96	0.47
1:C:1143:LEU:HB2	1:C:1154:LEU:HB2	1.96	0.47
1:A:82:VAL:HG22	1:A:204:MET:HG2	1.98	0.46
1:B:287:ILE:HG22	1:B:289:LYS:HE3	1.96	0.46
1:B:125:ILE:HG21	1:B:185:PHE:CZ	2.50	0.46
1:A:948:GLU:HG2	1:A:952:MET:HE2	1.97	0.46
1:A:390:VAL:HG11	1:B:639:THR:HG23	1.98	0.46
1:A:1221:VAL:HG21	1:C:987:LEU:HD21	1.98	0.46
1:B:744:CYS:HB3	1:B:757:CYS:HB2	1.84	0.46
1:C:742:SER:HA	6:C:1406:NAG:H82	1.98	0.46
1:B:515:ILE:HG12	1:B:536:ILE:HG23	1.98	0.46
1:A:109:LEU:HD12	1:A:123:LEU:HD13	1.97	0.46
1:B:536:ILE:HD13	1:B:590:VAL:HG12	1.97	0.46
1:B:173:VAL:HG13	1:B:183:PHE:HB2	1.98	0.45
1:C:544:VAL:HG21	1:C:549:PHE:HB3	1.96	0.45
1:B:822:LEU:O	1:B:825:GLN:HG2	2.17	0.45
1:B:1190:PHE:HE1	1:B:1205:SER:HB3	1.81	0.45
4:Q:1:NAG:H61	4:Q:2:NAG:C7	2.47	0.45
1:A:33:ARG:HH12	2:F:123:VAL:HG22	1.81	0.45
1:A:536:ILE:HD13	1:A:590:VAL:HG12	1.99	0.45
1:B:604:LEU:HD11	1:C:594:LEU:HD23	1.99	0.45
1:A:607:PRO:HG2	1:A:610:GLY:HA3	1.98	0.45
1:B:894:ARG:HD2	1:B:898:GLU:HB3	1.98	0.45
1:C:803:PRO:HG3	1:C:844:GLU:OE1	2.17	0.45
1:B:386:LYS:HG2	1:C:545:ASP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ILE:HG21	1:C:424:ILE:HG22	1.98	0.45
1:B:595:LEU:HD13	1:B:621:GLN:HB2	1.99	0.45
1:C:125:ILE:HG21	1:C:185:PHE:CZ	2.51	0.45
2:D:77:THR:HG21	2:D:89:MET:HB3	1.99	0.44
2:F:56:VAL:HG21	2:F:133:TRP:HZ3	1.81	0.44
1:A:958:ILE:HA	1:A:961:MET:HE2	1.99	0.44
1:B:31:ASN:HB3	1:B:34:ARG:HG2	1.98	0.44
1:B:82:VAL:HG22	1:B:204:MET:HG2	1.99	0.44
1:C:529:LEU:HD11	1:C:613:VAL:HG11	1.99	0.44
3:I:69:TYR:CZ	3:I:73:ASN:HB3	2.52	0.44
1:A:543:CYS:HA	1:A:589:CYS:HA	1.98	0.44
1:A:894:ARG:HD2	1:A:898:GLU:HB3	1.99	0.44
1:C:451:ILE:HG12	1:C:461:ILE:HG22	2.00	0.44
1:C:303:ILE:HG13	1:C:443:SER:HB2	1.99	0.44
4:L:1:NAG:H61	4:L:2:NAG:C7	2.48	0.44
1:A:529:LEU:HD11	1:A:613:VAL:HG11	1.99	0.44
1:B:771:GLN:HE21	1:B:1160:PRO:HD2	1.83	0.44
1:B:800:TYR:CZ	1:B:1149:GLN:HA	2.53	0.44
2:D:86:ARG:HH22	2:D:106:ARG:HD2	1.81	0.44
1:B:298:SER:HB3	1:B:301:GLN:HB2	1.99	0.44
1:C:572:CYS:HB2	1:C:599:CYS:HB3	1.87	0.44
1:C:644:MET:HE3	1:C:663:ILE:HG21	1.98	0.44
2:E:133:TRP:HB2	3:I:63:PRO:HB2	1.99	0.44
1:B:318:ALA:HA	1:B:401:THR:HA	2.00	0.43
1:A:466:ASP:HB2	1:A:469:SER:HB2	1.99	0.43
1:C:822:LEU:O	1:C:825:GLN:HG2	2.17	0.43
1:C:93:ILE:HA	1:C:194:THR:HG22	1.99	0.43
1:B:544:VAL:HG21	1:B:549:PHE:HB3	2.01	0.43
1:C:262:LEU:HD11	1:C:399:VAL:HG11	2.00	0.43
1:A:303:ILE:HD11	1:A:316:PRO:HG3	2.00	0.43
1:B:303:ILE:HD11	1:B:316:PRO:HG3	2.01	0.43
1:C:287:ILE:HG22	1:C:289:LYS:HE3	2.01	0.43
1:C:1187:LEU:HD23	1:C:1206:SER:HA	2.00	0.43
1:C:466:ASP:HB3	1:C:469:SER:HB2	2.01	0.43
1:A:287:ILE:HG22	1:A:289:LYS:HE3	2.01	0.42
1:B:109:LEU:HD12	1:B:123:LEU:HD13	2.01	0.42
1:B:468:VAL:HG22	1:B:713:ILE:HG13	2.01	0.42
2:E:133:TRP:CE2	3:I:64:PRO:HG2	2.54	0.42
4:V:1:NAG:H61	4:V:2:NAG:C7	2.50	0.42
1:A:31:ASN:HB3	1:A:34:ARG:HG2	2.01	0.42
1:B:314:ARG:HE	1:B:445:ASN:HD22	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:NH1	1:A:445:ASN:HD22	2.14	0.42
1:A:407:TYR:HA	1:A:412:GLY:H	1.84	0.42
1:A:572:CYS:HB2	1:A:599:CYS:HB3	1.86	0.42
2:F:25:GLU:HB2	2:F:136:GLY:HA2	2.01	0.42
1:A:515:ILE:HG12	1:A:536:ILE:HG23	2.01	0.42
1:A:788:PHE:CE2	1:A:1209:MET:HG2	2.55	0.42
1:A:817:SER:HA	1:A:820:LYS:HE3	2.01	0.42
1:A:468:VAL:HG22	1:A:713:ILE:HG13	2.02	0.42
1:A:803:PRO:HB2	1:A:941:LEU:HD12	2.02	0.42
1:A:1190:PHE:HE1	1:A:1205:SER:HB3	1.84	0.42
2:F:133:TRP:HB2	3:G:63:PRO:HB2	2.00	0.42
1:B:373:CYS:HB2	1:B:391:LEU:HD13	2.02	0.42
1:C:42:GLN:HG3	1:C:44:PRO:HD2	2.01	0.42
2:E:56:VAL:HG22	2:E:114:TYR:HB2	2.01	0.42
1:A:168:TRP:HB3	1:A:173:VAL:HG23	2.01	0.41
1:A:280:LEU:HD23	1:A:314:ARG:HH12	1.84	0.41
1:C:515:ILE:HG12	1:C:536:ILE:HG23	2.02	0.41
1:B:579:VAL:O	1:B:630:GLY:HA3	2.20	0.41
1:C:229:PRO:HG2	3:I:50:SER:HB2	2.02	0.41
1:C:373:CYS:HB2	1:C:391:LEU:HD13	2.01	0.41
1:B:510:HIS:CE1	1:B:634:PRO:HG3	2.56	0.41
1:A:834:GLU:O	1:A:838:GLN:HG2	2.20	0.41
1:C:406:VAL:HB	1:C:414:LEU:HB2	2.02	0.41
1:A:961:MET:HE1	1:A:1143:LEU:HD23	2.01	0.41
1:C:407:TYR:HA	1:C:412:GLY:H	1.85	0.41
1:A:262:LEU:HD11	1:A:399:VAL:HG11	2.02	0.41
1:B:36:PHE:HB3	1:B:215:LEU:HD21	2.02	0.41
1:B:216:ASN:HD22	4:O:1:NAG:H83	1.85	0.41
1:B:812:VAL:HG11	1:B:823:LEU:HD13	2.03	0.41
1:C:216:ASN:HD22	4:T:1:NAG:H83	1.85	0.41
2:F:41:CYS:HB2	2:F:55:TRP:CH2	2.55	0.41
1:A:510:HIS:ND1	1:A:634:PRO:HG3	2.36	0.41
2:F:55:TRP:CD2	2:F:100:LEU:HD22	2.56	0.41
1:B:31:ASN:HD22	1:B:34:ARG:HE	1.69	0.41
1:B:788:PHE:CE2	1:B:1209:MET:HG2	2.56	0.41
1:B:1143:LEU:HB2	1:B:1154:LEU:HB2	2.03	0.41
2:D:25:GLU:HB2	2:D:136:GLY:HA2	2.01	0.41
1:C:289:LYS:HD3	1:C:289:LYS:HA	1.91	0.41
1:A:553:LEU:HD22	1:A:576:LEU:HD13	2.03	0.41
1:C:543:CYS:HA	1:C:589:CYS:HA	2.03	0.41
1:C:788:PHE:CE2	1:C:1209:MET:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ARG:HE	1:C:445:ASN:HD22	1.70	0.40
3:I:113:THR:HB	3:I:116:ASN:HB3	2.04	0.40
1:C:803:PRO:HB2	1:C:941:LEU:HD12	2.03	0.40
3:I:55:TRP:CE2	3:I:93:LEU:HB2	2.56	0.40
1:B:278:PRO:HG2	1:B:320:ARG:NH1	2.36	0.40
1:C:278:PRO:HG2	1:C:320:ARG:NH1	2.37	0.40
1:C:800:TYR:CZ	1:C:1149:GLN:HA	2.56	0.40
1:A:216:ASN:HD22	4:J:1:NAG:H83	1.86	0.40
1:A:1035:LEU:HA	1:A:1035:LEU:HD23	1.87	0.40
1:B:744:CYS:HB2	1:B:761:SER:OG	2.22	0.40
1:C:510:HIS:CE1	1:C:634:PRO:HG3	2.57	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	1076/1327 (81%)	1037 (96%)	39 (4%)	0	100	100
1	B	1076/1327 (81%)	1041 (97%)	35 (3%)	0	100	100
1	C	1076/1327 (81%)	1039 (97%)	37 (3%)	0	100	100
2	D	115/144 (80%)	112 (97%)	3 (3%)	0	100	100
2	E	115/144 (80%)	111 (96%)	4 (4%)	0	100	100
2	F	115/144 (80%)	112 (97%)	3 (3%)	0	100	100
3	G	100/129 (78%)	95 (95%)	5 (5%)	0	100	100
3	H	100/129 (78%)	94 (94%)	6 (6%)	0	100	100
3	I	100/129 (78%)	95 (95%)	5 (5%)	0	100	100
All	All	3873/4800 (81%)	3736 (96%)	137 (4%)	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	946/1149 (82%)	946 (100%)	0	100	100
1	B	946/1149 (82%)	946 (100%)	0	100	100
1	C	946/1149 (82%)	946 (100%)	0	100	100
2	D	90/113 (80%)	90 (100%)	0	100	100
2	E	90/113 (80%)	90 (100%)	0	100	100
2	F	90/113 (80%)	90 (100%)	0	100	100
3	G	80/101 (79%)	80 (100%)	0	100	100
3	H	80/101 (79%)	80 (100%)	0	100	100
3	I	80/101 (79%)	80 (100%)	0	100	100
All	All	3348/4089 (82%)	3348 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	71	HIS
1	A	157	HIS
1	A	445	ASN
1	A	1095	ASN
1	A	1149	GLN
1	A	1222	GLN
2	F	84	ASN
1	B	31	ASN
1	B	110	HIS
1	B	257	ASN
1	B	301	GLN
1	B	636	GLN
1	B	771	GLN
1	B	821	GLN

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Mol	Chain	Res	Type
1	B	1095	ASN
1	B	1149	GLN
2	D	93	ASN
1	C	71	HIS
1	C	739	ASN
1	C	771	GLN
1	C	1033	HIS
1	C	1095	ASN
1	C	1128	GLN
1	C	1149	GLN
3	I	111	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

39 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	1	1,4	14,14,15	0.75	0	17,19,21	1.10	1 (5%)
4	NAG	J	2	4	14,14,15	0.70	0	17,19,21	0.85	0
4	NAG	K	1	1,4	14,14,15	0.75	0	17,19,21	0.93	0
4	NAG	K	2	4	14,14,15	0.74	0	17,19,21	0.97	0
4	NAG	L	1	1,4	14,14,15	0.83	1 (7%)	17,19,21	1.16	2 (11%)
4	NAG	L	2	4	14,14,15	0.71	0	17,19,21	1.36	1 (5%)
4	NAG	M	1	1,4	14,14,15	0.81	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	M	2	4	14,14,15	0.71	0	17,19,21	0.85	0
5	NAG	N	1	1,5	14,14,15	0.81	0	17,19,21	1.26	2 (11%)
5	NAG	N	2	5	14,14,15	0.83	0	17,19,21	0.91	0
5	BMA	N	3	5	11,11,12	1.00	0	15,15,17	2.79	5 (33%)
5	MAN	N	4	5	11,11,12	0.72	0	15,15,17	1.44	1 (6%)
5	MAN	N	5	5	11,11,12	0.72	0	15,15,17	1.46	2 (13%)
4	NAG	O	1	1,4	14,14,15	0.74	0	17,19,21	1.11	1 (5%)
4	NAG	O	2	4	14,14,15	0.70	0	17,19,21	0.84	0
4	NAG	P	1	1,4	14,14,15	0.75	0	17,19,21	0.97	0
4	NAG	P	2	4	14,14,15	0.74	0	17,19,21	0.93	0
4	NAG	Q	1	1,4	14,14,15	0.81	0	17,19,21	1.18	2 (11%)
4	NAG	Q	2	4	14,14,15	0.70	0	17,19,21	1.33	1 (5%)
4	NAG	R	1	1,4	14,14,15	0.81	0	17,19,21	1.06	1 (5%)
4	NAG	R	2	4	14,14,15	0.71	0	17,19,21	0.84	0
5	NAG	S	1	1,5	14,14,15	0.80	0	17,19,21	1.18	2 (11%)
5	NAG	S	2	5	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
5	BMA	S	3	5	11,11,12	0.99	0	15,15,17	2.82	5 (33%)
5	MAN	S	4	5	11,11,12	0.73	0	15,15,17	1.48	1 (6%)
5	MAN	S	5	5	11,11,12	0.71	0	15,15,17	1.41	2 (13%)
4	NAG	T	1	1,4	14,14,15	0.74	0	17,19,21	1.08	1 (5%)
4	NAG	T	2	4	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	U	1	1,4	14,14,15	0.75	0	17,19,21	1.01	1 (5%)
4	NAG	U	2	4	14,14,15	0.75	0	17,19,21	0.97	0
4	NAG	V	1	1,4	14,14,15	0.82	0	17,19,21	1.19	2 (11%)
4	NAG	V	2	4	14,14,15	0.71	0	17,19,21	1.33	1 (5%)
4	NAG	W	1	1,4	14,14,15	0.81	0	17,19,21	1.05	1 (5%)
4	NAG	W	2	4	14,14,15	0.70	0	17,19,21	0.86	0
5	NAG	X	1	1,5	14,14,15	0.78	0	17,19,21	1.22	2 (11%)
5	NAG	X	2	5	14,14,15	0.81	0	17,19,21	0.95	0
5	BMA	X	3	5	11,11,12	1.00	0	15,15,17	2.83	5 (33%)
5	MAN	X	4	5	11,11,12	0.71	0	15,15,17	1.50	1 (6%)
5	MAN	X	5	5	11,11,12	0.73	0	15,15,17	1.46	2 (13%)

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	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
5	MAN	N	4	5	-	0/2/19/22	0/1/1/1
5	MAN	N	5	5	-	0/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
5	NAG	S	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
5	MAN	S	4	5	-	1/2/19/22	0/1/1/1
5	MAN	S	5	5	-	0/2/19/22	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	1/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	1/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
5	NAG	X	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1
5	MAN	X	4	5	-	0/2/19/22	0/1/1/1
5	MAN	X	5	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1	NAG	O5-C1	-2.02	1.40	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	3	BMA	C1-O5-C5	8.17	123.26	112.19
5	S	3	BMA	C1-O5-C5	8.06	123.11	112.19
5	N	3	BMA	C1-O5-C5	7.94	122.95	112.19
5	X	4	MAN	C1-O5-C5	4.46	118.23	112.19
5	S	4	MAN	C1-O5-C5	4.36	118.09	112.19
5	N	4	MAN	C1-O5-C5	4.21	117.89	112.19
5	X	5	MAN	C1-O5-C5	4.06	117.69	112.19
5	S	5	MAN	C1-O5-C5	3.99	117.60	112.19
5	N	5	MAN	C1-O5-C5	3.98	117.58	112.19
5	N	3	BMA	C3-C4-C5	3.76	116.95	110.24
5	S	3	BMA	C2-C3-C4	3.73	117.35	110.89
4	L	2	NAG	C2-N2-C7	3.72	128.20	122.90
5	X	3	BMA	C3-C4-C5	3.71	116.86	110.24
4	V	2	NAG	C2-N2-C7	3.69	128.16	122.90
5	S	3	BMA	C3-C4-C5	3.67	116.78	110.24
4	Q	2	NAG	C2-N2-C7	3.64	128.08	122.90
5	X	3	BMA	C2-C3-C4	3.63	117.18	110.89
5	N	3	BMA	C2-C3-C4	3.60	117.12	110.89
4	J	1	NAG	C2-N2-C7	3.12	127.35	122.90
4	T	1	NAG	C2-N2-C7	2.99	127.16	122.90
4	O	1	NAG	C2-N2-C7	2.96	127.12	122.90
5	N	1	NAG	C2-N2-C7	2.95	127.11	122.90
5	S	1	NAG	C2-N2-C7	2.82	126.92	122.90
4	M	1	NAG	C2-N2-C7	2.77	126.85	122.90
4	R	1	NAG	C2-N2-C7	2.75	126.82	122.90
5	X	3	BMA	O5-C5-C4	2.74	117.49	110.83
5	X	1	NAG	C2-N2-C7	2.72	126.78	122.90
5	S	3	BMA	O5-C5-C4	2.72	117.44	110.83
4	W	1	NAG	C2-N2-C7	2.70	126.75	122.90
5	N	3	BMA	O5-C5-C4	2.67	117.31	110.83
4	V	1	NAG	O4-C4-C3	-2.67	104.19	110.35
5	X	5	MAN	C1-C2-C3	2.66	112.93	109.67
4	L	1	NAG	O4-C4-C3	-2.62	104.29	110.35
4	Q	1	NAG	O4-C4-C3	-2.59	104.36	110.35
5	N	5	MAN	C1-C2-C3	2.57	112.82	109.67
5	X	1	NAG	O3-C3-C2	-2.53	104.24	109.47
5	N	1	NAG	O3-C3-C2	-2.47	104.35	109.47
5	N	3	BMA	O4-C4-C3	-2.45	104.69	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	3	BMA	O4-C4-C3	-2.40	104.81	110.35
5	X	3	BMA	O4-C4-C3	-2.34	104.94	110.35
4	V	1	NAG	C2-N2-C7	2.32	126.20	122.90
5	S	1	NAG	O3-C3-C2	-2.28	104.74	109.47
5	S	5	MAN	C1-C2-C3	2.20	112.37	109.67
5	S	2	NAG	C1-O5-C5	2.19	115.16	112.19
4	Q	1	NAG	C2-N2-C7	2.09	125.89	122.90
4	U	1	NAG	C1-O5-C5	2.04	114.95	112.19
4	L	1	NAG	C2-N2-C7	2.01	125.76	122.90

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	Q	1	NAG	C8-C7-N2-C2
4	Q	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
4	P	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
5	S	4	MAN	O5-C5-C6-O6

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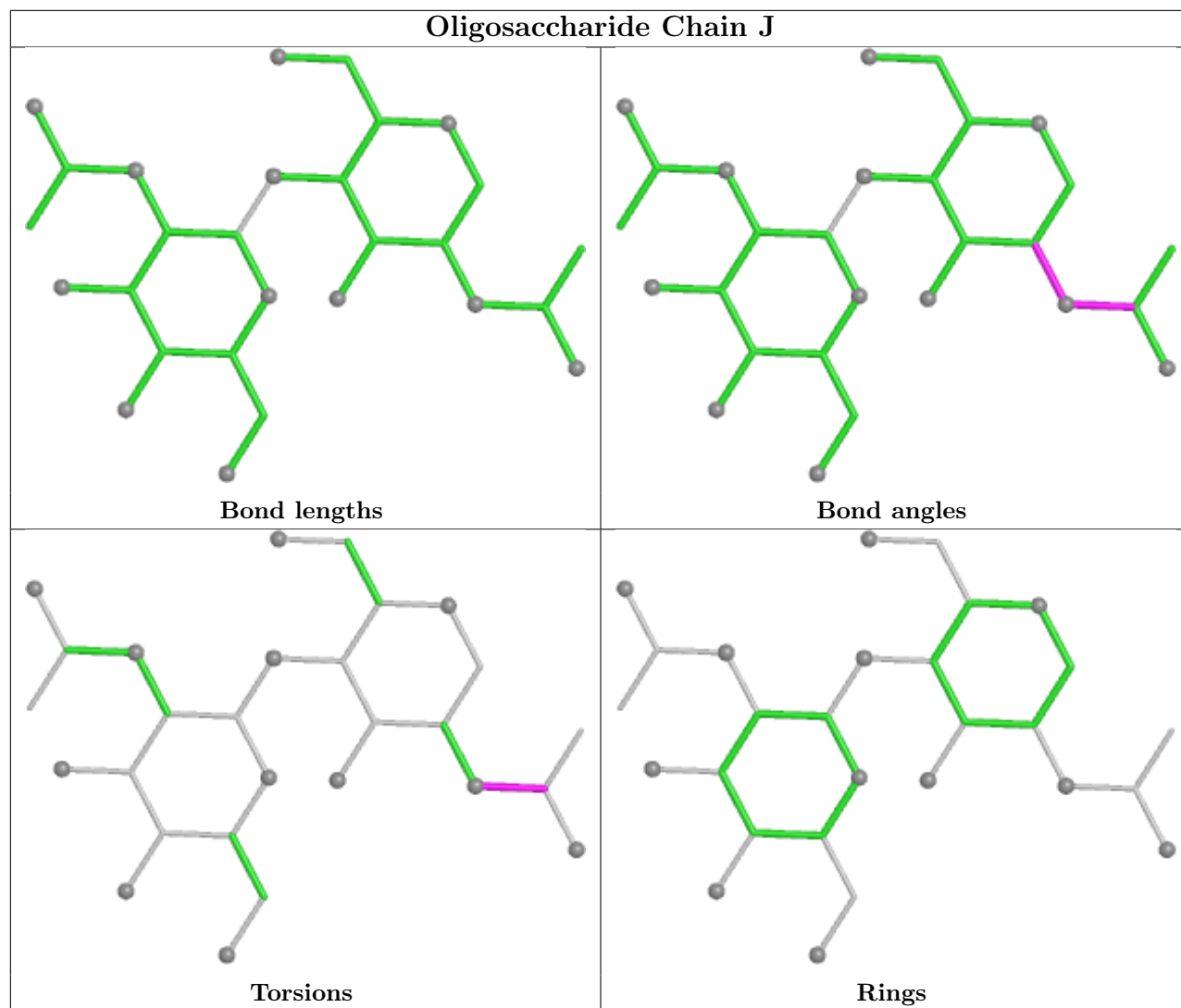
Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C3-C2-N2-C7
4	Q	2	NAG	C3-C2-N2-C7
4	V	2	NAG	C3-C2-N2-C7
4	Q	1	NAG	C4-C5-C6-O6

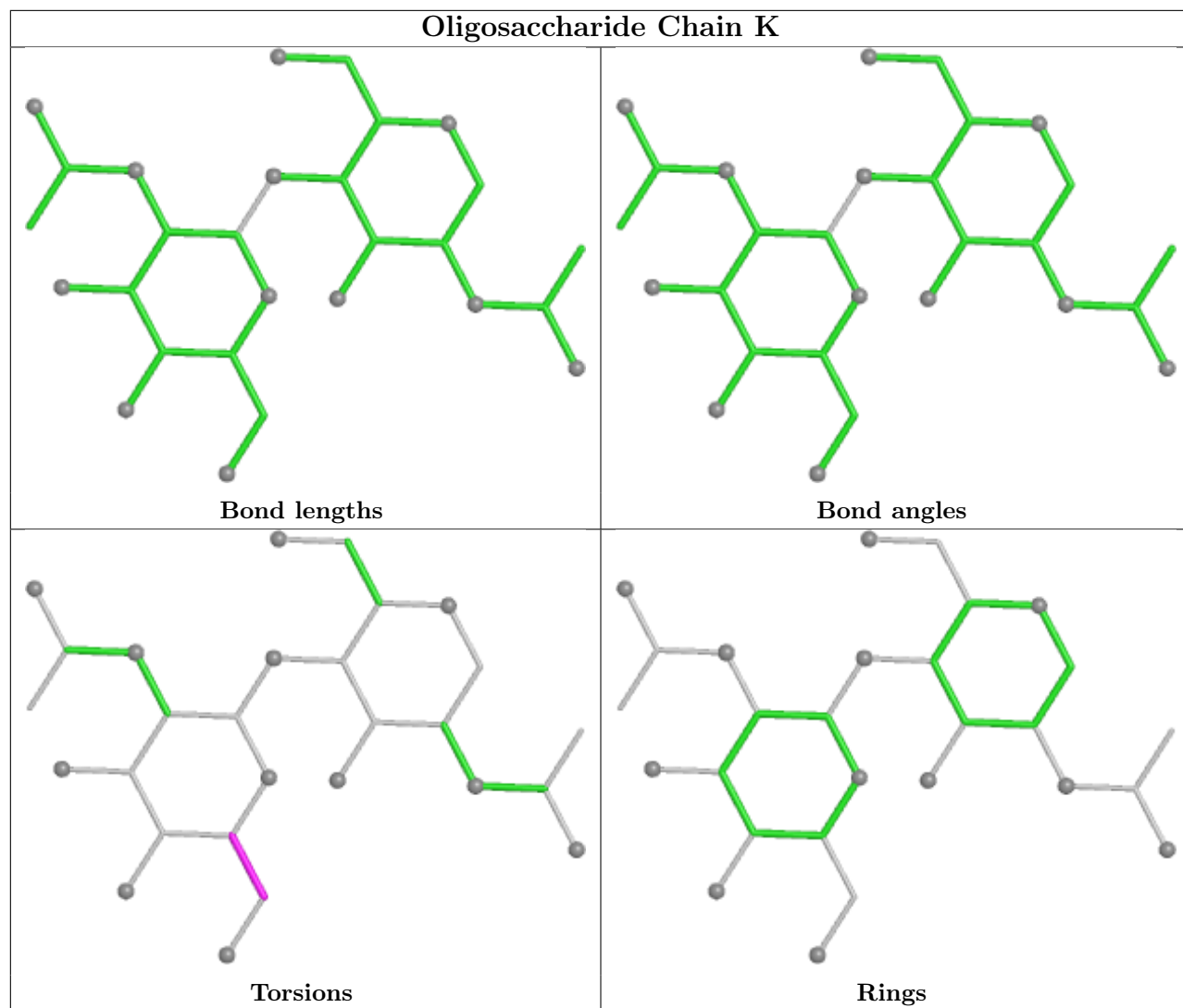
There are no ring outliers.

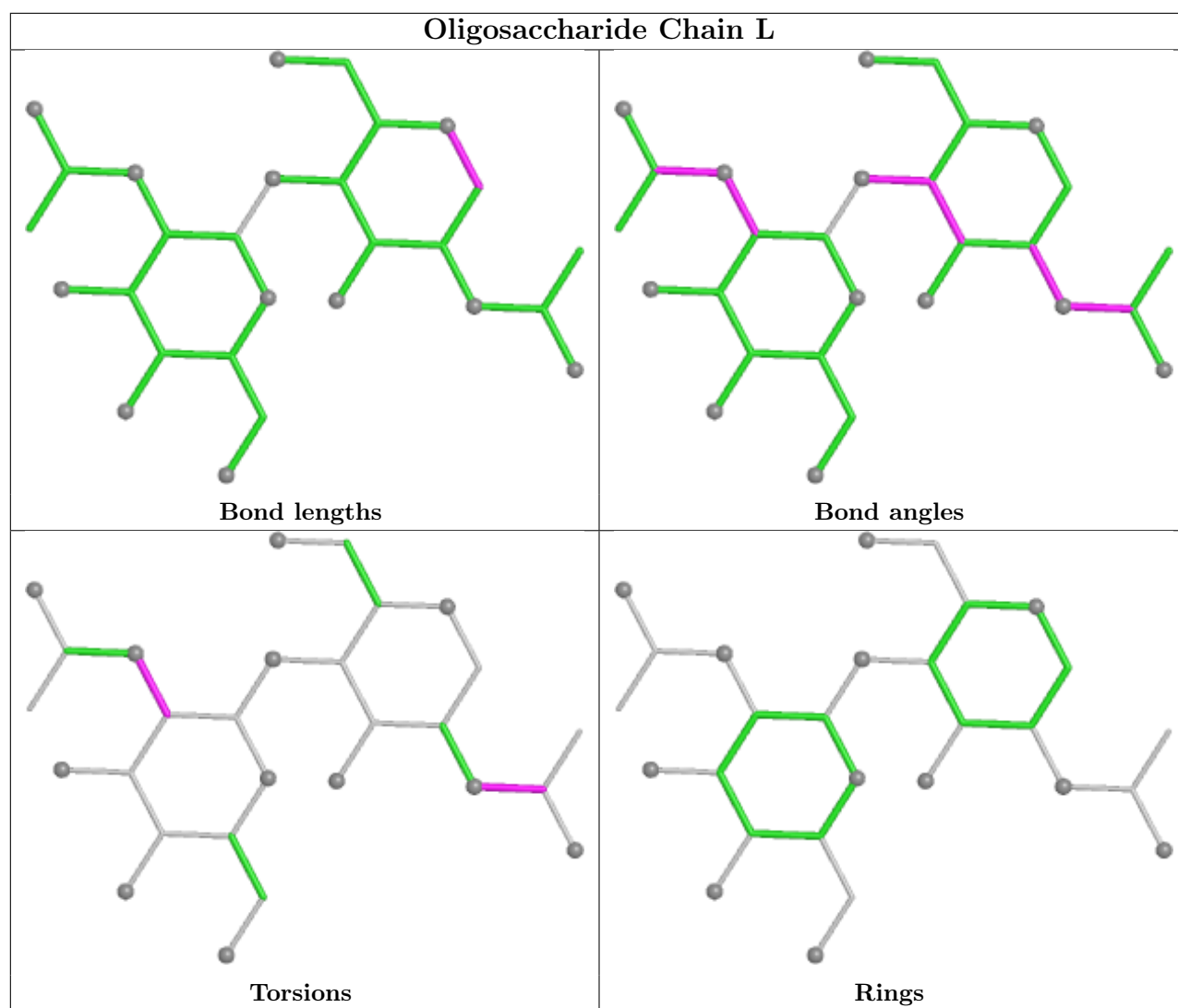
9 monomers are involved in 6 short contacts:

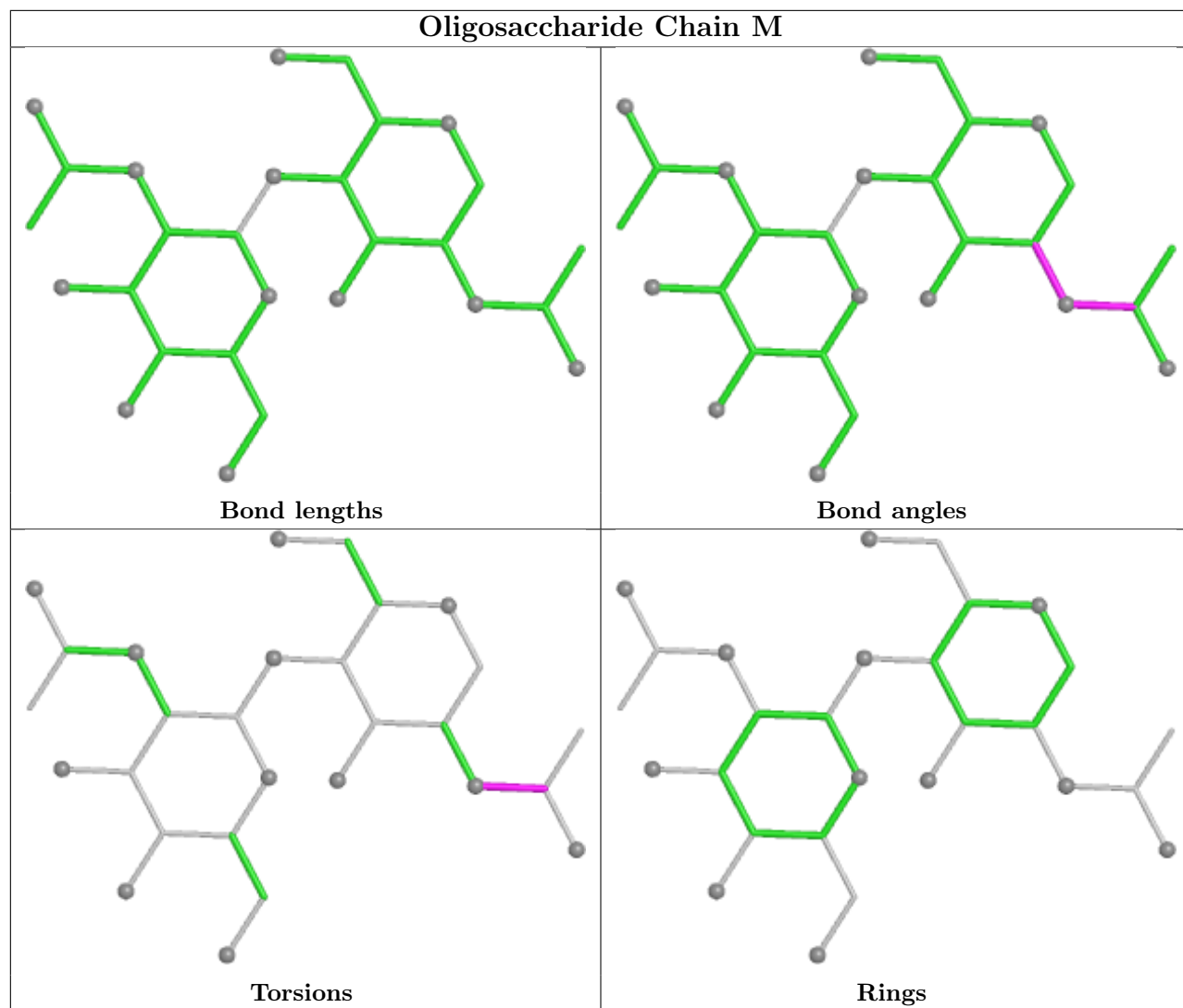
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	1	NAG	1	0
4	V	2	NAG	1	0
4	V	1	NAG	1	0
4	O	1	NAG	1	0
4	Q	2	NAG	1	0
4	J	1	NAG	1	0
4	L	2	NAG	1	0
4	L	1	NAG	1	0
4	T	1	NAG	1	0

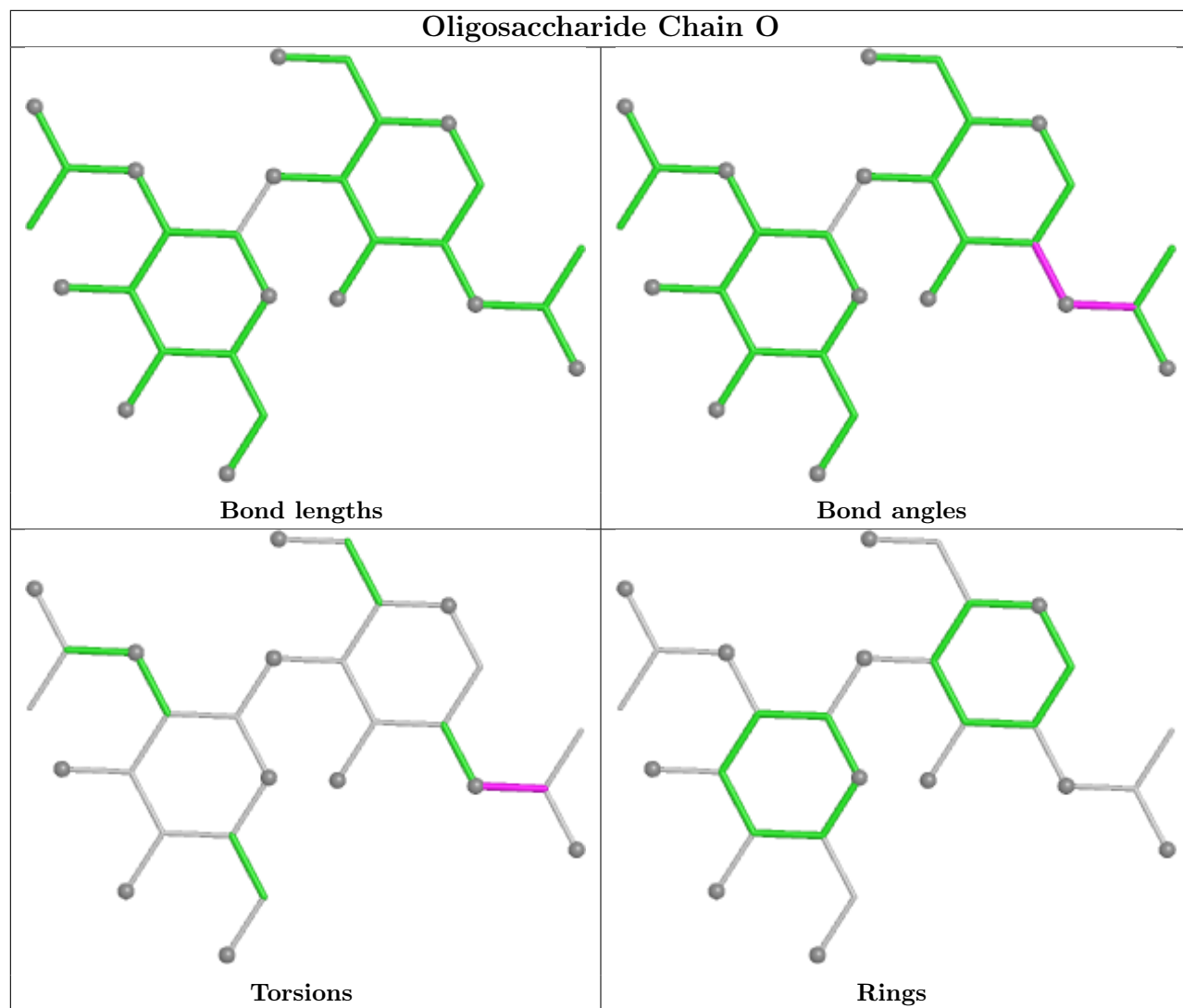
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

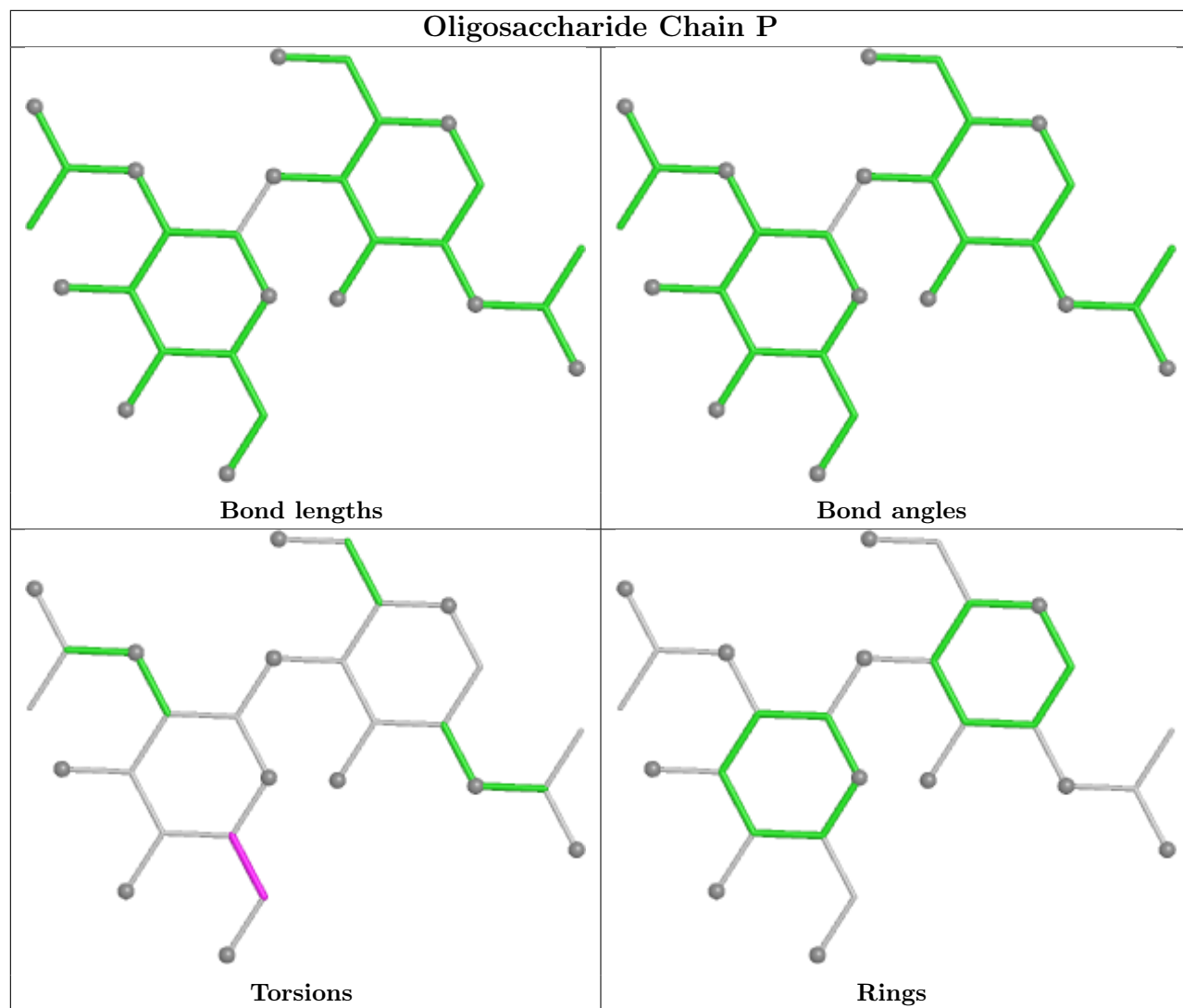


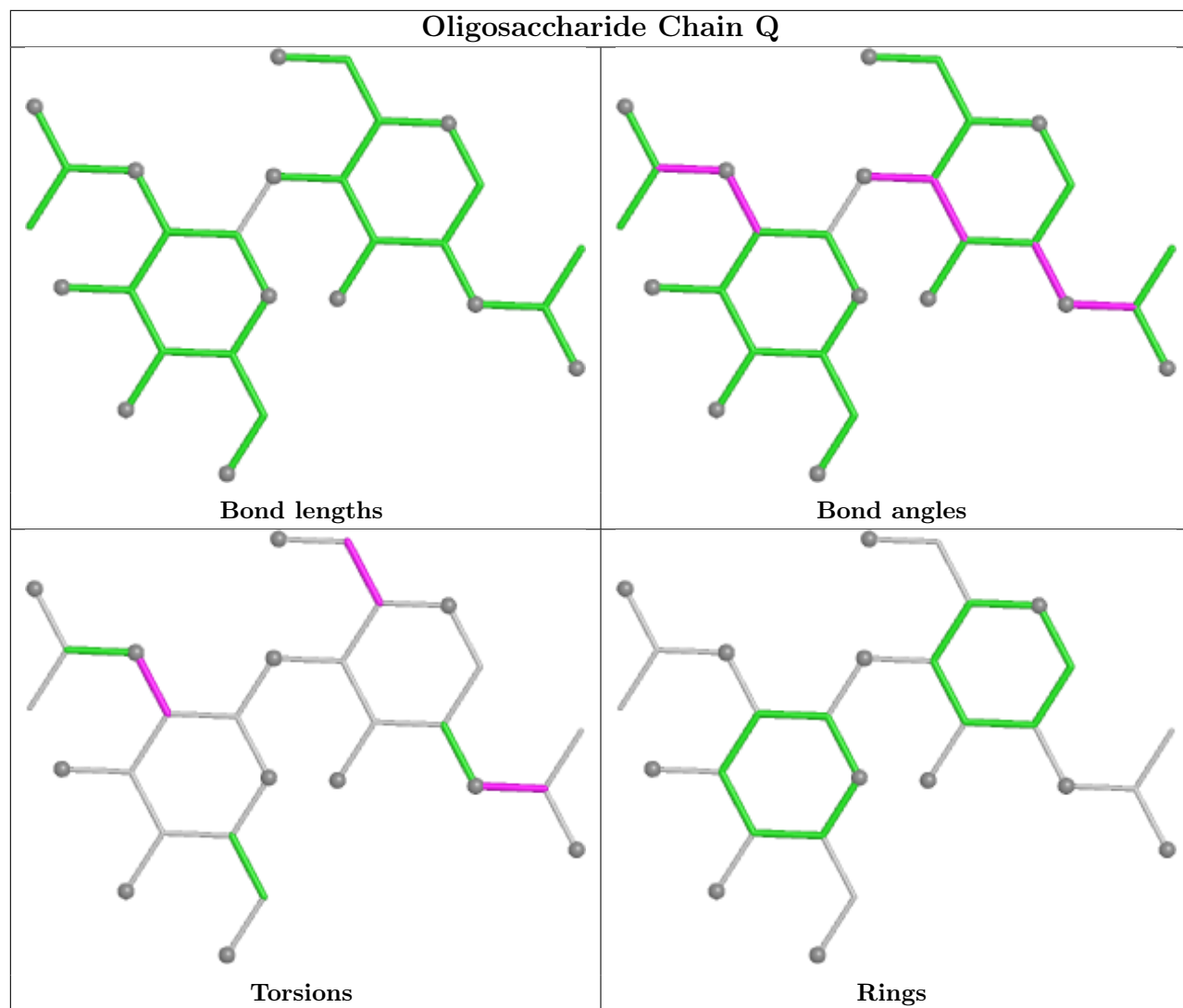


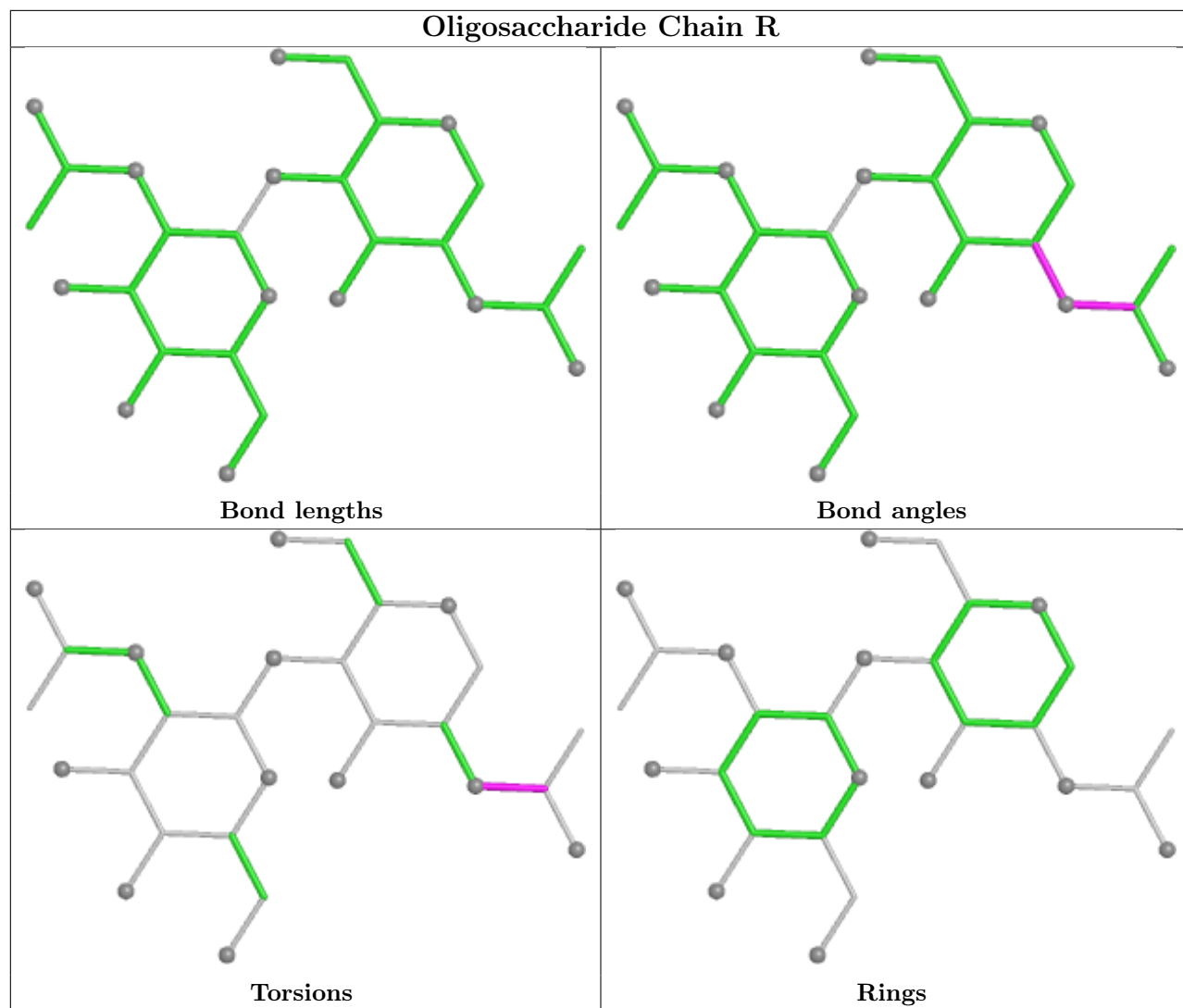


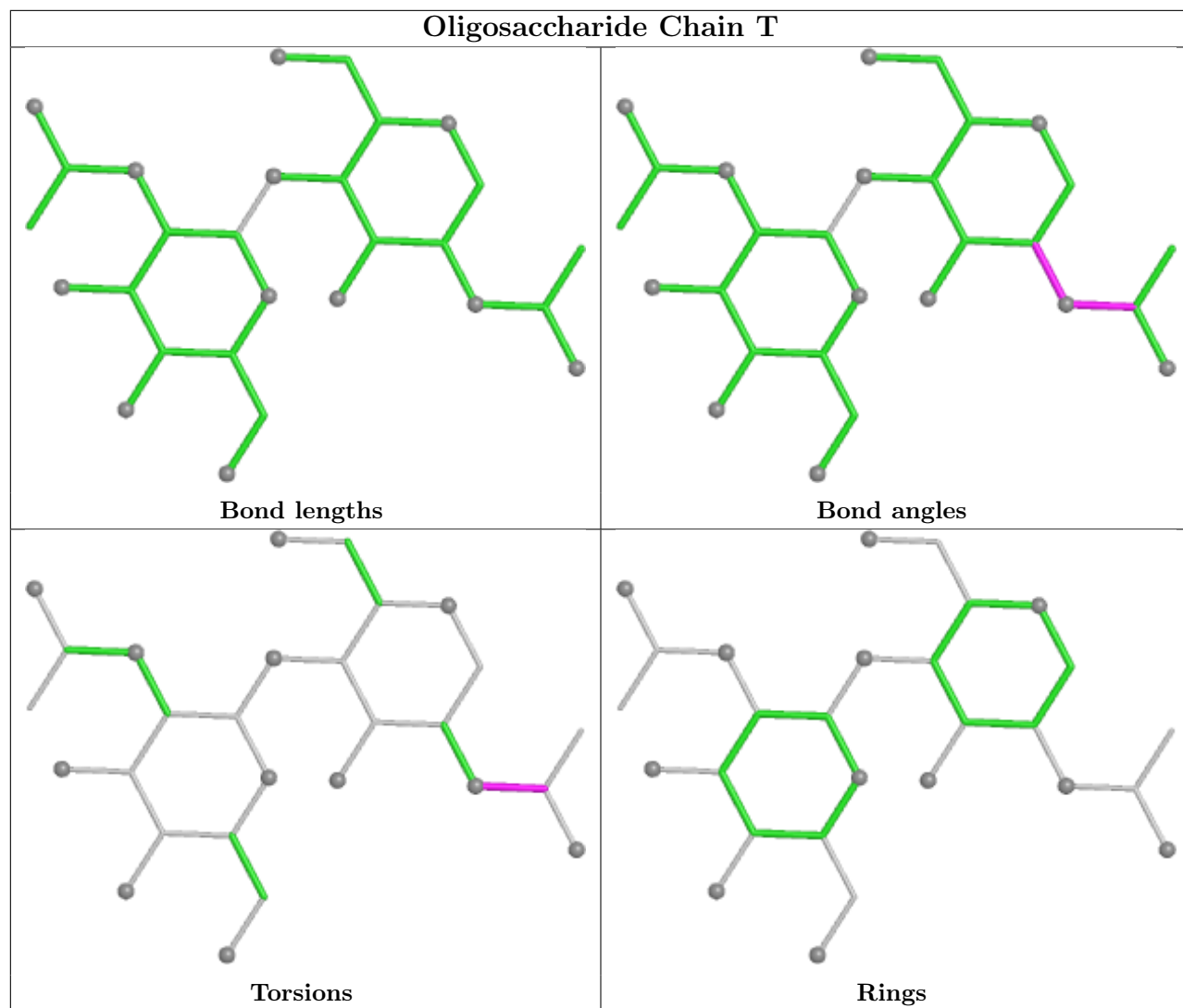


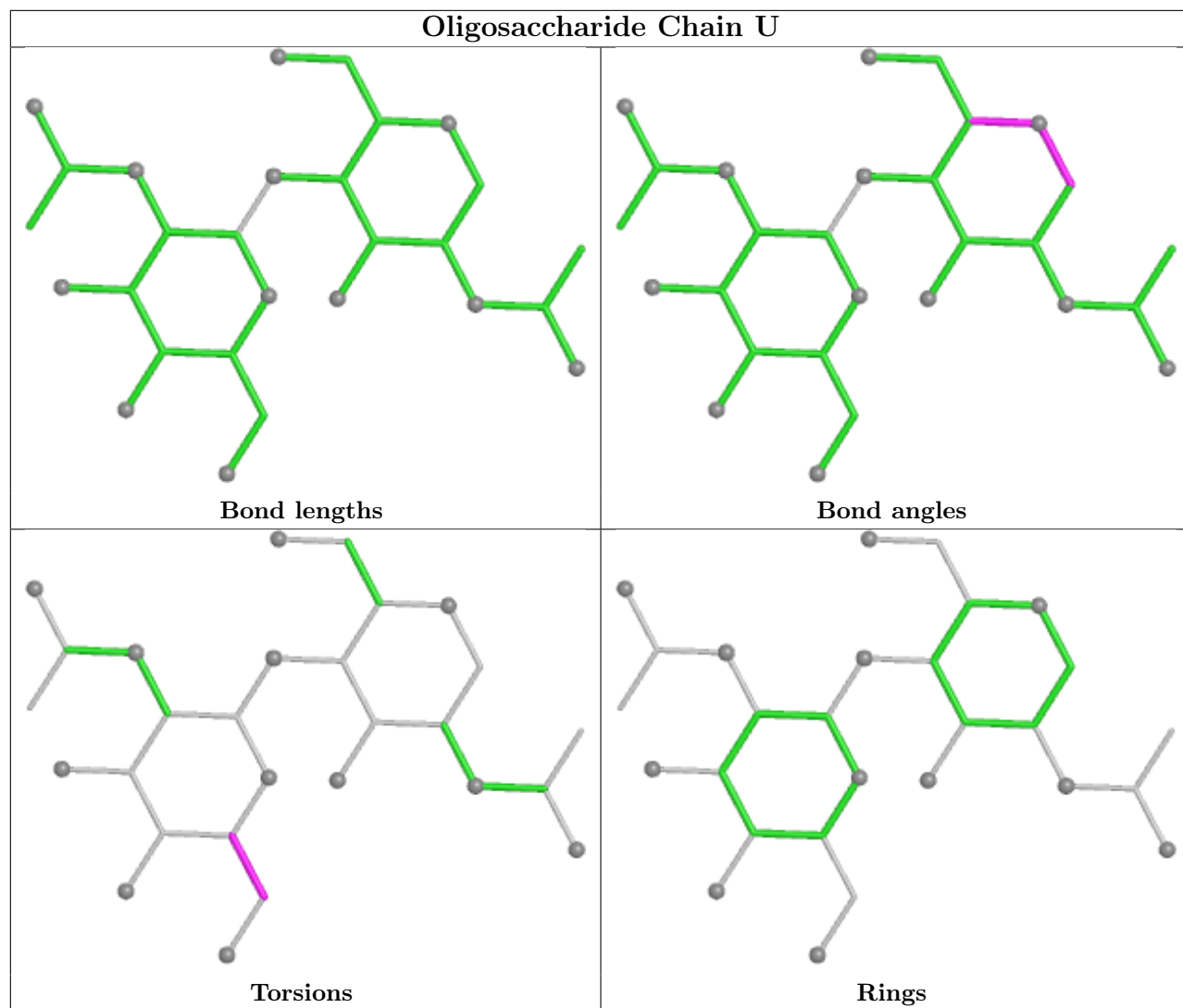


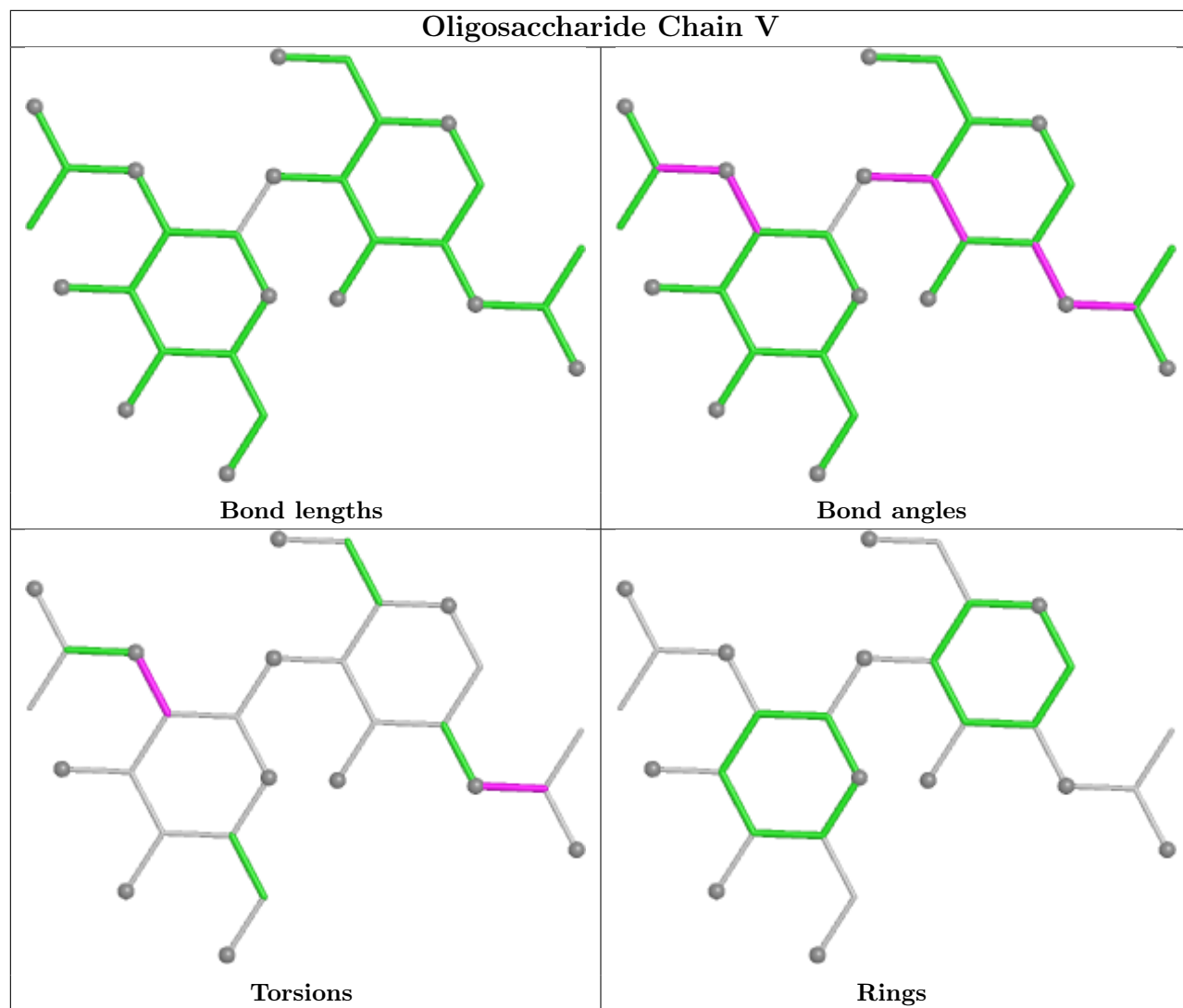


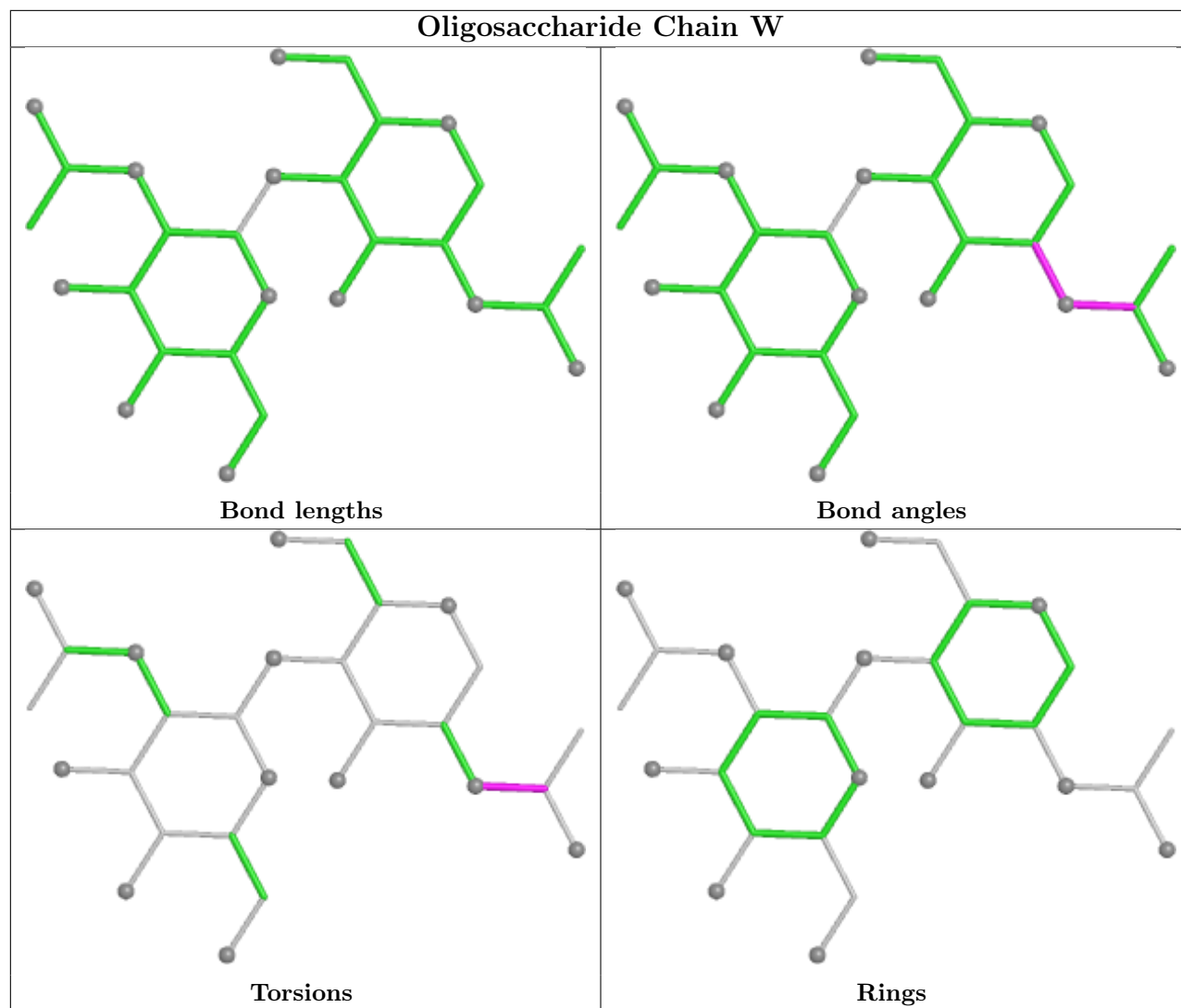


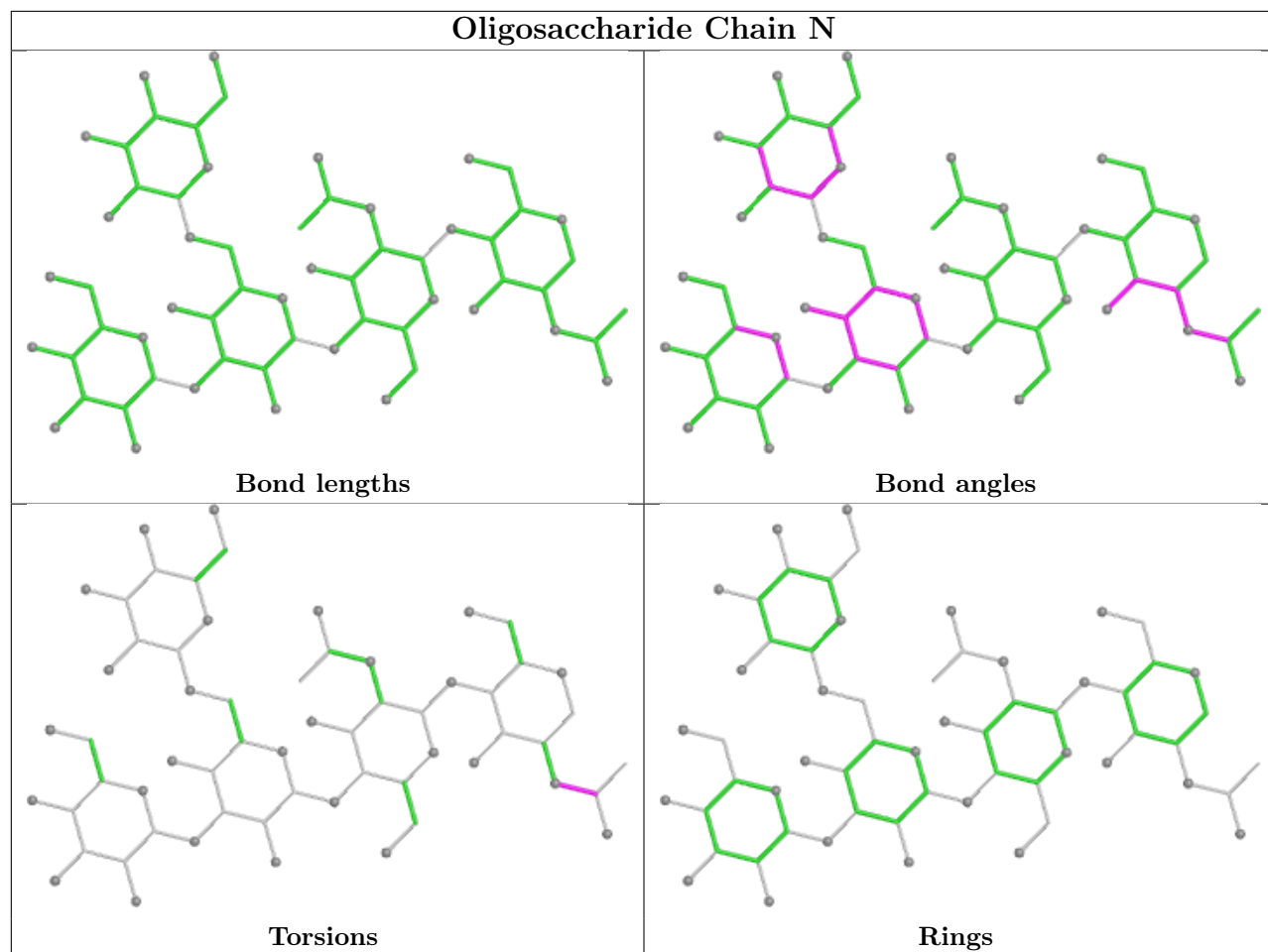


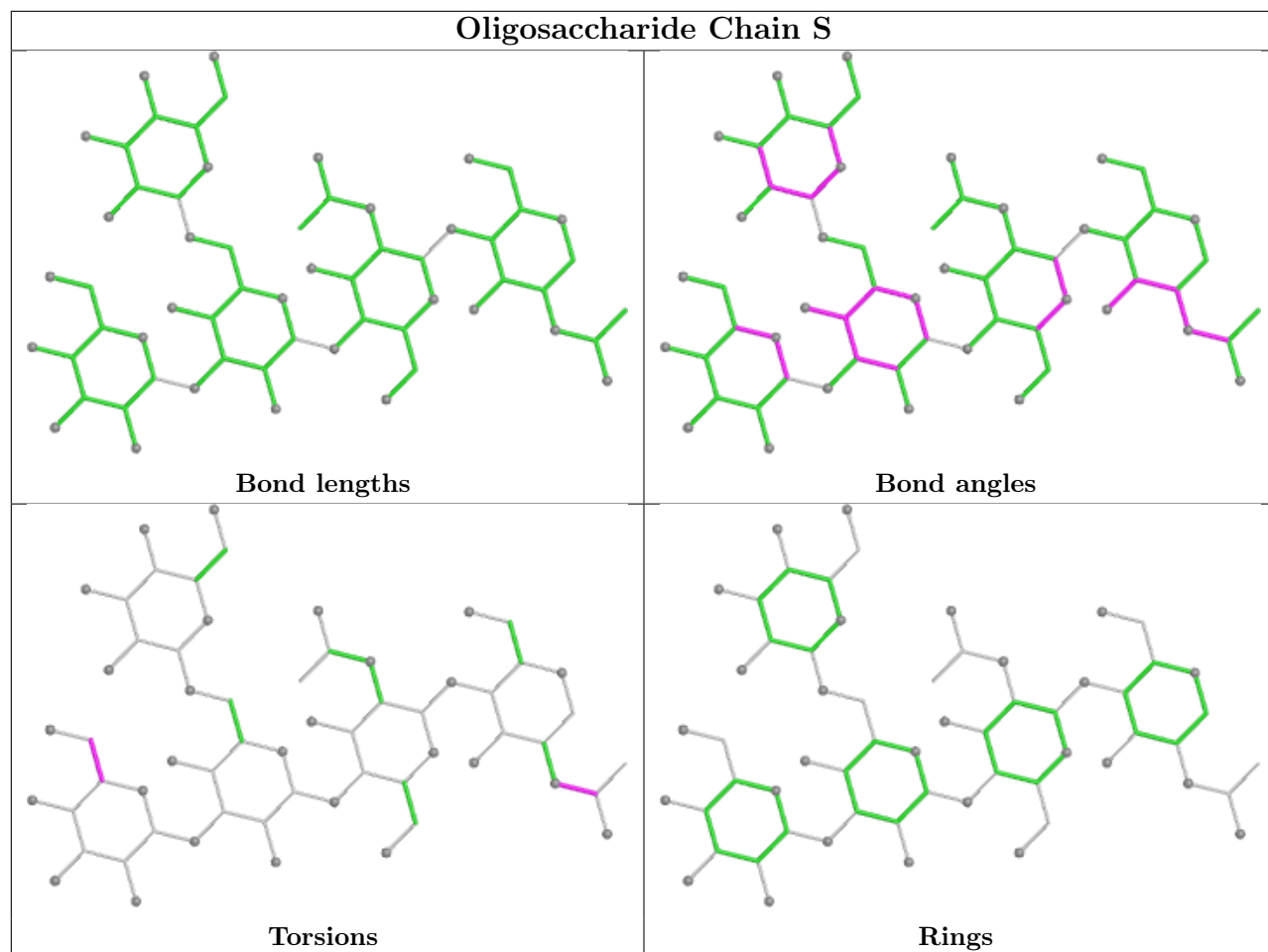


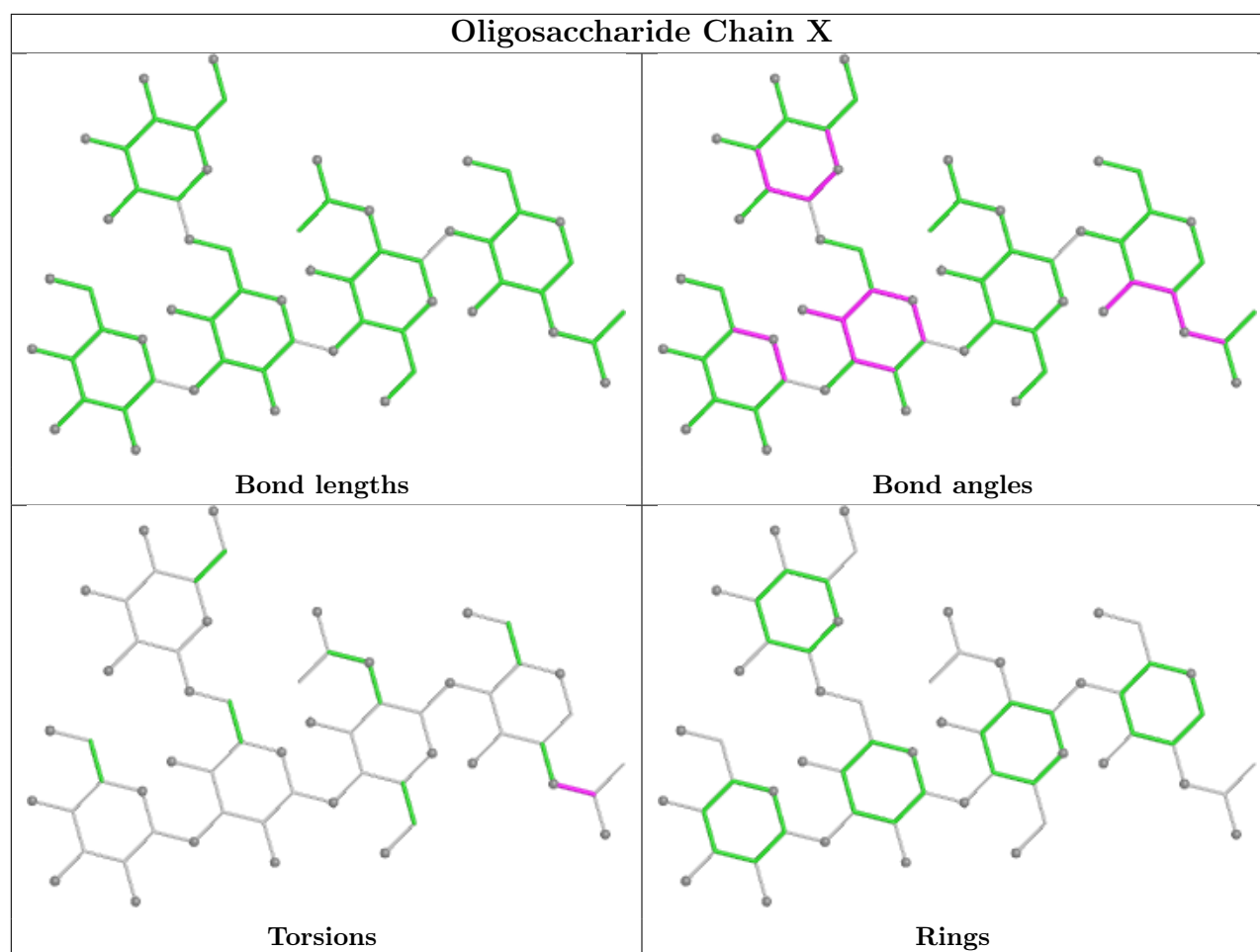












5.6 Ligand geometry [i](#)

39 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	A	1406	1	14,14,15	0.72	0	17,19,21	1.01	2 (11%)
6	NAG	C	1411	1	14,14,15	0.71	0	17,19,21	1.50	2 (11%)
6	NAG	A	1411	1	14,14,15	0.72	0	17,19,21	0.87	1 (5%)
7	PAM	A	1413	-	17,17,17	0.62	0	17,17,17	0.59	0
6	NAG	B	1412	1	14,14,15	0.71	0	17,19,21	0.78	0
7	PAM	C	1401	-	17,17,17	0.62	0	17,17,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1405	1	14,14,15	0.72	0	17,19,21	0.78	0
6	NAG	B	1407	1	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
7	PAM	B	1408	-	17,17,17	0.62	0	17,17,17	0.54	0
6	NAG	C	1412	1	14,14,15	0.73	0	17,19,21	0.85	0
6	NAG	C	1405	1	14,14,15	0.74	0	17,19,21	0.91	0
7	PAM	C	1409	-	17,17,17	0.62	0	17,17,17	0.56	0
6	NAG	A	1404	1	14,14,15	0.72	0	17,19,21	0.83	0
6	NAG	A	1401	1	14,14,15	0.72	0	17,19,21	0.93	0
6	NAG	B	1403	1	14,14,15	0.71	0	17,19,21	0.97	1 (5%)
6	NAG	B	1401	1	14,14,15	0.72	0	17,19,21	0.90	0
6	NAG	A	1409	1	14,14,15	0.70	0	17,19,21	2.37	5 (29%)
7	PAM	A	1408	-	17,17,17	0.61	0	17,17,17	0.59	0
6	NAG	C	1406	1	14,14,15	0.71	0	17,19,21	0.79	0
6	NAG	A	1403	1	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
6	NAG	B	1410	1	14,14,15	0.73	0	17,19,21	0.83	0
6	NAG	B	1405	1	14,14,15	0.73	0	17,19,21	0.80	0
6	NAG	A	1407	1	14,14,15	0.71	0	17,19,21	0.96	1 (5%)
6	NAG	C	1404	1	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
6	NAG	B	1402	1	14,14,15	0.75	0	17,19,21	1.30	1 (5%)
6	NAG	A	1402	1	14,14,15	0.75	0	17,19,21	1.38	1 (5%)
6	NAG	B	1409	1	14,14,15	0.74	0	17,19,21	1.51	3 (17%)
6	NAG	A	1410	1	14,14,15	0.63	0	17,19,21	1.54	2 (11%)
6	NAG	C	1407	1	14,14,15	0.73	0	17,19,21	1.00	1 (5%)
6	NAG	B	1411	1	14,14,15	0.69	0	17,19,21	0.76	0
6	NAG	C	1402	1	14,14,15	0.71	0	17,19,21	0.92	0
6	NAG	B	1404	1	14,14,15	0.72	0	17,19,21	0.84	0
6	NAG	C	1408	1	14,14,15	0.73	0	17,19,21	1.01	1 (5%)
6	NAG	C	1403	1	14,14,15	0.72	0	17,19,21	1.42	2 (11%)
6	NAG	A	1412	1	14,14,15	0.73	0	17,19,21	1.05	2 (11%)
7	PAM	B	1413	-	17,17,17	0.60	0	17,17,17	0.63	0
6	NAG	C	1413	1	14,14,15	0.71	0	17,19,21	0.78	0
6	NAG	C	1410	1	14,14,15	0.72	0	17,19,21	1.09	1 (5%)
6	NAG	B	1406	1	14,14,15	0.75	0	17,19,21	0.97	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	A	1406	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1411	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1411	1	-	2/6/23/26	0/1/1/1
7	PAM	A	1413	-	-	3/15/15/15	-
6	NAG	B	1412	1	-	0/6/23/26	0/1/1/1
7	PAM	C	1401	-	-	4/15/15/15	-
6	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
7	PAM	B	1408	-	-	3/15/15/15	-
6	NAG	C	1412	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
7	PAM	C	1409	-	-	4/15/15/15	-
6	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
7	PAM	A	1408	-	-	4/15/15/15	-
6	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1409	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1410	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1411	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1412	1	-	2/6/23/26	0/1/1/1
7	PAM	B	1413	-	-	4/15/15/15	-
6	NAG	C	1413	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1406	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1409	NAG	C1-O5-C5	6.74	121.32	112.19
6	A	1409	NAG	C2-N2-C7	4.77	129.69	122.90
6	A	1410	NAG	C2-N2-C7	4.29	129.01	122.90
6	B	1409	NAG	C2-N2-C7	4.22	128.91	122.90
6	A	1402	NAG	C2-N2-C7	4.21	128.89	122.90
6	C	1403	NAG	C2-N2-C7	4.16	128.83	122.90
6	B	1402	NAG	C2-N2-C7	4.16	128.83	122.90
6	C	1411	NAG	C2-N2-C7	3.77	128.27	122.90
6	C	1410	NAG	O5-C1-C2	-2.83	106.83	111.29
6	A	1409	NAG	C3-C4-C5	-2.76	105.32	110.24
6	B	1403	NAG	C1-O5-C5	2.39	115.43	112.19
6	A	1412	NAG	C2-N2-C7	2.35	126.25	122.90
6	B	1407	NAG	C1-O5-C5	2.35	115.37	112.19
6	A	1411	NAG	O5-C1-C2	-2.27	107.70	111.29
6	A	1412	NAG	C1-O5-C5	2.27	115.27	112.19
6	B	1406	NAG	C2-N2-C7	2.26	126.12	122.90
6	C	1411	NAG	O5-C1-C2	-2.26	107.73	111.29
6	A	1410	NAG	O5-C1-C2	-2.25	107.74	111.29
6	C	1408	NAG	C1-O5-C5	2.25	115.23	112.19
6	C	1404	NAG	C1-O5-C5	2.22	115.21	112.19
6	C	1407	NAG	C2-N2-C7	2.11	125.91	122.90
6	B	1409	NAG	O5-C1-C2	-2.10	107.97	111.29
6	B	1409	NAG	C1-C2-N2	2.10	114.07	110.49
6	A	1409	NAG	O7-C7-N2	2.06	125.74	121.95
6	A	1406	NAG	C1-O5-C5	2.05	114.98	112.19
6	A	1407	NAG	C1-O5-C5	2.03	114.94	112.19
6	A	1406	NAG	C2-N2-C7	2.02	125.78	122.90
6	A	1409	NAG	C4-C3-C2	2.02	113.98	111.02
6	A	1403	NAG	C1-O5-C5	2.01	114.91	112.19
6	C	1403	NAG	O7-C7-N2	2.00	125.63	121.95

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1409	NAG	C1-C2-N2-C7
6	C	1410	NAG	C4-C5-C6-O6
6	C	1410	NAG	O5-C5-C6-O6
6	A	1402	NAG	C8-C7-N2-C2
6	A	1402	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	1406	NAG	C8-C7-N2-C2
6	A	1406	NAG	O7-C7-N2-C2
6	A	1412	NAG	C8-C7-N2-C2
6	A	1412	NAG	O7-C7-N2-C2
6	B	1402	NAG	C8-C7-N2-C2
6	B	1402	NAG	O7-C7-N2-C2
6	B	1406	NAG	C8-C7-N2-C2
6	B	1406	NAG	O7-C7-N2-C2
6	C	1407	NAG	C8-C7-N2-C2
6	C	1407	NAG	O7-C7-N2-C2
6	B	1406	NAG	O5-C5-C6-O6
6	C	1407	NAG	O5-C5-C6-O6
6	A	1406	NAG	O5-C5-C6-O6
7	A	1408	PAM	C4-C5-C6-C7
7	C	1401	PAM	C4-C5-C6-C7
7	A	1408	PAM	C6-C7-C8-C9
7	A	1408	PAM	C2-C3-C4-C5
7	C	1401	PAM	C5-C6-C7-C8
7	B	1408	PAM	C4-C5-C6-C7
6	B	1411	NAG	O5-C5-C6-O6
6	C	1411	NAG	O5-C5-C6-O6
6	A	1411	NAG	C4-C5-C6-O6
7	A	1413	PAM	C6-C7-C8-C9
7	C	1409	PAM	C7-C8-C9-C10
6	A	1411	NAG	O5-C5-C6-O6
7	B	1413	PAM	C12-C13-C14-C15
7	B	1413	PAM	C13-C14-C15-C16
6	B	1406	NAG	C4-C5-C6-O6
7	C	1409	PAM	C4-C5-C6-C7
7	A	1408	PAM	C10-C11-C12-C13
7	B	1413	PAM	C6-C7-C8-C9
7	B	1408	PAM	C7-C8-C9-C10
7	C	1401	PAM	C7-C8-C9-C10
6	A	1409	NAG	C3-C2-N2-C7
6	A	1410	NAG	C3-C2-N2-C7
6	C	1403	NAG	C3-C2-N2-C7
6	C	1411	NAG	C3-C2-N2-C7
7	A	1413	PAM	C7-C8-C9-C10
6	B	1409	NAG	C4-C5-C6-O6
7	C	1401	PAM	C6-C7-C8-C9
7	B	1408	PAM	C3-C4-C5-C6
7	A	1413	PAM	C10-C11-C12-C13

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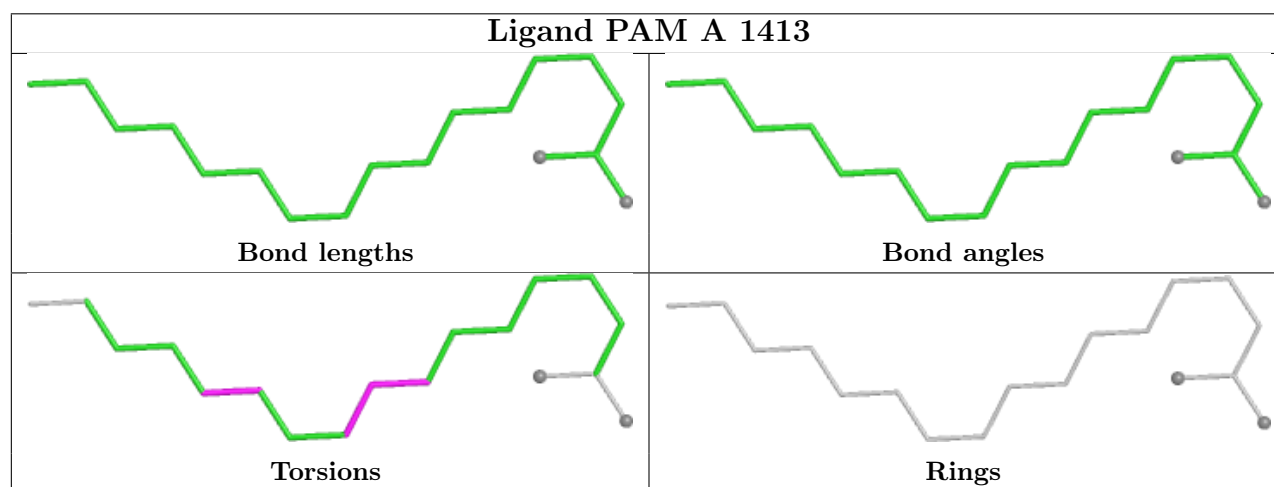
Mol	Chain	Res	Type	Atoms
7	B	1413	PAM	C7-C8-C9-C10
6	B	1409	NAG	C3-C2-N2-C7
6	B	1409	NAG	C1-C2-N2-C7
7	C	1409	PAM	O1-C1-C2-C3
7	C	1409	PAM	C2-C3-C4-C5

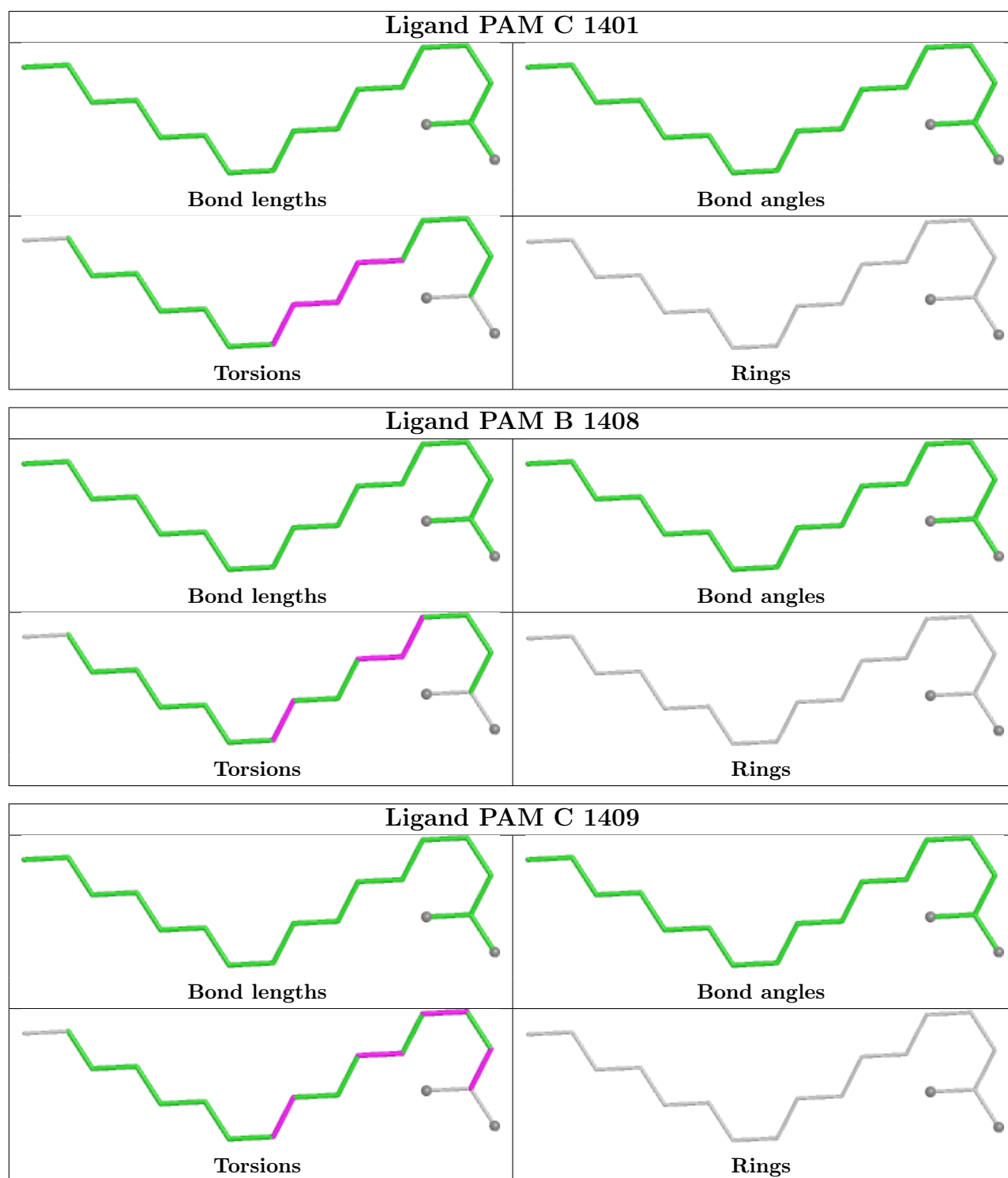
There are no ring outliers.

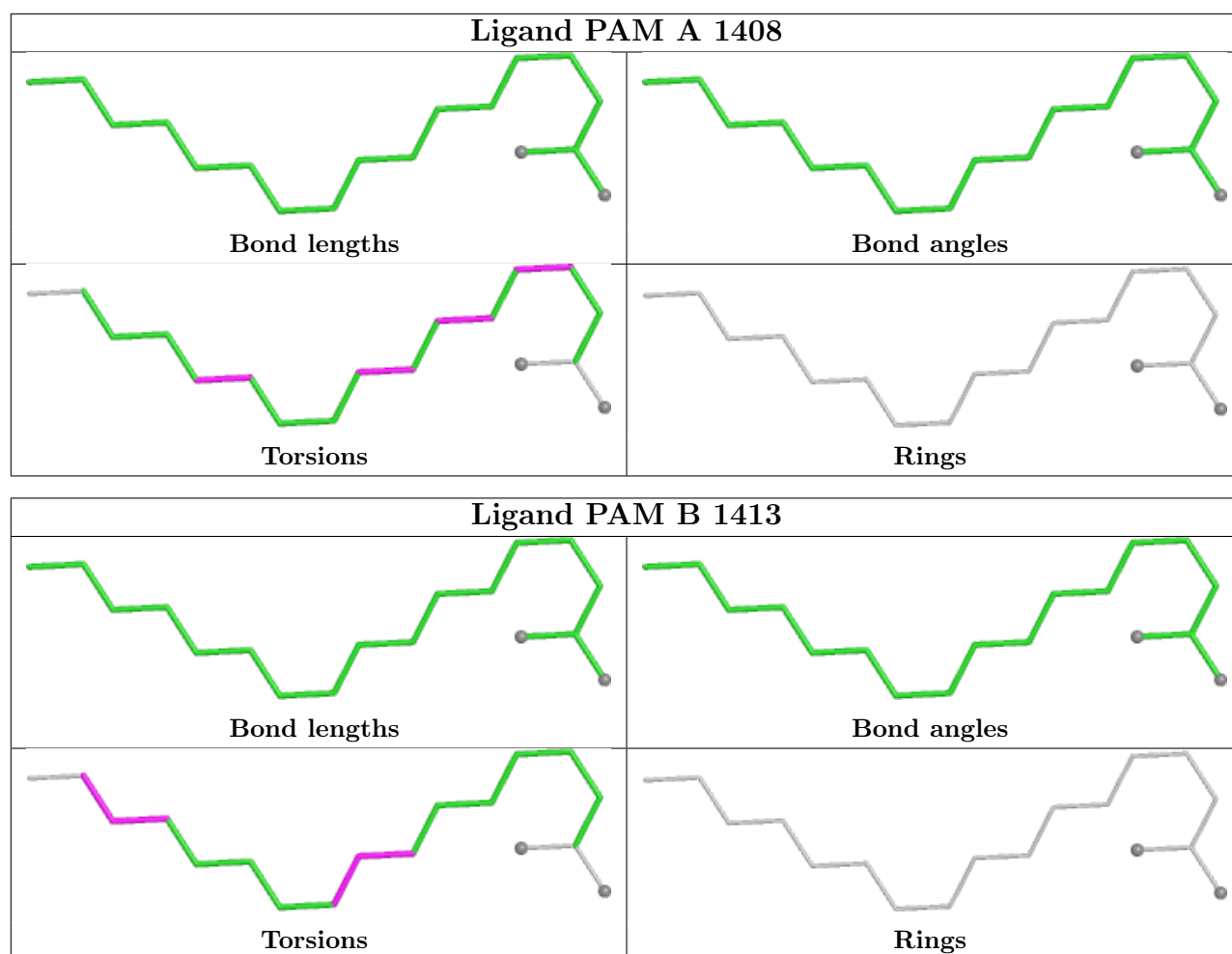
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1408	PAM	1	0
6	C	1406	NAG	1	0
6	B	1411	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

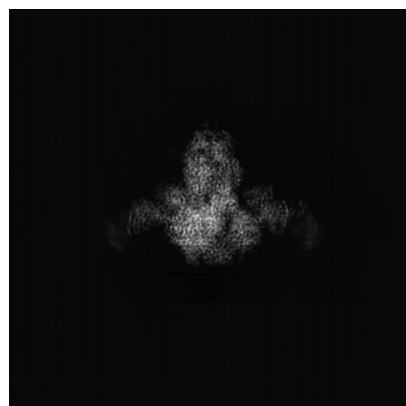
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67065. 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](#)

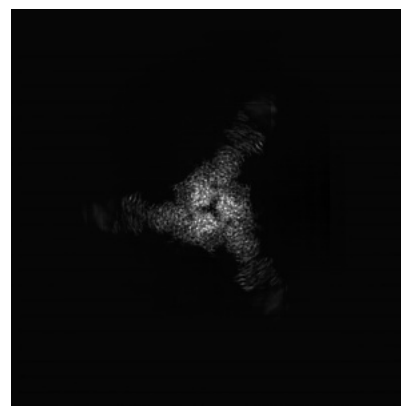
6.1.1 Primary map



X

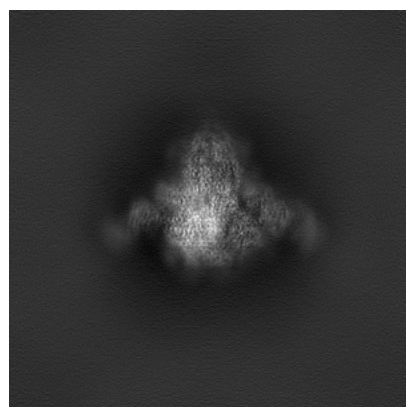


Y

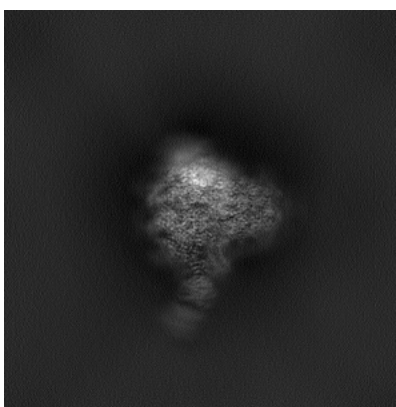


Z

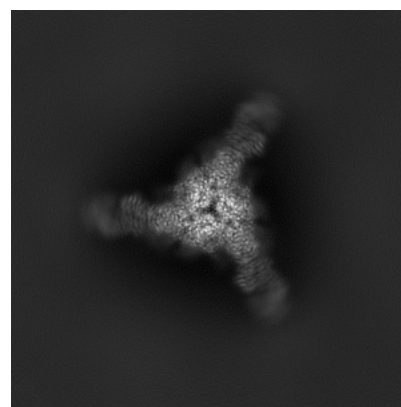
6.1.2 Raw map



X



Y



Z

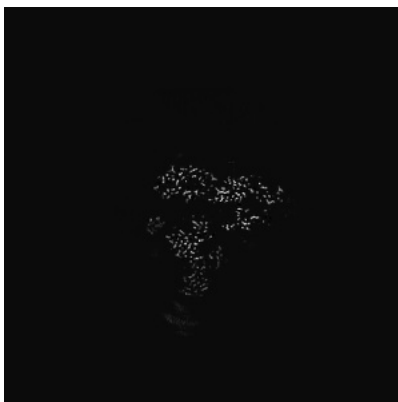
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225

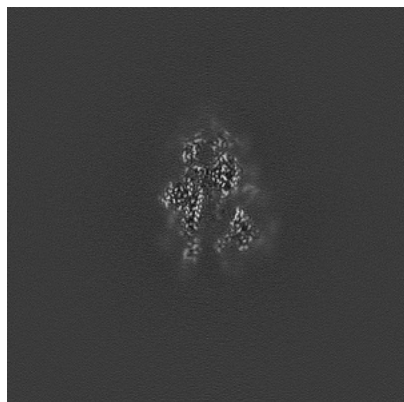


Y Index: 225



Z Index: 225

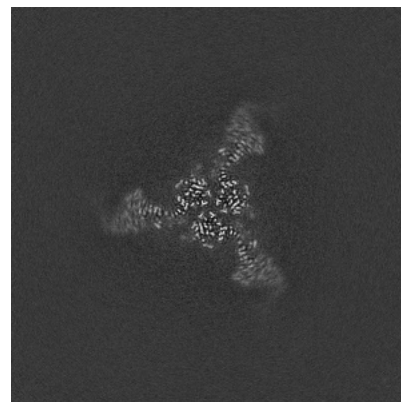
6.2.2 Raw map



X Index: 225



Y Index: 225



Z Index: 225

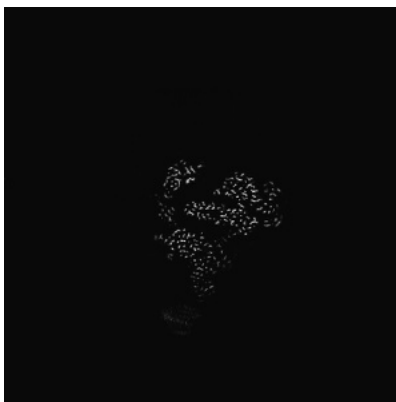
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 209

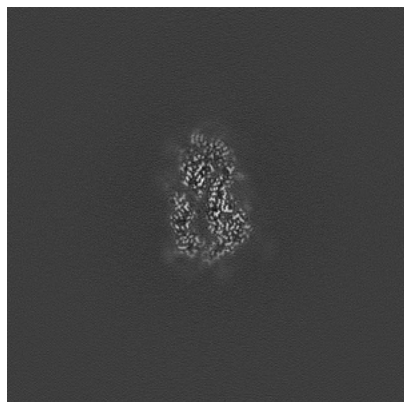


Y Index: 215

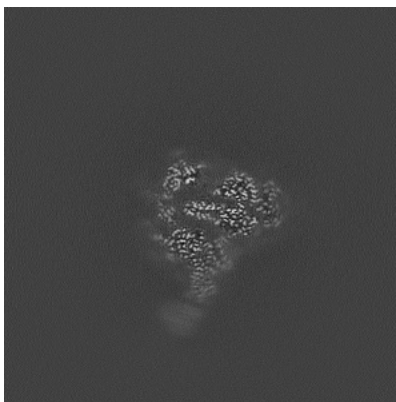


Z Index: 214

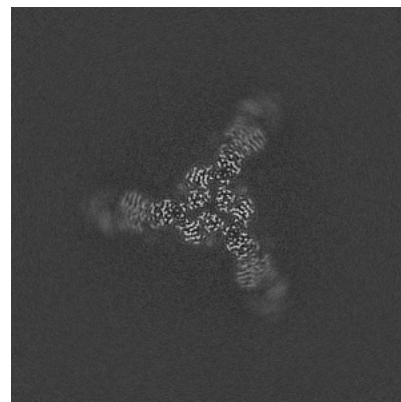
6.3.2 Raw map



X Index: 209



Y Index: 215

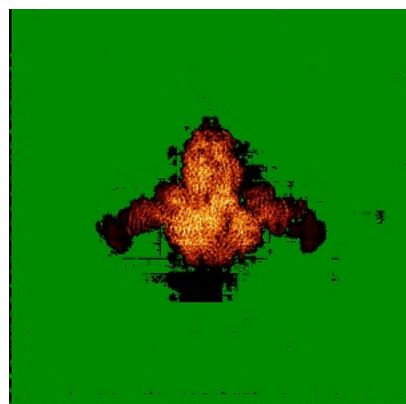


Z Index: 213

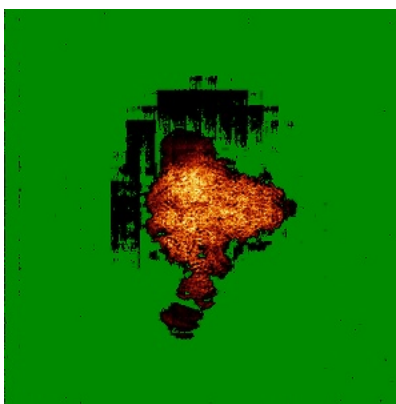
The images above show the largest variance slices of the map in three orthogonal directions.

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

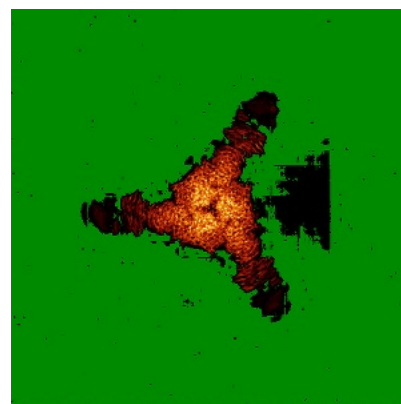
6.4.1 Primary map



X

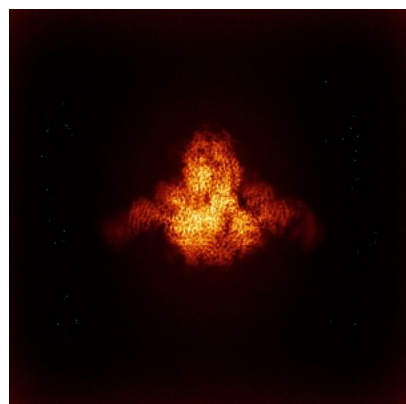


Y

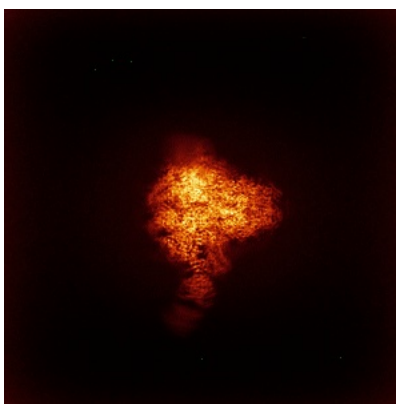


Z

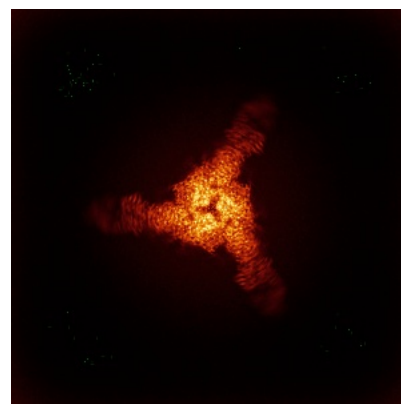
6.4.2 Raw map



X



Y

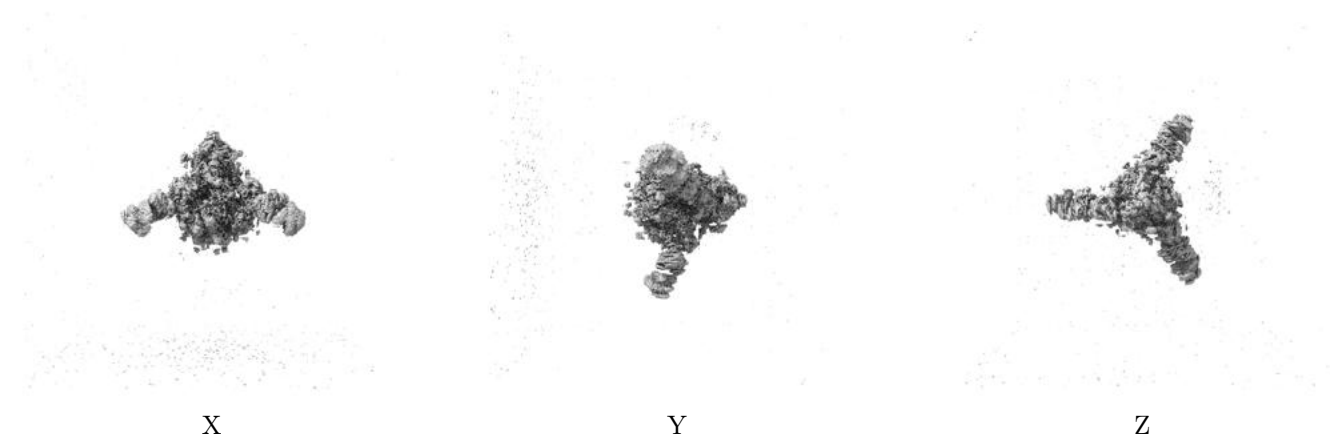


Z

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.

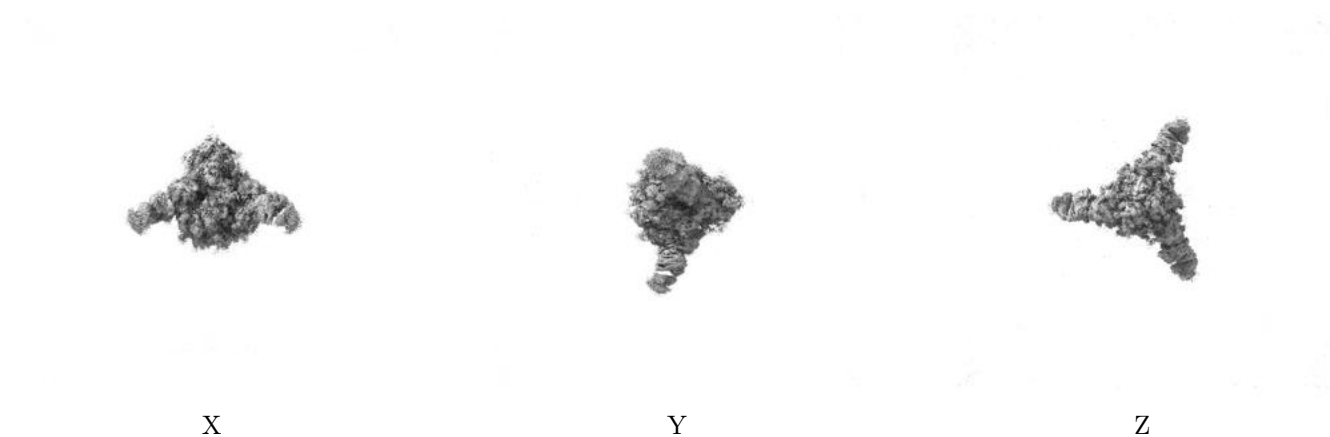
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

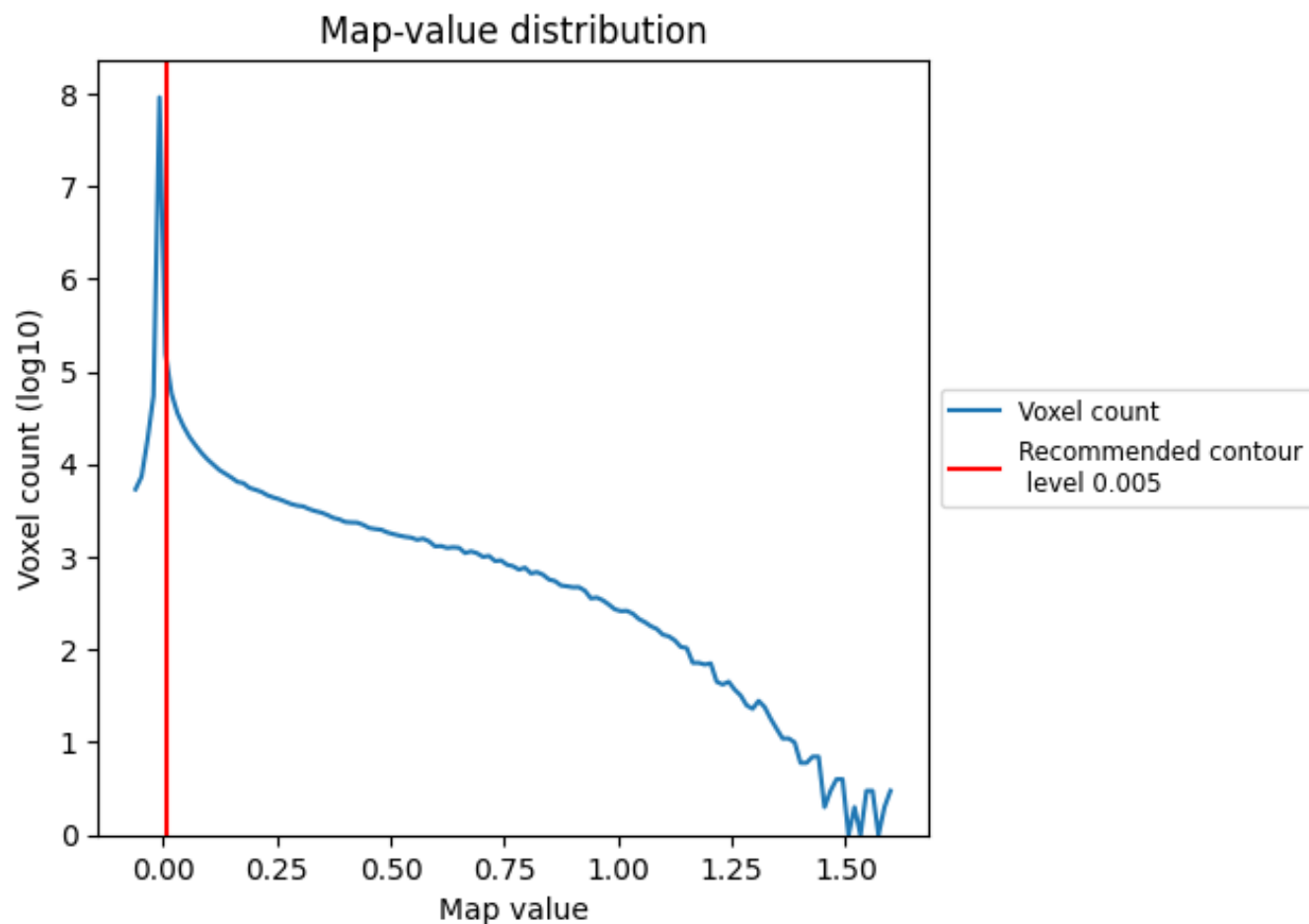
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

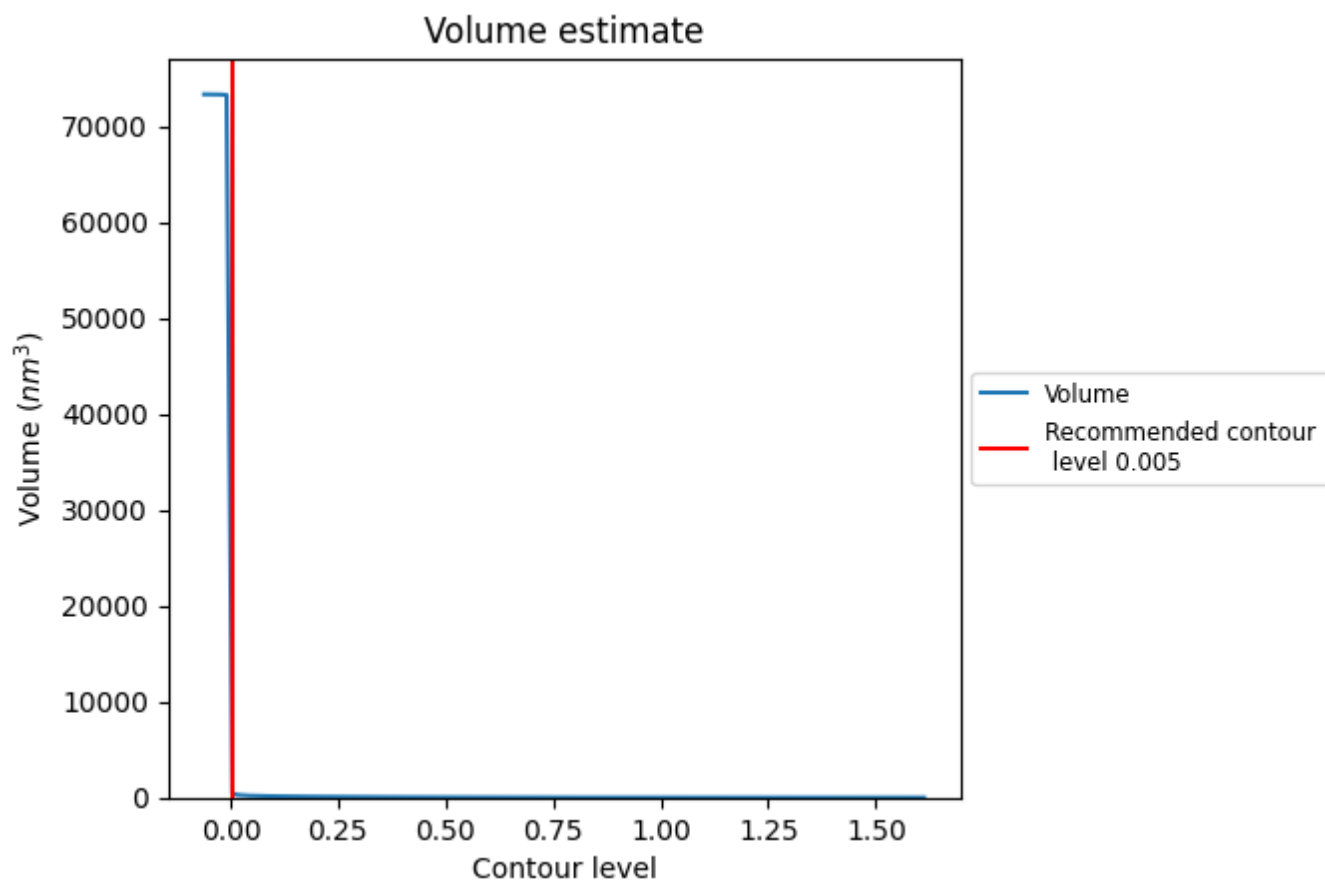
This section contains the results of statistical analysis of the map.

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.

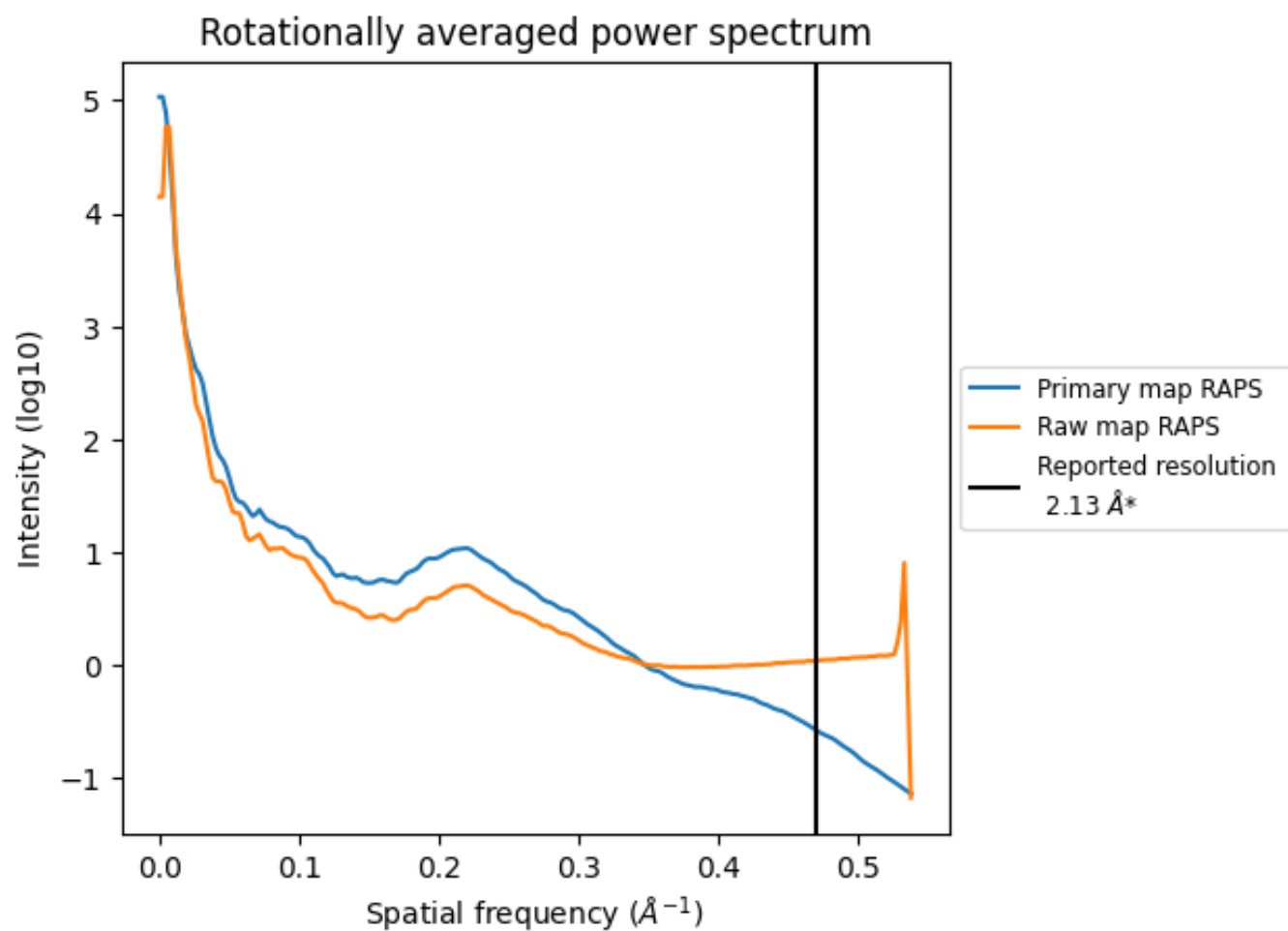
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm³; this corresponds to an approximate mass of 365 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 ⓘ

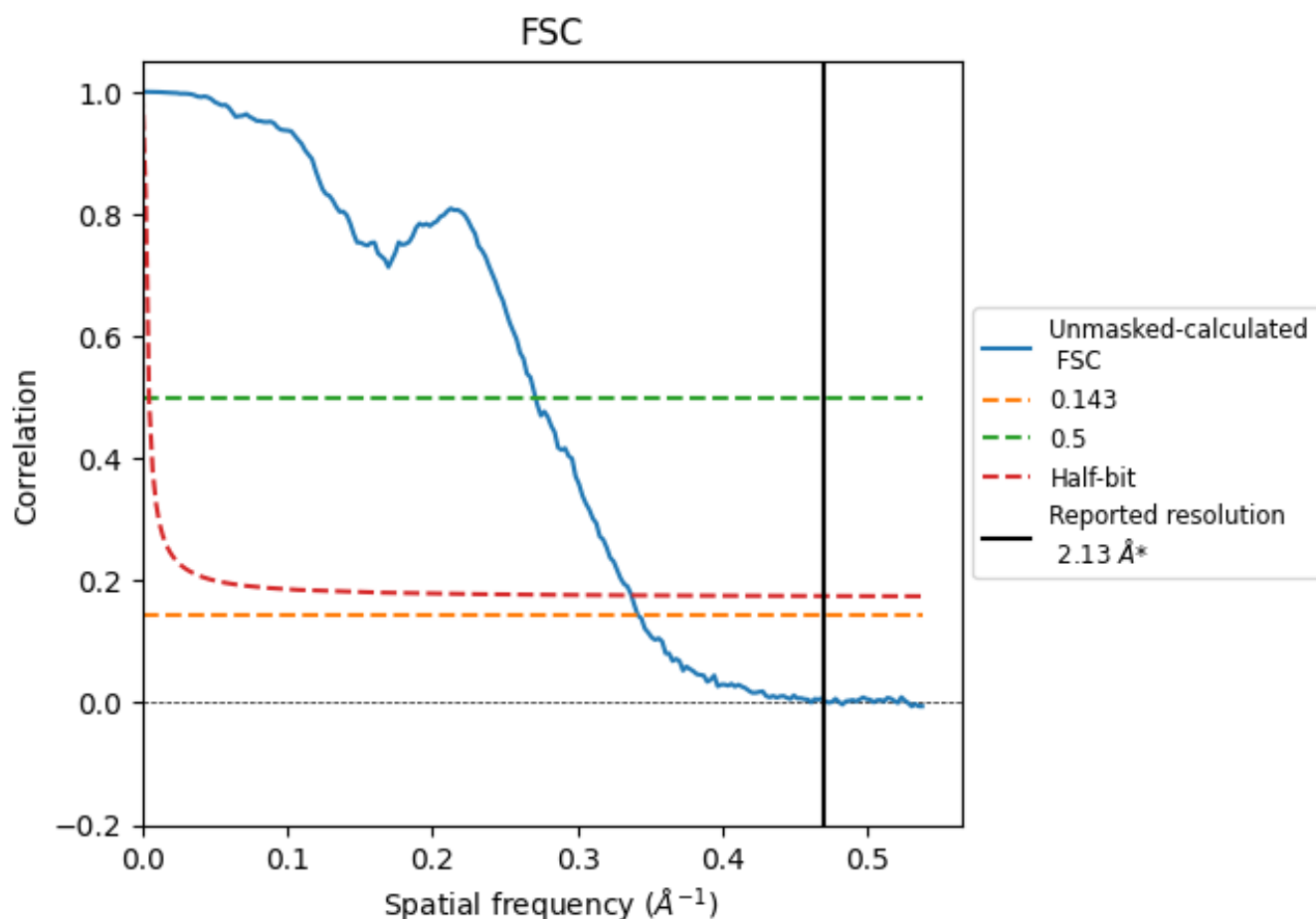


*Reported resolution corresponds to spatial frequency of 0.469 Å⁻¹

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 $0.469 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

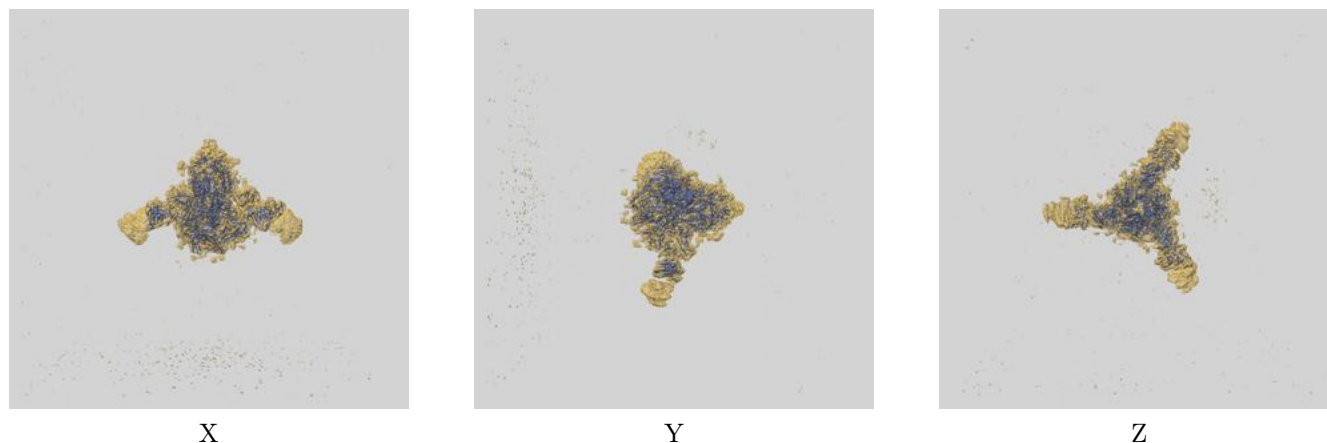
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.93	3.69	2.97

*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 2.93 differs from the reported value 2.13 by more than 10 %

9 Map-model fit [i](#)

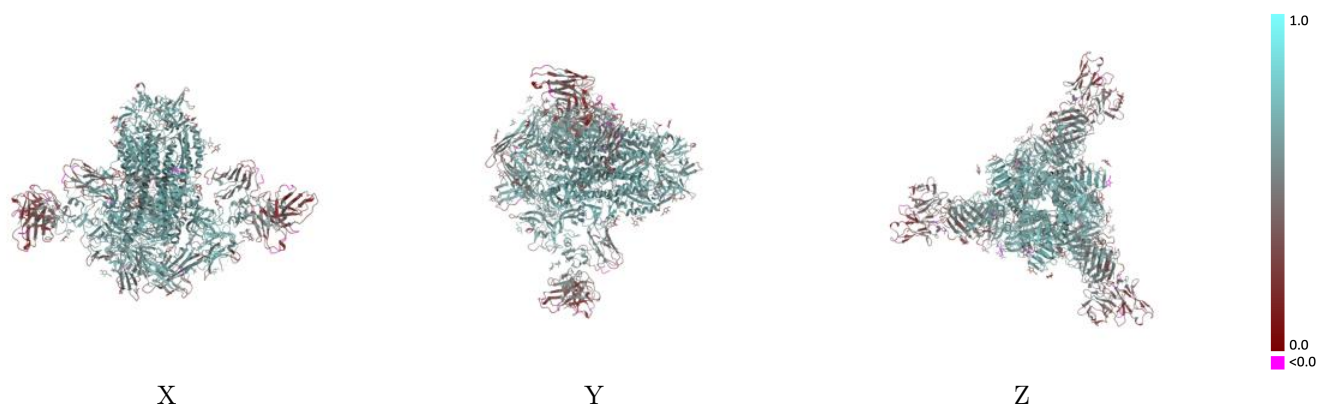
This section contains information regarding the fit between EMDB map EMD-67065 and PDB model 9XO0. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



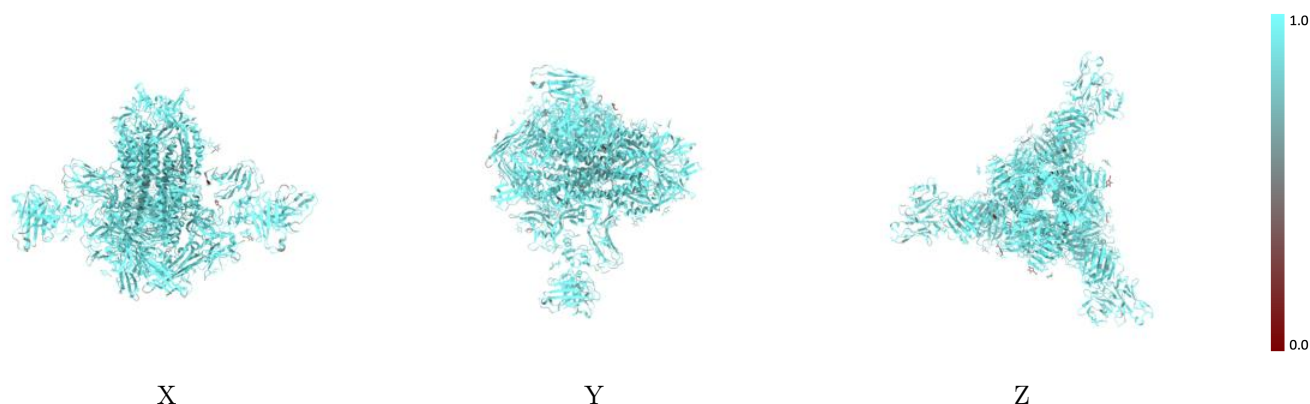
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



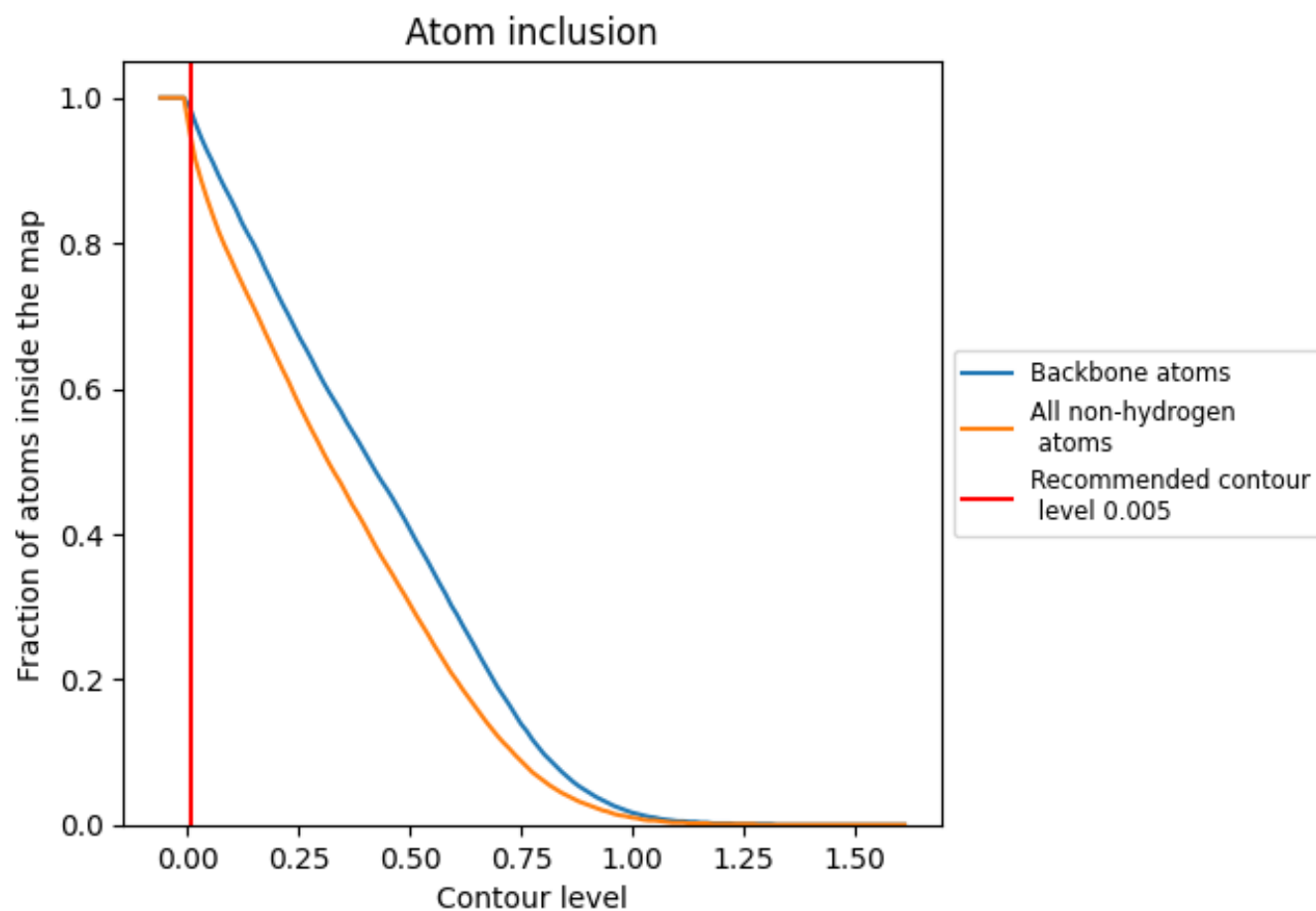
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9510	 0.5540
A	 0.9620	 0.5940
B	 0.9570	 0.5890
C	 0.9620	 0.5940
D	 0.9100	 0.3600
E	 0.8960	 0.3590
F	 0.9060	 0.3600
G	 0.9270	 0.3480
H	 0.9070	 0.3530
I	 0.8810	 0.3360
J	 0.8930	 0.4690
K	 0.9640	 0.4960
L	 1.0000	 0.5980
M	 0.8570	 0.4070
N	 0.9840	 0.6100
O	 0.7500	 0.3880
P	 1.0000	 0.5120
Q	 1.0000	 0.5720
R	 0.7860	 0.3460
S	 0.9840	 0.6150
T	 0.8570	 0.4750
U	 0.9640	 0.5090
V	 1.0000	 0.5630
W	 0.8570	 0.3580
X	 0.9840	 0.6020

