



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 05:32 PM EDT

PDB ID : 11HO / pdb_000011ho
EMDB ID : EMD-75698
Title : 1332D4 Spike KP3.1.1 Complex
Authors : Kizziah, J.L.; Walter, M.R.
Deposited on : 2026-02-24
Resolution : 3.26 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:

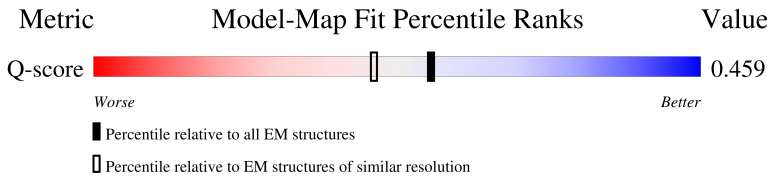
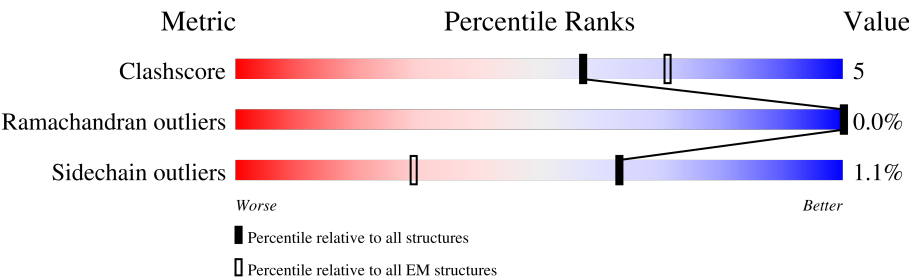
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.26 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.



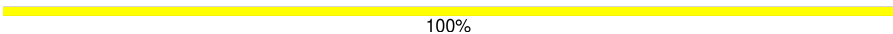
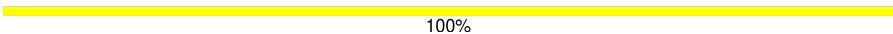
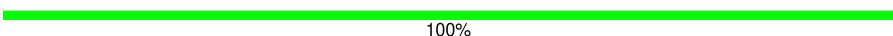
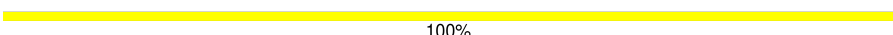
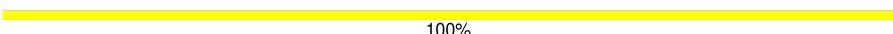
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14557 (2.76 - 3.76)

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	D	240	
2	E	234	
3	A	1218	
3	B	1218	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	1218	 74%11%15%
4	F	2	 50%50%
4	G	2	 100%
4	H	2	 50%50%
4	I	2	 50%50%
4	J	2	 100%
4	K	2	 100%
4	L	2	 100%
4	M	2	 50%50%
4	N	2	 50%50%
4	O	2	 50%50%
4	P	2	 50%50%
4	Q	2	 100%
4	R	2	 50%50%
4	S	2	 100%
4	T	2	 100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26756 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 1332D4 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	120	Total	C	N	O	S	0	0
			941	602	154	180	5		

- Molecule 2 is a protein called 1332D4 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	109	Total	C	N	O	S	0	0
			843	530	147	164	2		

- Molecule 3 is a protein called SARS-CoV-2 KP3.1.1 variant.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1032	Total	C	N	O	S	0	0
			8086	5182	1340	1529	35		
3	B	1032	Total	C	N	O	S	0	0
			8086	5182	1340	1529	35		
3	C	1032	Total	C	N	O	S	0	0
			8086	5182	1340	1529	35		

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



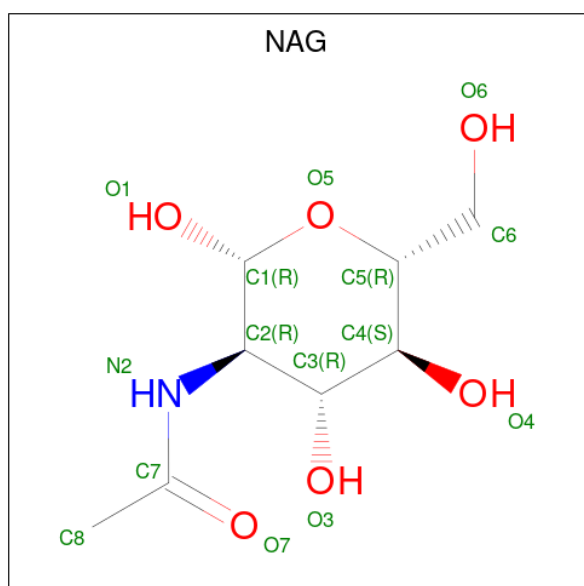
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

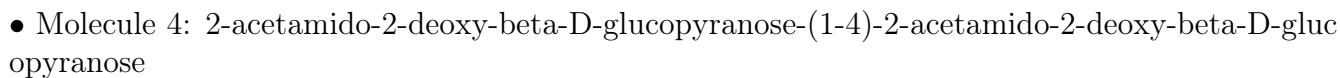
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
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	N	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	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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



NAG1
NAG2

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

NAG1
NAG2

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

	NAG1	NAG2
1	0.0000	0.0000
2	0.0000	0.0000
3	0.0000	0.0000
4	0.0000	0.0000
5	0.0000	0.0000
6	0.0000	0.0000
7	0.0000	0.0000
8	0.0000	0.0000
9	0.0000	0.0000
10	0.0000	0.0000
11	0.0000	0.0000
12	0.0000	0.0000
13	0.0000	0.0000
14	0.0000	0.0000
15	0.0000	0.0000
16	0.0000	0.0000
17	0.0000	0.0000
18	0.0000	0.0000
19	0.0000	0.0000
20	0.0000	0.0000
21	0.0000	0.0000
22	0.0000	0.0000
23	0.0000	0.0000
24	0.0000	0.0000
25	0.0000	0.0000
26	0.0000	0.0000
27	0.0000	0.0000
28	0.0000	0.0000
29	0.0000	0.0000
30	0.0000	0.0000
31	0.0000	0.0000
32	0.0000	0.0000
33	0.0000	0.0000
34	0.0000	0.0000
35	0.0000	0.0000
36	0.0000	0.0000
37	0.0000	0.0000
38	0.0000	0.0000
39	0.0000	0.0000
40	0.0000	0.0000
41	0.0000	0.0000
42	0.0000	0.0000
43	0.0000	0.0000
44	0.0000	0.0000
45	0.0000	0.0000
46	0.0000	0.0000
47	0.0000	0.0000
48	0.0000	0.0000
49	0.0000	0.0000
50	0.0000	0.0000
51	0.0000	0.0000
52	0.0000	0.0000
53	0.0000	0.0000
54	0.0000	0.0000
55	0.0000	0.0000
56	0.0000	0.0000
57	0.0000	0.0000
58	0.0000	0.0000
59	0.0000	0.0000
60	0.0000	0.0000
61	0.0000	0.0000
62	0.0000	0.0000
63	0.0000	0.0000
64	0.0000	0.0000
65	0.0000	0.0000
66	0.0000	0.0000
67	0.0000	0.0000
68	0.0000	0.0000
69	0.0000	0.0000
70	0.0000	0.0000
71	0.0000	0.0000
72	0.0000	0.0000
73	0.0000	0.0000
74	0.0000	0.0000
75	0.0000	0.0000
76	0.0000	0.0000
77	0.0000	0.0000
78	0.0000	0.0000
79	0.0000	0.0000
80	0.0000	0.0000
81	0.0000	0.0000
82	0.0000	0.0000
83	0.0000	0.0000
84	0.0000	0.0000
85	0.0000	0.0000
86	0.0000	0.0000
87	0.0000	0.0000
88	0.0000	0.0000
89	0.0000	0.0000
90	0.0000	0.0000
91	0.0000	0.0000
92	0.0000	0.0000
93	0.0000	0.0000
94	0.0000	0.0000
95	0.0000	0.0000
96	0.0000	0.0000
97	0.0000	0.0000
98	0.0000	0.0000
99	0.0000	0.0000
100	0.0000	0.0000

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

Chain I:  50% 50%

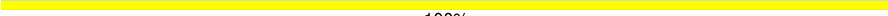
MAG1
MAG2

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

Chain J:  100%

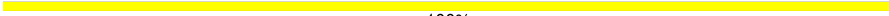
MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

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

Chain N:  50% 50%

MAG1
MAG2

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

Chain O:  50% 50%

MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

- 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% 50%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

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

Chain T:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124495	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.530	Depositor
Minimum map value	-0.247	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	367.104, 367.104, 367.104	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95600003, 0.95600003, 0.95600003	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

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	D	0.17	0/968	0.47	0/1318
2	E	0.15	0/864	0.40	0/1176
3	A	0.17	0/8282	0.32	0/11274
3	B	0.17	0/8282	0.34	0/11274
3	C	0.16	0/8282	0.32	0/11274
All	All	0.17	0/26678	0.34	0/36316

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	941	0	903	30	0
2	E	843	0	823	11	0
3	A	8086	0	7895	79	0
3	B	8086	0	7896	71	0
3	C	8086	0	7895	73	0
4	F	28	0	25	1	0
4	G	28	0	25	0	0
4	H	28	0	25	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
5	A	98	0	91	2	0
5	B	98	0	91	1	0
5	C	98	0	91	1	0
All	All	26756	0	26060	251	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 5.

All (251) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:425:LEU:HD12	3:C:426:PRO:HD2	1.53	0.90
3:A:417:ASN:HD21	3:A:455:SER:HA	1.49	0.78
3:C:67:ALA:HB3	3:C:259:ALA:HB3	1.69	0.74
3:C:391:CYS:HB2	3:C:525:CYS:HA	1.71	0.72
1:D:59:THR:HG21	1:D:71:ILE:HB	1.71	0.72
3:C:383:SER:HB3	3:C:386:LYS:HG2	1.71	0.71
3:B:985:ASP:HB3	3:B:987:PRO:HD2	1.73	0.69
1:D:3:GLN:HE22	1:D:5:VAL:HG12	1.58	0.69
1:D:106:TRP:CD1	2:E:96:TYR:HH	2.11	0.68
3:C:858:LEU:HD13	3:C:959:LEU:HD22	1.76	0.67
3:B:977:LEU:HD11	3:B:993:ILE:HG12	1.75	0.67
3:B:29:THR:HG22	3:B:61:ASN:HA	1.78	0.65
1:D:49:MET:HE1	1:D:65:PHE:HB2	1.78	0.65
3:B:124:VAL:HG23	3:B:171:PRO:HA	1.77	0.65
3:C:456:LEU:HB2	3:C:491:PRO:HA	1.80	0.64
3:C:433:VAL:HG12	3:C:512:VAL:HG22	1.78	0.64
3:B:902:MET:HE1	3:B:1049:LEU:HD13	1.79	0.63
3:A:1074:ASN:HB3	5:A:1306:NAG:N2	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:196:GLY:HA2	3:A:228:GLY:HA2	1.81	0.62
3:A:383:SER:HB3	3:A:386:LYS:HG2	1.82	0.62
3:C:196:GLY:HA2	3:C:228:GLY:HA2	1.81	0.62
3:C:377:PHE:C	3:C:378:LYS:HD3	2.25	0.62
3:A:736:VAL:HG11	3:A:1004:LEU:HD21	1.83	0.61
3:B:431:GLY:HA2	3:B:515:PHE:CE2	2.37	0.59
3:A:104:PHE:HB3	3:A:231:ILE:HD12	1.85	0.59
3:C:116:LEU:HD11	3:C:118:VAL:HG23	1.83	0.59
3:C:124:VAL:HG23	3:C:171:PRO:HA	1.85	0.59
3:A:350:VAL:HG22	3:A:422:ASN:HB3	1.84	0.59
3:A:326:ILE:HD11	3:A:534:VAL:HB	1.84	0.58
3:A:124:VAL:HG23	3:A:171:PRO:HA	1.84	0.58
3:B:869:MET:HE3	3:C:699:LEU:HD21	1.84	0.58
3:B:986:PRO:O	3:B:990:GLU:HG2	2.04	0.58
3:C:742:ILE:HG12	3:C:1000:ARG:HB3	1.85	0.58
3:B:196:GLY:HA2	3:B:228:GLY:HA2	1.87	0.57
3:A:409:GLN:HB3	3:A:419:ALA:HB2	1.85	0.57
3:C:320:VAL:HG23	3:C:590:CYS:HB3	1.85	0.57
1:D:19:ARG:HH21	1:D:83:GLN:HB2	1.70	0.57
3:C:458:LYS:HA	3:C:473:TYR:HE1	1.70	0.56
3:C:931:ILE:O	3:C:934:ILE:HG22	2.05	0.56
3:A:98:ILE:HG12	3:A:238:LEU:HD22	1.86	0.56
3:B:418:ILE:HD12	3:B:418:ILE:H	1.71	0.56
3:A:1103:PHE:HZ	4:H:1:NAG:H62	1.71	0.56
3:C:393:THR:HA	3:C:522:ALA:HA	1.89	0.55
3:C:28:TYR:HD1	3:C:29:THR:H	1.56	0.54
3:C:382:VAL:HG21	3:C:387:LEU:HD21	1.89	0.54
3:C:1006:THR:O	3:C:1010:GLN:HG2	2.07	0.54
3:A:99:ILE:HD11	3:A:187:ARG:HH21	1.73	0.53
3:B:409:GLN:HA	3:B:414:GLN:HG2	1.89	0.53
3:C:1129:VAL:HB	3:C:1132:ILE:HD11	1.91	0.53
3:A:425:LEU:HD21	3:A:429:PHE:CD2	2.43	0.53
3:A:1110:TYR:CZ	3:A:1112:PRO:HG3	2.44	0.53
3:B:1110:TYR:CZ	3:B:1112:PRO:HG3	2.44	0.53
3:C:391:CYS:CB	3:C:525:CYS:HA	2.39	0.53
3:C:726:ILE:HG12	3:C:1061:VAL:HG22	1.90	0.53
3:A:318:PHE:HD2	3:A:629:LEU:HD11	1.74	0.52
2:E:13:VAL:HG11	2:E:19:ALA:HB2	1.91	0.52
3:C:103:ILE:HG12	3:C:237:LEU:HD21	1.92	0.52
1:D:29:PHE:HE2	1:D:75:LYS:HA	1.75	0.52
3:B:439:ASN:HA	3:B:507:PRO:HG2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD21	1:D:119:VAL:HB	1.91	0.52
3:B:736:VAL:HG11	3:B:1004:LEU:HD21	1.91	0.52
3:C:984:LEU:HB2	3:C:989:ALA:HB2	1.91	0.52
3:A:193:ASN:HD22	3:A:198:PHE:HD1	1.58	0.52
3:A:485:GLY:H	3:A:488:CYS:HB3	1.75	0.52
3:B:1114:ILE:HD12	3:B:1114:ILE:H	1.76	0.51
3:A:902:MET:HE3	3:A:1049:LEU:HD13	1.92	0.51
1:D:92:THR:HG23	1:D:118:THR:HA	1.92	0.51
3:C:977:LEU:HD11	3:C:993:ILE:HG12	1.92	0.51
3:C:425:LEU:HD11	3:C:429:PHE:CD1	2.46	0.51
3:A:194:ILE:HG23	3:A:195:ASP:OD2	2.11	0.51
3:B:1086:LYS:HE2	3:B:1122:VAL:HG21	1.91	0.51
2:E:100:GLN:H	2:E:100:GLN:CD	2.20	0.50
3:B:303:LEU:HD12	3:B:308:VAL:HG12	1.92	0.50
3:C:378:LYS:HD3	3:C:378:LYS:N	2.27	0.50
3:A:763:LEU:HG	3:A:1008:VAL:HG21	1.93	0.50
3:B:555:SER:HB3	3:B:584:ILE:HG23	1.93	0.50
3:C:736:VAL:HG11	3:C:1004:LEU:HD21	1.94	0.50
1:D:37:TRP:CZ3	1:D:97:CYS:HB3	2.47	0.50
3:B:498:ARG:H	3:B:501:TYR:HE1	1.60	0.50
3:A:715:PRO:HA	3:A:1072:GLU:HA	1.94	0.49
3:A:598:ILE:HG23	3:A:664:ILE:HG21	1.93	0.49
3:B:103:ILE:HD11	3:B:237:LEU:HD23	1.94	0.49
3:A:804:GLN:NE2	4:F:1:NAG:H62	2.27	0.49
3:C:434:ILE:HB	3:C:511:VAL:HG13	1.95	0.49
3:C:497:PHE:CE1	3:C:507:PRO:HB3	2.48	0.49
3:A:109:ASP:HB3	3:A:111:LYS:NZ	2.27	0.49
3:C:207:ILE:HD11	3:C:213:PRO:HD3	1.95	0.49
3:C:551:VAL:HG22	3:C:588:THR:HB	1.93	0.49
2:E:94(A):PRO:N	2:E:95:PRO:HD2	2.27	0.48
3:A:599:THR:HG22	3:A:601:GLY:H	1.78	0.48
3:C:225:LEU:HB3	3:C:227:ILE:HD11	1.95	0.48
1:D:49:MET:HE3	1:D:49:MET:O	2.13	0.48
3:B:452:TRP:CD2	3:B:494:SER:HB3	2.48	0.48
3:B:878:LEU:HD21	3:B:1052:PHE:HB3	1.95	0.48
3:C:878:LEU:HD21	3:C:1052:PHE:HB3	1.95	0.48
3:A:1107:ARG:HG2	3:C:904:TYR:OH	2.14	0.48
3:C:1140:PRO:O	3:C:1144:GLU:HG2	2.14	0.48
3:A:109:ASP:HB3	3:A:111:LYS:HZ2	1.79	0.48
3:C:341:VAL:HG13	3:C:342:PHE:HD1	1.79	0.47
3:B:452:TRP:CE2	3:B:494:SER:HB3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:PRO:HA	1:D:66:GLN:HG2	1.97	0.47
3:A:977:LEU:O	3:A:981:LEU:HG	2.14	0.47
3:B:119:ASN:ND2	3:B:173:LEU:H	2.10	0.47
3:B:722:VAL:HG22	3:B:1065:VAL:HG22	1.97	0.47
3:C:763:LEU:HD22	3:C:1008:VAL:HG21	1.95	0.47
1:D:34:TRP:O	1:D:100:PRO:HD2	2.14	0.47
3:C:106:THR:HB	5:C:1301:NAG:H61	1.97	0.47
3:B:276:ASN:HD21	5:B:1302:NAG:H83	1.80	0.47
3:B:555:SER:HB2	3:B:586:ASP:HB2	1.97	0.47
3:B:959:LEU:O	3:B:963:VAL:HG23	2.15	0.47
3:A:823:PHE:HD1	3:A:1057:PRO:HG3	1.79	0.46
3:C:433:VAL:C	3:C:434:ILE:HD13	2.40	0.46
3:B:127:LYS:HD3	3:B:166:GLU:OE2	2.15	0.46
3:A:272:LEU:HD11	3:A:304:LYS:HA	1.98	0.46
3:A:411:ALA:HB3	3:A:414:GLN:HG3	1.98	0.46
3:B:671:CYS:SG	3:B:697:MET:HE2	2.56	0.46
2:E:66:GLY:HA3	2:E:71:PHE:HA	1.97	0.46
3:B:764:LYS:HZ3	3:C:314:GLN:HG2	1.81	0.46
2:E:30:THR:HG23	2:E:31:THR:H	1.80	0.46
3:A:118:VAL:HG13	3:A:125:PHE:HB2	1.97	0.46
3:A:462:LYS:HD2	3:A:463:PRO:HD2	1.98	0.46
3:B:659:SER:HB3	3:B:698:SER:HB2	1.98	0.45
3:C:402:ILE:HD11	3:C:407:VAL:HA	1.98	0.45
3:A:198:PHE:HE2	3:A:200:ILE:HD11	1.82	0.45
3:C:1080:ALA:HB3	3:C:1132:ILE:HD13	1.97	0.45
1:D:6:GLN:H	1:D:113:GLN:HG3	1.81	0.45
3:A:740:MET:HE1	3:B:319:ARG:NE	2.31	0.45
3:A:1074:ASN:OD1	3:A:1074:ASN:C	2.60	0.45
3:C:130:GLU:HB2	3:C:161:ASN:O	2.16	0.45
3:B:330:PRO:HD3	3:B:544:ASN:OD1	2.17	0.45
3:B:379:CYS:HA	3:B:432:CYS:HA	1.99	0.45
3:C:379:CYS:SG	3:C:384:PRO:HG3	2.57	0.45
3:C:1141:LEU:O	3:C:1145:LEU:HG	2.16	0.45
3:A:983:ARG:HG3	3:B:382:VAL:HG13	1.99	0.45
3:C:116:LEU:HD12	3:C:117:ILE:N	2.32	0.45
1:D:99:ARG:HD2	1:D:109:VAL:HG21	1.99	0.44
3:B:116:LEU:HD21	3:B:118:VAL:HG13	1.98	0.44
3:B:740:MET:HE2	3:B:740:MET:HB2	1.89	0.44
3:C:127:LYS:HG2	3:C:129:CYS:SG	2.57	0.44
3:C:365:TYR:O	3:C:368:LEU:HG	2.17	0.44
1:D:10:GLU:HB2	1:D:12:LYS:HZ1	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:309:GLU:OE2	3:A:309:GLU:HA	2.17	0.44
3:A:326:ILE:HD12	3:A:539:VAL:HG21	2.00	0.44
3:B:186:LEU:HD12	3:B:187:ARG:N	2.32	0.44
3:C:167:TYR:CE1	3:C:169:SER:HB2	2.53	0.44
3:B:763:LEU:HD22	3:B:1008:VAL:HG21	2.00	0.44
3:A:869:MET:HE1	3:B:697:MET:HG3	2.00	0.44
1:D:48:TRP:HE1	1:D:51:ILE:HG23	1.83	0.44
3:A:129:CYS:HB3	3:A:131:PHE:CE2	2.52	0.43
3:B:636:TYR:CZ	3:B:638:THR:HG22	2.53	0.43
3:A:802:PHE:HD1	3:A:805:ILE:HD11	1.83	0.43
3:B:94:GLU:HB2	3:B:187:ARG:NH2	2.33	0.43
3:B:129:CYS:HB2	3:B:131:PHE:CE2	2.53	0.43
2:E:24:ARG:HE	2:E:70:GLU:HB3	1.84	0.43
3:A:462:LYS:HD3	3:A:462:LYS:HA	1.69	0.43
3:B:617:CYS:HB2	3:B:649:CYS:HB2	1.84	0.43
3:C:113:GLN:OE1	3:C:128:VAL:HG12	2.18	0.43
3:A:948:LEU:O	3:A:951:VAL:HG12	2.19	0.43
3:B:715:PRO:HA	3:B:1072:GLU:HA	1.99	0.43
3:C:402:ILE:HG12	3:C:510:VAL:HG11	2.00	0.43
1:D:95:TYR:O	1:D:114:GLY:HA2	2.19	0.43
3:A:295:PRO:HG3	3:A:633:TRP:CZ3	2.54	0.43
3:A:708:SER:HB3	3:A:711:SER:HB3	2.00	0.43
3:C:335:LEU:HD12	3:C:335:LEU:HA	1.82	0.43
3:B:474:GLN:HA	3:B:488:CYS:SG	2.59	0.43
3:C:350:VAL:HG11	3:C:418:ILE:HD11	2.01	0.43
3:C:56:LEU:HD12	3:C:57:PRO:HD2	2.01	0.43
1:D:19:ARG:CD	1:D:81:TYR:HB3	2.48	0.43
1:D:98:VAL:HG22	1:D:99:ARG:H	1.83	0.43
3:A:1030:SER:HB3	3:B:1041:ASP:HB2	2.01	0.43
3:A:104:PHE:HB2	3:A:115:LEU:HB3	2.00	0.42
3:B:309:GLU:N	3:B:309:GLU:OE2	2.52	0.42
3:B:986:PRO:N	3:B:987:PRO:HD2	2.33	0.42
3:A:240:LEU:HD22	3:A:256:ALA:HB3	2.02	0.42
3:B:127:LYS:HD2	3:B:165:PHE:O	2.20	0.42
3:B:453:TYR:CZ	3:B:493:GLU:HG3	2.55	0.42
3:B:675:GLN:HG3	3:B:693:ILE:HD11	2.02	0.42
1:D:33:PHE:CE1	3:A:499:PRO:HB2	2.54	0.42
3:C:905:ARG:HD3	3:C:1049:LEU:O	2.19	0.42
1:D:18:LEU:HD12	1:D:19:ARG:H	1.83	0.42
3:B:916:LEU:HD12	3:B:923:ILE:HD13	2.01	0.42
3:C:187:ARG:HG2	3:C:204:HIS:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:770:ILE:O	3:C:774:GLN:HG2	2.20	0.42
1:D:105:ASP:O	2:E:91:TYR:HB2	2.20	0.42
3:B:934:ILE:HD13	3:B:934:ILE:HA	1.85	0.42
3:C:376:ALA:HB3	3:C:435:ALA:HB3	2.00	0.42
3:B:378:LYS:HB2	3:B:380:TYR:HE1	1.84	0.42
3:A:452:TRP:CE2	3:A:494:SER:HB2	2.55	0.42
3:A:420:ASP:O	3:A:461:LEU:HG	2.18	0.42
3:B:380:TYR:CE2	3:B:412:PRO:HD2	2.55	0.42
3:C:724:THR:OG1	3:C:934:ILE:HD11	2.20	0.42
3:A:395:VAL:HG23	3:A:524:VAL:HG11	2.00	0.42
3:A:736:VAL:HG22	3:A:858:LEU:HD22	2.02	0.42
3:A:742:ILE:HG12	3:A:1000:ARG:HB3	2.01	0.42
1:D:34:TRP:C	1:D:35:ILE:HD13	2.45	0.41
3:A:327:VAL:HG12	3:A:542:ASN:HB3	2.02	0.41
2:E:94:TRP:CE3	2:E:94:TRP:HA	2.55	0.41
3:A:722:VAL:HG22	3:A:1065:VAL:HG22	2.02	0.41
3:C:431:GLY:HA2	3:C:515:PHE:CD2	2.55	0.41
3:A:484:LYS:HZ3	3:A:490:PHE:H	1.68	0.41
3:A:858:LEU:HD13	3:A:959:LEU:HD22	2.01	0.41
3:C:743:CYS:HB3	3:C:749:CYS:HB3	1.81	0.41
3:A:125:PHE:CD1	3:A:125:PHE:N	2.86	0.41
3:A:555:SER:HB2	3:A:586:ASP:HB2	2.03	0.41
3:B:792:PRO:HG3	3:C:707:TYR:HB3	2.01	0.41
3:A:1073:LYS:HE3	3:A:1075:PHE:CZ	2.56	0.41
1:D:30:THR:O	1:D:55:ASP:HB2	2.21	0.41
3:A:431:GLY:HA2	3:A:515:PHE:CD2	2.55	0.41
3:B:350:VAL:HG22	3:B:422:ASN:HB3	2.02	0.41
3:C:330:PRO:HD3	3:C:544:ASN:OD1	2.21	0.41
1:D:19:ARG:HD2	1:D:81:TYR:HB3	2.03	0.41
3:A:1118:ASP:OD1	3:A:1118:ASP:C	2.64	0.41
3:B:528:LYS:HE2	3:B:528:LYS:HB2	1.90	0.41
3:B:1029:MET:HE2	3:B:1029:MET:HB2	1.93	0.41
1:D:5:VAL:HG13	1:D:23:LYS:HB2	2.03	0.41
1:D:6:GLN:HB2	1:D:113:GLN:NE2	2.35	0.41
3:C:902:MET:HE3	3:C:1049:LEU:HD13	2.03	0.41
1:D:34:TRP:O	1:D:35:ILE:HD13	2.20	0.41
1:D:101:ASP:HA	3:A:445:HIS:ND1	2.36	0.41
2:E:33:LEU:HG	2:E:71:PHE:CD1	2.56	0.41
3:A:110:SER:HB3	3:A:132:GLN:HB2	2.03	0.41
3:A:961:THR:O	3:A:965:GLN:HG2	2.21	0.41
3:A:963:VAL:HB	3:B:570:VAL:HG21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1074:ASN:HB3	5:A:1306:NAG:C7	2.50	0.41
3:B:419:ALA:O	3:B:424:LYS:HE3	2.20	0.41
3:B:497:PHE:CE2	3:B:507:PRO:HB3	2.55	0.41
3:B:344:ALA:HB3	3:B:347:PHE:CE1	2.56	0.41
3:C:431:GLY:HA2	3:C:515:PHE:CE2	2.54	0.41
3:A:113:GLN:HG2	3:A:229:ILE:HD12	2.02	0.40
3:A:128:VAL:HB	3:A:165:PHE:HB3	2.03	0.40
3:A:916:LEU:HD12	3:A:923:ILE:HD12	2.03	0.40
3:C:54:LEU:HD13	3:C:86:ASP:HB3	2.03	0.40
3:C:529:LYS:HD2	3:C:530:SER:N	2.37	0.40
3:C:986:PRO:N	3:C:987:PRO:HD2	2.36	0.40
1:D:27:TYR:OH	1:D:35:ILE:HD11	2.21	0.40
3:A:388:ASN:HB2	3:A:527:PRO:HD2	2.03	0.40
3:A:730:SER:O	3:A:1058:HIS:HB3	2.22	0.40
3:B:855:PHE:HB2	3:B:858:LEU:HB2	2.02	0.40
3:B:900:MET:HE2	3:B:900:MET:HB3	1.94	0.40
3:C:57:PRO:HB3	3:C:269:ARG:NH1	2.35	0.40
3:C:749:CYS:HB2	3:C:977:LEU:HD21	2.03	0.40
3:A:826:VAL:HB	3:A:1057:PRO:HG2	2.03	0.40
3:A:985:ASP:HB3	3:A:987:PRO:HD2	2.04	0.40
3:B:65:PHE:CZ	3:B:82:LEU:HD21	2.56	0.40
3:B:342:PHE:CZ	3:B:511:VAL:HG11	2.56	0.40
3:B:752:LEU:HD21	3:B:994:ASP:OD1	2.21	0.40
3:B:974:SER:HB3	3:B:980:ILE:HD11	2.02	0.40
3:C:502:GLY:O	3:C:506:GLN:HG3	2.21	0.40
3:A:751:ASN:OD1	3:A:751:ASN:C	2.64	0.40
3:A:1086:LYS:HD2	3:A:1122:VAL:HG21	2.03	0.40
2:E:73:LEU:HG	2:E:75:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	118/240 (49%)	108 (92%)	10 (8%)	0	100	100
2	E	107/234 (46%)	100 (94%)	7 (6%)	0	100	100
3	A	1018/1218 (84%)	993 (98%)	25 (2%)	0	100	100
3	B	1018/1218 (84%)	982 (96%)	36 (4%)	0	100	100
3	C	1018/1218 (84%)	978 (96%)	39 (4%)	1 (0%)	48	76
All	All	3279/4128 (79%)	3161 (96%)	117 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	136	ASP

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	D	102/204 (50%)	101 (99%)	1 (1%)	68	75
2	E	91/201 (45%)	89 (98%)	2 (2%)	45	65
3	A	904/1059 (85%)	896 (99%)	8 (1%)	70	76
3	B	904/1059 (85%)	893 (99%)	11 (1%)	63	74
3	C	904/1059 (85%)	895 (99%)	9 (1%)	68	75
All	All	2905/3582 (81%)	2874 (99%)	31 (1%)	63	75

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	64	SER
2	E	29	VAL
2	E	93	HIS
3	A	136	ASP
3	A	236	THR
3	A	754	LEU
3	A	762	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	763	LEU
3	A	1010	GLN
3	A	1074	ASN
3	A	1122	VAL
3	B	32	PHE
3	B	51	THR
3	B	66	HIS
3	B	382	VAL
3	B	432	CYS
3	B	510	VAL
3	B	515	PHE
3	B	524	VAL
3	B	584	ILE
3	B	645	THR
3	B	1136	THR
3	C	392	PHE
3	C	511	VAL
3	C	524	VAL
3	C	645	THR
3	C	723	THR
3	C	738	CYS
3	C	780	GLU
3	C	791	THR
3	C	976	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3	GLN
1	D	40	GLN
3	A	66	HIS
3	A	185	ASN
3	A	204	HIS
3	A	267	GLN
3	A	317	ASN
3	A	417	ASN
3	A	606	ASN
3	A	762	GLN
3	A	957	GLN
3	A	965	GLN
3	A	1054	GLN
3	A	1083	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1106	GLN
3	B	49	HIS
3	B	79	ASN
3	B	235	GLN
3	B	417	ASN
3	B	506	GLN
3	B	804	GLN
3	B	907	ASN
3	C	97	ASN
3	C	123	ASN
3	C	162	ASN
3	C	445	HIS
3	C	690	GLN
3	C	762	GLN
3	C	935	GLN
3	C	1083	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 ⓘ

30 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	F	1	4,3	14,14,15	0.74	0	17,19,21	1.17	1 (5%)
4	NAG	F	2	4	14,14,15	0.73	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	1	4,3	14,14,15	0.79	0	17,19,21	0.91	0
4	NAG	G	2	4	14,14,15	0.72	0	17,19,21	0.87	0
4	NAG	H	1	4,3	14,14,15	0.74	0	17,19,21	0.82	0
4	NAG	H	2	4	14,14,15	0.71	0	17,19,21	0.78	0
4	NAG	I	1	4,3	14,14,15	0.75	0	17,19,21	0.83	0
4	NAG	I	2	4	14,14,15	0.76	0	17,19,21	2.35	3 (17%)
4	NAG	J	1	4,3	14,14,15	0.75	0	17,19,21	0.80	0
4	NAG	J	2	4	14,14,15	0.72	0	17,19,21	0.81	0
4	NAG	K	1	4,3	14,14,15	0.83	0	17,19,21	1.37	1 (5%)
4	NAG	K	2	4	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
4	NAG	L	1	4,3	14,14,15	0.80	0	17,19,21	1.08	1 (5%)
4	NAG	L	2	4	14,14,15	0.69	0	17,19,21	1.18	2 (11%)
4	NAG	M	1	4,3	14,14,15	0.75	0	17,19,21	1.33	2 (11%)
4	NAG	M	2	4	14,14,15	0.74	0	17,19,21	0.82	0
4	NAG	N	1	4,3	14,14,15	0.71	0	17,19,21	0.93	0
4	NAG	N	2	4	14,14,15	0.73	0	17,19,21	1.13	1 (5%)
4	NAG	O	1	4,3	14,14,15	0.74	0	17,19,21	0.82	1 (5%)
4	NAG	O	2	4	14,14,15	0.71	0	17,19,21	0.86	0
4	NAG	P	1	4,3	14,14,15	0.76	0	17,19,21	0.95	0
4	NAG	P	2	4	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
4	NAG	Q	1	4,3	14,14,15	0.75	0	17,19,21	0.88	0
4	NAG	Q	2	4	14,14,15	0.72	0	17,19,21	0.79	0
4	NAG	R	1	4,3	14,14,15	0.81	0	17,19,21	2.11	7 (41%)
4	NAG	R	2	4	14,14,15	0.74	0	17,19,21	0.87	0
4	NAG	S	1	4,3	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
4	NAG	S	2	4	14,14,15	0.72	0	17,19,21	1.14	1 (5%)
4	NAG	T	1	4,3	14,14,15	0.71	0	17,19,21	1.38	2 (11%)
4	NAG	T	2	4	14,14,15	0.78	0	17,19,21	2.36	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	5/6/23/26	0/1/1/1
4	NAG	J	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
4	NAG	P	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C2-N2-C7	8.35	134.09	122.90
4	T	2	NAG	C2-N2-C7	8.30	134.02	122.90
4	K	1	NAG	C1-O5-C5	4.48	118.19	112.19
4	M	1	NAG	O5-C1-C2	-4.04	105.04	111.29
4	R	1	NAG	O5-C1-C2	-3.66	105.63	111.29
4	R	1	NAG	C2-N2-C7	3.54	127.65	122.90
4	R	1	NAG	C1-O5-C5	-3.51	107.49	112.19
4	T	1	NAG	C2-N2-C7	3.38	127.43	122.90
4	L	2	NAG	C2-N2-C7	3.13	127.10	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2	NAG	C2-N2-C7	3.09	127.04	122.90
4	F	1	NAG	C2-N2-C7	3.08	127.02	122.90
4	R	1	NAG	C1-C2-N2	3.00	115.16	110.43
4	R	1	NAG	C3-C4-C5	2.96	115.60	110.23
4	N	2	NAG	C2-N2-C7	2.95	126.86	122.90
4	T	2	NAG	C8-C7-N2	2.67	120.54	116.12
4	R	1	NAG	C4-C3-C2	2.65	114.89	111.02
4	T	1	NAG	O5-C1-C2	-2.58	107.30	111.29
4	I	2	NAG	C8-C7-N2	2.57	120.38	116.12
4	M	1	NAG	O4-C4-C3	-2.47	104.55	110.38
4	R	1	NAG	O4-C4-C3	-2.43	104.64	110.38
4	T	2	NAG	C1-C2-N2	2.34	114.11	110.43
4	O	1	NAG	O5-C1-C2	-2.20	107.88	111.29
4	S	1	NAG	C1-O5-C5	2.13	115.04	112.19
4	L	1	NAG	O4-C4-C3	-2.11	105.40	110.38
4	K	2	NAG	O5-C1-C2	-2.05	108.12	111.29
4	L	2	NAG	O5-C1-C2	-2.04	108.14	111.29
4	P	2	NAG	O5-C1-C2	-2.02	108.16	111.29
4	I	2	NAG	C1-C2-N2	2.01	113.61	110.43

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
4	P	2	NAG	C8-C7-N2-C2
4	P	2	NAG	O7-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
4	P	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

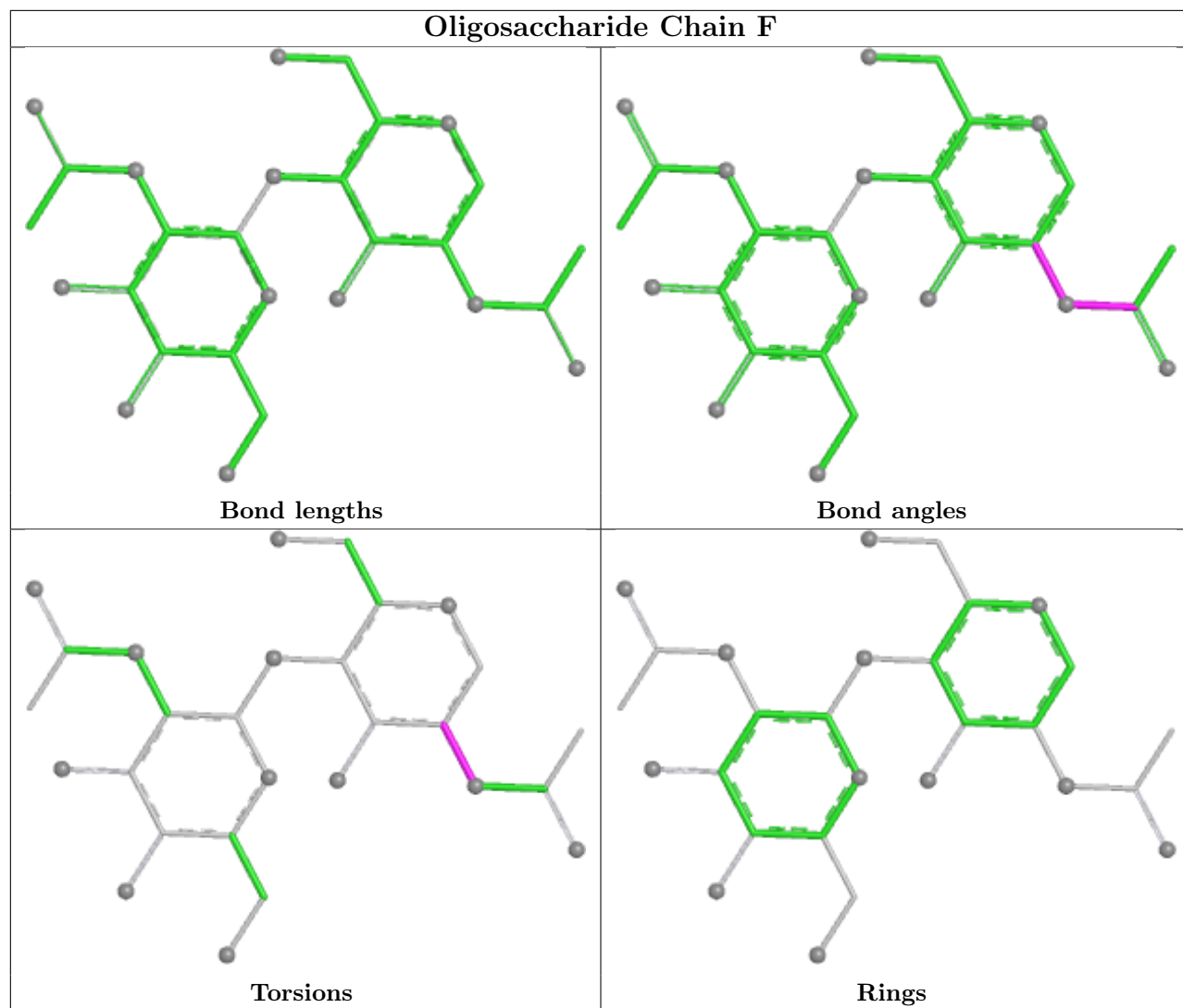
Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C1-C2-N2-C7
4	N	2	NAG	C1-C2-N2-C7
4	R	1	NAG	C1-C2-N2-C7
4	S	2	NAG	C1-C2-N2-C7
4	T	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
4	L	2	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	F	1	NAG	C1-C2-N2-C7
4	I	2	NAG	C1-C2-N2-C7
4	T	2	NAG	C1-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C3-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7

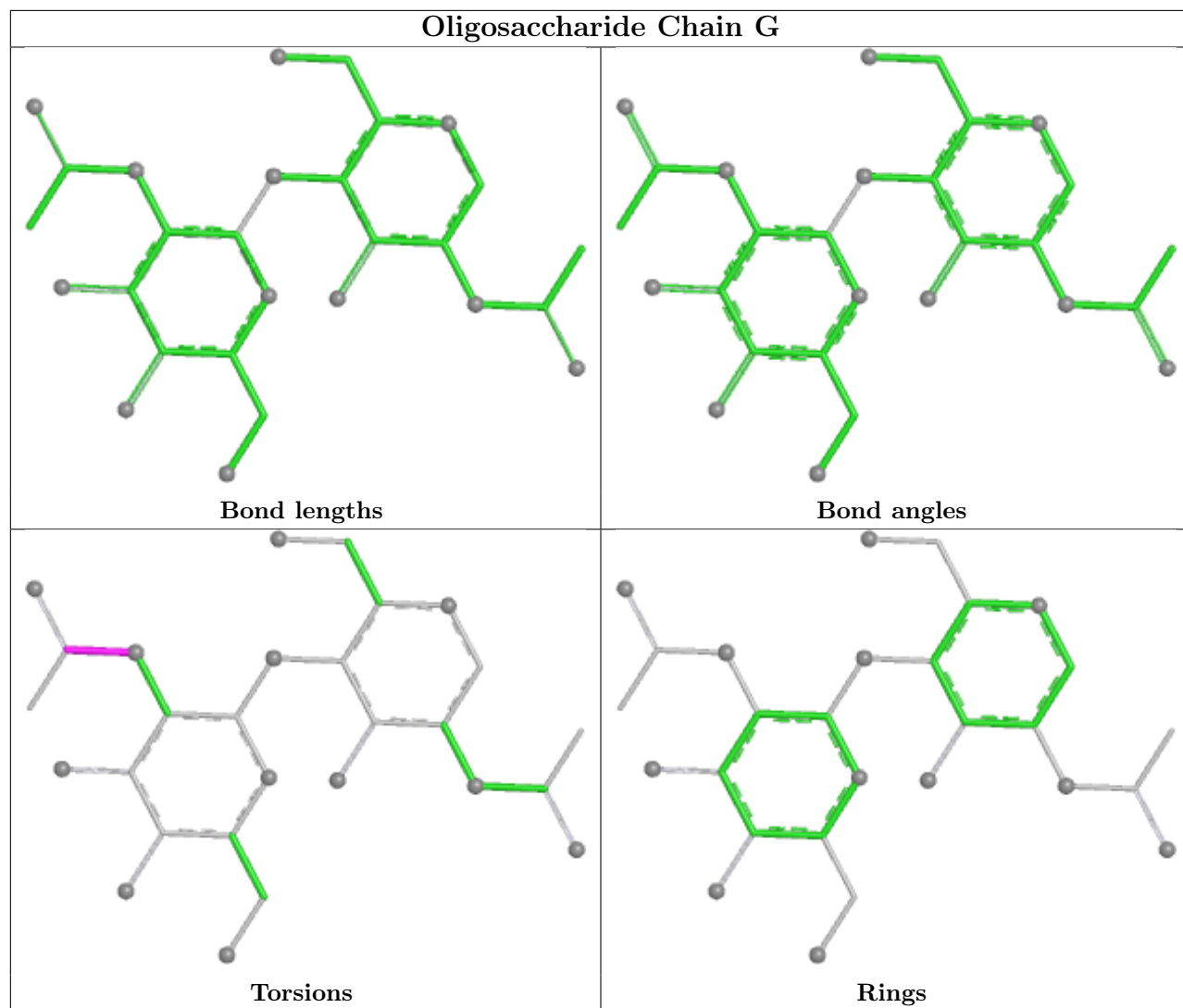
There are no ring outliers.

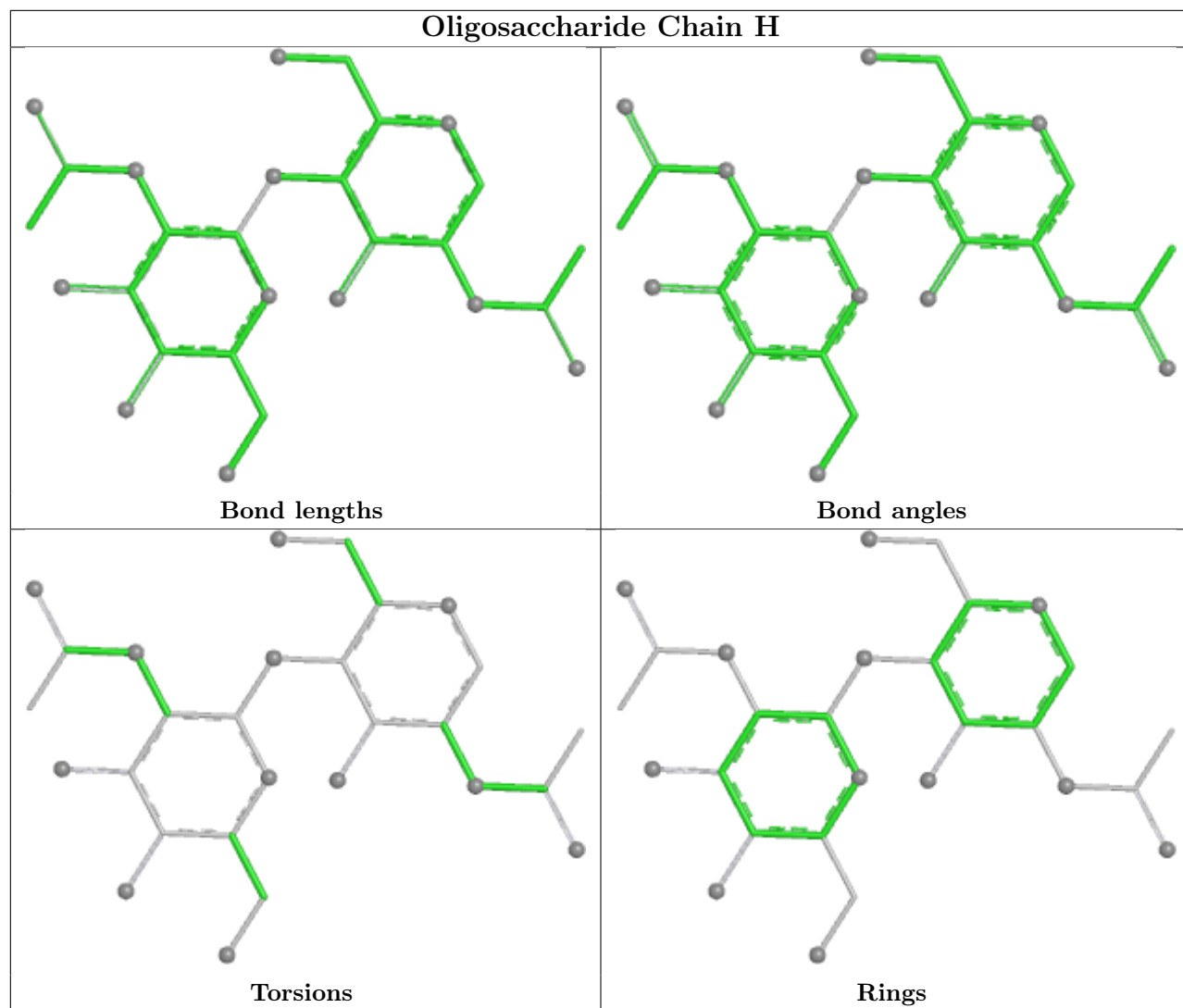
2 monomers are involved in 2 short contacts:

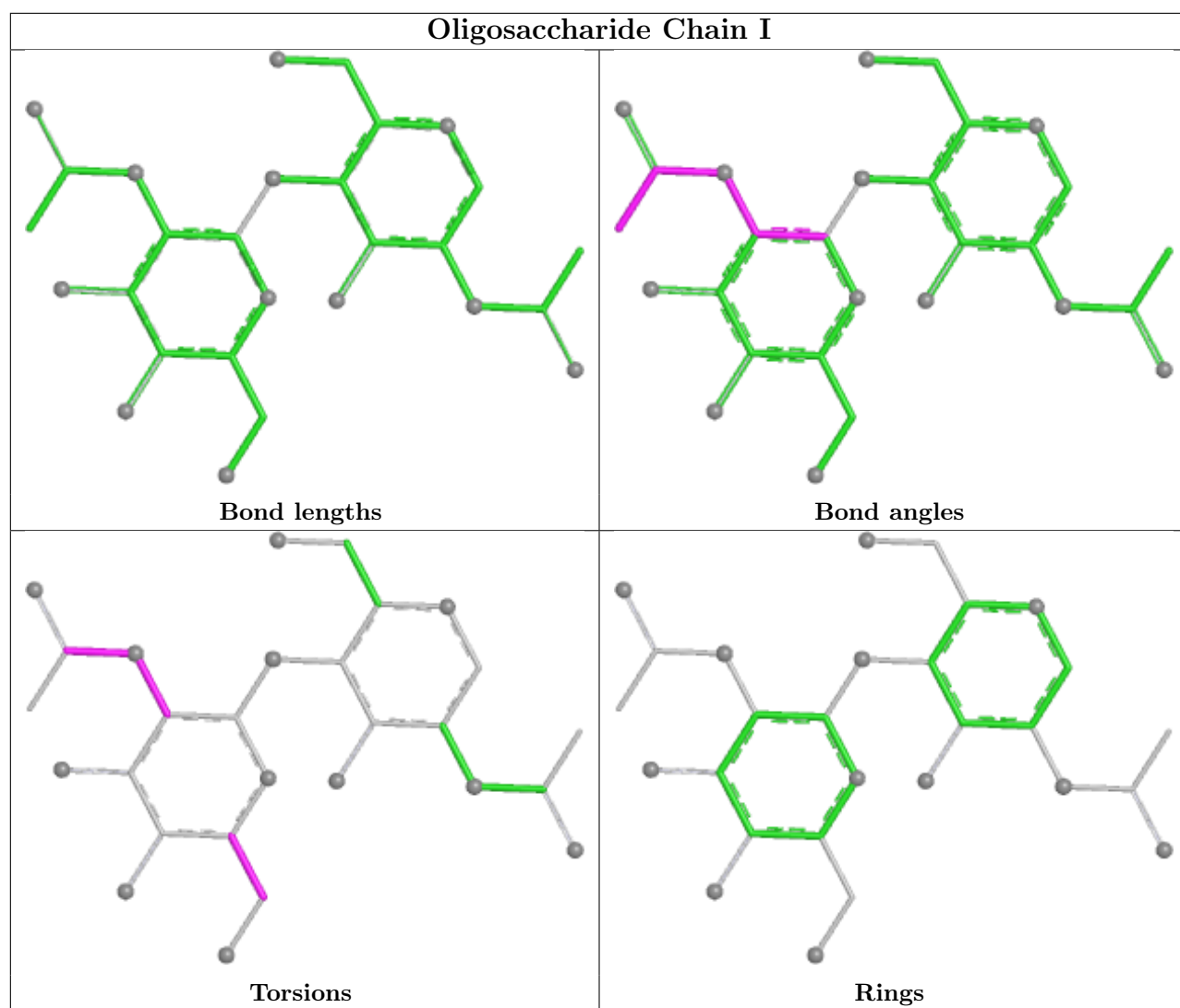
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0
4	F	1	NAG	1	0

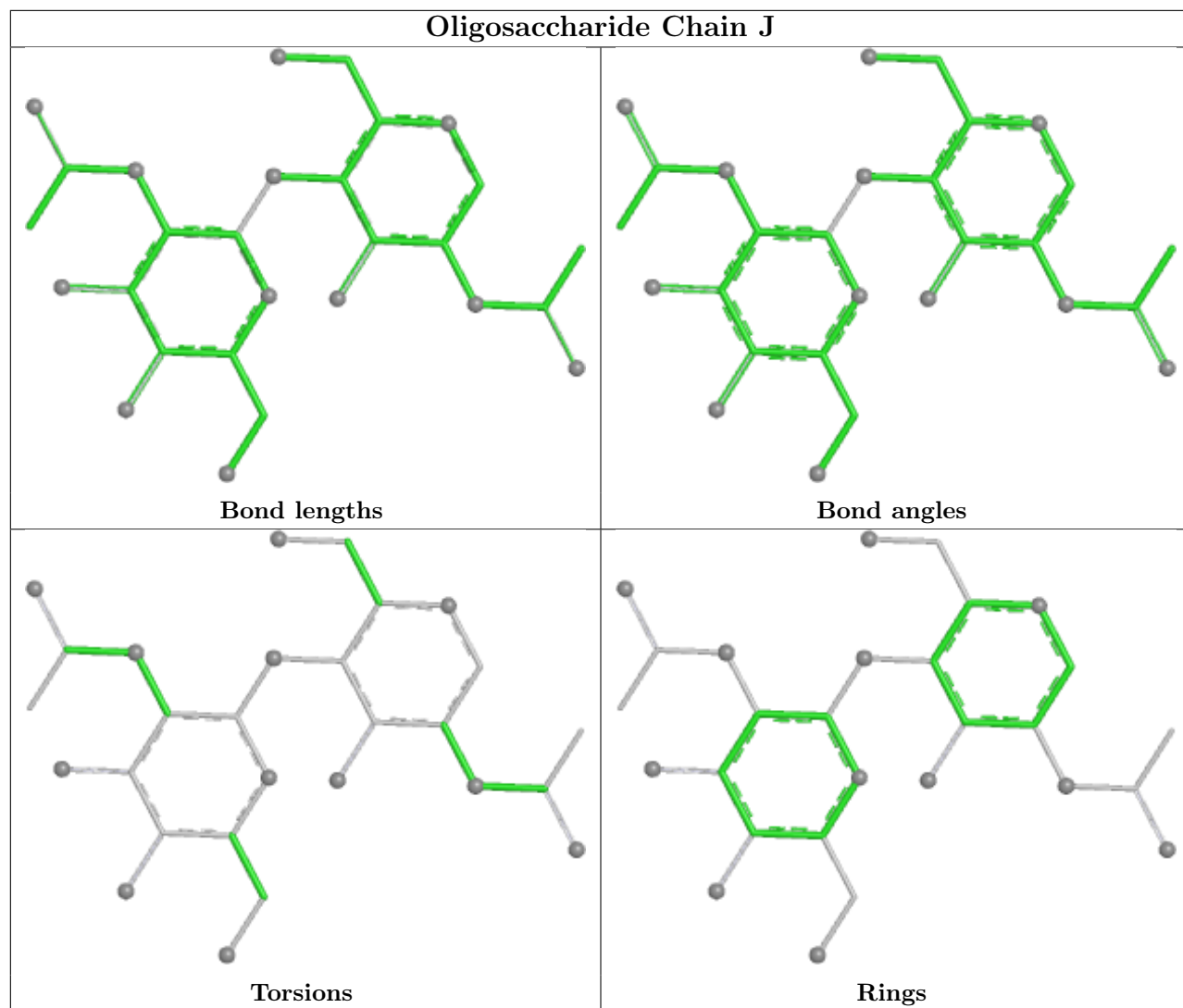
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

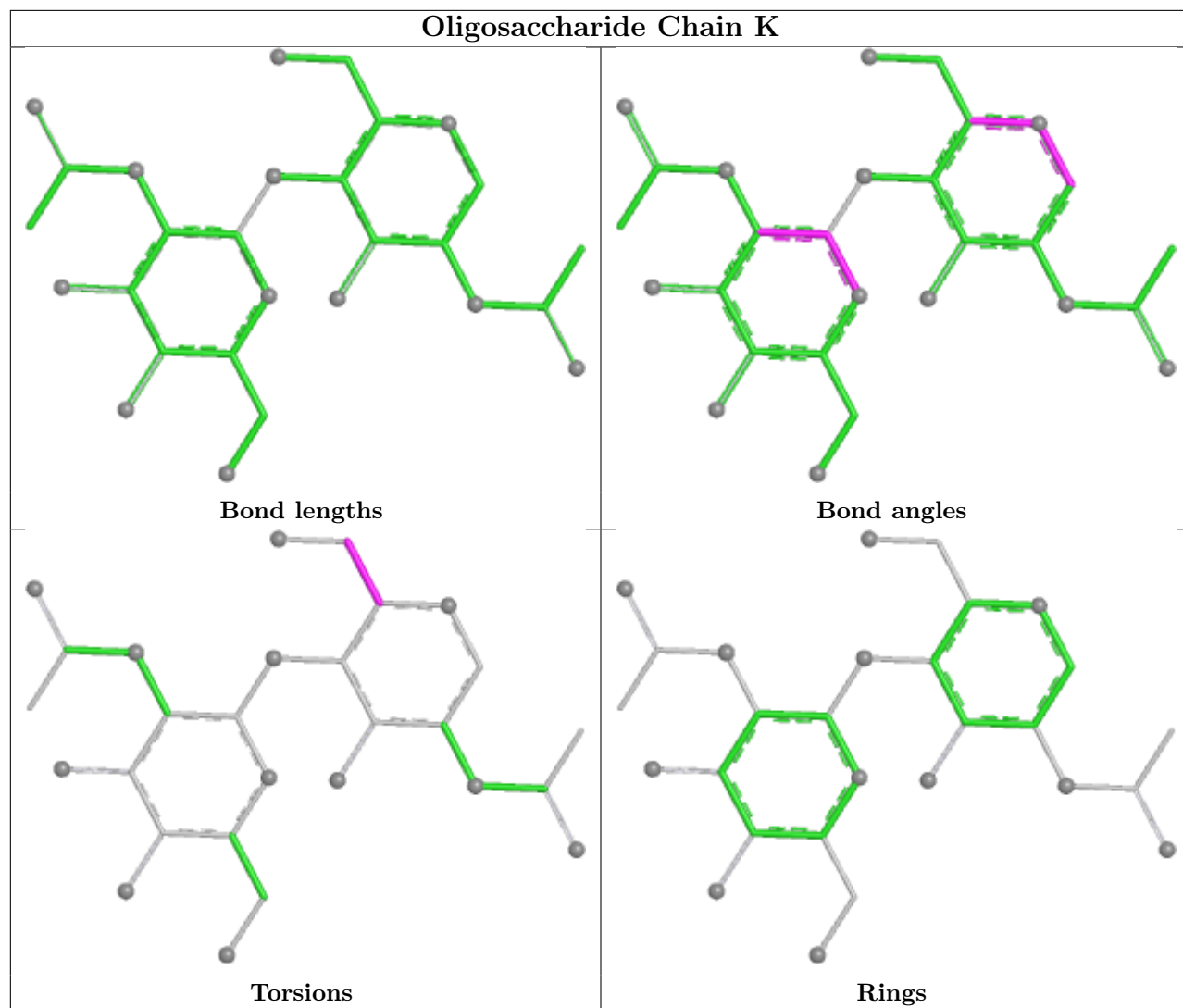


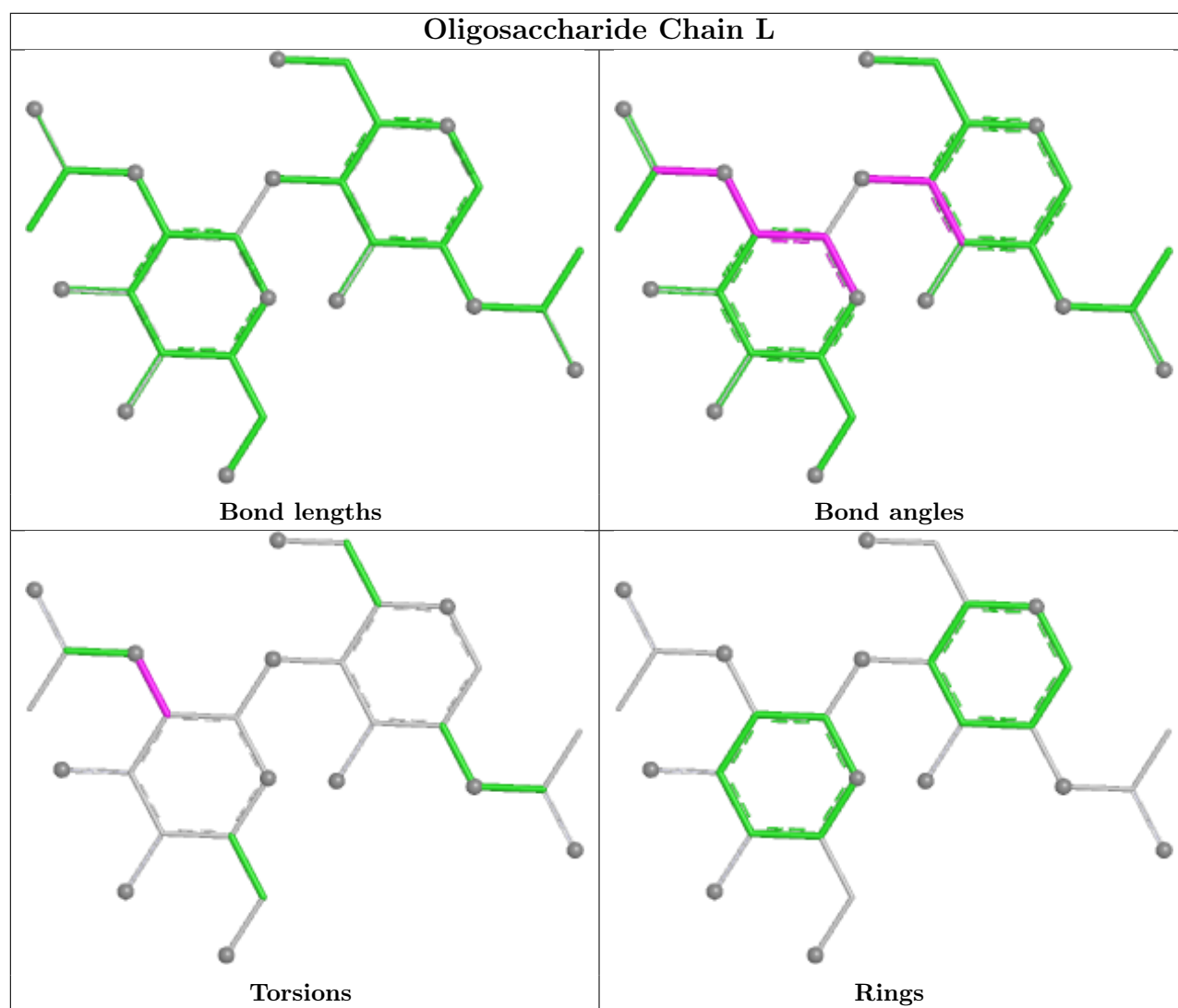


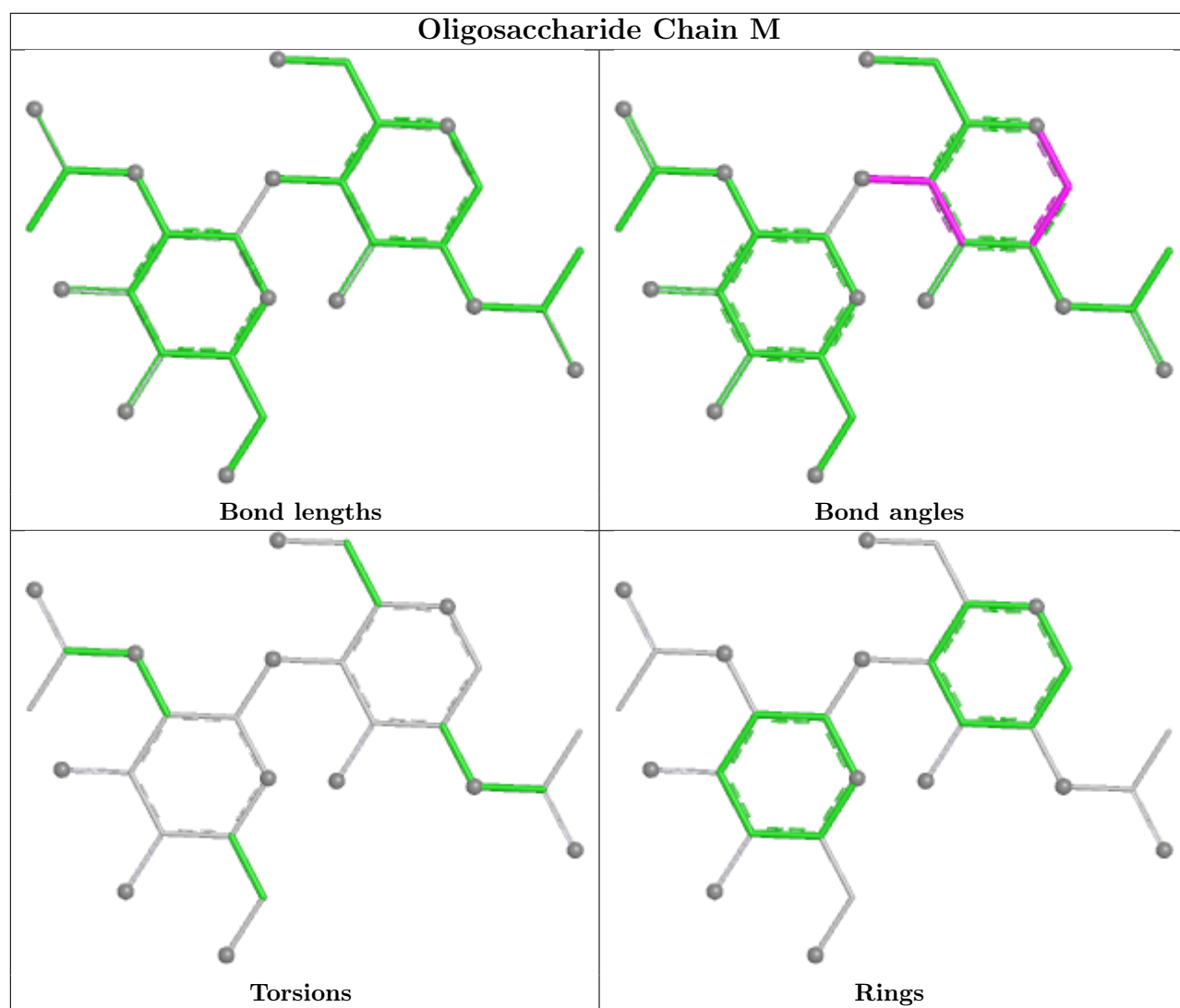


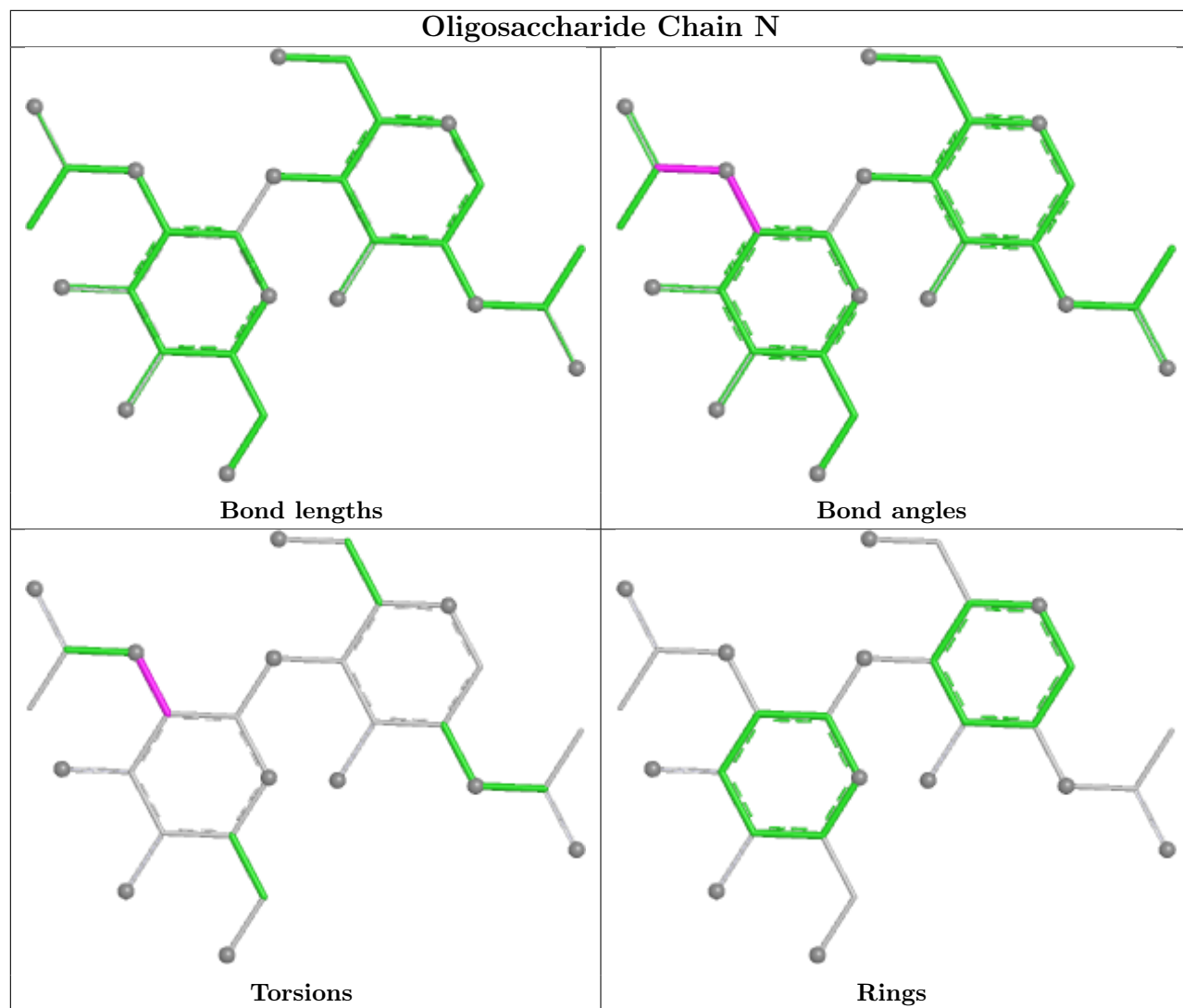


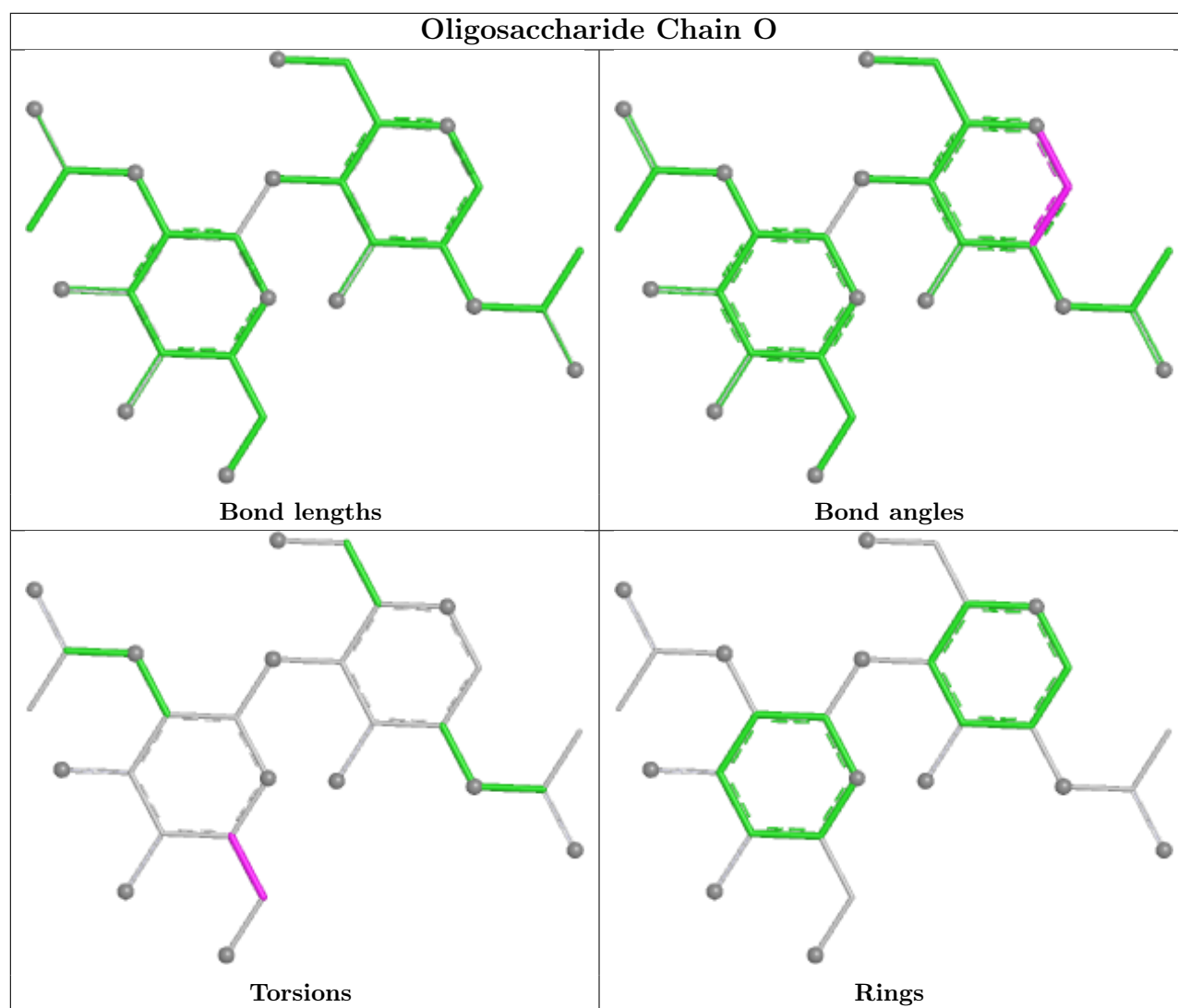


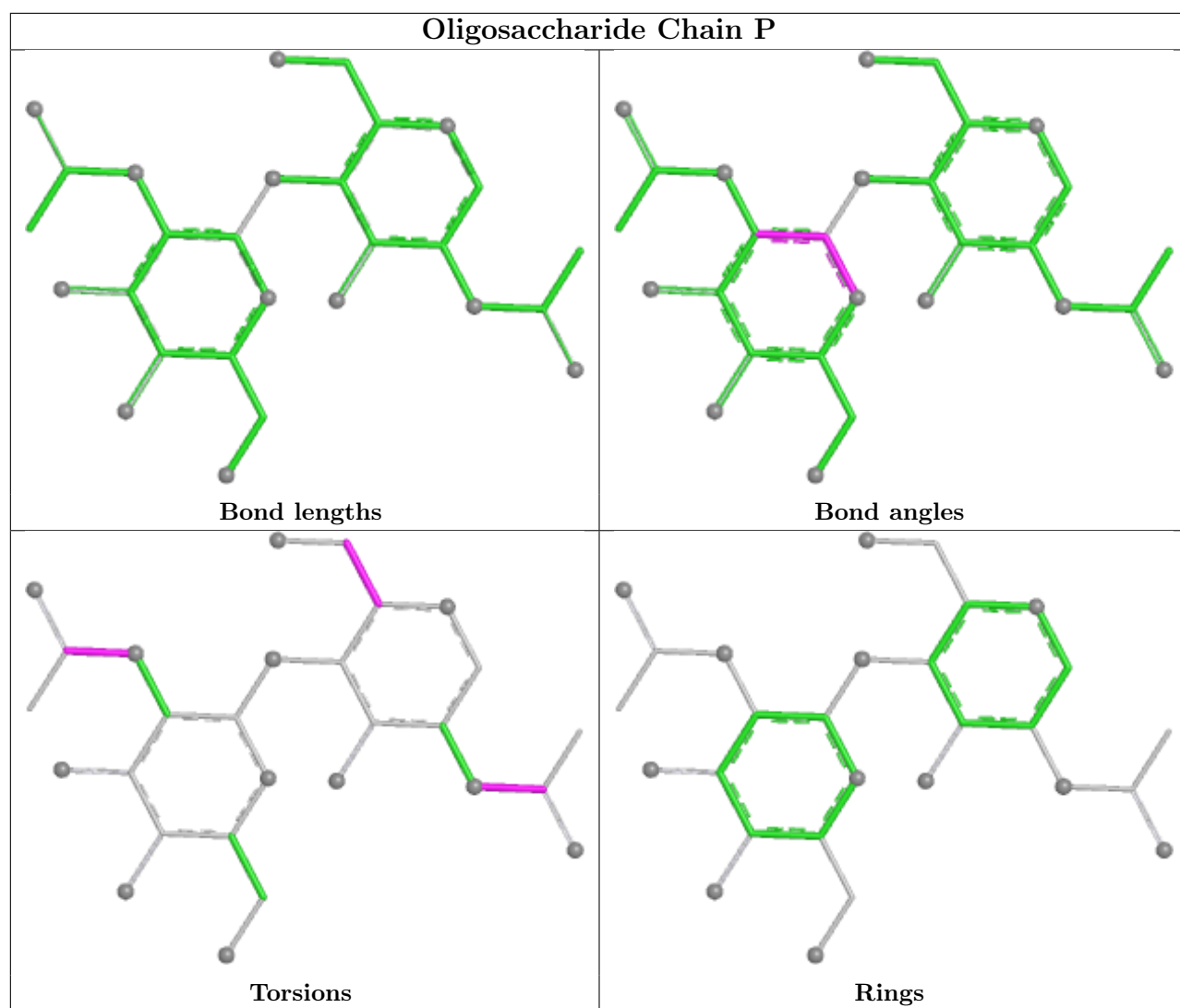


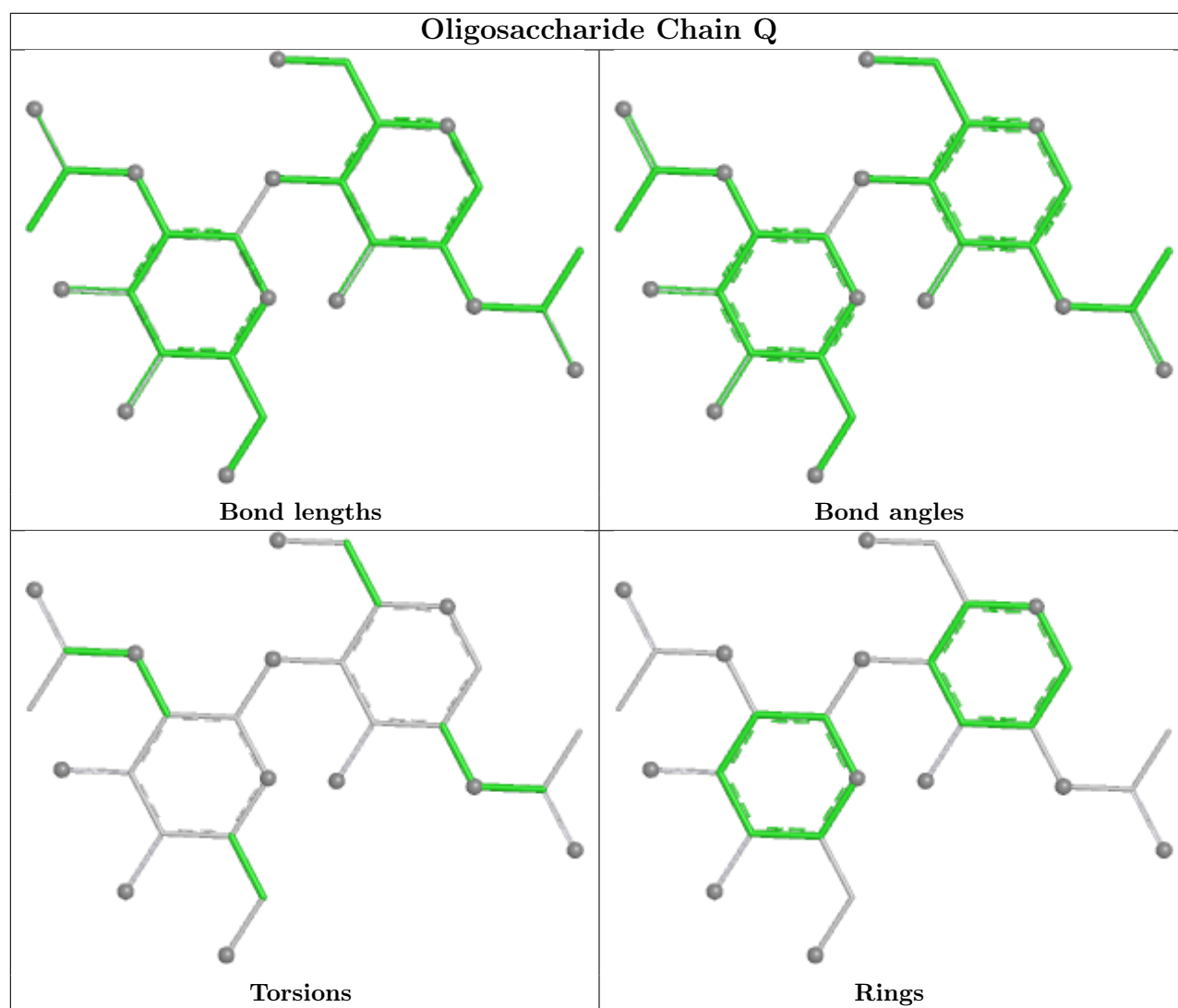


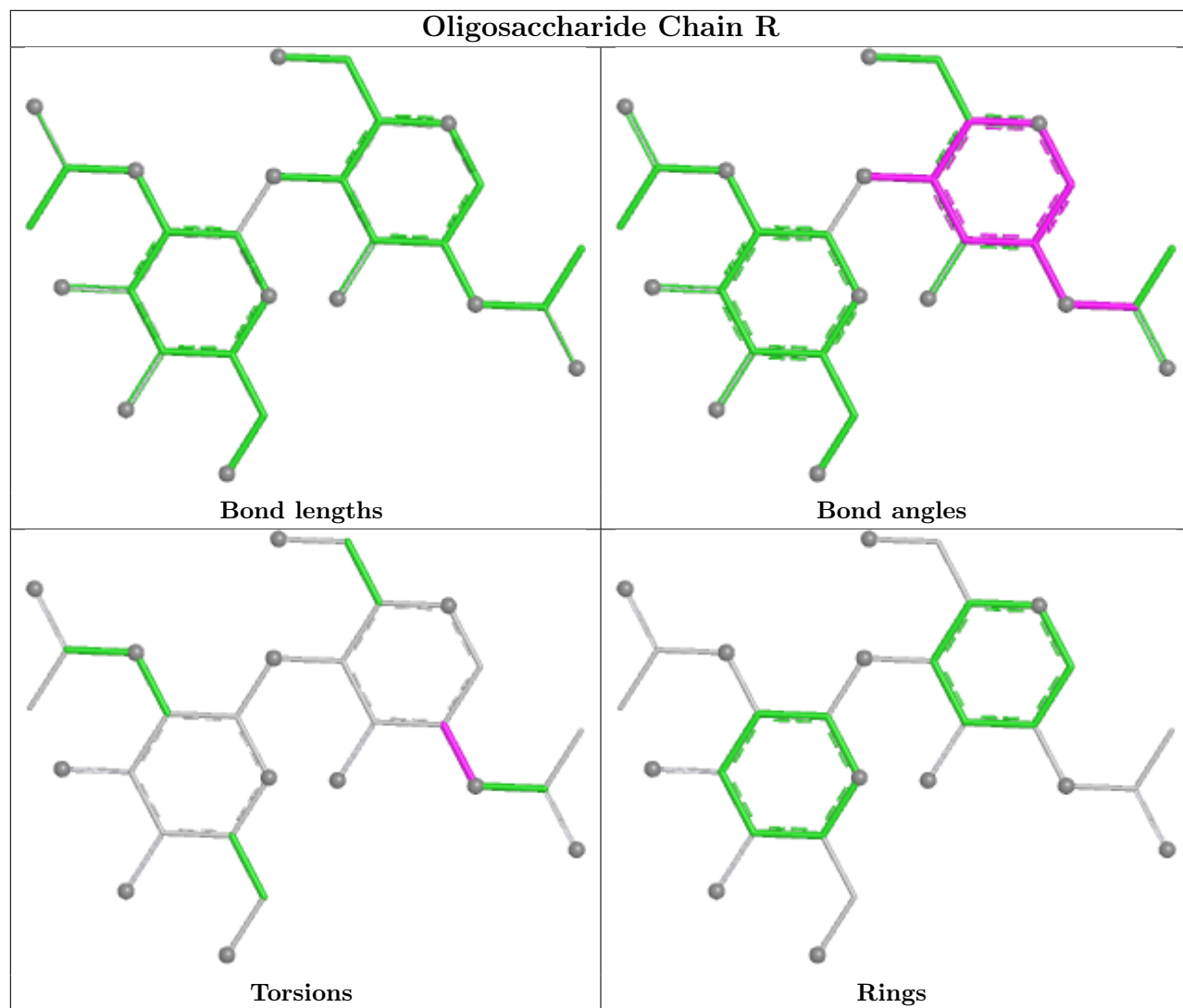


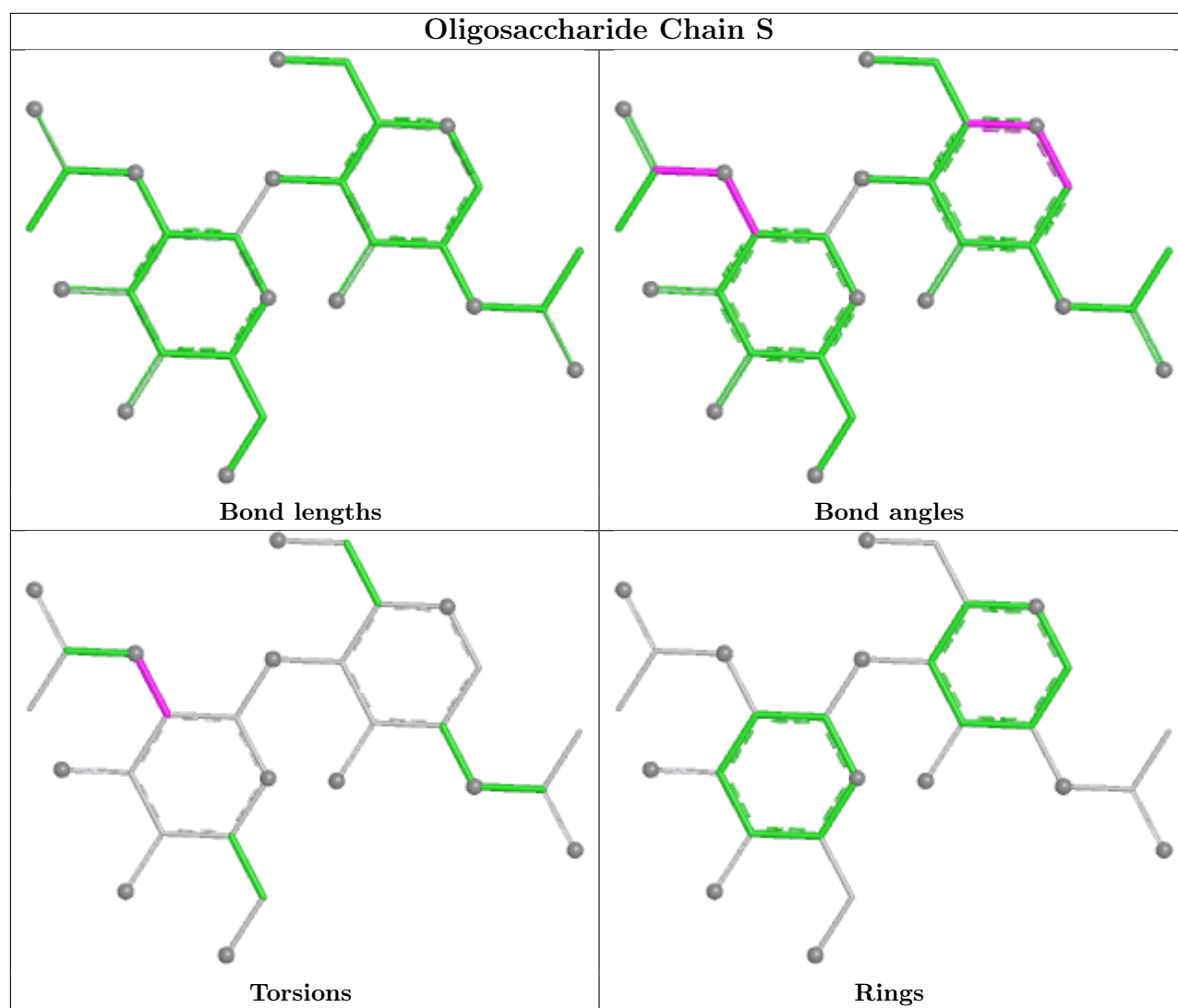


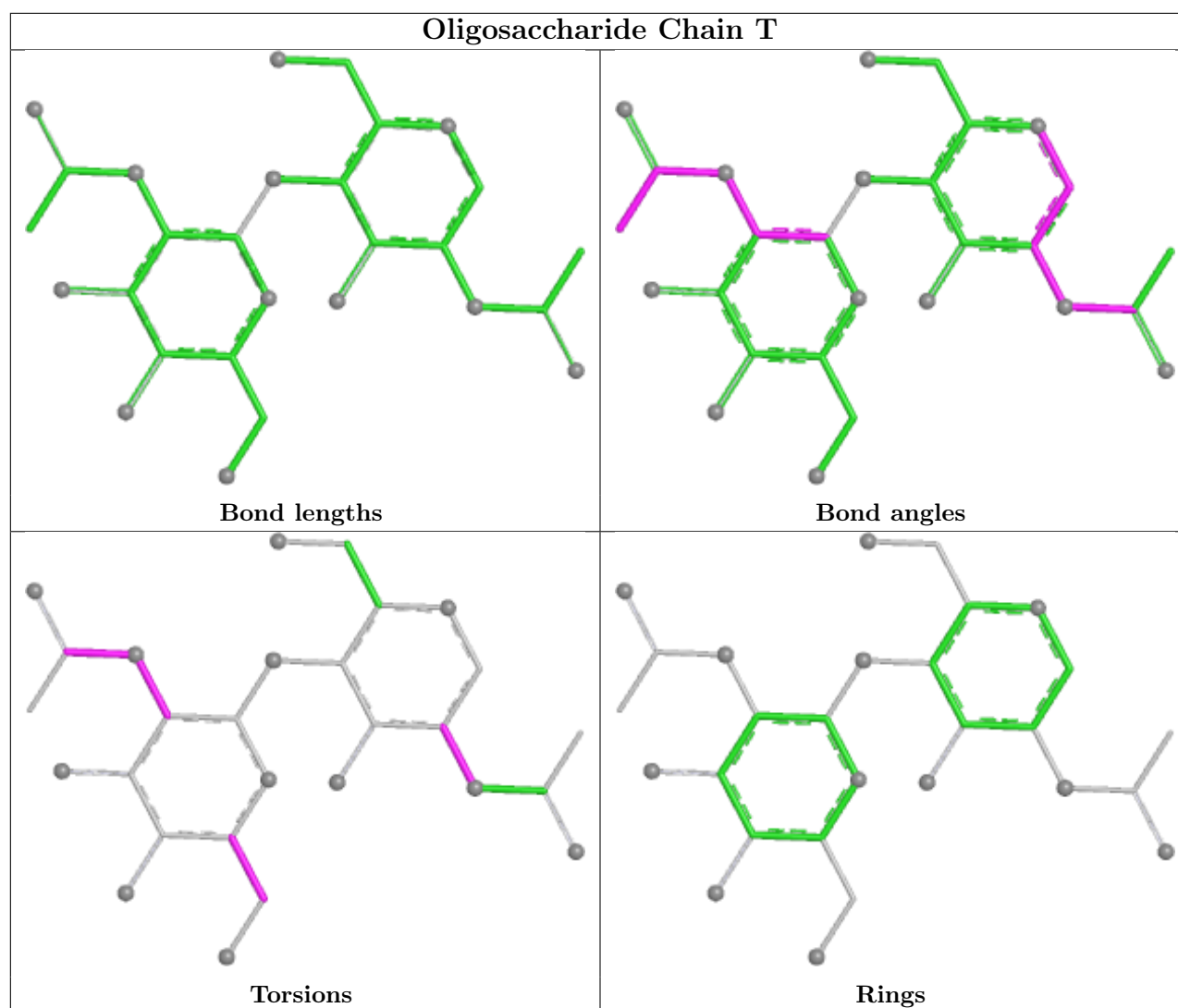












5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1304	3	14,14,15	0.72	0	17,19,21	0.90	0
5	NAG	B	1303	3	14,14,15	0.73	0	17,19,21	0.82	0
5	NAG	A	1306	3	14,14,15	0.83	1 (7%)	17,19,21	1.89	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1307	3	14,14,15	0.68	0	17,19,21	1.56	2 (11%)
5	NAG	B	1301	3	14,14,15	0.72	0	17,19,21	0.82	0
5	NAG	C	1304	3	14,14,15	0.71	0	17,19,21	0.77	0
5	NAG	A	1303	3	14,14,15	0.83	0	17,19,21	0.96	1 (5%)
5	NAG	A	1301	3	14,14,15	0.69	0	17,19,21	1.25	1 (5%)
5	NAG	C	1305	3	14,14,15	0.70	0	17,19,21	1.23	1 (5%)
5	NAG	C	1303	3	14,14,15	0.69	0	17,19,21	0.79	0
5	NAG	B	1305	3	14,14,15	0.69	0	17,19,21	1.13	1 (5%)
5	NAG	C	1301	3	14,14,15	0.73	0	17,19,21	0.89	0
5	NAG	C	1302	3	14,14,15	0.73	0	17,19,21	2.35	3 (17%)
5	NAG	A	1307	3	14,14,15	0.75	0	17,19,21	1.11	1 (5%)
5	NAG	B	1302	3	14,14,15	0.74	0	17,19,21	1.18	1 (5%)
5	NAG	A	1305	3	14,14,15	0.73	0	17,19,21	0.79	0
5	NAG	B	1306	3	14,14,15	0.70	0	17,19,21	0.83	0
5	NAG	B	1304	3	14,14,15	0.76	0	17,19,21	0.99	0
5	NAG	C	1306	3	14,14,15	0.71	0	17,19,21	1.22	1 (5%)
5	NAG	B	1307	3	14,14,15	1.15	1 (7%)	17,19,21	1.68	2 (11%)
5	NAG	A	1302	3	14,14,15	0.71	0	17,19,21	2.40	4 (23%)

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
5	NAG	A	1304	3	-	3/6/23/26	0/1/1/1
5	NAG	B	1303	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	3	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	3	-	3/6/23/26	0/1/1/1
5	NAG	B	1301	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	3	-	3/6/23/26	0/1/1/1
5	NAG	C	1305	3	-	3/6/23/26	0/1/1/1
5	NAG	C	1303	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	3	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	3	-	1/6/23/26	0/1/1/1
5	NAG	C	1302	3	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1307	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	3	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1306	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1304	3	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	3	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	3	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1307	NAG	C1-C2	3.41	1.57	1.52
5	A	1306	NAG	C1-C2	2.03	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1302	NAG	C2-N2-C7	8.41	134.17	122.90
5	A	1302	NAG	C2-N2-C7	8.37	134.12	122.90
5	B	1307	NAG	C1-O5-C5	4.88	118.73	112.19
5	A	1306	NAG	C1-O5-C5	4.36	118.02	112.19
5	C	1307	NAG	O5-C1-C2	-4.04	105.03	111.29
5	A	1306	NAG	C2-N2-C7	3.42	127.48	122.90
5	C	1307	NAG	C2-N2-C7	3.40	127.45	122.90
5	C	1305	NAG	C2-N2-C7	3.30	127.32	122.90
5	A	1306	NAG	C1-C2-N2	3.18	115.44	110.43
5	C	1306	NAG	C2-N2-C7	3.17	127.15	122.90
5	A	1301	NAG	C2-N2-C7	3.17	127.15	122.90
5	B	1305	NAG	C2-N2-C7	3.10	127.05	122.90
5	B	1307	NAG	C3-C4-C5	-3.04	104.72	110.23
5	B	1302	NAG	C2-N2-C7	2.97	126.88	122.90
5	A	1307	NAG	C1-O5-C5	2.95	116.14	112.19
5	A	1302	NAG	C1-C2-N2	2.65	114.61	110.43
5	C	1302	NAG	C8-C7-N2	2.61	120.44	116.12
5	A	1306	NAG	O5-C1-C2	-2.60	107.26	111.29
5	A	1302	NAG	C8-C7-N2	2.58	120.39	116.12
5	A	1303	NAG	O5-C1-C2	-2.31	107.71	111.29
5	C	1302	NAG	C1-C2-N2	2.29	114.04	110.43
5	A	1302	NAG	O5-C1-C2	-2.06	108.11	111.29

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1302	NAG	C8-C7-N2-C2
5	A	1302	NAG	O7-C7-N2-C2
5	A	1304	NAG	C8-C7-N2-C2
5	A	1304	NAG	O7-C7-N2-C2
5	B	1307	NAG	C8-C7-N2-C2
5	B	1307	NAG	O7-C7-N2-C2
5	C	1302	NAG	C8-C7-N2-C2
5	C	1302	NAG	O7-C7-N2-C2
5	C	1301	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	A	1301	NAG	C1-C2-N2-C7
5	B	1302	NAG	C1-C2-N2-C7
5	B	1305	NAG	C1-C2-N2-C7
5	C	1305	NAG	C1-C2-N2-C7
5	C	1307	NAG	C1-C2-N2-C7
5	A	1301	NAG	C3-C2-N2-C7
5	A	1306	NAG	C3-C2-N2-C7
5	B	1302	NAG	C3-C2-N2-C7
5	C	1306	NAG	C3-C2-N2-C7
5	A	1302	NAG	C1-C2-N2-C7
5	A	1306	NAG	C1-C2-N2-C7
5	C	1302	NAG	C1-C2-N2-C7
5	C	1306	NAG	C1-C2-N2-C7
5	A	1302	NAG	C3-C2-N2-C7
5	B	1305	NAG	C3-C2-N2-C7
5	C	1302	NAG	C3-C2-N2-C7
5	C	1305	NAG	C3-C2-N2-C7
5	C	1307	NAG	C3-C2-N2-C7
5	A	1305	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1306	NAG	2	0
5	C	1301	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1302	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

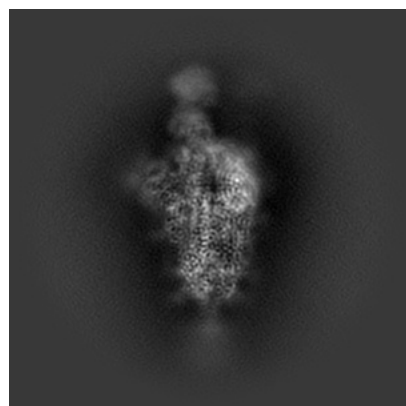
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75698. These allow visual inspection of the internal detail of the map and identification of artifacts.

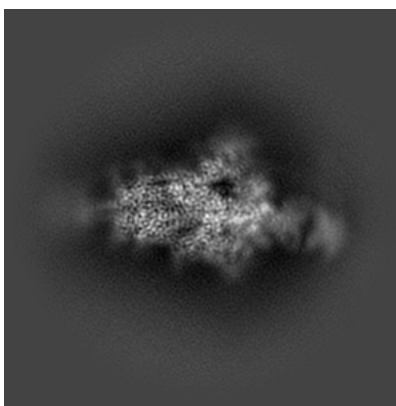
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

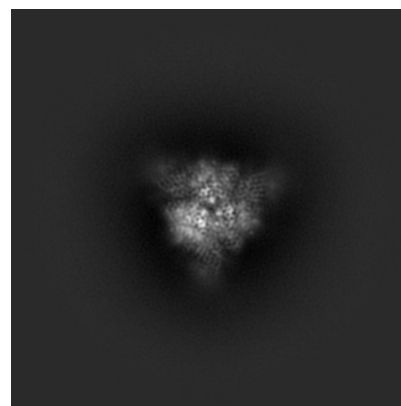
6.1.1 Primary map



X

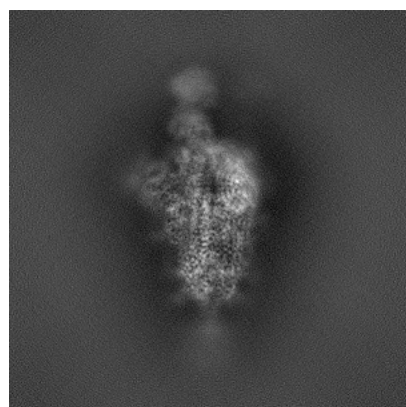


Y

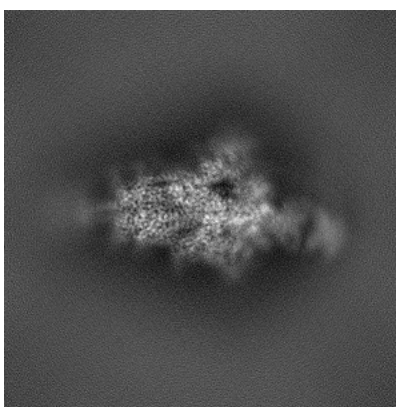


Z

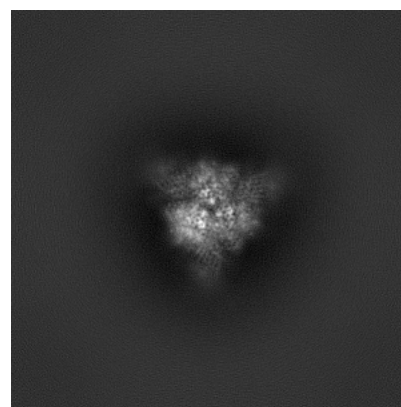
6.1.2 Raw map



X



Y

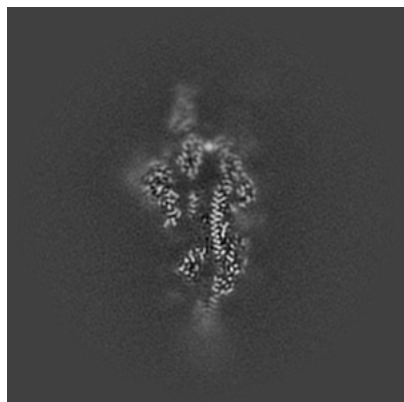


Z

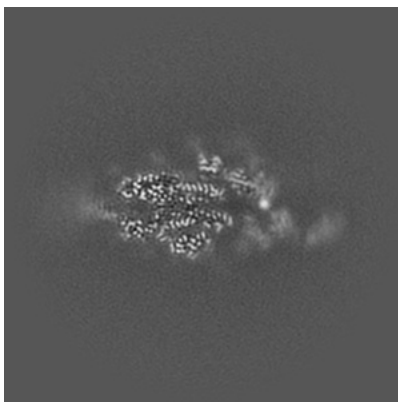
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

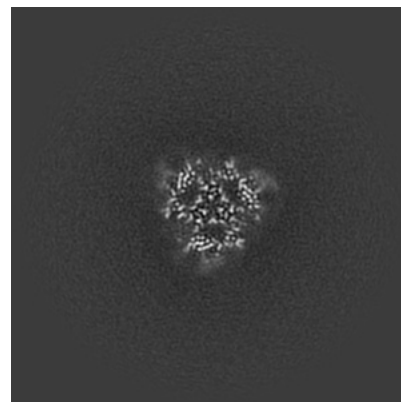
6.2.1 Primary map



X Index: 192

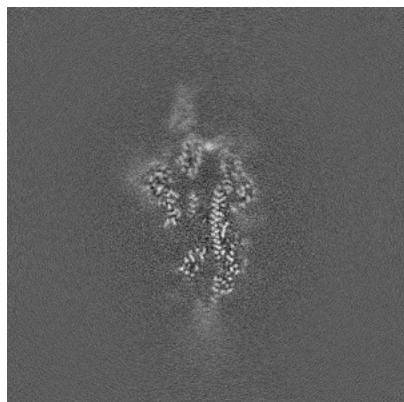


Y Index: 192

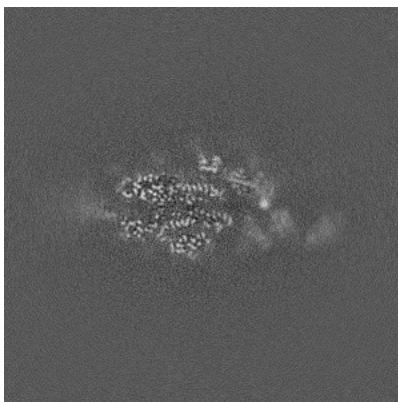


Z Index: 192

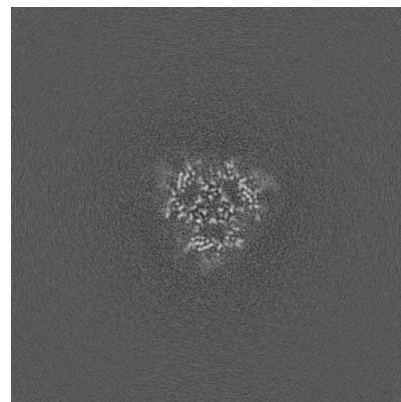
6.2.2 Raw map



X Index: 192



Y Index: 192

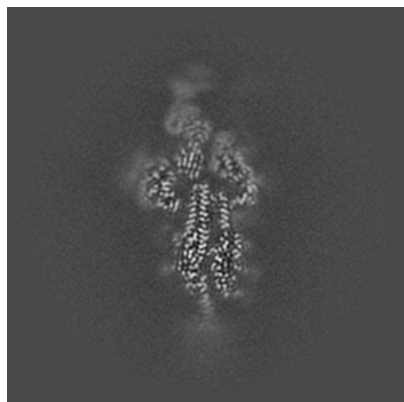


Z Index: 192

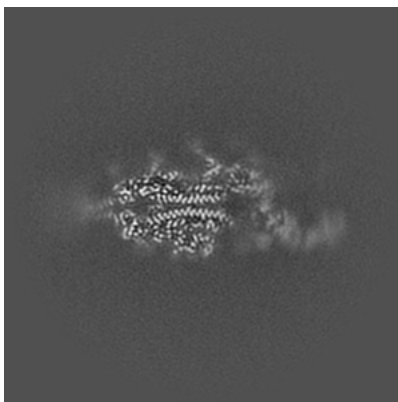
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

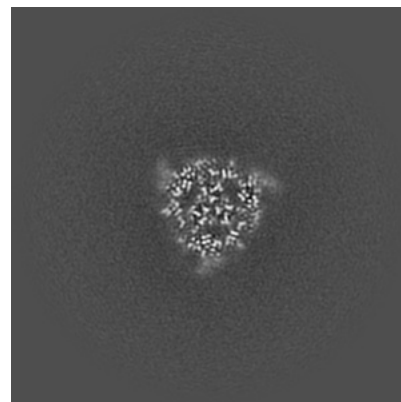
6.3.1 Primary map



X Index: 184

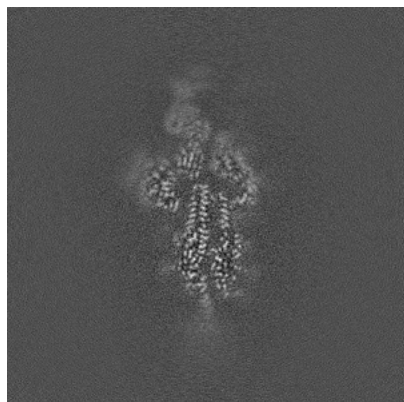


Y Index: 188

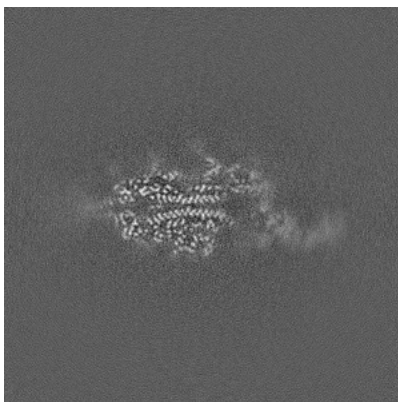


Z Index: 194

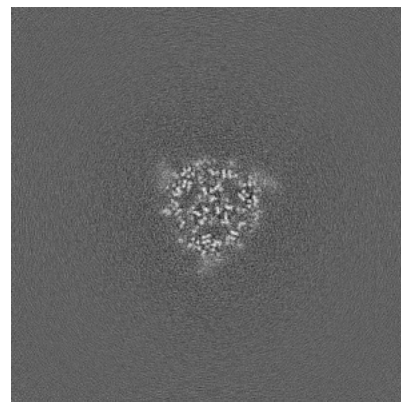
6.3.2 Raw map



X Index: 184



Y Index: 188

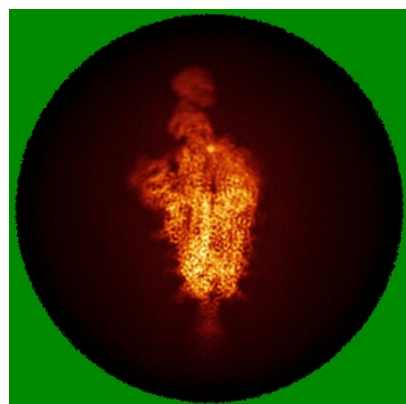


Z Index: 194

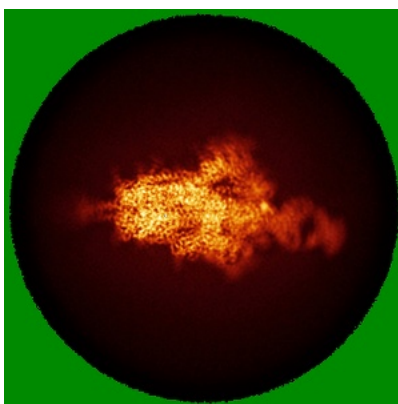
The images above show the largest variance slices of the map in three orthogonal directions.

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

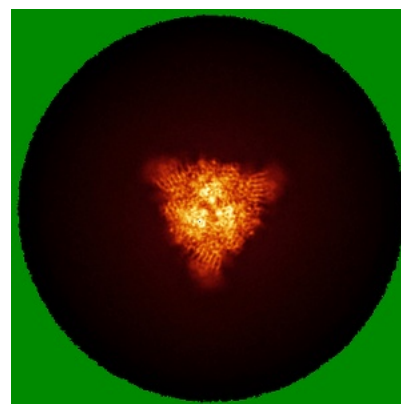
6.4.1 Primary map



X



Y

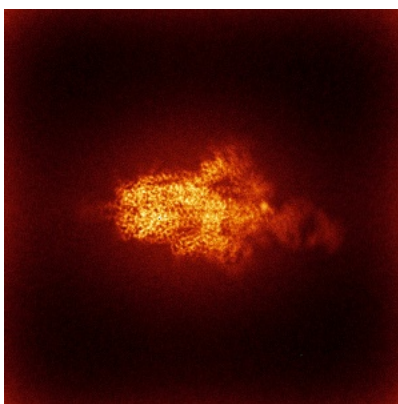


Z

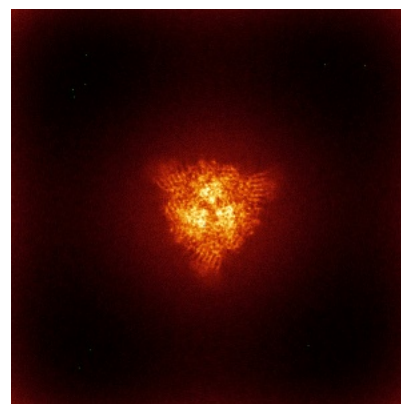
6.4.2 Raw map



X



Y

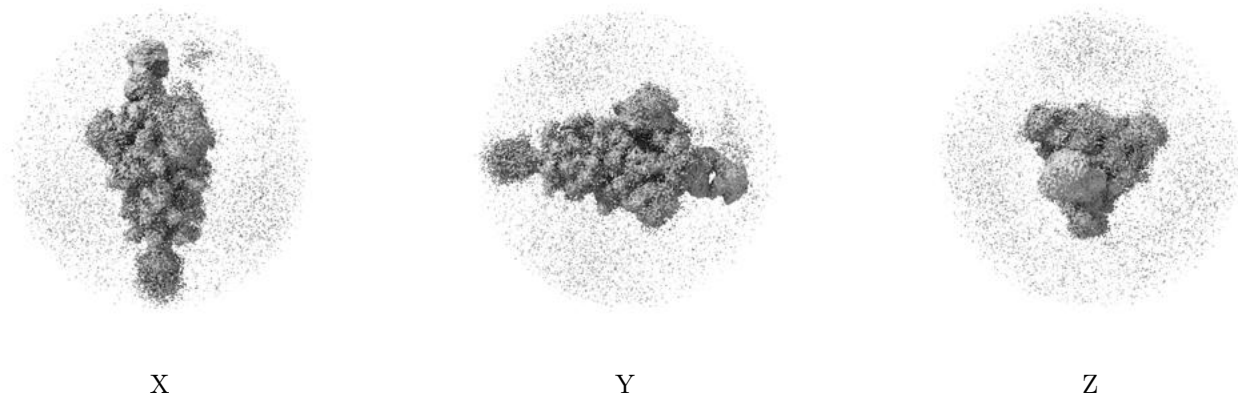


Z

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.

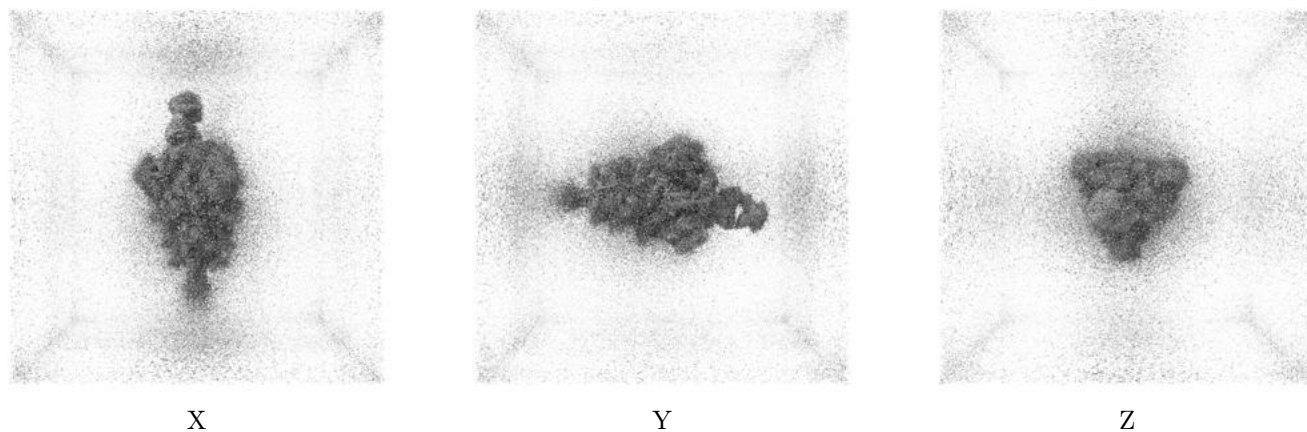
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

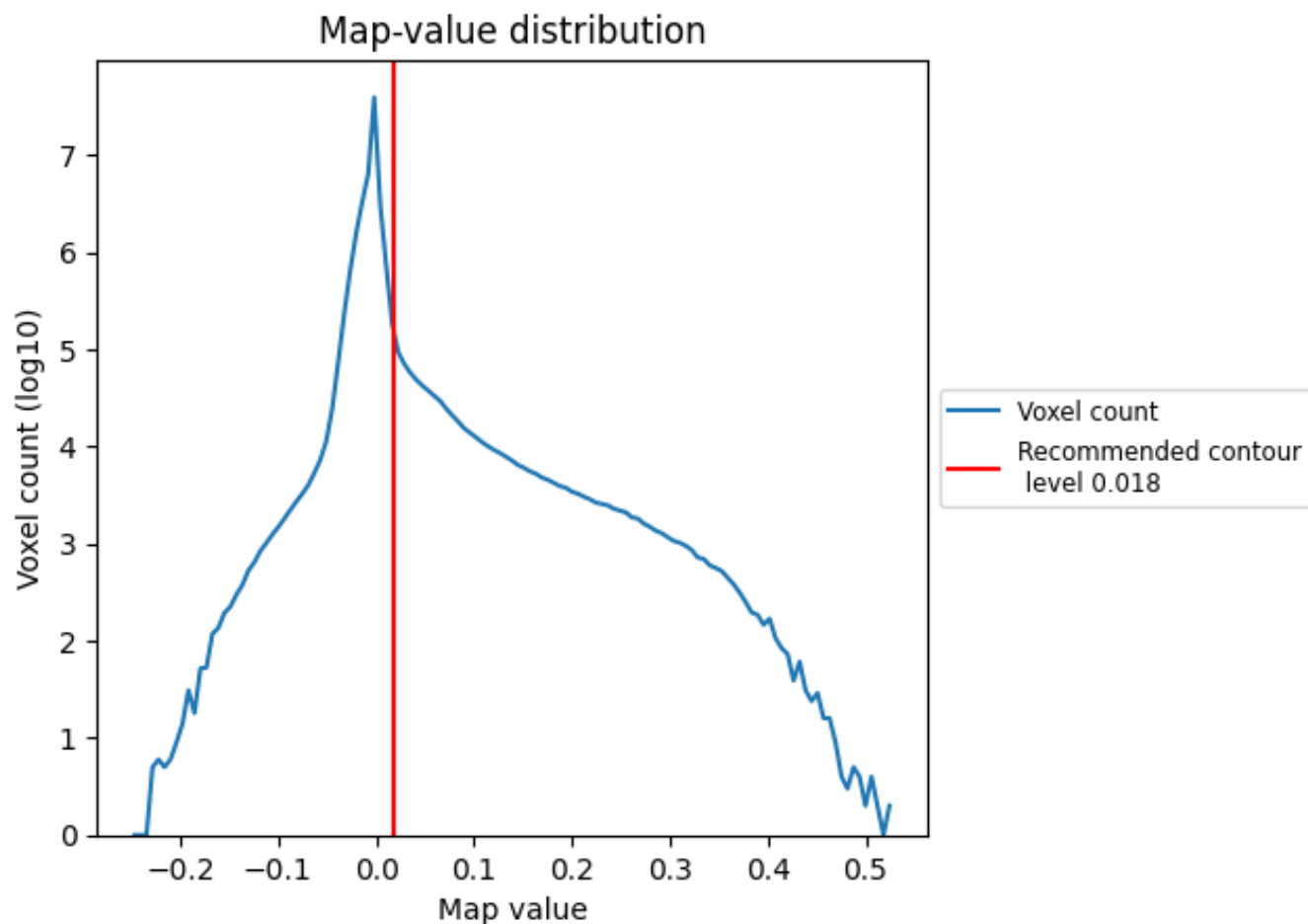
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

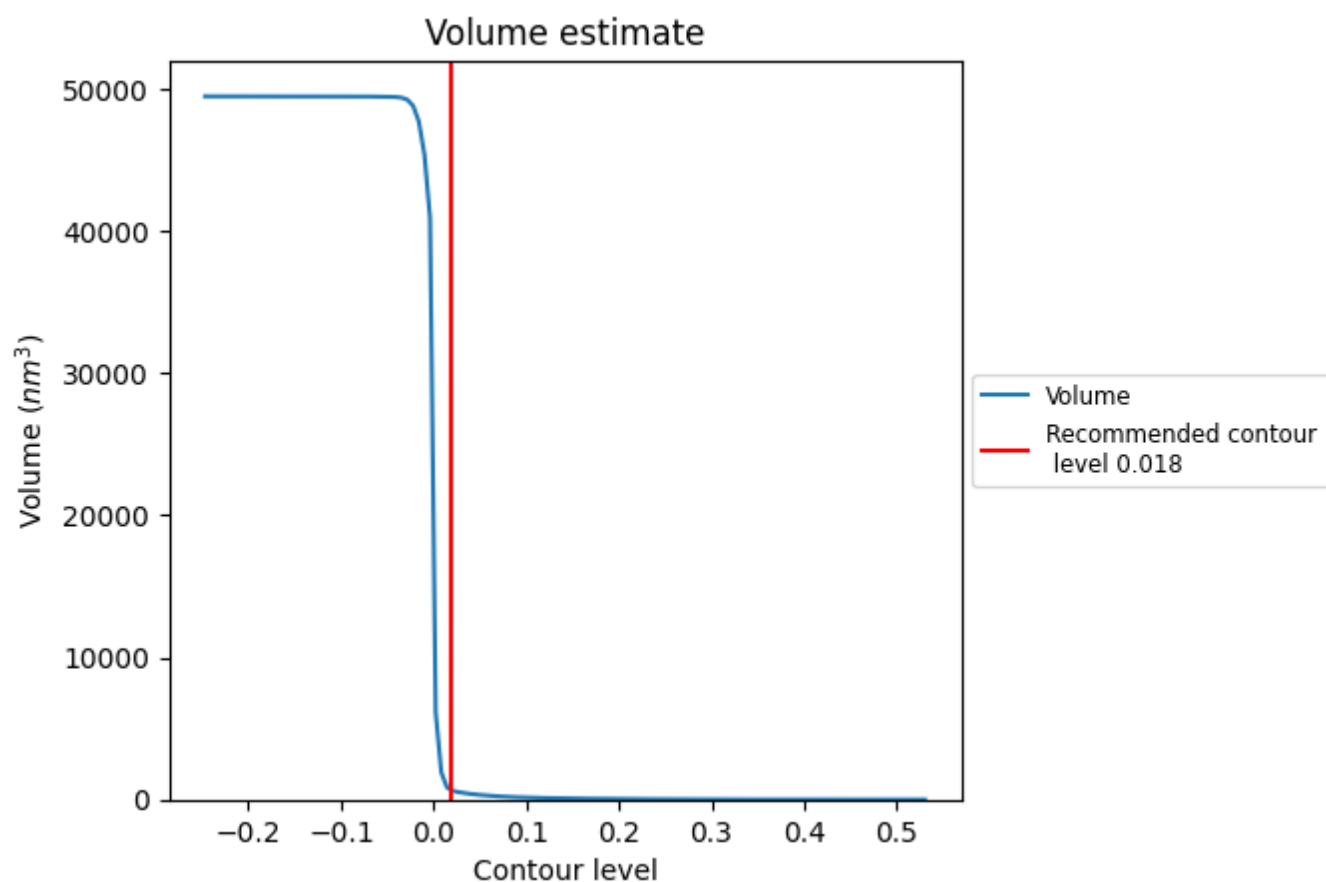
This section contains the results of statistical analysis of the map.

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.

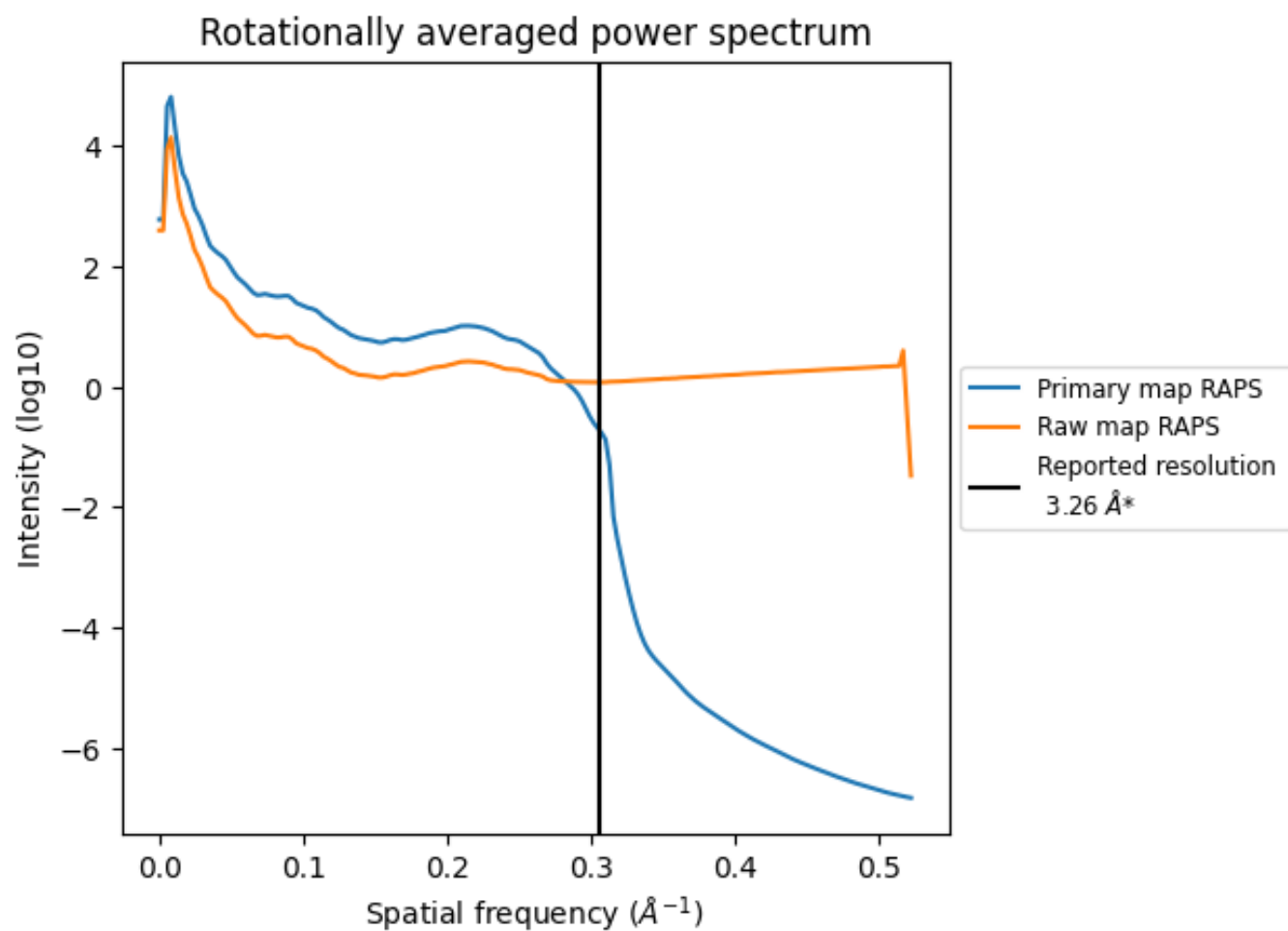
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 716 nm^3 ; this corresponds to an approximate mass of 647 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 ⓘ

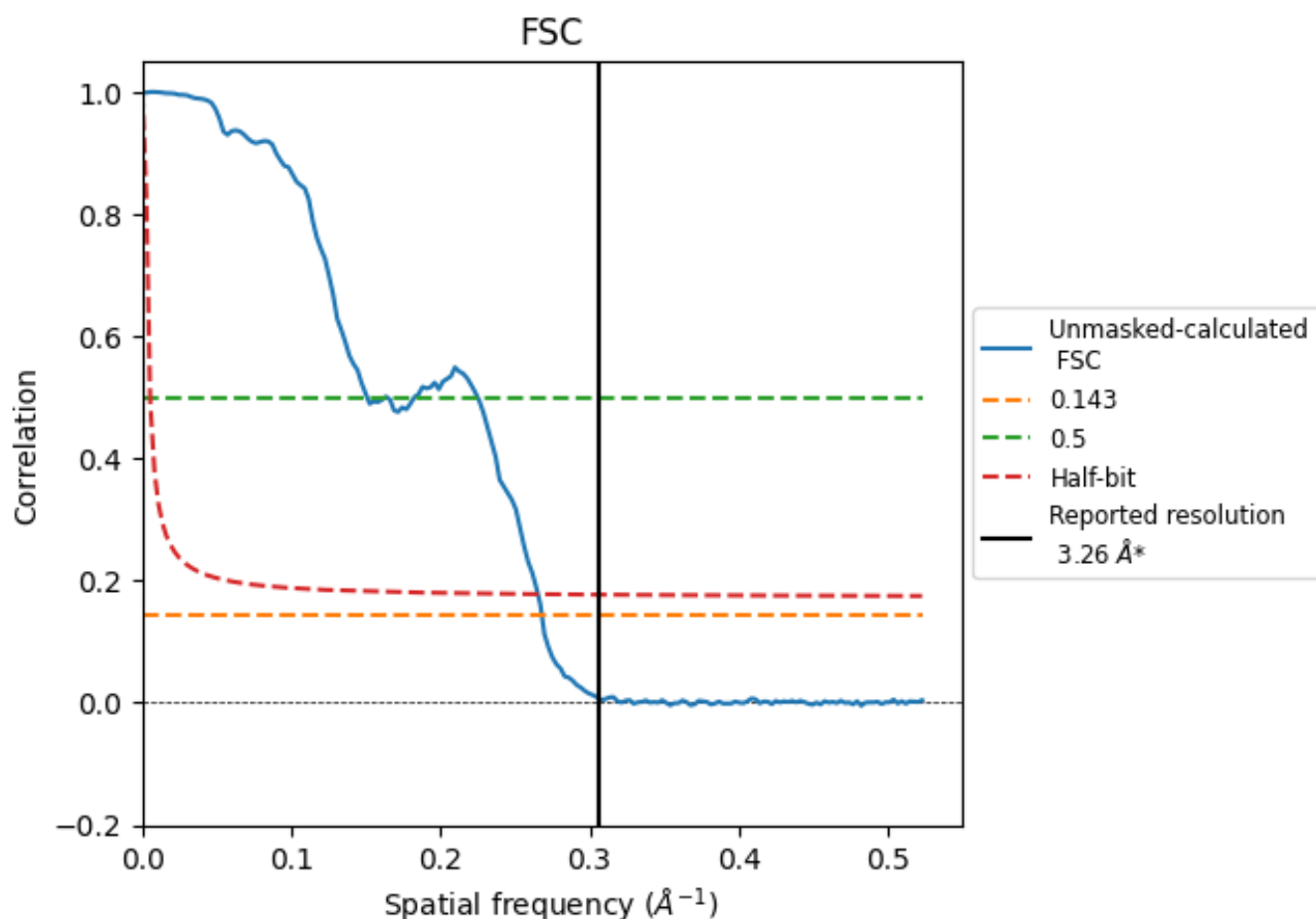


*Reported resolution corresponds to spatial frequency of 0.307 $\text{\AA}^{-1}$

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 $0.307 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

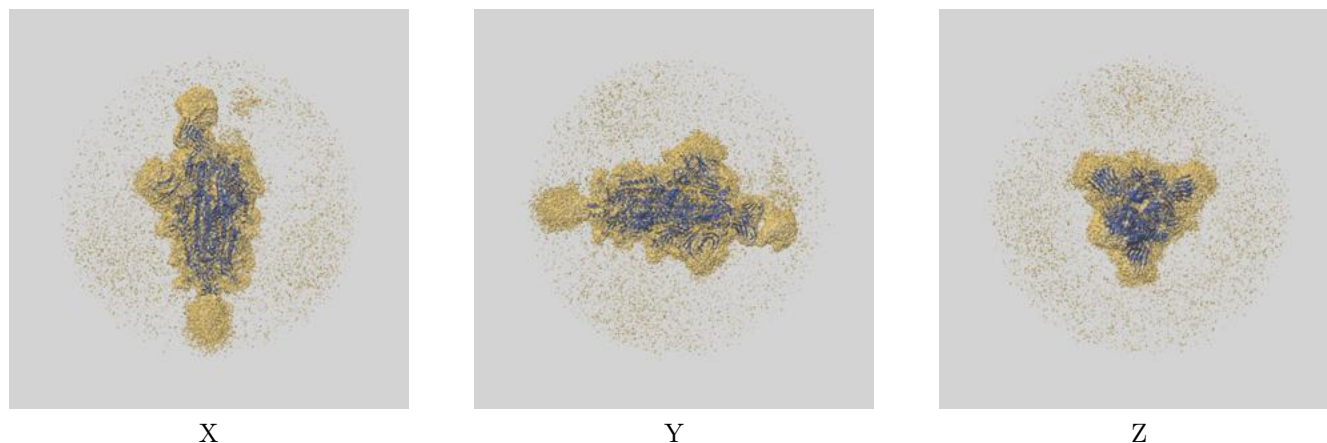
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	6.63	3.77

*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 3.73 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

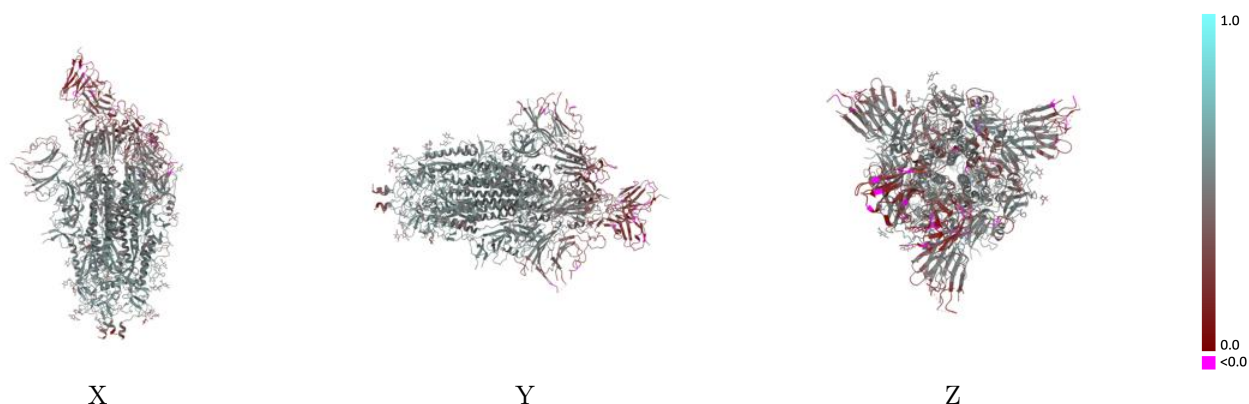
This section contains information regarding the fit between EMDB map EMD-75698 and PDB model 11HO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.018 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](#)



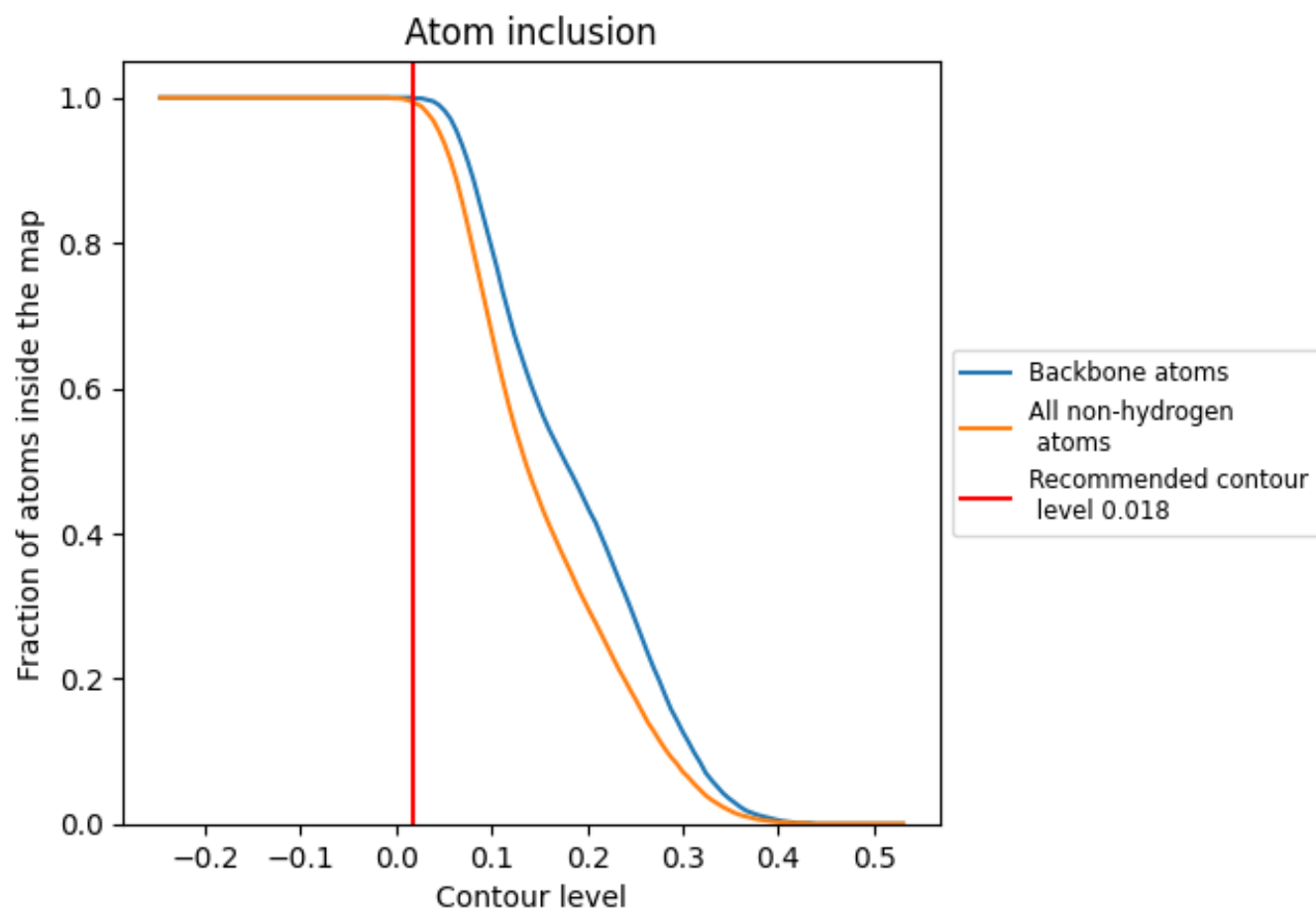
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9940	 0.4590
A	 0.9960	 0.4850
B	 0.9940	 0.4700
C	 0.9940	 0.4760
D	 0.9830	 0.2520
E	 0.9870	 0.1820
F	 1.0000	 0.4180
G	 1.0000	 0.4860
H	 0.9640	 0.4070
I	 1.0000	 0.4160
J	 1.0000	 0.4670
K	 1.0000	 0.4460
L	 1.0000	 0.4470
M	 0.9640	 0.3410
N	 1.0000	 0.3580
O	 1.0000	 0.4410
P	 1.0000	 0.4070
Q	 1.0000	 0.4830
R	 1.0000	 0.4110
S	 1.0000	 0.3800
T	 1.0000	 0.4290

