



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:56 AM UTC

PDB ID : 7Y6V / pdb_00007y6v
EMDB ID : EMD-33649
Title : Symmetry-expanded and locally refined protomer structure of IPEC-J2 cell-derived PEDV PT52 S with a CTD-open conformation
Authors : Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on : 2022-06-21
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

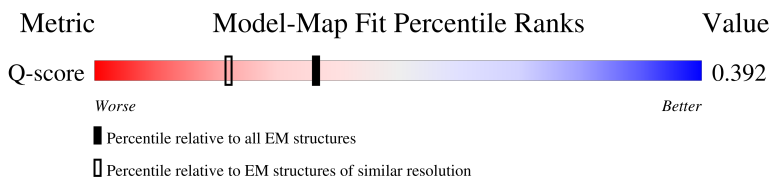
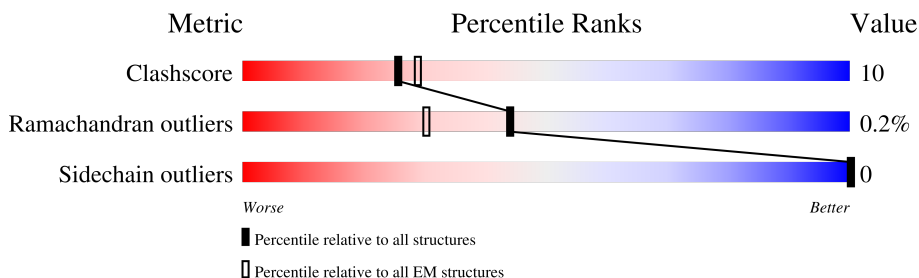
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



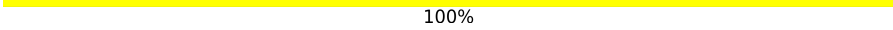
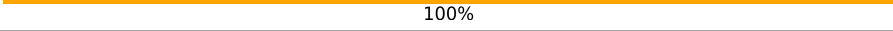
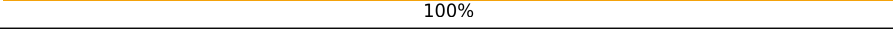
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	1402	 25% 67% 20% 13%
2	B	4	 100%
3	C	5	 20% 80%
4	D	2	 50% 50%

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Mol	Chain	Length	Quality of chain
4	G	2	 50% 50%
5	E	3	 33% 67%
5	H	3	 67% 33%
5	K	3	 67% 33%
5	M	3	 67% 33%
6	F	2	 100%
6	I	2	 50% 50%
6	J	2	 100%
6	L	2	 50% 50%
6	N	2	 100%
7	O	3	 33% 67%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9974 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	1224	Total	C	N	O	S	0	0
			9398	5972	1556	1829	41		

There are 77 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1076	PRO	ILE	conflict	UNP A0A1Y0DD46
A	1077	PRO	LEU	conflict	UNP A0A1Y0DD46
A	1328	GLU	-	expression tag	UNP A0A1Y0DD46
A	1329	PHE	-	expression tag	UNP A0A1Y0DD46
A	1330	GLY	-	expression tag	UNP A0A1Y0DD46
A	1331	SER	-	expression tag	UNP A0A1Y0DD46
A	1332	GLY	-	expression tag	UNP A0A1Y0DD46
A	1333	GLY	-	expression tag	UNP A0A1Y0DD46
A	1334	TYR	-	expression tag	UNP A0A1Y0DD46
A	1335	ILE	-	expression tag	UNP A0A1Y0DD46
A	1336	PRO	-	expression tag	UNP A0A1Y0DD46
A	1337	GLU	-	expression tag	UNP A0A1Y0DD46
A	1338	ALA	-	expression tag	UNP A0A1Y0DD46
A	1339	PRO	-	expression tag	UNP A0A1Y0DD46
A	1340	ARG	-	expression tag	UNP A0A1Y0DD46
A	1341	ASP	-	expression tag	UNP A0A1Y0DD46
A	1342	GLY	-	expression tag	UNP A0A1Y0DD46
A	1343	GLN	-	expression tag	UNP A0A1Y0DD46
A	1344	ALA	-	expression tag	UNP A0A1Y0DD46
A	1345	TYR	-	expression tag	UNP A0A1Y0DD46
A	1346	VAL	-	expression tag	UNP A0A1Y0DD46
A	1347	ARG	-	expression tag	UNP A0A1Y0DD46
A	1348	LYS	-	expression tag	UNP A0A1Y0DD46
A	1349	ASP	-	expression tag	UNP A0A1Y0DD46
A	1350	GLY	-	expression tag	UNP A0A1Y0DD46
A	1351	GLU	-	expression tag	UNP A0A1Y0DD46
A	1352	TRP	-	expression tag	UNP A0A1Y0DD46
A	1353	VAL	-	expression tag	UNP A0A1Y0DD46

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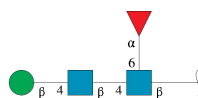
Chain	Residue	Modelled	Actual	Comment	Reference
A	1354	LEU	-	expression tag	UNP A0A1Y0DD46
A	1355	LEU	-	expression tag	UNP A0A1Y0DD46
A	1356	SER	-	expression tag	UNP A0A1Y0DD46
A	1357	THR	-	expression tag	UNP A0A1Y0DD46
A	1358	PHE	-	expression tag	UNP A0A1Y0DD46
A	1359	LEU	-	expression tag	UNP A0A1Y0DD46
A	1360	LYS	-	expression tag	UNP A0A1Y0DD46
A	1361	GLY	-	expression tag	UNP A0A1Y0DD46
A	1362	GLN	-	expression tag	UNP A0A1Y0DD46
A	1363	ASP	-	expression tag	UNP A0A1Y0DD46
A	1364	ASN	-	expression tag	UNP A0A1Y0DD46
A	1365	SER	-	expression tag	UNP A0A1Y0DD46
A	1366	ALA	-	expression tag	UNP A0A1Y0DD46
A	1367	ASP	-	expression tag	UNP A0A1Y0DD46
A	1368	ILE	-	expression tag	UNP A0A1Y0DD46
A	1369	GLN	-	expression tag	UNP A0A1Y0DD46
A	1370	HIS	-	expression tag	UNP A0A1Y0DD46
A	1371	SER	-	expression tag	UNP A0A1Y0DD46
A	1372	GLY	-	expression tag	UNP A0A1Y0DD46
A	1373	ARG	-	expression tag	UNP A0A1Y0DD46
A	1374	PRO	-	expression tag	UNP A0A1Y0DD46
A	1375	LEU	-	expression tag	UNP A0A1Y0DD46
A	1376	GLU	-	expression tag	UNP A0A1Y0DD46
A	1377	SER	-	expression tag	UNP A0A1Y0DD46
A	1378	ARG	-	expression tag	UNP A0A1Y0DD46
A	1379	GLY	-	expression tag	UNP A0A1Y0DD46
A	1380	PRO	-	expression tag	UNP A0A1Y0DD46
A	1381	PHE	-	expression tag	UNP A0A1Y0DD46
A	1382	GLU	-	expression tag	UNP A0A1Y0DD46
A	1383	GLN	-	expression tag	UNP A0A1Y0DD46
A	1384	LYS	-	expression tag	UNP A0A1Y0DD46
A	1385	LEU	-	expression tag	UNP A0A1Y0DD46
A	1386	ILE	-	expression tag	UNP A0A1Y0DD46
A	1387	SER	-	expression tag	UNP A0A1Y0DD46
A	1388	GLU	-	expression tag	UNP A0A1Y0DD46
A	1389	GLU	-	expression tag	UNP A0A1Y0DD46
A	1390	ASP	-	expression tag	UNP A0A1Y0DD46
A	1391	LEU	-	expression tag	UNP A0A1Y0DD46
A	1392	ASN	-	expression tag	UNP A0A1Y0DD46
A	1393	MET	-	expression tag	UNP A0A1Y0DD46
A	1394	HIS	-	expression tag	UNP A0A1Y0DD46
A	1395	THR	-	expression tag	UNP A0A1Y0DD46

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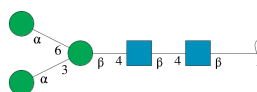
Chain	Residue	Modelled	Actual	Comment	Reference
A	1396	GLY	-	expression tag	UNP A0A1Y0DD46
A	1397	HIS	-	expression tag	UNP A0A1Y0DD46
A	1398	HIS	-	expression tag	UNP A0A1Y0DD46
A	1399	HIS	-	expression tag	UNP A0A1Y0DD46
A	1400	HIS	-	expression tag	UNP A0A1Y0DD46
A	1401	HIS	-	expression tag	UNP A0A1Y0DD46
A	1402	HIS	-	expression tag	UNP A0A1Y0DD46

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	4	Total	C	N	O	0	0
			49	28	2	19		

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



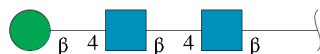
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	5	Total	C	N	O	0	0
			61	34	2	25		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			24	14	1	9		
4	G	2	Total	C	N	O	0	0
			24	14	1	9		

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



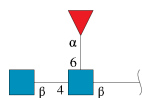
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	H	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		
5	M	3	Total	C	N	O	0	0
			39	22	2	15		

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



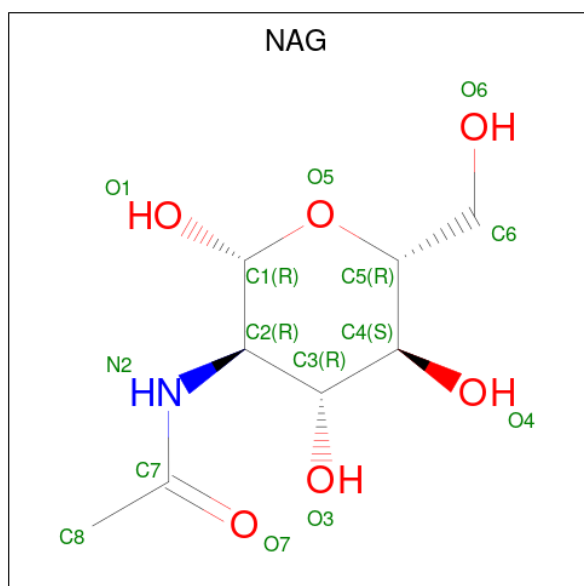
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	L	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	3	Total	C	N	O	0	0
			38	22	2	14		

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

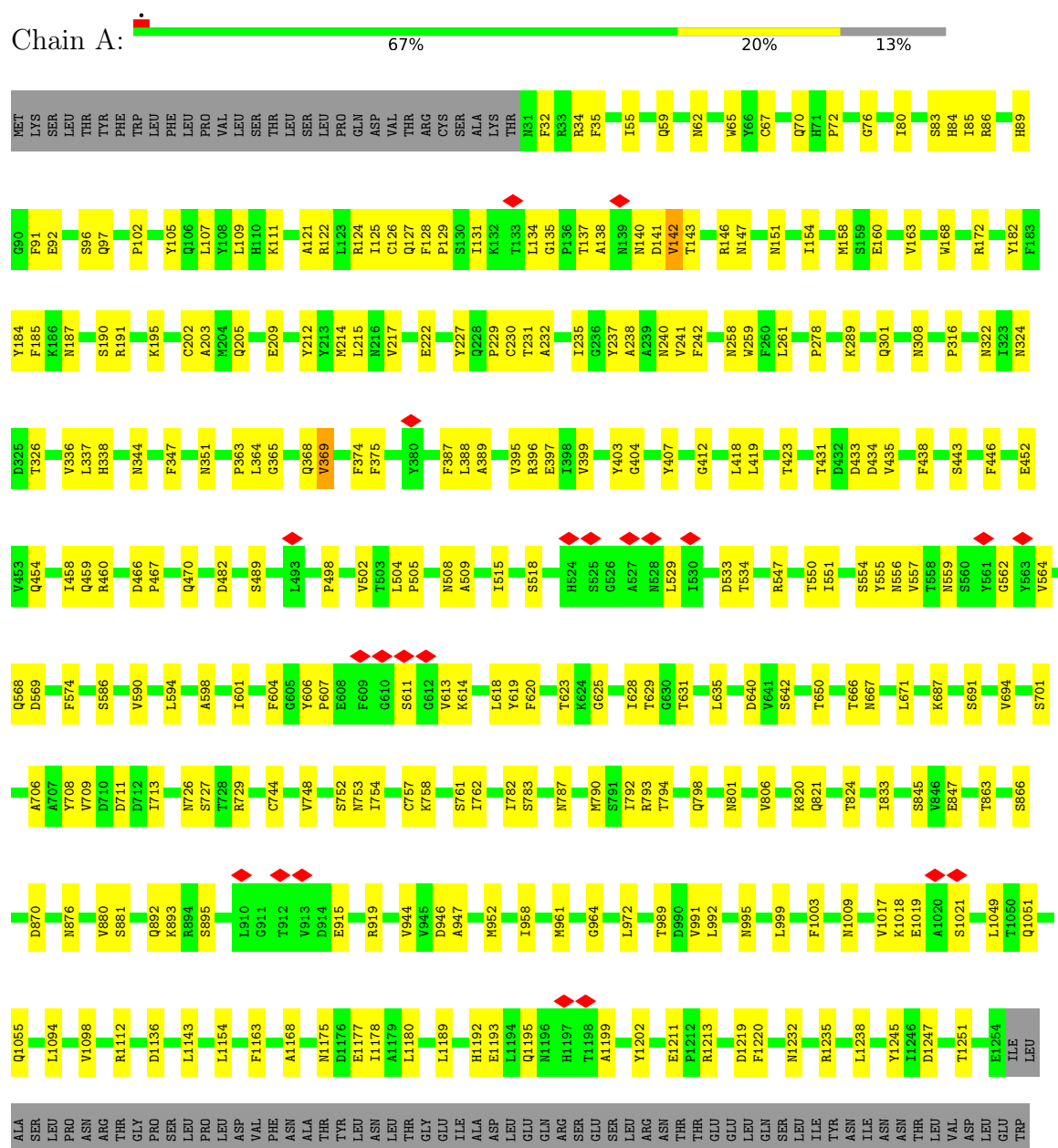


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	

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



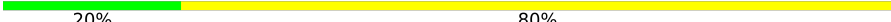
LEU	ASN	ARG	VAL	GLU	THR	TYR	ILE	LYS	PRO	GLU	PHE	GLY	SER	LEU	GLY	GLY	GLY	TYR	ILE	PRO	GLU	ALA	HIS	PRO	ARG	ASP	GLY	GLN	VAL	TYR	ARG	LYS	ASP	GLY	GLY	TRP	VAL	LEU	LEU	SER	THR	PHE	LEU	LYS	GLY	GLN	ASP	ASN	SER	ALA	ASP	ILE	HIS	HIS	SER	GLY	ARG	PRO	LEU	GLU
SER	ARG	GLY	PRO	PHE	GLU	GLN	LYS	LEU	ILE	SER	PRO	GLU	GLY	ASP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

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

Chain B:  25% 100%



- Molecule 3: 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 C:  20% 80%



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

Chain D:  50% 50%

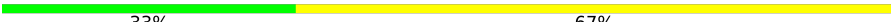


- Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%



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

Chain E:  33% 67%

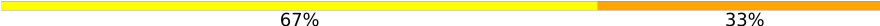


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%



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

Chain K:  67% 33%

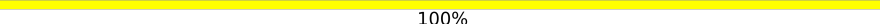
MAG1
MAG2
BMA3

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

Chain M:  67% 33%

MAG1
MAG2
BMA3

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

Chain F:  100%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  33% 67%

MAG1
MAG2
FUC3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	124142, 124142, 124142, 124142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.358	Depositor
Minimum map value	-0.437	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	385.83997, 385.83997, 385.83997	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	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: FUC, BMA, MAN, 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	A	0.14	0/9610	0.35	0/13097

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	A	9398	0	9082	190	0
2	B	49	0	43	0	0
3	C	61	0	52	1	0
4	D	24	0	22	1	0
4	G	24	0	22	6	0
5	E	39	0	34	1	0
5	H	39	0	34	1	0
5	K	39	0	34	4	0
5	M	39	0	34	0	0
6	F	28	0	25	1	0
6	I	28	0	25	1	0
6	J	28	0	25	3	0
6	L	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	28	0	25	2	0
7	O	38	0	34	2	0
8	A	84	0	78	3	0
All	All	9974	0	9594	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (201) 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:518:SER:HA	1:A:556:ASN:HB2	1.44	0.97
1:A:1177:GLU:HG3	1:A:1178:ILE:HD12	1.53	0.88
1:A:364:LEU:HB2	4:G:1:NAG:H61	1.62	0.79
1:A:137:THR:O	1:A:140:ASN:ND2	2.18	0.77
1:A:729:ARG:HH22	6:L:1:NAG:H62	1.51	0.75
1:A:134:LEU:HD21	1:A:195:LYS:HD2	1.67	0.75
1:A:142:VAL:HG13	1:A:146:ARG:HE	1.52	0.73
1:A:337:LEU:HB3	1:A:419:LEU:HD11	1.72	0.72
1:A:126:CYS:HB2	1:A:128:PHE:HB2	1.71	0.72
1:A:404:GLY:HA2	1:A:419:LEU:HD23	1.73	0.71
1:A:564:VAL:HG22	1:A:607:PRO:HA	1.72	0.70
1:A:92:GLU:HB2	1:A:195:LYS:HB3	1.74	0.70
1:A:642:SER:HB2	5:K:1:NAG:H81	1.73	0.70
1:A:231:THR:HG22	1:A:232:ALA:H	1.56	0.70
1:A:363:PRO:HG2	4:G:1:NAG:H5	1.74	0.69
1:A:529:LEU:HD11	1:A:613:VAL:HG11	1.75	0.69
1:A:59:GLN:HG3	1:A:229:PRO:HG3	1.73	0.69
1:A:102:PRO:O	1:A:146:ARG:NH2	2.26	0.68
1:A:1189:LEU:HD11	1:A:1202:TYR:HB3	1.76	0.67
1:A:726:ASN:OD1	1:A:727:SER:N	2.29	0.65
1:A:96:SER:O	1:A:191:ARG:HB3	1.97	0.64
1:A:509:ALA:H	1:A:547:ARG:HH22	1.43	0.64
1:A:83:SER:OG	1:A:202:CYS:O	2.15	0.64
1:A:240:ASN:ND2	1:A:438:PHE:O	2.25	0.63
1:A:289:LYS:HB2	1:A:435:VAL:H	1.64	0.62
1:A:1213:ARG:NH2	1:A:1219:ASP:OD2	2.33	0.62
1:A:326:THR:HG22	1:A:395:VAL:H	1.64	0.62
1:A:375:PHE:CE2	1:A:388:LEU:HD12	2.36	0.61
6:J:1:NAG:H82	6:J:2:NAG:H83	1.83	0.61
1:A:821:GLN:O	1:A:824:THR:OG1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ASP:O	1:A:470:GLN:N	2.31	0.60
1:A:351:ASN:OD1	4:G:1:NAG:N2	2.34	0.60
1:A:322:ASN:ND2	1:A:397:GLU:OE2	2.34	0.60
1:A:790:MET:HB2	1:A:999:LEU:HD22	1.83	0.60
1:A:794:THR:HG22	1:A:1154:LEU:HD22	1.84	0.60
1:A:798:GLN:NE2	1:A:801:ASN:OD1	2.36	0.59
1:A:1195:GLN:HB2	1:A:1199:ALA:HB3	1.83	0.59
1:A:847:GLU:OE1	1:A:1112:ARG:NH1	2.36	0.59
1:A:127:GLN:OE1	1:A:146:ARG:NH1	2.38	0.57
1:A:744:CYS:SG	1:A:757:CYS:N	2.77	0.57
1:A:833:ILE:HG23	1:A:1098:VAL:HG21	1.85	0.57
1:A:316:PRO:HB3	1:A:443:SER:OG	2.05	0.57
1:A:127:GLN:HB2	1:A:147:ASN:HB3	1.86	0.57
1:A:964:GLY:HA3	1:A:972:LEU:HD13	1.86	0.57
1:A:508:ASN:ND2	1:A:635:LEU:O	2.27	0.57
1:A:482:ASP:HA	1:A:708:TYR:O	2.04	0.56
1:A:569:ASP:HB2	1:A:604:PHE:HE1	1.70	0.56
1:A:55:ILE:H	1:A:205:GLN:HE22	1.52	0.56
1:A:787:ASN:OD1	8:A:1505:NAG:N2	2.38	0.56
1:A:215:LEU:HB3	1:A:217:VAL:HG23	1.88	0.56
1:A:433:ASP:HB2	5:E:2:NAG:HN2	1.70	0.56
6:N:1:NAG:H83	6:N:1:NAG:H3	1.86	0.56
6:J:1:NAG:H3	6:J:1:NAG:H83	1.88	0.56
5:K:1:NAG:H83	5:K:1:NAG:H3	1.88	0.56
1:A:958:ILE:HA	1:A:961:MET:HE3	1.87	0.55
6:N:2:NAG:H3	6:N:2:NAG:H83	1.87	0.55
1:A:258:ASN:HB2	1:A:322:ASN:HD21	1.72	0.55
1:A:1192:HIS:CG	1:A:1193:GLU:H	2.23	0.55
1:A:793:ARG:NH1	1:A:1136:ASP:O	2.39	0.55
1:A:586:SER:HB3	1:A:625:GLY:HA3	1.89	0.55
1:A:754:ILE:HD12	1:A:762:ILE:HD11	1.88	0.55
1:A:498:PRO:O	1:A:650:THR:OG1	2.21	0.54
1:A:586:SER:N	1:A:623:THR:O	2.35	0.54
1:A:1051:GLN:NE2	1:A:1055:GLN:OE1	2.40	0.54
1:A:518:SER:HA	1:A:556:ASN:CB	2.30	0.54
1:A:65:TRP:HB3	1:A:202:CYS:HA	1.90	0.54
1:A:301:GLN:NE2	4:D:1:NAG:O7	2.39	0.53
1:A:482:ASP:HB3	1:A:709:VAL:HG12	1.88	0.53
1:A:322:ASN:HA	1:A:397:GLU:HG2	1.90	0.53
1:A:870:ASP:N	1:A:870:ASP:OD1	2.42	0.53
1:A:242:PHE:O	1:A:308:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LEU:O	1:A:687:LYS:NZ	2.41	0.53
1:A:238:ALA:HB3	1:A:241:VAL:HG22	1.91	0.53
7:O:1:NAG:H4	7:O:3:FUC:H5	1.90	0.52
1:A:184:TYR:CE2	5:H:1:NAG:H3	2.45	0.52
1:A:32:PHE:HB2	1:A:227:TYR:CZ	2.46	0.51
1:A:568:GLN:NE2	1:A:569:ASP:O	2.43	0.51
1:A:946:ASP:OD1	1:A:947:ALA:N	2.42	0.51
1:A:172:ARG:NH1	1:A:182:TYR:OH	2.34	0.51
1:A:185:PHE:O	1:A:187:ASN:ND2	2.44	0.51
1:A:278:PRO:HA	1:A:446:PHE:HA	1.92	0.50
1:A:554:SER:HB3	6:I:1:NAG:H83	1.93	0.50
1:A:128:PHE:CD1	1:A:129:PRO:HD2	2.47	0.50
1:A:324:ASN:O	1:A:396:ARG:NE	2.41	0.50
1:A:214:MET:HE1	1:A:237:TYR:CG	2.47	0.50
1:A:598:ALA:HB1	1:A:619:TYR:HB3	1.93	0.50
1:A:666:THR:HG23	1:A:694:VAL:HG23	1.92	0.50
1:A:121:ALA:N	1:A:154:ILE:O	2.45	0.50
1:A:76:GLY:H	1:A:190:SER:HB2	1.76	0.49
1:A:881:SER:HA	1:A:892:GLN:HA	1.94	0.49
1:A:129:PRO:HA	1:A:141:ASP:O	2.12	0.49
4:G:1:NAG:O4	4:G:2:FUC:O5	2.22	0.49
1:A:706:ALA:HB1	1:A:713:ILE:HD12	1.94	0.49
1:A:547:ARG:O	1:A:629:THR:N	2.39	0.49
1:A:667:ASN:HB2	8:A:1504:NAG:N2	2.28	0.49
1:A:138:ALA:O	1:A:140:ASN:ND2	2.46	0.49
1:A:1192:HIS:CG	1:A:1193:GLU:N	2.81	0.49
1:A:454:GLN:NE2	1:A:459:GLN:OE1	2.45	0.49
1:A:783:SER:HB3	1:A:1163:PHE:HB3	1.95	0.48
3:C:1:NAG:O6	3:C:2:NAG:N2	2.45	0.48
1:A:67:CYS:HA	1:A:203:ALA:HB3	1.95	0.48
1:A:782:ILE:HD12	1:A:1168:ALA:HB2	1.96	0.48
1:A:992:LEU:HB2	1:A:995:ASN:HB2	1.95	0.48
1:A:431:THR:HA	1:A:434:ASP:OD2	2.14	0.48
1:A:1143:LEU:HD11	1:A:1154:LEU:HD12	1.95	0.48
1:A:129:PRO:HB3	1:A:140:ASN:CG	2.38	0.48
1:A:559:ASN:HB3	1:A:562:GLY:O	2.14	0.48
1:A:35:PHE:HB2	1:A:163:VAL:HB	1.96	0.47
1:A:618:LEU:HD21	1:A:620:PHE:CE1	2.49	0.47
1:A:231:THR:HG22	1:A:232:ALA:N	2.27	0.47
1:A:124:ARG:HD2	1:A:128:PHE:CE1	2.50	0.47
1:A:86:ARG:HB3	1:A:89:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD13	1:A:125:ILE:HG12	1.97	0.47
1:A:261:LEU:HB3	1:A:458:ILE:HD11	1.97	0.47
1:A:598:ALA:HA	1:A:620:PHE:O	2.14	0.47
6:J:1:NAG:H5	6:J:2:NAG:C7	2.45	0.47
1:A:752:SER:OG	1:A:753:ASN:N	2.38	0.47
1:A:131:ILE:HG12	1:A:138:ALA:HB3	1.96	0.46
1:A:792:ILE:HD11	1:A:1003:PHE:CD1	2.51	0.46
1:A:989:THR:HG23	1:A:1211:GLU:HB3	1.97	0.46
1:A:508:ASN:HA	1:A:547:ARG:HH12	1.81	0.46
6:F:1:NAG:H62	6:F:2:NAG:HN2	1.80	0.46
1:A:407:TYR:CD1	1:A:412:GLY:HA2	2.51	0.46
1:A:845:SER:HA	1:A:944:VAL:HG11	1.97	0.46
1:A:820:LYS:O	1:A:824:THR:HG23	2.16	0.46
1:A:1192:HIS:O	1:A:1193:GLU:HG2	2.15	0.46
1:A:34:ARG:NE	1:A:222:GLU:OE2	2.49	0.45
1:A:84:HIS:CE1	1:A:86:ARG:HD2	2.51	0.45
1:A:559:ASN:HB2	1:A:564:VAL:HG23	1.97	0.45
5:K:2:NAG:H4	5:K:3:BMA:H2	1.60	0.45
1:A:1238:LEU:HD22	1:A:1245:TYR:CD2	2.51	0.45
1:A:70:GLN:HG3	1:A:72:PRO:HD3	1.98	0.45
1:A:991:VAL:HG13	1:A:991:VAL:O	2.16	0.45
1:A:55:ILE:H	1:A:205:GLN:NE2	2.15	0.45
1:A:212:TYR:CD2	1:A:235:ILE:HD11	2.52	0.45
1:A:607:PRO:HG2	1:A:611:SER:H	1.82	0.45
1:A:502:VAL:HA	1:A:642:SER:HB3	1.99	0.45
1:A:363:PRO:HG2	4:G:1:NAG:C5	2.47	0.44
1:A:1232:ASN:OD1	7:O:1:NAG:N2	2.50	0.44
1:A:336:VAL:HB	1:A:423:THR:OG1	2.18	0.44
1:A:399:VAL:CG1	1:A:407:TYR:HB2	2.47	0.44
1:A:504:LEU:HD12	1:A:505:PRO:HD2	2.00	0.44
1:A:604:PHE:CZ	1:A:614:LYS:HE2	2.52	0.44
1:A:326:THR:CG2	1:A:395:VAL:H	2.29	0.44
1:A:467:PRO:HA	1:A:470:GLN:HB2	1.98	0.44
1:A:1180:LEU:HG	1:A:1220:PHE:HB3	1.99	0.44
1:A:863:THR:HG23	1:A:866:SER:H	1.83	0.44
1:A:55:ILE:HG12	1:A:205:GLN:NE2	2.33	0.44
1:A:489:SER:HB2	1:A:701:SER:HB2	1.99	0.44
1:A:590:VAL:HG13	1:A:620:PHE:HE1	1.83	0.44
1:A:915:GLU:OE1	1:A:919:ARG:NH2	2.49	0.44
1:A:1019:GLU:C	1:A:1021:SER:H	2.25	0.44
1:A:1009:ASN:OD1	8:A:1506:NAG:N2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:HE1	1:A:388:LEU:HD13	1.82	0.43
1:A:1247:ASP:O	1:A:1251:THR:HG23	2.18	0.43
1:A:135:GLY:HA3	1:A:138:ALA:HB2	2.00	0.43
1:A:97:GLN:NE2	1:A:105:TYR:O	2.51	0.43
1:A:564:VAL:HG13	1:A:606:TYR:C	2.43	0.43
1:A:880:VAL:O	1:A:893:LYS:N	2.51	0.43
1:A:363:PRO:HB2	4:G:2:FUC:H3	2.01	0.43
1:A:452:GLU:HB3	1:A:460:ARG:HG2	2.00	0.43
1:A:594:LEU:HA	1:A:619:TYR:CE2	2.54	0.43
1:A:748:VAL:HG21	1:A:758:LYS:HB3	2.01	0.43
1:A:1175:ASN:CG	1:A:1235:ARG:HG2	2.44	0.43
1:A:129:PRO:HD3	1:A:143:THR:O	2.18	0.43
1:A:368:GLN:O	1:A:369:VAL:HG12	2.19	0.43
1:A:550:THR:OG1	1:A:631:THR:O	2.35	0.43
1:A:876:ASN:O	1:A:895:SER:OG	2.36	0.43
1:A:515:ILE:HG13	1:A:551:ILE:HD11	2.01	0.42
1:A:691:SER:HB3	5:K:1:NAG:H62	2.00	0.42
1:A:91:PHE:HB3	1:A:111:LYS:HG3	2.02	0.42
1:A:338:HIS:ND1	1:A:344:ASN:OD1	2.41	0.42
1:A:374:PHE:CE1	1:A:387:PHE:HD1	2.38	0.42
1:A:547:ARG:HA	1:A:628:ILE:HA	2.02	0.42
1:A:80:ILE:HG23	1:A:168:TRP:HH2	1.84	0.42
1:A:91:PHE:HE2	1:A:109:LEU:HD23	1.84	0.42
1:A:403:TYR:HA	1:A:418:LEU:HD23	2.02	0.42
1:A:557:VAL:HG11	1:A:564:VAL:HG11	2.02	0.42
1:A:388:LEU:HD23	1:A:389:ALA:HB3	2.01	0.42
1:A:952:MET:HE2	1:A:952:MET:HB2	1.92	0.42
1:A:55:ILE:HB	1:A:62:ASN:ND2	2.35	0.41
1:A:209:GLU:OE1	1:A:209:GLU:N	2.54	0.41
1:A:555:TYR:HD1	1:A:555:TYR:HA	1.79	0.41
1:A:122:ARG:HH12	1:A:151:ASN:C	2.25	0.41
1:A:86:ARG:HA	1:A:160:GLU:OE1	2.21	0.41
1:A:128:PHE:CG	1:A:129:PRO:HD2	2.55	0.41
1:A:214:MET:HB2	1:A:230:CYS:SG	2.60	0.41
1:A:744:CYS:HB2	1:A:761:SER:C	2.46	0.41
1:A:1049:LEU:HD23	1:A:1049:LEU:HA	1.87	0.41
1:A:85:ILE:HG13	1:A:158:MET:SD	2.61	0.41
1:A:958:ILE:O	1:A:961:MET:HG2	2.20	0.41
1:A:259:TRP:O	1:A:458:ILE:HD12	2.20	0.41
1:A:708:TYR:CZ	1:A:711:ASP:HA	2.56	0.41
1:A:86:ARG:HB3	1:A:89:HIS:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:ASP:OD1	1:A:534:THR:N	2.54	0.41
1:A:574:PHE:HE1	1:A:620:PHE:HD2	1.68	0.41
1:A:1017:VAL:O	1:A:1018:LYS:HG3	2.20	0.41
1:A:806:VAL:HG11	1:A:1094:LEU:HD11	2.02	0.40
1:A:365:GLY:O	1:A:368:GLN:NE2	2.41	0.40
1:A:124:ARG:HD2	1:A:128:PHE:HE1	1.86	0.40
1:A:569:ASP:O	1:A:601:ILE:HG23	2.22	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	A	1222/1402 (87%)	1149 (94%)	70 (6%)	3 (0%)	43 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	VAL
1	A	369	VAL
1	A	640	ASP

5.3.2 Protein sidechains [i](#)

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	1049/1209 (87%)	1049 (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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	258	ASN
1	A	415	HIS
1	A	454	GLN
1	A	459	GLN
1	A	577	GLN
1	A	705	GLN
1	A	768	GLN
1	A	798	GLN
1	A	814	ASN
1	A	988	GLN
1	A	1145	GLN

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 ⓘ

38 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
2	NAG	B	1	2,1	14,14,15	0.32	0	17,19,21	0.57	0
2	NAG	B	2	2	14,14,15	0.26	0	17,19,21	0.43	0
2	BMA	B	3	2	11,11,12	0.54	0	15,15,17	0.73	0
2	FUC	B	4	2	10,10,11	0.53	0	14,14,16	0.75	0
3	NAG	C	1	1,3	14,14,15	0.30	0	17,19,21	0.43	0
3	NAG	C	2	3	14,14,15	0.26	0	17,19,21	0.44	0
3	BMA	C	3	3	11,11,12	0.72	0	15,15,17	0.95	0
3	MAN	C	4	3	11,11,12	0.75	0	15,15,17	0.98	1 (6%)
3	MAN	C	5	3	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
4	NAG	D	1	4,1	14,14,15	0.18	0	17,19,21	0.47	0
4	FUC	D	2	4	10,10,11	0.84	0	14,14,16	0.90	0
5	NAG	E	1	5,1	14,14,15	0.42	0	17,19,21	0.41	0
5	NAG	E	2	5	14,14,15	0.16	0	17,19,21	0.50	0
5	BMA	E	3	5	11,11,12	0.66	0	15,15,17	1.32	2 (13%)
6	NAG	F	1	6,1	14,14,15	0.21	0	17,19,21	0.47	0
6	NAG	F	2	6	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	G	1	4,1	14,14,15	0.85	2 (14%)	17,19,21	0.78	1 (5%)
4	FUC	G	2	4	10,10,11	0.64	0	14,14,16	0.90	0
5	NAG	H	1	5,1	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	H	2	5	14,14,15	0.17	0	17,19,21	0.42	0
5	BMA	H	3	5	11,11,12	0.56	0	15,15,17	0.75	0
6	NAG	I	1	6,1	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	I	2	6	14,14,15	0.24	0	17,19,21	0.40	0
6	NAG	J	1	6,1	14,14,15	0.66	1 (7%)	17,19,21	1.75	3 (17%)
6	NAG	J	2	6	14,14,15	0.47	0	17,19,21	0.67	1 (5%)
5	NAG	K	1	5,1	14,14,15	0.47	0	17,19,21	1.36	2 (11%)
5	NAG	K	2	5	14,14,15	0.28	0	17,19,21	0.59	0
5	BMA	K	3	5	11,11,12	0.66	0	15,15,17	0.68	0
6	NAG	L	1	6,1	14,14,15	0.52	0	17,19,21	0.76	0
6	NAG	L	2	6	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	M	1	5,1	14,14,15	0.50	0	17,19,21	0.69	0
5	NAG	M	2	5	14,14,15	0.26	0	17,19,21	0.53	0
5	BMA	M	3	5	11,11,12	0.97	0	15,15,17	0.98	1 (6%)
6	NAG	N	1	6,1	14,14,15	0.73	1 (7%)	17,19,21	1.46	2 (11%)
6	NAG	N	2	6	14,14,15	0.45	0	17,19,21	1.29	2 (11%)
7	NAG	O	1	7,1	14,14,15	0.38	0	17,19,21	0.60	0
7	NAG	O	2	7	14,14,15	0.24	0	17,19,21	0.49	0
7	FUC	O	3	7	10,10,11	0.65	0	14,14,16	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	FUC	B	4	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1
5	NAG	E	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	1/2/19/22	0/1/1/1
6	NAG	F	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	6,1	-	6/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	6/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
6	NAG	L	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,1	-	6/6/23/26	0/1/1/1
6	NAG	N	2	6	-	5/6/23/26	0/1/1/1
7	NAG	O	1	7,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	O	2	7	-	4/6/23/26	0/1/1/1
7	FUC	O	3	7	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	1	NAG	O5-C1	-2.54	1.39	1.43
4	G	1	NAG	O5-C1	2.24	1.47	1.43
4	G	1	NAG	C1-C2	2.12	1.55	1.52
6	J	1	NAG	O5-C1	-2.10	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1	NAG	C2-N2-C7	4.91	129.47	122.90
6	N	1	NAG	C2-N2-C7	4.65	129.13	122.90
5	K	1	NAG	C2-N2-C7	4.57	129.03	122.90
6	N	2	NAG	C2-N2-C7	4.49	128.92	122.90
5	E	3	BMA	C1-O5-C5	3.19	116.46	112.19
6	J	1	NAG	C1-C2-N2	2.83	114.89	110.43
3	C	5	MAN	C1-O5-C5	2.47	115.50	112.19
4	G	1	NAG	C1-O5-C5	2.43	115.45	112.19
6	J	1	NAG	C3-C4-C5	2.42	114.63	110.23
5	K	1	NAG	C1-C2-N2	2.33	114.10	110.43
5	M	3	BMA	C2-C3-C4	2.28	114.88	110.86
3	C	4	MAN	O2-C2-C3	-2.26	105.47	110.15
6	N	1	NAG	C1-C2-N2	2.23	113.95	110.43
3	C	5	MAN	O2-C2-C3	-2.16	105.69	110.15
5	E	3	BMA	C1-C2-C3	2.16	112.78	109.64
6	J	2	NAG	C1-O5-C5	2.06	114.95	112.19
6	N	2	NAG	C1-C2-N2	2.02	113.61	110.43

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	1	NAG	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	M	1	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
6	F	2	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C4-C5-C6-O6
6	N	1	NAG	C1-C2-N2-C7
5	E	2	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7
5	M	1	NAG	C3-C2-N2-C7
6	I	1	NAG	C3-C2-N2-C7
6	J	2	NAG	C3-C2-N2-C7
6	L	1	NAG	C3-C2-N2-C7
7	O	1	NAG	C3-C2-N2-C7
5	K	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7
5	K	1	NAG	C1-C2-N2-C7
5	M	1	NAG	C1-C2-N2-C7
6	I	1	NAG	C1-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
6	J	2	NAG	C1-C2-N2-C7
6	L	1	NAG	C1-C2-N2-C7
6	N	2	NAG	C1-C2-N2-C7
7	O	1	NAG	C1-C2-N2-C7
3	C	3	BMA	C4-C5-C6-O6
5	K	1	NAG	C3-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7
6	N	1	NAG	C3-C2-N2-C7
6	N	2	NAG	C3-C2-N2-C7
5	K	1	NAG	O5-C5-C6-O6

There are no ring outliers.

20 monomers are involved in 24 short contacts:

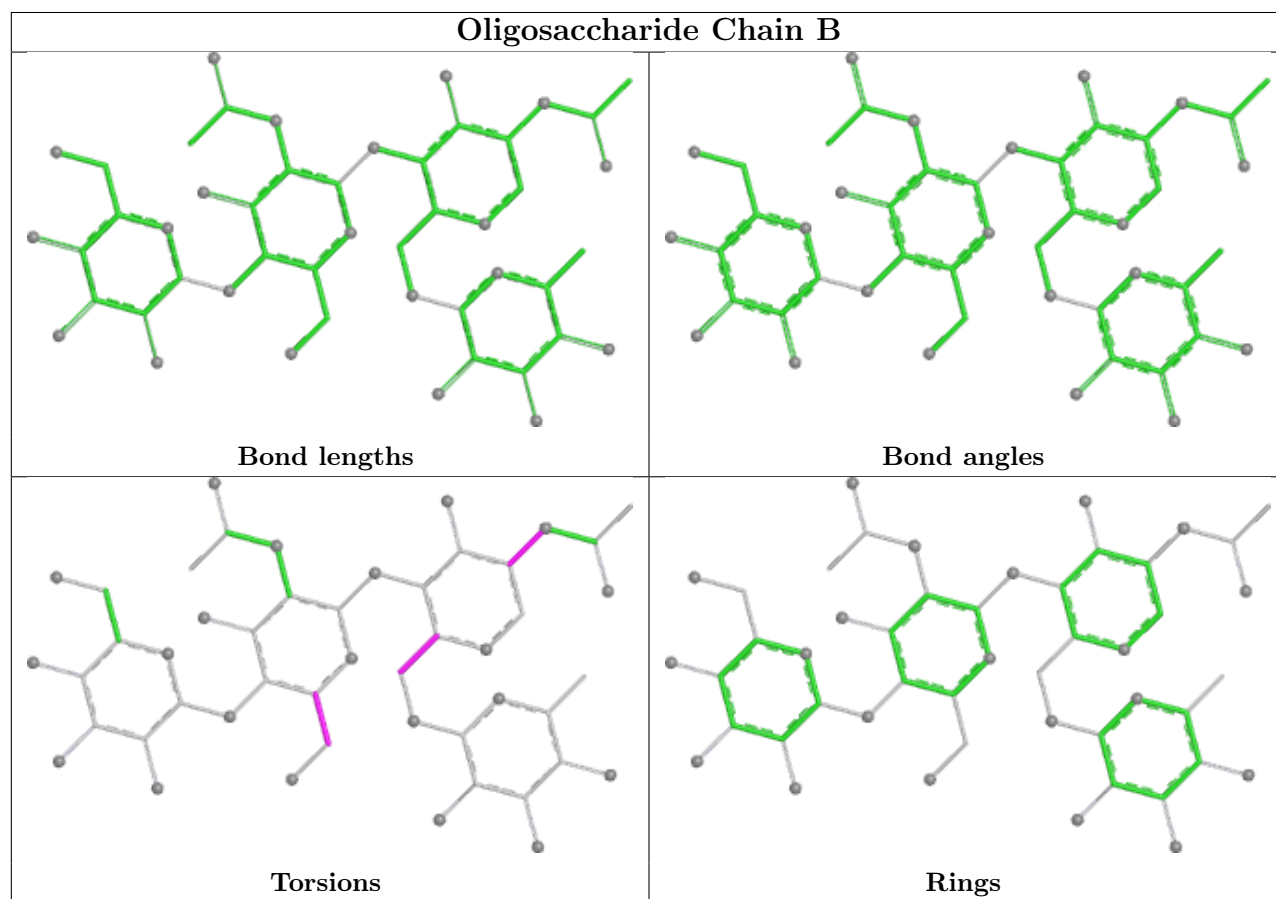
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	2	NAG	1	0
3	C	2	NAG	1	0
6	J	1	NAG	3	0
6	J	2	NAG	2	0
6	F	2	NAG	1	0
6	N	2	NAG	1	0
3	C	1	NAG	1	0

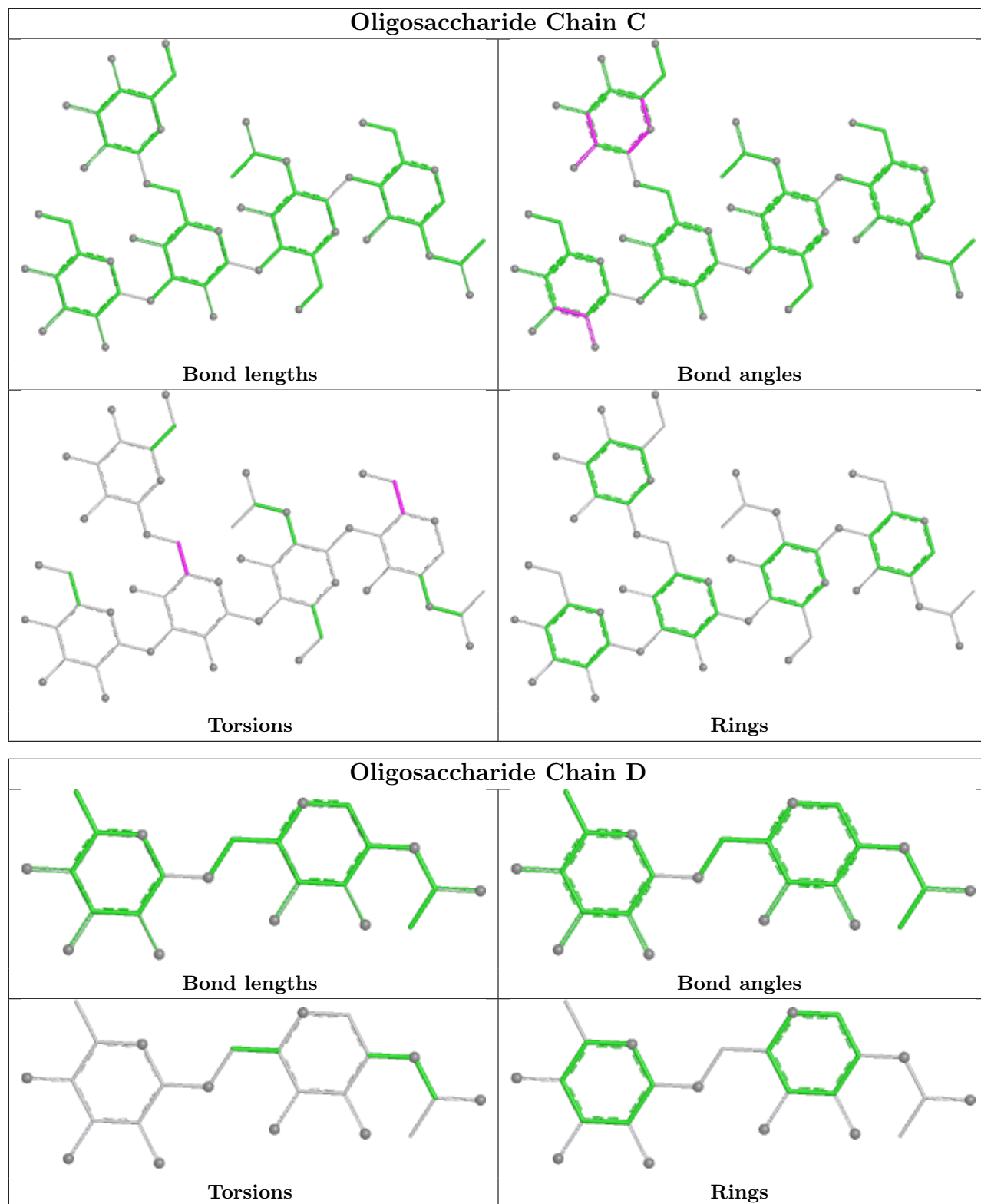
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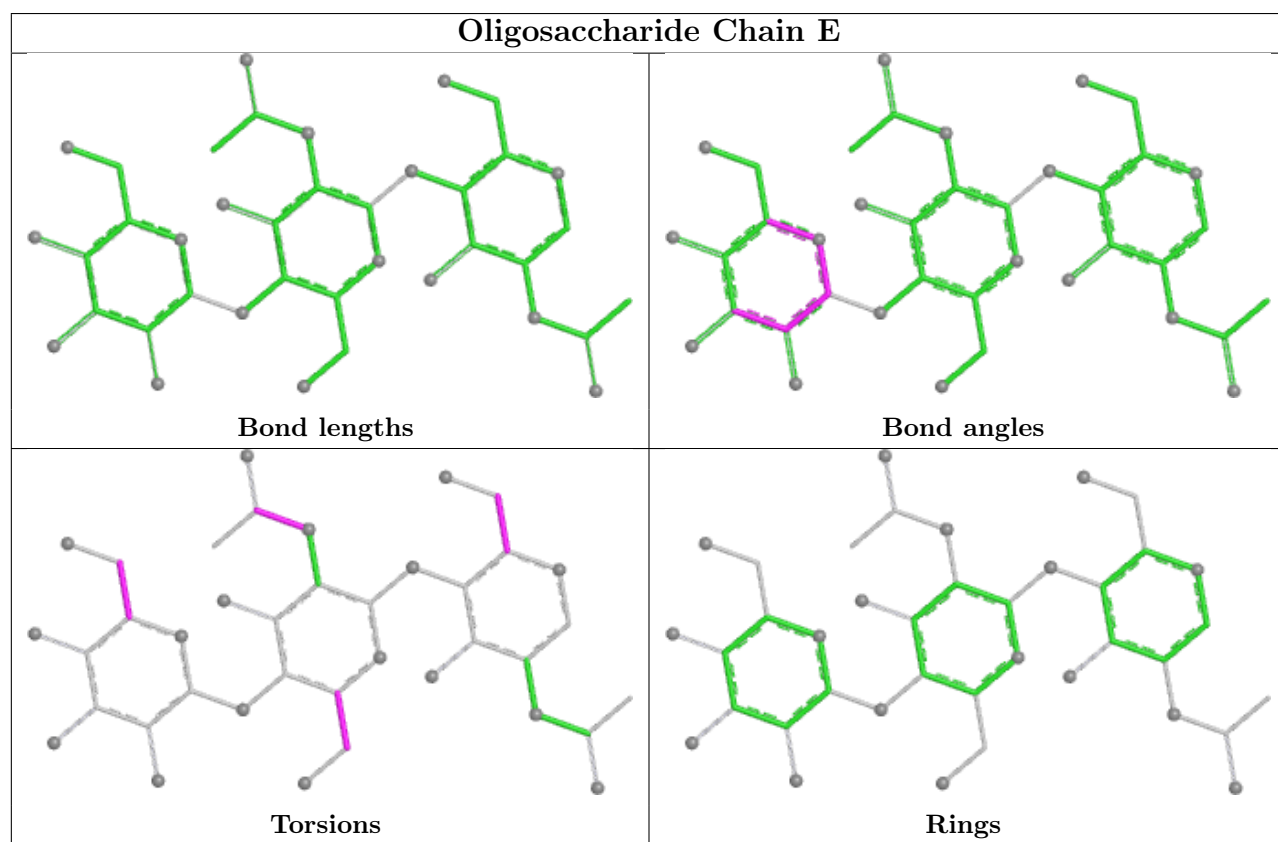
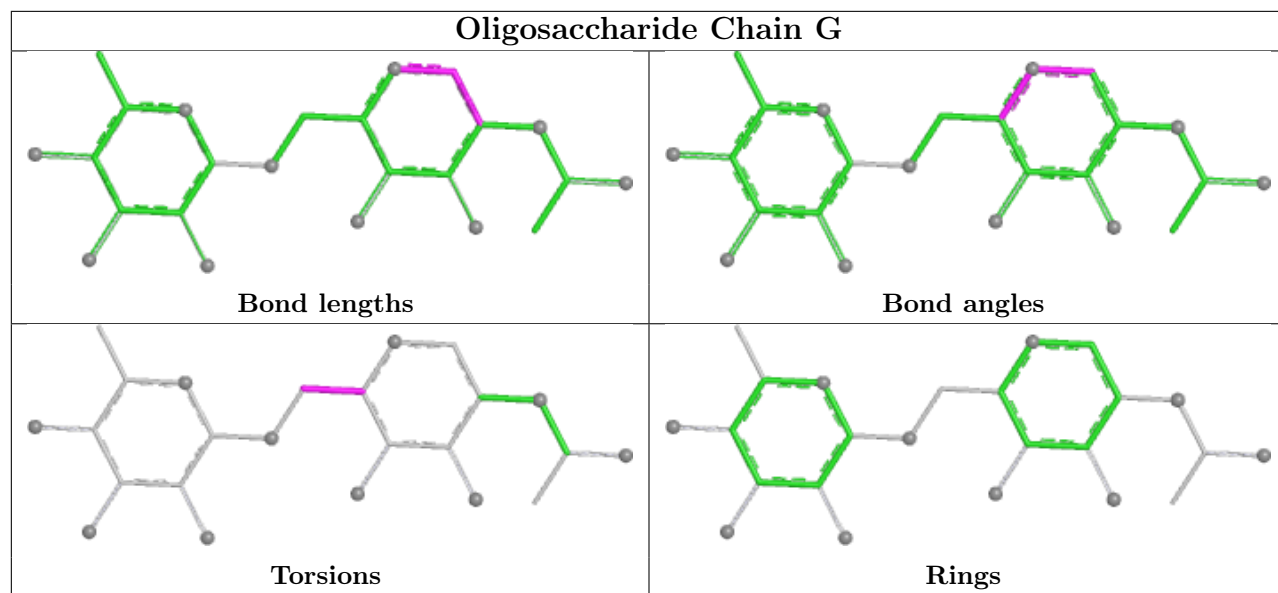
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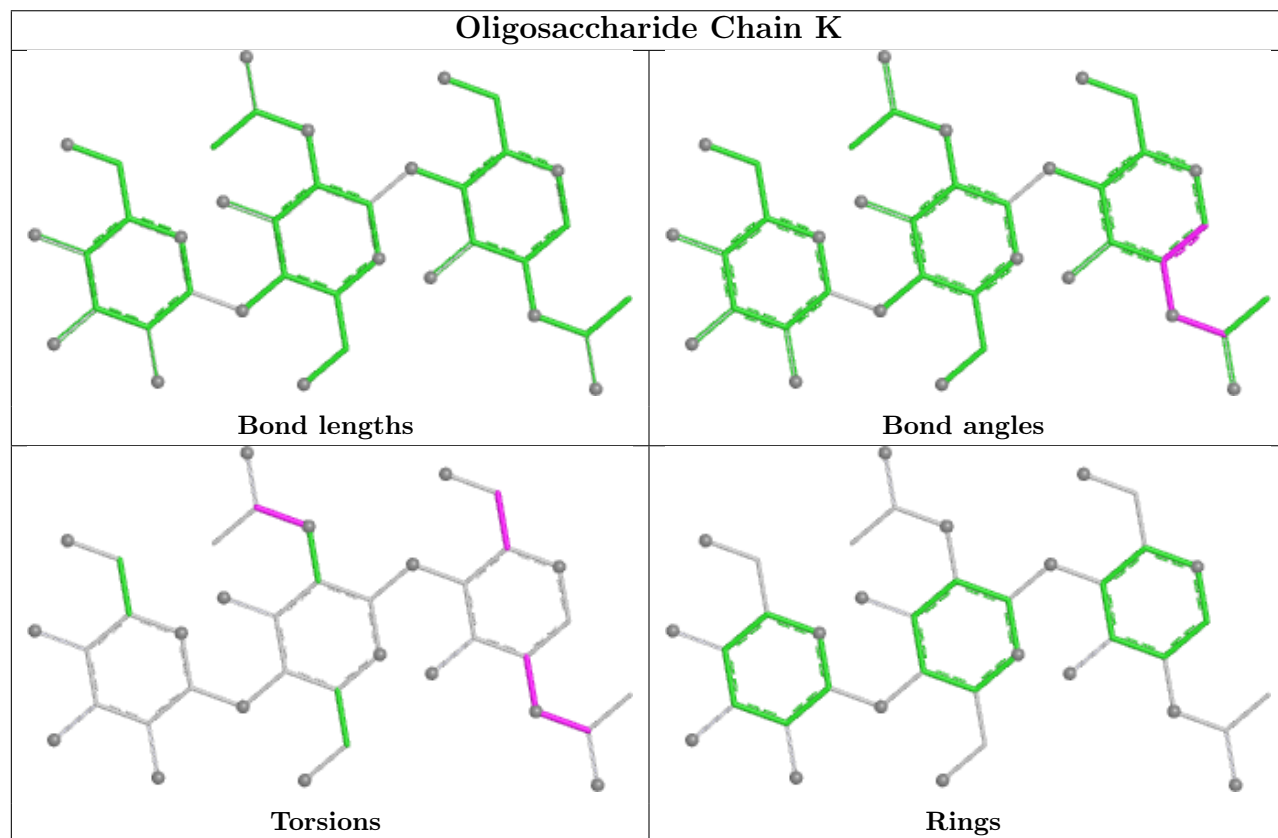
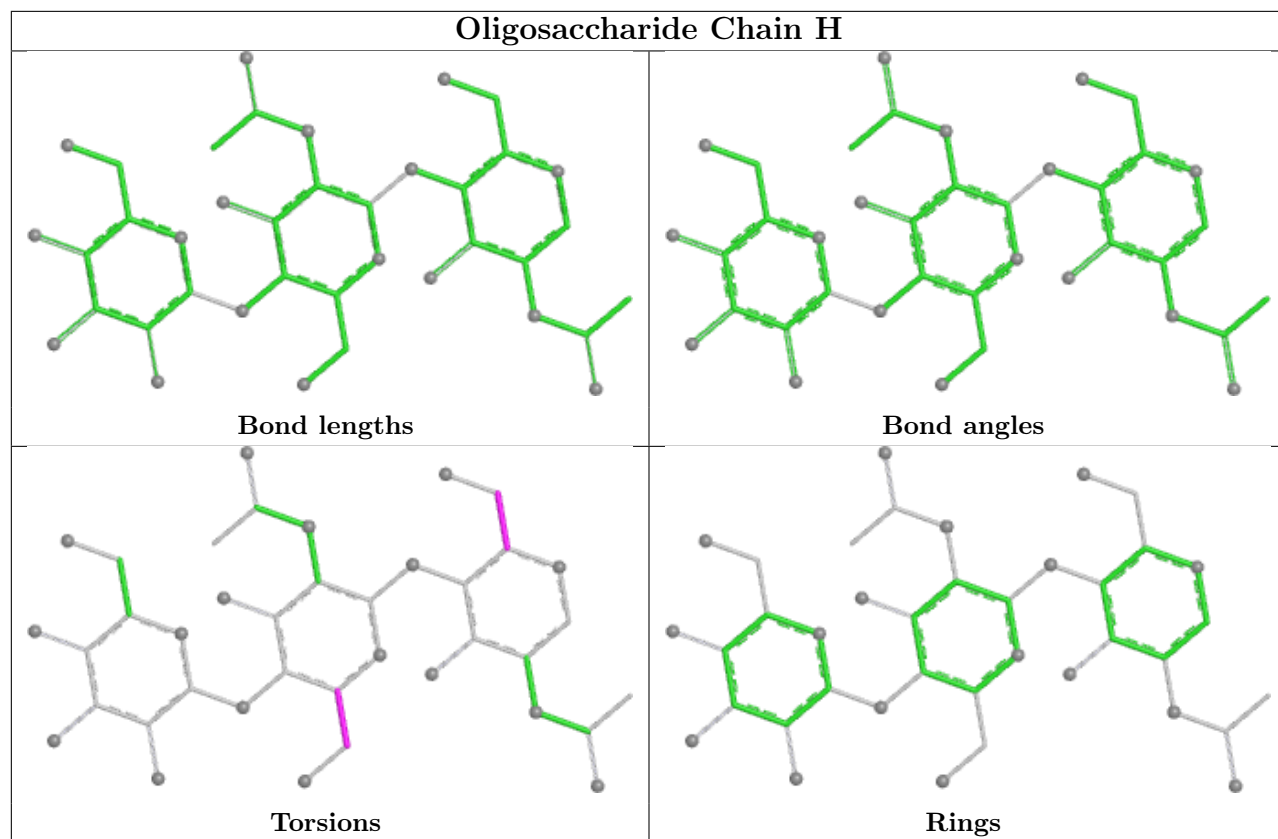
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	1	0
4	D	1	NAG	1	0
7	O	3	FUC	1	0
5	K	1	NAG	3	0
5	H	1	NAG	1	0
6	F	1	NAG	1	0
5	E	2	NAG	1	0
5	K	3	BMA	1	0
7	O	1	NAG	2	0
4	G	2	FUC	2	0
6	L	1	NAG	1	0
4	G	1	NAG	5	0
6	N	1	NAG	1	0

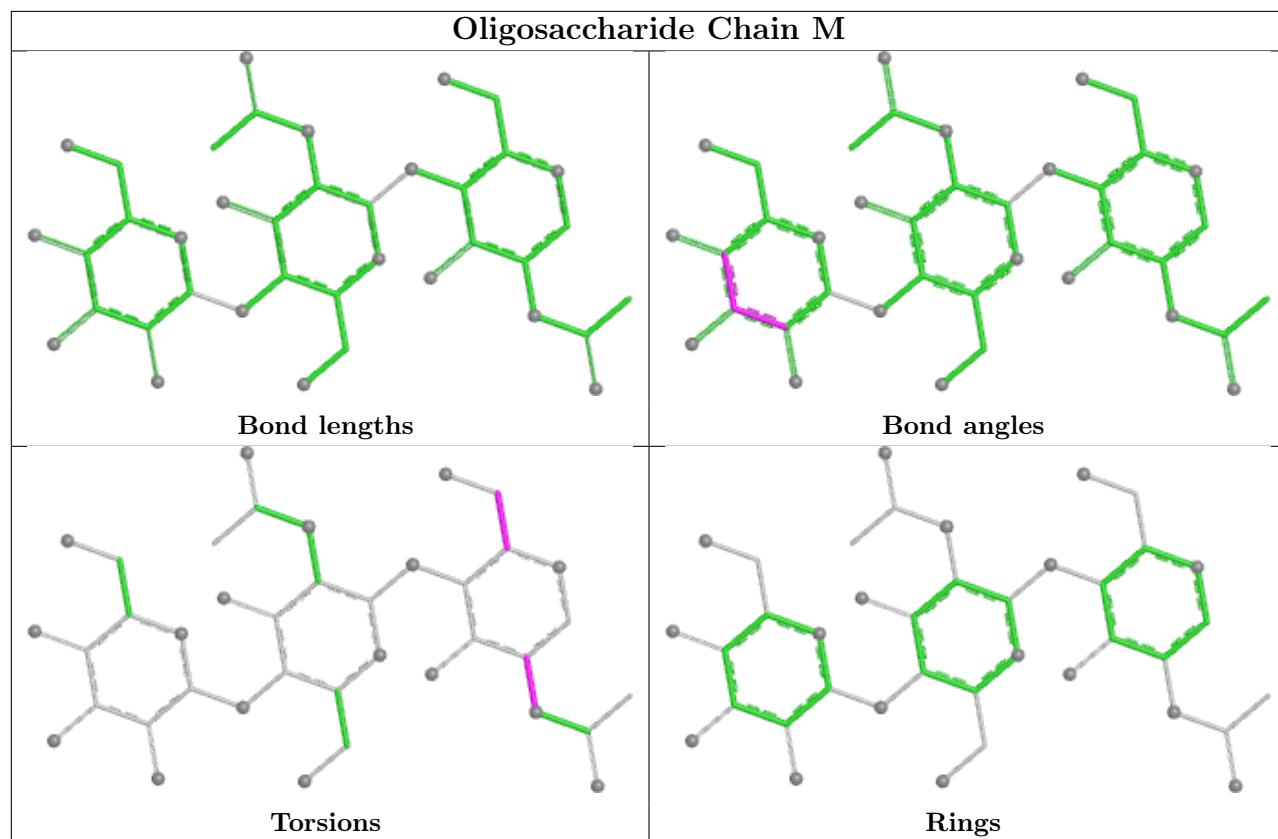
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

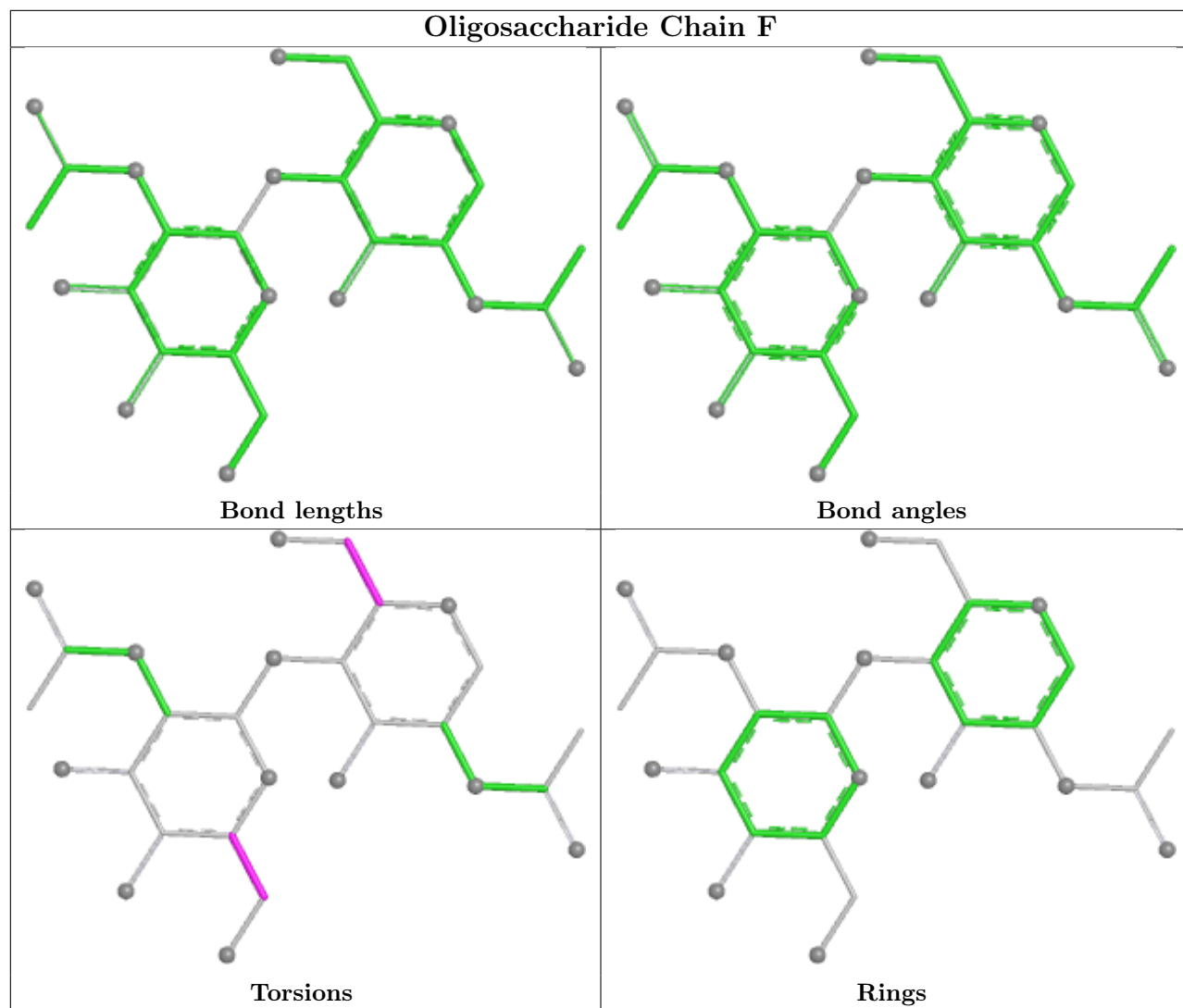


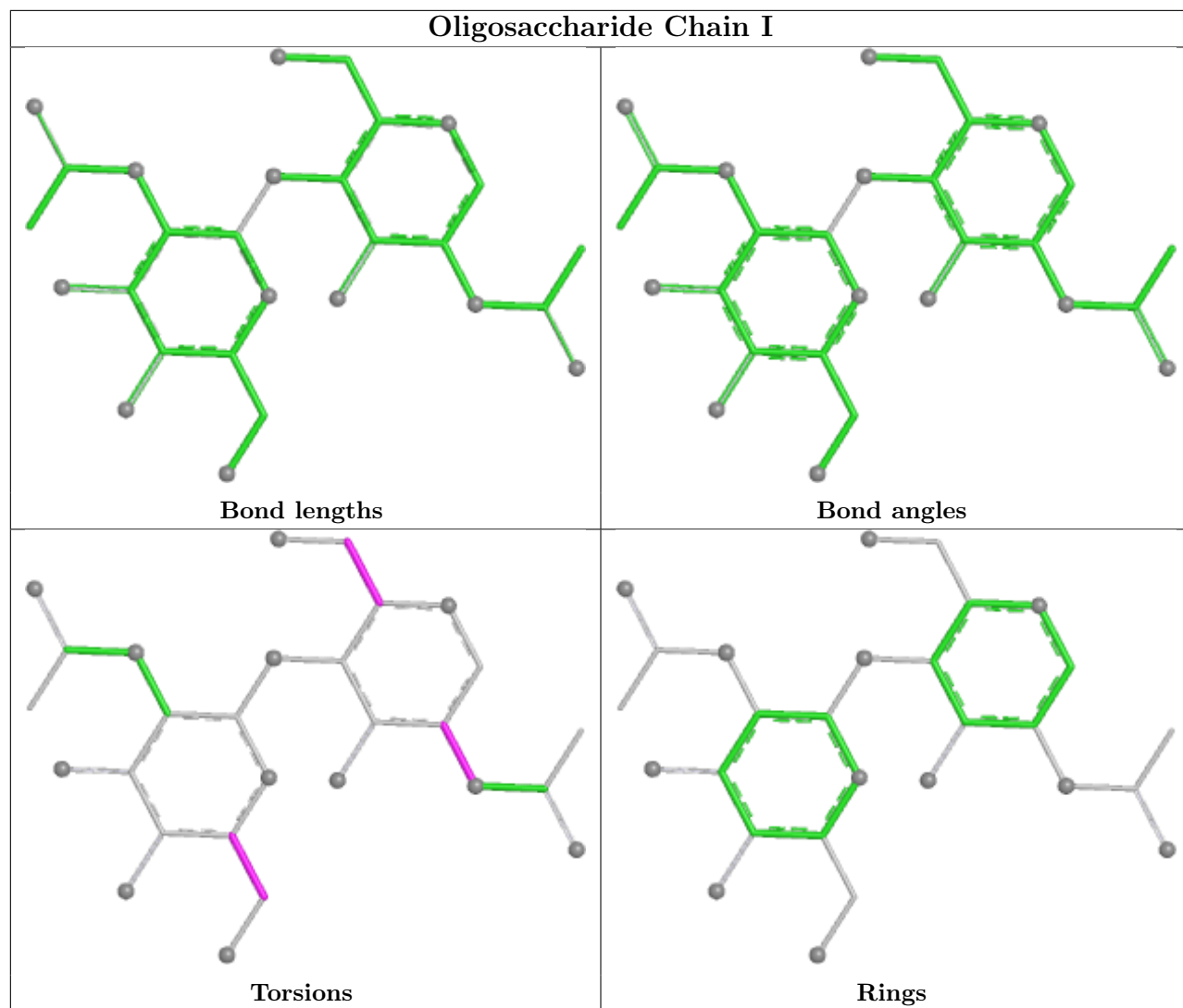


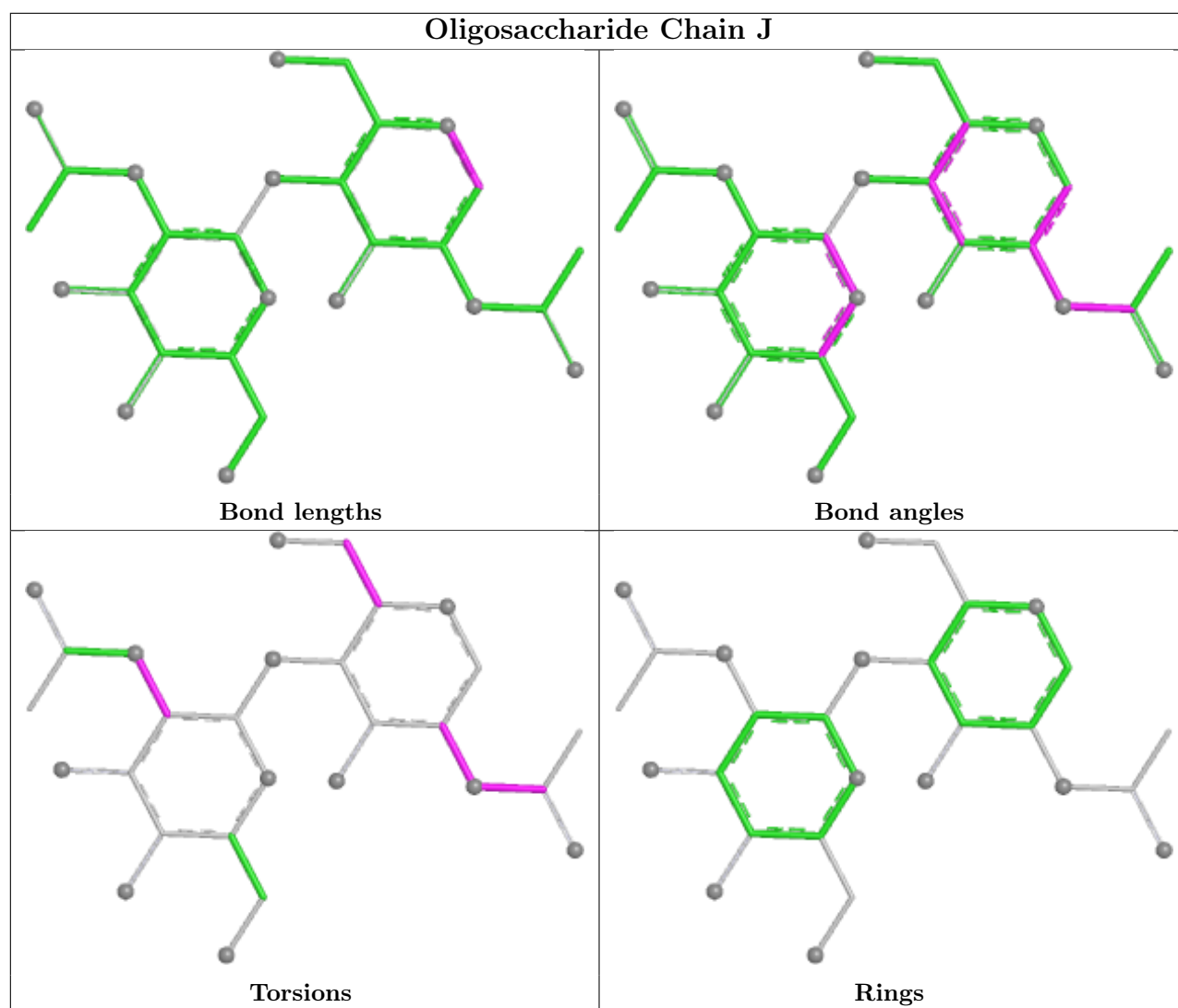


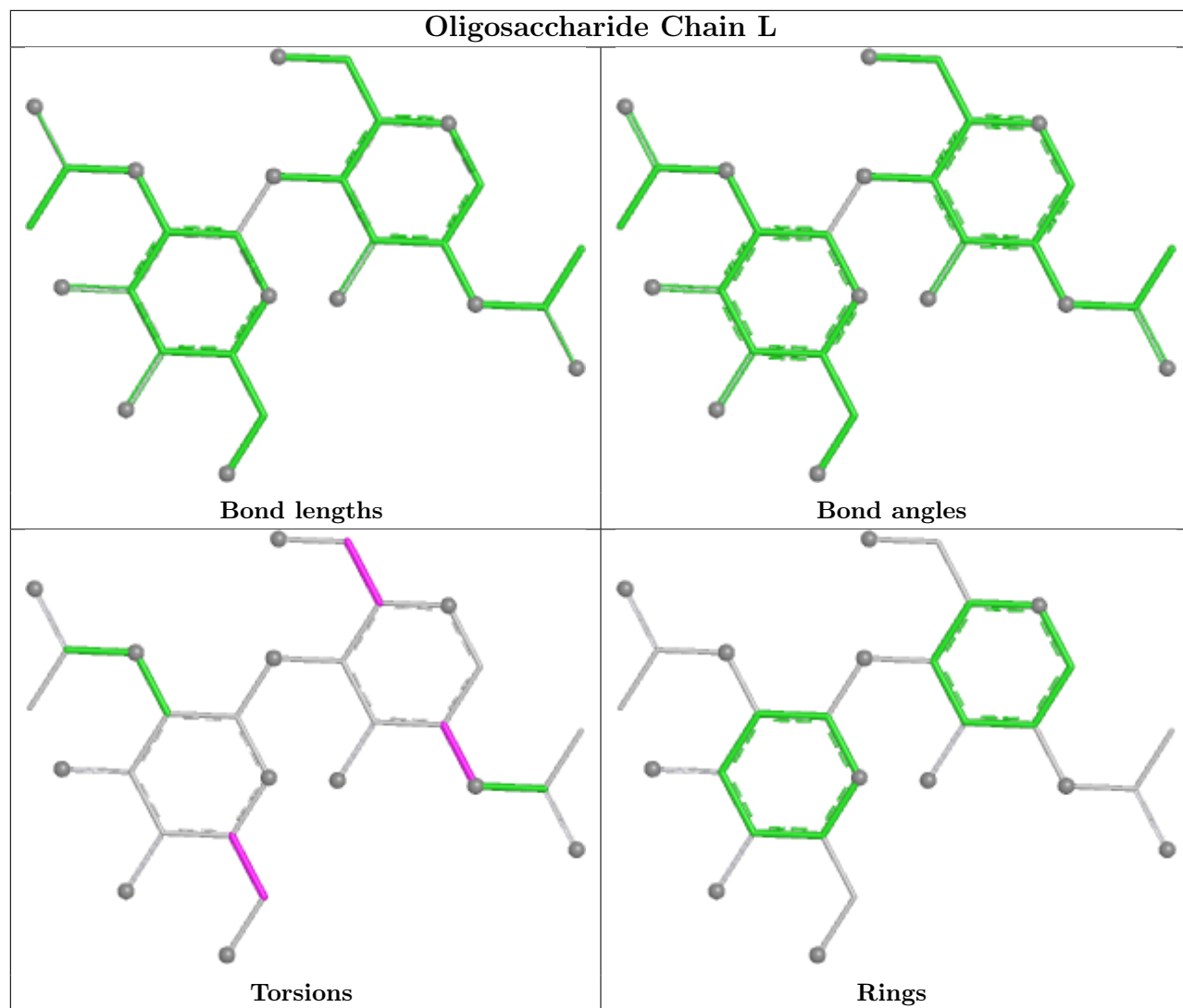


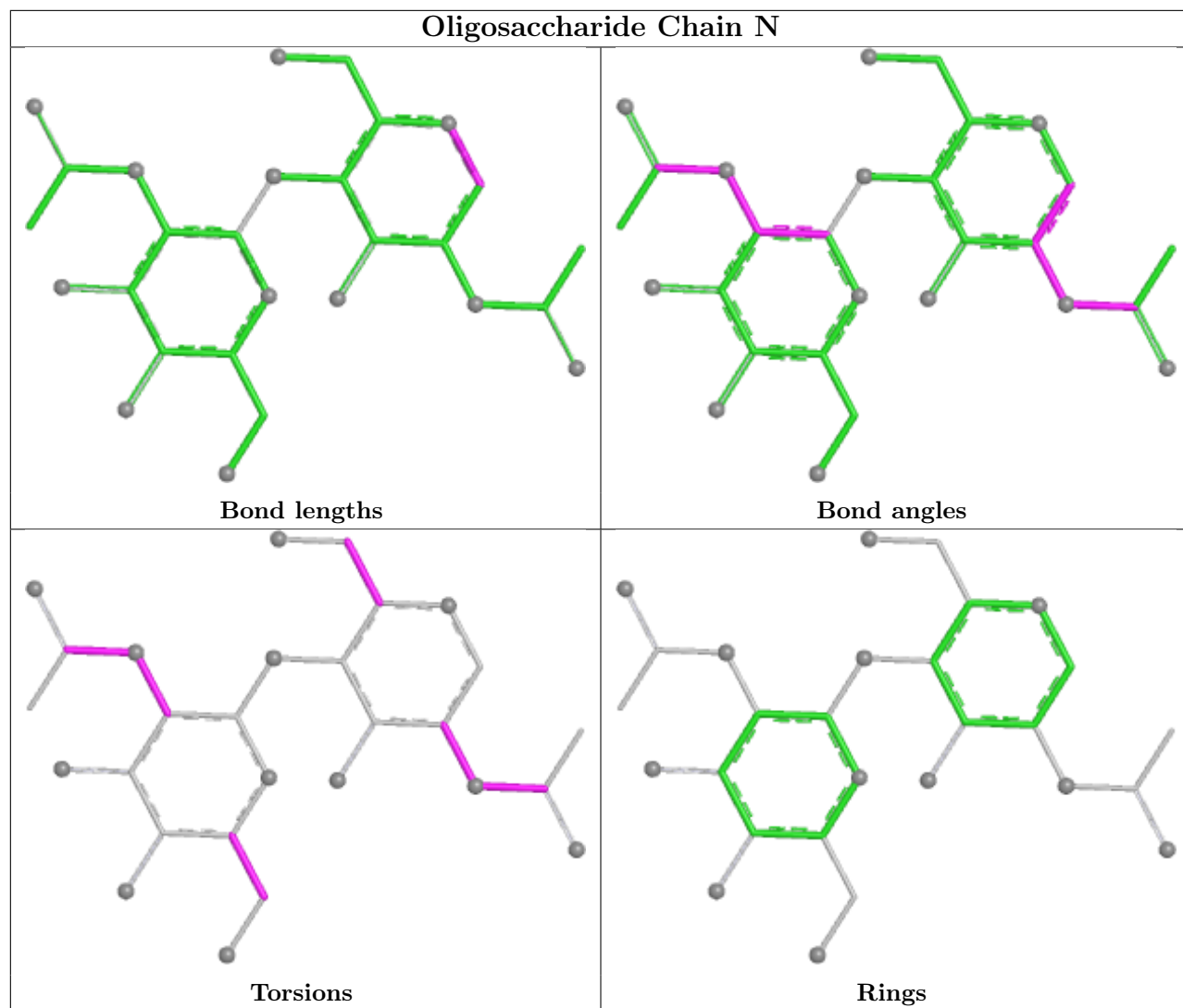


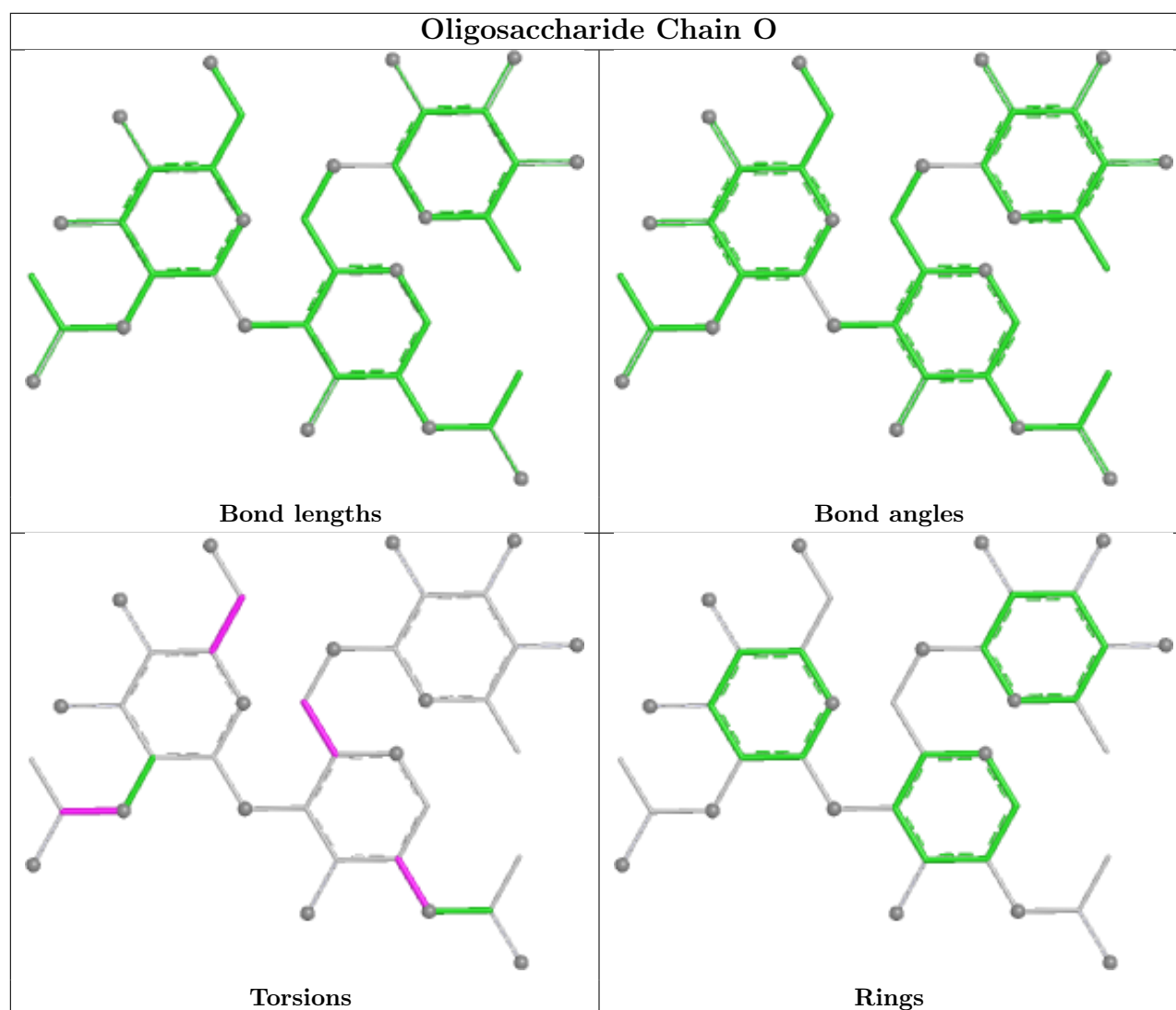












5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	A	1505	1	14,14,15	0.40	0	17,19,21	0.55	0
8	NAG	A	1501	1	14,14,15	0.22	0	17,19,21	0.45	0
8	NAG	A	1506	1	14,14,15	0.35	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	1503	1	14,14,15	0.23	0	17,19,21	0.88	1 (5%)
8	NAG	A	1502	1	14,14,15	0.30	0	17,19,21	0.48	0
8	NAG	A	1504	1	14,14,15	0.62	1 (7%)	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1505	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1506	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1503	1	-	3/6/23/26	0/1/1/1
8	NAG	A	1502	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1504	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1504	NAG	C1-C2	2.18	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1503	NAG	C1-O5-C5	-2.22	109.22	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1505	NAG	O5-C5-C6-O6
8	A	1505	NAG	C4-C5-C6-O6
8	A	1502	NAG	O5-C5-C6-O6
8	A	1503	NAG	O5-C5-C6-O6
8	A	1504	NAG	O5-C5-C6-O6
8	A	1503	NAG	C1-C2-N2-C7
8	A	1505	NAG	C3-C2-N2-C7
8	A	1505	NAG	C1-C2-N2-C7
8	A	1503	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1505	NAG	1	0
8	A	1506	NAG	1	0
8	A	1504	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.

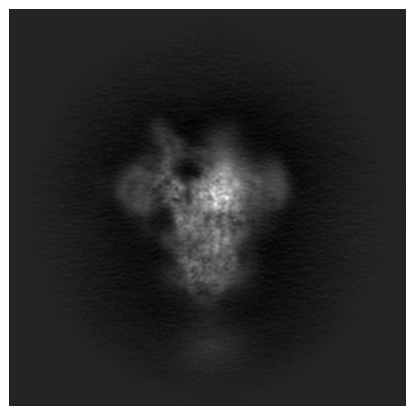
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33649. These allow visual inspection of the internal detail of the map and identification of artifacts.

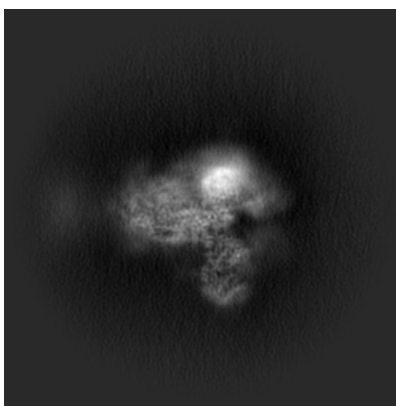
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

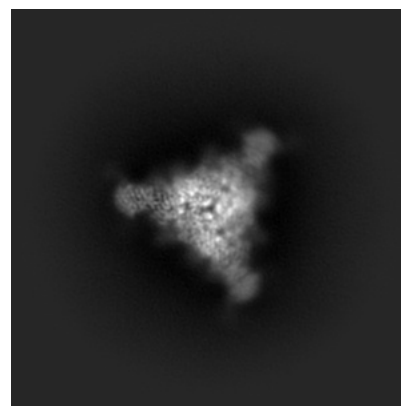
6.1.1 Primary map



X

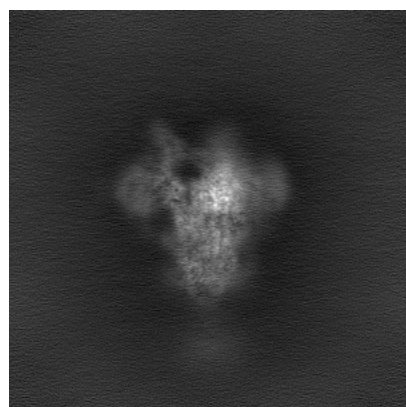


Y

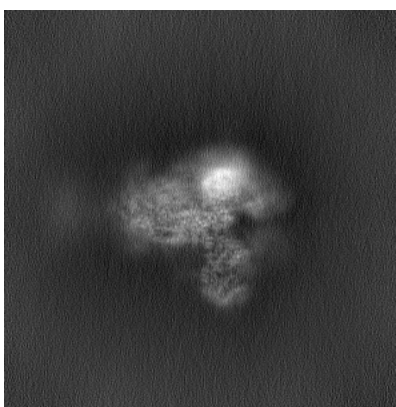


Z

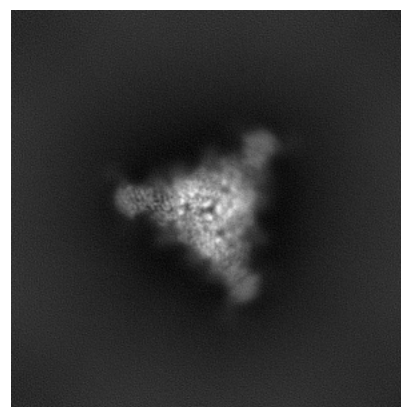
6.1.2 Raw map



X



Y

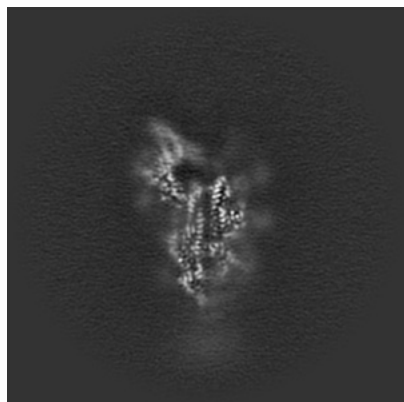


Z

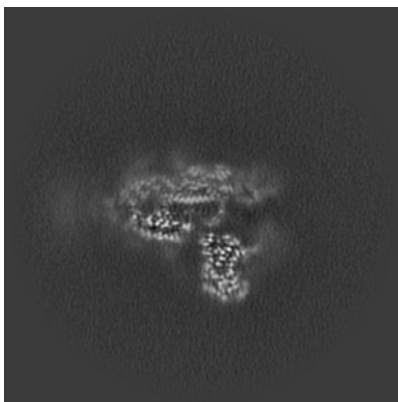
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

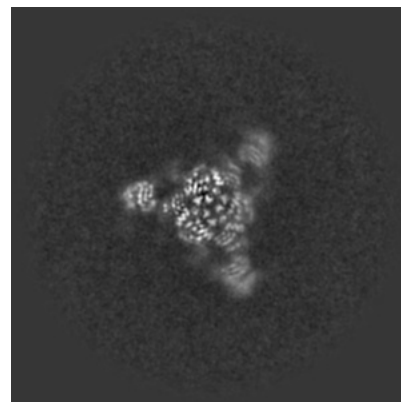
6.2.1 Primary map



X Index: 182

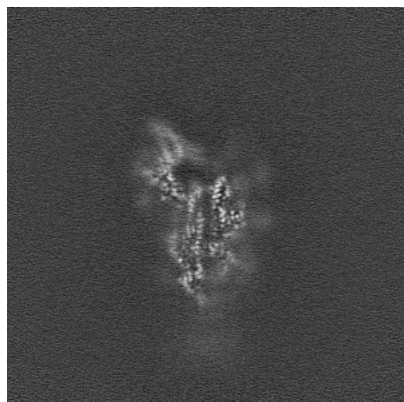


Y Index: 182



Z Index: 182

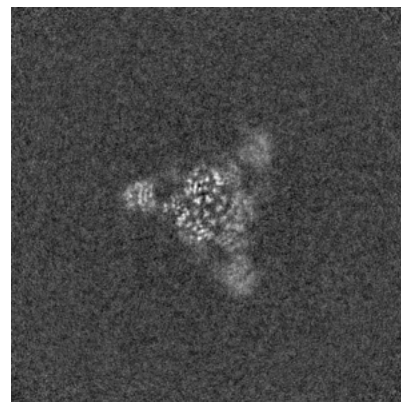
6.2.2 Raw map



X Index: 182



Y Index: 182

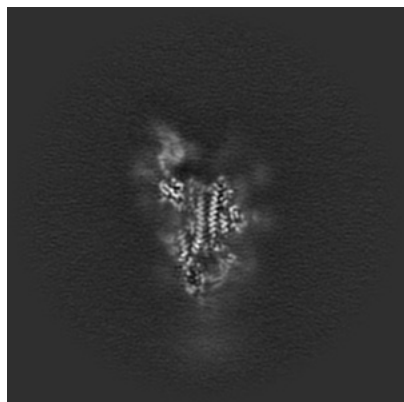


Z Index: 182

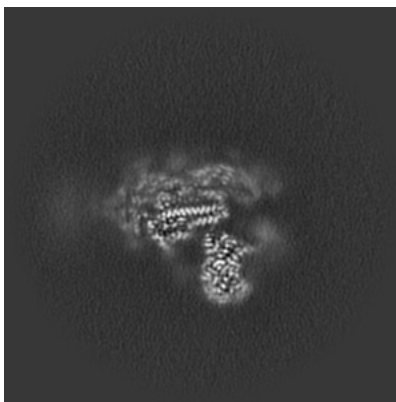
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

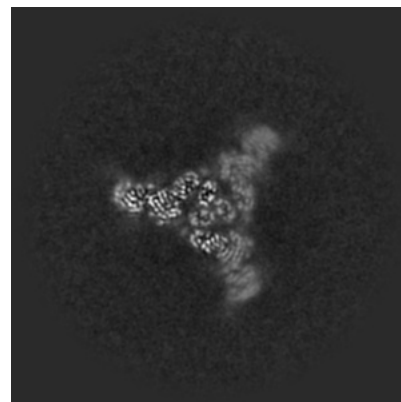
6.3.1 Primary map



X Index: 179

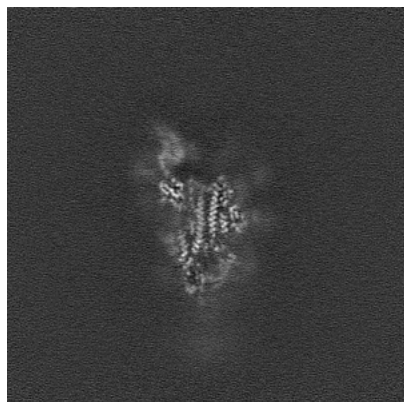


Y Index: 187

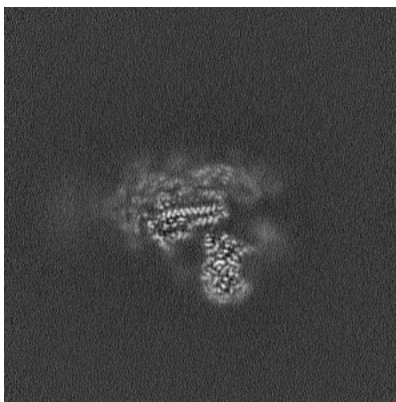


Z Index: 196

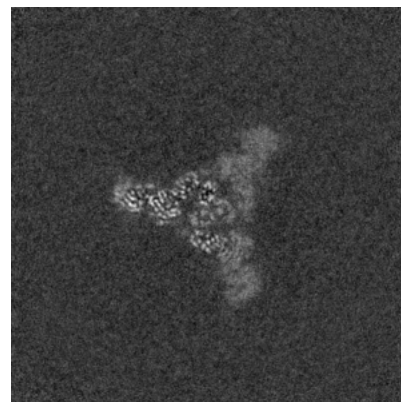
6.3.2 Raw map



X Index: 179



Y Index: 187

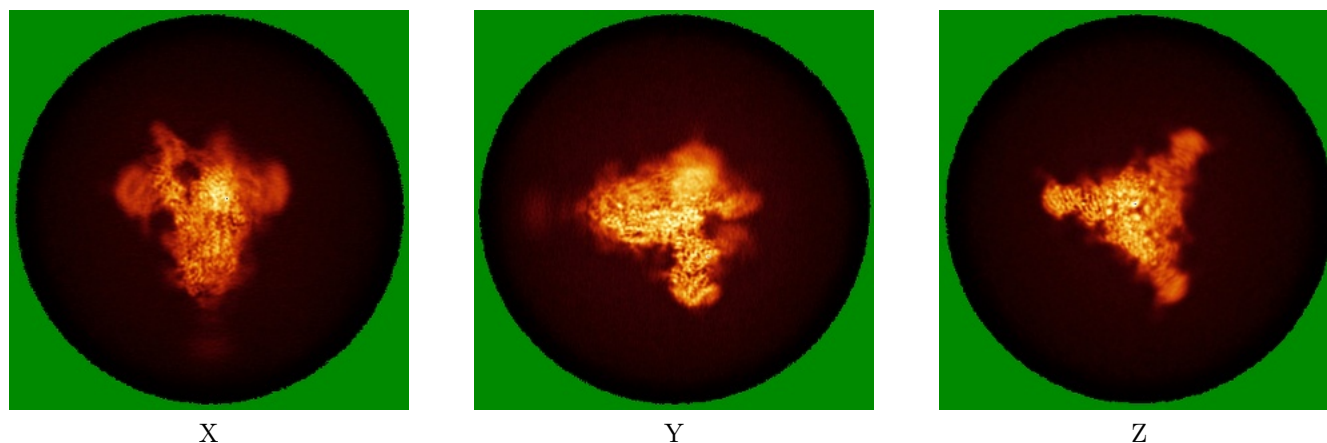


Z Index: 196

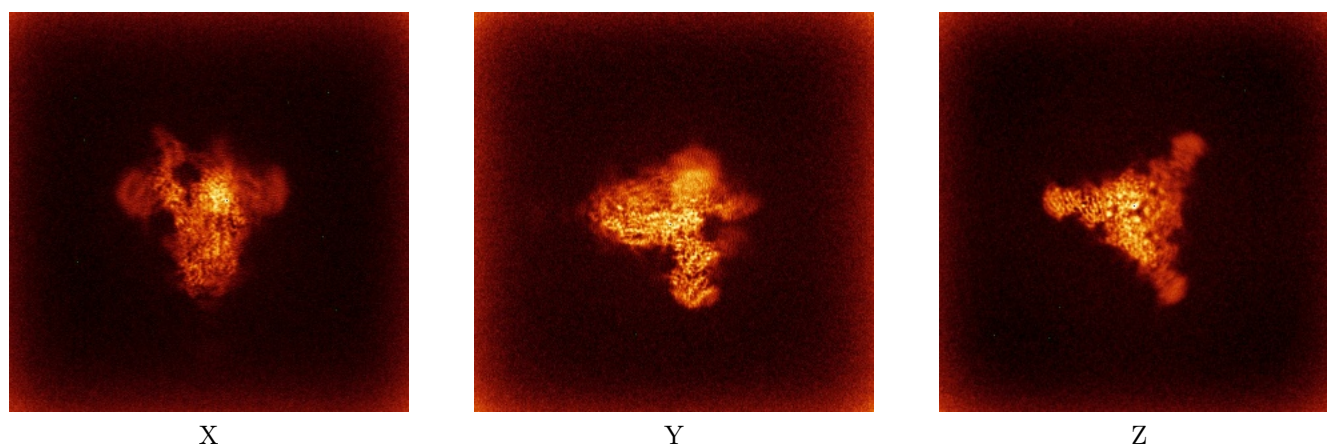
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

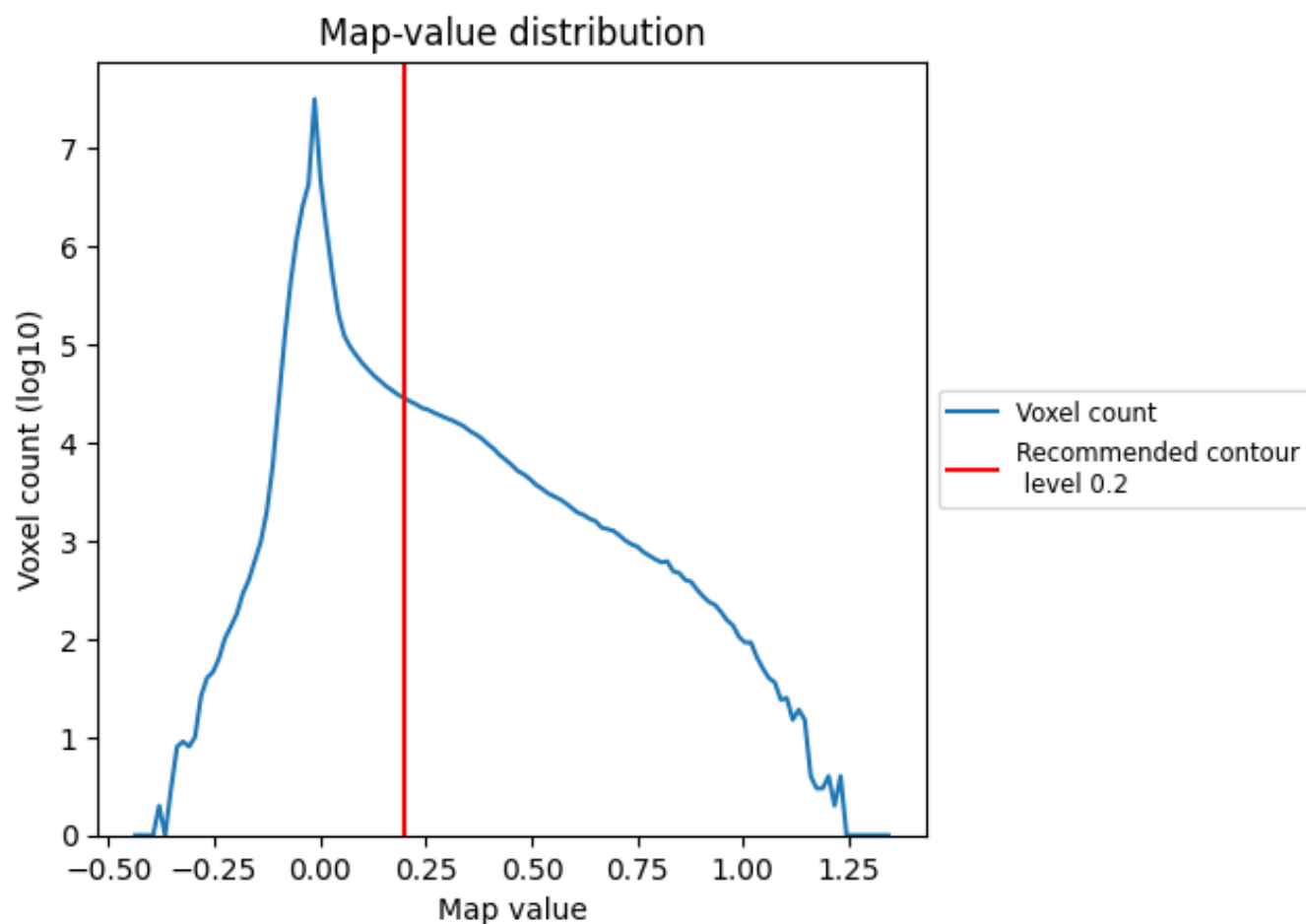
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

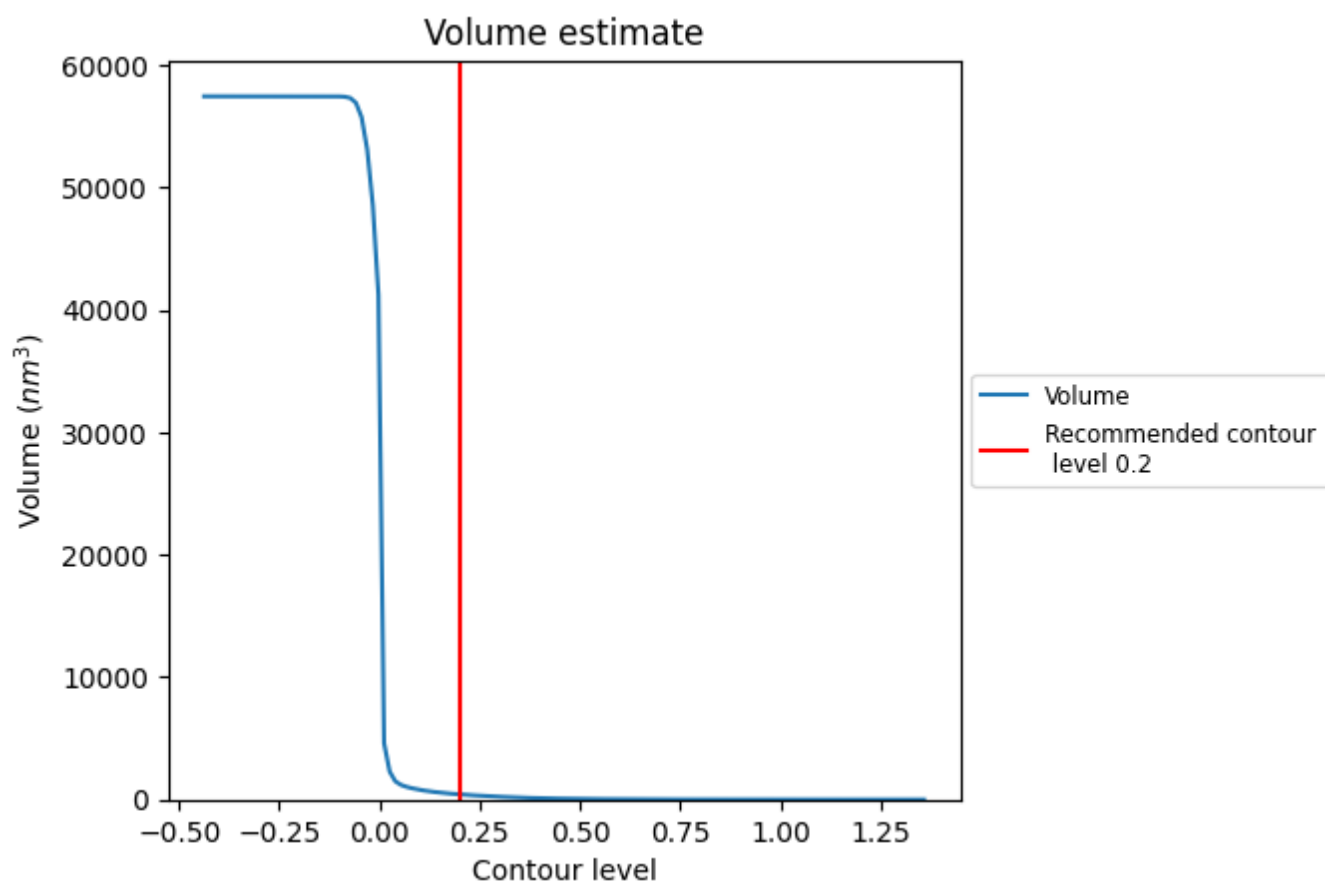
This section contains the results of statistical analysis of the map.

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.

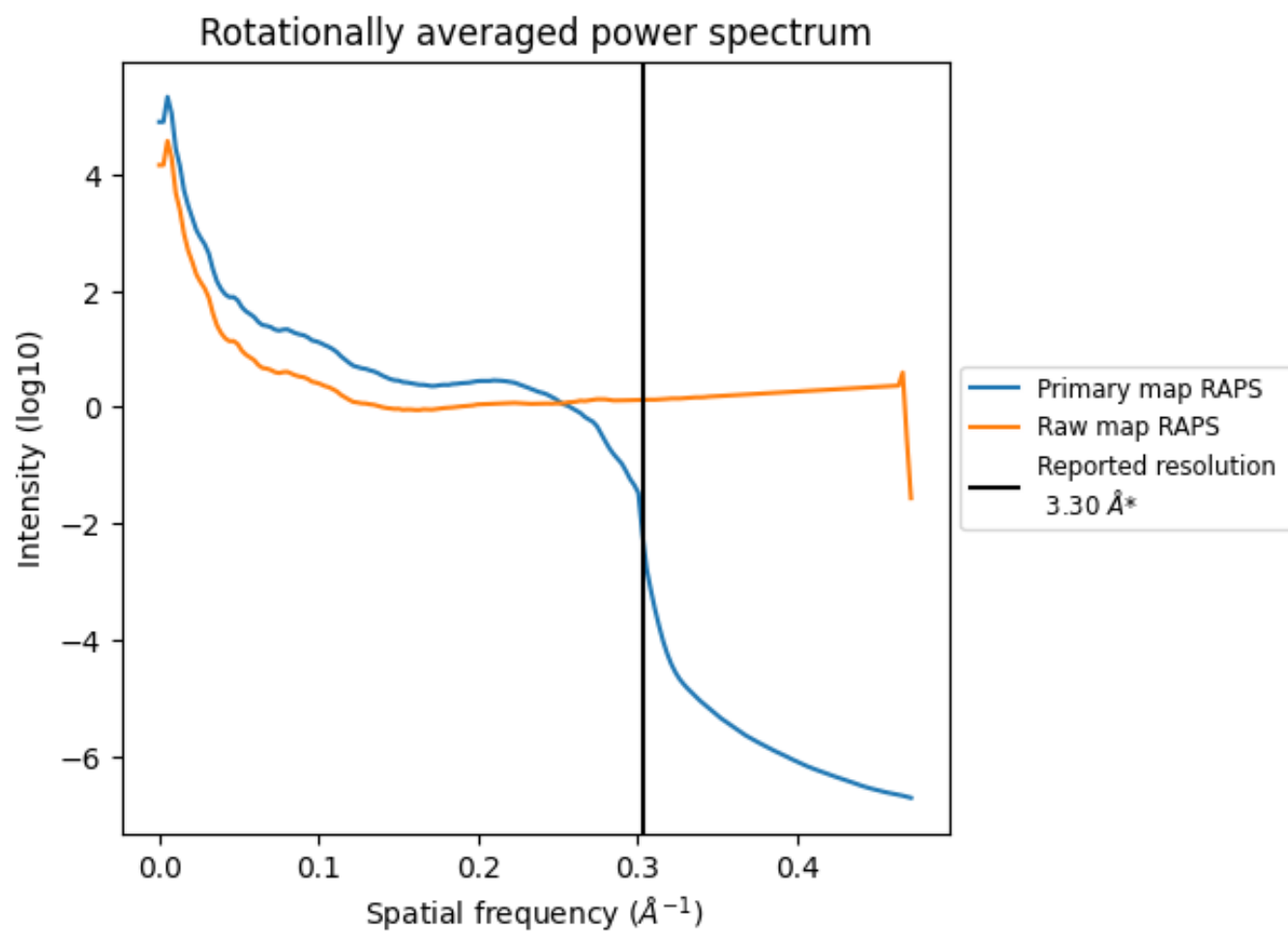
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 425 nm³; this corresponds to an approximate mass of 384 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

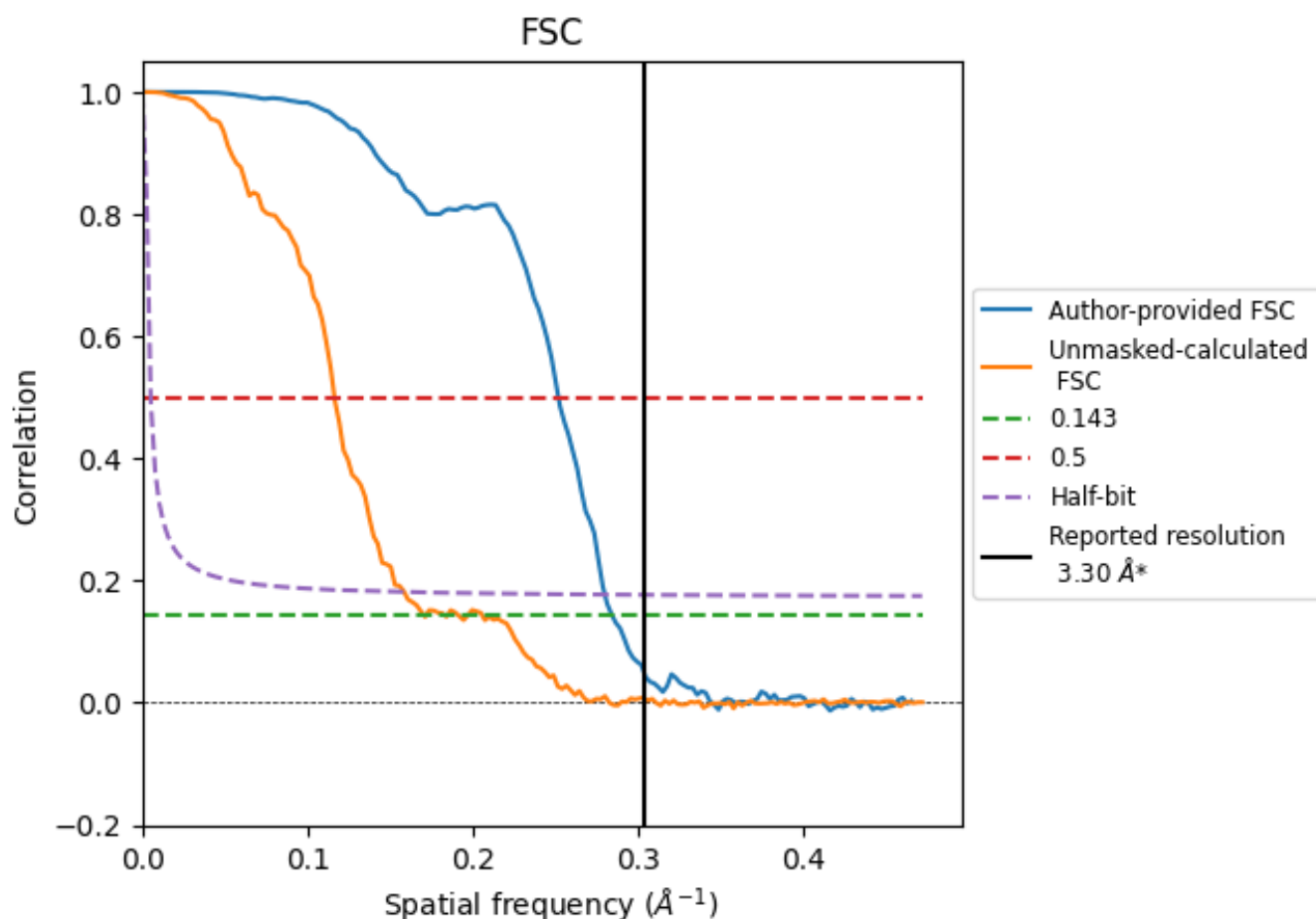


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.52	3.97	3.57
Unmasked-calculated*	5.87	8.60	6.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

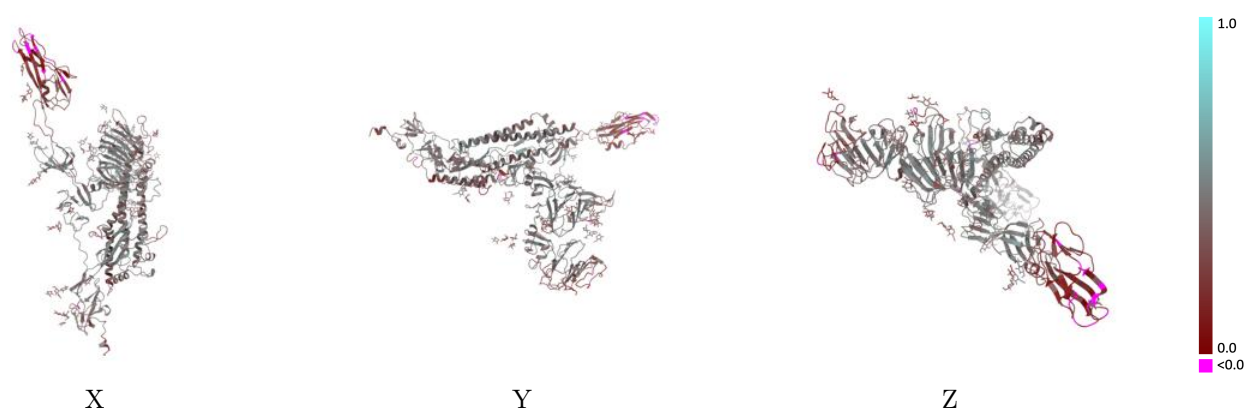
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-33649 and PDB model 7Y6V. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

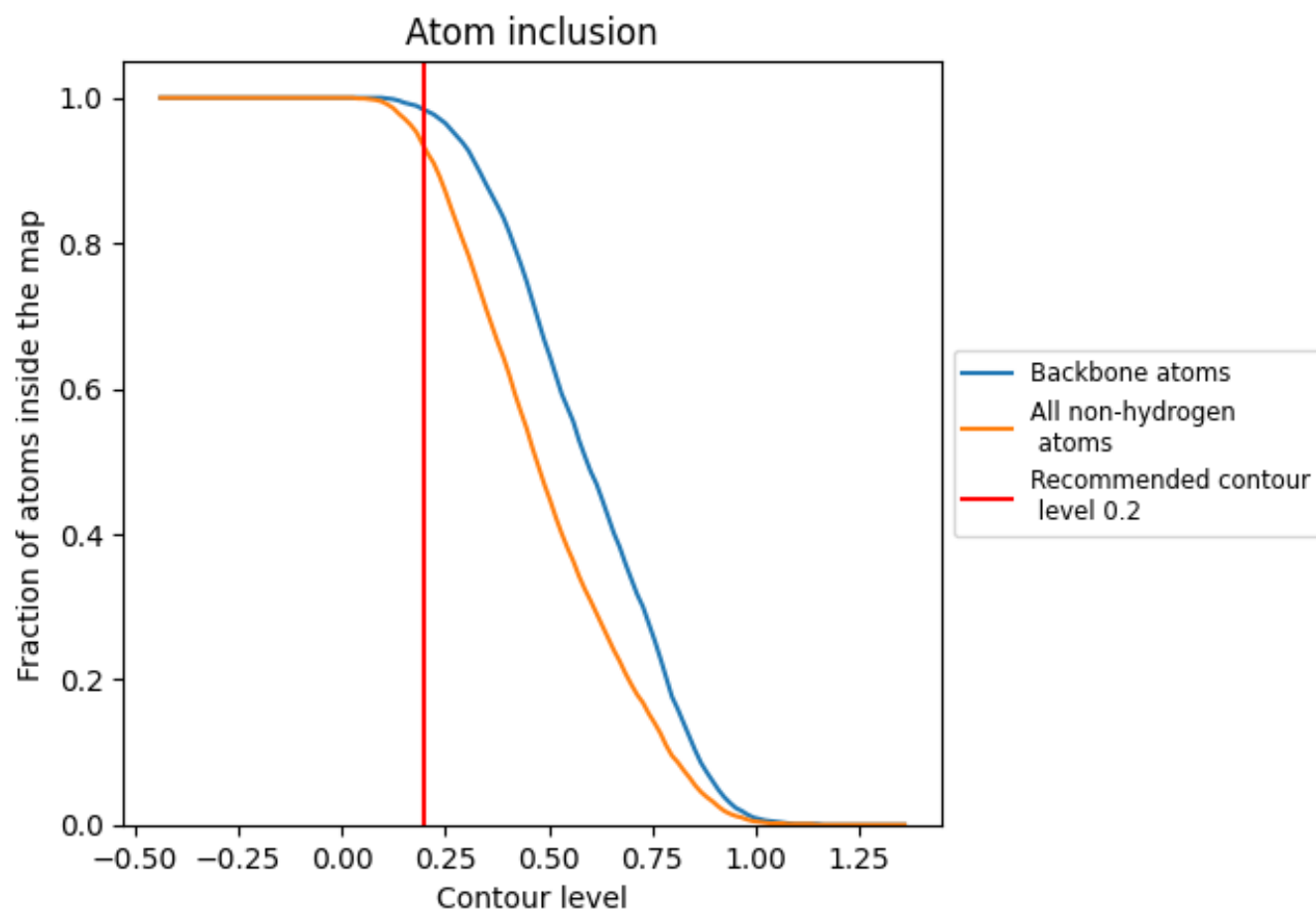


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.3920
A	0.9330	0.3940
B	0.7750	0.3050
C	0.9670	0.4440
D	0.7500	0.3160
E	0.8970	0.2750
F	0.8570	0.3420
G	0.9580	0.3000
H	0.8970	0.3900
I	0.7860	0.2420
J	0.8930	0.2850
K	0.8970	0.4300
L	0.9290	0.2730
M	0.9230	0.3240
N	0.9290	0.3510
O	0.8950	0.3380

1.0

0.0

<0.0