



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2022 – 01:15 pm BST

PDB ID : 7O7O  
EMDB ID : EMD-12751  
Title : (h-alpha2M)4 semiactivated II state  
Authors : Luque, D.; Goulas, T.; Mata, C.P.; Mendes, S.R.; Gomis-Ruth, F.X.; Caston, J.R.  
Deposited on : 2021-04-13  
Resolution : 4.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

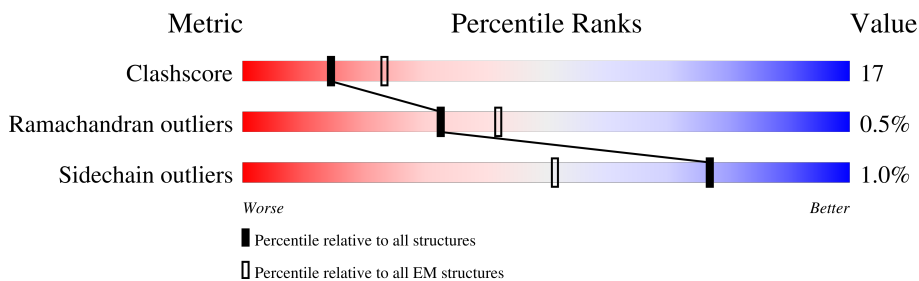
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1474	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">45%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">58%</div> <div style="text-align: center;">28%</div> <div style="text-align: center;">13%</div> </div>
1	B	1474	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">25%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">59%</div> <div style="text-align: center;">35%</div> <div style="text-align: center;">..</div> </div>
1	C	1474	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">45%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">58%</div> <div style="text-align: center;">28%</div> <div style="text-align: center;">13%</div> </div>
1	D	1474	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">25%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">59%</div> <div style="text-align: center;">35%</div> <div style="text-align: center;">..</div> </div>
2	E	2	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">100%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">50%</div> <div style="text-align: center;">50%</div> </div>
2	G	2	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">100%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">50%</div> <div style="text-align: center;">50%</div> </div>
2	J	2	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">100%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">100%</div> </div>
2	K	2	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">100%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">50%</div> <div style="text-align: center;">50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	M	2	<p>100% 50% 50%</p>
2	P	2	<p>100% 100%</p>
3	F	4	<p>100% 25% 75%</p>
3	H	4	<p>100% 25% 50% 25%</p>
3	L	4	<p>100% 25% 25% 50%</p>
3	N	4	<p>100% 25% 50% 25%</p>
4	I	3	<p>67% 33% 33% 33%</p>
4	O	3	<p>67% 33% 33% 33%</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 42642 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 Alpha-2-macroglobulin.

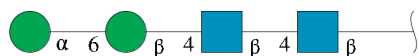
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1278	9968	6336	1674	1915	43	0	0
1	B	1410	11004	6999	1840	2117	48	0	0
1	C	1278	9968	6336	1674	1915	43	0	0
1	D	1410	11004	6999	1840	2117	48	0	0

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



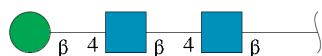
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	E	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	J	2	28	16	2	10	0	0
2	K	2	28	16	2	10	0	0
2	M	2	28	16	2	10	0	0
2	P	2	28	16	2	10	0	0

- Molecule 3 is an oligosaccharide called 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
			Total	C	N	O		
3	F	4	50	28	2	20	0	0
3	H	4	50	28	2	20	0	0
3	L	4	50	28	2	20	0	0
3	N	4	50	28	2	20	0	0

- Molecule 4 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
			Total	C	N	O		
4	I	3	39	22	2	15	0	0
4	O	3	39	22	2	15	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
5	A	1	70	40	5	25	0
5	A	1	70	40	5	25	0
5	A	1	70	40	5	25	0
5	A	1	70	40	5	25	0
5	A	1	70	40	5	25	0
5	B	1	56	32	4	20	0
5	B	1	56	32	4	20	0
5	B	1	56	32	4	20	0
5	B	1	56	32	4	20	0
5	C	1	70	40	5	25	0
5	C	1	70	40	5	25	0
5	C	1	70	40	5	25	0
5	C	1	70	40	5	25	0
5	C	1	70	40	5	25	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	D	1	Total 56	C 32	N 4	O 20	0
5	D	1	Total 56	C 32	N 4	O 20	0
5	D	1	Total 56	C 32	N 4	O 20	0
5	D	1	Total 56	C 32	N 4	O 20	0

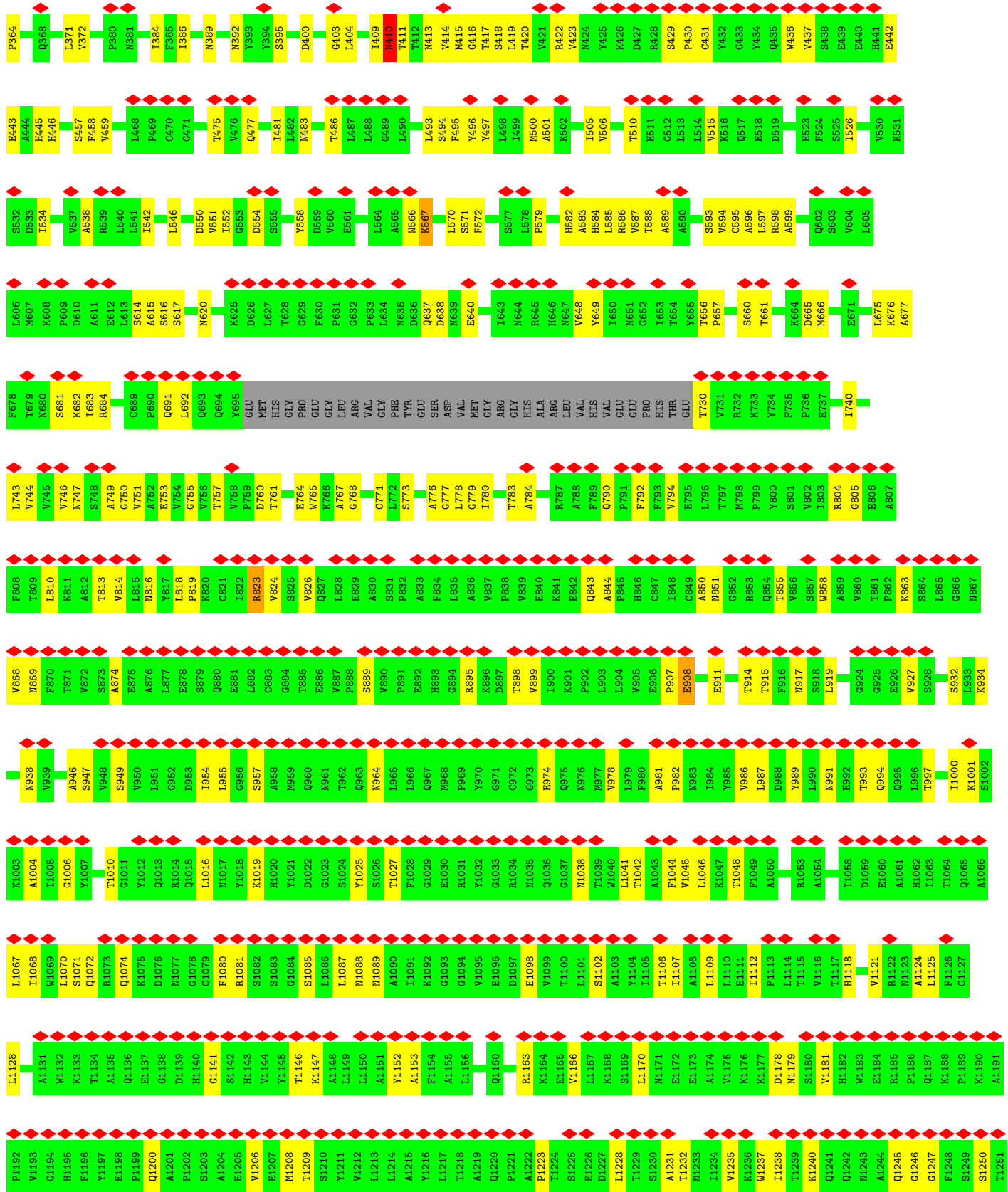








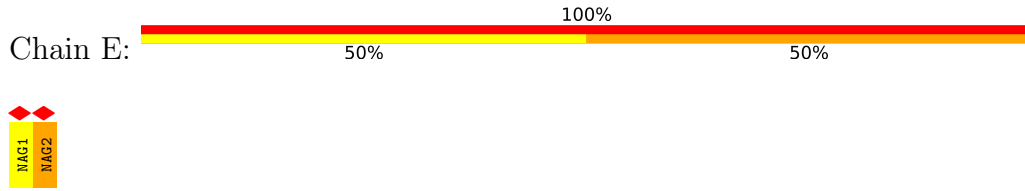








● Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

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



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



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



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

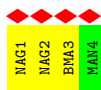


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

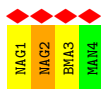


- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

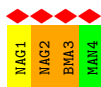
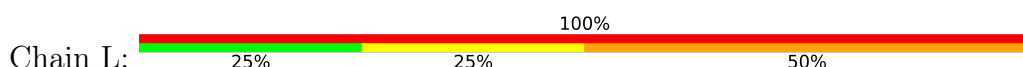




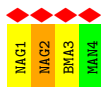
- Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	185640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	39.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	47775	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size ( $\text{\AA}$ )	335.04, 335.04, 335.04	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.047, 1.047, 1.047	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: 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	0.48	3/10189 (0.0%)	0.66	3/13842 (0.0%)
1	B	0.55	8/11249 (0.1%)	0.75	17/15286 (0.1%)
1	C	0.48	3/10189 (0.0%)	0.66	3/13842 (0.0%)
1	D	0.56	7/11249 (0.1%)	0.74	16/15286 (0.1%)
All	All	0.52	21/42876 (0.0%)	0.71	39/58256 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
All	All	0	6

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	LEU	C-N	-20.66	0.86	1.34
1	C	54	LEU	C-N	-20.66	0.86	1.34
1	D	968	MET	C-N	17.99	1.68	1.34
1	B	968	MET	C-N	17.97	1.68	1.34
1	D	969	PRO	N-CA	13.55	1.70	1.47

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	990	LEU	O-C-N	13.04	143.56	122.70
1	D	990	LEU	O-C-N	13.04	143.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	975	GLN	CG-CD-OE1	-12.60	96.40	121.60
1	B	990	LEU	C-N-CA	-11.02	94.14	121.70
1	D	990	LEU	C-N-CA	-11.02	94.14	121.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	ASN	Mainchain
1	A	54	LEU	Mainchain
1	A	869	ASN	Mainchain
1	C	410	ASN	Mainchain
1	C	54	LEU	Mainchain

## 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	9968	0	9864	318	0
1	B	11004	0	10888	408	0
1	C	9968	0	9864	315	0
1	D	11004	0	10888	409	0
2	E	28	0	25	2	0
2	G	28	0	25	1	0
2	J	28	0	25	0	0
2	K	28	0	25	2	0
2	M	28	0	25	1	0
2	P	28	0	25	0	0
3	F	50	0	43	0	0
3	H	50	0	43	3	0
3	L	50	0	43	1	0
3	N	50	0	43	3	0
4	I	39	0	34	1	0
4	O	39	0	34	2	0
5	A	70	0	65	0	0
5	B	56	0	52	2	0
5	C	70	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	56	0	52	2	0
All	All	42642	0	42128	1446	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 17.

The worst 5 of 1446 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:D:968:MET:C	1:D:969:PRO:N	1.68	1.46
1:D:969:PRO:N	1:D:969:PRO:CA	1.70	1.45
1:C:54:LEU:C	1:C:55:ASN:CA	1.87	1.43
1:B:968:MET:C	1:B:969:PRO:N	1.68	1.42
1:B:969:PRO:N	1:B:969:PRO:CA	1.70	1.41

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	1274/1474 (86%)	1067 (84%)	203 (16%)	4 (0%)	41	76
1	B	1406/1474 (95%)	1135 (81%)	263 (19%)	8 (1%)	25	65
1	C	1274/1474 (86%)	1067 (84%)	203 (16%)	4 (0%)	41	76
1	D	1406/1474 (95%)	1134 (81%)	263 (19%)	9 (1%)	25	65
All	All	5360/5896 (91%)	4403 (82%)	932 (17%)	25 (0%)	32	68

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	PRO

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Mol	Chain	Res	Type
1	A	908	GLU
1	A	1333	LEU
1	B	800	TYR
1	B	808	PHE

### 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	1115/1290 (86%)	1108 (99%)	7 (1%)	86	92
1	B	1236/1290 (96%)	1221 (99%)	15 (1%)	71	84
1	C	1115/1290 (86%)	1108 (99%)	7 (1%)	86	92
1	D	1236/1290 (96%)	1220 (99%)	16 (1%)	69	82
All	All	4702/5160 (91%)	4657 (99%)	45 (1%)	77	86

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1001	LYS
1	D	975	GLN
1	D	278	CYS
1	D	811	LYS
1	D	1184	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1035	ASN
1	D	1065	GLN
1	B	1013	GLN
1	B	963	GLN
1	D	1072	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

34 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	E	1	2,1	14,14,15	0.35	0	17,19,21	0.75	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.94	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.46	0	17,19,21	1.37	2 (11%)
3	NAG	F	2	3	14,14,15	0.35	0	17,19,21	1.12	2 (11%)
3	BMA	F	3	3	11,11,12	0.26	0	15,15,17	1.01	1 (6%)
3	MAN	F	4	3	11,11,12	0.25	0	15,15,17	0.70	0
2	NAG	G	1	2,1	14,14,15	0.32	0	17,19,21	1.13	3 (17%)
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	0.85	0
3	NAG	H	1	1,3	14,14,15	0.38	0	17,19,21	0.56	0
3	NAG	H	2	3	14,14,15	0.38	0	17,19,21	1.07	1 (5%)
3	BMA	H	3	3	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
3	MAN	H	4	3	11,11,12	0.23	0	15,15,17	0.58	0
4	NAG	I	1	1,4	14,14,15	0.51	0	17,19,21	1.21	1 (5%)
4	NAG	I	2	4	14,14,15	0.33	0	17,19,21	0.56	0
4	BMA	I	3	4	11,11,12	0.21	0	15,15,17	0.60	0
2	NAG	J	1	2,1	14,14,15	0.31	0	17,19,21	0.54	0
2	NAG	J	2	2	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	K	1	2,1	14,14,15	0.35	0	17,19,21	0.75	0
2	NAG	K	2	2	14,14,15	0.37	0	17,19,21	0.94	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.46	0	17,19,21	1.37	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	L	2	3	14,14,15	0.35	0	17,19,21	1.12	2 (11%)
3	BMA	L	3	3	11,11,12	0.26	0	15,15,17	1.01	1 (6%)
3	MAN	L	4	3	11,11,12	0.25	0	15,15,17	0.70	0
2	NAG	M	1	2,1	14,14,15	0.32	0	17,19,21	1.13	3 (17%)
2	NAG	M	2	2	14,14,15	0.30	0	17,19,21	0.85	0
3	NAG	N	1	1,3	14,14,15	0.38	0	17,19,21	0.56	0
3	NAG	N	2	3	14,14,15	0.38	0	17,19,21	1.07	1 (5%)
3	BMA	N	3	3	11,11,12	0.23	0	15,15,17	0.77	1 (6%)
3	MAN	N	4	3	11,11,12	0.23	0	15,15,17	0.58	0
4	NAG	O	1	1,4	14,14,15	0.51	0	17,19,21	1.21	1 (5%)
4	NAG	O	2	4	14,14,15	0.33	0	17,19,21	0.56	0
4	BMA	O	3	4	11,11,12	0.21	0	15,15,17	0.60	0
2	NAG	P	1	2,1	14,14,15	0.31	0	17,19,21	0.54	0
2	NAG	P	2	2	14,14,15	0.31	0	17,19,21	0.50	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	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	MAN	H	4	3	-	1/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
4	BMA	I	3	4	-	1/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	MAN	L	4	3	-	0/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	BMA	N	3	3	-	1/2/19/22	0/1/1/1
3	MAN	N	4	3	-	1/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	4/6/23/26	0/1/1/1
4	BMA	O	3	4	-	1/2/19/22	0/1/1/1
2	NAG	P	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	P	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C3-C4-C5	3.49	116.46	110.24
3	L	1	NAG	C3-C4-C5	3.49	116.46	110.24
3	H	2	NAG	C1-O5-C5	3.42	116.83	112.19
3	N	2	NAG	C1-O5-C5	3.42	116.83	112.19
4	I	1	NAG	C3-C4-C5	3.15	115.86	110.24

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2

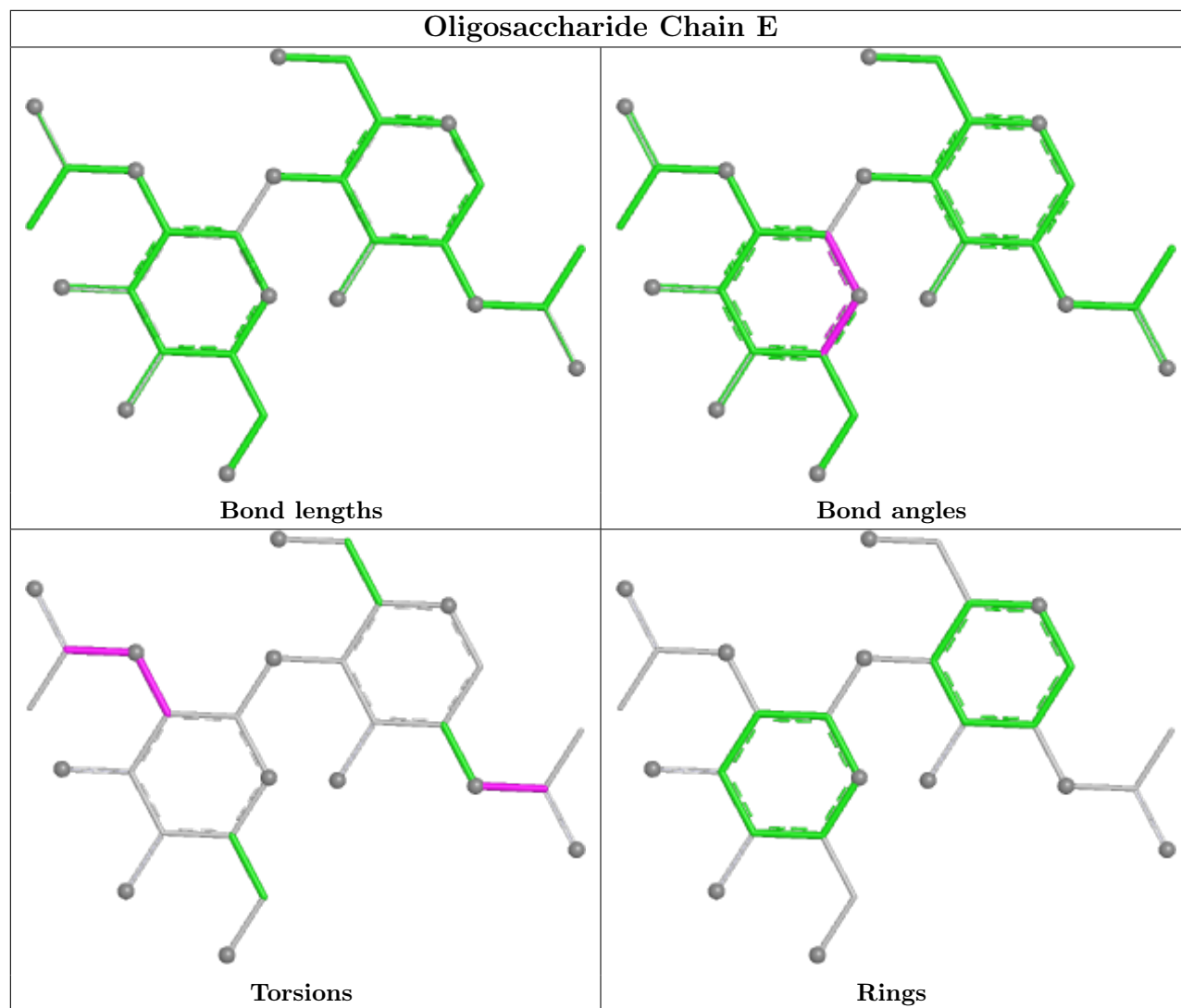
There are no ring outliers.

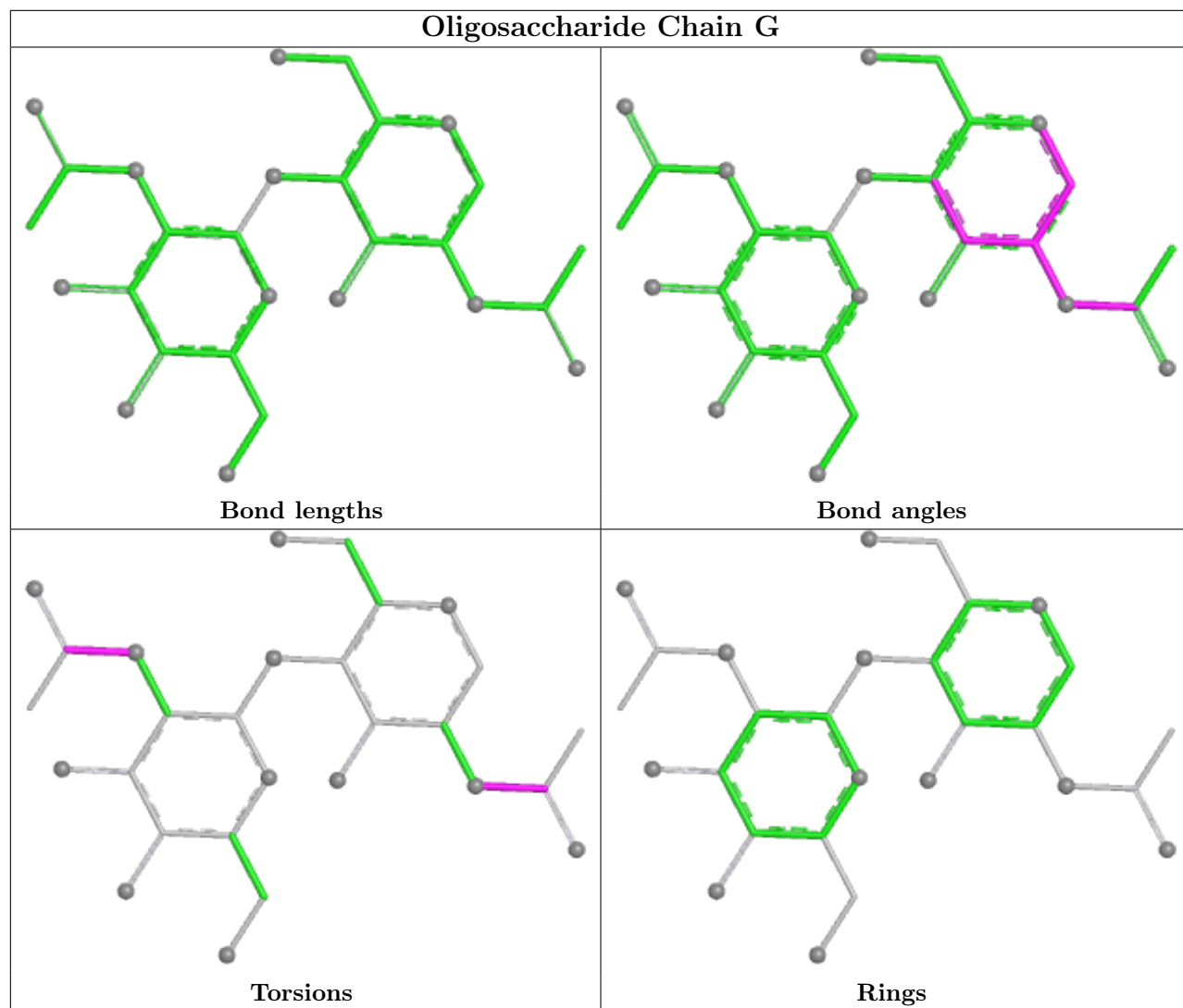


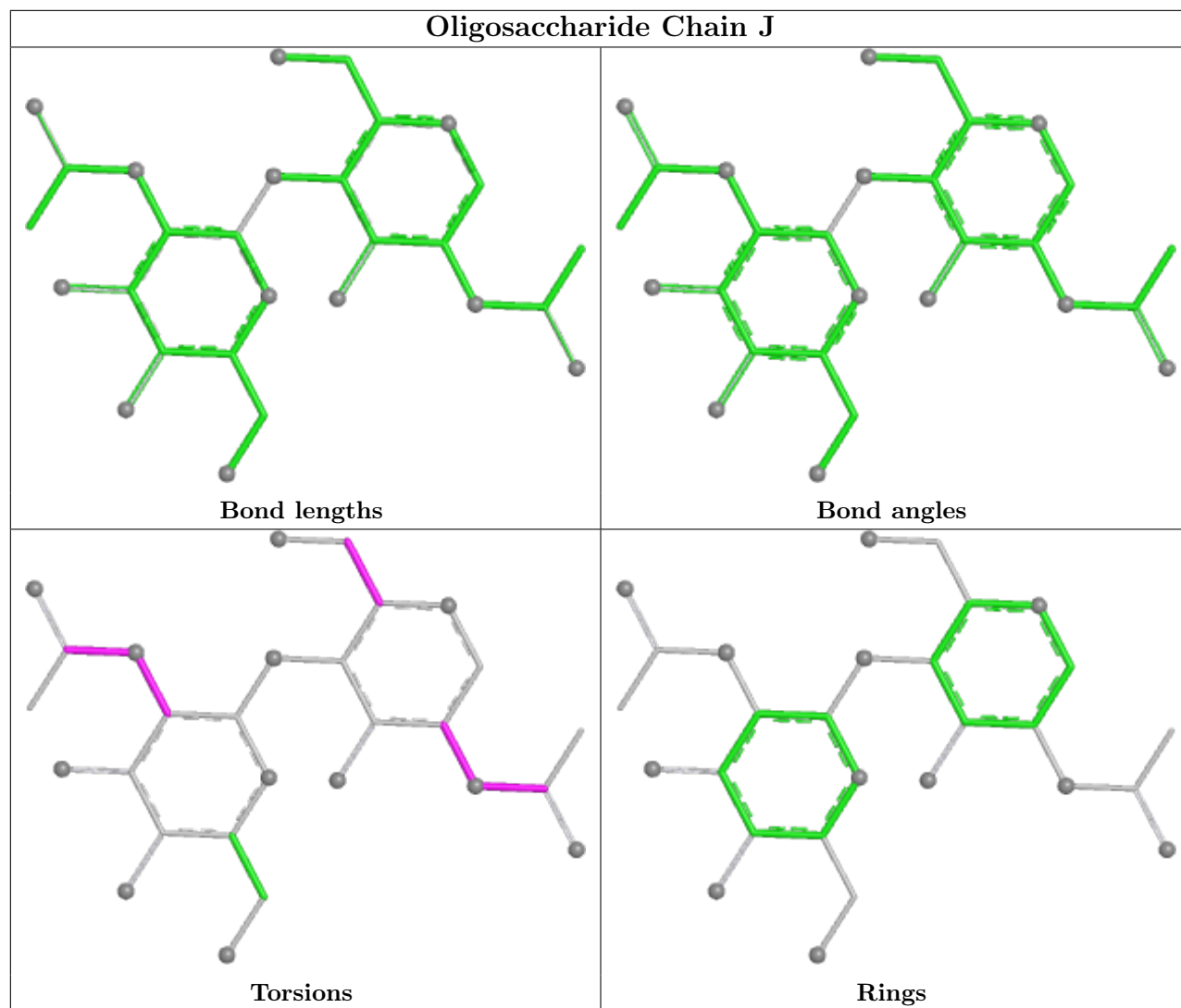
16 monomers are involved in 16 short contacts:

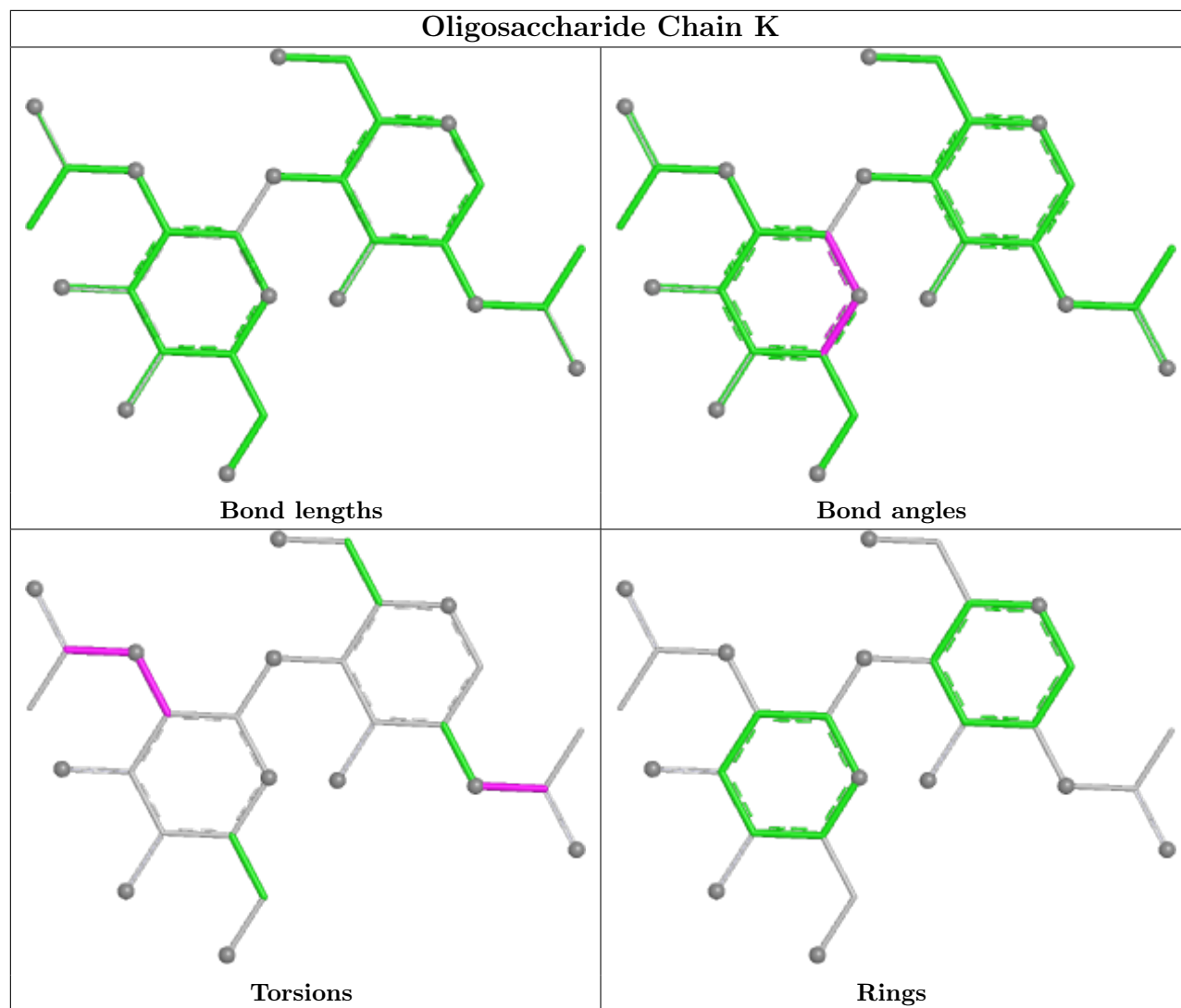
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	2	NAG	1	0
3	H	2	NAG	2	0
3	N	2	NAG	2	0
2	K	2	NAG	2	0
3	L	3	BMA	1	0
3	H	1	NAG	1	0
4	O	1	NAG	2	0
4	O	2	NAG	1	0
4	I	1	NAG	1	0
2	E	2	NAG	2	0
4	I	2	NAG	1	0
3	N	1	NAG	1	0
2	E	1	NAG	1	0
2	G	1	NAG	1	0
2	K	1	NAG	1	0
2	M	1	NAG	1	0

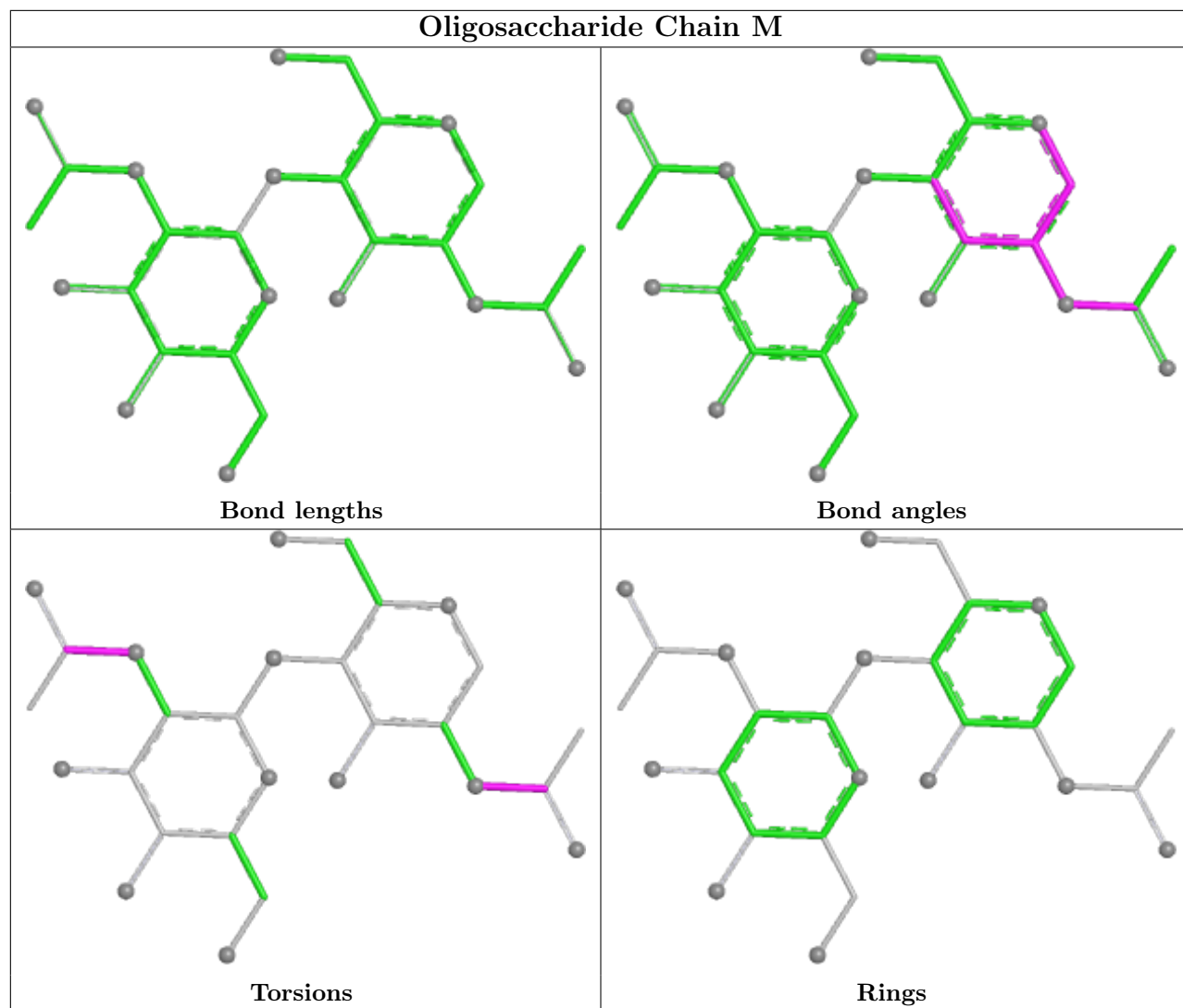
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

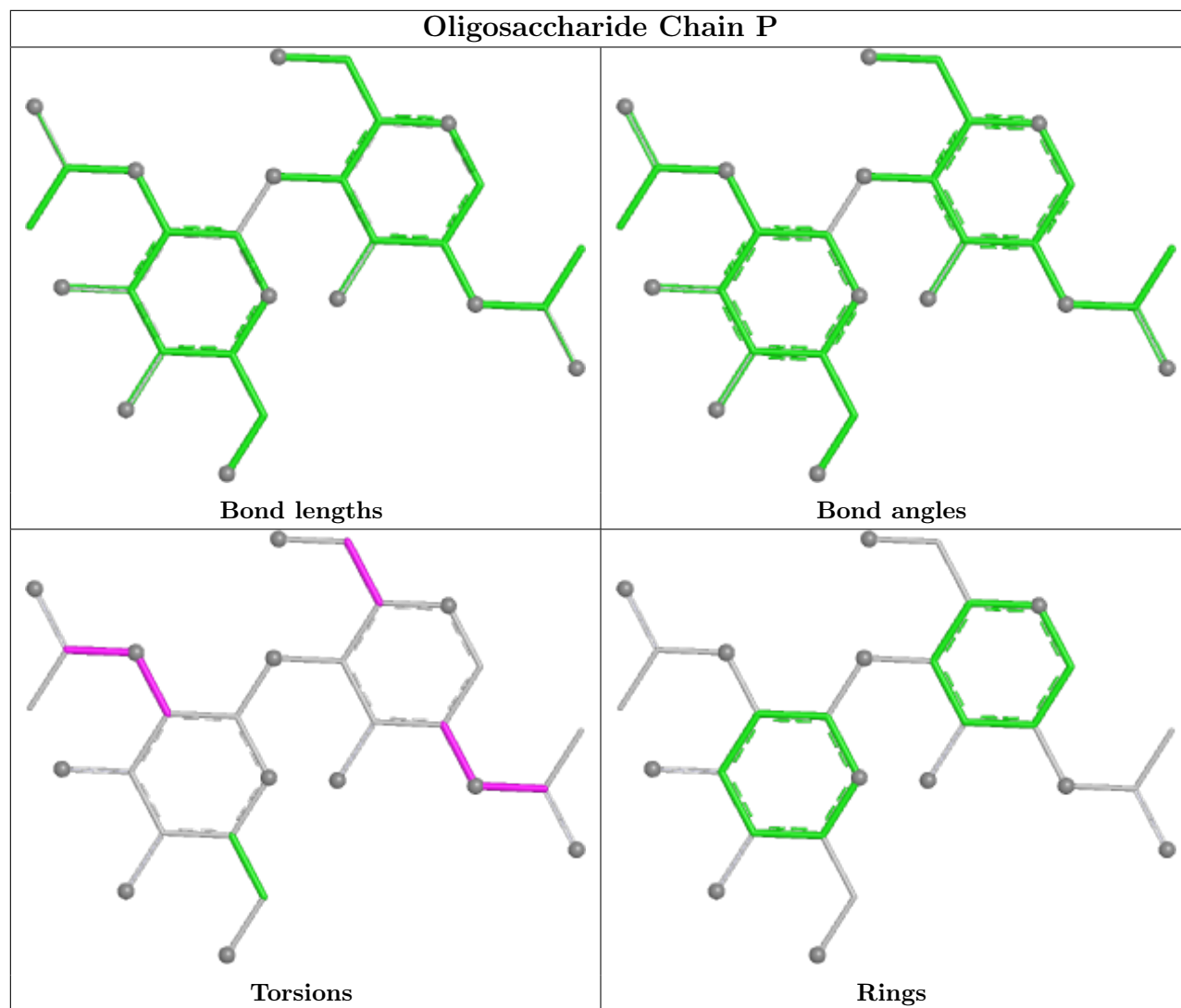


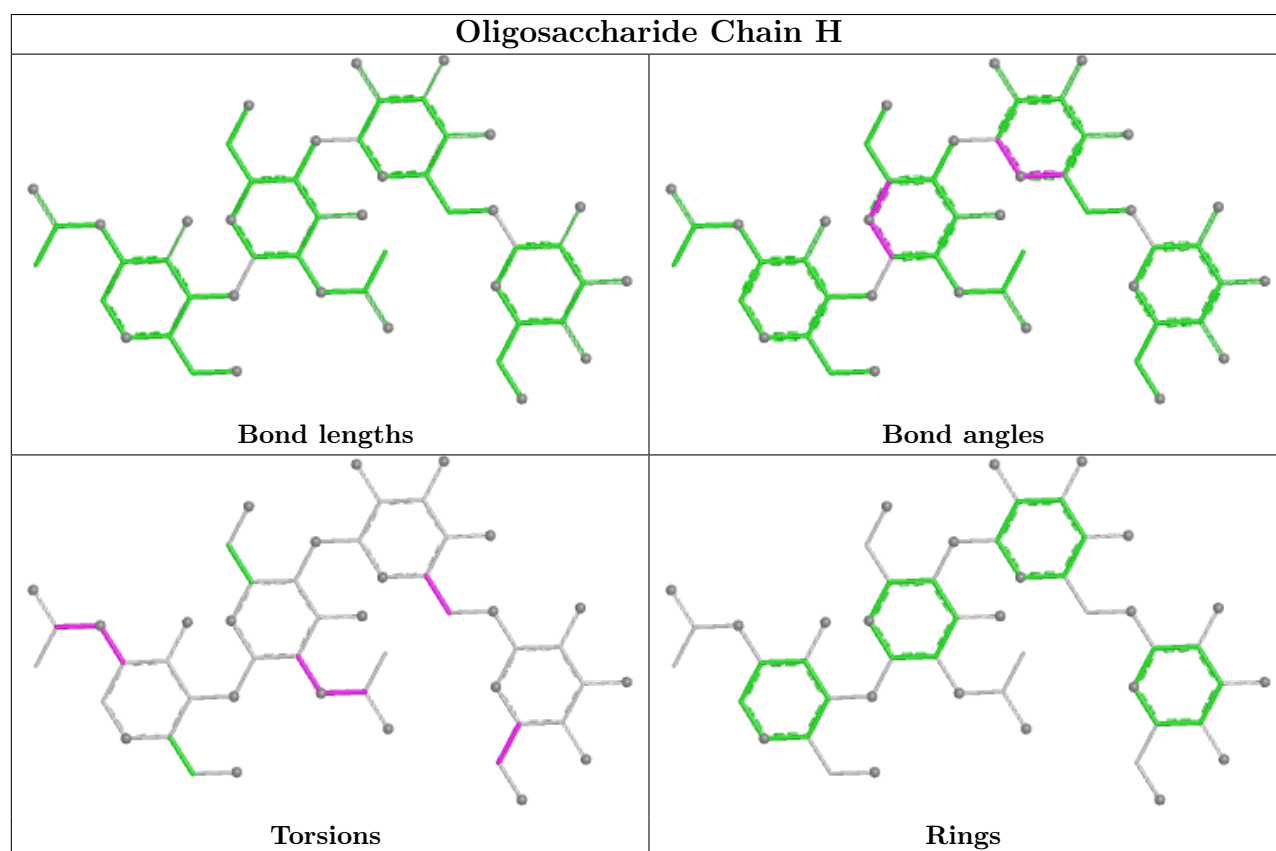
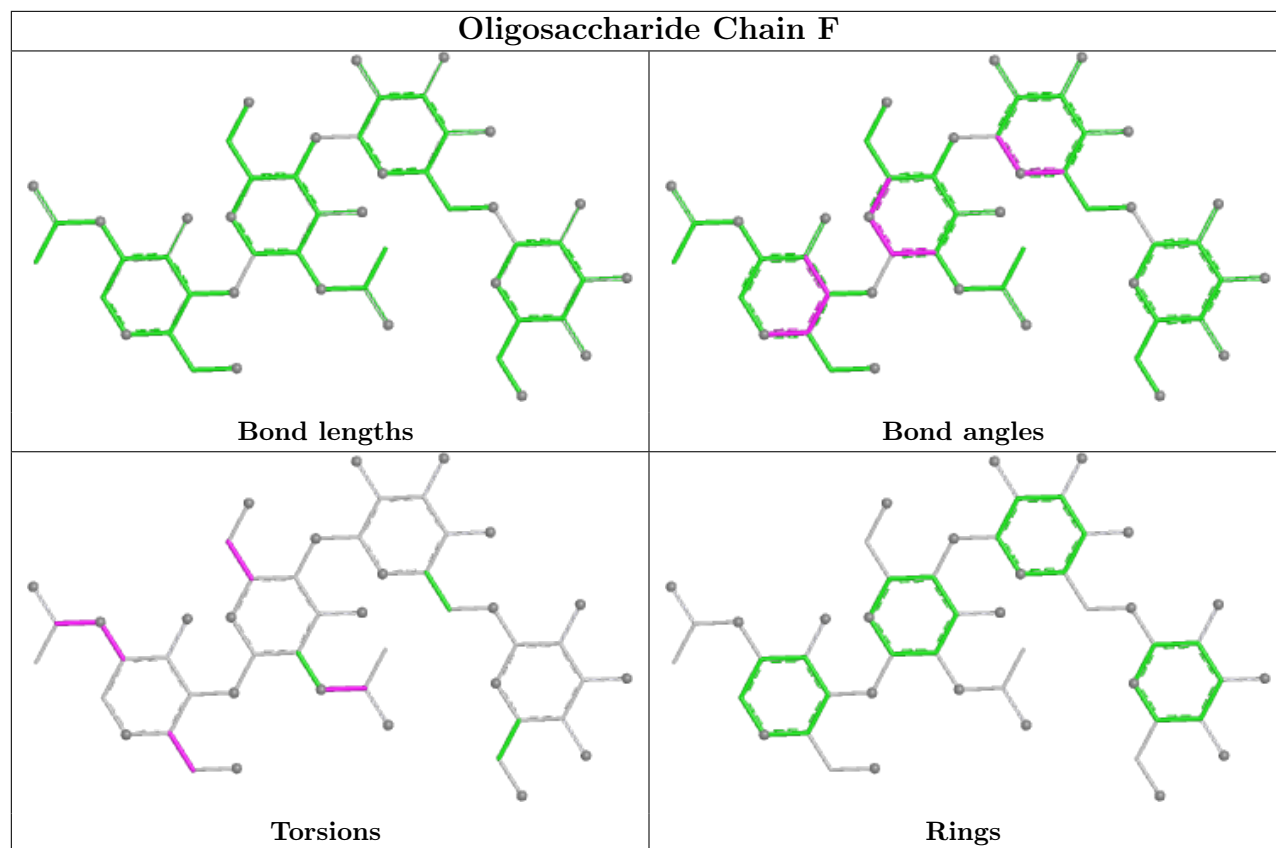




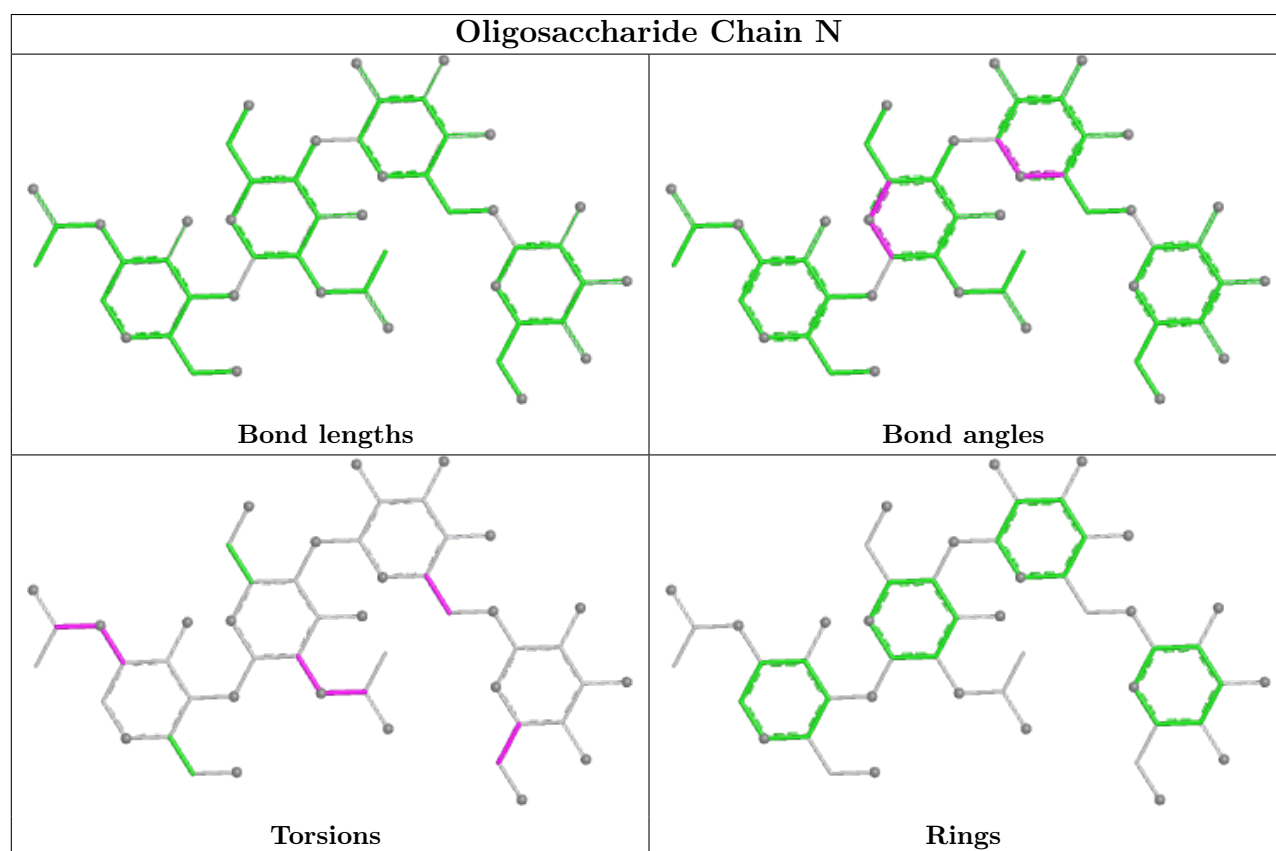
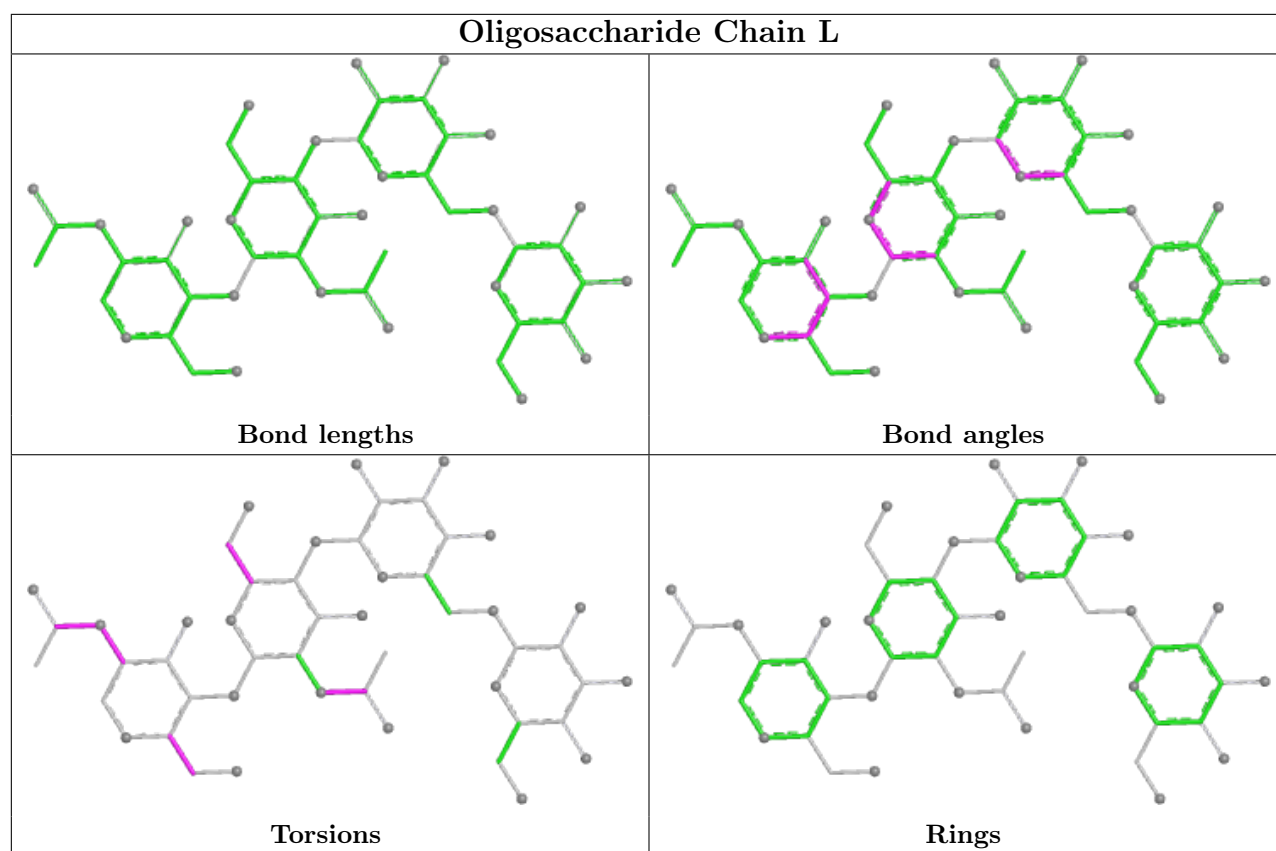


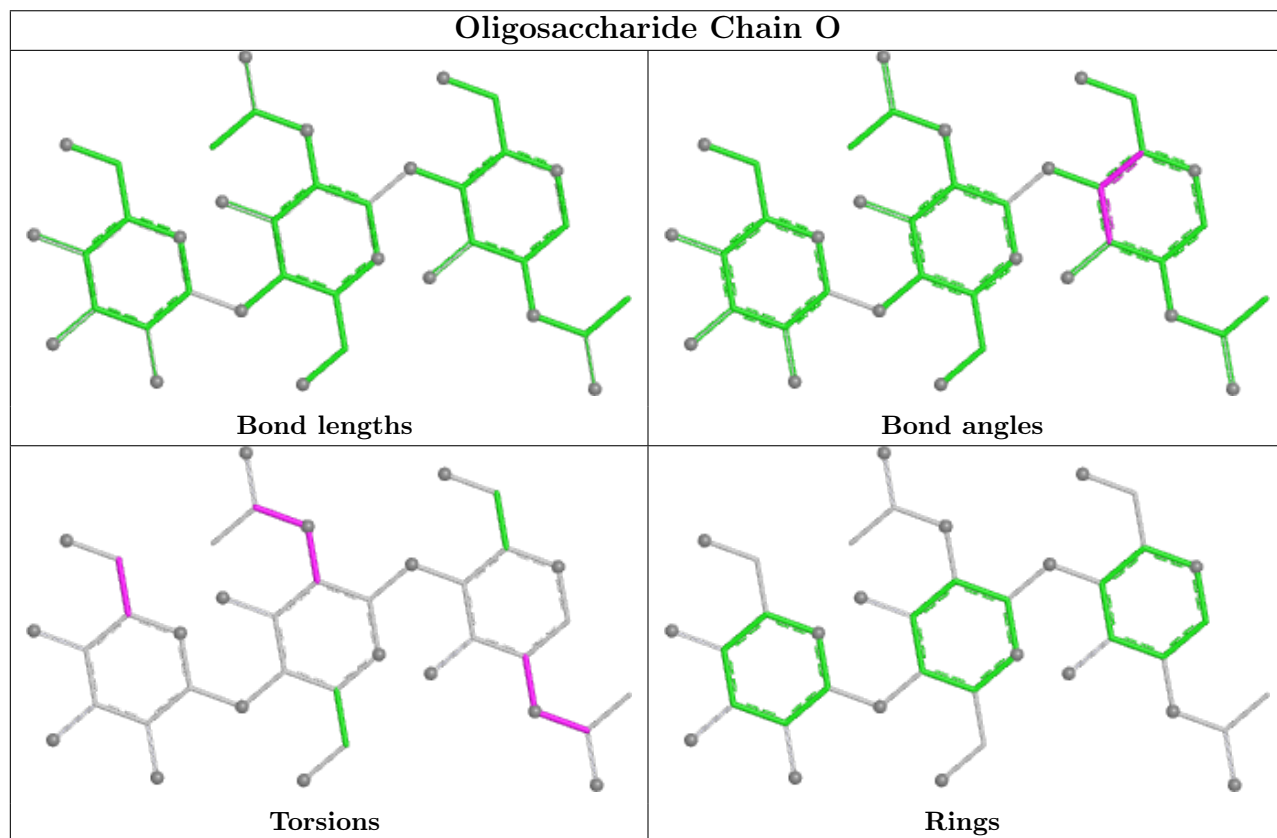
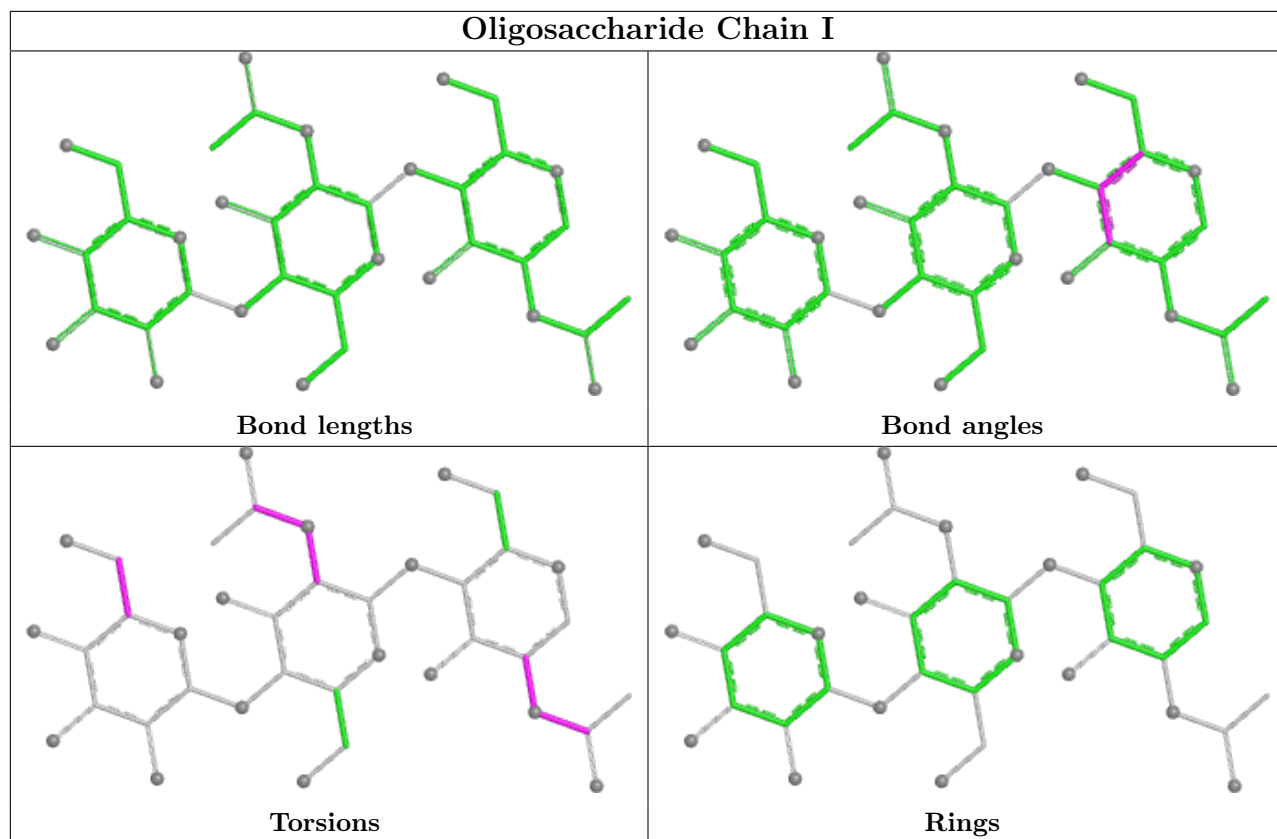












## 5.6 Ligand geometry

18 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	D	2003	1	14,14,15	0.32	0	17,19,21	0.73	0
5	NAG	B	2002	1	14,14,15	0.33	0	17,19,21	0.77	0
5	NAG	A	2005	1	14,14,15	0.30	0	17,19,21	0.64	0
5	NAG	C	2003	1	14,14,15	0.29	0	17,19,21	0.73	0
5	NAG	B	2001	1	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	C	2002	1	14,14,15	1.85	4 (28%)	17,19,21	0.91	0
5	NAG	C	2004	1	14,14,15	0.34	0	17,19,21	0.75	1 (5%)
5	NAG	A	2001	1	14,14,15	1.87	3 (21%)	17,19,21	1.11	2 (11%)
5	NAG	D	2001	1	14,14,15	0.27	0	17,19,21	1.26	2 (11%)
5	NAG	D	2004	1	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
5	NAG	C	2001	1	14,14,15	1.87	3 (21%)	17,19,21	1.11	2 (11%)
5	NAG	B	2004	1	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
5	NAG	C	2005	1	14,14,15	0.30	0	17,19,21	0.64	0
5	NAG	A	2004	1	14,14,15	0.34	0	17,19,21	0.75	1 (5%)
5	NAG	A	2003	1	14,14,15	0.29	0	17,19,21	0.73	0
5	NAG	A	2002	1	14,14,15	1.85	4 (28%)	17,19,21	0.91	0
5	NAG	B	2003	1	14,14,15	0.32	0	17,19,21	0.73	0
5	NAG	D	2002	1	14,14,15	0.33	0	17,19,21	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
5	NAG	D	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2002	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2005	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2001	1	-	1/6/23/26	0/1/1/1
5	NAG	C	2002	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	D	2001	1	-	1/6/23/26	0/1/1/1
5	NAG	D	2004	1	-	5/6/23/26	0/1/1/1
5	NAG	C	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2004	1	-	5/6/23/26	0/1/1/1
5	NAG	C	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2004	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2002	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	D	2002	1	-	4/6/23/26	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	NAG	O5-C1	4.28	1.50	1.43
5	C	2001	NAG	O5-C1	4.28	1.50	1.43
5	A	2002	NAG	O5-C1	3.97	1.50	1.43
5	C	2002	NAG	O5-C1	3.97	1.50	1.43
5	A	2002	NAG	C7-N2	3.37	1.45	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2001	NAG	C1-O5-C5	3.86	117.42	112.19
5	D	2001	NAG	C1-O5-C5	3.86	117.42	112.19
5	B	2004	NAG	C1-O5-C5	2.47	115.54	112.19
5	D	2004	NAG	C1-O5-C5	2.47	115.54	112.19
5	A	2001	NAG	C2-N2-C7	-2.30	119.63	122.90

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2003	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	B	2002	NAG	C3-C2-N2-C7
5	B	2002	NAG	C8-C7-N2-C2
5	B	2002	NAG	O7-C7-N2-C2
5	B	2003	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2003	NAG	1	0
5	B	2002	NAG	1	0
5	B	2004	NAG	1	0
5	D	2002	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	A	3
1	C	3
1	B	2

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	968:MET	C	969:PRO	N	1.68
1	D	968:MET	C	969:PRO	N	1.68
1	D	978:VAL	C	979:LEU	N	1.61
1	A	409:ILE	C	410:ASN	N	1.16
1	C	409:ILE	C	410:ASN	N	1.16

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12751. These allow visual inspection of the internal detail of the map and identification of artifacts.

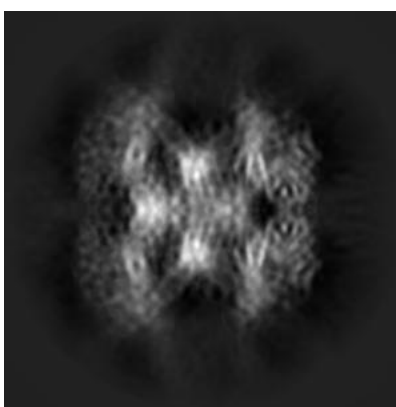
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

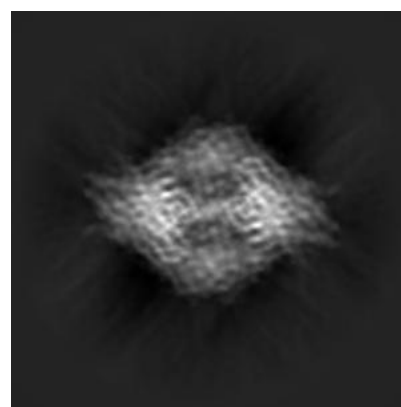
#### 6.1.1 Primary map



X



Y



Z

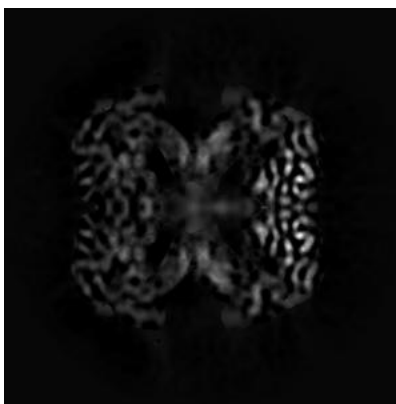
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

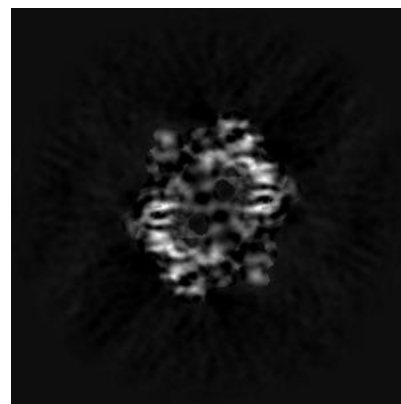
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

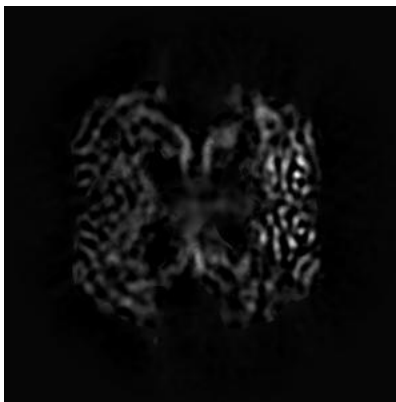
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

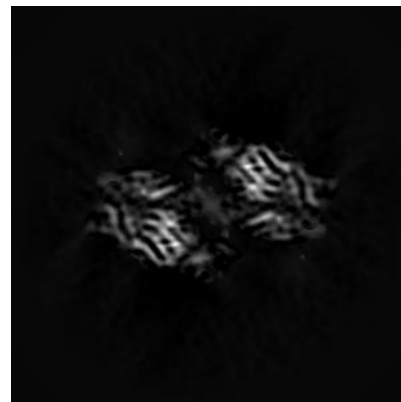
### 6.3.1 Primary map



X Index: 196



Y Index: 157

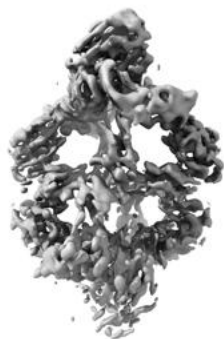


Z Index: 196

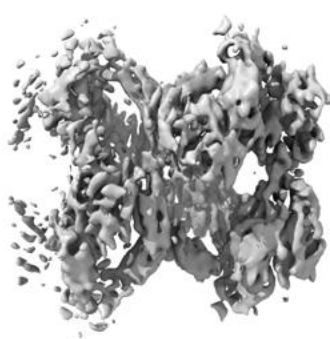
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

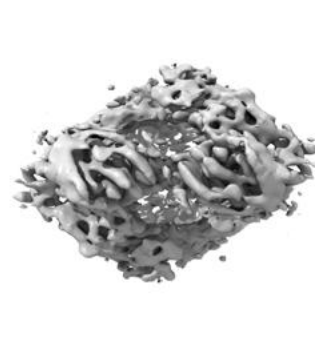
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

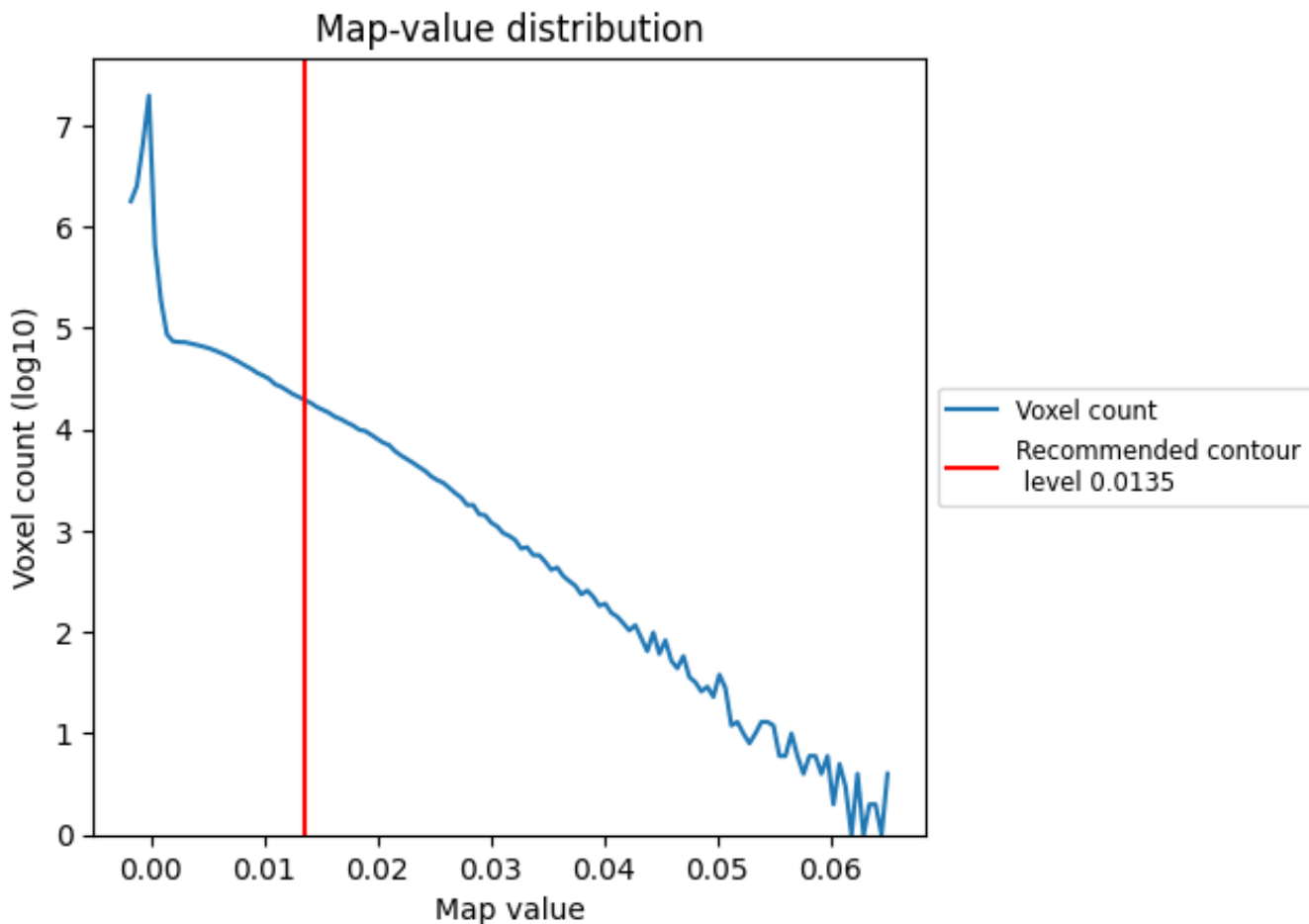
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

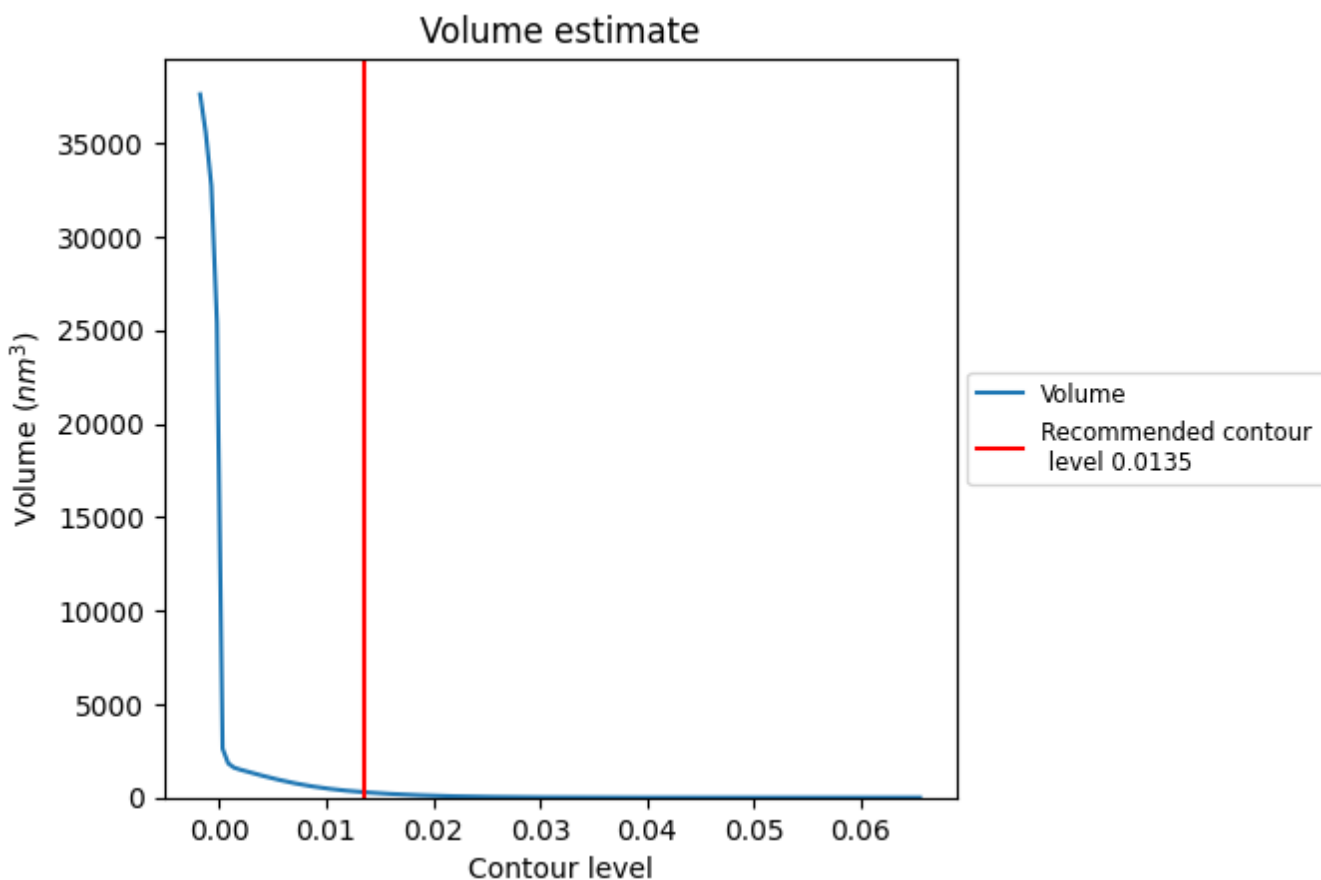
This section contains the results of statistical analysis of the map.

### 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.

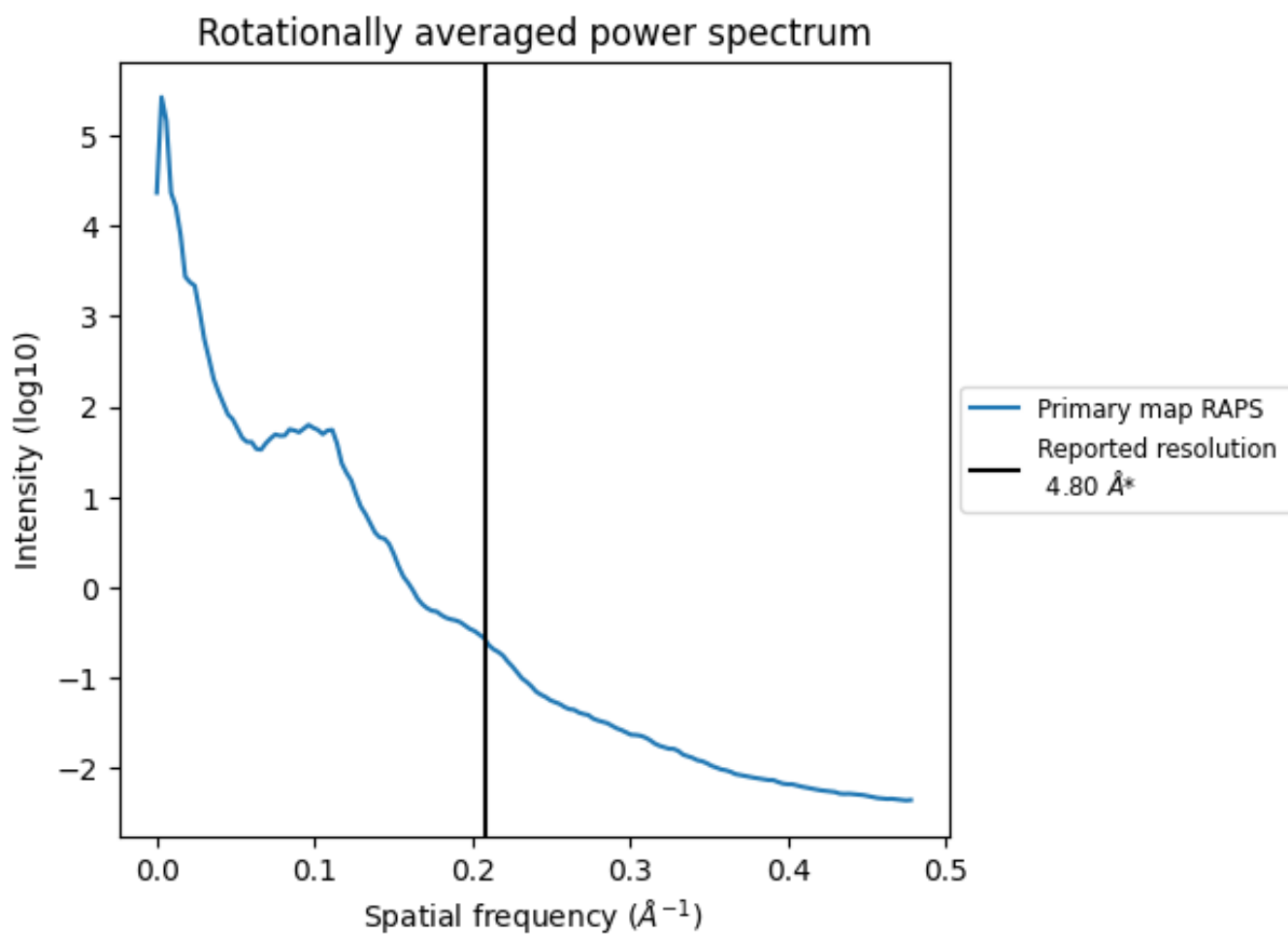
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 289 nm<sup>3</sup>; this corresponds to an approximate mass of 261 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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.208 Å<sup>-1</sup>

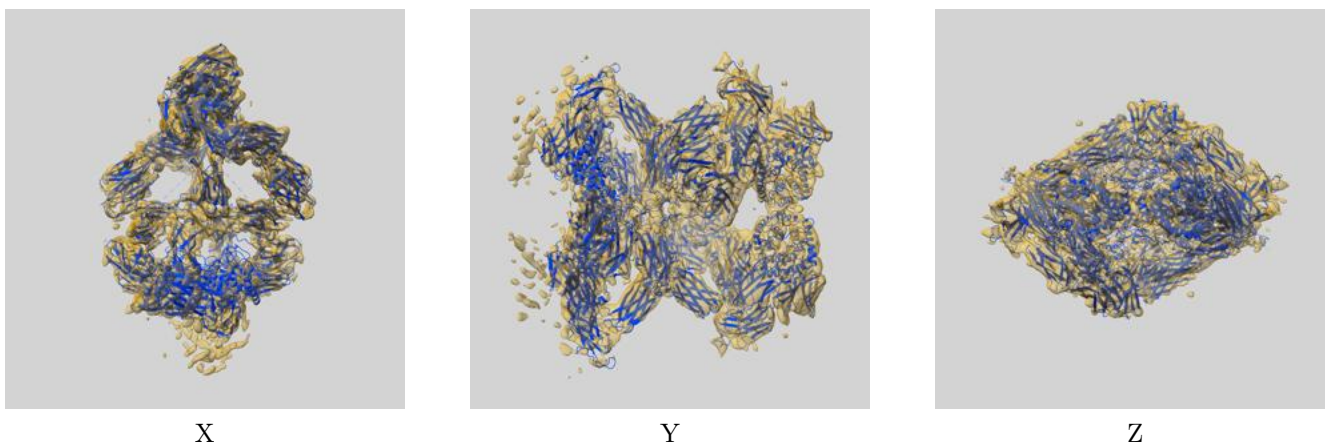
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

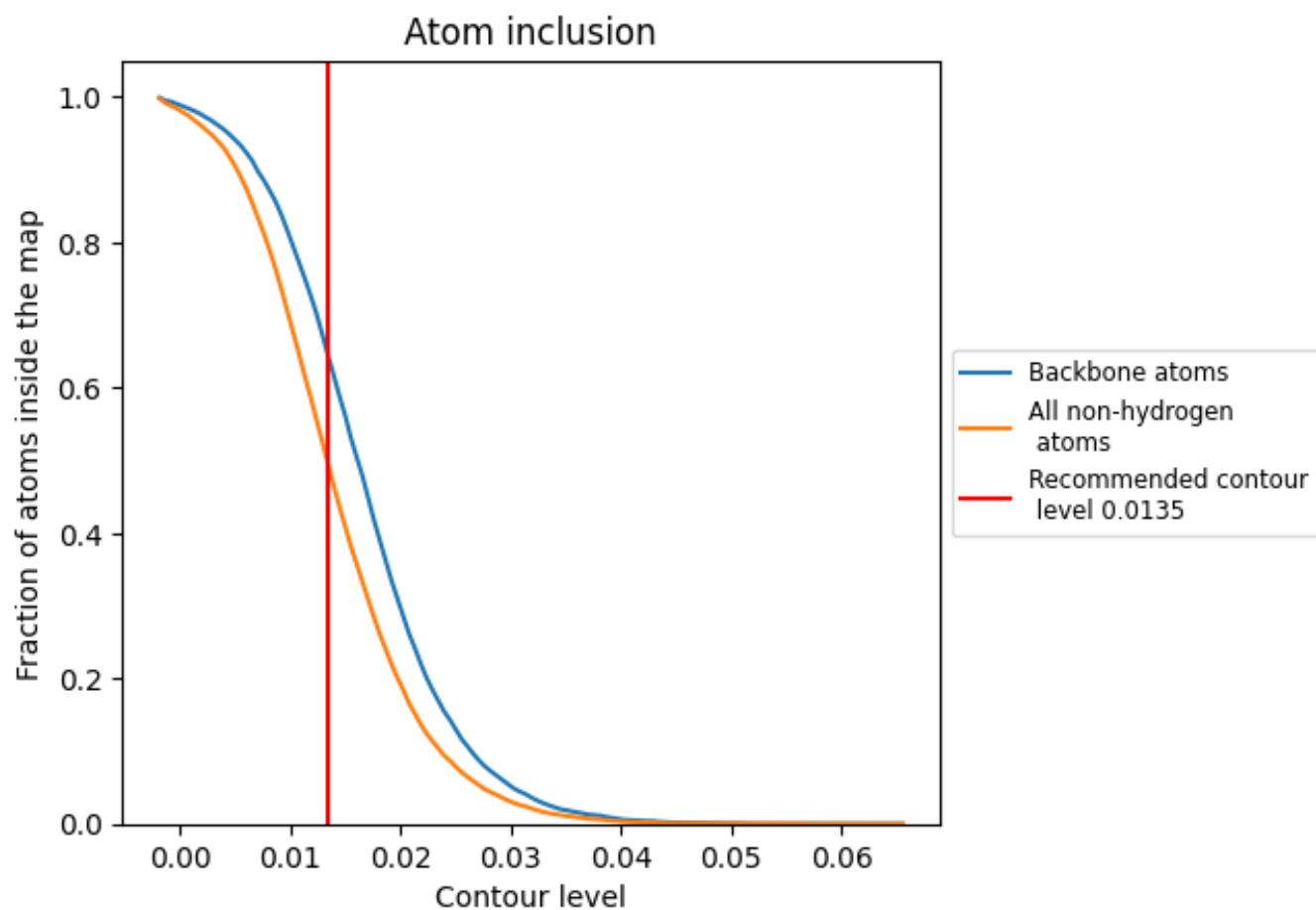
This section contains information regarding the fit between EMDB map EMD-12751 and PDB model 7O7O. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0135 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 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.