



wwPDB EM Validation Summary Report ⓘ

Apr 10, 2022 – 07:08 am BST

PDB ID : 7QNB
EMDB ID : EMD-14073
Title : Cryo-EM structure of human full-length beta3gamma2 GABA(A)R in complex with GABA and nanobody Nb25
Authors : Sente, A.; Desai, R.; Naydenova, K.; Malinauskas, T.; Jounaidi, Y.; Miehling, J.; Zhou, X.; Masiulis, S.; Hardwick, S.W.; Chirgadze, D.Y.; Miller, K.W.; Aricescu, A.R.
Deposited on : 2021-12-20
Resolution : 3.10 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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
buster-report : 1.1.7 (2018)
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

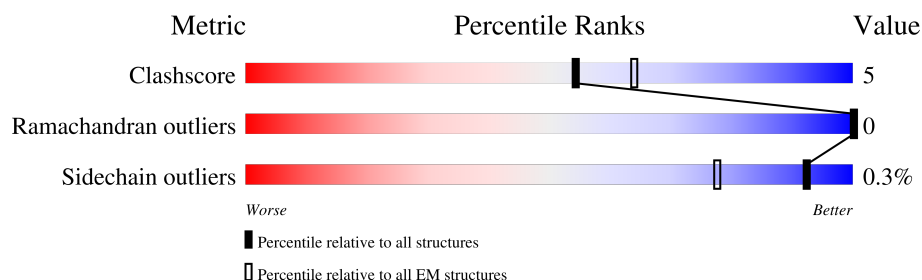
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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 ≥ 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	487	
1	C	487	
2	B	473	
2	D	473	
2	E	473	
3	N	121	
4	b	2	
4	d	2	

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Mol	Chain	Length	Quality of chain
4	e	2	 100%
5	F	5	 60% 40%
5	G	5	 80% 20%
5	H	5	 80% 20%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14793 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 Gamma-aminobutyric acid type A receptor subunit gamma2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	328	Total	C	N	O	S	0	0
			2701	1766	443	477	15		
1	C	328	Total	C	N	O	S	0	0
			2701	1766	443	477	15		

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP A0A2K5TLN2
A	-29	GLY	-	expression tag	UNP A0A2K5TLN2
A	-28	ILE	-	expression tag	UNP A0A2K5TLN2
A	-27	LEU	-	expression tag	UNP A0A2K5TLN2
A	-26	PRO	-	expression tag	UNP A0A2K5TLN2
A	-25	SER	-	expression tag	UNP A0A2K5TLN2
A	-24	PRO	-	expression tag	UNP A0A2K5TLN2
A	-23	GLY	-	expression tag	UNP A0A2K5TLN2
A	-22	MET	-	expression tag	UNP A0A2K5TLN2
A	-21	PRO	-	expression tag	UNP A0A2K5TLN2
A	-20	ALA	-	expression tag	UNP A0A2K5TLN2
A	-19	LEU	-	expression tag	UNP A0A2K5TLN2
A	-18	LEU	-	expression tag	UNP A0A2K5TLN2
A	-17	SER	-	expression tag	UNP A0A2K5TLN2
A	-16	LEU	-	expression tag	UNP A0A2K5TLN2
A	-15	VAL	-	expression tag	UNP A0A2K5TLN2
A	-14	SER	-	expression tag	UNP A0A2K5TLN2
A	-13	LEU	-	expression tag	UNP A0A2K5TLN2
A	-12	LEU	-	expression tag	UNP A0A2K5TLN2
A	-11	SER	-	expression tag	UNP A0A2K5TLN2
A	-10	VAL	-	expression tag	UNP A0A2K5TLN2
A	-9	LEU	-	expression tag	UNP A0A2K5TLN2
A	-8	LEU	-	expression tag	UNP A0A2K5TLN2
A	-7	MET	-	expression tag	UNP A0A2K5TLN2
A	-6	GLY	-	expression tag	UNP A0A2K5TLN2
A	-5	CYS	-	expression tag	UNP A0A2K5TLN2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	VAL	-	expression tag	UNP A0A2K5TLN2
A	-3	ALA	-	expression tag	UNP A0A2K5TLN2
A	-2	GLU	-	expression tag	UNP A0A2K5TLN2
A	-1	THR	-	expression tag	UNP A0A2K5TLN2
A	0	GLY	-	expression tag	UNP A0A2K5TLN2
A	1	GLN	-	expression tag	UNP A0A2K5TLN2
A	2	LYS	-	expression tag	UNP A0A2K5TLN2
A	3	SER	-	expression tag	UNP A0A2K5TLN2
A	4	ASP	-	expression tag	UNP A0A2K5TLN2
A	5	ASP	-	expression tag	UNP A0A2K5TLN2
A	6	ASP	-	expression tag	UNP A0A2K5TLN2
A	7	TYR	-	expression tag	UNP A0A2K5TLN2
A	8	GLU	-	expression tag	UNP A0A2K5TLN2
A	9	ASP	-	expression tag	UNP A0A2K5TLN2
A	10	TYR	-	expression tag	UNP A0A2K5TLN2
A	11	THR	-	expression tag	UNP A0A2K5TLN2
A	437	GLY	-	expression tag	UNP A0A2K5TLN2
A	438	THR	-	expression tag	UNP A0A2K5TLN2
A	439	GLY	-	expression tag	UNP A0A2K5TLN2
A	440	GLY	-	expression tag	UNP A0A2K5TLN2
A	441	SER	-	expression tag	UNP A0A2K5TLN2
A	442	GLY	-	expression tag	UNP A0A2K5TLN2
A	443	GLY	-	expression tag	UNP A0A2K5TLN2
A	444	SER	-	expression tag	UNP A0A2K5TLN2
A	445	GLY	-	expression tag	UNP A0A2K5TLN2
A	446	GLY	-	expression tag	UNP A0A2K5TLN2
A	447	SER	-	expression tag	UNP A0A2K5TLN2
A	448	THR	-	expression tag	UNP A0A2K5TLN2
A	449	GLU	-	expression tag	UNP A0A2K5TLN2
A	450	THR	-	expression tag	UNP A0A2K5TLN2
A	451	SER	-	expression tag	UNP A0A2K5TLN2
A	452	GLN	-	expression tag	UNP A0A2K5TLN2
A	453	VAL	-	expression tag	UNP A0A2K5TLN2
A	454	ALA	-	expression tag	UNP A0A2K5TLN2
A	455	PRO	-	expression tag	UNP A0A2K5TLN2
A	456	ALA	-	expression tag	UNP A0A2K5TLN2
C	-30	MET	-	initiating methionine	UNP A0A2K5TLN2
C	-29	GLY	-	expression tag	UNP A0A2K5TLN2
C	-28	ILE	-	expression tag	UNP A0A2K5TLN2
C	-27	LEU	-	expression tag	UNP A0A2K5TLN2
C	-26	PRO	-	expression tag	UNP A0A2K5TLN2
C	-25	SER	-	expression tag	UNP A0A2K5TLN2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	PRO	-	expression tag	UNP A0A2K5TLN2
C	-23	GLY	-	expression tag	UNP A0A2K5TLN2
C	-22	MET	-	expression tag	UNP A0A2K5TLN2
C	-21	PRO	-	expression tag	UNP A0A2K5TLN2
C	-20	ALA	-	expression tag	UNP A0A2K5TLN2
C	-19	LEU	-	expression tag	UNP A0A2K5TLN2
C	-18	LEU	-	expression tag	UNP A0A2K5TLN2
C	-17	SER	-	expression tag	UNP A0A2K5TLN2
C	-16	LEU	-	expression tag	UNP A0A2K5TLN2
C	-15	VAL	-	expression tag	UNP A0A2K5TLN2
C	-14	SER	-	expression tag	UNP A0A2K5TLN2
C	-13	LEU	-	expression tag	UNP A0A2K5TLN2
C	-12	LEU	-	expression tag	UNP A0A2K5TLN2
C	-11	SER	-	expression tag	UNP A0A2K5TLN2
C	-10	VAL	-	expression tag	UNP A0A2K5TLN2
C	-9	LEU	-	expression tag	UNP A0A2K5TLN2
C	-8	LEU	-	expression tag	UNP A0A2K5TLN2
C	-7	MET	-	expression tag	UNP A0A2K5TLN2
C	-6	GLY	-	expression tag	UNP A0A2K5TLN2
C	-5	CYS	-	expression tag	UNP A0A2K5TLN2
C	-4	VAL	-	expression tag	UNP A0A2K5TLN2
C	-3	ALA	-	expression tag	UNP A0A2K5TLN2
C	-2	GLU	-	expression tag	UNP A0A2K5TLN2
C	-1	THR	-	expression tag	UNP A0A2K5TLN2
C	0	GLY	-	expression tag	UNP A0A2K5TLN2
C	1	GLN	-	expression tag	UNP A0A2K5TLN2
C	2	LYS	-	expression tag	UNP A0A2K5TLN2
C	3	SER	-	expression tag	UNP A0A2K5TLN2
C	4	ASP	-	expression tag	UNP A0A2K5TLN2
C	5	ASP	-	expression tag	UNP A0A2K5TLN2
C	6	ASP	-	expression tag	UNP A0A2K5TLN2
C	7	TYR	-	expression tag	UNP A0A2K5TLN2
C	8	GLU	-	expression tag	UNP A0A2K5TLN2
C	9	ASP	-	expression tag	UNP A0A2K5TLN2
C	10	TYR	-	expression tag	UNP A0A2K5TLN2
C	11	THR	-	expression tag	UNP A0A2K5TLN2
C	437	GLY	-	expression tag	UNP A0A2K5TLN2
C	438	THR	-	expression tag	UNP A0A2K5TLN2
C	439	GLY	-	expression tag	UNP A0A2K5TLN2
C	440	GLY	-	expression tag	UNP A0A2K5TLN2
C	441	SER	-	expression tag	UNP A0A2K5TLN2
C	442	GLY	-	expression tag	UNP A0A2K5TLN2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	443	GLY	-	expression tag	UNP A0A2K5TLN2
C	444	SER	-	expression tag	UNP A0A2K5TLN2
C	445	GLY	-	expression tag	UNP A0A2K5TLN2
C	446	GLY	-	expression tag	UNP A0A2K5TLN2
C	447	SER	-	expression tag	UNP A0A2K5TLN2
C	448	THR	-	expression tag	UNP A0A2K5TLN2
C	449	GLU	-	expression tag	UNP A0A2K5TLN2
C	450	THR	-	expression tag	UNP A0A2K5TLN2
C	451	SER	-	expression tag	UNP A0A2K5TLN2
C	452	GLN	-	expression tag	UNP A0A2K5TLN2
C	453	VAL	-	expression tag	UNP A0A2K5TLN2
C	454	ALA	-	expression tag	UNP A0A2K5TLN2
C	455	PRO	-	expression tag	UNP A0A2K5TLN2
C	456	ALA	-	expression tag	UNP A0A2K5TLN2

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	330	Total	C	N	O	S	1	0
			2714	1780	440	478	16		
2	D	330	Total	C	N	O	S	1	0
			2721	1784	441	480	16		
2	E	330	Total	C	N	O	S	1	0
			2714	1780	440	478	16		

- Molecule 3 is a protein called Nanobody Nb25.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	121	Total	C	N	O	S	0	0
			940	593	161	182	4		

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



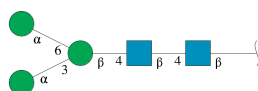
Mol	Chain	Residues	Atoms				AltConf	Trace
4	b	2	Total	C	N	O	0	0
			28	16	2	10		

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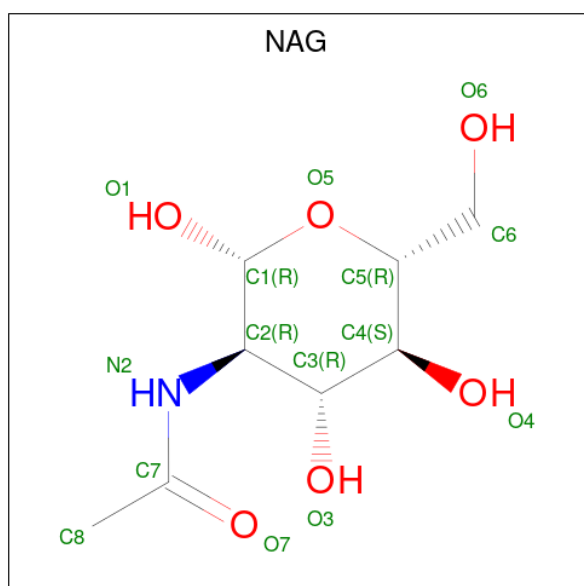
Mol	Chain	Residues	Atoms				AltConf	Trace
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		

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



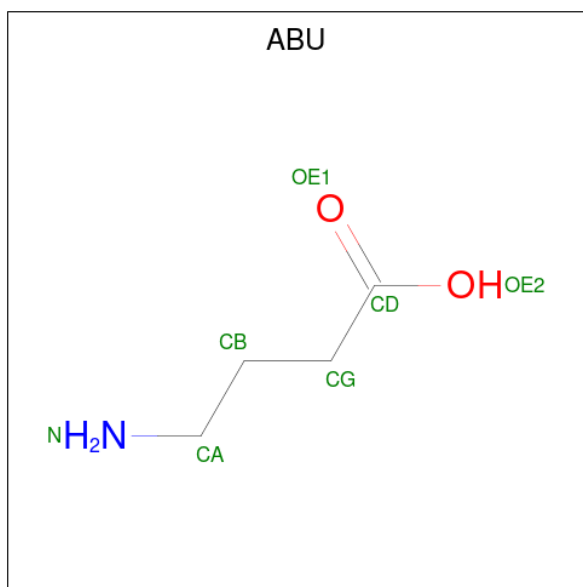
Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	5	Total	C	N	O	0	0
			61	34	2	25		
5	G	5	Total	C	N	O	0	0
			61	34	2	25		
5	H	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: $C_4H_9NO_2$) (labeled as "Ligand of Interest" by depositor).




Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			7	4	1	2	

Chain E: 61% 9% 30%

Position	Residue	Category
1	GLN	Conserved
2	ASP	Conserved
3	ASP	Conserved
4	ASP	Conserved
5	ASP	Conserved
6	ASP	Conserved
7	ASP	Conserved
8	ASP	Conserved
9	ASP	Conserved
10	ASP	Conserved
11	ASP	Conserved
12	ASP	Conserved
13	ASP	Conserved
14	ASP	Conserved
15	ASP	Conserved
16	ASP	Conserved
17	ASP	Conserved
18	ASP	Conserved
19	ASP	Conserved
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22	ASP	Conserved
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153	ASP	Conserved
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155	ASP	Conserved
156	ASP	Conserved
157	ASP	Conserved
158	ASP	Conserved
159	ASP	Conserved
160	ASP	Conserved
161	ASP	Conserved
162		

- Molecule 3: Nanobody Nb25

Chain N:  78% 22%



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

Chain b:  100%



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

Chain d:  50% 100%



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

Chain e:  100%




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

Chain F:  60% 40%




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

Chain G:  80% 20%



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

Chain H:  80% 20%

MAG1
MAG2
EMA3
MAN4
MAN5

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.46	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	259.84, 259.84, 259.84	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89599997, 0.89599997, 0.89599997	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: MAN, BMA, ABU, 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	0.24	0/2775	0.46	0/3779
1	C	0.24	0/2775	0.46	0/3779
2	B	0.25	0/2789	0.46	0/3795
2	D	0.25	0/2794	0.46	0/3802
2	E	0.25	0/2789	0.46	0/3795
3	N	0.25	0/963	0.47	0/1304
All	All	0.24	0/14885	0.46	0/20254

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	2701	0	2693	26	0
1	C	2701	0	2693	33	0
2	B	2714	0	2709	33	0
2	D	2721	0	2706	41	0
2	E	2714	0	2709	31	0
3	N	940	0	887	15	0
4	b	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	28	0	25	0	0
4	e	28	0	25	0	0
5	F	61	0	52	2	0
5	G	61	0	52	1	0
5	H	61	0	52	2	0
6	A	14	0	13	0	0
6	C	14	0	13	0	0
7	B	7	0	5	1	0
All	All	14793	0	14659	159	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.

The worst 5 of 159 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)
2:B:272:LEU:HD13	2:B:279:LYS:HE3	1.67	0.77
2:D:272:LEU:HD13	2:D:279:LYS:HE3	1.67	0.75
2:E:272:LEU:HD13	2:E:279:LYS:HE3	1.67	0.75
3:N:478:THR:HG22	3:N:510:VAL:H	1.57	0.68
2:B:44[A]:ILE:HD12	2:B:59:LEU:HD11	1.76	0.67

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	324/487 (66%)	312 (96%)	12 (4%)	0	100	100
1	C	324/487 (66%)	312 (96%)	12 (4%)	0	100	100
2	B	327/473 (69%)	326 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	327/473 (69%)	326 (100%)	1 (0%)	0	100	100
2	E	327/473 (69%)	326 (100%)	1 (0%)	0	100	100
3	N	117/121 (97%)	115 (98%)	2 (2%)	0	100	100
All	All	1746/2514 (70%)	1717 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/437 (69%)	303 (100%)	0	100	100
1	C	303/437 (69%)	303 (100%)	0	100	100
2	B	298/417 (72%)	297 (100%)	1 (0%)	92	96
2	D	298/417 (72%)	297 (100%)	1 (0%)	92	96
2	E	298/417 (72%)	297 (100%)	1 (0%)	92	96
3	N	97/97 (100%)	96 (99%)	1 (1%)	76	90
All	All	1597/2222 (72%)	1593 (100%)	4 (0%)	92	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	275	ILE
2	D	275	ILE
2	E	275	ILE
3	N	459	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	323	ASN
1	C	323	ASN
2	D	267	HIS

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](#)

21 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	$\# Z > 2$
5	NAG	F	1	2,5	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	F	2	5	14,14,15	0.22	0	17,19,21	0.47	0
5	BMA	F	3	5	11,11,12	0.60	0	15,15,17	0.78	0
5	MAN	F	4	5	11,11,12	0.19	0	15,15,17	0.25	0
5	MAN	F	5	5	11,11,12	0.20	0	15,15,17	0.25	0
5	NAG	G	1	2,5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.48	0
5	BMA	G	3	5	11,11,12	0.62	0	15,15,17	0.84	0
5	MAN	G	4	5	11,11,12	0.21	0	15,15,17	0.23	0
5	MAN	G	5	5	11,11,12	0.21	0	15,15,17	0.23	0
5	NAG	H	1	2,5	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	H	2	5	14,14,15	0.24	0	17,19,21	0.55	0
5	BMA	H	3	5	11,11,12	0.68	0	15,15,17	0.93	0
5	MAN	H	4	5	11,11,12	0.21	0	15,15,17	0.26	0
5	MAN	H	5	5	11,11,12	0.19	0	15,15,17	0.24	0
4	NAG	b	1	2,4	14,14,15	0.23	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	b	2	4	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	d	1	2,4	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	d	2	4	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	e	1	2,4	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	e	2	4	14,14,15	0.23	0	17,19,21	0.40	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	F	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	NAG	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
5	NAG	H	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
4	NAG	b	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	NAG	d	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	NAG	e	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	3	BMA	C4-C5-C6-O6

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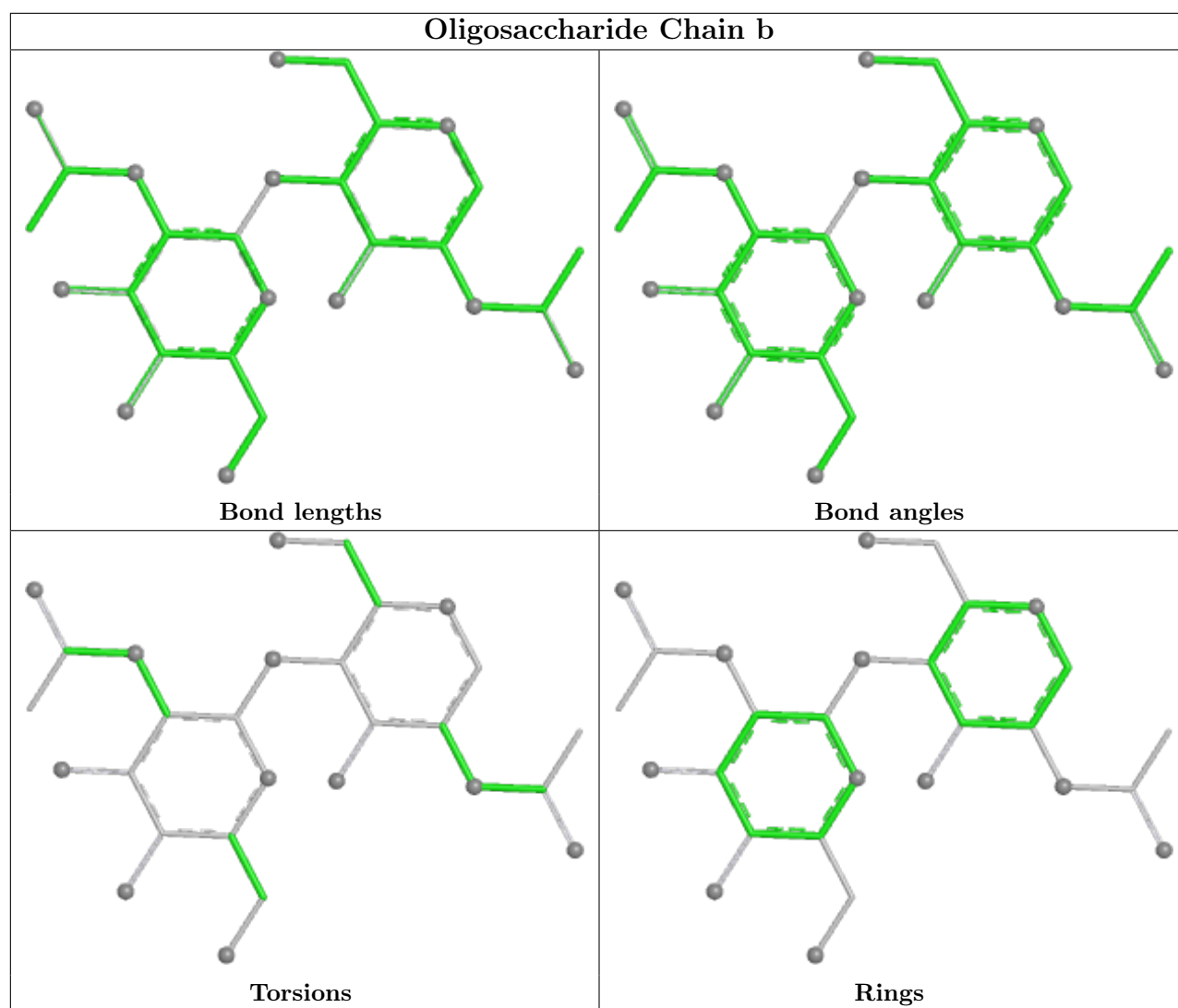
Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
5	H	3	BMA	C4-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6

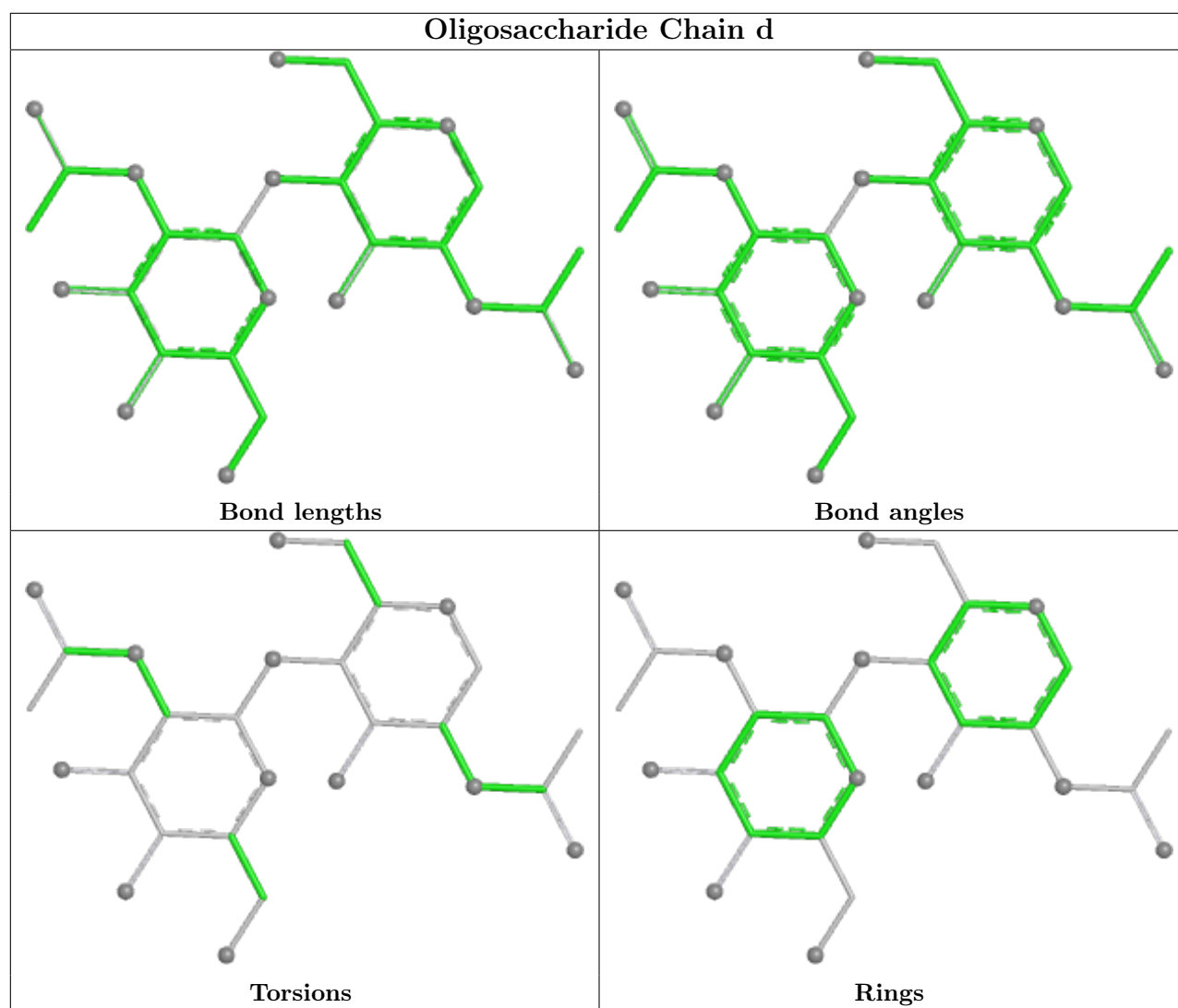
There are no ring outliers.

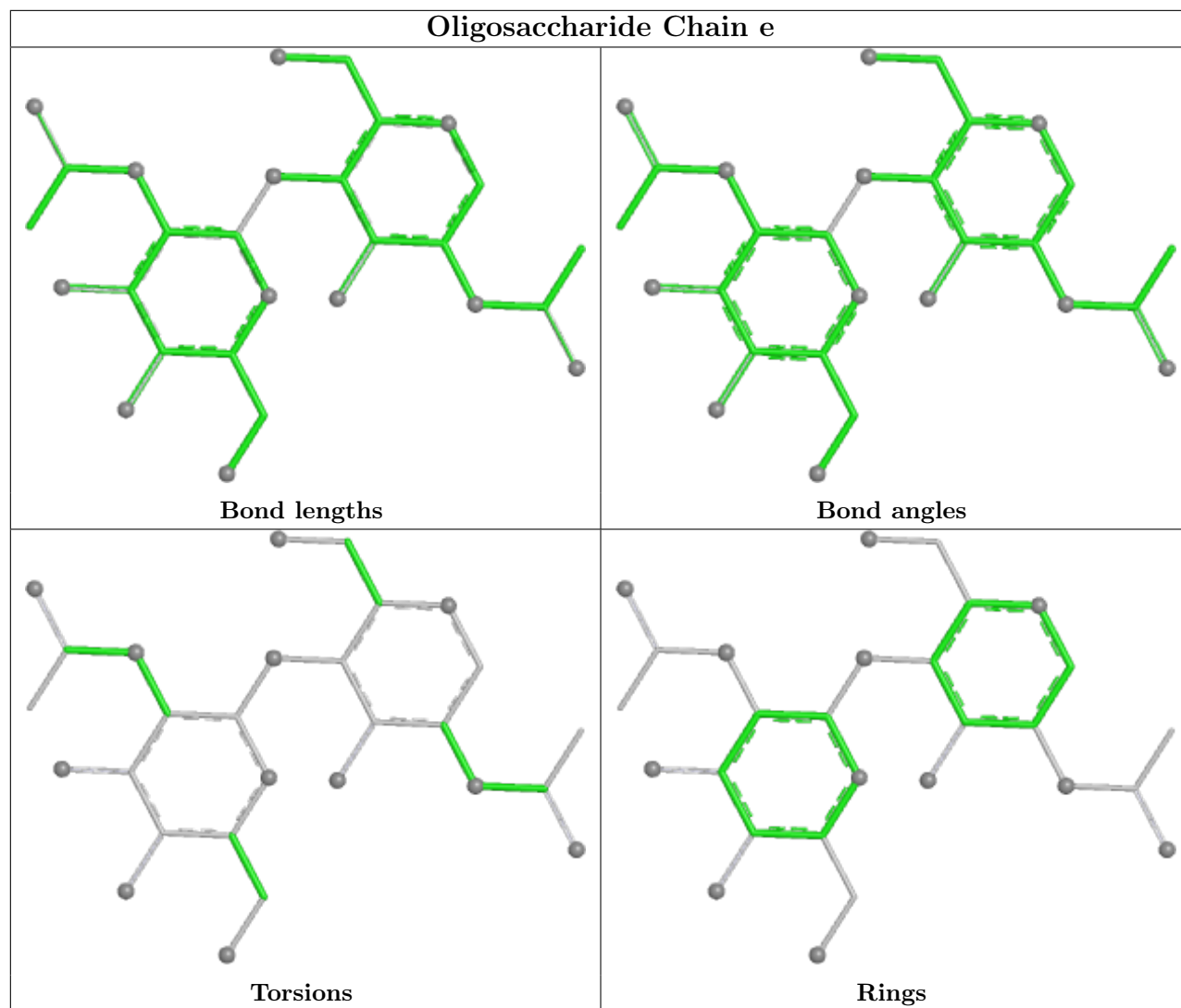
4 monomers are involved in 5 short contacts:

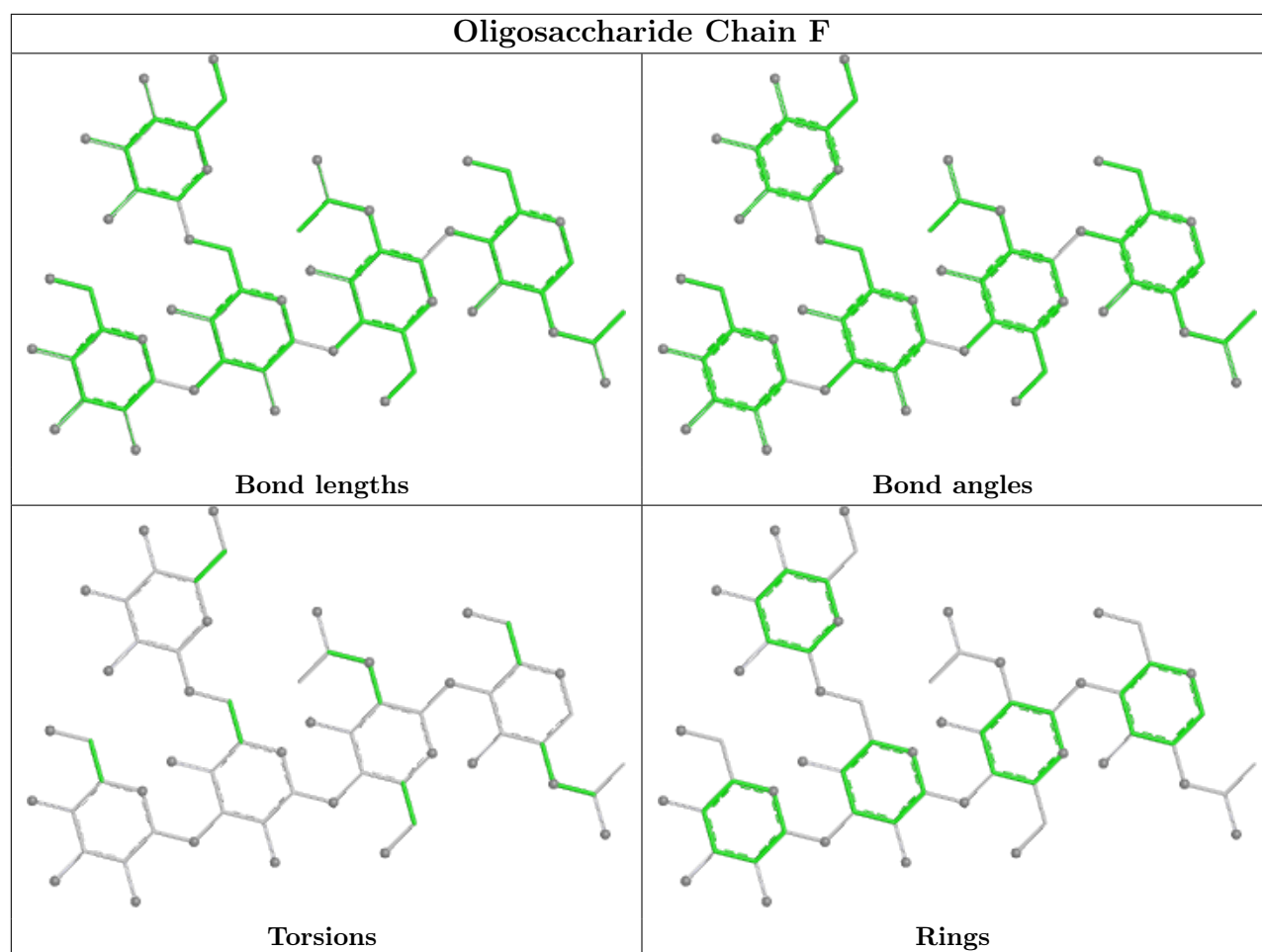
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	1	0
5	F	1	NAG	1	0
5	F	2	NAG	1	0
5	H	1	NAG	2	0

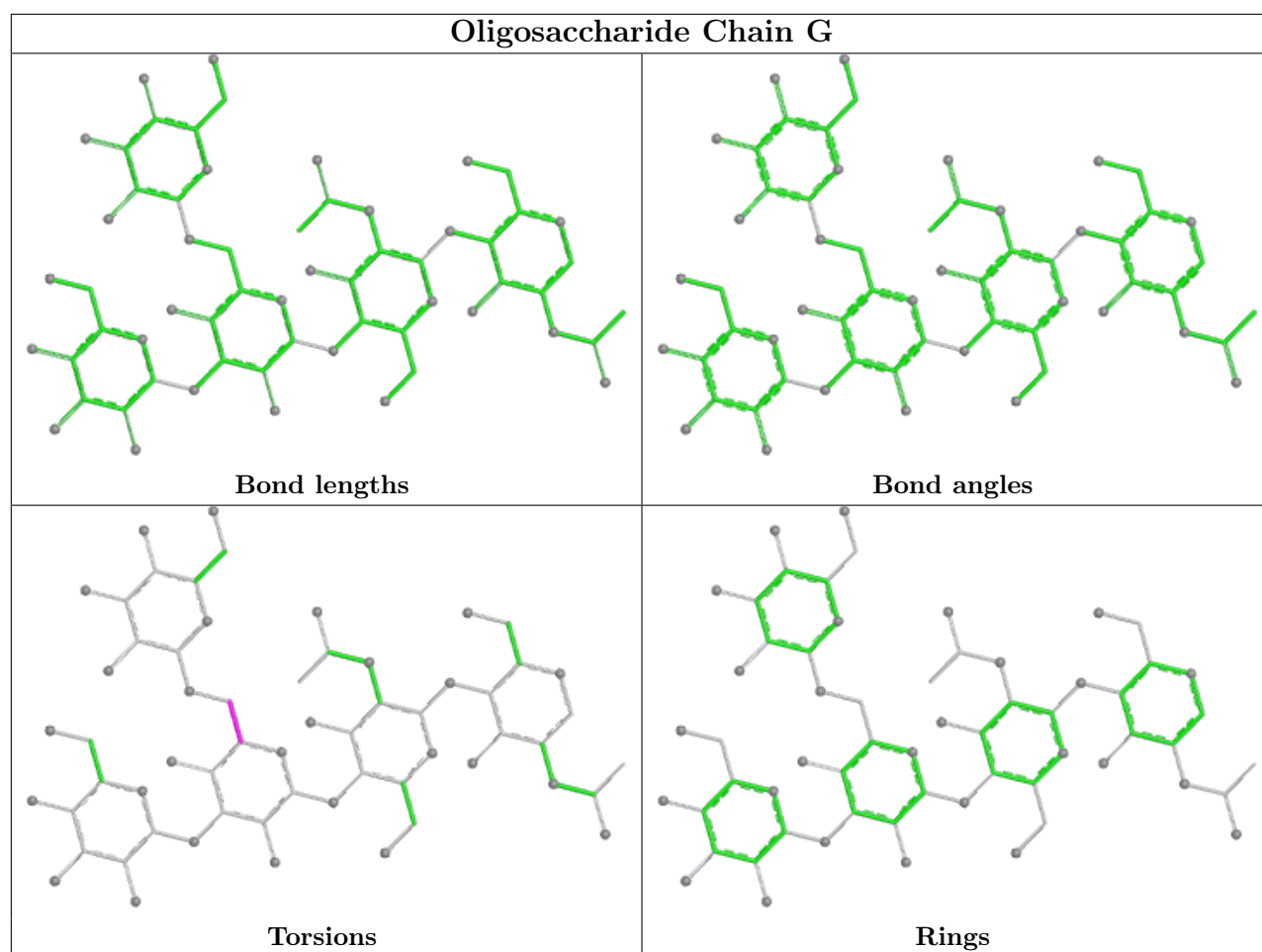
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

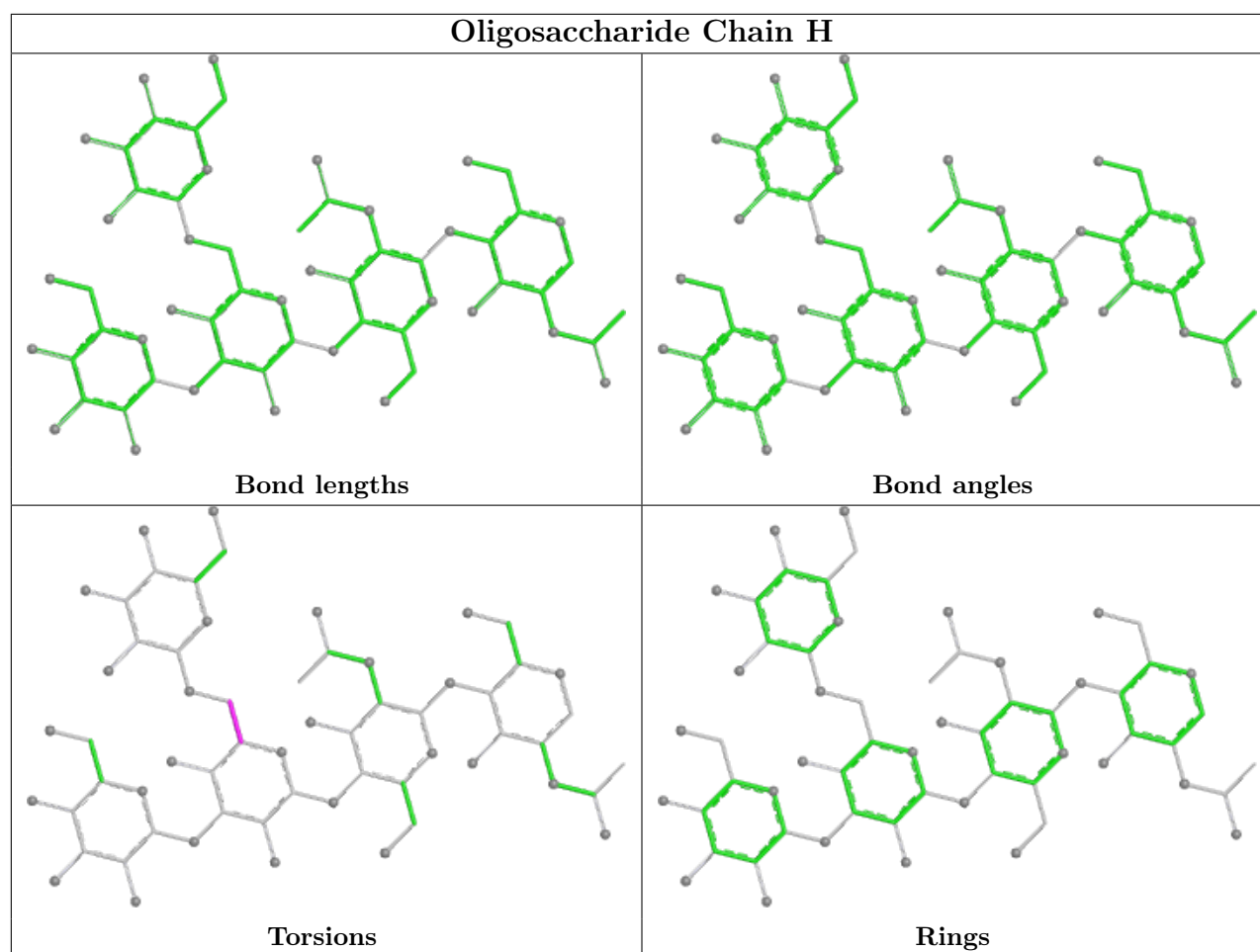












5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
7	ABU	B	501	-	3,6,6	0.13	0	2,6,6	0.03	0
6	NAG	A	501	1	14,14,15	0.21	0	17,19,21	0.49	0
6	NAG	C	501	1	14,14,15	0.22	0	17,19,21	0.46	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
7	ABU	B	501	-	-	0/2/4/4	-
6	NAG	A	501	1	-	1/6/23/26	0/1/1/1
6	NAG	C	501	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

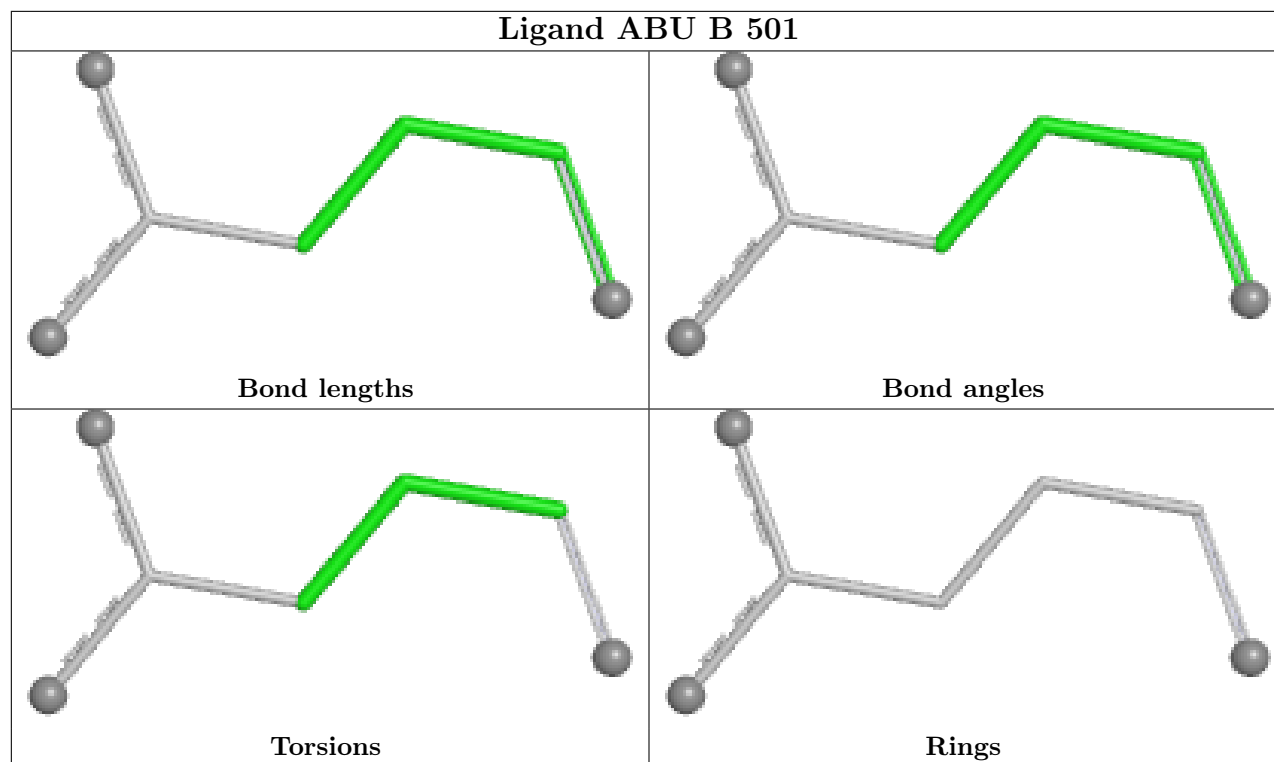
Mol	Chain	Res	Type	Atoms
6	C	501	NAG	O5-C5-C6-O6
6	A	501	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	ABU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	13:GLN	C	403:GLY	N	5.63

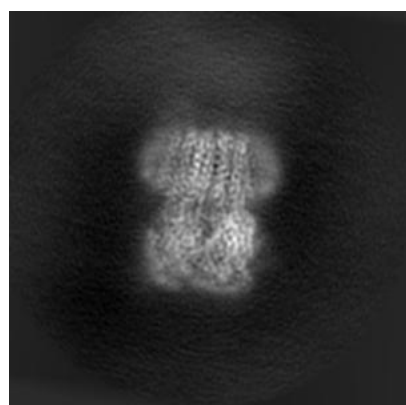
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14073. These allow visual inspection of the internal detail of the map and identification of artifacts.

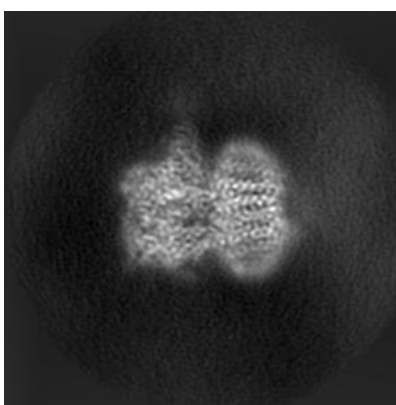
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

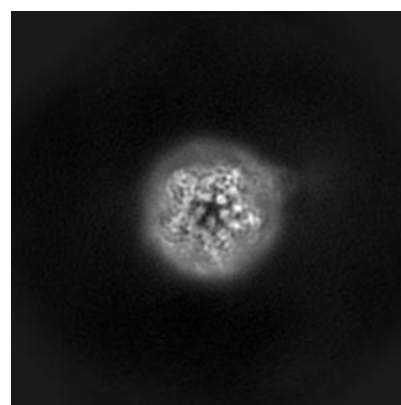
6.1.1 Primary map



X



Y

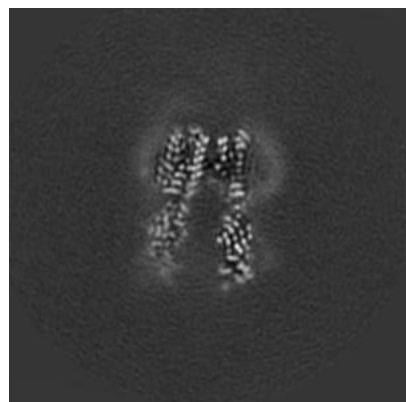


Z

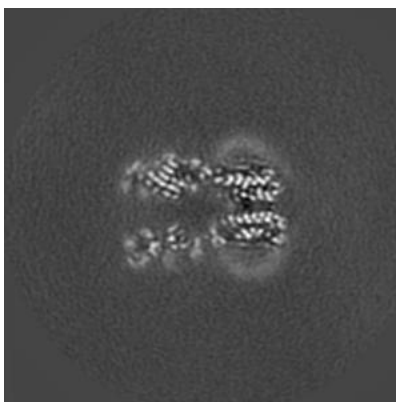
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

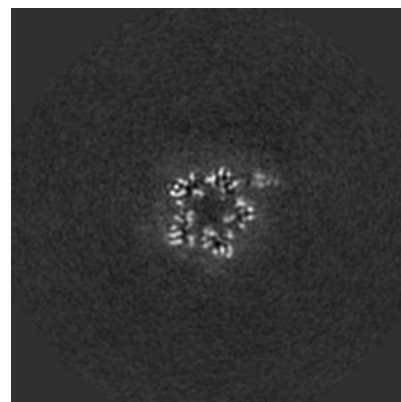
6.2.1 Primary map



X Index: 145



Y Index: 145

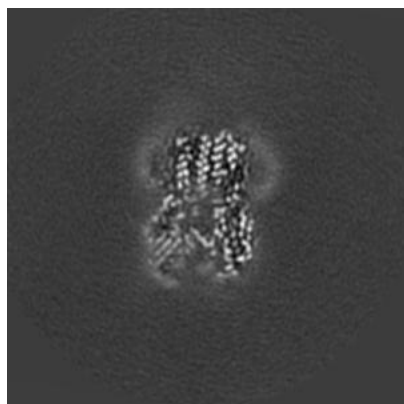


Z Index: 145

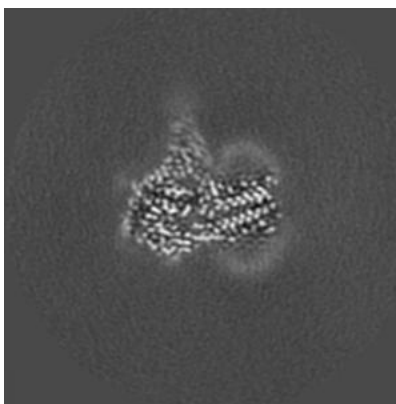
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

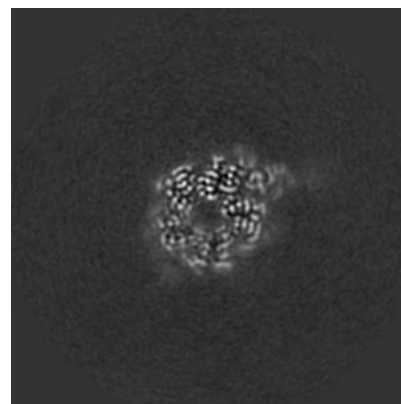
6.3.1 Primary map



X Index: 154



Y Index: 164



Z Index: 121

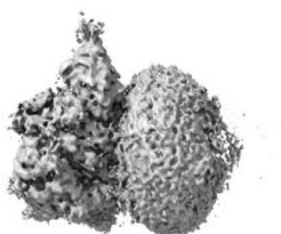
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

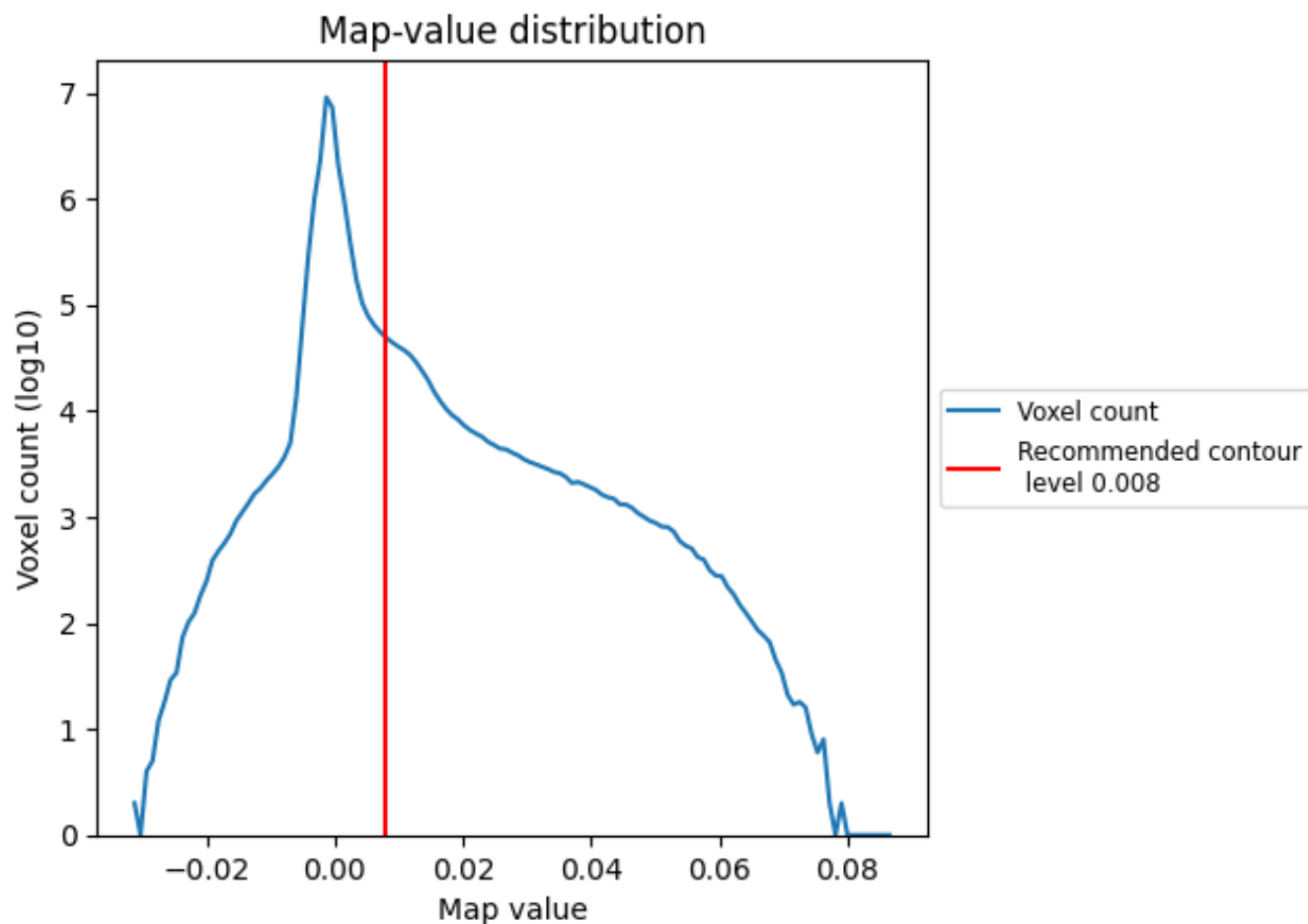
6.5 Mask visualisation

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

7 Map analysis [i](#)

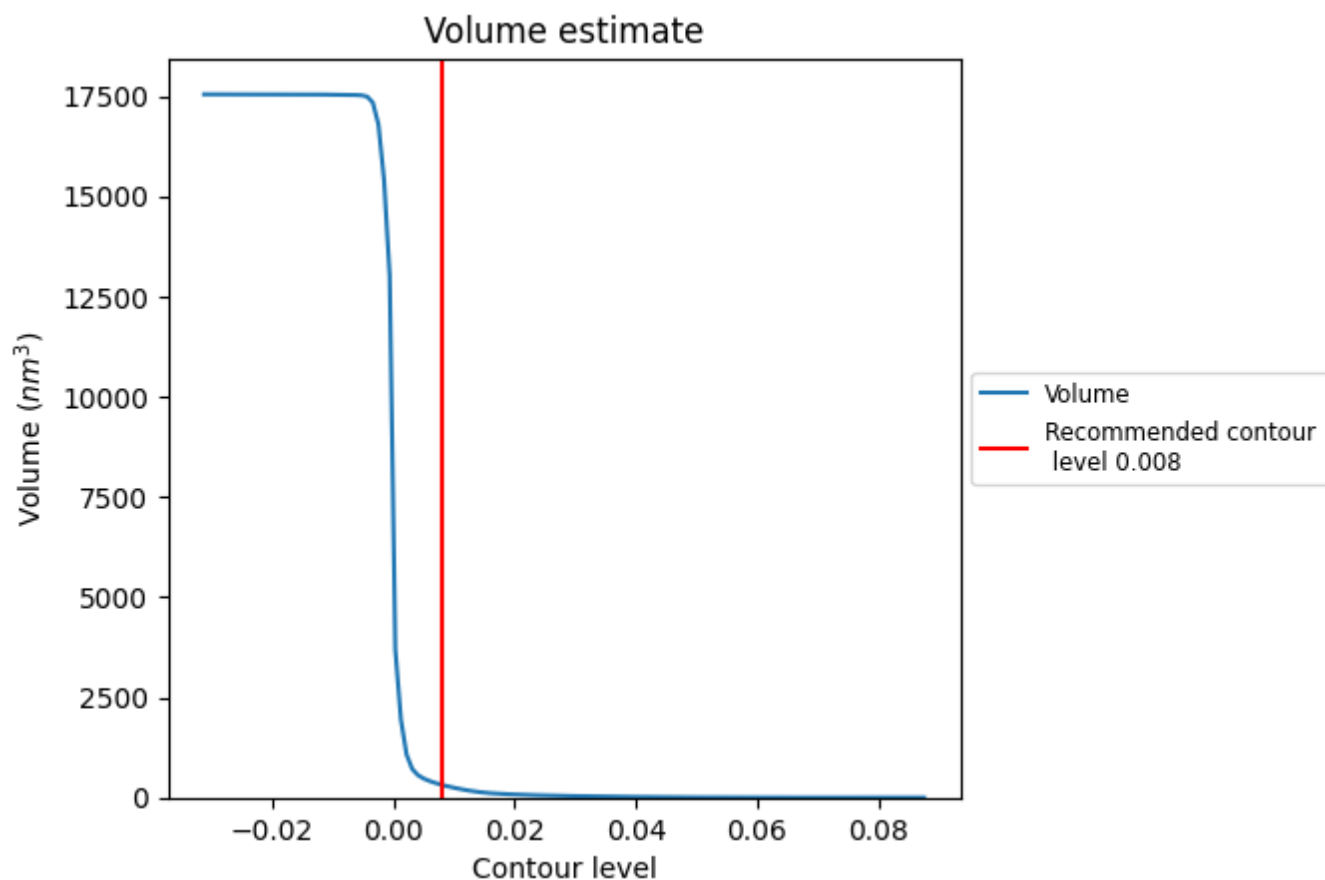
This section contains the results of statistical analysis of the map.

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.

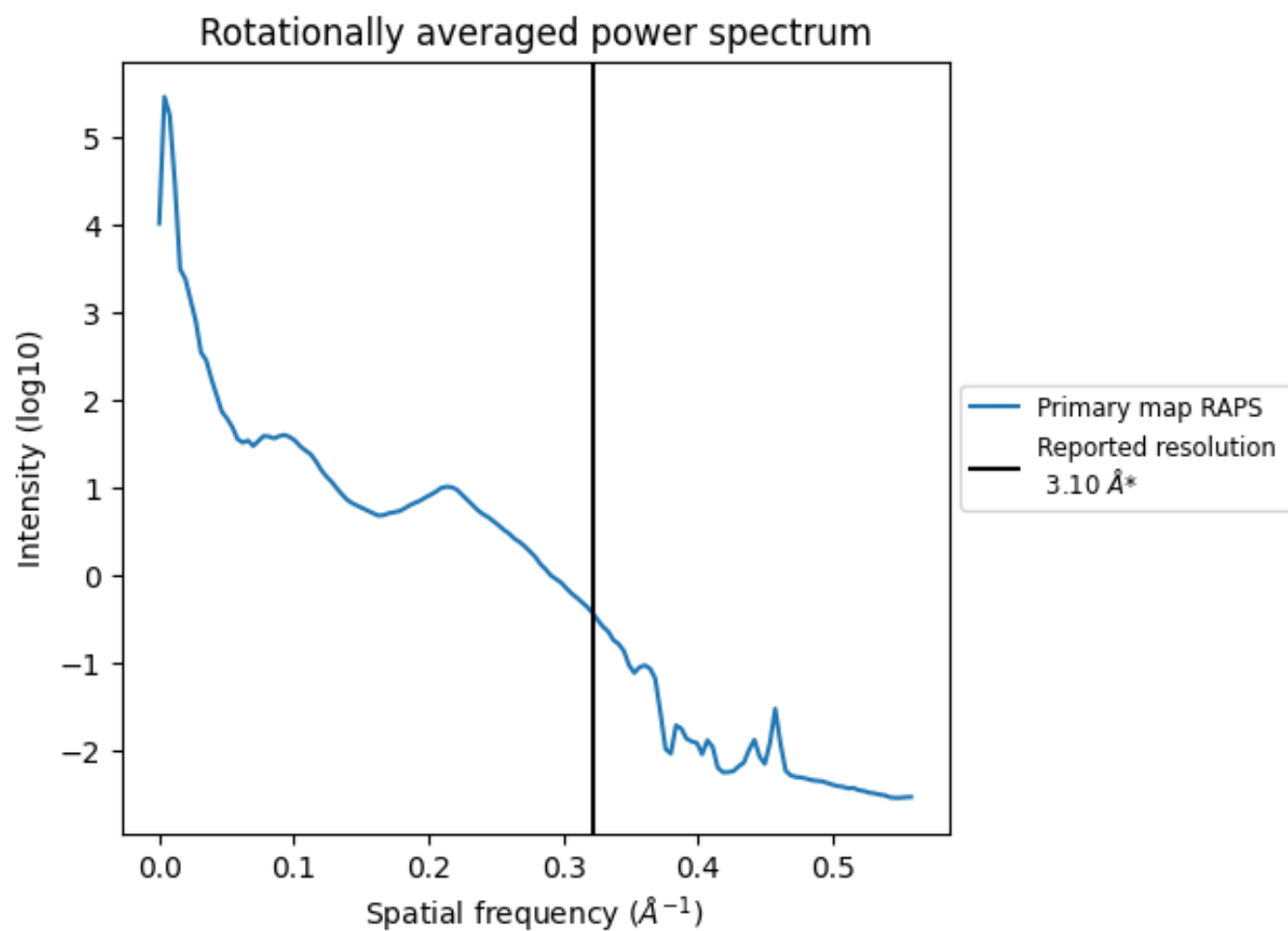
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 317 nm³; this corresponds to an approximate mass of 286 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 ⓘ

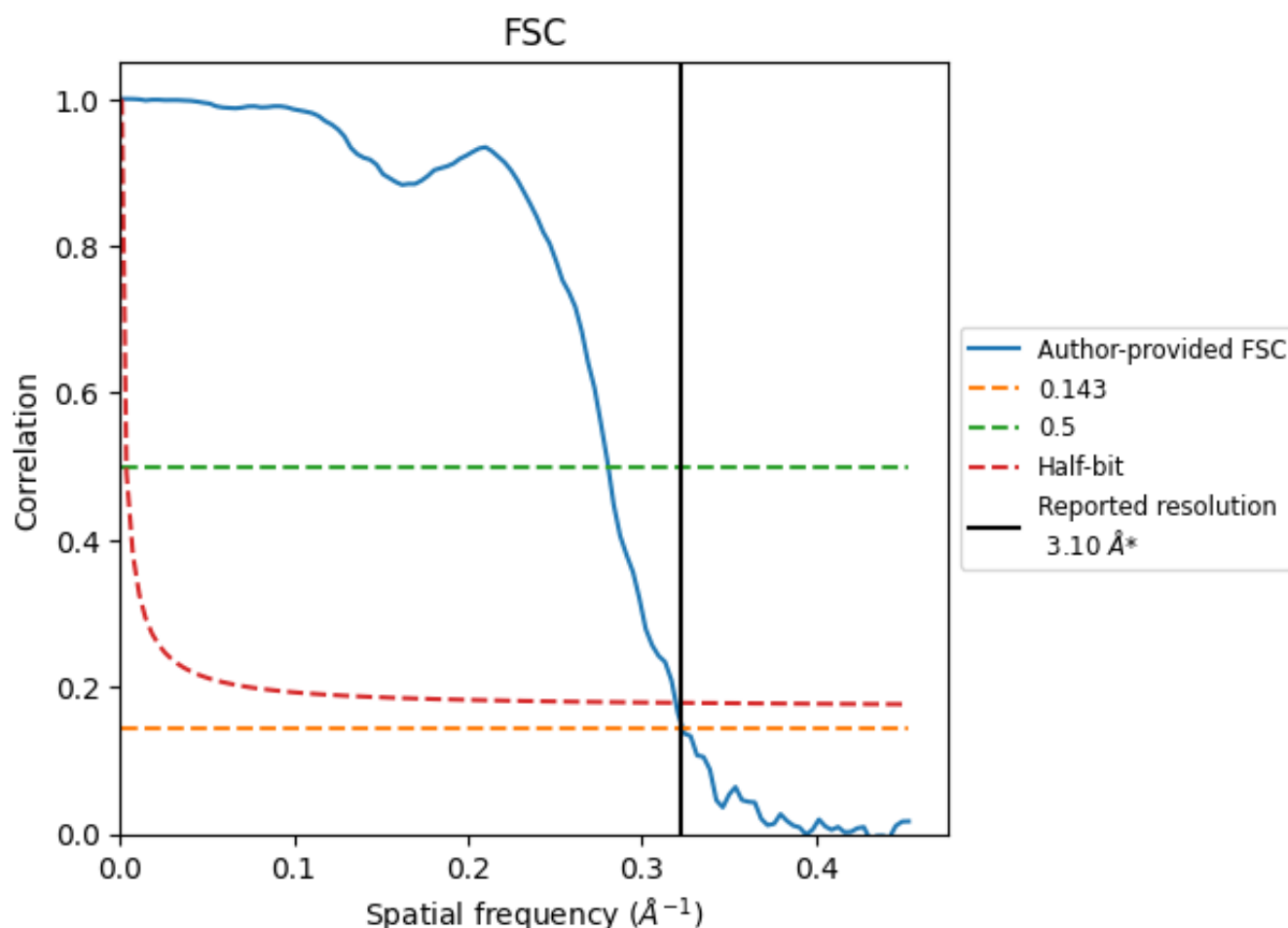


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

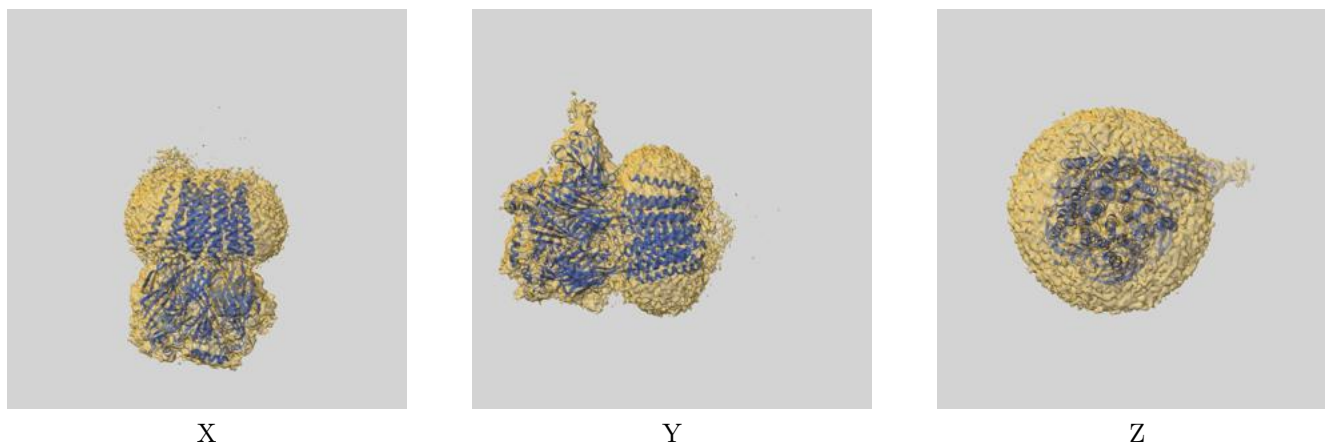
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.09	3.56	3.13
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

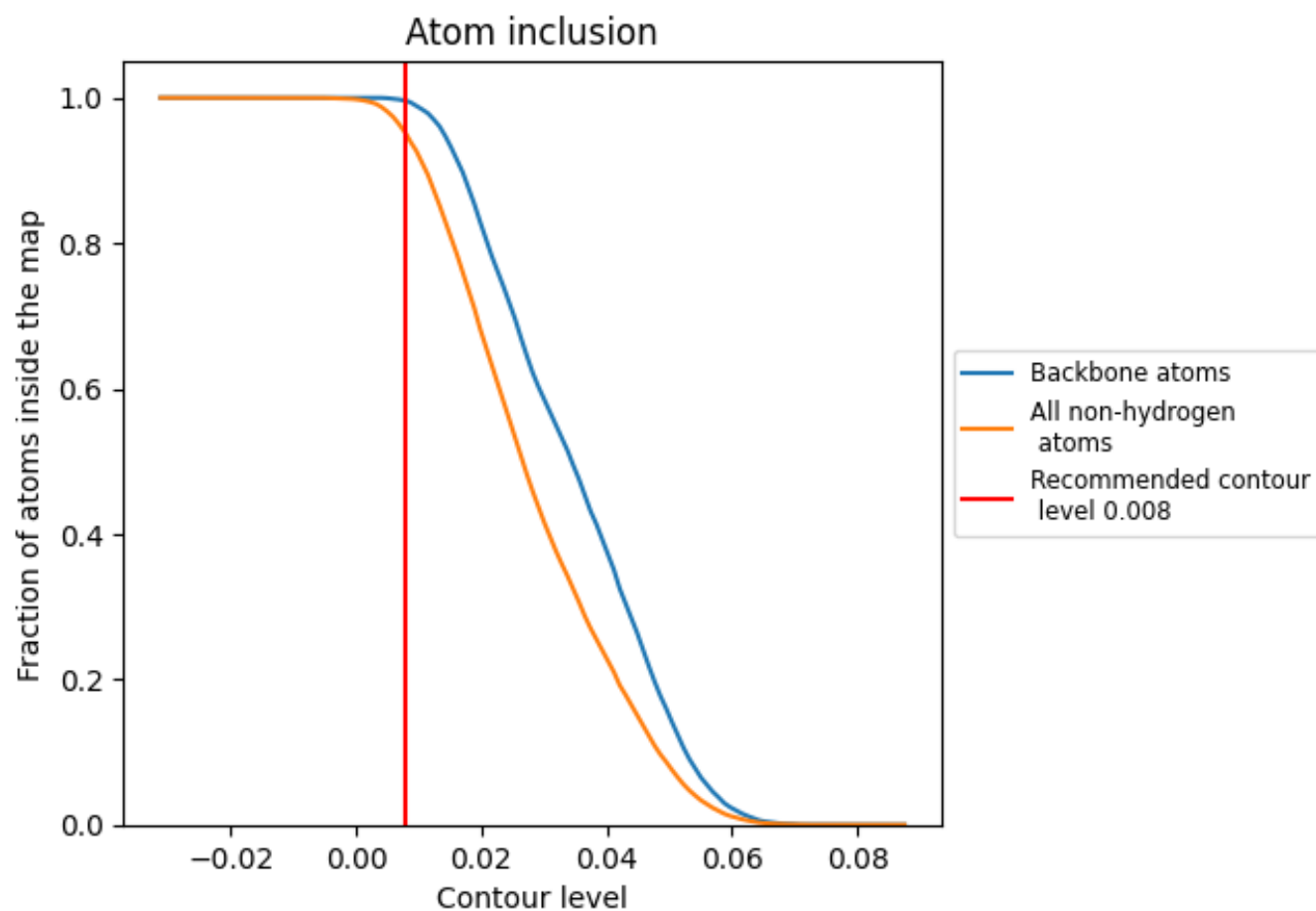
This section contains information regarding the fit between EMDB map EMD-14073 and PDB model 7QNB. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.008 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, 100% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.