



## Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 02:35 PM EDT

PDB ID : 7UAI / pdb\_00007uai  
EMDB ID : EMD-26426  
Title : Meprin alpha helix in complex with fetuin-B  
Authors : Bayly-Jones, C.; Lupton, C.J.; Fritz, C.; Schlenzig, D.; Whisstock, J.C.  
Deposited on : 2022-03-13  
Resolution : 2.80 Å (reported)  
Based on initial models : 7UAB, 7AUW

This is a Full wwPDB EM Validation 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.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

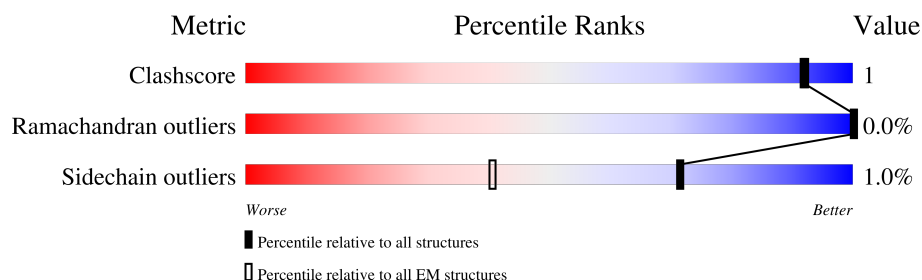
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	587	
1	C	587	
1	D	587	
1	E	587	
2	A	388	
2	H	388	
3	F	3	
3	L	3	

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Mol	Chain	Length	Quality of chain
3	R	3	 100%
4	G	2	 100%
4	J	2	 100%
4	K	2	 100%
4	M	2	 100%
4	O	2	 100%
4	P	2	 100%
4	S	2	 100%
4	U	2	 100%
5	I	4	 100%
5	N	4	 25%  75%
5	Q	4	 25%  75%
5	T	4	 100%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21936 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 Meprin A subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	535	Total	C	N	O	S	0	0
			4280	2706	725	828	21		
1	B	535	Total	C	N	O	S	0	0
			4296	2715	731	829	21		
1	C	529	Total	C	N	O	S	0	0
			4250	2688	721	820	21		
1	D	535	Total	C	N	O	S	0	0
			4300	2717	731	831	21		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	14	TRP	-	expression tag	UNP Q16819
E	15	SER	-	expression tag	UNP Q16819
E	16	HIS	-	expression tag	UNP Q16819
E	17	PRO	-	expression tag	UNP Q16819
E	18	GLN	-	expression tag	UNP Q16819
E	19	PHE	-	expression tag	UNP Q16819
E	20	GLU	-	expression tag	UNP Q16819
E	21	LYS	-	expression tag	UNP Q16819
B	14	TRP	-	expression tag	UNP Q16819
B	15	SER	-	expression tag	UNP Q16819
B	16	HIS	-	expression tag	UNP Q16819
B	17	PRO	-	expression tag	UNP Q16819
B	18	GLN	-	expression tag	UNP Q16819
B	19	PHE	-	expression tag	UNP Q16819
B	20	GLU	-	expression tag	UNP Q16819
B	21	LYS	-	expression tag	UNP Q16819
C	14	TRP	-	expression tag	UNP Q16819
C	15	SER	-	expression tag	UNP Q16819
C	16	HIS	-	expression tag	UNP Q16819
C	17	PRO	-	expression tag	UNP Q16819
C	18	GLN	-	expression tag	UNP Q16819
C	19	PHE	-	expression tag	UNP Q16819

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLU	-	expression tag	UNP Q16819
C	21	LYS	-	expression tag	UNP Q16819
D	14	TRP	-	expression tag	UNP Q16819
D	15	SER	-	expression tag	UNP Q16819
D	16	HIS	-	expression tag	UNP Q16819
D	17	PRO	-	expression tag	UNP Q16819
D	18	GLN	-	expression tag	UNP Q16819
D	19	PHE	-	expression tag	UNP Q16819
D	20	GLU	-	expression tag	UNP Q16819
D	21	LYS	-	expression tag	UNP Q16819

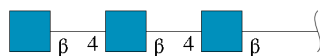
- Molecule 2 is a protein called Fetuin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	274	Total	C	N	O	S	0	0
			2004	1272	333	386	13		
2	H	282	Total	C	N	O	S	0	0
			2192	1406	359	413	14		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	HIS	-	expression tag	UNP Q9UGM5
A	384	HIS	-	expression tag	UNP Q9UGM5
A	385	HIS	-	expression tag	UNP Q9UGM5
A	386	HIS	-	expression tag	UNP Q9UGM5
A	387	HIS	-	expression tag	UNP Q9UGM5
A	388	HIS	-	expression tag	UNP Q9UGM5
H	383	HIS	-	expression tag	UNP Q9UGM5
H	384	HIS	-	expression tag	UNP Q9UGM5
H	385	HIS	-	expression tag	UNP Q9UGM5
H	386	HIS	-	expression tag	UNP Q9UGM5
H	387	HIS	-	expression tag	UNP Q9UGM5
H	388	HIS	-	expression tag	UNP Q9UGM5

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



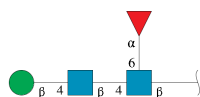
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			42	24	3	15		
3	L	3	Total	C	N	O	0	0
			42	24	3	15		
3	R	3	Total	C	N	O	0	0
			42	24	3	15		

- 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	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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
5	I	4	Total	C	N	O	0	0
			49	28	2	19		

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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	E	2	Total	Ca	0
			2	2	
6	B	2	Total	Ca	0
			2	2	
6	C	2	Total	Ca	0
			2	2	
6	D	2	Total	Ca	0
			2	2	

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total	Zn	0
			1	1	
7	A	1	Total	Zn	0
			1	1	
7	B	1	Total	Zn	0
			1	1	
7	C	1	Total	Zn	0
			1	1	

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



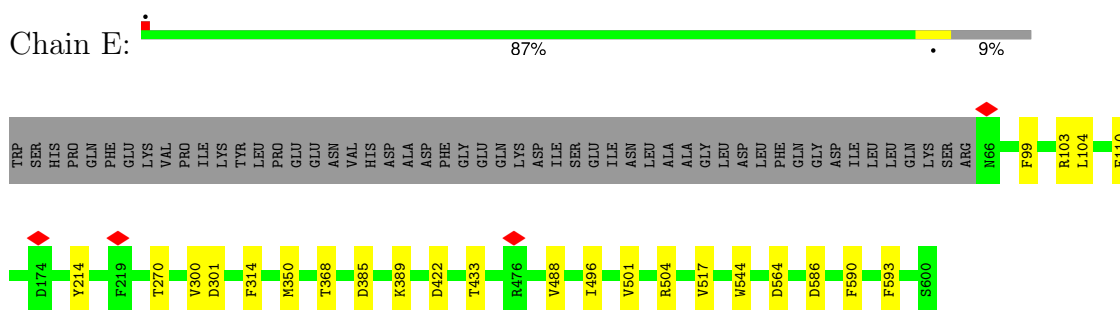
Mol	Chain	Residues	Atoms				AltConf
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	



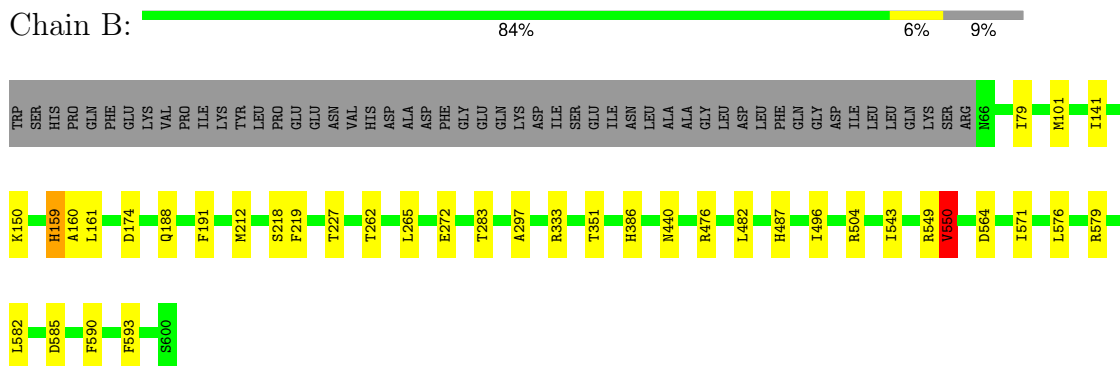
### 3 Residue-property plots

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.

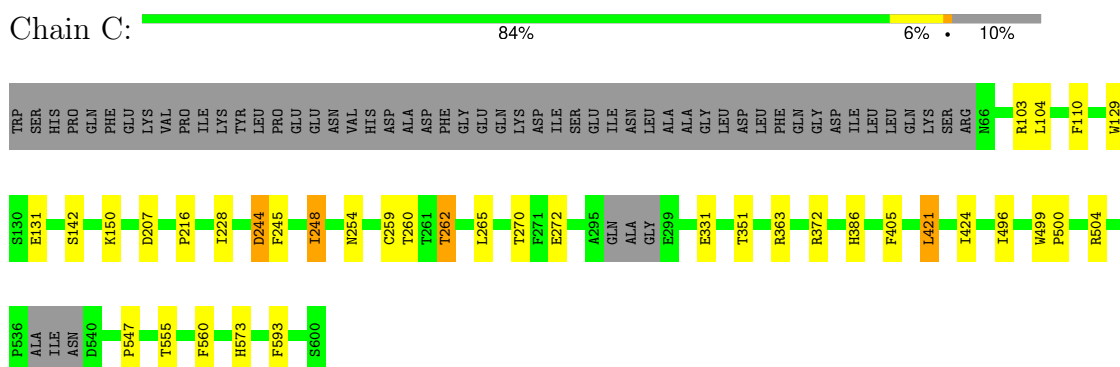
- Molecule 1: Meprin A subunit alpha



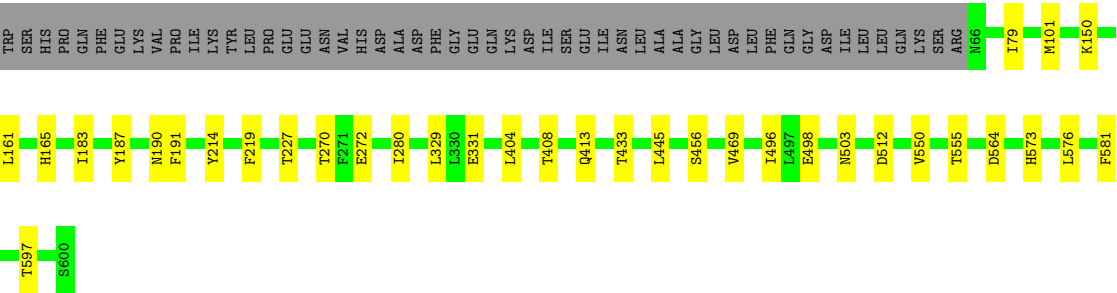
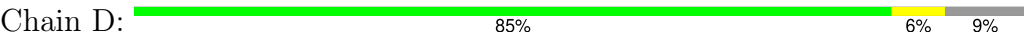
- Molecule 1: Meprin A subunit alpha



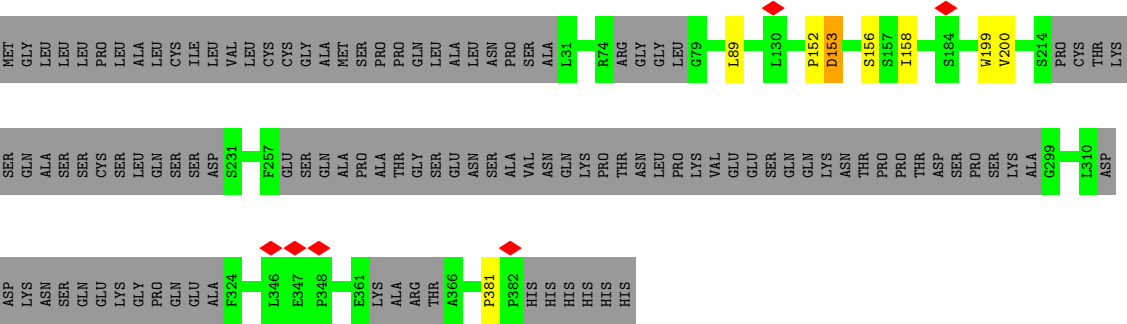
- Molecule 1: Meprin A subunit alpha



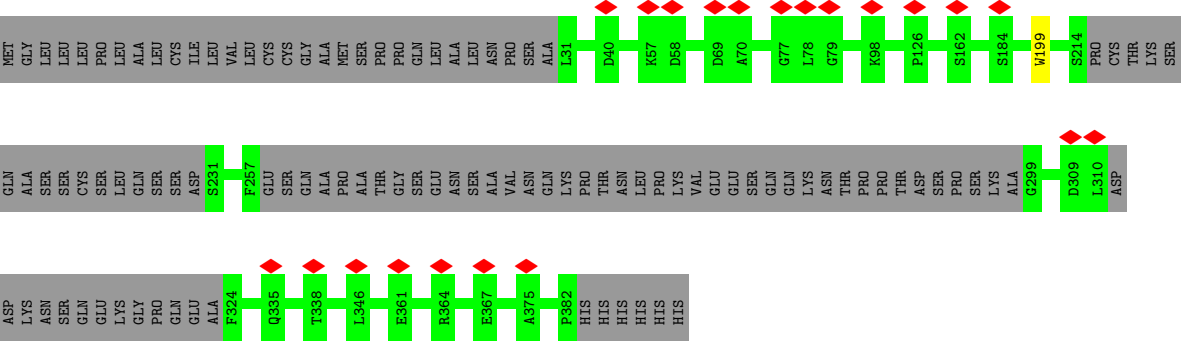
• Molecule 1: Meprin A subunit alpha



• Molecule 2: Fetuin-B



• Molecule 2: Fetuin-B



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




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

Chain L:  100%

NAG1  
NAG2  
NAG3

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

Chain R:  100%


NAG1  
NAG2  
NAG3

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

Chain G:  100%

NAG1  
NAG2

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

Chain J:  100%

NAG1  
NAG2

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

Chain K:  100%

NAG1  
NAG2

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

Chain M:  100%

NAG1  
NAG2

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

Chain O:  100%

NAG1  
NAG2

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

Chain P:  100%

NAG1  
NAG2

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

Chain S:  100%

NAG1  
NAG2

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

Chain U:  100%

NAG1  
NAG2

- Molecule 5: 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 I:  100%

NAG1  
NAG2  
BMA3  
FUC4

- Molecule 5: 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 N:  25% 75%

NAG1  
NAG2  
BMA3  
FUC4

- Molecule 5: 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 Q:  25% 75%

NAG1  
NAG2  
BMA3  
FUC4

- Molecule 5: 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 T:

100%

MAG1  
MAG2  
BMA3  
FUC4

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	115951	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 ( $e^-/\text{\AA}^2$ )	44.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.155	Depositor
Minimum map value	-1.103	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	305.27927, 305.27927, 305.27927	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.41333, 1.41333, 1.41333	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, BMA, CA, ZN

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	B	0.79	2/4406 (0.0%)	1.26	12/5980 (0.2%)
1	C	0.79	0/4358	1.24	5/5912 (0.1%)
1	D	0.80	0/4410	1.25	7/5985 (0.1%)
1	E	0.76	1/4390 (0.0%)	1.25	8/5961 (0.1%)
2	A	0.79	1/2044 (0.0%)	1.24	0/2785
2	H	0.77	0/2244	1.23	0/3050
All	All	0.78	4/21852 (0.0%)	1.25	32/29673 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	300	VAL	C-N	-7.95	1.22	1.33
1	B	550	VAL	C-N	5.81	1.40	1.33
2	A	381	PRO	CA-C	5.79	1.55	1.51
1	B	549	ARG	C-N	-5.65	1.25	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	550	VAL	CA-C-N	-7.24	114.84	122.30
1	B	550	VAL	C-N-CA	-7.24	114.84	122.30
1	D	564	ASP	CA-CB-CG	6.99	119.59	112.60
1	B	590	PHE	CA-CB-CG	6.82	120.62	113.80
1	B	174	ASP	CA-CB-CG	6.02	118.62	112.60
1	D	512	ASP	N-CA-C	-5.92	99.55	108.96
1	E	586	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	297	ALA	N-CA-C	5.70	117.50	111.28
1	B	333	ARG	N-CA-C	-5.62	102.96	110.55
1	D	413	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	E	564	ASP	CA-CB-CG	5.54	118.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	THR	N-CA-C	-5.46	107.27	114.31
1	B	476	ARG	CA-C-N	5.41	128.07	120.28
1	B	476	ARG	C-N-CA	5.41	128.07	120.28
1	C	245	PHE	CB-CA-C	-5.38	100.78	109.72
1	E	99	PHE	CA-CB-CG	5.38	119.18	113.80
1	E	368	THR	CB-CA-C	-5.33	101.70	110.72
1	D	433	THR	CA-C-N	5.33	125.86	122.18
1	D	433	THR	C-N-CA	5.33	125.86	122.18
1	B	564	ASP	CA-CB-CG	5.25	117.84	112.60
1	B	159	HIS	CB-CG-CD2	-5.18	124.46	131.20
1	B	487	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	C	573	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	C	260	THR	N-CA-C	-5.14	106.95	113.43
1	C	555	THR	CA-C-N	5.14	127.68	120.28
1	C	555	THR	C-N-CA	5.14	127.68	120.28
1	E	433	THR	CA-C-N	5.11	125.12	121.65
1	E	433	THR	C-N-CA	5.11	125.12	121.65
1	E	590	PHE	CA-CB-CG	5.10	118.90	113.80
1	E	300	VAL	O-C-N	-5.10	116.32	122.59
1	D	555	THR	CA-C-N	5.10	128.83	120.63
1	D	555	THR	C-N-CA	5.10	128.83	120.63

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4296	0	4047	16	0
1	C	4250	0	3995	18	0
1	D	4300	0	4051	14	0
1	E	4280	0	4017	12	0
2	A	2004	0	1801	4	0
2	H	2192	0	2135	2	0
3	F	42	0	37	0	0
3	L	42	0	37	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	42	0	37	0	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	S	28	0	25	0	0
4	U	28	0	25	0	0
5	I	49	0	43	0	0
5	N	49	0	43	0	0
5	Q	49	0	43	0	0
5	T	49	0	43	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	14	0	13	0	0
8	C	14	0	13	0	0
8	D	14	0	13	0	0
8	E	14	0	13	0	0
All	All	21936	0	20581	61	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 1.

All (61) 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:C:262:THR:HG22	1:C:265:LEU:H	1.48	0.77
1:C:254:ASN:HA	1:C:259:CYS:HB2	1.75	0.67
1:C:103:ARG:HH21	1:C:110:PHE:HB2	1.62	0.64
1:B:351:THR:HG22	1:B:386:HIS:HB3	1.79	0.63
1:E:103:ARG:HH21	1:E:110:PHE:HB2	1.65	0.61
1:C:262:THR:CG2	1:C:265:LEU:H	2.15	0.59
1:B:440:ASN:HA	1:B:585:ASP:HB3	1.88	0.56
1:B:101:MET:HG3	1:B:150:LYS:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:THR:HG22	1:C:386:HIS:HB3	1.87	0.55
2:A:199:TRP:CG	1:D:219:PHE:H	2.26	0.54
1:E:301:ASP:HB3	1:E:314:PHE:HD1	1.71	0.54
1:E:501:VAL:HG11	1:E:593:PHE:CZ	2.44	0.53
2:A:153:ASP:HB3	2:A:200:VAL:HG11	1.90	0.53
1:D:280:ILE:HG13	1:D:331:GLU:HB3	1.89	0.53
1:C:150:LYS:NZ	1:C:244:ASP:HB3	2.23	0.53
1:C:103:ARG:O	1:C:262:THR:HG23	2.09	0.52
1:E:301:ASP:HB2	1:E:422:ASP:OD2	2.09	0.52
1:B:141:ILE:HD11	1:B:160:ALA:HB2	1.92	0.52
1:E:301:ASP:HB3	1:E:314:PHE:CD1	2.45	0.51
1:B:262:THR:OG1	1:B:265:LEU:HB3	2.10	0.50
1:D:503:ASN:HB2	1:D:597:THR:OG1	2.12	0.50
1:D:79:ILE:HD11	1:D:161:LEU:HD21	1.95	0.49
1:C:104:LEU:O	1:C:262:THR:HG21	2.11	0.49
1:D:329:LEU:HD22	1:D:404:LEU:HD23	1.95	0.49
1:E:501:VAL:HG11	1:E:593:PHE:HZ	1.77	0.48
1:B:504:ARG:HB3	1:B:593:PHE:CE1	2.48	0.48
1:E:104:LEU:HG	1:E:517:VAL:HG11	1.94	0.48
1:C:129:TRP:CE2	1:C:142:SER:HB2	2.49	0.47
1:D:191:PHE:CZ	1:D:227:THR:HG21	2.49	0.47
1:D:183:ILE:HG12	1:D:227:THR:HG23	1.97	0.47
1:C:405:PHE:CG	1:C:421:LEU:HD11	2.49	0.46
1:D:187:TYR:HD1	1:D:190:ASN:HD21	1.64	0.46
1:B:79:ILE:HD11	1:B:161:LEU:HD21	1.97	0.45
1:C:207:ASP:HB2	1:C:248:ILE:HD12	1.97	0.45
2:A:156:SER:HB3	1:D:187:TYR:HE1	1.81	0.45
1:B:582:LEU:HD23	1:B:582:LEU:HA	1.80	0.45
1:C:547:PRO:HB3	1:C:560:PHE:O	2.17	0.44
1:B:579:ARG:HD2	1:B:579:ARG:HA	1.87	0.44
1:C:421:LEU:HD22	1:C:424:ILE:HD11	2.00	0.44
1:D:456:SER:HB3	1:D:469:VAL:H	1.83	0.44
1:B:159:HIS:NE2	1:B:212:MET:HE1	2.33	0.43
2:A:152:PRO:HB2	1:D:165:HIS:CE1	2.53	0.43
1:B:571:ILE:HG21	1:B:576:LEU:HD13	2.00	0.43
1:E:501:VAL:HG12	1:E:504:ARG:HB2	1.99	0.43
1:D:576:LEU:O	1:D:581:PHE:HB2	2.19	0.43
1:C:499:TRP:HA	1:C:500:PRO:C	2.44	0.42
1:B:218:SER:HA	2:H:199:TRP:CD1	2.54	0.42
1:C:331:GLU:CD	1:C:363:ARG:HH21	2.28	0.42
1:C:504:ARG:HB3	1:C:593:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:MET:HE3	1:D:150:LYS:HE3	2.01	0.42
1:B:219:PHE:H	2:H:199:TRP:CG	2.39	0.41
1:B:543:ILE:O	1:B:550:VAL:HG11	2.21	0.41
1:B:482:LEU:HD23	1:B:482:LEU:C	2.46	0.41
1:D:445:LEU:HD11	1:D:573:HIS:CE1	2.55	0.41
1:B:191:PHE:CZ	1:B:227:THR:HG21	2.55	0.41
1:C:363:ARG:HD2	1:C:372:ARG:HA	2.03	0.41
1:E:488:VAL:HG21	1:E:501:VAL:HG21	2.03	0.40
1:E:350:MET:HE2	1:E:350:MET:HB3	2.00	0.40
1:C:216:PRO:HA	1:C:228:ILE:HG23	2.03	0.40
1:E:385:ASP:HB3	1:E:389:LYS:HE3	2.03	0.40
1:E:501:VAL:HG23	1:E:544:TRP:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	533/587 (91%)	507 (95%)	26 (5%)	0	100	100
1	C	523/587 (89%)	502 (96%)	20 (4%)	1 (0%)	44	73
1	D	533/587 (91%)	507 (95%)	26 (5%)	0	100	100
1	E	533/587 (91%)	513 (96%)	20 (4%)	0	100	100
2	A	262/388 (68%)	253 (97%)	9 (3%)	0	100	100
2	H	274/388 (71%)	265 (97%)	9 (3%)	0	100	100
All	All	2658/3124 (85%)	2547 (96%)	110 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	244	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	472/523 (90%)	468 (99%)	4 (1%)	79	93
1	C	467/523 (89%)	460 (98%)	7 (2%)	60	86
1	D	473/523 (90%)	466 (98%)	7 (2%)	60	86
1	E	469/523 (90%)	466 (99%)	3 (1%)	84	95
2	A	200/343 (58%)	197 (98%)	3 (2%)	60	86
2	H	244/343 (71%)	244 (100%)	0	100	100
All	All	2325/2778 (84%)	2301 (99%)	24 (1%)	71	91

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	214	TYR
1	E	270	THR
1	E	496	ILE
2	A	89	LEU
2	A	153	ASP
2	A	158	ILE
1	B	188	GLN
1	B	272	GLU
1	B	496	ILE
1	B	550	VAL
1	C	131	GLU
1	C	248	ILE
1	C	262	THR
1	C	270	THR
1	C	272	GLU
1	C	421	LEU
1	C	496	ILE
1	D	214	TYR
1	D	270	THR
1	D	272	GLU
1	D	408	THR
1	D	496	ILE

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Mol	Chain	Res	Type
1	D	498	GLU
1	D	550	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	381	GLN
1	E	386	HIS
1	E	399	GLN
1	E	554	HIS
1	E	584	ASN
2	A	37	ASN
1	B	66	ASN
1	B	145	GLN
1	B	268	HIS
1	B	503	ASN
1	B	554	HIS
1	B	558	ASN
1	C	86	ASN
1	C	123	GLN
1	C	145	GLN
1	C	275	ASN
1	C	341	GLN
1	C	386	HIS
1	C	455	GLN
1	D	66	ASN
1	D	90	ASN
1	D	124	GLN
1	D	182	GLN
1	D	275	ASN
1	D	341	GLN
1	D	455	GLN
1	D	503	ASN
2	H	116	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 ⓘ

41 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
3	NAG	F	1	1,3	14,14,15	1.32	2 (14%)	17,19,21	0.69	0
3	NAG	F	2	3	14,14,15	1.42	3 (21%)	17,19,21	0.57	0
3	NAG	F	3	3	14,14,15	1.34	2 (14%)	17,19,21	0.93	0
4	NAG	G	1	4,1	14,14,15	1.30	2 (14%)	17,19,21	0.67	0
4	NAG	G	2	4	14,14,15	1.34	2 (14%)	17,19,21	0.91	1 (5%)
5	NAG	I	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	0.80	0
5	NAG	I	2	5	14,14,15	1.16	2 (14%)	17,19,21	0.88	0
5	BMA	I	3	5	11,11,12	1.10	1 (9%)	15,15,17	1.09	1 (6%)
5	FUC	I	4	5	10,10,11	1.08	1 (10%)	14,14,16	0.69	0
4	NAG	J	1	4,1	14,14,15	1.16	2 (14%)	17,19,21	1.06	1 (5%)
4	NAG	J	2	4	14,14,15	0.95	1 (7%)	17,19,21	1.44	3 (17%)
4	NAG	K	1	4,1	14,14,15	1.15	1 (7%)	17,19,21	0.83	0
4	NAG	K	2	4	14,14,15	1.22	1 (7%)	17,19,21	0.90	1 (5%)
3	NAG	L	1	1,3	14,14,15	1.17	2 (14%)	17,19,21	0.76	0
3	NAG	L	2	3	14,14,15	1.46	3 (21%)	17,19,21	0.88	1 (5%)
3	NAG	L	3	3	14,14,15	1.33	3 (21%)	17,19,21	0.93	0
4	NAG	M	1	4,1	14,14,15	1.14	1 (7%)	17,19,21	0.84	0
4	NAG	M	2	4	14,14,15	1.21	2 (14%)	17,19,21	0.76	0
5	NAG	N	1	1,5	14,14,15	1.18	1 (7%)	17,19,21	0.82	0
5	NAG	N	2	5	14,14,15	1.06	0	17,19,21	0.84	0
5	BMA	N	3	5	11,11,12	1.13	1 (9%)	15,15,17	0.96	1 (6%)
5	FUC	N	4	5	10,10,11	1.08	1 (10%)	14,14,16	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	O	1	4,1	14,14,15	1.05	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	O	2	4	14,14,15	1.28	2 (14%)	17,19,21	0.79	1 (5%)
4	NAG	P	1	4,1	14,14,15	1.12	1 (7%)	17,19,21	0.61	0
4	NAG	P	2	4	14,14,15	1.16	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	Q	1	1,5	14,14,15	1.04	0	17,19,21	0.85	0
5	NAG	Q	2	5	14,14,15	1.21	2 (14%)	17,19,21	0.69	0
5	BMA	Q	3	5	11,11,12	1.13	1 (9%)	15,15,17	1.20	1 (6%)
5	FUC	Q	4	5	10,10,11	1.11	1 (10%)	14,14,16	0.71	0
3	NAG	R	1	1,3	14,14,15	1.19	2 (14%)	17,19,21	0.90	0
3	NAG	R	2	3	14,14,15	1.39	3 (21%)	17,19,21	0.58	0
3	NAG	R	3	3	14,14,15	1.32	2 (14%)	17,19,21	0.94	0
4	NAG	S	1	4,1	14,14,15	1.19	1 (7%)	17,19,21	0.67	0
4	NAG	S	2	4	14,14,15	1.14	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	T	1	1,5	14,14,15	1.10	1 (7%)	17,19,21	0.70	0
5	NAG	T	2	5	14,14,15	1.06	1 (7%)	17,19,21	0.83	1 (5%)
5	BMA	T	3	5	11,11,12	1.19	1 (9%)	15,15,17	0.85	1 (6%)
5	FUC	T	4	5	10,10,11	1.15	2 (20%)	14,14,16	0.79	0
4	NAG	U	1	4,1	14,14,15	1.05	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	U	2	4	14,14,15	1.23	1 (7%)	17,19,21	1.05	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	3	3	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	FUC	I	4	5	-	-	0/1/1/1
4	NAG	J	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	3	3	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
5	FUC	N	4	5	-	-	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	0/2/19/22	0/1/1/1
5	FUC	Q	4	5	-	-	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	3	3	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
5	FUC	T	4	5	-	-	0/1/1/1
4	NAG	U	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2	NAG	O5-C5	3.10	1.49	1.43
4	G	2	NAG	O5-C5	3.02	1.49	1.43
4	O	2	NAG	O5-C5	2.97	1.49	1.43
4	K	2	NAG	O5-C5	2.89	1.49	1.43
4	U	2	NAG	O5-C5	2.87	1.49	1.43
4	G	1	NAG	O5-C5	2.87	1.49	1.43
4	M	2	NAG	O5-C5	2.85	1.49	1.43
3	L	3	NAG	O5-C5	2.79	1.48	1.43
3	R	2	NAG	O5-C5	2.78	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	3	BMA	O5-C5	2.73	1.48	1.43
3	F	2	NAG	O5-C5	2.72	1.48	1.43
3	F	3	NAG	C1-C2	2.71	1.56	1.52
4	S	2	NAG	O5-C5	2.63	1.48	1.43
3	R	3	NAG	O5-C5	2.62	1.48	1.43
3	R	3	NAG	C1-C2	2.58	1.55	1.52
3	F	3	NAG	O5-C5	2.57	1.48	1.43
4	J	1	NAG	O5-C5	2.53	1.48	1.43
5	Q	3	BMA	O5-C5	2.53	1.48	1.43
4	K	1	NAG	O5-C5	2.52	1.48	1.43
4	M	1	NAG	O5-C5	2.51	1.48	1.43
5	I	3	BMA	O5-C5	2.50	1.48	1.43
3	R	2	NAG	O4-C4	2.49	1.49	1.43
3	L	2	NAG	O4-C4	2.48	1.49	1.43
4	P	2	NAG	O5-C5	2.46	1.48	1.43
3	F	1	NAG	O5-C5	2.43	1.48	1.43
4	U	1	NAG	O5-C5	2.43	1.48	1.43
4	J	2	NAG	O5-C5	2.42	1.48	1.43
4	O	1	NAG	O5-C5	2.38	1.48	1.43
5	N	3	BMA	O5-C5	2.37	1.48	1.43
3	R	1	NAG	O5-C5	2.35	1.48	1.43
3	F	2	NAG	O4-C4	2.34	1.48	1.43
5	T	4	FUC	O5-C1	2.33	1.47	1.43
5	Q	2	NAG	O5-C5	2.32	1.48	1.43
5	I	2	NAG	O5-C5	2.32	1.48	1.43
4	J	1	NAG	O4-C4	2.32	1.48	1.43
3	F	1	NAG	C1-C2	2.31	1.55	1.52
5	T	1	NAG	O5-C5	2.31	1.47	1.43
5	N	1	NAG	O5-C5	2.28	1.47	1.43
3	L	3	NAG	C1-C2	2.28	1.55	1.52
4	G	2	NAG	O5-C1	2.28	1.47	1.43
5	T	2	NAG	O5-C5	2.28	1.47	1.43
3	L	1	NAG	O5-C5	2.23	1.47	1.43
5	I	1	NAG	O5-C5	2.20	1.47	1.43
4	S	1	NAG	O5-C5	2.18	1.47	1.43
4	O	2	NAG	O5-C1	2.18	1.47	1.43
3	R	2	NAG	O5-C1	2.17	1.47	1.43
5	N	4	FUC	O5-C5	2.16	1.47	1.43
5	I	2	NAG	O4-C4	2.15	1.48	1.43
3	F	2	NAG	O5-C1	2.10	1.47	1.43
5	Q	2	NAG	O4-C4	2.10	1.48	1.43
4	G	1	NAG	O4-C4	2.09	1.48	1.43

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2	NAG	O5-C1	2.08	1.47	1.43
3	R	1	NAG	C1-C2	2.08	1.55	1.52
3	L	3	NAG	O5-C1	2.07	1.47	1.43
3	L	1	NAG	C1-C2	2.07	1.55	1.52
5	Q	4	FUC	O5-C1	2.06	1.47	1.43
5	I	4	FUC	O5-C1	2.06	1.47	1.43
4	M	2	NAG	O5-C1	2.06	1.47	1.43
5	T	4	FUC	O5-C5	2.01	1.47	1.43
4	P	1	NAG	O5-C5	2.00	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	3	BMA	C1-O5-C5	3.91	117.43	112.19
4	J	2	NAG	C1-O5-C5	3.82	117.30	112.19
5	I	3	BMA	C1-O5-C5	3.66	117.09	112.19
4	S	2	NAG	C1-O5-C5	3.48	116.84	112.19
4	U	2	NAG	C1-O5-C5	3.37	116.70	112.19
4	P	2	NAG	C1-O5-C5	3.09	116.33	112.19
4	O	1	NAG	C1-O5-C5	2.80	115.94	112.19
5	N	3	BMA	C1-O5-C5	2.71	115.82	112.19
4	J	1	NAG	O5-C1-C2	-2.56	107.33	111.29
4	K	2	NAG	C1-O5-C5	2.46	115.49	112.19
4	G	2	NAG	C1-O5-C5	2.46	115.48	112.19
5	T	3	BMA	C1-O5-C5	2.36	115.35	112.19
4	J	2	NAG	C4-C3-C2	-2.36	107.56	111.02
3	L	2	NAG	C1-O5-C5	2.33	115.31	112.19
4	O	2	NAG	C1-O5-C5	2.17	115.10	112.19
4	J	2	NAG	O4-C4-C3	-2.11	105.40	110.38
4	U	1	NAG	O5-C1-C2	-2.09	108.06	111.29
5	T	2	NAG	O5-C1-C2	-2.06	108.10	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C3-C2-N2-C7
4	U	1	NAG	C1-C2-N2-C7

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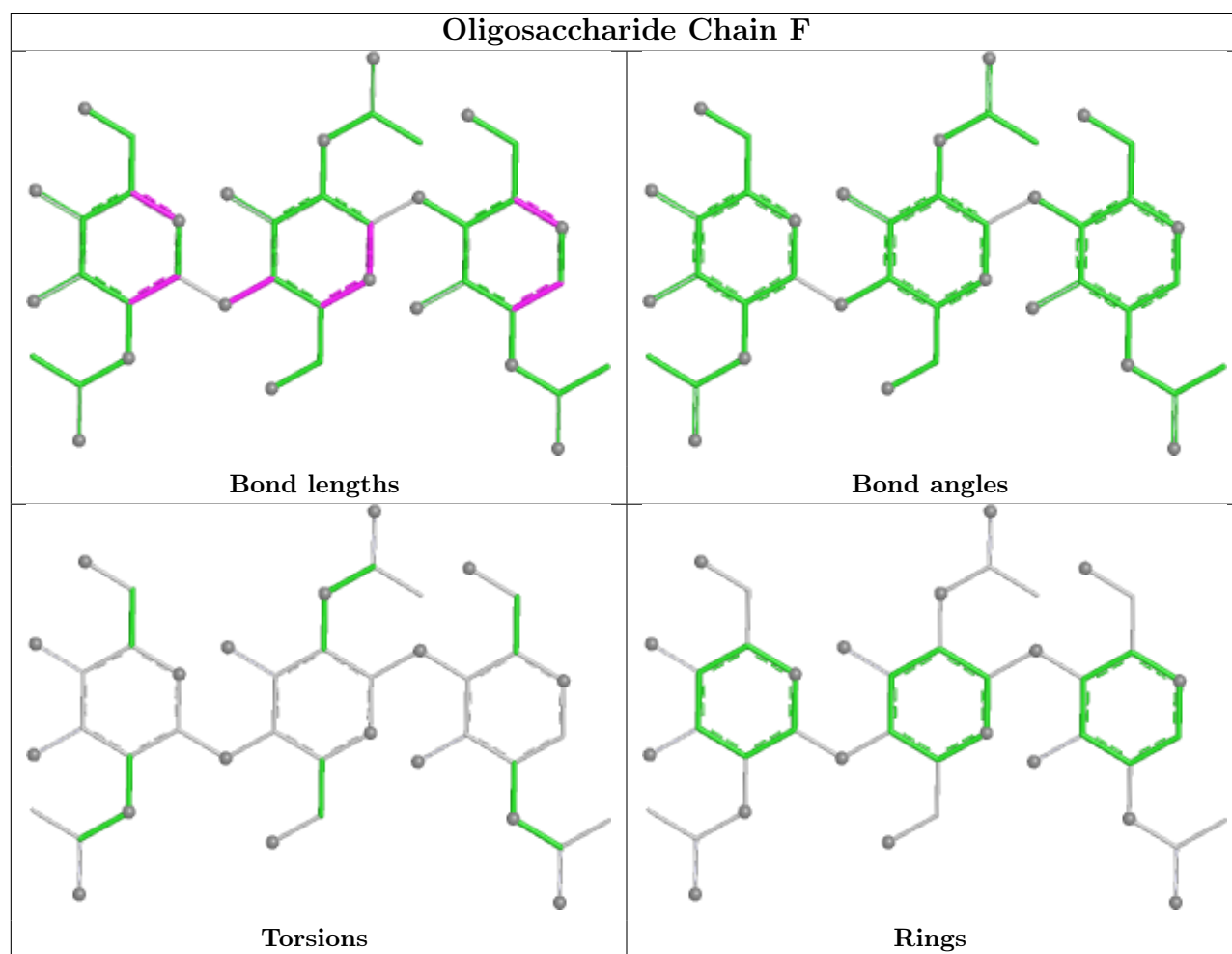
Continued from previous page...

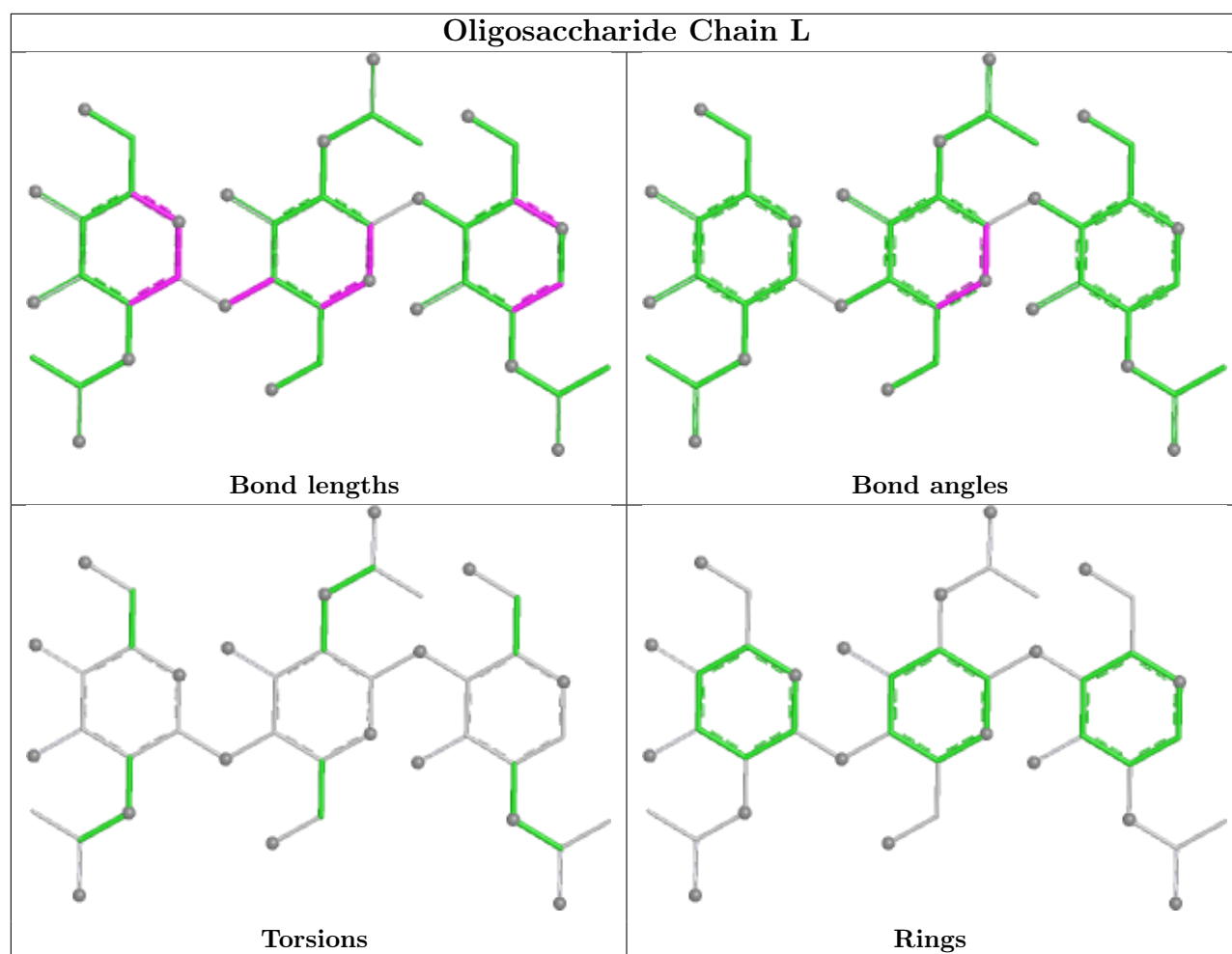
Mol	Chain	Res	Type	Atoms
5	Q	1	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C1-C2-N2-C7
4	O	2	NAG	C1-C2-N2-C7
5	T	1	NAG	C1-C2-N2-C7
4	U	1	NAG	C3-C2-N2-C7

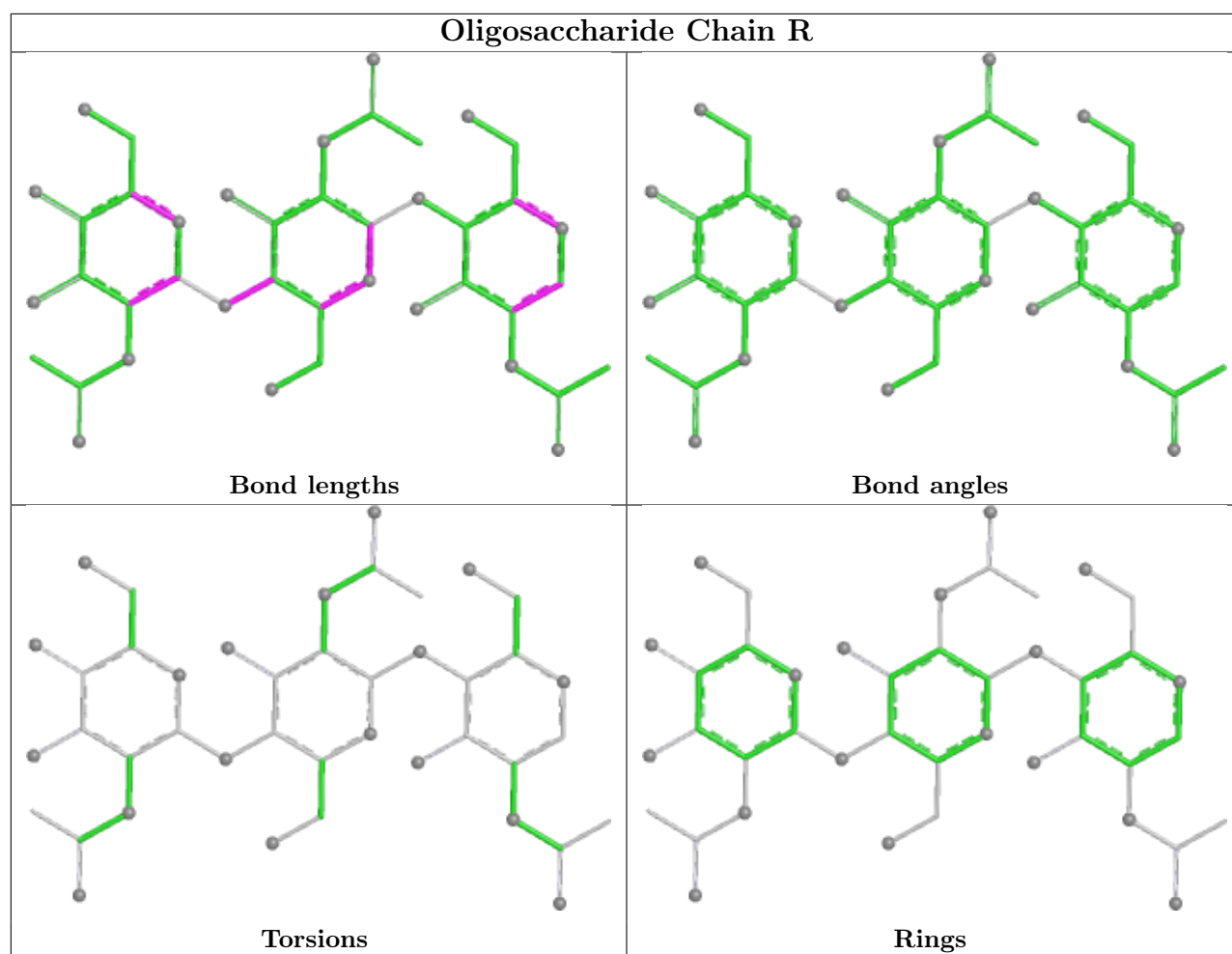
There are no ring outliers.

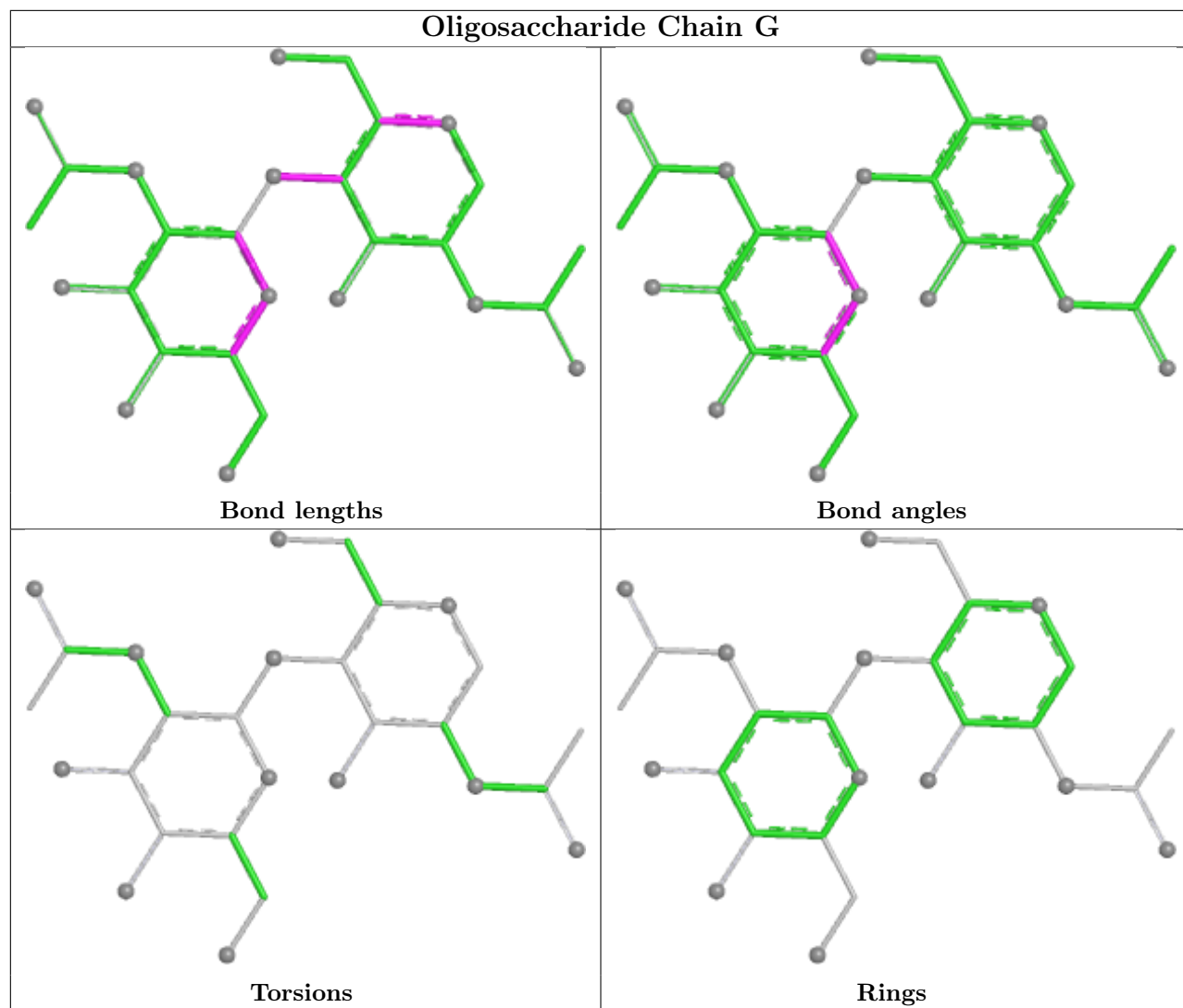
No monomer is involved in short contacts.

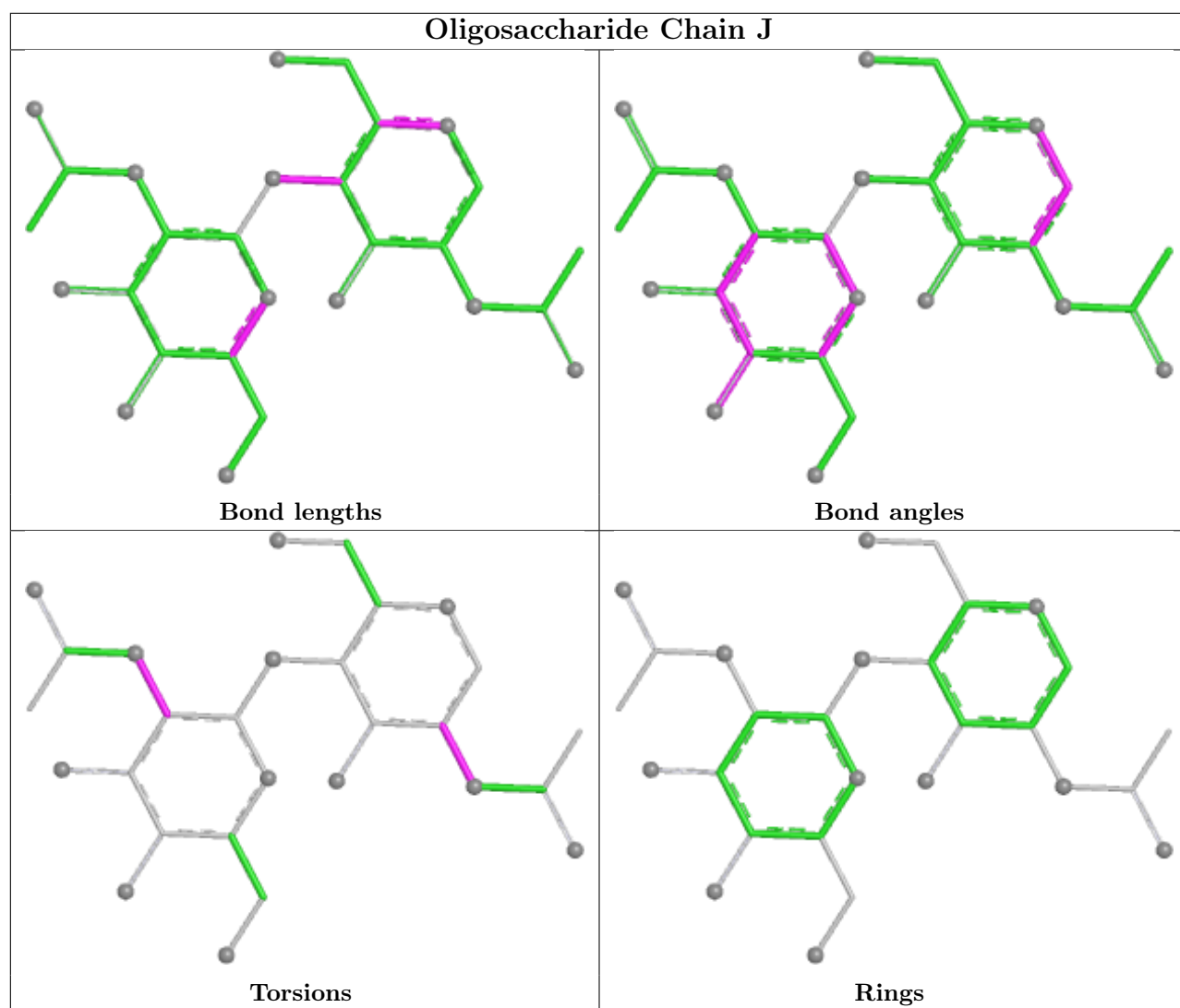
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

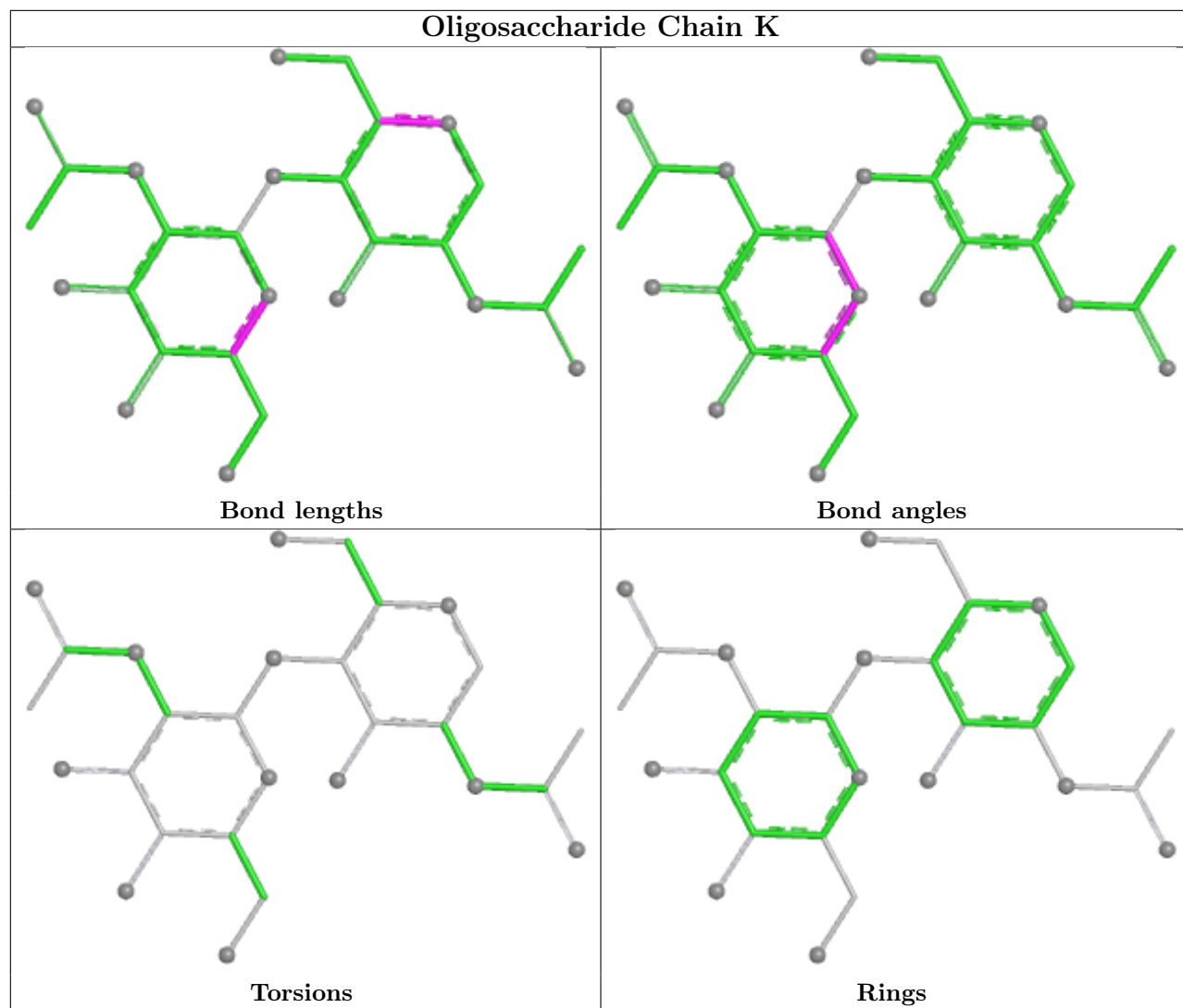




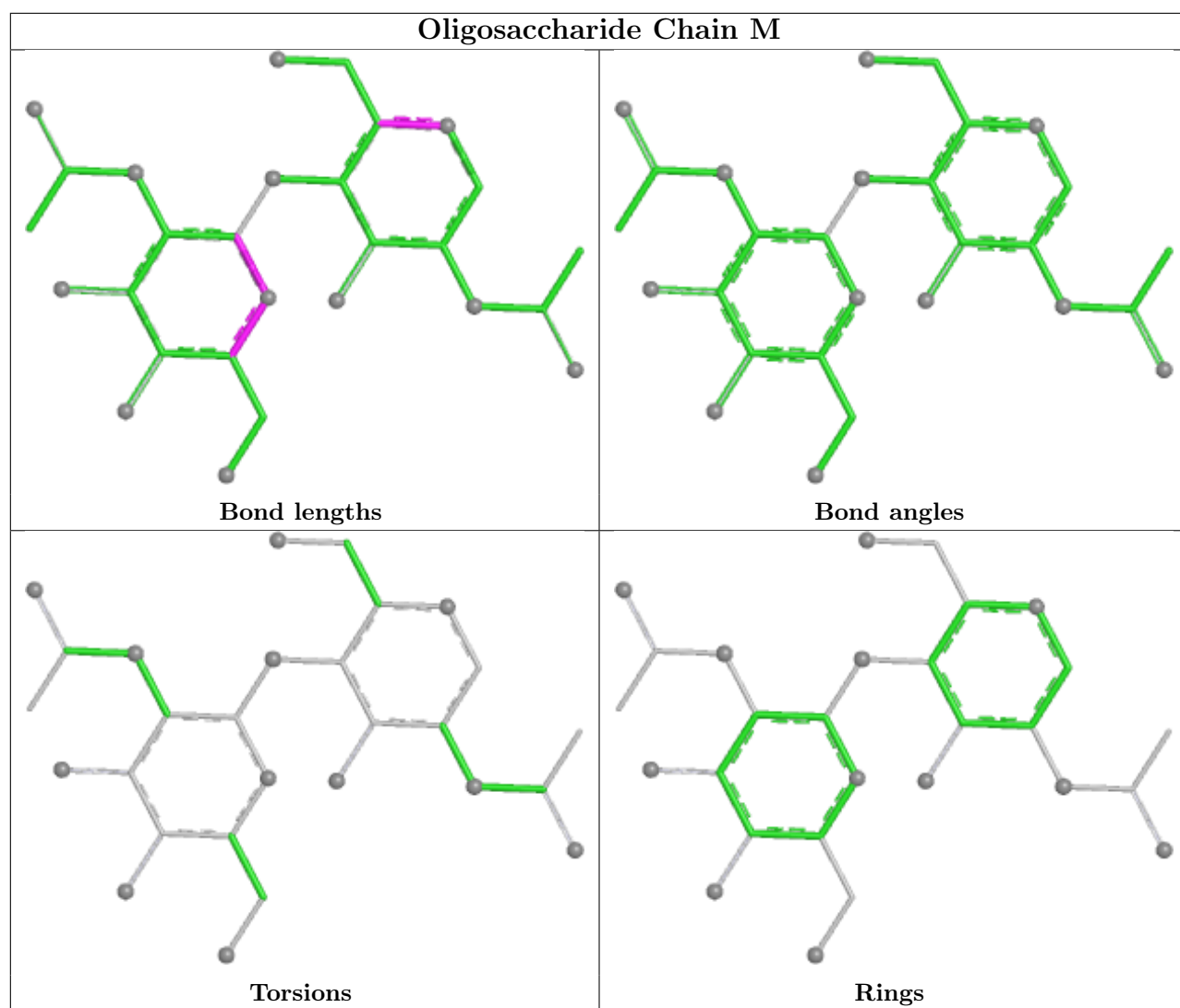


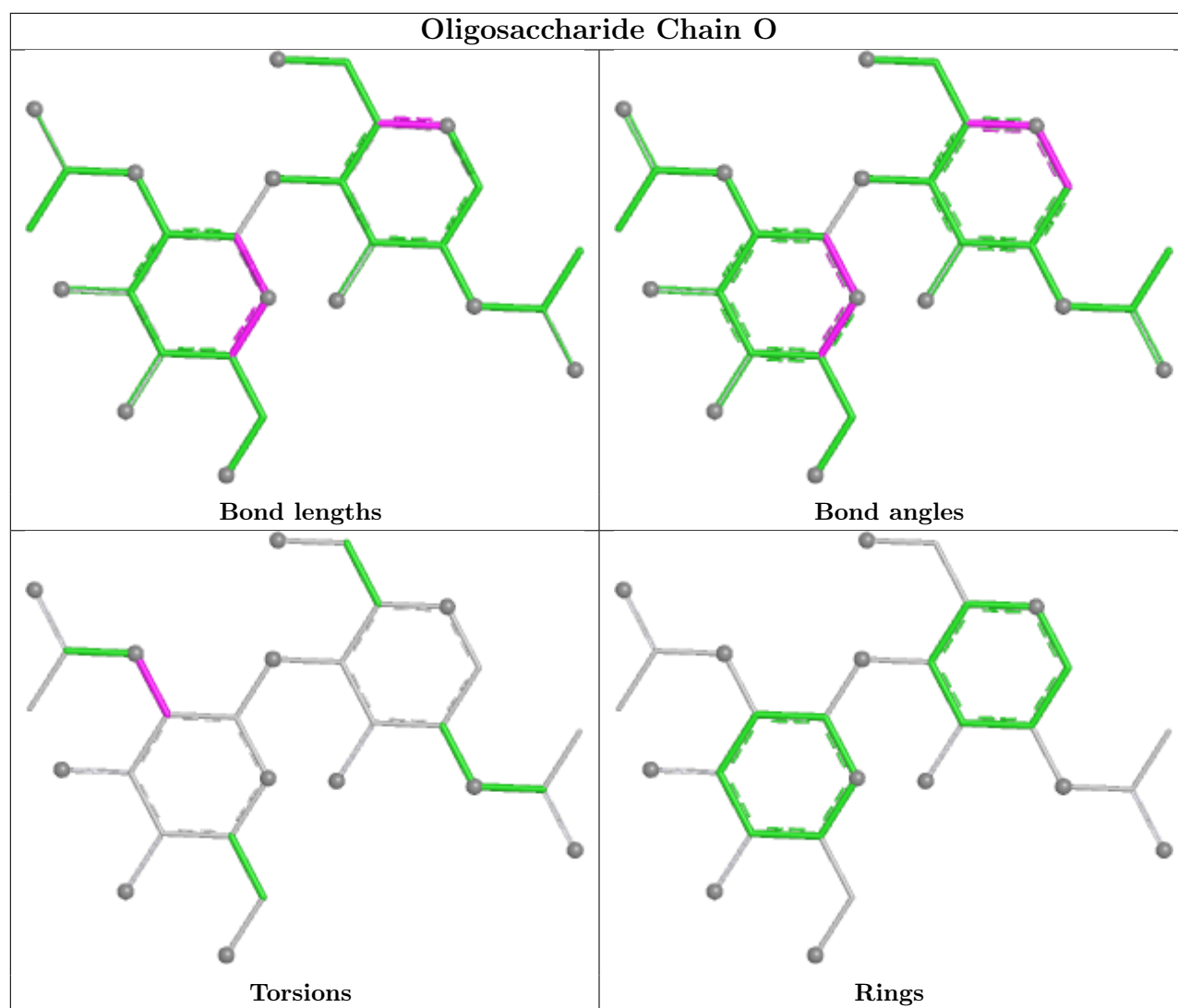


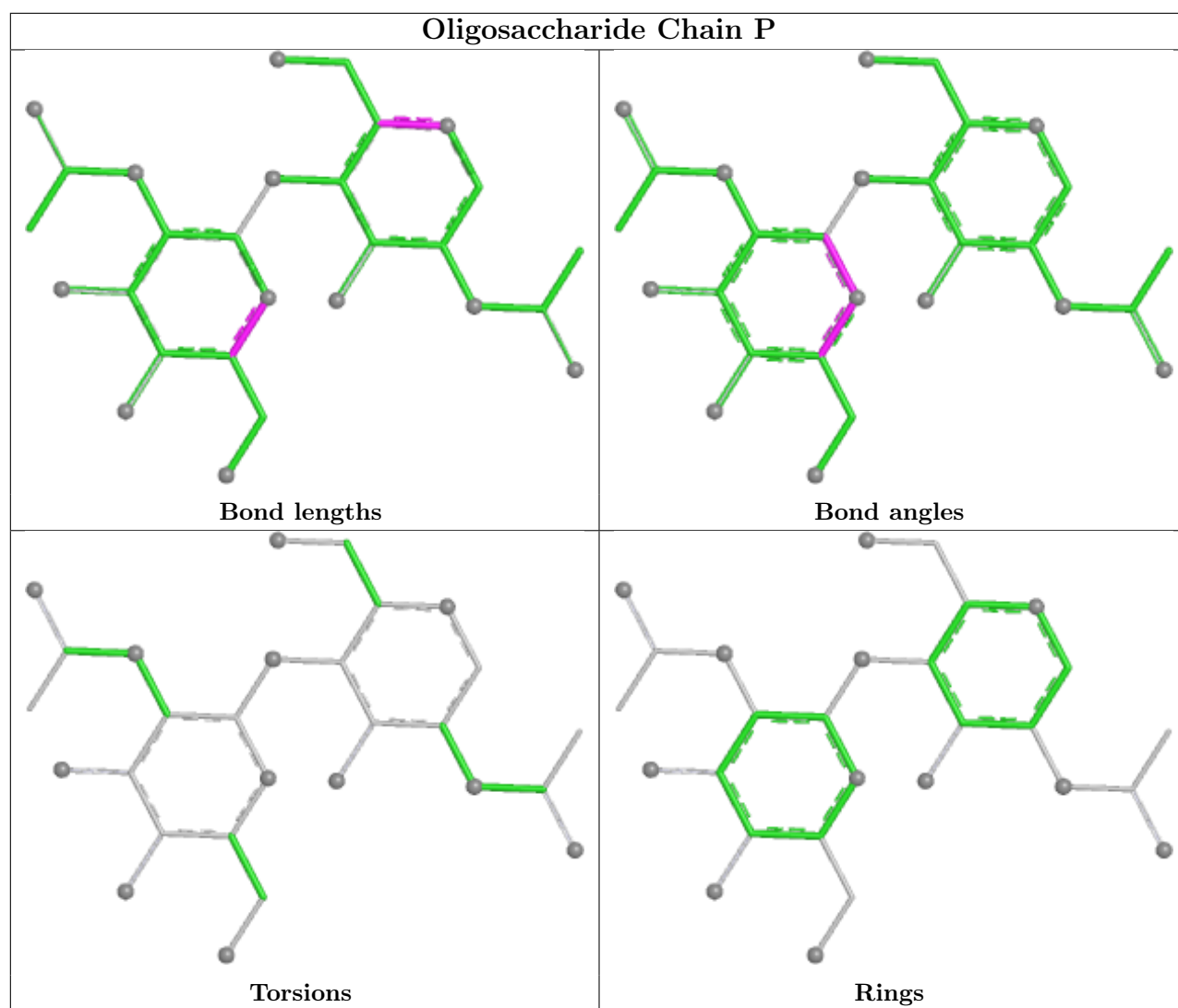


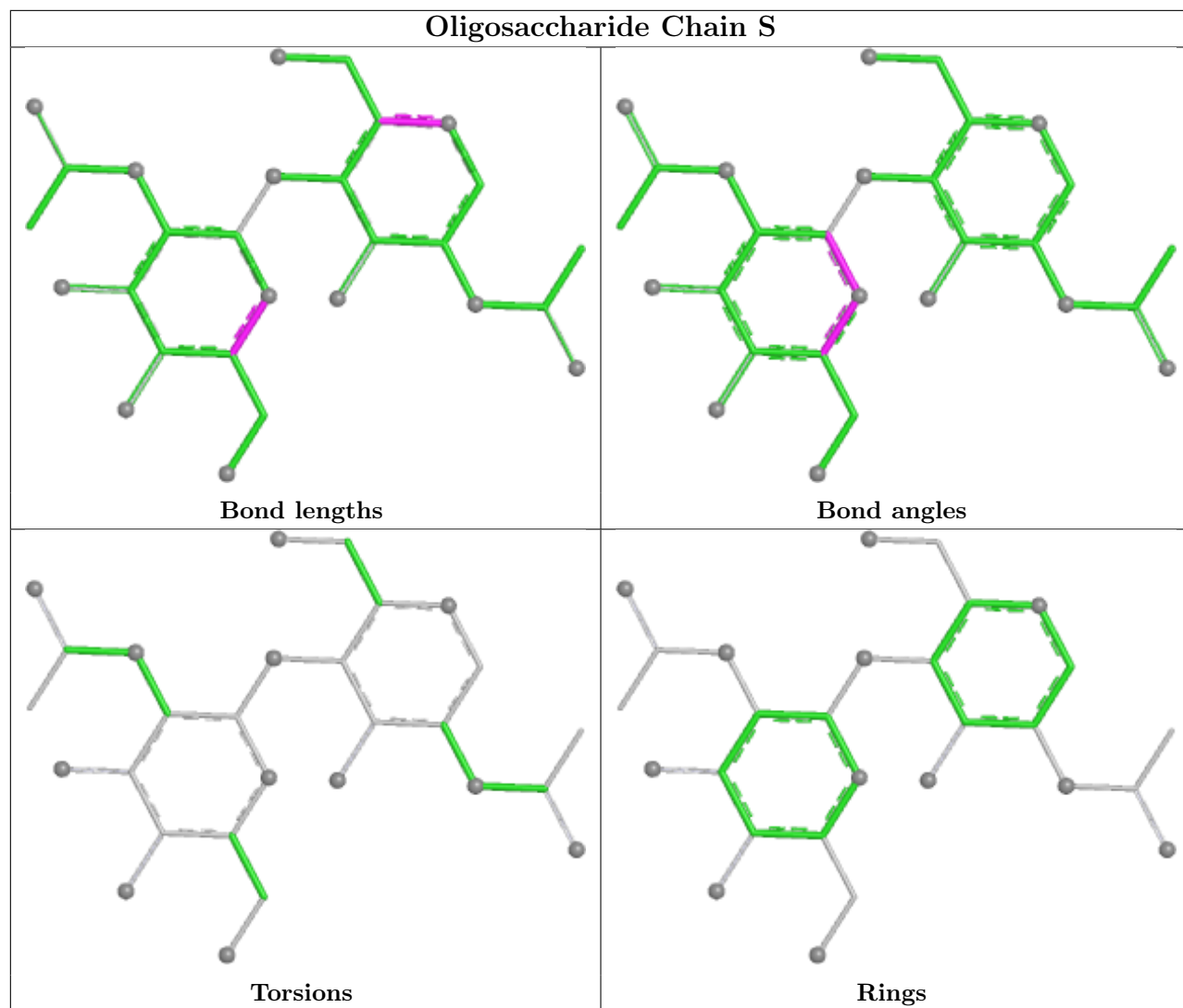


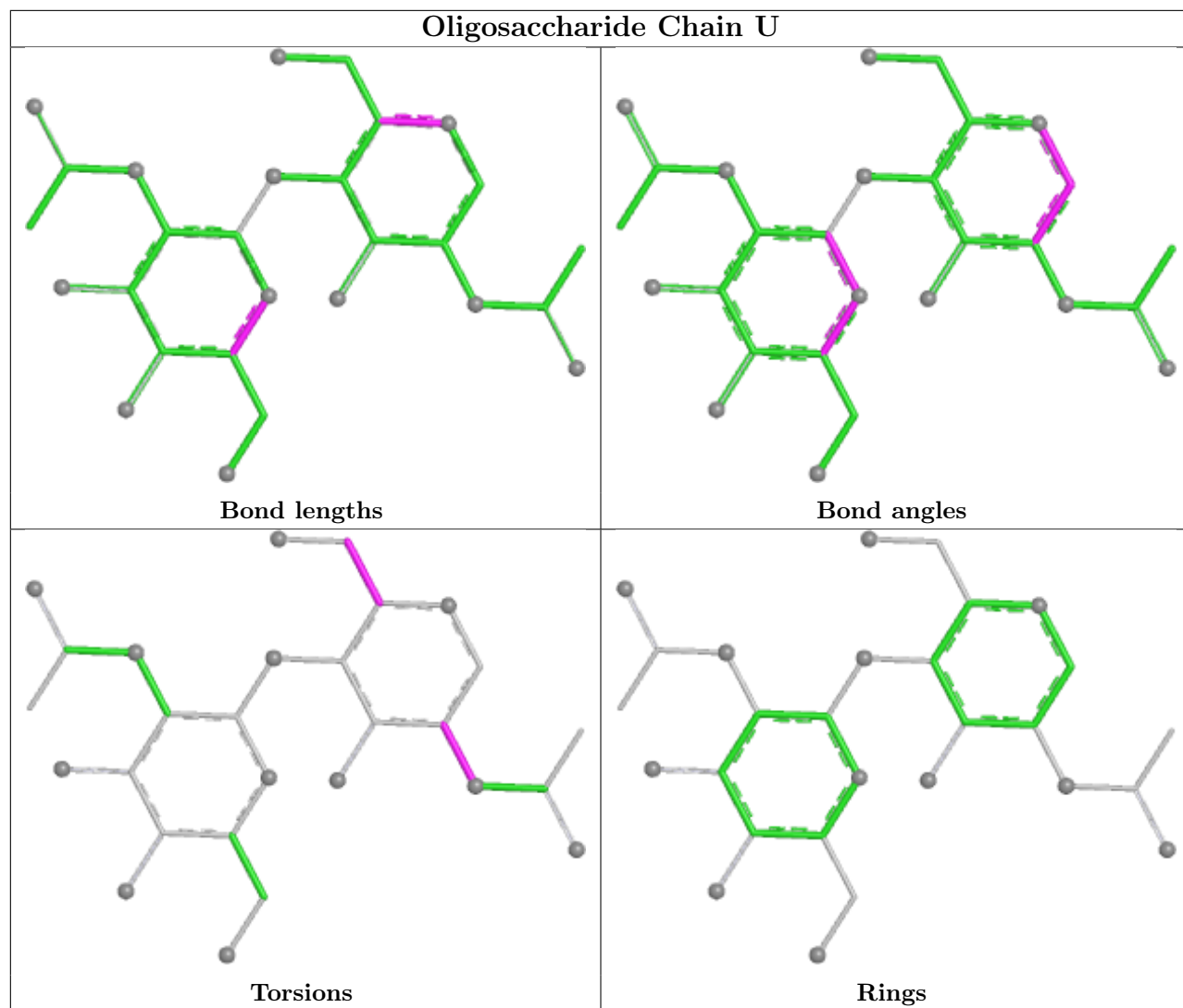


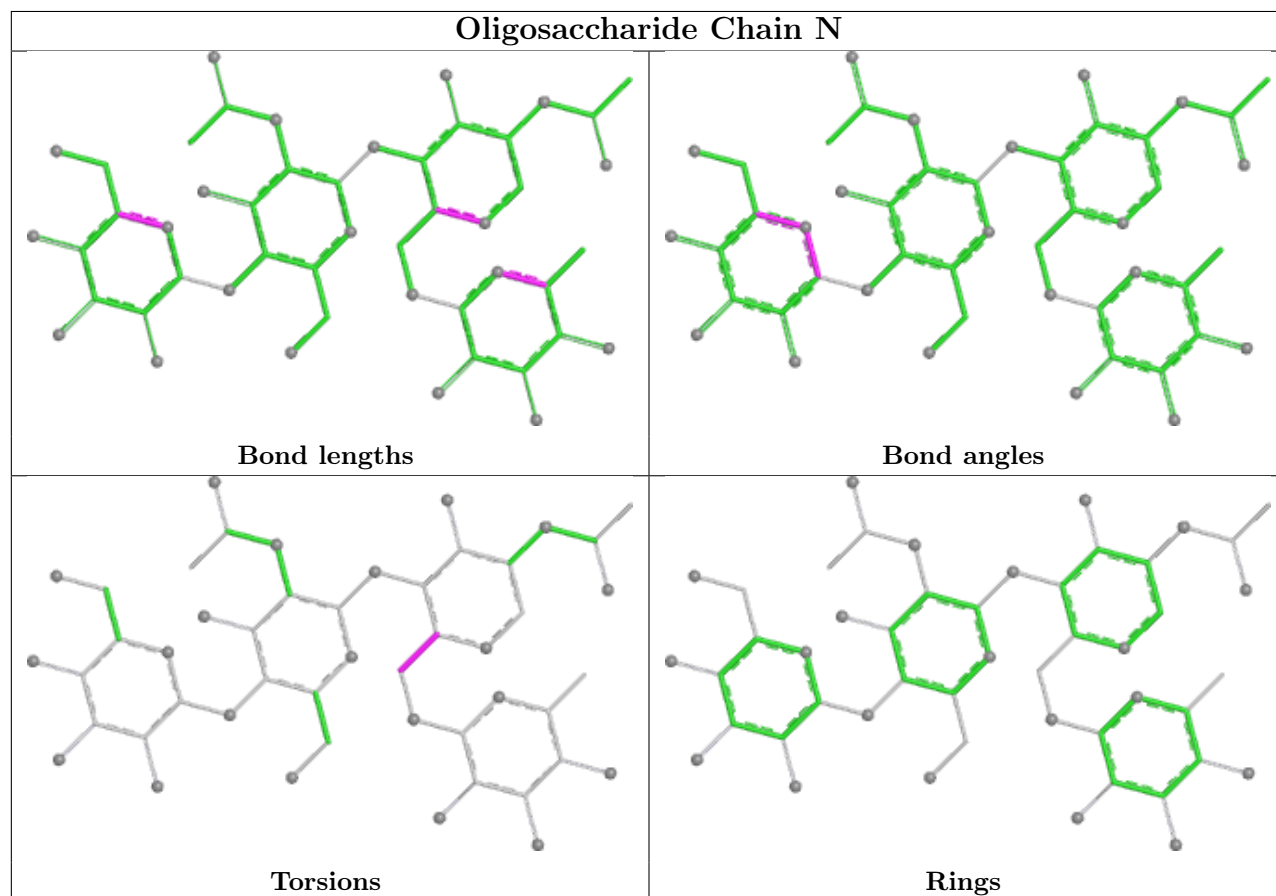
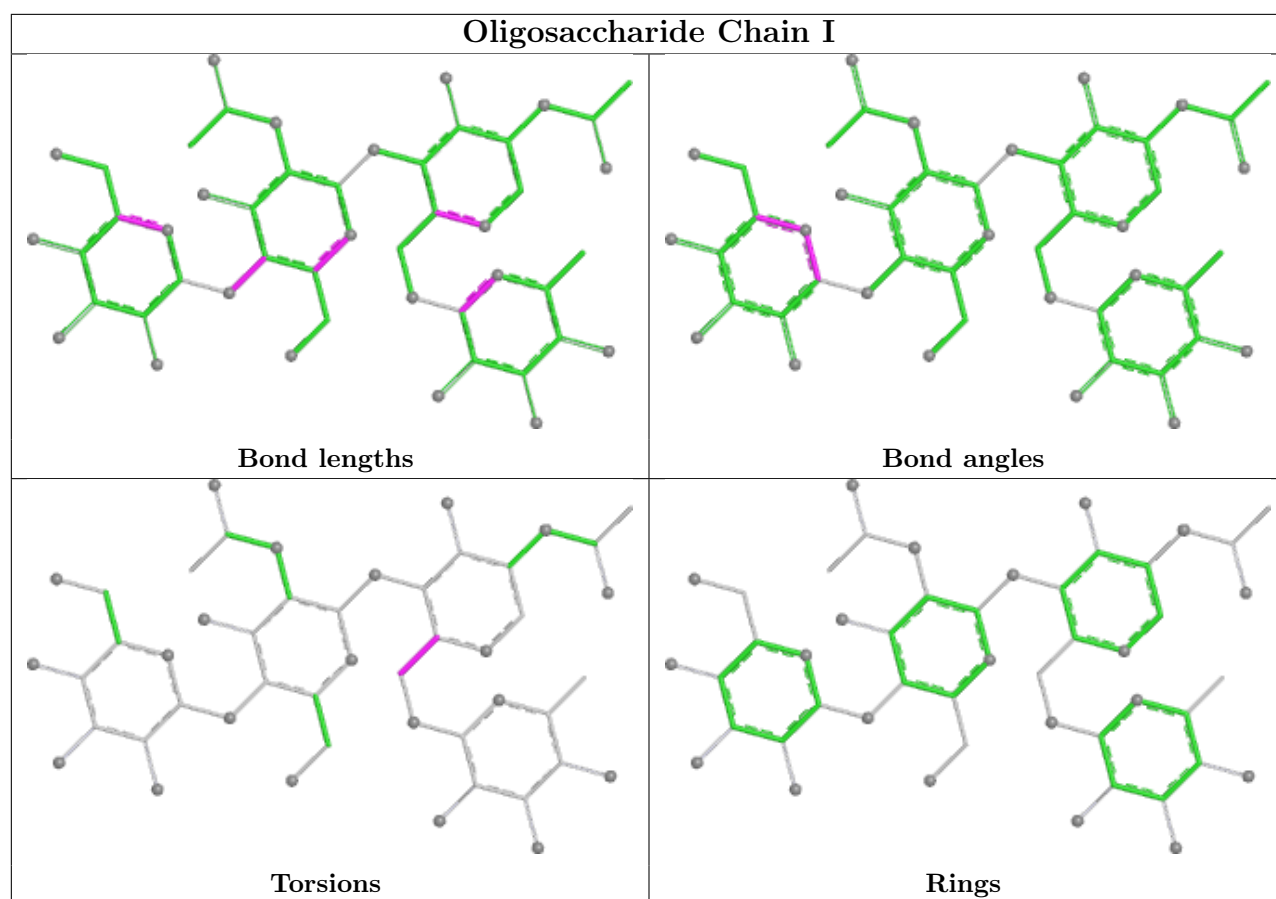


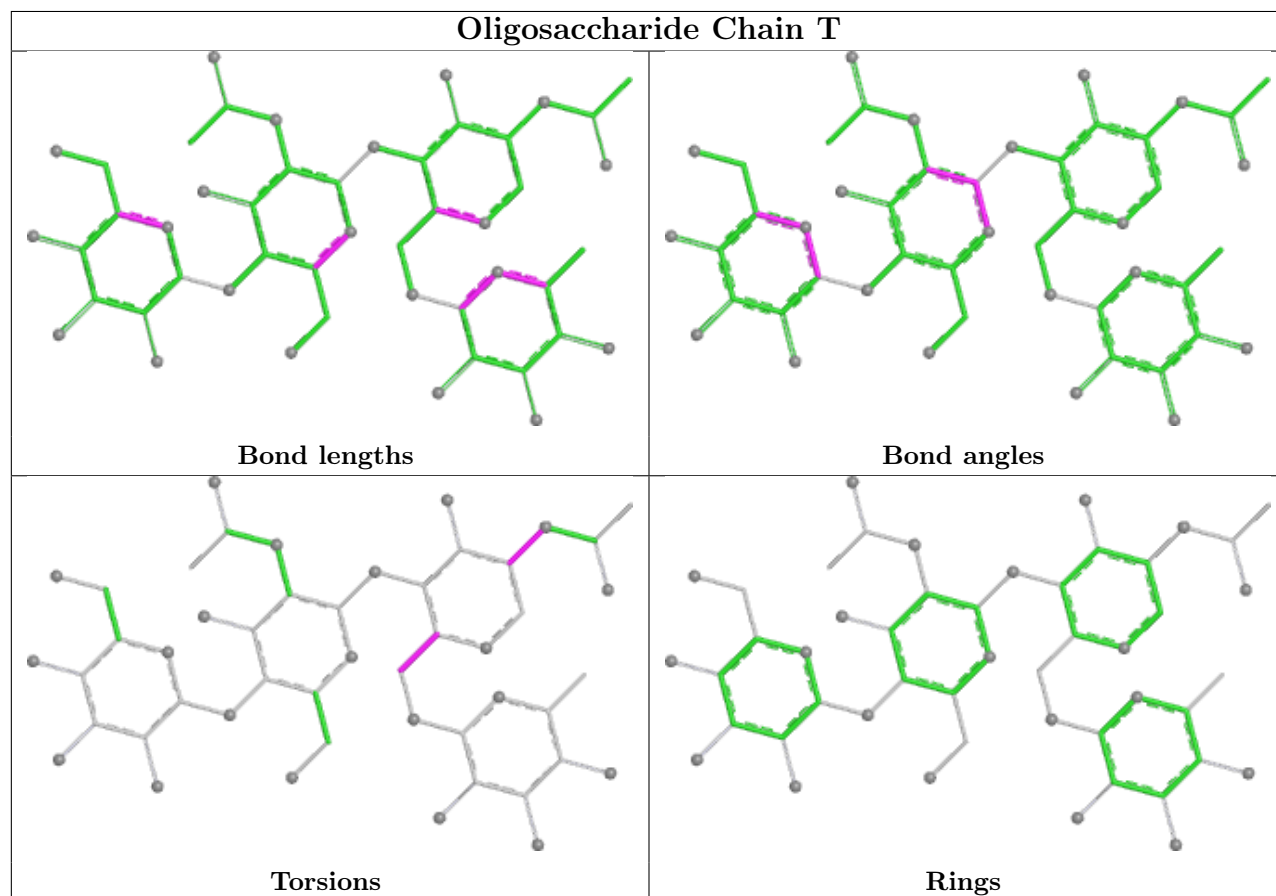
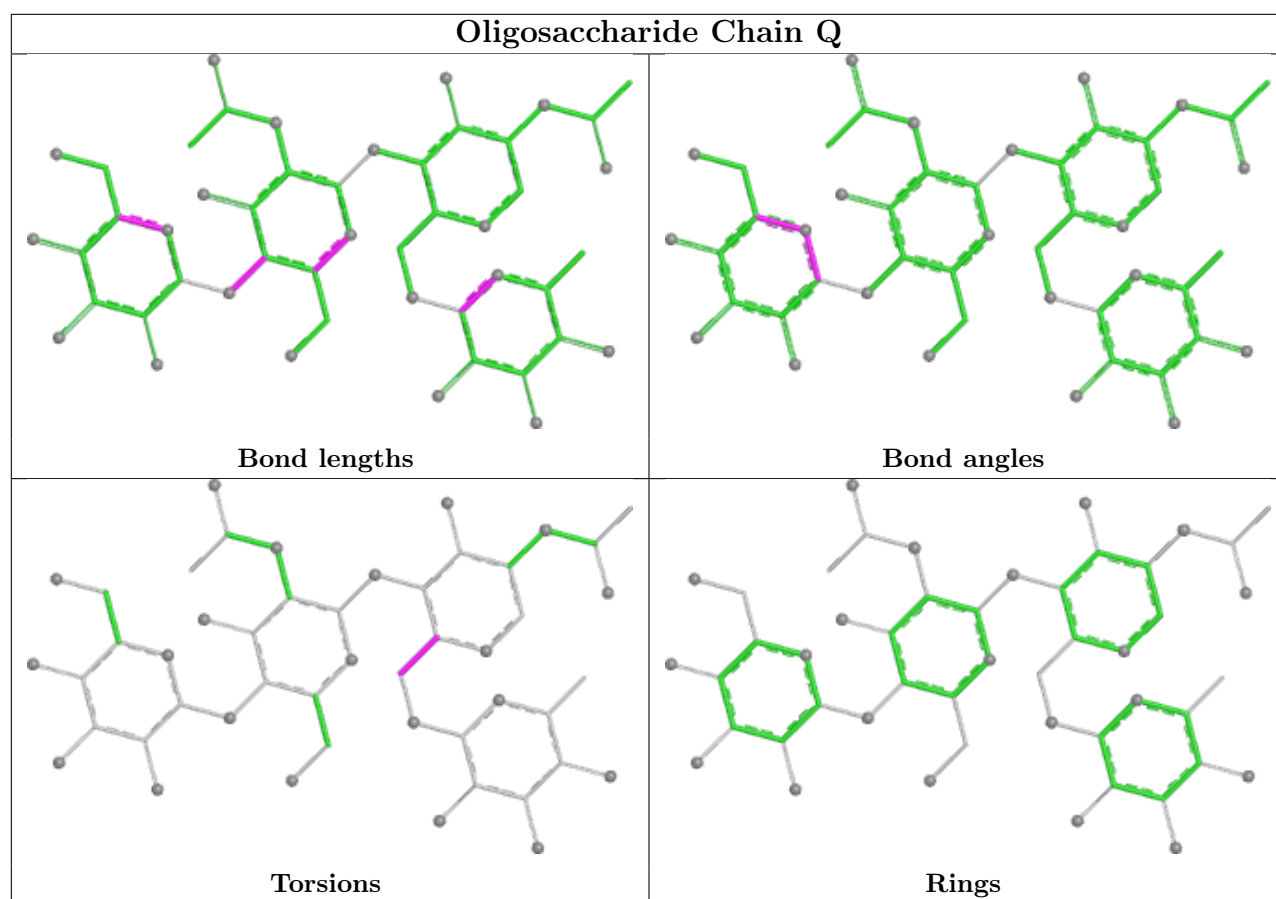












## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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	B	704	1	14,14,15	1.16	2 (14%)	17,19,21	1.16	1 (5%)
8	NAG	C	704	1	14,14,15	1.19	2 (14%)	17,19,21	0.91	1 (5%)
8	NAG	E	704	1	14,14,15	1.36	3 (21%)	17,19,21	0.79	1 (5%)
8	NAG	D	703	1	14,14,15	1.26	1 (7%)	17,19,21	0.81	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	704	1	-	1/6/23/26	0/1/1/1
8	NAG	C	704	1	-	0/6/23/26	0/1/1/1
8	NAG	E	704	1	-	0/6/23/26	0/1/1/1
8	NAG	D	703	1	-	0/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	703	NAG	O5-C5	3.07	1.49	1.43
8	E	704	NAG	O5-C5	3.05	1.49	1.43
8	C	704	NAG	O5-C5	2.64	1.48	1.43
8	E	704	NAG	C1-C2	2.35	1.55	1.52
8	E	704	NAG	O5-C1	2.33	1.47	1.43
8	B	704	NAG	C1-C2	2.28	1.55	1.52
8	B	704	NAG	O5-C5	2.25	1.47	1.43
8	C	704	NAG	C1-C2	2.09	1.55	1.52

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
8	B	704	NAG	C1-O5-C5	4.31	117.96	112.19
8	C	704	NAG	C1-O5-C5	2.62	115.70	112.19
8	E	704	NAG	C1-O5-C5	2.21	115.15	112.19
8	D	703	NAG	C1-O5-C5	2.15	115.07	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	704	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

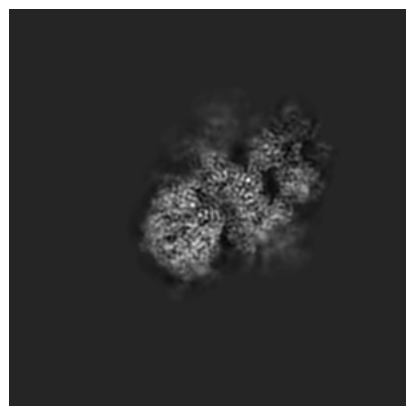
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26426. These allow visual inspection of the internal detail of the map and identification of artifacts.

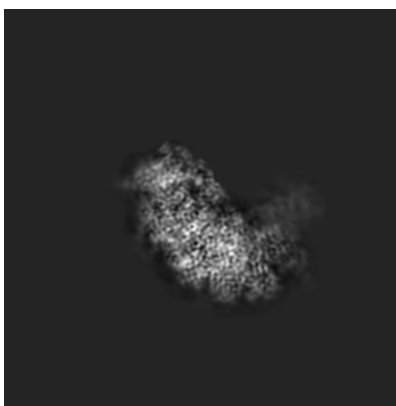
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

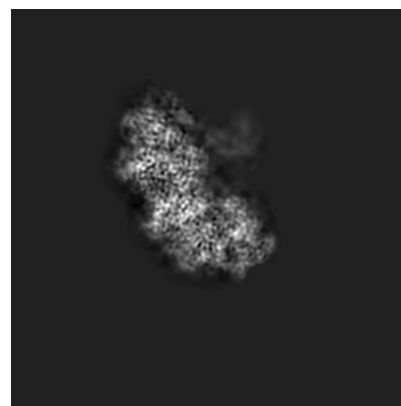
#### 6.1.1 Primary map



X

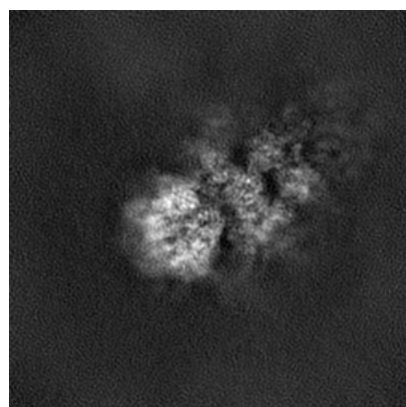


Y

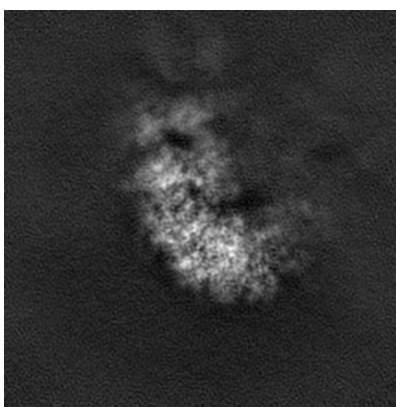


Z

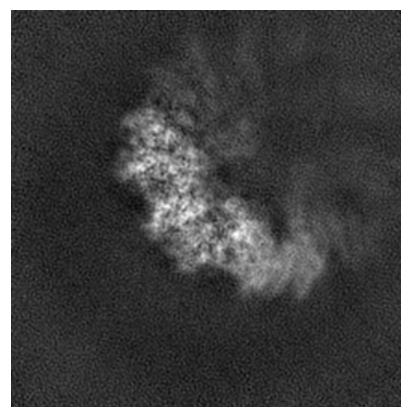
#### 6.1.2 Raw map



X



Y

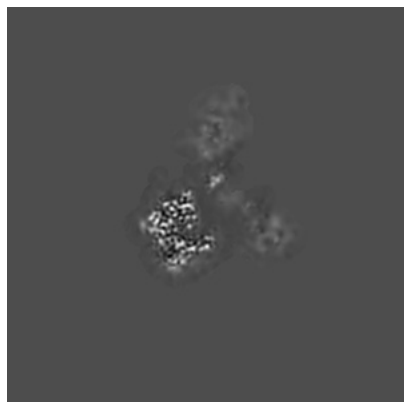


Z

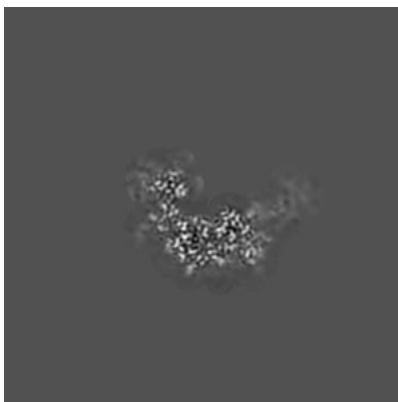
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

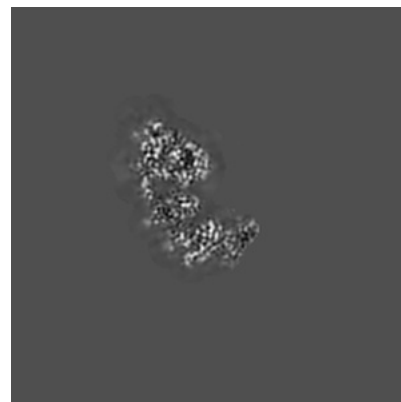
### 6.2.1 Primary map



X Index: 108

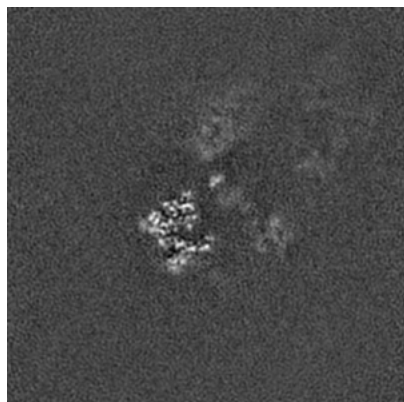


Y Index: 108

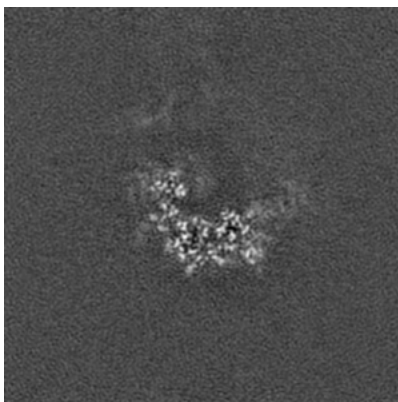


Z Index: 108

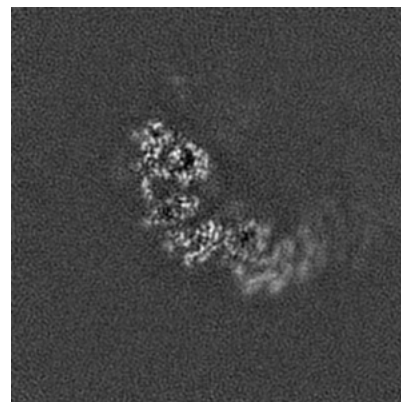
### 6.2.2 Raw map



X Index: 108



Y Index: 108

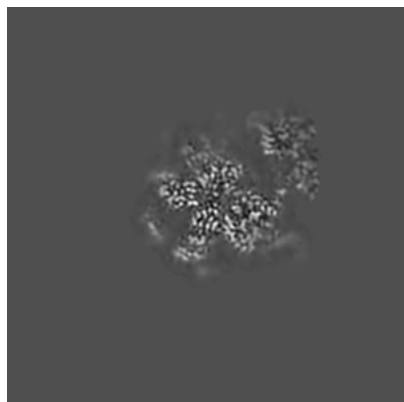


Z Index: 108

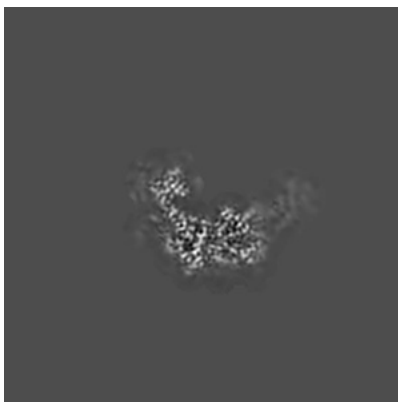
The images above show central slices of the map in three orthogonal directions.

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

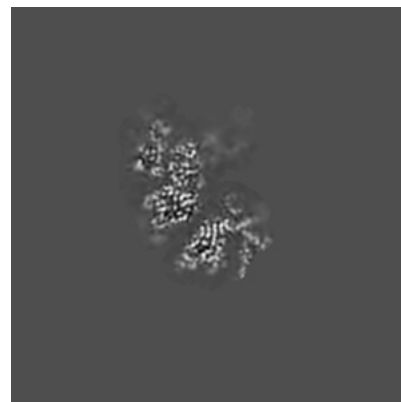
### 6.3.1 Primary map



X Index: 91

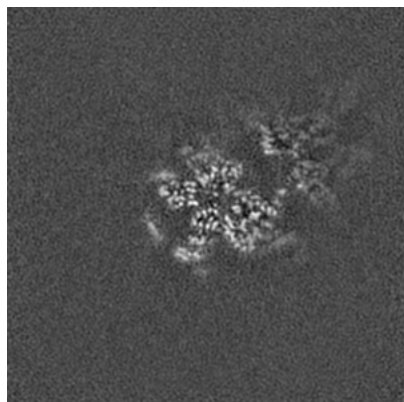


Y Index: 109

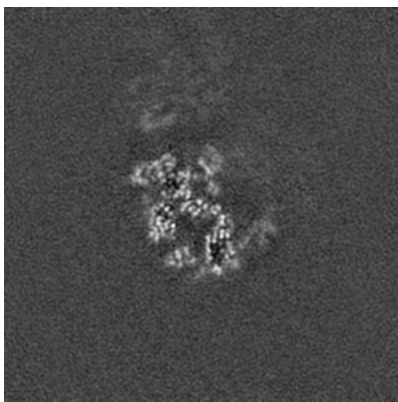


Z Index: 99

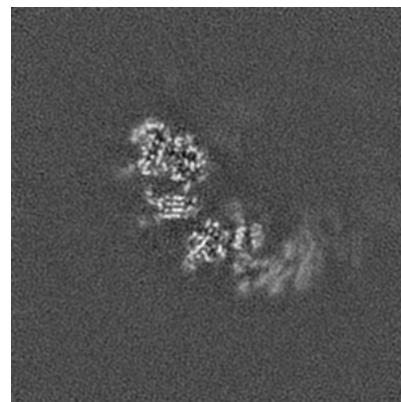
### 6.3.2 Raw map



X Index: 91



Y Index: 98

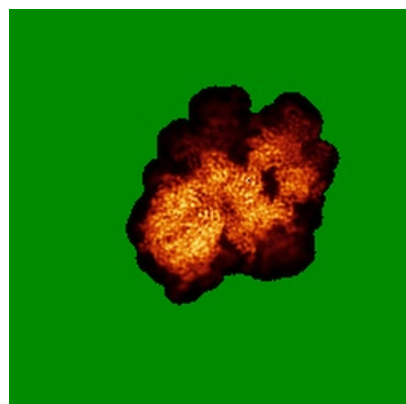


Z Index: 105

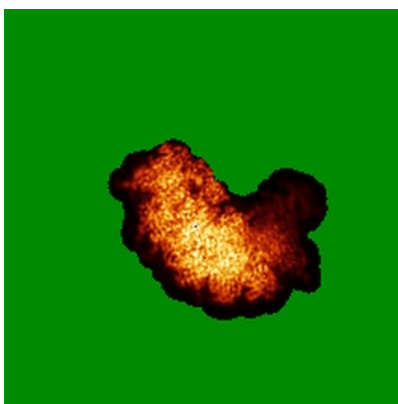
The images above show the largest variance slices of the map in three orthogonal directions.

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

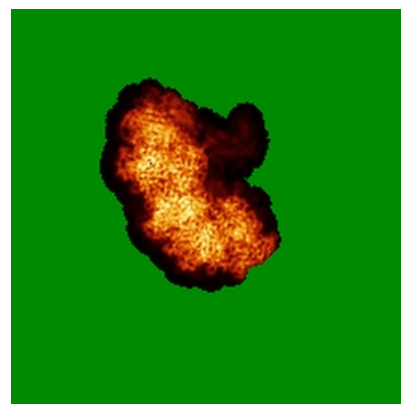
### 6.4.1 Primary map



X

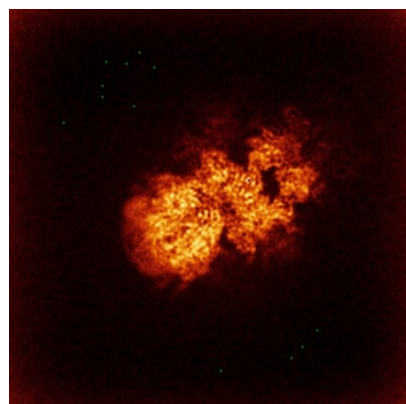


Y

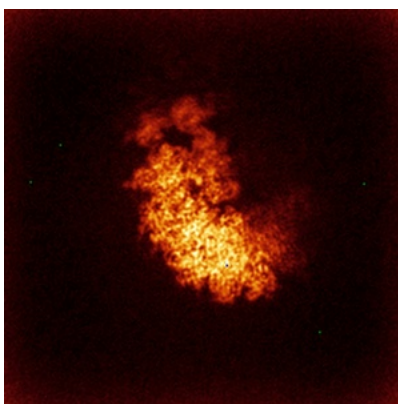


Z

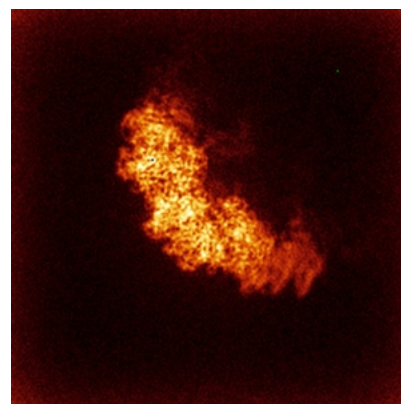
### 6.4.2 Raw map



X



Y

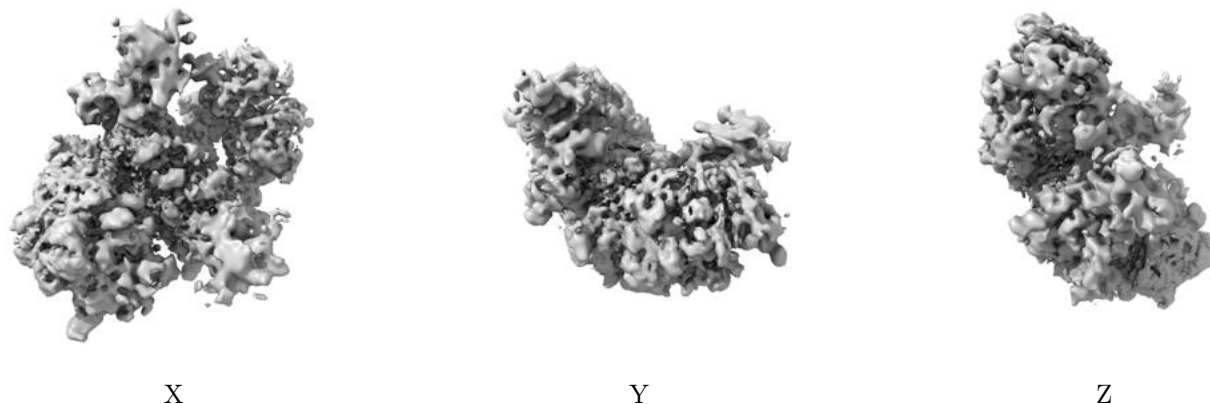


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

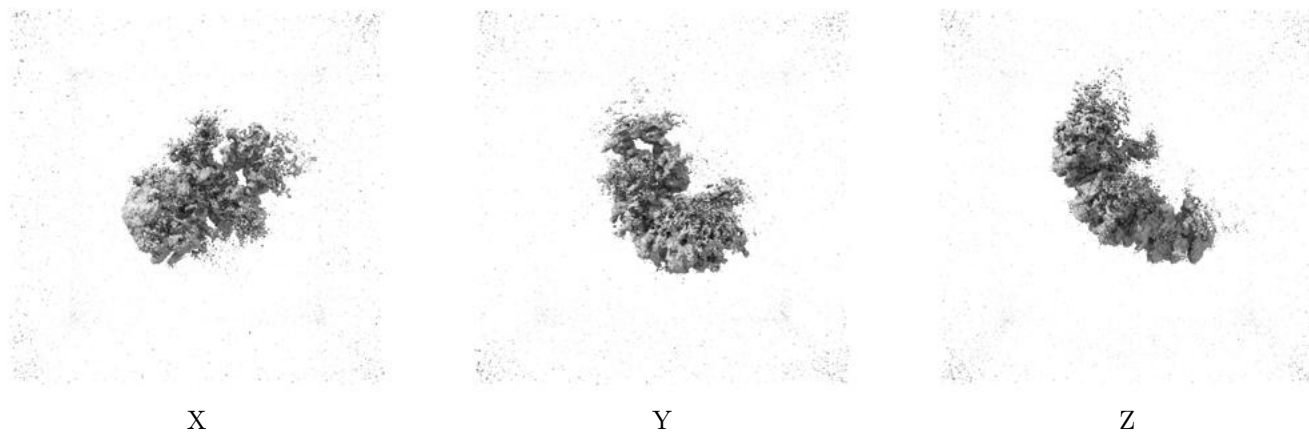
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

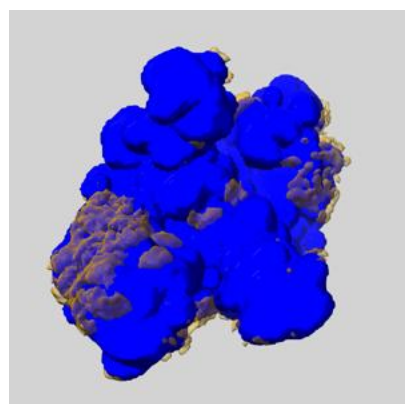
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

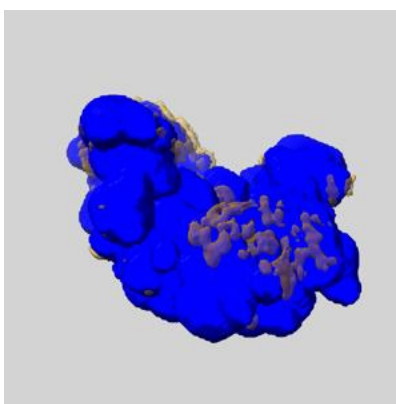
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

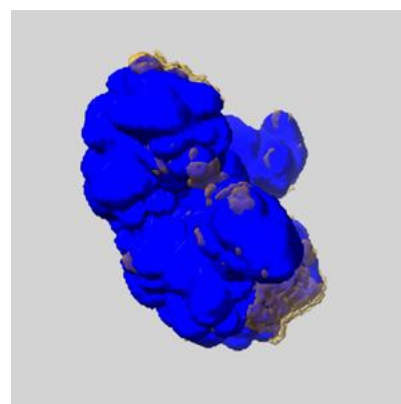
### 6.6.1 emd\_26426\_msk\_1.map [i](#)



X



Y



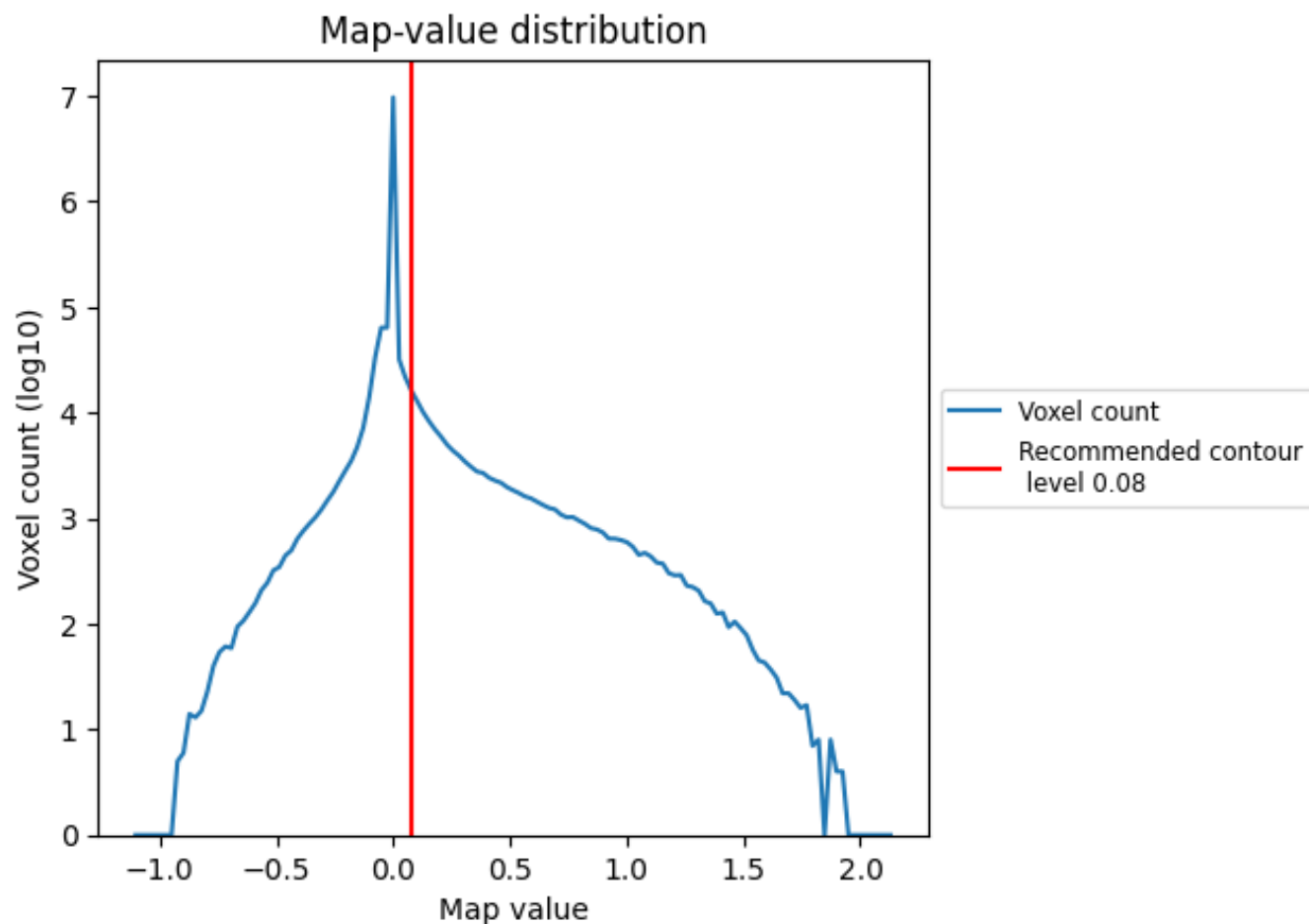
Z



## 7 Map analysis [i](#)

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

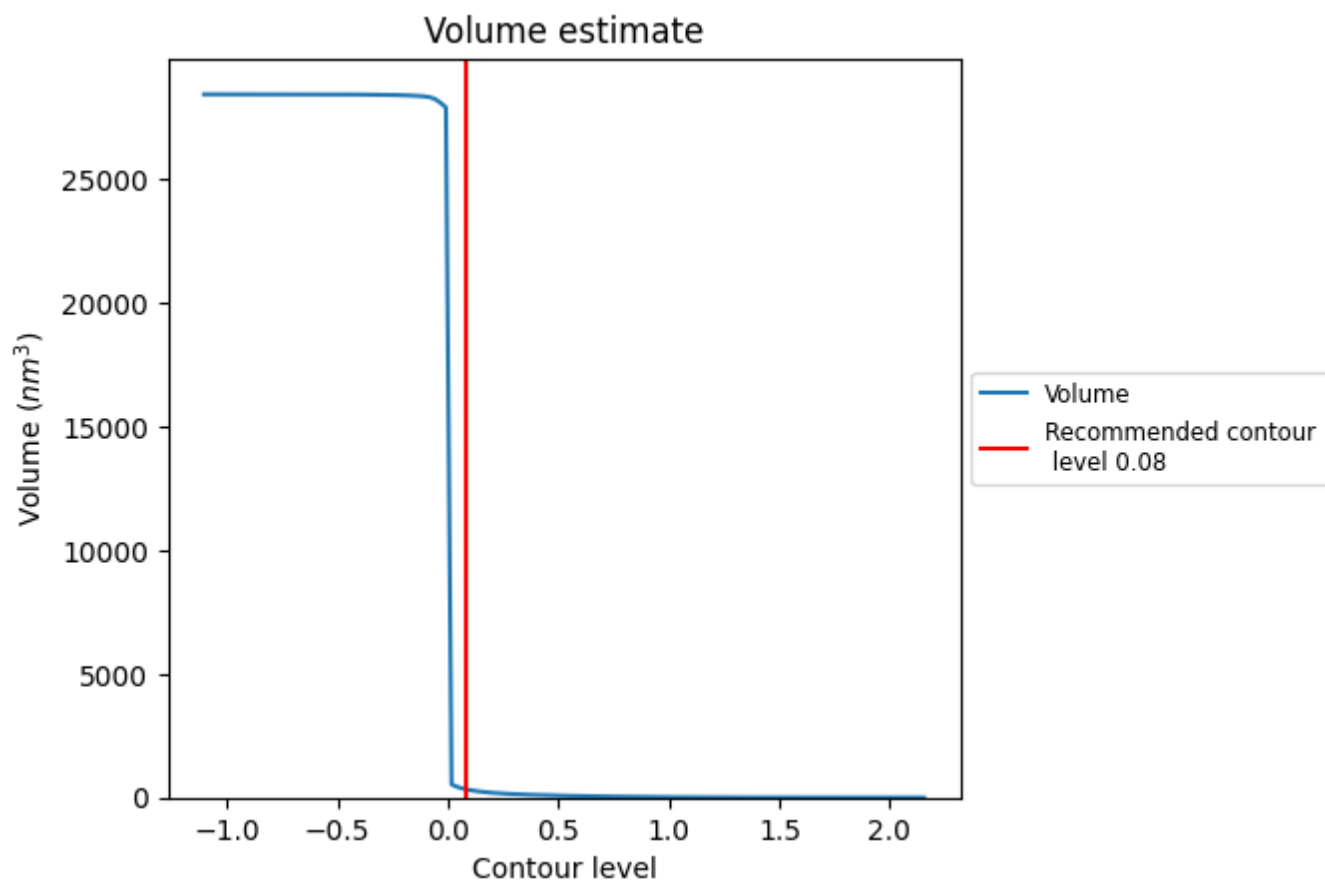
### 7.1 Map-value distribution [i](#)



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.



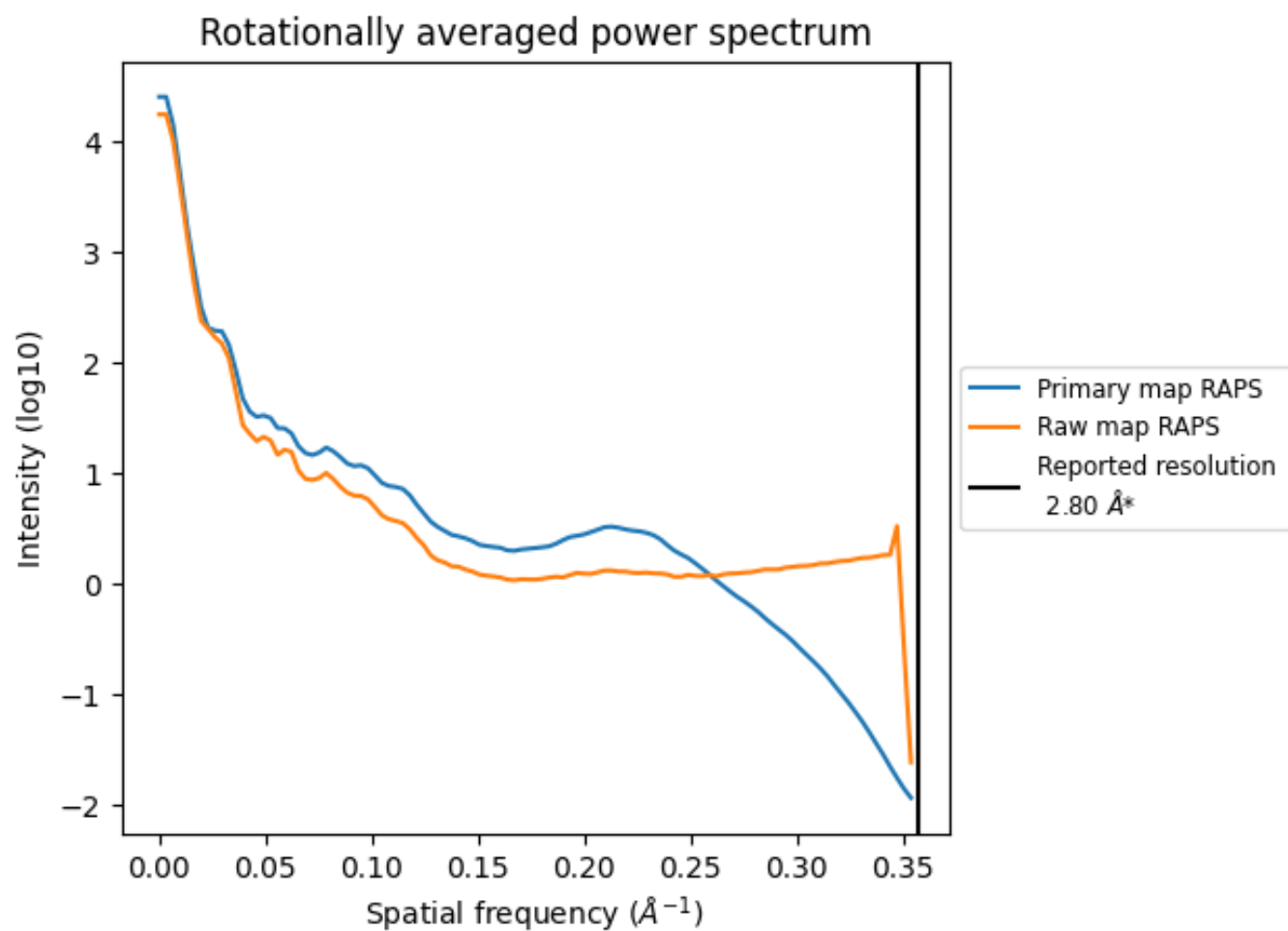
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339  $\text{nm}^3$ ; this corresponds to an approximate mass of 306 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 ⓘ

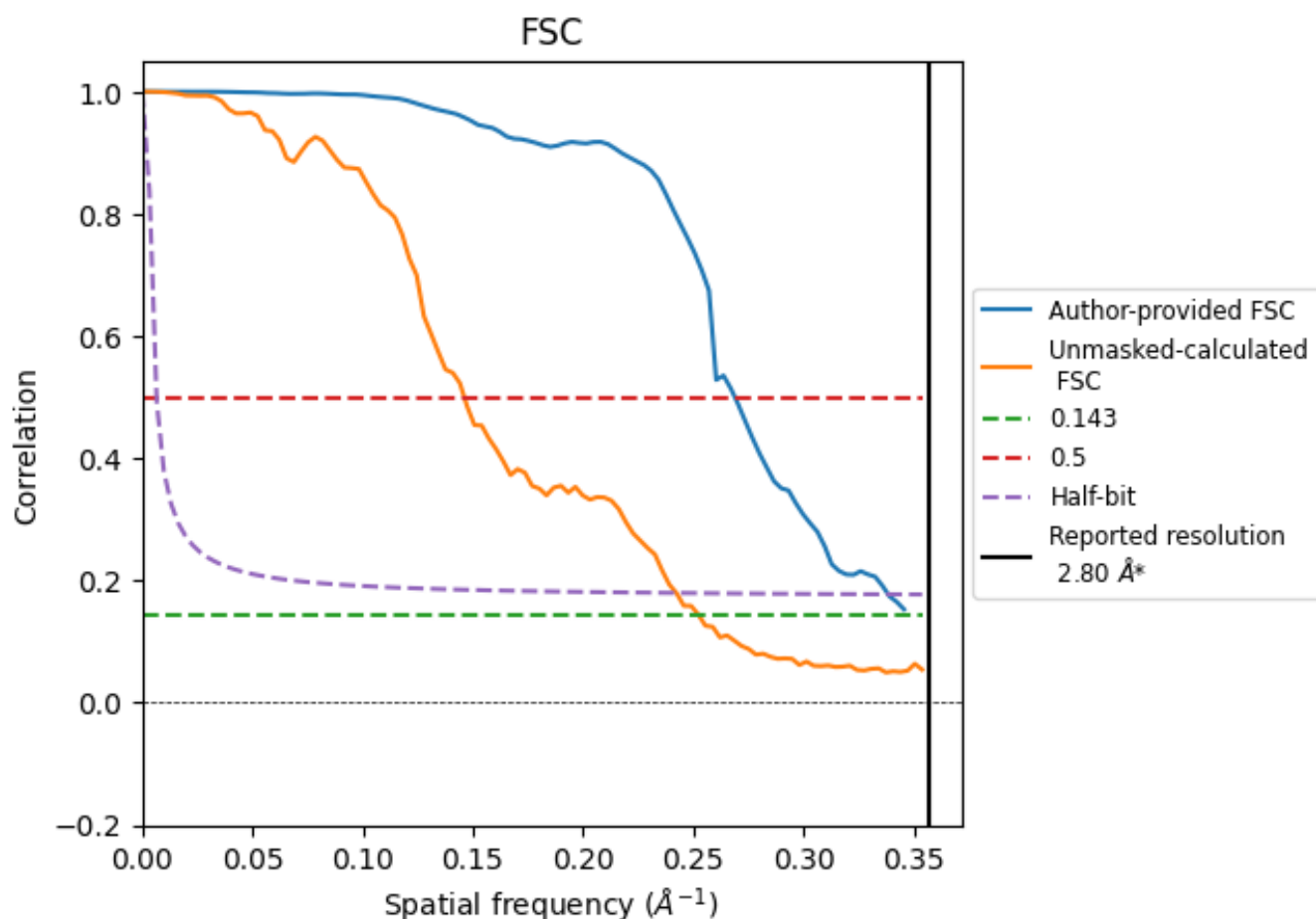


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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 0.357 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

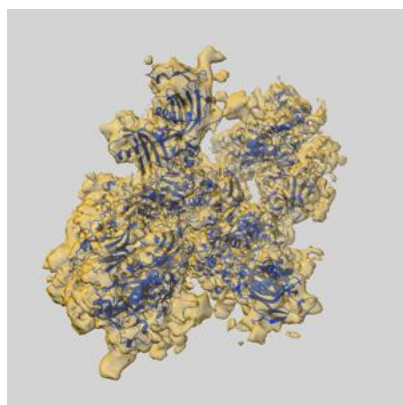
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	3.72	2.96
Unmasked-calculated*	3.96	6.84	4.13

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 2.8 by more than 10 %

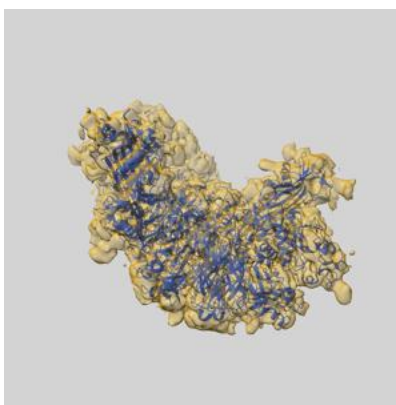
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26426 and PDB model 7UAI. Per-residue inclusion information can be found in section [3](#) on page [9](#).

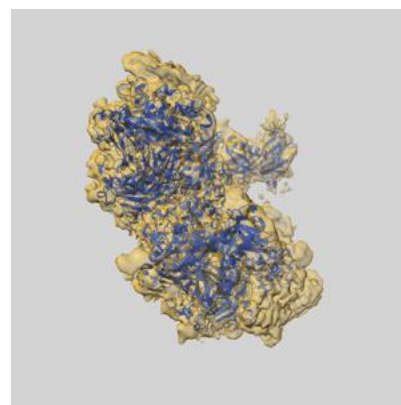
### 9.1 Map-model overlay [i](#)



X



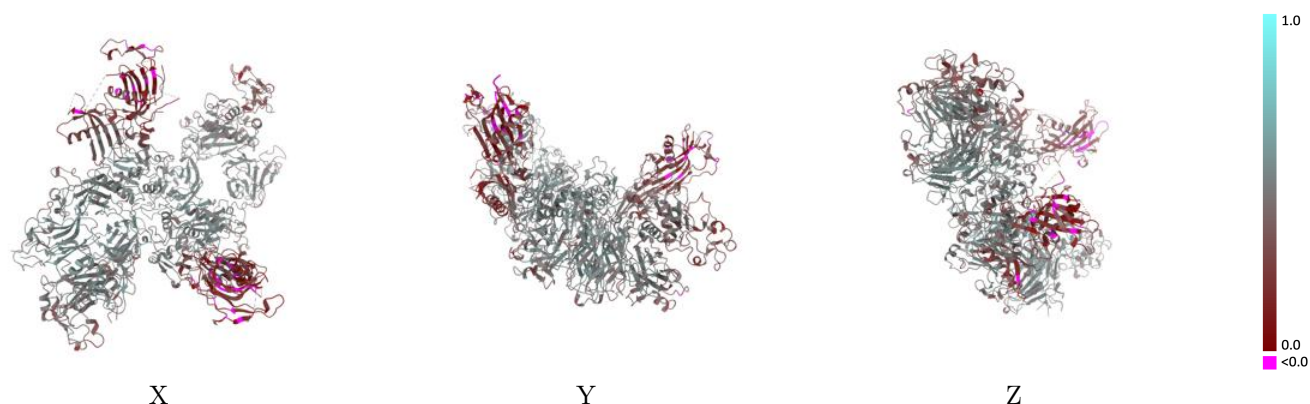
Y



Z

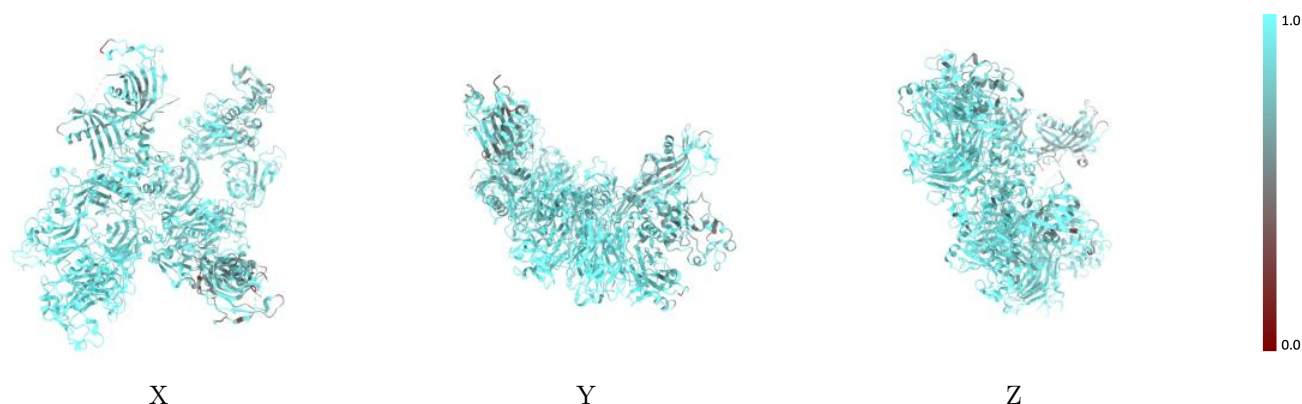
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



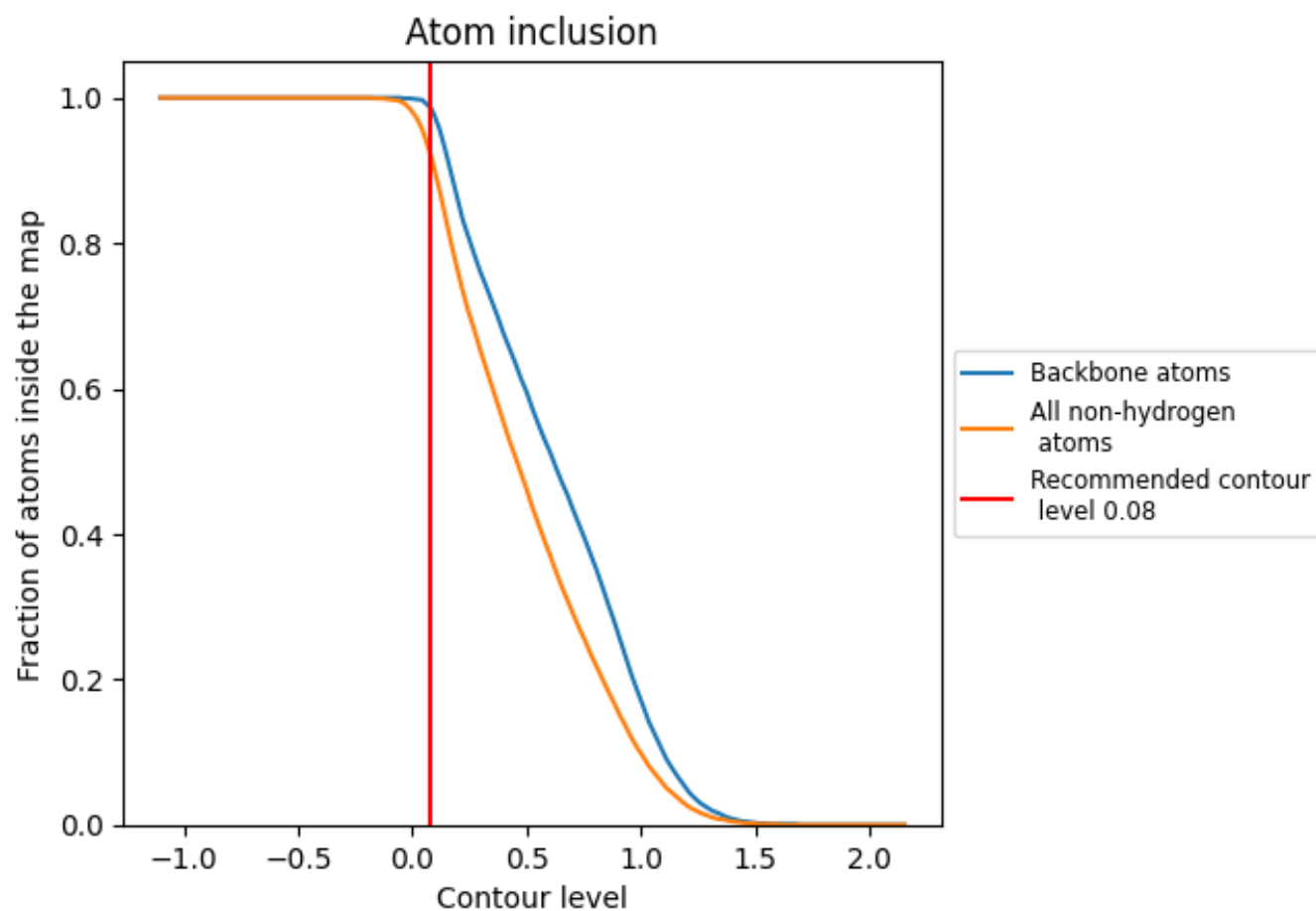
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9210	 0.4250
A	 0.8300	 0.2500
B	 0.9760	 0.4910
C	 0.9720	 0.4810
D	 0.9770	 0.4950
E	 0.8890	 0.4300
F	 0.1910	 0.1390
G	 0.6790	 0.3040
H	 0.7520	 0.2160
I	 0.9590	 0.3940
J	 0.8930	 0.3140
K	 1.0000	 0.3600
L	 0.9520	 0.3690
M	 0.9640	 0.3640
N	 0.9800	 0.4480
O	 0.9640	 0.3870
P	 1.0000	 0.3340
Q	 1.0000	 0.4060
R	 1.0000	 0.4200
S	 1.0000	 0.3770
T	 0.9800	 0.3790
U	 1.0000	 0.3380

