



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:30 AM UTC

PDB ID : 9G2F / pdb\_00009g2f  
EMDB ID : EMD-50975  
Title : Mouse Teneurin2 dimer variant A1B1  
Authors : Berbeira-Santana, M.; Zhou, J.C.; el Omari, K.; Baker, L.; Seiradake, E.  
Deposited on : 2024-07-10  
Resolution : 2.80 Å (reported)  
Based on initial model : .

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:

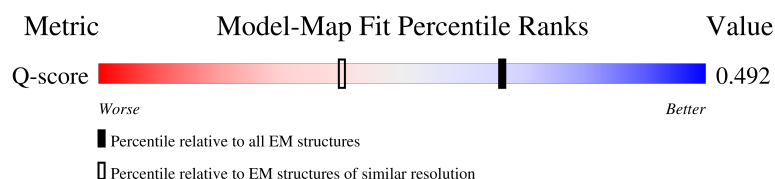
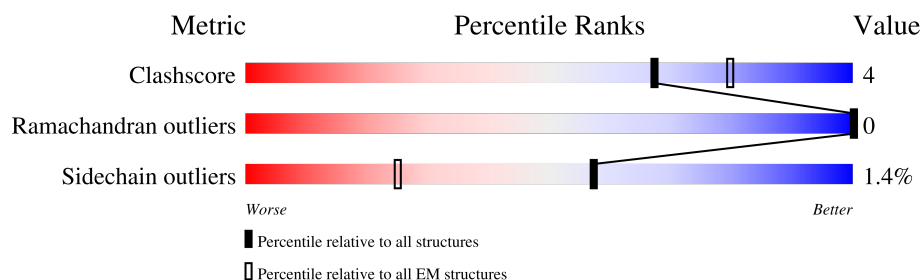
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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.







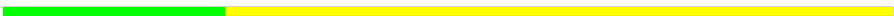
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 ( 2.30 - 3.30 )

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	2410	 5% 65% 8% 27%
1	B	2410	 6% 64% 9% 27%
2	C	2	 100%
2	F	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%
2	K	2	 50% 50%
2	L	2	 50% 50%
3	D	5	 60% 40%
3	I	5	 20% 60% 20%
4	E	4	 50% 50%
4	J	4	 25% 75%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28158 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 Teneurin transmembrane protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1752	Total	C	N	O	S	0	0
			13842	8734	2397	2656	55		
1	B	1752	Total	C	N	O	S	0	0
			13842	8734	2397	2656	55		

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	GLU	-	expression tag	UNP A0A0A0MQB7
A	368	THR	-	expression tag	UNP A0A0A0MQB7
A	369	GLY	-	expression tag	UNP A0A0A0MQB7
A	370	HIS	-	expression tag	UNP A0A0A0MQB7
A	371	HIS	-	expression tag	UNP A0A0A0MQB7
A	372	HIS	-	expression tag	UNP A0A0A0MQB7
A	373	HIS	-	expression tag	UNP A0A0A0MQB7
A	374	HIS	-	expression tag	UNP A0A0A0MQB7
A	375	HIS	-	expression tag	UNP A0A0A0MQB7
A	376	ARG	-	expression tag	UNP A0A0A0MQB7
A	377	GLY	-	expression tag	UNP A0A0A0MQB7
A	378	GLY	-	expression tag	UNP A0A0A0MQB7
A	379	LEU	-	expression tag	UNP A0A0A0MQB7
A	380	ASN	-	expression tag	UNP A0A0A0MQB7
A	381	ASP	-	expression tag	UNP A0A0A0MQB7
A	382	ILE	-	expression tag	UNP A0A0A0MQB7
A	383	PHE	-	expression tag	UNP A0A0A0MQB7
A	384	GLU	-	expression tag	UNP A0A0A0MQB7
A	385	ALA	-	expression tag	UNP A0A0A0MQB7
A	386	GLN	-	expression tag	UNP A0A0A0MQB7
A	387	LYS	-	expression tag	UNP A0A0A0MQB7
A	388	ILE	-	expression tag	UNP A0A0A0MQB7
A	389	GLU	-	expression tag	UNP A0A0A0MQB7
A	390	TRP	-	expression tag	UNP A0A0A0MQB7
A	391	HIS	-	expression tag	UNP A0A0A0MQB7
A	392	GLU	-	expression tag	UNP A0A0A0MQB7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	393	GLY	-	expression tag	UNP A0A0A0MQB7
A	394	GLY	-	expression tag	UNP A0A0A0MQB7
A	395	SER	-	expression tag	UNP A0A0A0MQB7
A	396	THR	-	expression tag	UNP A0A0A0MQB7
A	397	GLY	-	expression tag	UNP A0A0A0MQB7
A	737	GLU	-	insertion	UNP A0A0A0MQB7
A	799	GLY	-	insertion	UNP A0A0A0MQB7
A	800	ARG	-	insertion	UNP A0A0A0MQB7
A	801	GLN	-	insertion	UNP A0A0A0MQB7
A	802	THR	-	insertion	UNP A0A0A0MQB7
A	803	ALA	-	insertion	UNP A0A0A0MQB7
A	804	GLY	-	insertion	UNP A0A0A0MQB7
A	805	THR	-	insertion	UNP A0A0A0MQB7
A	806	GLU	-	insertion	UNP A0A0A0MQB7
A	807	THR	-	insertion	UNP A0A0A0MQB7
A	2775	GLY	-	expression tag	UNP A0A0A0MQB7
A	2776	THR	-	expression tag	UNP A0A0A0MQB7
B	367	GLU	-	expression tag	UNP A0A0A0MQB7
B	368	THR	-	expression tag	UNP A0A0A0MQB7
B	369	GLY	-	expression tag	UNP A0A0A0MQB7
B	370	HIS	-	expression tag	UNP A0A0A0MQB7
B	371	HIS	-	expression tag	UNP A0A0A0MQB7
B	372	HIS	-	expression tag	UNP A0A0A0MQB7
B	373	HIS	-	expression tag	UNP A0A0A0MQB7
B	374	HIS	-	expression tag	UNP A0A0A0MQB7
B	375	HIS	-	expression tag	UNP A0A0A0MQB7
B	376	ARG	-	expression tag	UNP A0A0A0MQB7
B	377	GLY	-	expression tag	UNP A0A0A0MQB7
B	378	GLY	-	expression tag	UNP A0A0A0MQB7
B	379	LEU	-	expression tag	UNP A0A0A0MQB7
B	380	ASN	-	expression tag	UNP A0A0A0MQB7
B	381	ASP	-	expression tag	UNP A0A0A0MQB7
B	382	ILE	-	expression tag	UNP A0A0A0MQB7
B	383	PHE	-	expression tag	UNP A0A0A0MQB7
B	384	GLU	-	expression tag	UNP A0A0A0MQB7
B	385	ALA	-	expression tag	UNP A0A0A0MQB7
B	386	GLN	-	expression tag	UNP A0A0A0MQB7
B	387	LYS	-	expression tag	UNP A0A0A0MQB7
B	388	ILE	-	expression tag	UNP A0A0A0MQB7
B	389	GLU	-	expression tag	UNP A0A0A0MQB7
B	390	TRP	-	expression tag	UNP A0A0A0MQB7
B	391	HIS	-	expression tag	UNP A0A0A0MQB7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	392	GLU	-	expression tag	UNP A0A0A0MQB7
B	393	GLY	-	expression tag	UNP A0A0A0MQB7
B	394	GLY	-	expression tag	UNP A0A0A0MQB7
B	395	SER	-	expression tag	UNP A0A0A0MQB7
B	396	THR	-	expression tag	UNP A0A0A0MQB7
B	397	GLY	-	expression tag	UNP A0A0A0MQB7
B	737	GLU	-	insertion	UNP A0A0A0MQB7
B	799	GLY	-	insertion	UNP A0A0A0MQB7
B	800	ARG	-	insertion	UNP A0A0A0MQB7
B	801	GLN	-	insertion	UNP A0A0A0MQB7
B	802	THR	-	insertion	UNP A0A0A0MQB7
B	803	ALA	-	insertion	UNP A0A0A0MQB7
B	804	GLY	-	insertion	UNP A0A0A0MQB7
B	805	THR	-	insertion	UNP A0A0A0MQB7
B	806	GLU	-	insertion	UNP A0A0A0MQB7
B	807	THR	-	insertion	UNP A0A0A0MQB7
B	2775	GLY	-	expression tag	UNP A0A0A0MQB7
B	2776	THR	-	expression tag	UNP A0A0A0MQB7

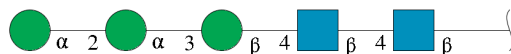
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

cetamido-2-deoxy-beta-D-glucopyranose.



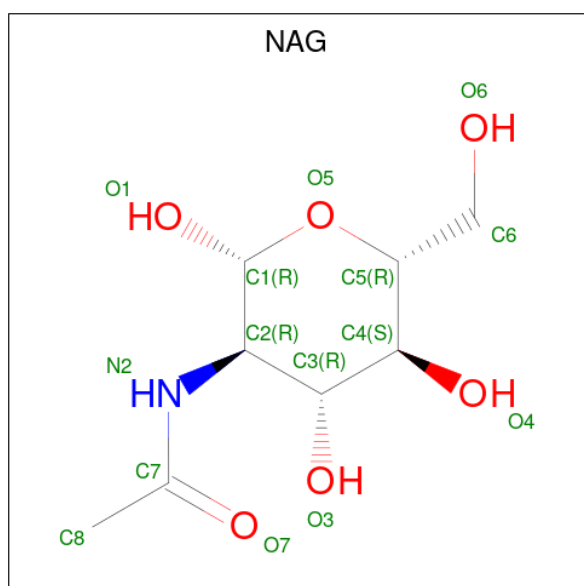
Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	5	Total	C	N	O	0	0
			61	34	2	25		
3	I	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
4	E	4	Total	C	N	O	0	0
			50	28	2	20		
4	J	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 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
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	











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

Chain F:



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

Chain G:



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

Chain H:



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

Chain K:



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

Chain L:



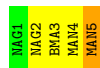
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain I: 

  
NAG1  
NAG2  
BMA3  
MAN4  
MAN5

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

Chain E: 

  
NAG1  
NAG2  
BMA3  
MAN4

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

Chain J: 

  
NAG1  
NAG2  
BMA3  
MAN4

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	19620	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 ( $e^-/\text{\AA}^2$ )	42.303	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.622	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	290.5, 290.5, 290.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.17	0/14138	0.42	0/19177
1	B	0.17	0/14138	0.41	0/19177
All	All	0.17	0/28276	0.42	0/38354

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	4
1	B	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1343	ARG	Sidechain
1	A	1777	ARG	Sidechain
1	A	1805	ARG	Sidechain
1	A	2428	ARG	Sidechain
1	B	1343	ARG	Sidechain
1	B	1805	ARG	Sidechain
1	B	2499	ARG	Sidechain

## 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	A	13842	0	13588	94	0
1	B	13842	0	13589	115	0
2	C	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
3	D	61	0	52	0	0
3	I	61	0	52	1	0
4	E	50	0	43	0	0
4	J	50	0	43	0	0
5	A	42	0	39	0	0
5	B	42	0	39	1	0
All	All	28158	0	27595	209	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 4.

All (209) 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:B:1098:ARG:HB2	1:B:1149:GLU:HB3	1.76	0.68
1:A:1081:SER:HB3	1:A:1166:LEU:HD22	1.77	0.65
1:A:1826:GLU:HB2	1:A:1834:ILE:HB	1.79	0.65
1:B:2043:ASP:HB3	1:B:2047:GLY:H	1.61	0.64
1:B:1372:VAL:HG22	1:B:1377:ILE:HG12	1.79	0.64
1:B:1846:LEU:HD12	1:B:1847:LEU:HB2	1.81	0.63
1:A:1372:VAL:HG22	1:A:1377:ILE:HG12	1.79	0.63
1:A:1846:LEU:HD12	1:A:1847:LEU:HB2	1.79	0.63
1:A:1245:VAL:HG23	1:A:1550:ALA:HB1	1.82	0.62
1:B:1245:VAL:HG23	1:B:1550:ALA:HB1	1.83	0.61
1:B:1239:ALA:HB3	1:B:1256:PHE:HB2	1.82	0.60
1:A:2043:ASP:HB3	1:A:2047:GLY:H	1.66	0.60
1:A:1782:ASN:HA	1:A:2046:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1845:ASN:ND2	1:A:1863:ASP:OD2	2.32	0.59
1:B:1826:GLU:HB2	1:B:1834:ILE:HB	1.84	0.59
1:B:1782:ASN:HA	1:B:2046:THR:HG23	1.84	0.59
1:A:1819:ILE:HG12	1:A:1841:VAL:HG22	1.85	0.58
1:A:1098:ARG:HB2	1:A:1149:GLU:HB3	1.85	0.58
1:B:1824:ARG:NH2	1:B:1850:ASP:OD1	2.37	0.58
1:A:1099:VAL:HB	1:A:1114:PHE:HB2	1.85	0.58
1:B:1362:ALA:HB1	1:B:1422:VAL:HG23	1.86	0.58
1:A:2165:TYR:HB3	1:A:2173:TYR:HB3	1.86	0.57
1:A:2092:THR:HG23	1:A:2101:ALA:HB3	1.86	0.57
1:B:2073:ASP:HA	1:B:2091:TYR:HB2	1.86	0.57
1:B:1032:ILE:HB	1:B:1084:LYS:HB3	1.86	0.57
1:A:1362:ALA:HB1	1:A:1422:VAL:HG23	1.86	0.57
1:B:1217:ASN:ND2	1:B:1234:GLY:O	2.37	0.57
1:A:1534:ASP:OD1	1:A:1568:ARG:NH1	2.38	0.57
1:A:1586:ALA:H	1:A:1800:THR:HG21	1.70	0.56
1:B:2134:VAL:HG22	1:B:2143:ILE:HG12	1.86	0.56
1:B:1534:ASP:OD1	1:B:1568:ARG:NH1	2.38	0.56
1:B:1173:PRO:HB3	1:B:1186:THR:HB	1.88	0.55
1:B:2704:LEU:HD23	1:B:2763:ILE:HD13	1.88	0.55
1:A:2456:ASN:HB3	1:A:2459:MET:HB3	1.89	0.55
1:A:2390:GLN:HB2	1:A:2399:TYR:HB3	1.88	0.55
1:A:2185:VAL:HG23	1:A:2467:SER:HB3	1.88	0.55
1:B:2576:ILE:HG12	1:B:2581:VAL:HG22	1.89	0.55
1:A:2048:VAL:HB	1:A:2067:LYS:HD2	1.88	0.55
1:A:2192:LEU:HD21	1:A:2376:LEU:HB3	1.89	0.55
1:B:1695:GLU:OE2	1:B:2554:ARG:NH1	2.40	0.55
1:A:2576:ILE:HG12	1:A:2581:VAL:HG22	1.88	0.54
1:B:2048:VAL:HB	1:B:2067:LYS:HD2	1.88	0.54
1:B:2192:LEU:HD21	1:B:2376:LEU:HB3	1.88	0.54
1:A:2592:ASP:HB3	1:A:2643:LEU:HD13	1.90	0.53
1:B:2311:TYR:HD2	1:B:2319:LEU:HB2	1.74	0.53
1:B:1632:ASN:OD1	1:B:1878:ARG:NH1	2.41	0.53
1:B:1637:LYS:HD2	1:B:1639:ARG:HH12	1.72	0.53
1:B:2128:HIS:NE2	1:B:2130:GLY:O	2.41	0.53
1:B:2165:TYR:HB3	1:B:2173:TYR:HB3	1.91	0.53
1:B:2185:VAL:HG23	1:B:2467:SER:HB3	1.91	0.53
1:B:1586:ALA:H	1:B:1800:THR:HG21	1.73	0.53
1:A:2428:ARG:NH2	1:A:2439:SER:O	2.42	0.52
1:B:1703:ASP:HB3	5:B:2802:NAG:H83	1.91	0.52
1:A:2073:ASP:HA	1:A:2091:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1099:VAL:HB	1:B:1114:PHE:HB2	1.91	0.52
1:B:1745:THR:HB	1:B:1760:VAL:HB	1.91	0.52
1:A:1239:ALA:HB3	1:A:1256:PHE:HB2	1.92	0.52
1:B:2456:ASN:HB3	1:B:2459:MET:HB3	1.90	0.52
1:A:1632:ASN:OD1	1:A:1878:ARG:NH1	2.41	0.51
1:A:2084:MET:HE1	1:A:2310:SER:HB2	1.92	0.51
1:A:2301:ARG:HB3	1:A:2310:SER:HB3	1.91	0.51
1:A:1549:LEU:HD13	1:A:1557:ILE:HD11	1.93	0.51
1:B:1549:LEU:HD13	1:B:1557:ILE:HD11	1.92	0.51
1:A:1026:ARG:NH2	1:A:1159:TRP:O	2.43	0.51
1:A:1695:GLU:OE2	1:A:2554:ARG:NH1	2.44	0.51
1:A:2074:LYS:HE3	1:A:2076:ILE:HD11	1.91	0.51
1:A:2604:TYR:HB2	1:A:2622:VAL:HG23	1.92	0.51
1:B:1786:VAL:HG22	1:B:1808:ILE:HG23	1.92	0.51
1:B:1794:VAL:HG22	1:B:1825:LYS:HG2	1.93	0.51
1:B:2100:ILE:HD11	1:B:2326:LEU:HD12	1.92	0.51
1:B:1026:ARG:NH2	1:B:1159:TRP:O	2.44	0.50
1:B:2233:HIS:HA	1:B:2246:LEU:HB2	1.93	0.50
1:A:2742:TYR:OH	1:A:2767:ARG:NH2	2.44	0.50
1:A:1173:PRO:HB3	1:A:1186:THR:HB	1.93	0.50
1:B:2631:LEU:HD21	1:B:2651:VAL:HG11	1.92	0.50
1:A:1308:ARG:HB2	1:A:1333:GLY:HA2	1.94	0.50
1:A:1714:THR:HG23	1:A:1720:VAL:HG22	1.92	0.50
1:B:1754:GLU:HG3	1:B:1771:CYS:HA	1.94	0.50
1:B:2390:GLN:HB2	1:B:2399:TYR:HB3	1.94	0.50
1:B:1098:ARG:HH21	1:B:1113:SER:HB3	1.76	0.49
1:B:1905:GLN:OE1	1:B:1912:ARG:NH2	2.44	0.49
1:B:2276:ASP:OD1	1:B:2291:ASN:ND2	2.46	0.49
1:A:1312:ARG:HG3	1:A:1329:VAL:HG21	1.94	0.49
1:A:2166:GLU:HG2	1:A:2171:LEU:HA	1.95	0.49
1:A:2311:TYR:HD2	1:A:2319:LEU:HB2	1.77	0.49
1:A:2210:GLN:OE1	1:A:2463:ASN:ND2	2.39	0.49
1:B:1335:GLN:HG3	1:B:1356:MET:HA	1.93	0.49
1:B:1813:GLU:O	3:I:5:MAN:O3	2.31	0.49
1:B:2085:ILE:HD13	1:B:2108:SER:HB2	1.94	0.49
1:A:1947:SER:O	1:A:1947:SER:OG	2.30	0.49
1:A:2005:ARG:NH2	1:A:2026:SER:O	2.46	0.49
1:B:1312:ARG:HG3	1:B:1329:VAL:HG21	1.94	0.48
1:B:1255:ASP:O	1:B:1289:TYR:OH	2.26	0.48
1:B:2732:GLN:HB3	1:B:2739:VAL:HG12	1.95	0.48
1:A:1145:SER:HB3	1:A:1161:LYS:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2691:GLU:OE1	1:B:2694:ARG:NH1	2.46	0.48
1:A:1906:ARG:NH1	1:A:2474:ASN:O	2.46	0.48
1:B:2732:GLN:NE2	1:B:2740:GLN:OE1	2.44	0.48
1:B:1906:ARG:NH1	1:B:2474:ASN:O	2.46	0.47
1:A:2085:ILE:HD13	1:A:2108:SER:HB2	1.96	0.47
1:B:2277:ILE:HG12	1:B:2719:ARG:HG2	1.96	0.47
1:A:1941:MET:HE1	1:A:2452:PRO:HG2	1.96	0.47
1:B:2634:LEU:O	1:B:2641:LYS:NZ	2.39	0.47
1:B:2634:LEU:HD13	1:B:2649:VAL:HG11	1.97	0.47
1:A:2233:HIS:HA	1:A:2246:LEU:HB2	1.97	0.47
1:B:2222:TRP:NE1	1:B:2238:GLY:O	2.42	0.46
1:B:2478:ASP:N	1:B:2478:ASP:OD1	2.48	0.46
1:A:1366:ASN:O	1:A:1382:GLN:NE2	2.48	0.46
1:B:2263:LYS:HB2	1:B:2272:GLN:HB3	1.97	0.46
1:B:2604:TYR:HB2	1:B:2622:VAL:HG23	1.96	0.46
1:A:1997:ILE:HB	1:A:2010:SER:HB2	1.98	0.46
1:B:1346:ASP:OD1	1:B:1378:ARG:NH2	2.40	0.46
1:B:2592:ASP:HB3	1:B:2643:LEU:HD13	1.98	0.46
1:B:1788:PHE:HD1	1:B:1803:ILE:HG21	1.80	0.46
1:A:1966:MET:HE2	1:A:1966:MET:HB3	1.84	0.46
1:A:2556:LYS:HB3	1:A:2559:HIS:HB2	1.98	0.46
1:B:1587:SER:O	1:B:1587:SER:OG	2.34	0.46
1:B:1308:ARG:HB2	1:B:1333:GLY:HA2	1.97	0.46
1:B:2084:MET:HE1	1:B:2310:SER:HB2	1.97	0.46
1:B:2138:ASP:OD1	1:B:2139:ILE:N	2.49	0.46
1:A:1305:THR:HG21	1:A:1359:ARG:HE	1.81	0.45
1:B:1027:PRO:HG3	1:B:1148:PHE:CG	2.51	0.45
1:B:1366:ASN:O	1:B:1382:GLN:NE2	2.45	0.45
1:A:2100:ILE:HD11	1:A:2326:LEU:HD12	1.98	0.45
1:B:1021:LEU:HD11	1:B:1156:LEU:HD23	1.97	0.45
1:B:1525:ASP:HB3	1:B:1528:CYS:HB2	1.98	0.45
1:B:1429:LEU:HD23	1:B:1440:ILE:HD12	1.97	0.45
1:B:1958:SER:OG	1:B:1960:ARG:NH1	2.49	0.45
1:A:1932:TRP:HB3	1:A:1943:LEU:HD11	1.98	0.45
1:B:1390:LEU:HD13	1:B:1409:VAL:HG12	1.99	0.45
1:B:1997:ILE:HB	1:B:2010:SER:HB2	1.99	0.45
1:B:2003:ASP:OD1	1:B:2003:ASP:N	2.47	0.45
1:B:2251:ARG:HE	1:B:2251:ARG:HB3	1.56	0.45
1:A:2081:GLU:OE2	1:A:2301:ARG:NH1	2.50	0.45
1:A:2347:TYR:HE2	1:A:2358:GLU:HB2	1.81	0.45
1:B:2301:ARG:HB3	1:B:2310:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1221:ARG:NH2	1:B:1257:ASN:OD1	2.45	0.44
1:B:1714:THR:HG23	1:B:1720:VAL:HG22	1.98	0.44
1:B:1605:THR:HG22	1:B:1615:TYR:HB2	2.00	0.44
1:A:1525:ASP:HB3	1:A:1528:CYS:HB2	1.99	0.44
1:B:2014:THR:OG1	1:B:2267:ASP:OD2	2.28	0.44
1:A:2014:THR:OG1	1:A:2267:ASP:OD2	2.29	0.44
1:A:2251:ARG:HE	1:A:2251:ARG:HB3	1.57	0.44
1:A:2138:ASP:OD1	1:A:2139:ILE:N	2.50	0.43
1:B:1375:THR:HG22	1:B:1417:PRO:HD2	2.00	0.43
1:B:1170:GLU:OE2	1:B:1201:ASN:ND2	2.51	0.43
1:A:1027:PRO:HG3	1:A:1148:PHE:CG	2.52	0.43
1:B:2347:TYR:HE2	1:B:2358:GLU:HB2	1.82	0.43
1:A:1429:LEU:HD23	1:A:1440:ILE:HD12	1.99	0.43
1:A:2732:GLN:HB3	1:A:2739:VAL:HG12	2.00	0.43
1:B:1262:ILE:HG12	1:B:1268:VAL:HG22	2.00	0.43
1:B:1664:ASN:OD1	1:B:1664:ASN:N	2.52	0.43
1:A:1375:THR:HG22	1:A:1417:PRO:HD2	2.00	0.43
1:A:1390:LEU:HD13	1:A:1409:VAL:HG12	2.00	0.43
1:B:1305:THR:O	1:B:1308:ARG:NH1	2.46	0.43
1:A:1893:VAL:HG12	1:A:1904:LEU:HD23	2.01	0.43
1:B:2638:ILE:HD13	1:B:2638:ILE:HA	1.90	0.43
1:A:2278:PHE:HE2	1:A:2420:THR:HB	1.83	0.43
1:B:1958:SER:OG	1:B:1958:SER:O	2.34	0.43
1:B:1776:LEU:HB3	1:B:1788:PHE:HB2	2.01	0.42
1:B:1657:ILE:HG12	1:B:1672:THR:HG22	2.00	0.42
1:A:2415:LEU:HD23	1:A:2415:LEU:HA	1.86	0.42
1:B:1095:ASN:HB2	1:B:1150:TYR:HD2	1.84	0.42
1:B:2278:PHE:HE2	1:B:2420:THR:HB	1.85	0.42
1:A:1860:ILE:HD13	1:A:1869:LEU:HD23	2.01	0.42
1:B:2631:LEU:HD23	1:B:2637:THR:HA	2.00	0.42
1:A:1627:GLU:HG3	1:A:1637:LYS:HG2	2.01	0.42
1:A:2227:ASP:OD1	1:A:2228:LEU:N	2.48	0.42
1:B:1947:SER:O	1:B:1947:SER:OG	2.31	0.42
1:A:2066:ARG:HD3	1:A:2074:LYS:HE2	2.01	0.42
1:A:2180:ASP:OD1	1:A:2184:ARG:N	2.52	0.42
1:B:1377:ILE:HD12	1:B:1390:LEU:HD21	2.02	0.42
1:A:1053:THR:O	1:A:1079:TYR:OH	2.35	0.42
1:A:1414:LEU:HD22	1:A:1433:GLU:HG3	2.02	0.42
1:A:1294:ASP:HB2	1:A:1301:TYR:HE2	1.85	0.42
1:A:2638:ILE:HD13	1:A:2638:ILE:HA	1.90	0.42
1:A:2084:MET:HE3	1:A:2084:MET:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1664:ASN:OD1	1:A:1664:ASN:N	2.53	0.41
1:A:1258:TYR:HE1	1:A:1322:LEU:HD13	1.85	0.41
1:B:1941:MET:HE1	1:B:2452:PRO:HG2	2.02	0.41
1:B:2066:ARG:NH2	1:B:2073:ASP:OD2	2.44	0.41
1:B:1085:ILE:HD12	1:B:1144:VAL:HG21	2.02	0.41
1:B:1952:ILE:HB	1:B:1965:THR:HB	2.02	0.41
1:A:1928:ASP:OD2	1:A:2184:ARG:NH2	2.53	0.41
1:B:1080:LYS:HD2	1:B:1127:ASP:HA	2.01	0.41
1:B:1932:TRP:HB3	1:B:1943:LEU:HD11	2.01	0.41
1:B:1101:LEU:HB3	1:B:1112:LYS:HB3	2.02	0.41
1:A:1300:LEU:HD23	1:A:1313:VAL:HG21	2.01	0.41
1:A:1346:ASP:OD1	1:A:1378:ARG:NH2	2.39	0.41
1:A:1377:ILE:HD12	1:A:1390:LEU:HD21	2.02	0.41
1:B:1294:ASP:HB2	1:B:1301:TYR:HE2	1.85	0.41
1:B:1300:LEU:HD23	1:B:1313:VAL:HG21	2.02	0.41
1:B:2084:MET:HE3	1:B:2084:MET:HB3	1.85	0.41
1:B:1840:ARG:NH2	1:B:1843:GLY:O	2.54	0.41
1:A:2175:MET:HE2	1:A:2175:MET:HB3	1.99	0.40
1:B:1942:VAL:HG22	1:B:1952:ILE:HG12	2.03	0.40
1:B:2415:LEU:HD23	1:B:2415:LEU:HA	1.91	0.40
1:A:1085:ILE:HD12	1:A:1144:VAL:HG21	2.03	0.40
1:A:1749:ASN:HD22	1:A:1749:ASN:HA	1.66	0.40
1:B:1860:ILE:HD13	1:B:1869:LEU:HD23	2.03	0.40
1:A:1166:LEU:HD23	1:A:1166:LEU:HA	1.97	0.40
1:A:2147:VAL:HG12	1:A:2167:MET:HB2	2.04	0.40
1:B:2122:ILE:HD13	1:B:2122:ILE:HA	1.93	0.40
1:B:2549:LEU:HD23	1:B:2549:LEU:HA	1.95	0.40
1:A:1305:THR:O	1:A:1308:ARG:NH1	2.48	0.40
1:B:1127:ASP:OD1	1:B:1127:ASP:N	2.45	0.40
1:A:1974:MET:HB3	1:A:2561:PHE:CG	2.56	0.40
1:A:2323:TYR:CE2	1:A:2332:ILE:HG12	2.57	0.40
1:B:1742:ASP:OD1	1:B:1742:ASP:N	2.52	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	A	1750/2410 (73%)	1687 (96%)	63 (4%)	0	100	100
1	B	1750/2410 (73%)	1689 (96%)	61 (4%)	0	100	100
All	All	3500/4820 (73%)	3376 (96%)	124 (4%)	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	1521/2069 (74%)	1498 (98%)	23 (2%)	57	84
1	B	1521/2069 (74%)	1500 (99%)	21 (1%)	59	85
All	All	3042/4138 (74%)	2998 (99%)	44 (1%)	57	85

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1139	LEU
1	A	1144	VAL
1	A	1146	VAL
1	A	1208	PRO
1	A	1337	LEU
1	A	1340	ASP
1	A	1343	ARG
1	A	1457	GLN
1	A	1458	VAL
1	A	1465	LEU
1	A	1562	LEU
1	A	1604	TYR
1	A	1749	ASN
1	A	1941	MET

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Mol	Chain	Res	Type
1	A	1969	VAL
1	A	2122	ILE
1	A	2149	THR
1	A	2428	ARG
1	A	2559	HIS
1	A	2573	MET
1	A	2583	THR
1	A	2655	THR
1	A	2657	LEU
1	B	1069	LEU
1	B	1123	THR
1	B	1337	LEU
1	B	1340	ASP
1	B	1341	GLU
1	B	1343	ARG
1	B	1457	GLN
1	B	1458	VAL
1	B	1465	LEU
1	B	1562	LEU
1	B	1749	ASN
1	B	1931	VAL
1	B	1941	MET
1	B	1969	VAL
1	B	2128	HIS
1	B	2172	MET
1	B	2499	ARG
1	B	2559	HIS
1	B	2655	THR
1	B	2656	LEU
1	B	2657	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1281	HIS
1	A	1366	ASN
1	A	1457	GLN
1	A	1673	GLN
1	A	1737	ASN
1	A	1749	ASN
1	A	1761	GLN
1	A	1766	ASN

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Mol	Chain	Res	Type
1	A	1977	HIS
1	A	2327	HIS
1	A	2521	GLN
1	A	2550	HIS
1	A	2698	GLN
1	B	1281	HIS
1	B	1366	ASN
1	B	1457	GLN
1	B	1673	GLN
1	B	1749	ASN
1	B	1761	GLN
1	B	1977	HIS
1	B	2053	ASN
1	B	2353	HIS
1	B	2390	GLN
1	B	2464	ASN
1	B	2521	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 ⓘ

30 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	1	2,1	14,14,15	0.18	0	17,19,21	0.50	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.52	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	1	3,1	14,14,15	0.30	0	17,19,21	0.65	0
3	NAG	D	2	3	14,14,15	0.20	0	17,19,21	0.66	0
3	BMA	D	3	3	11,11,12	0.94	0	15,15,17	0.84	0
3	MAN	D	4	3	11,11,12	1.27	1 (9%)	15,15,17	1.54	2 (13%)
3	MAN	D	5	3	11,11,12	0.82	1 (9%)	15,15,17	1.00	1 (6%)
4	NAG	E	1	4,1	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	E	2	4	14,14,15	0.40	0	17,19,21	0.48	0
4	BMA	E	3	4	11,11,12	0.55	0	15,15,17	0.85	1 (6%)
4	MAN	E	4	4	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
2	NAG	F	1	2,1	14,14,15	0.18	0	17,19,21	0.80	1 (5%)
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	0.56	0
2	NAG	G	1	2,1	14,14,15	0.24	0	17,19,21	0.61	0
2	NAG	G	2	2	14,14,15	0.35	0	17,19,21	0.52	0
2	NAG	H	1	2,1	14,14,15	0.19	0	17,19,21	0.50	0
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.54	0
3	NAG	I	1	3,1	14,14,15	0.26	0	17,19,21	0.60	0
3	NAG	I	2	3	14,14,15	0.30	0	17,19,21	1.07	1 (5%)
3	BMA	I	3	3	11,11,12	0.63	0	15,15,17	0.81	1 (6%)
3	MAN	I	4	3	11,11,12	0.66	0	15,15,17	0.99	2 (13%)
3	MAN	I	5	3	11,11,12	0.66	0	15,15,17	0.95	2 (13%)
4	NAG	J	1	4,1	14,14,15	0.24	0	17,19,21	0.76	1 (5%)
4	NAG	J	2	4	14,14,15	0.45	0	17,19,21	0.52	0
4	BMA	J	3	4	11,11,12	0.54	0	15,15,17	0.84	1 (6%)
4	MAN	J	4	4	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
2	NAG	K	1	2,1	14,14,15	0.18	0	17,19,21	0.78	1 (5%)
2	NAG	K	2	2	14,14,15	0.42	0	17,19,21	0.50	0
2	NAG	L	1	2,1	14,14,15	0.28	0	17,19,21	0.59	0
2	NAG	L	2	2	14,14,15	0.42	0	17,19,21	1.00	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	MAN	C1-C2	2.43	1.58	1.52
3	D	5	MAN	C1-C2	2.12	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-O5-C5	4.66	118.42	112.19
3	I	2	NAG	C2-N2-C7	3.02	126.95	122.90
2	L	2	NAG	C2-N2-C7	3.01	126.93	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	MAN	C1-O5-C5	2.98	116.17	112.19
4	E	4	MAN	C1-O5-C5	2.90	116.08	112.19
4	J	4	MAN	C1-O5-C5	2.84	115.99	112.19
2	F	1	NAG	C1-O5-C5	2.71	115.81	112.19
3	I	4	MAN	C1-O5-C5	2.60	115.67	112.19
2	K	1	NAG	C1-O5-C5	2.58	115.64	112.19
3	I	5	MAN	C1-O5-C5	2.47	115.50	112.19
4	E	3	BMA	C1-O5-C5	2.30	115.28	112.19
4	J	1	NAG	C1-O5-C5	2.30	115.26	112.19
3	D	4	MAN	O2-C2-C1	2.28	114.44	109.22
4	J	3	BMA	C1-O5-C5	2.28	115.24	112.19
3	I	3	BMA	C1-O5-C5	2.23	115.17	112.19
3	I	5	MAN	O2-C2-C3	-2.10	105.79	110.15
4	E	4	MAN	O2-C2-C3	-2.10	105.81	110.15
4	J	4	MAN	O2-C2-C3	-2.05	105.90	110.15
3	I	4	MAN	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2

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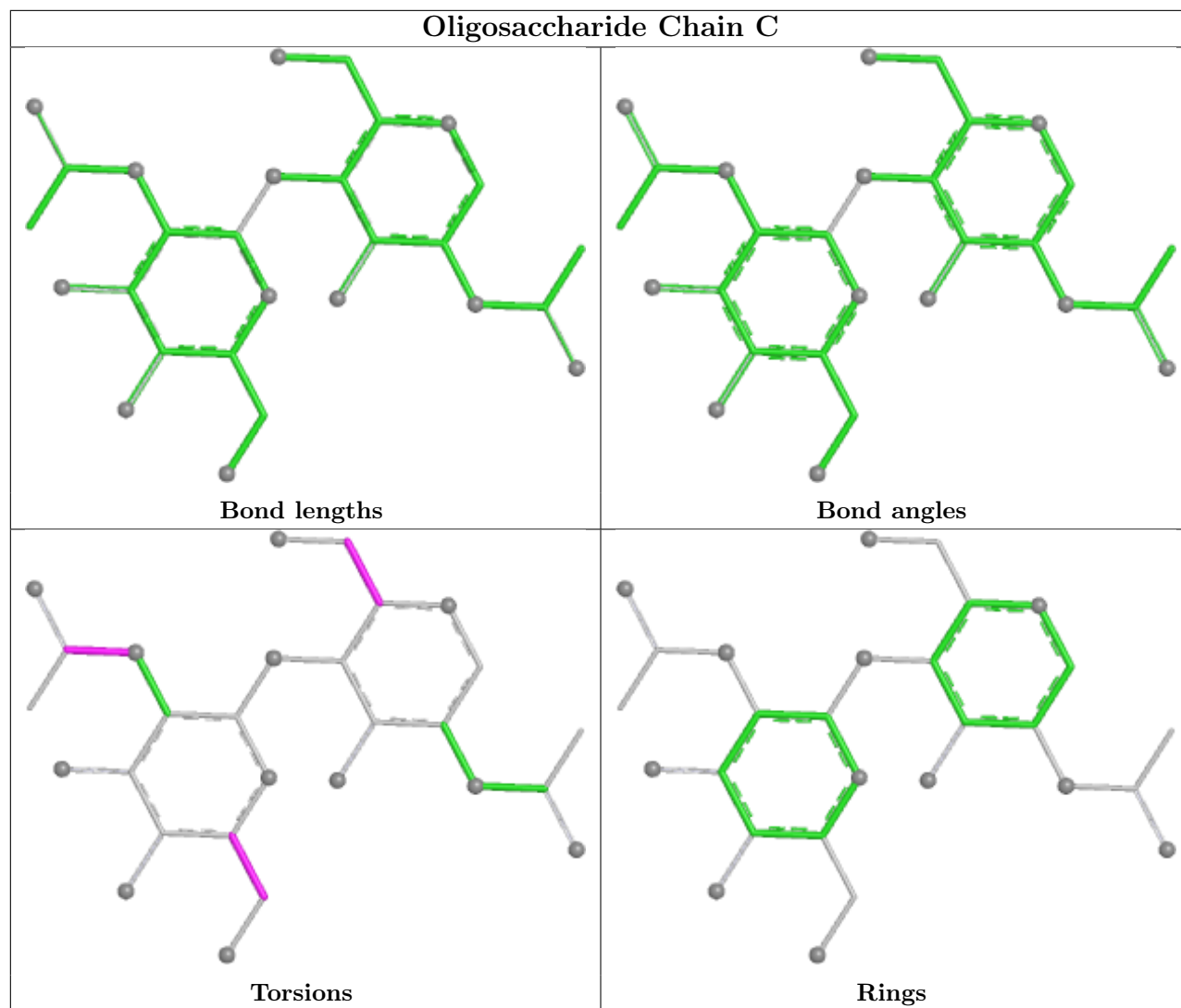
Mol	Chain	Res	Type	Atoms
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
3	D	4	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7
2	K	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C1-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
3	D	4	MAN	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

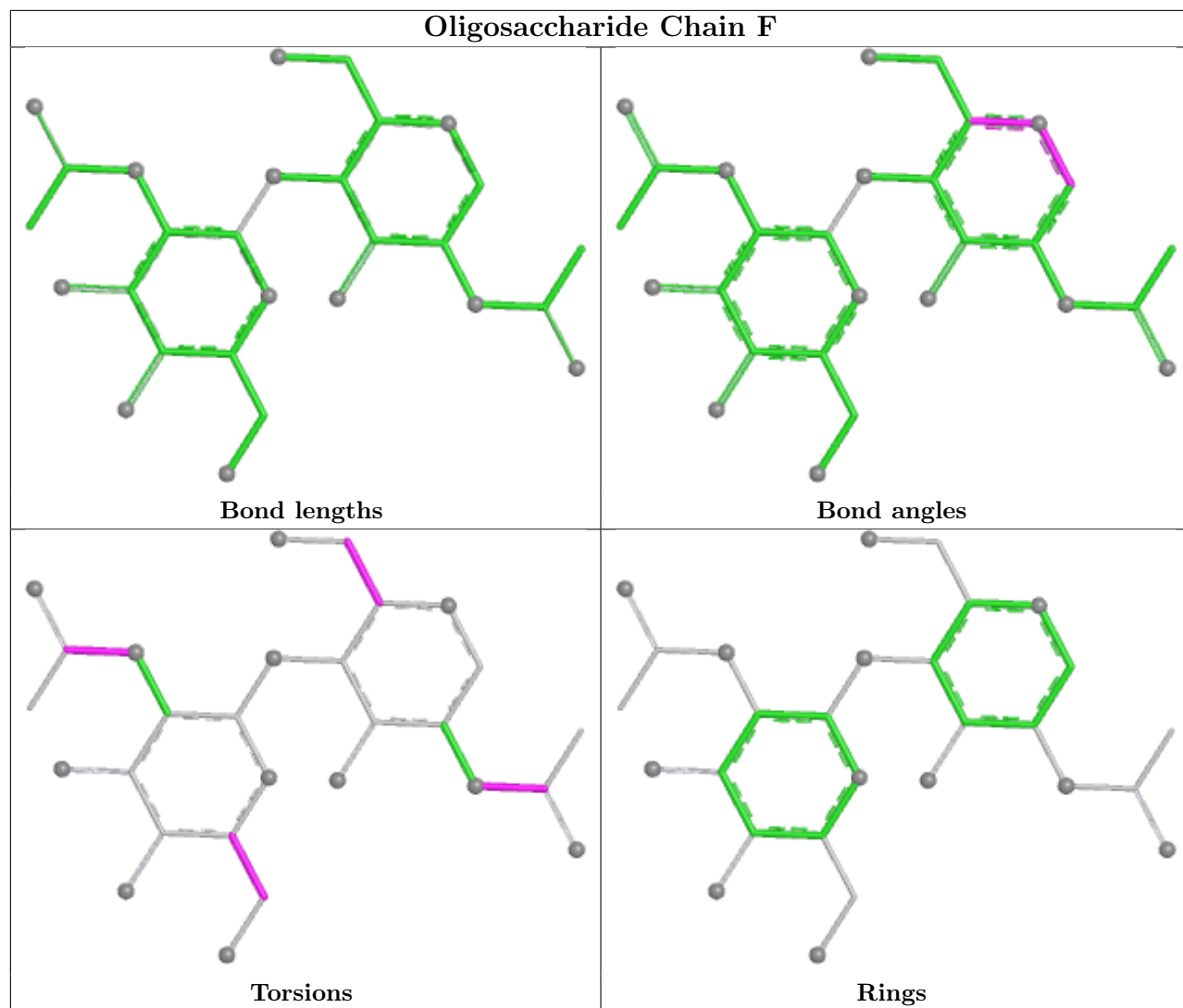
There are no ring outliers.

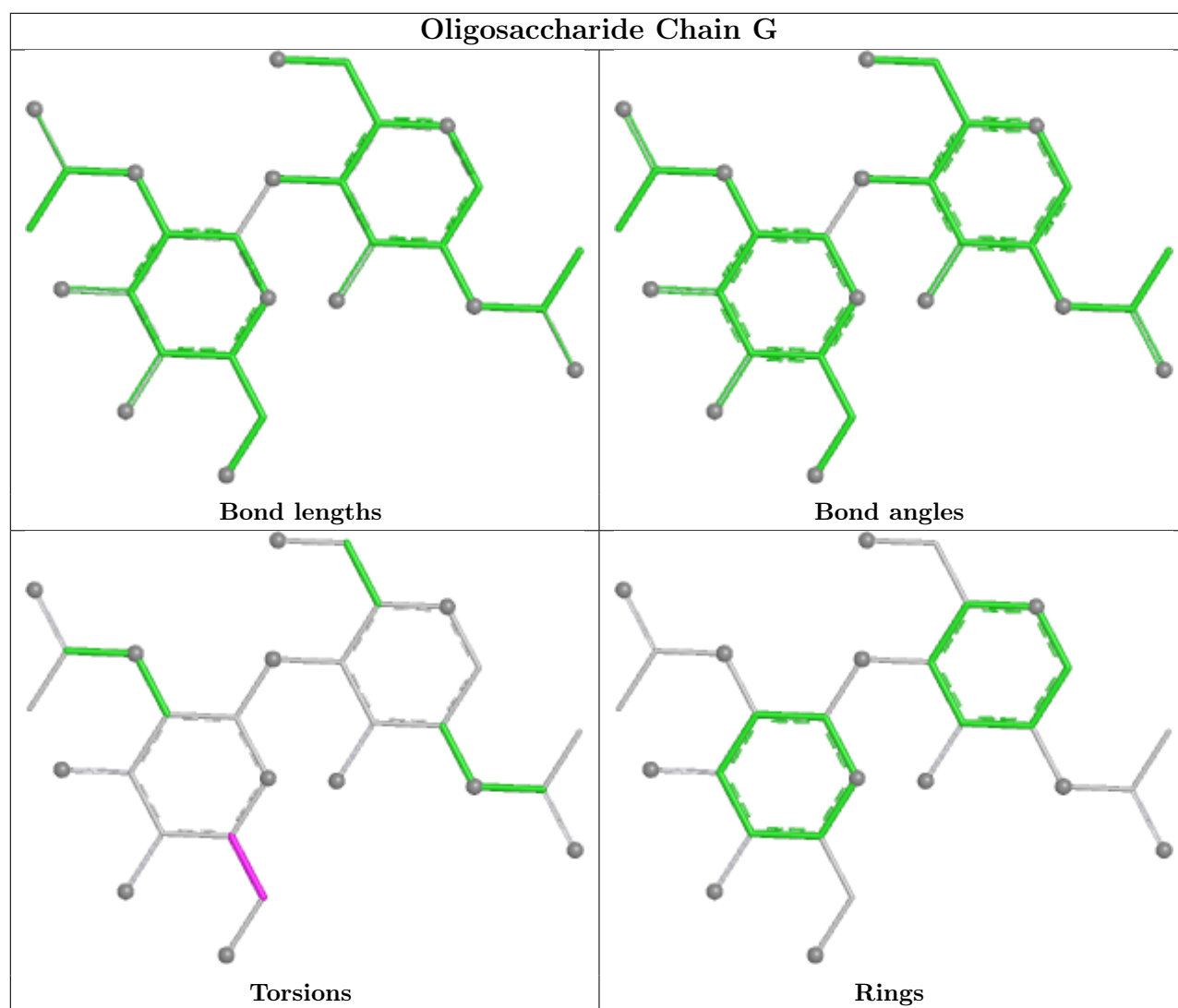
1 monomer is involved in 1 short contact:

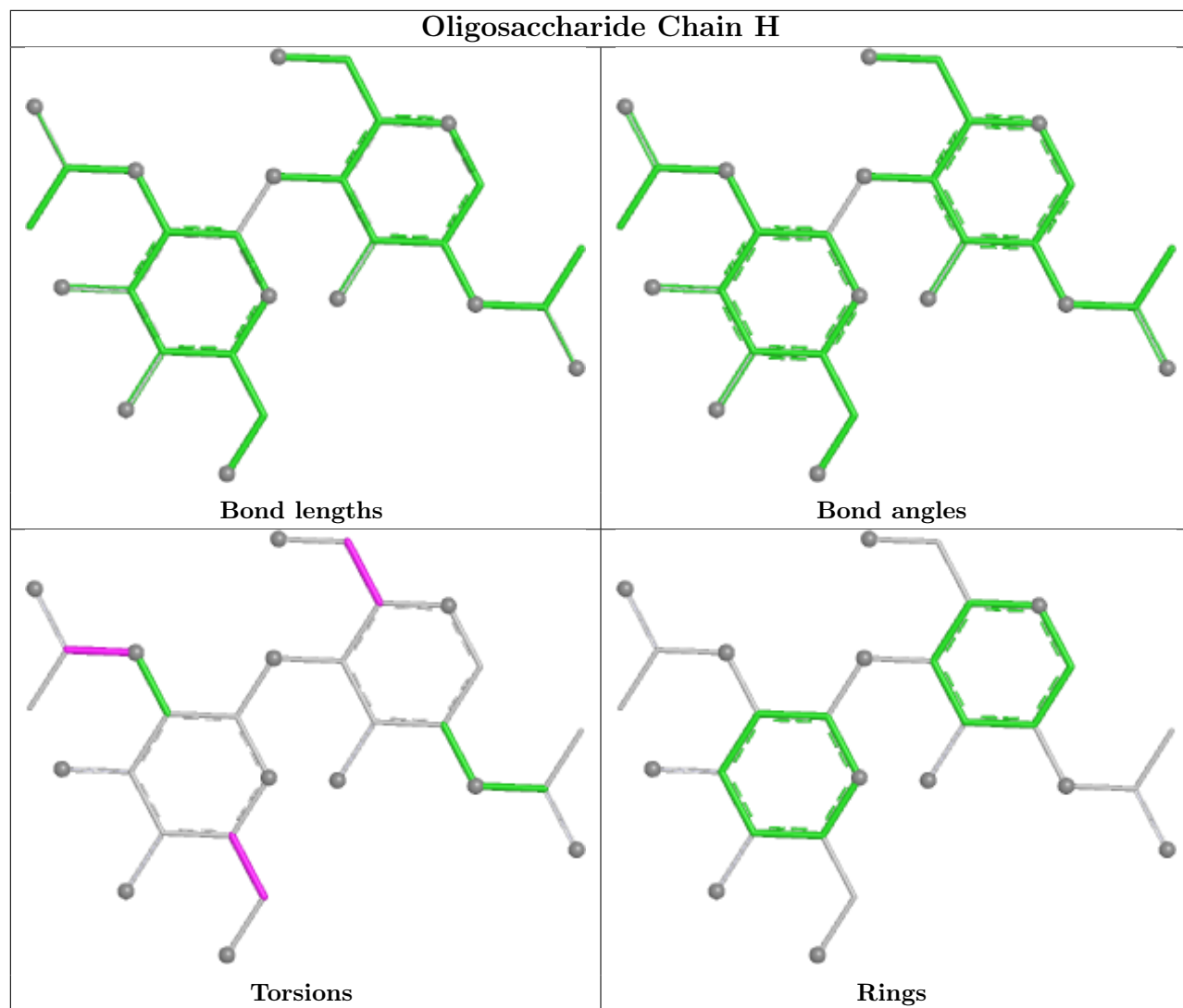
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	5	MAN	1	0

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

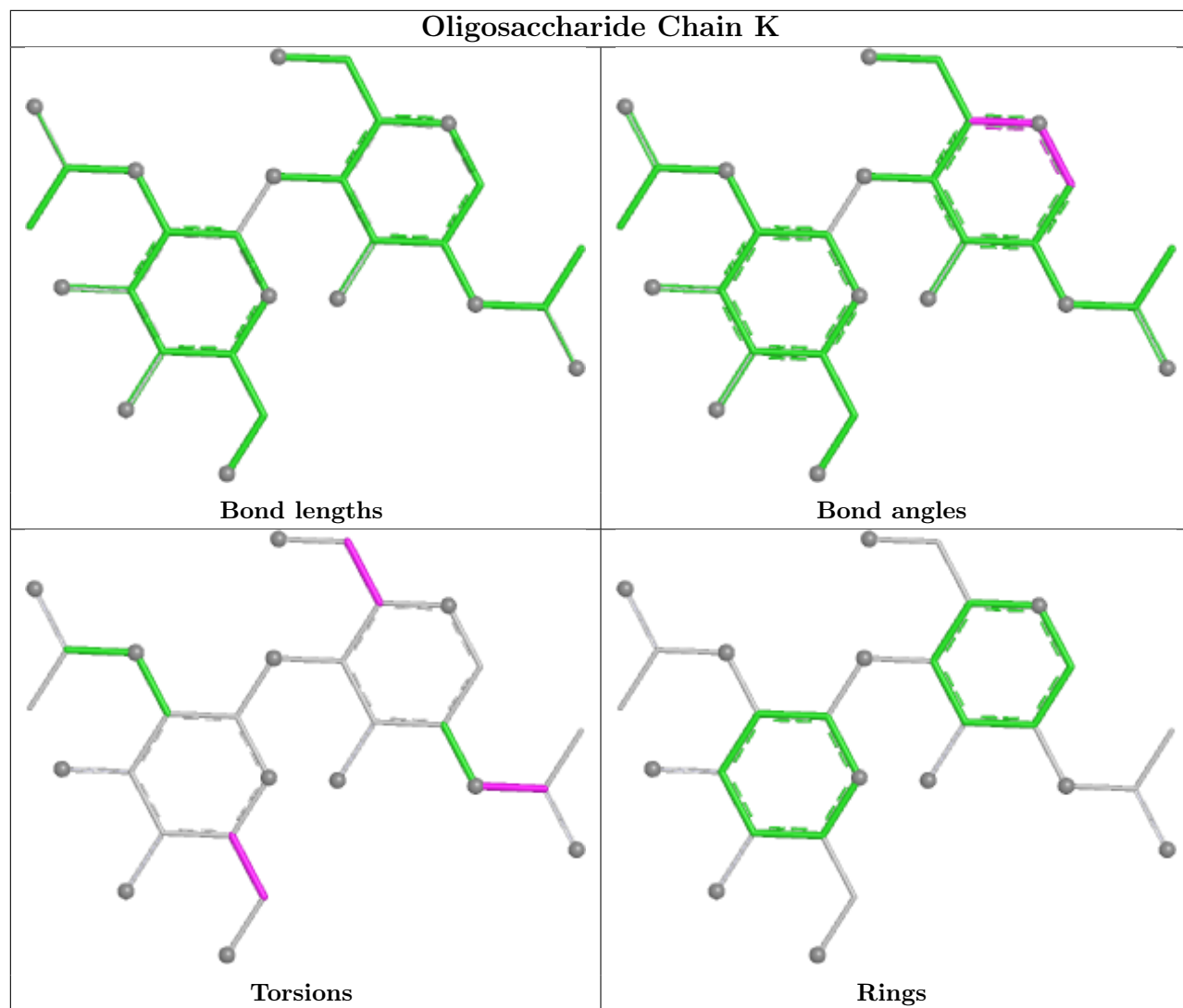


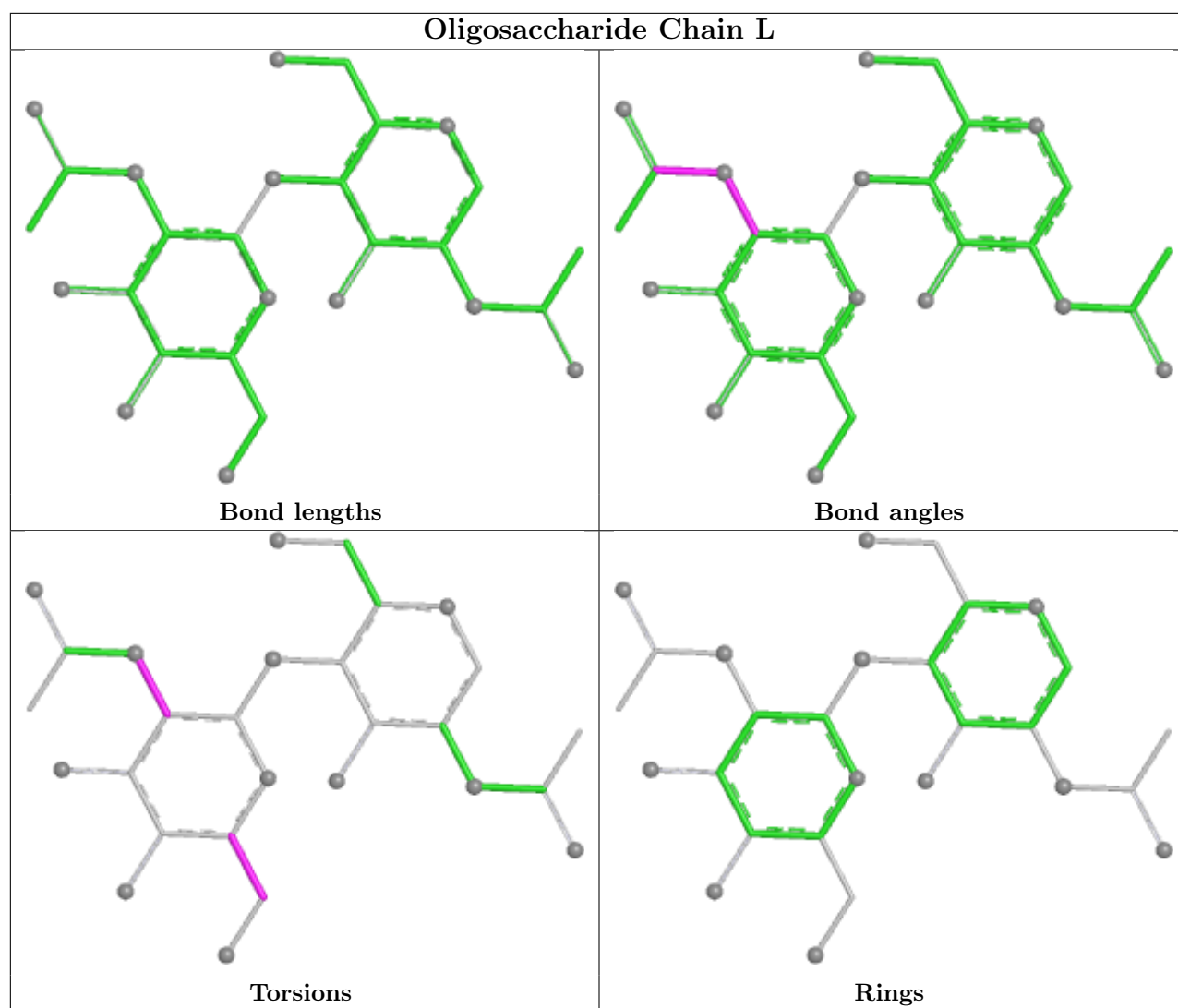


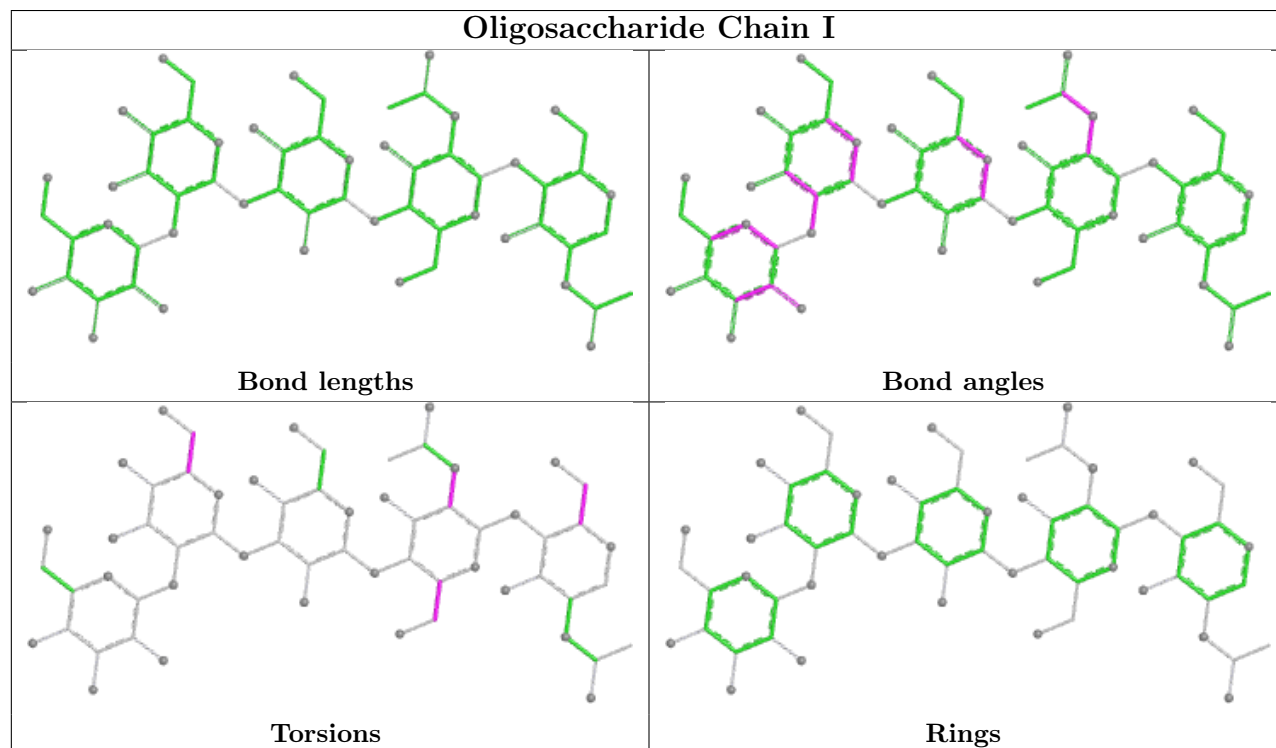
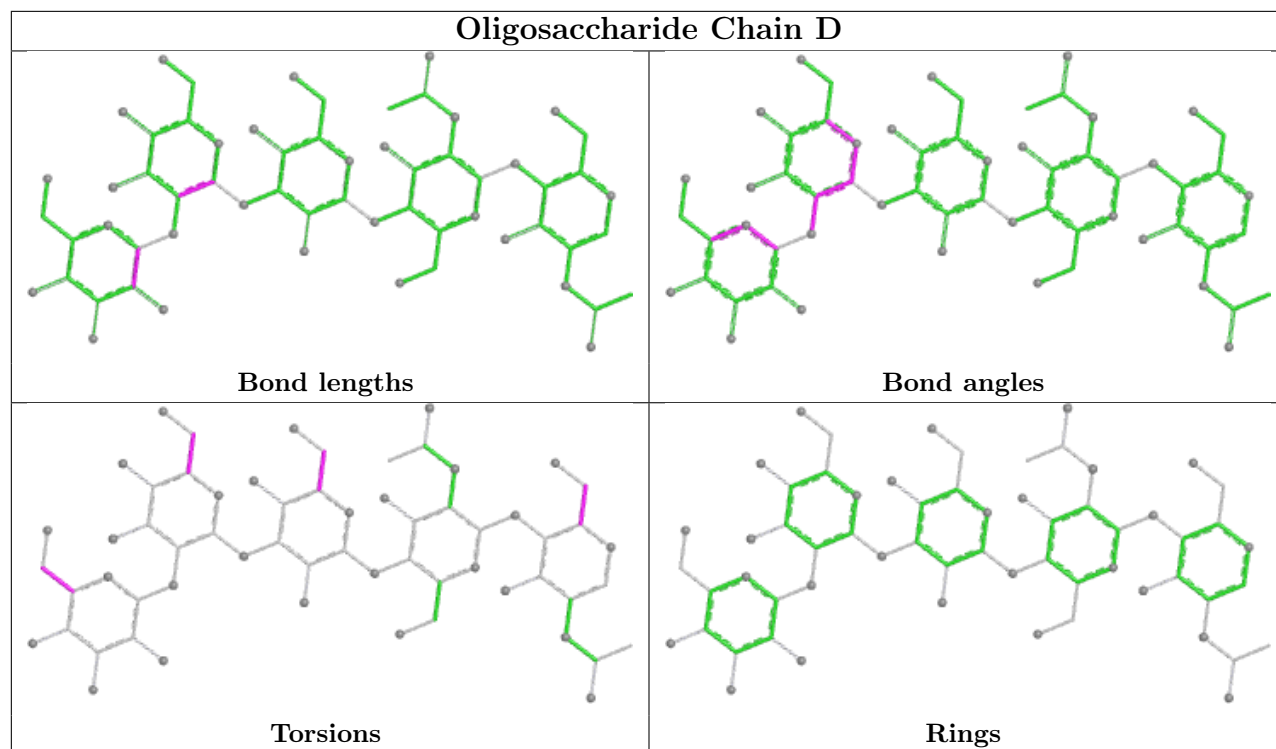


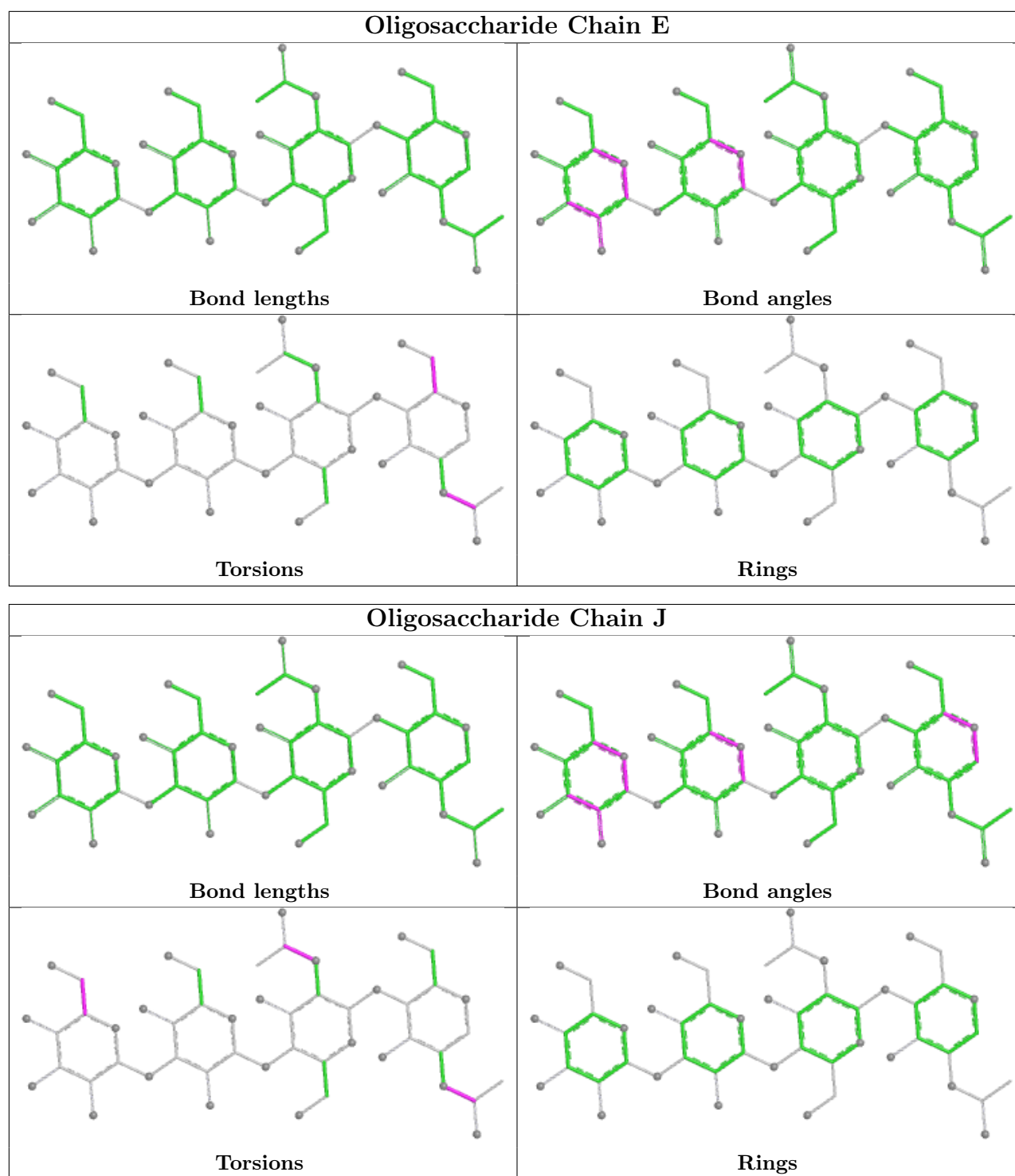












## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	B	2803	1	14,14,15	0.41	0	17,19,21	0.97	1 (5%)
5	NAG	A	2801	1	14,14,15	0.34	0	17,19,21	0.58	0
5	NAG	B	2802	1	14,14,15	0.47	0	17,19,21	0.65	0
5	NAG	B	2801	1	14,14,15	0.34	0	17,19,21	0.58	0
5	NAG	A	2803	1	14,14,15	0.55	0	17,19,21	0.93	1 (5%)
5	NAG	A	2802	1	14,14,15	0.76	1 (7%)	17,19,21	0.58	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	B	2803	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2801	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2802	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2801	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2803	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2802	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2802	NAG	C1-C2	2.16	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2803	NAG	C2-N2-C7	2.97	126.89	122.90
5	A	2803	NAG	C2-N2-C7	2.95	126.85	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2802	NAG	O5-C5-C6-O6
5	A	2803	NAG	O5-C5-C6-O6
5	B	2803	NAG	O5-C5-C6-O6
5	B	2802	NAG	C4-C5-C6-O6
5	A	2801	NAG	C8-C7-N2-C2
5	A	2801	NAG	O7-C7-N2-C2
5	A	2802	NAG	C8-C7-N2-C2
5	A	2802	NAG	O7-C7-N2-C2
5	B	2801	NAG	C8-C7-N2-C2
5	B	2801	NAG	O7-C7-N2-C2
5	B	2802	NAG	C8-C7-N2-C2
5	B	2802	NAG	O7-C7-N2-C2
5	A	2803	NAG	C4-C5-C6-O6
5	B	2803	NAG	C4-C5-C6-O6
5	A	2802	NAG	O5-C5-C6-O6
5	A	2803	NAG	C1-C2-N2-C7
5	B	2803	NAG	C1-C2-N2-C7
5	A	2803	NAG	C3-C2-N2-C7
5	B	2803	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2802	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

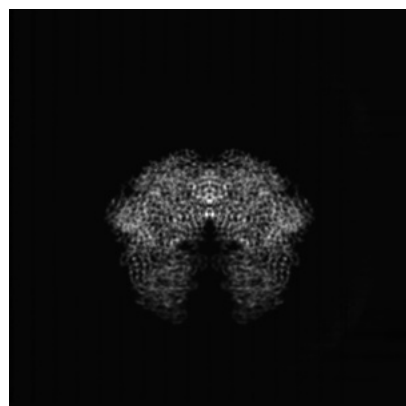
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50975. These allow visual inspection of the internal detail of the map and identification of artifacts.

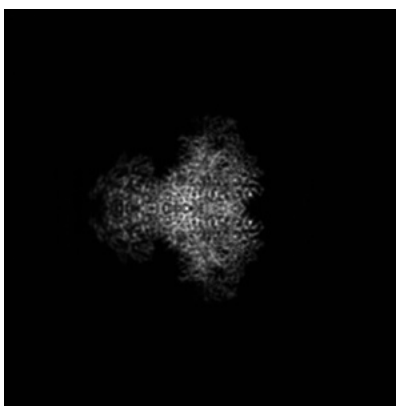
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

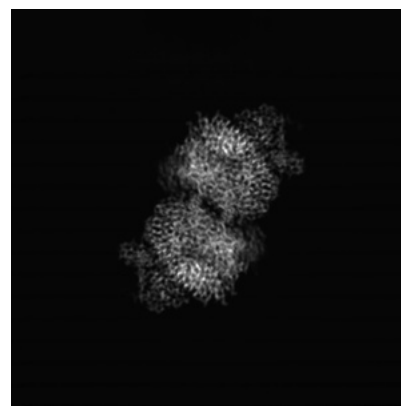
#### 6.1.1 Primary map



X

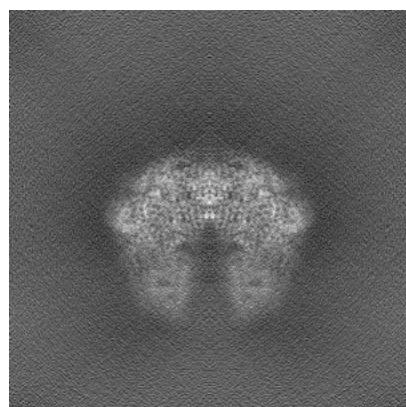


Y

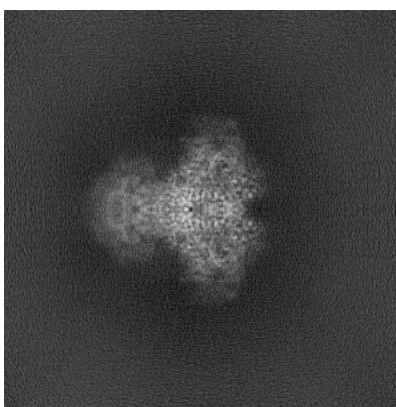


Z

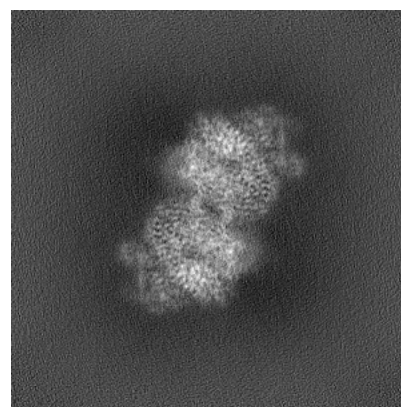
#### 6.1.2 Raw map



X



Y



Z

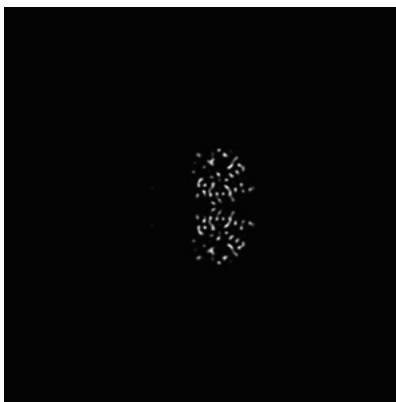
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 175

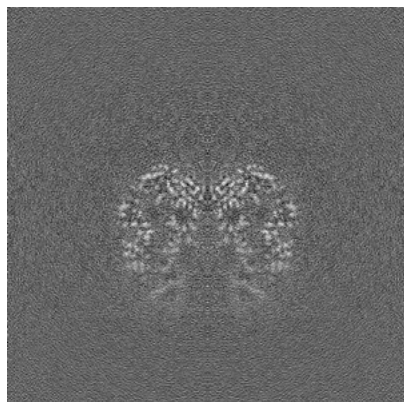


Y Index: 175

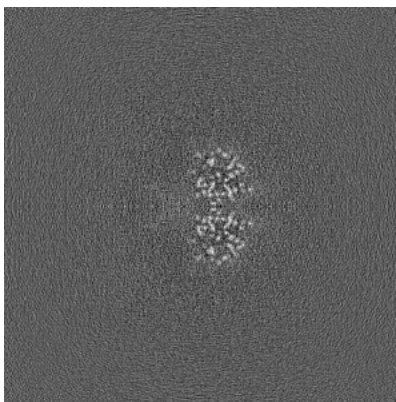


Z Index: 175

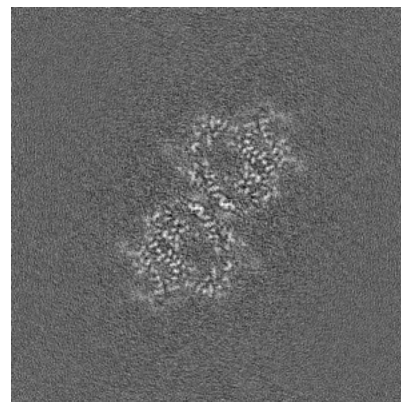
### 6.2.2 Raw map



X Index: 175



Y Index: 175



Z Index: 175

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: 185

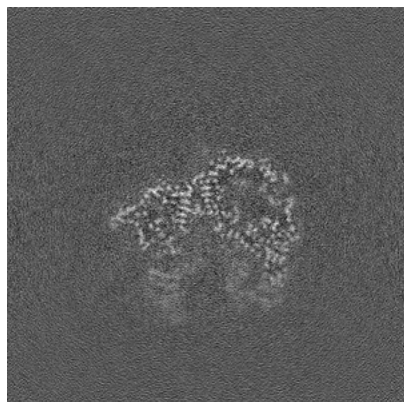


Y Index: 118

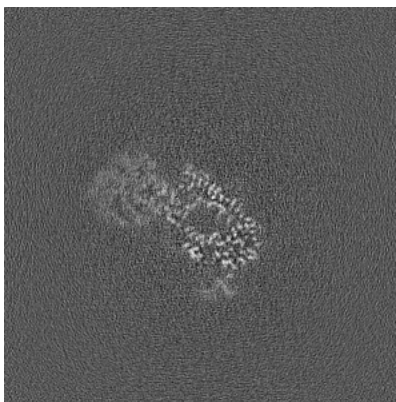


Z Index: 169

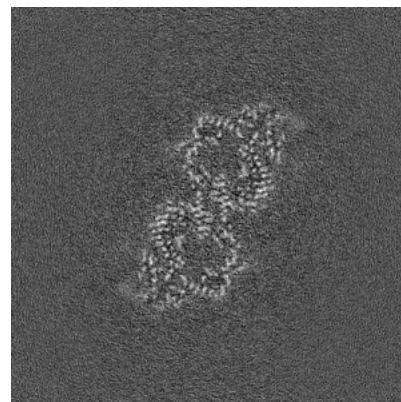
### 6.3.2 Raw map



X Index: 186



Y Index: 144

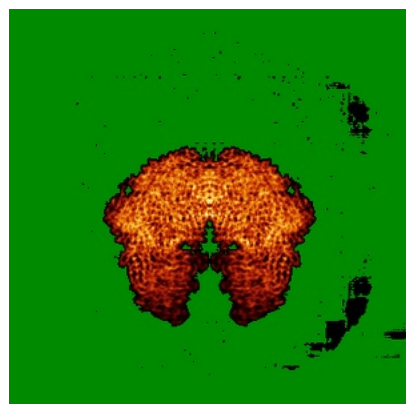


Z Index: 169

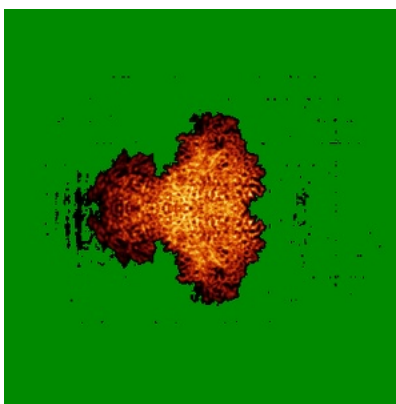
The images above show the largest variance slices of the map in three orthogonal directions.

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

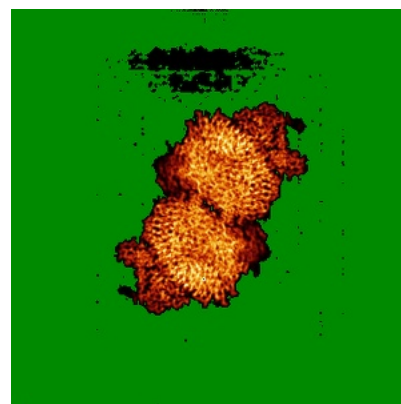
### 6.4.1 Primary map



X

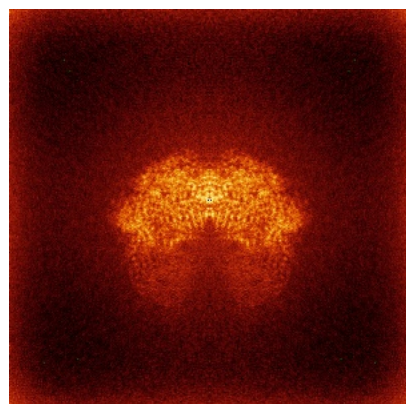


Y

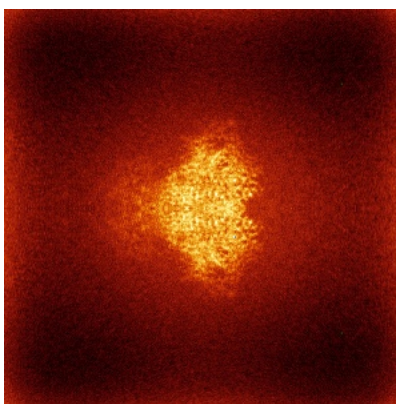


Z

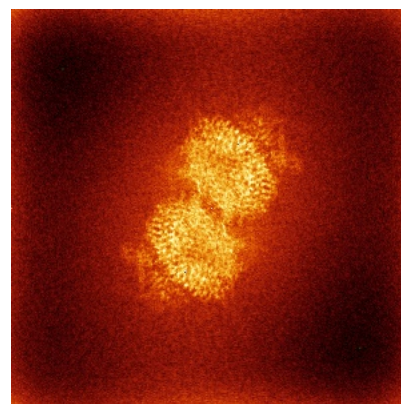
### 6.4.2 Raw map



X



Y

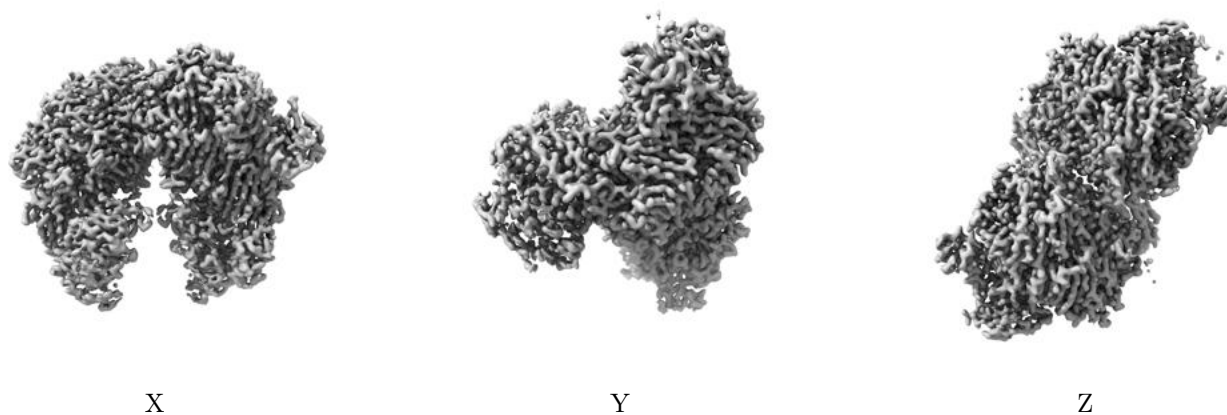


Z

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.

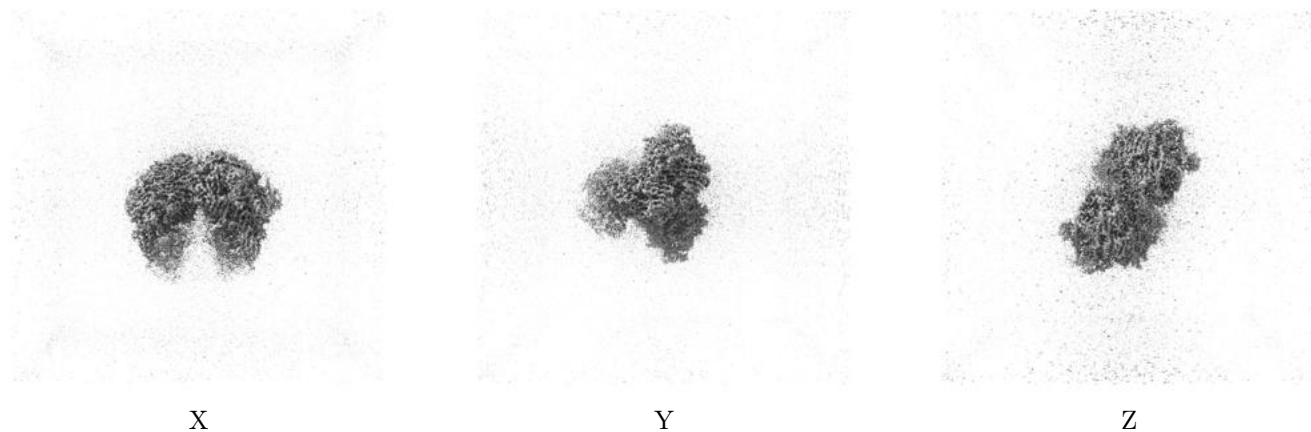
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

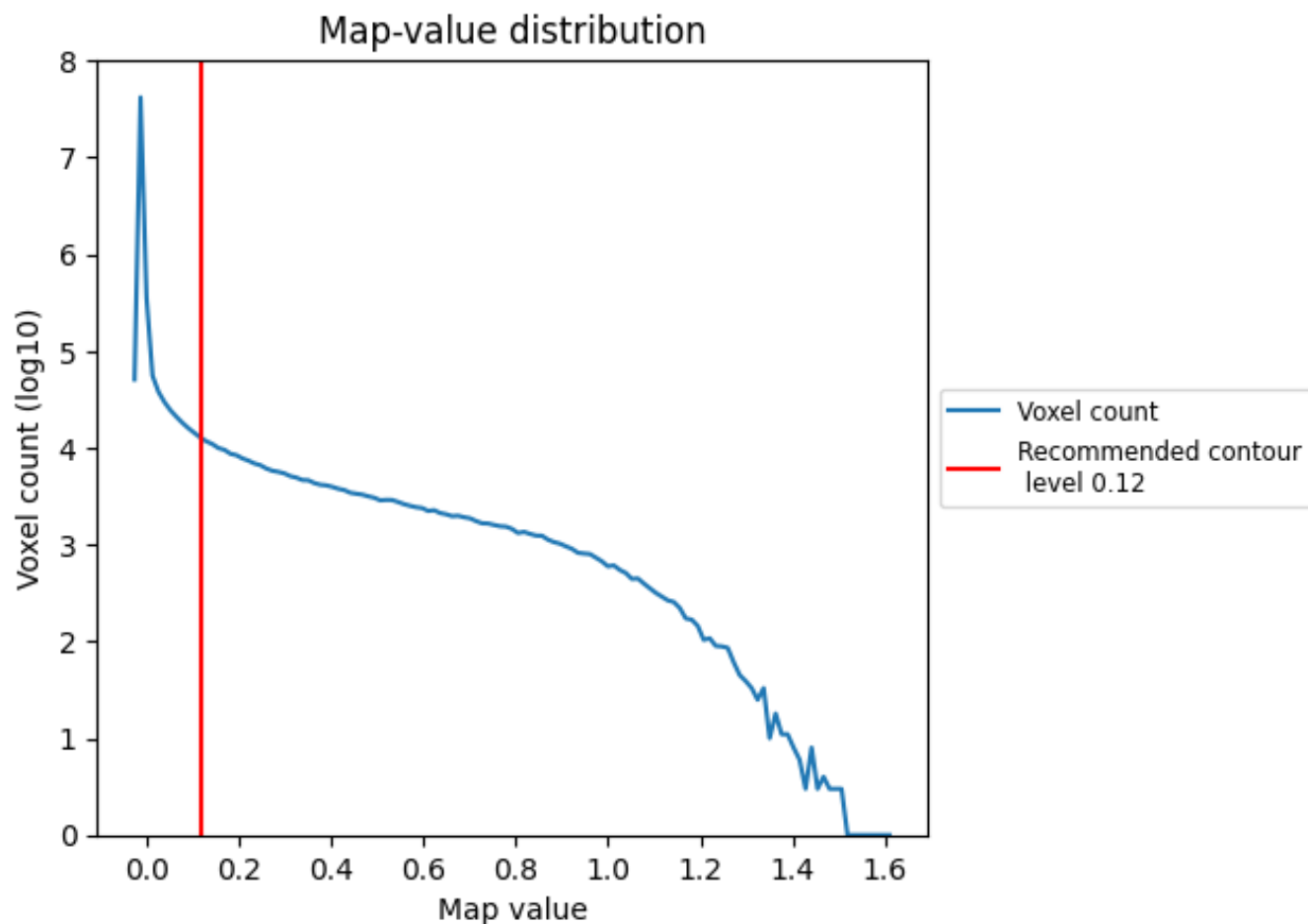
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

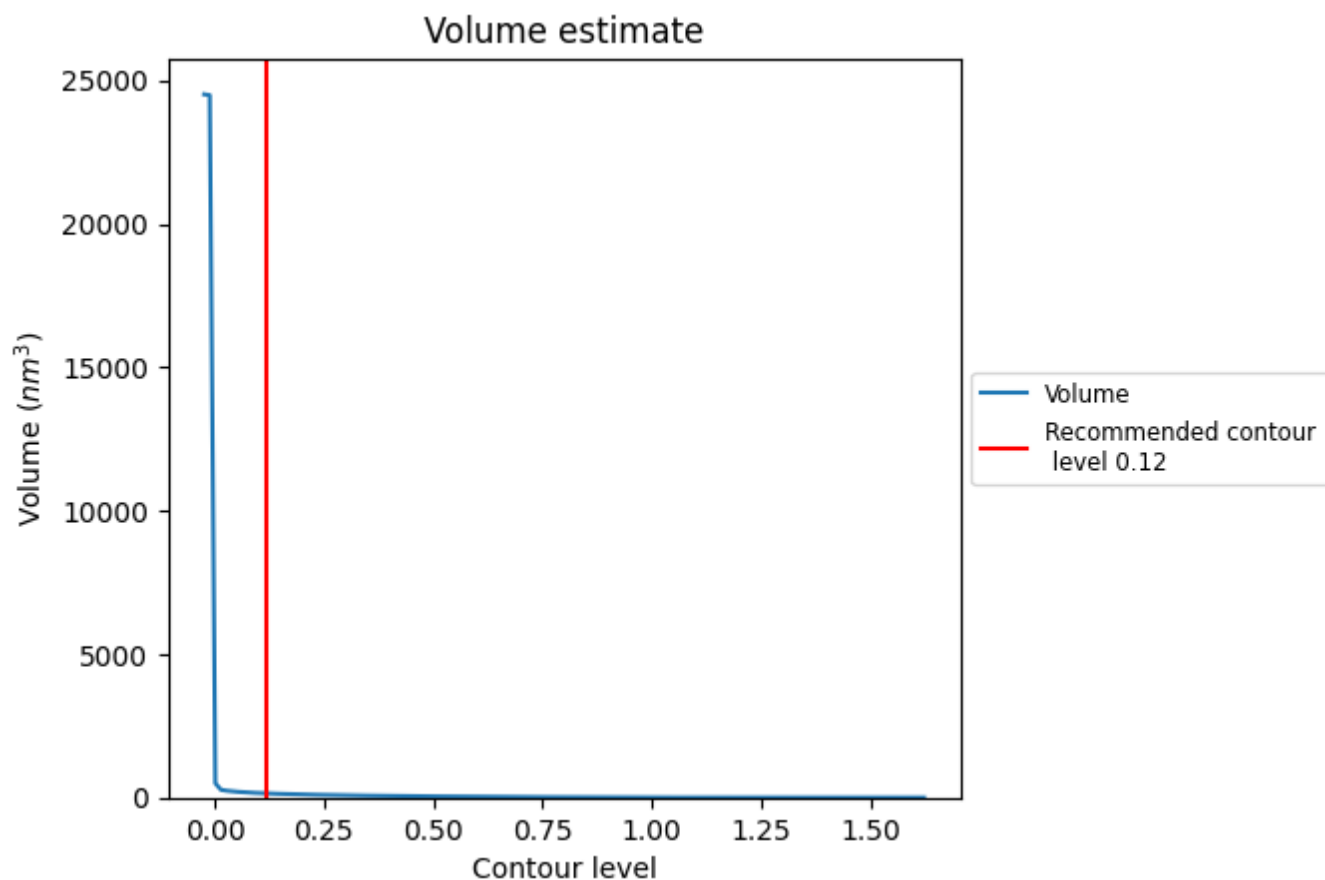
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

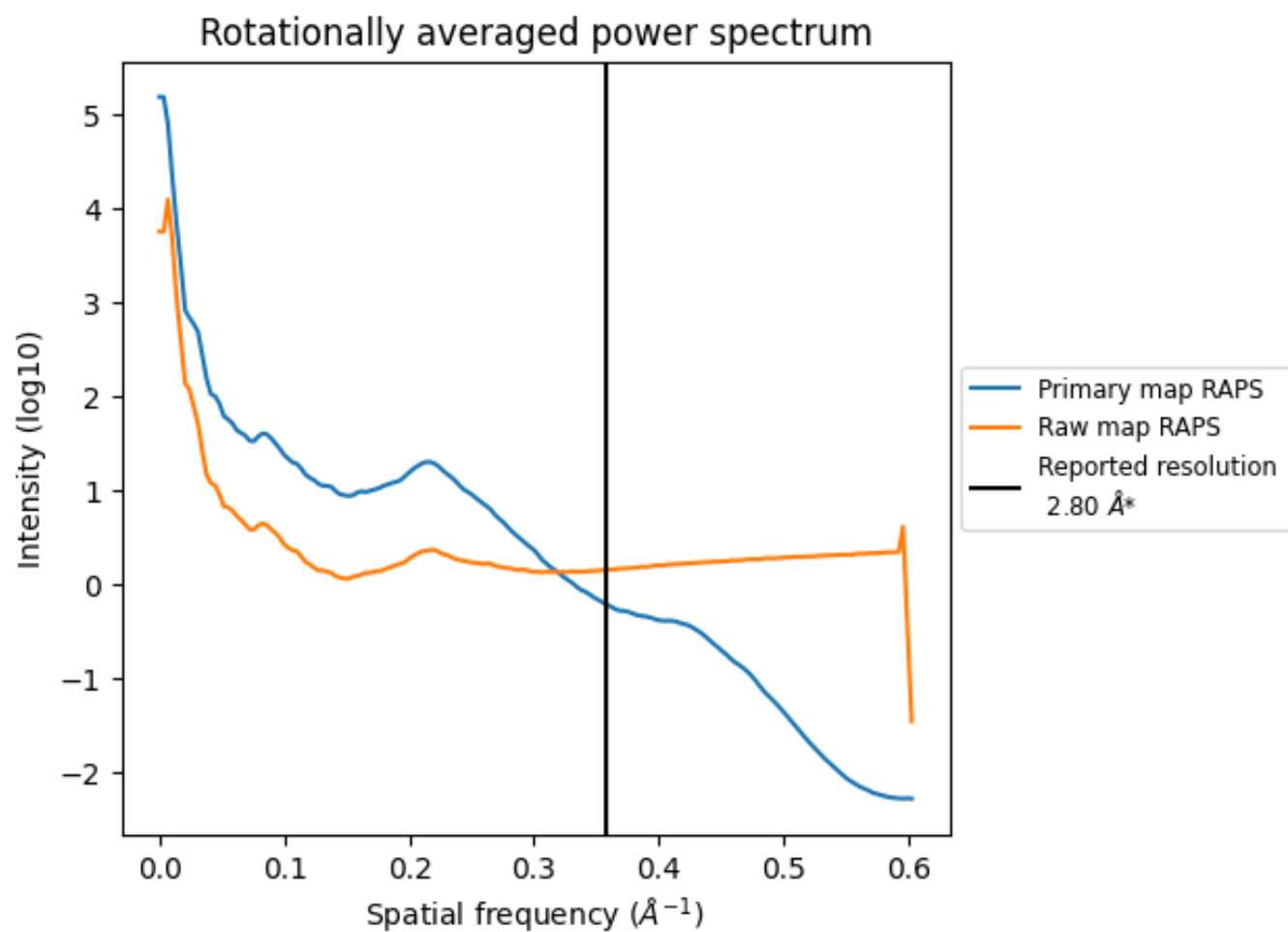
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 145  $\text{nm}^3$ ; this corresponds to an approximate mass of 131 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 ⓘ

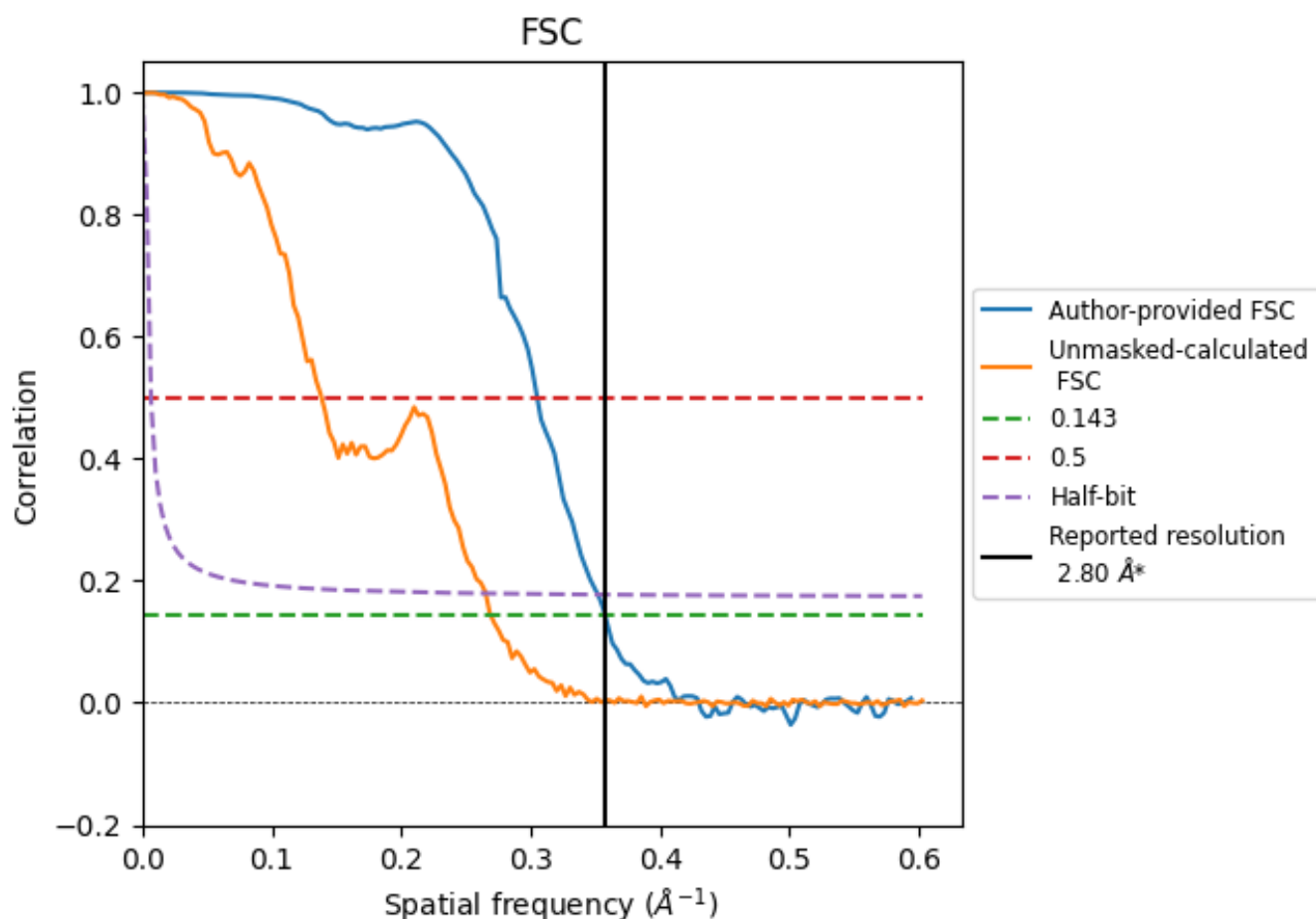


\*Reported resolution corresponds to spatial frequency of 0.357  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.28	2.84
Unmasked-calculated*	3.71	7.22	3.77

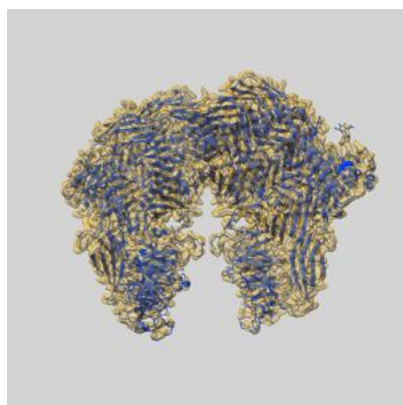
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.71 differs from the reported value 2.8 by more than 10 %



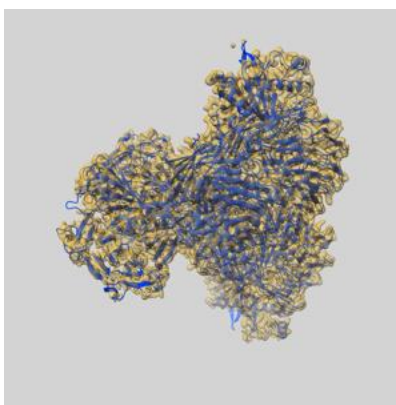
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50975 and PDB model 9G2F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

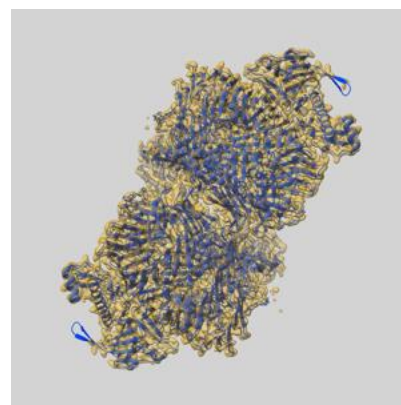
### 9.1 Map-model overlay [i](#)



X



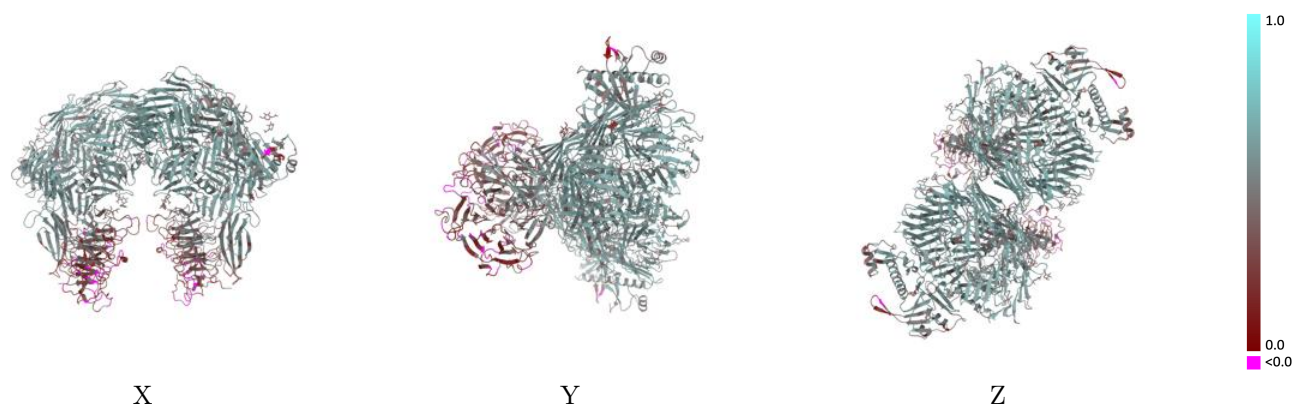
Y



Z

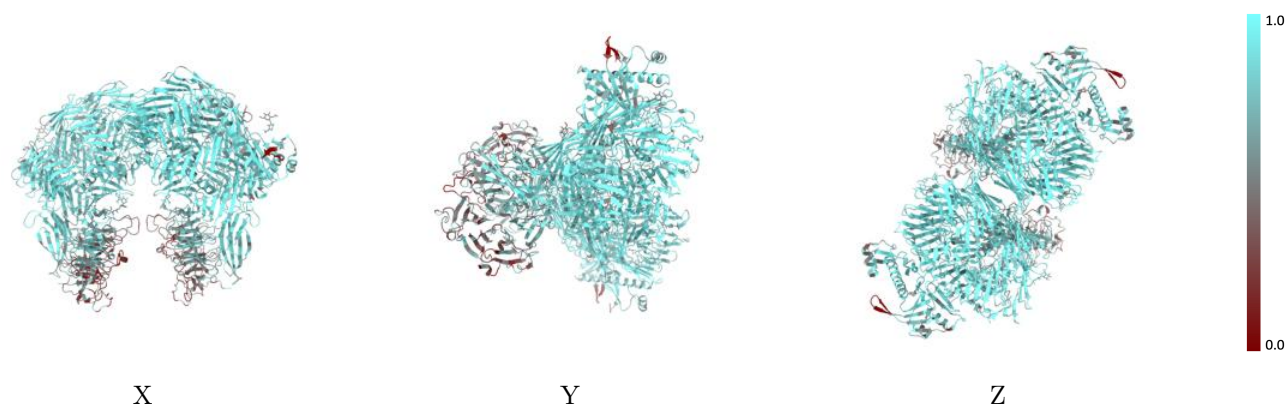
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



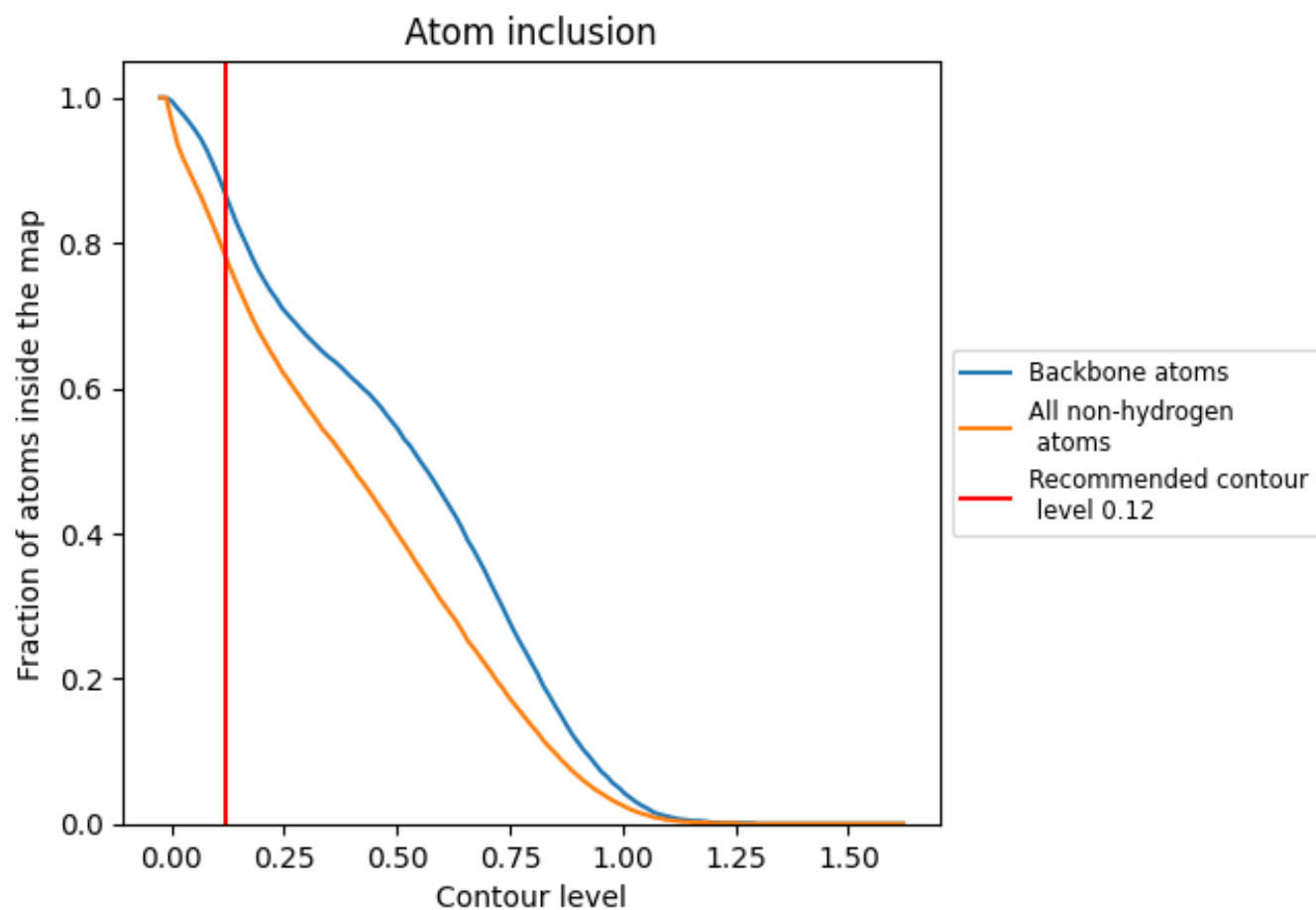
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7820	<div></div> 0.4920
A	<div></div> 0.7830	<div></div> 0.4930
B	<div></div> 0.7830	<div></div> 0.4930
C	<div></div> 0.7140	<div></div> 0.3910
D	<div></div> 0.6390	<div></div> 0.3960
E	<div></div> 0.8200	<div></div> 0.4960
F	<div></div> 0.7500	<div></div> 0.4620
G	<div></div> 0.5360	<div></div> 0.3760
H	<div></div> 0.7140	<div></div> 0.3940
I	<div></div> 0.5900	<div></div> 0.3910
J	<div></div> 0.7800	<div></div> 0.4980
K	<div></div> 0.7860	<div></div> 0.4610
L	<div></div> 0.5710	<div></div> 0.3880

