



## Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 06:54 pm GMT

PDB ID : 6TQL  
EMDB ID : EMD-10554  
Title : Cryo-EM of elastase-treated human uromodulin (UMOD)/Tamm-Horsfall protein (THP) filament  
Authors : Stsiapanava, A.; Xu, C.; Carroni, M.; Wu, B.; Jovine, L.  
Deposited on : 2019-12-16  
Resolution : 3.96 Å(reported)  
Based on initial model : 6TQK

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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.39

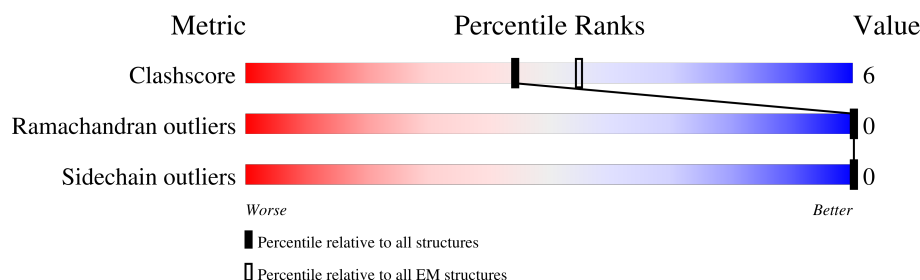
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.96 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	A	296	<div> <div>10%</div> <div>86%</div> <div>13%</div> </div>
1	B	296	<div> <div>43%</div> <div>52%</div> </div>
1	C	296	<div> <div>9%</div> <div>44%</div> <div>8%</div> <div>48%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>
3	E	10	<div> <div>30%</div> <div>50%</div> <div>20%</div> </div>
4	G	8	<div> <div>25%</div> <div>38%</div> <div>38%</div> </div>

## 2 Entry composition [i](#)

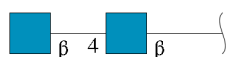
There are 5 unique types of molecules in this entry. The entry contains 9547 atoms, of which 4658 are hydrogens and 0 are deuteriums.

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 Uromodulin.

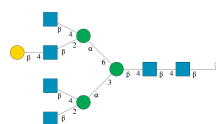
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	293	Total	C	H	N	O	S	0	0
			4474	1420	2190	389	449	26		
1	B	141	Total	C	H	N	O	S	0	0
			2137	685	1045	182	213	12		
1	C	153	Total	C	H	N	O	S	0	0
			2348	738	1150	208	238	14		

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



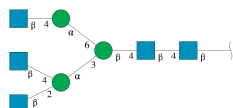
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
2	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

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



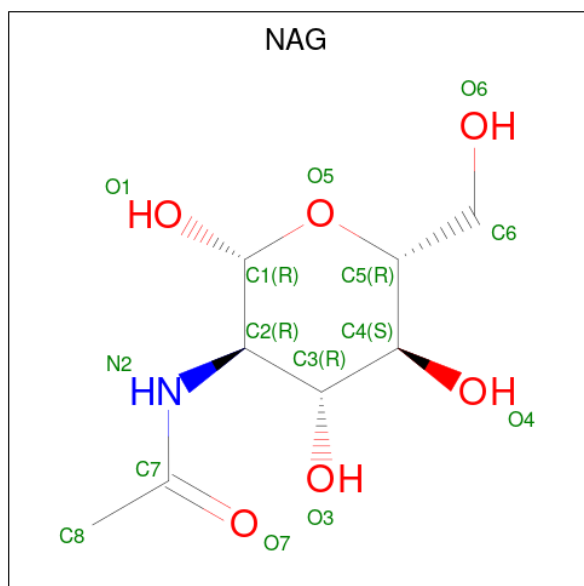
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	10	Total	C	H	N	O	0	0
			237	72	109	6	50		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	8	Total	C	H	N	O	0	0
			191	58	88	5	40		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).




Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
5	B	1	Total	C	H	N	O	0
			27	8	13	1	5	



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

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

Chain D: 

MAG1	MAG2
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- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

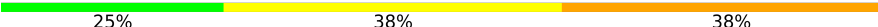
MAG1	MAG2
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- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 

MAG1	MAG2	BMA3	MAN4	MAG5	GAL6	MAG7	MAG8	MAG9	MAG10
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- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

MAG1	MAG2	BMA3	MAN4	MAG5	MAG6	MAG7	MAG8
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-179.9°, rise=62.7 Å, axial sym=C1	Depositor
Number of segments used	94937	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	45	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	20.389	Depositor
Minimum map value	-15.694	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	110.7, 68.88, 286.18	wwPDB
Map dimensions	349, 84, 135	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, MAN, NAG, 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	0.25	0/2327	0.53	0/3149
1	B	0.25	0/1115	0.51	0/1511
1	C	0.24	0/1217	0.52	0/1643
All	All	0.25	0/4659	0.52	0/6303

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2284	2190	2190	31	0
1	B	1092	1045	1044	8	0
1	C	1198	1150	1150	22	0
2	D	28	25	25	2	0
2	F	28	25	25	2	0
3	E	128	109	109	3	0
4	G	103	88	88	6	0
5	A	14	13	13	0	0
5	B	14	13	13	0	0
All	All	4889	4658	4657	59	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 6.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:OD1	1:C:420:LYS:CG	2.26	0.84
1:A:447:ASN:OD1	1:C:420:LYS:HG2	1.83	0.78
1:A:494:GLY:N	1:C:338:ASN:OD1	2.22	0.72
1:A:322:ASN:OD1	2:D:1:NAG:N2	2.26	0.69
1:A:469:THR:OG1	1:A:470:GLN:OE1	2.03	0.69
1:C:322:ASN:OD1	2:F:1:NAG:N2	2.26	0.69
4:G:8:NAG:H3	4:G:8:NAG:H83	1.75	0.68
1:B:469:THR:OG1	1:B:470:GLN:OE1	2.03	0.66
1:A:447:ASN:OD1	1:C:420:LYS:HG3	2.03	0.59
1:A:447:ASN:HD21	1:C:420:LYS:CE	2.18	0.57
3:E:10:NAG:H83	3:E:10:NAG:H3	1.87	0.57
1:A:326:ILE:O	1:A:330:GLU:N	2.41	0.54
1:C:326:ILE:O	1:C:330:GLU:N	2.41	0.53
1:C:355:ASP:OD1	1:C:356:LYS:N	2.41	0.53
1:B:554:ARG:NH2	1:B:560:ASP:OD1	2.42	0.53
1:A:554:ARG:NH2	1:A:560:ASP:OD1	2.42	0.53
1:A:296:THR:OG1	1:A:298:GLU:OE1	2.21	0.53
1:A:447:ASN:OD1	1:C:420:LYS:CE	2.57	0.52
1:A:447:ASN:ND2	1:C:420:LYS:HE3	2.25	0.52
1:C:404:ASN:OD1	1:C:405:THR:N	2.43	0.52
1:A:355:ASP:OD1	1:A:356:LYS:N	2.41	0.52
1:C:294:GLU:OE1	1:C:294:GLU:N	2.43	0.52
3:E:3:BMA:H61	3:E:5:NAG:H83	1.92	0.52
1:A:294:GLU:N	1:A:294:GLU:OE1	2.43	0.51
1:A:307:LYS:N	1:A:314:HIS:O	2.44	0.51
1:C:307:LYS:N	1:C:314:HIS:O	2.44	0.51
1:A:421:ILE:CD1	1:B:448:ILE:HD11	2.41	0.51
1:A:404:ASN:OD1	1:A:405:THR:N	2.43	0.50
3:E:5:NAG:O3	3:E:5:NAG:H82	2.12	0.50
1:A:338:ASN:OD1	1:B:494:GLY:N	2.45	0.50
1:B:543:SER:OG	1:B:544:SER:N	2.45	0.49
1:C:343:SER:C	1:C:344:LEU:HD12	2.33	0.49
1:A:343:SER:C	1:A:344:LEU:HD12	2.33	0.49
1:A:447:ASN:ND2	1:C:420:LYS:CE	2.76	0.48
1:A:543:SER:OG	1:A:544:SER:N	2.45	0.48
1:A:447:ASN:HD21	1:C:420:LYS:HE2	1.78	0.48
4:G:6:NAG:H82	4:G:6:NAG:C1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ARG:NH2	1:C:393:LEU:HD13	2.29	0.47
1:A:308:SER:HG	1:A:313:TRP:HE1	1.61	0.47
1:A:537:VAL:HG12	1:A:548:PHE:CB	2.47	0.45
1:B:537:VAL:HG12	1:B:548:PHE:CB	2.47	0.45
1:C:363:ASP:OD1	1:C:365:ARG:NE	2.43	0.45
1:A:363:ASP:OD1	1:A:365:ARG:NE	2.43	0.45
1:C:308:SER:HG	1:C:313:TRP:HE1	1.63	0.45
1:C:361:LEU:HD12	1:C:389:CYS:SG	2.58	0.44
1:A:333:LEU:HD23	1:A:334:GLU:N	2.34	0.43
1:A:393:LEU:HD13	1:B:498:ARG:NH2	2.34	0.43
1:C:333:LEU:HD23	1:C:334:GLU:N	2.34	0.43
1:A:361:LEU:HD12	1:A:389:CYS:SG	2.58	0.43
4:G:7:MAN:H5	4:G:8:NAG:H82	1.99	0.42
4:G:8:NAG:H3	4:G:8:NAG:C8	2.46	0.42
2:F:1:NAG:C6	2:F:2:NAG:C1	2.98	0.42
1:B:491:LEU:HD11	1:B:501:LEU:HD13	2.02	0.42
4:G:6:NAG:H83	4:G:6:NAG:H3	2.02	0.42
2:D:1:NAG:C6	2:D:2:NAG:C1	2.98	0.41
1:A:491:LEU:HD11	1:A:501:LEU:HD13	2.02	0.41
1:A:376:ASP:N	1:A:376:ASP:OD1	2.54	0.41
4:G:6:NAG:C1	4:G:6:NAG:C8	2.98	0.41
1:C:376:ASP:N	1:C:376:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/296 (98%)	285 (98%)	6 (2%)	0	100	100
1	B	139/296 (47%)	138 (99%)	1 (1%)	0	100	100
1	C	151/296 (51%)	146 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	581/888 (65%)	569 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/264 (99%)	261 (100%)	0	100	100
1	B	123/264 (47%)	123 (100%)	0	100	100
1	C	139/264 (53%)	139 (100%)	0	100	100
All	All	523/792 (66%)	523 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

22 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	D	1	1,2	14,14,15	0.25	0	17,19,21	0.88	1 (5%)
2	NAG	D	2	2	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	E	1	1,3	14,14,15	0.19	0	17,19,21	0.49	0
3	NAG	E	10	3	14,14,15	0.31	0	17,19,21	1.19	2 (11%)
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	BMA	E	3	3	11,11,12	0.63	0	15,15,17	0.81	0
3	MAN	E	4	3	11,11,12	1.17	1 (9%)	15,15,17	1.34	3 (20%)
3	NAG	E	5	3	14,14,15	0.66	1 (7%)	17,19,21	0.86	1 (5%)
3	GAL	E	6	3	11,11,12	0.65	0	15,15,17	1.29	1 (6%)
3	NAG	E	7	3	14,14,15	1.08	2 (14%)	17,19,21	0.77	0
3	MAN	E	8	3	11,11,12	0.67	0	15,15,17	1.05	2 (13%)
3	NAG	E	9	3	14,14,15	0.54	0	17,19,21	0.70	0
2	NAG	F	1	1,2	14,14,15	0.25	0	17,19,21	0.89	1 (5%)
2	NAG	F	2	2	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	G	1	1,4	14,14,15	0.26	0	17,19,21	0.55	0
4	NAG	G	2	4	14,14,15	0.21	0	17,19,21	0.61	0
4	BMA	G	3	4	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
4	MAN	G	4	4	11,11,12	0.81	0	15,15,17	1.15	2 (13%)
4	NAG	G	5	4	14,14,15	0.63	0	17,19,21	0.75	1 (5%)
4	NAG	G	6	4	14,14,15	0.46	0	17,19,21	1.11	1 (5%)
4	MAN	G	7	4	11,11,12	0.87	0	15,15,17	1.74	4 (26%)
4	NAG	G	8	4	14,14,15	0.41	0	17,19,21	1.11	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	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	10	3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	5	3	-	2/6/23/26	0/1/1/1
3	GAL	E	6	3	-	0/2/19/22	0/1/1/1
3	NAG	E	7	3	-	2/6/23/26	0/1/1/1
3	MAN	E	8	3	-	0/2/19/22	0/1/1/1
3	NAG	E	9	3	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	NAG	G	5	4	-	3/6/23/26	0/1/1/1
4	NAG	G	6	4	-	3/6/23/26	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1
4	NAG	G	8	4	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	7	NAG	O5-C1	-3.24	1.38	1.43
3	E	4	MAN	C1-C2	2.88	1.58	1.52
3	E	5	NAG	C1-C2	2.03	1.55	1.52
3	E	7	NAG	C1-C2	2.02	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	7	MAN	C1-O5-C5	4.70	118.56	112.19
4	G	8	NAG	C2-N2-C7	3.52	127.91	122.90
3	E	10	NAG	C2-N2-C7	3.51	127.90	122.90
4	G	6	NAG	C2-N2-C7	3.32	127.63	122.90
3	E	6	GAL	C1-O5-C5	3.23	116.56	112.19
4	G	4	MAN	C1-O5-C5	2.86	116.06	112.19
3	E	4	MAN	O2-C2-C3	-2.83	104.47	110.14
3	E	4	MAN	C1-O5-C5	2.77	115.94	112.19
3	E	4	MAN	O2-C2-C1	2.66	114.59	109.15
3	E	5	NAG	C2-N2-C7	2.53	126.51	122.90
4	G	7	MAN	O4-C4-C5	2.51	115.53	109.30
3	E	8	MAN	O2-C2-C3	-2.41	105.31	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	4	MAN	O2-C2-C3	-2.38	105.38	110.14
3	E	8	MAN	C1-O5-C5	2.35	115.37	112.19
2	F	1	NAG	C1-O5-C5	2.28	115.28	112.19
4	G	7	MAN	O5-C5-C6	-2.27	103.64	107.20
2	D	1	NAG	C1-O5-C5	2.27	115.27	112.19
4	G	3	BMA	C1-C2-C3	-2.26	106.88	109.67
4	G	7	MAN	O2-C2-C3	-2.13	105.86	110.14
4	G	5	NAG	C1-O5-C5	-2.12	109.32	112.19
3	E	10	NAG	C1-C2-N2	2.04	113.97	110.49

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	7	NAG	C1-C2-N2-C7
2	D	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	5	NAG	C8-C7-N2-C2
3	E	5	NAG	O7-C7-N2-C2
3	E	10	NAG	C8-C7-N2-C2
3	E	10	NAG	O7-C7-N2-C2
4	G	6	NAG	C8-C7-N2-C2
4	G	6	NAG	O7-C7-N2-C2
4	G	8	NAG	C8-C7-N2-C2
4	G	8	NAG	O7-C7-N2-C2
4	G	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
4	G	5	NAG	O5-C5-C6-O6
4	G	5	NAG	C4-C5-C6-O6
3	E	9	NAG	C1-C2-N2-C7
3	E	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	G	6	NAG	C1-C2-N2-C7
4	G	5	NAG	C1-C2-N2-C7
3	E	7	NAG	C3-C2-N2-C7
3	E	10	NAG	C3-C2-N2-C7
4	G	8	NAG	C3-C2-N2-C7
2	D	1	NAG	C1-C2-N2-C7
2	F	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
3	E	9	NAG	C3-C2-N2-C7

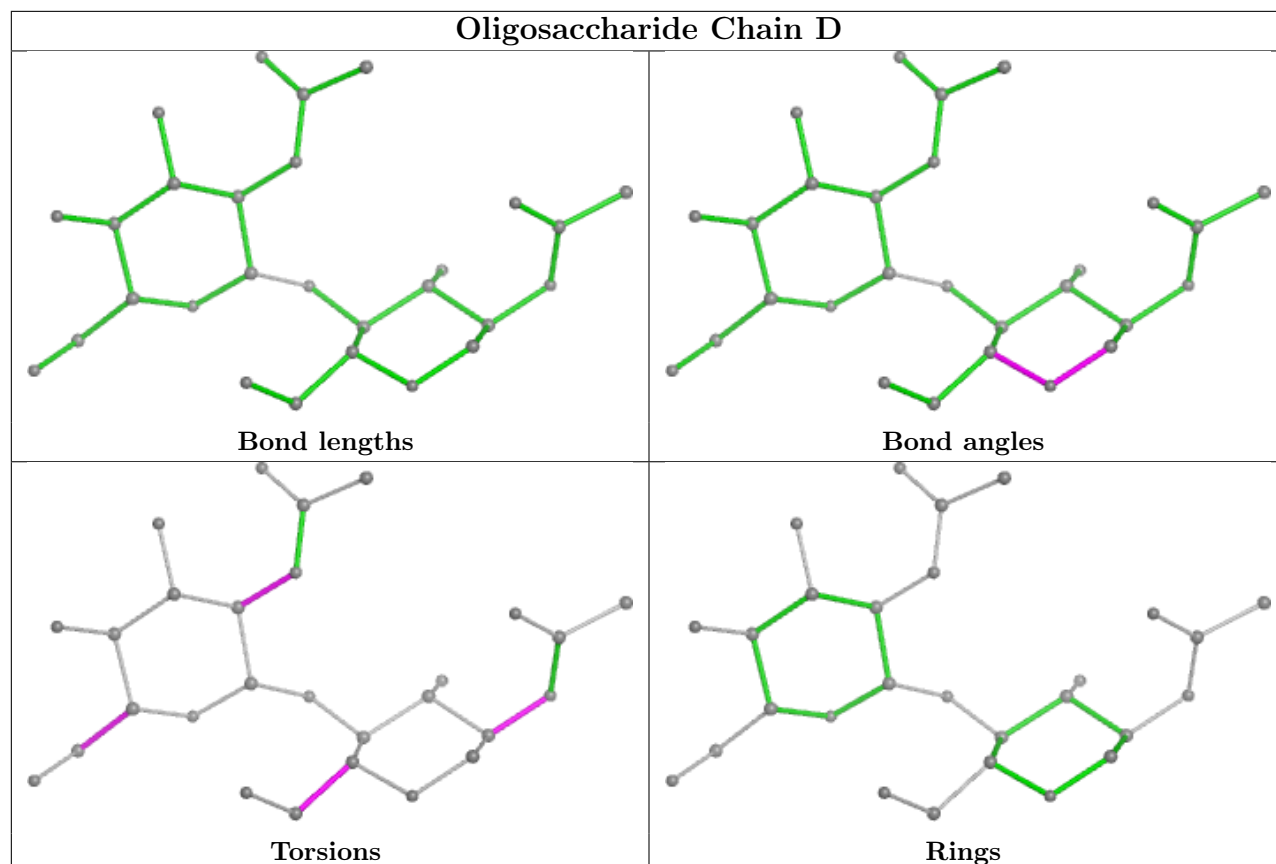
There are no ring outliers.

10 monomers are involved in 13 short contacts:

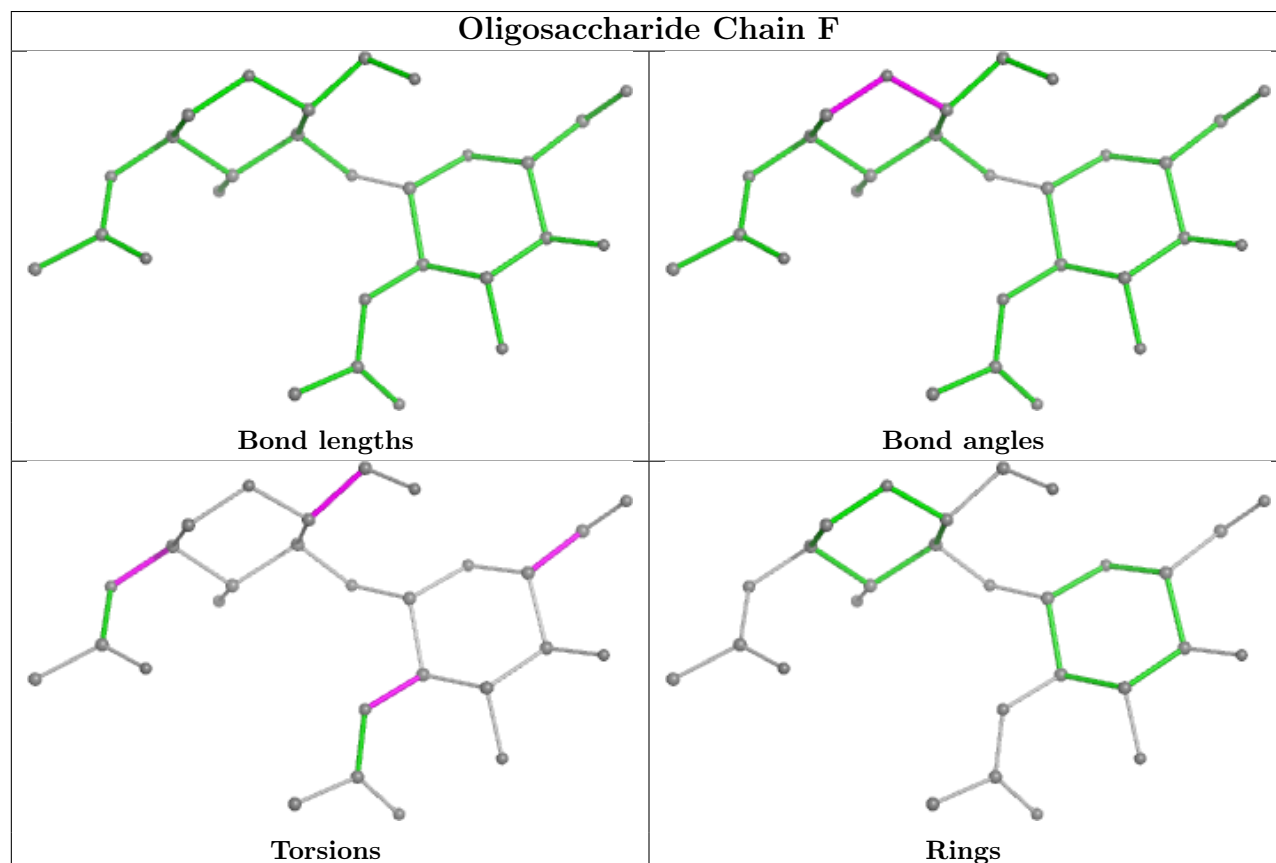
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	1	0
2	D	2	NAG	1	0
4	G	7	MAN	1	0
3	E	3	BMA	1	0
4	G	6	NAG	3	0
4	G	8	NAG	3	0
2	F	1	NAG	2	0
3	E	5	NAG	2	0
3	E	10	NAG	1	0
2	D	1	NAG	2	0

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

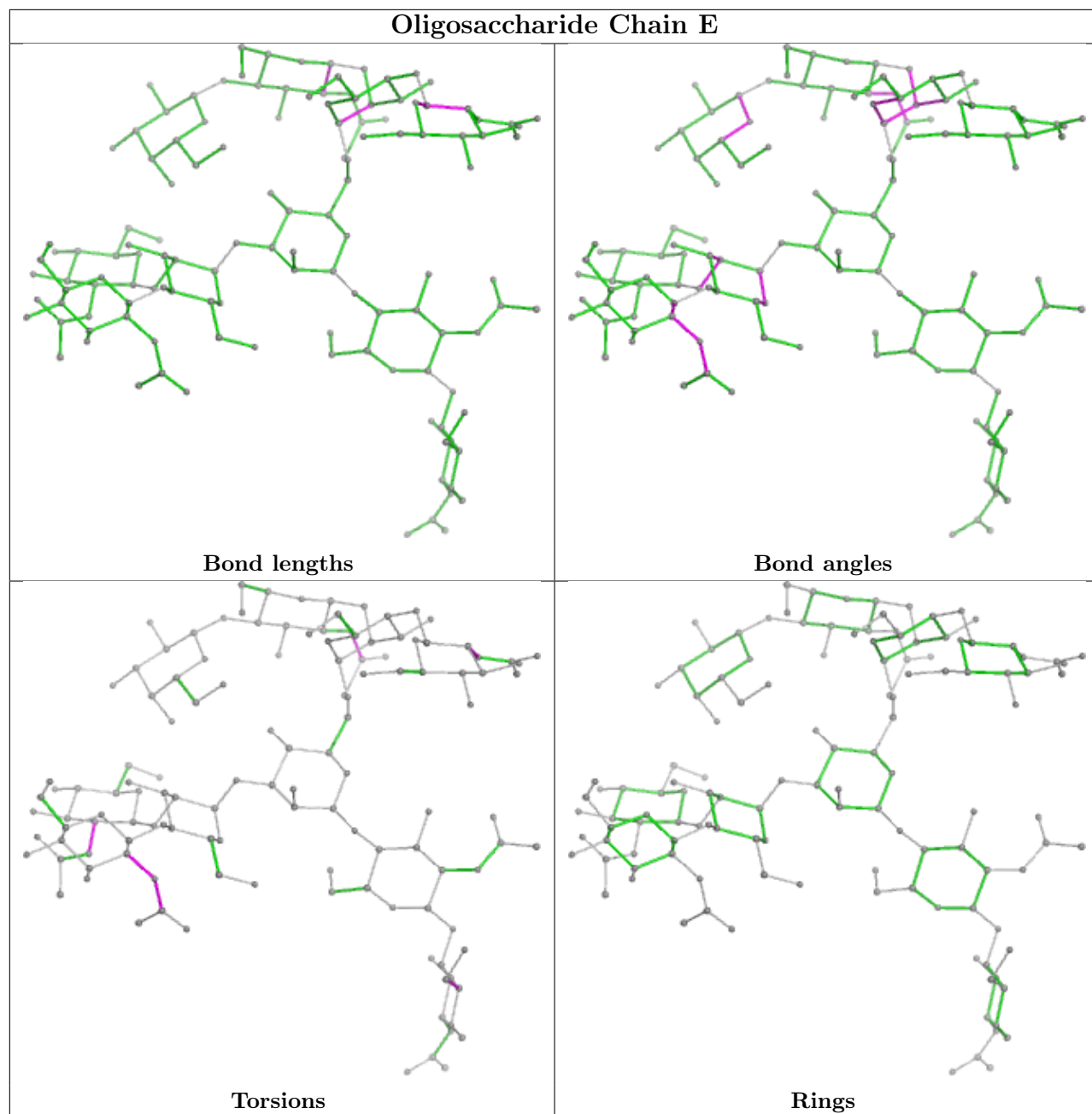
## Oligosaccharide Chain D

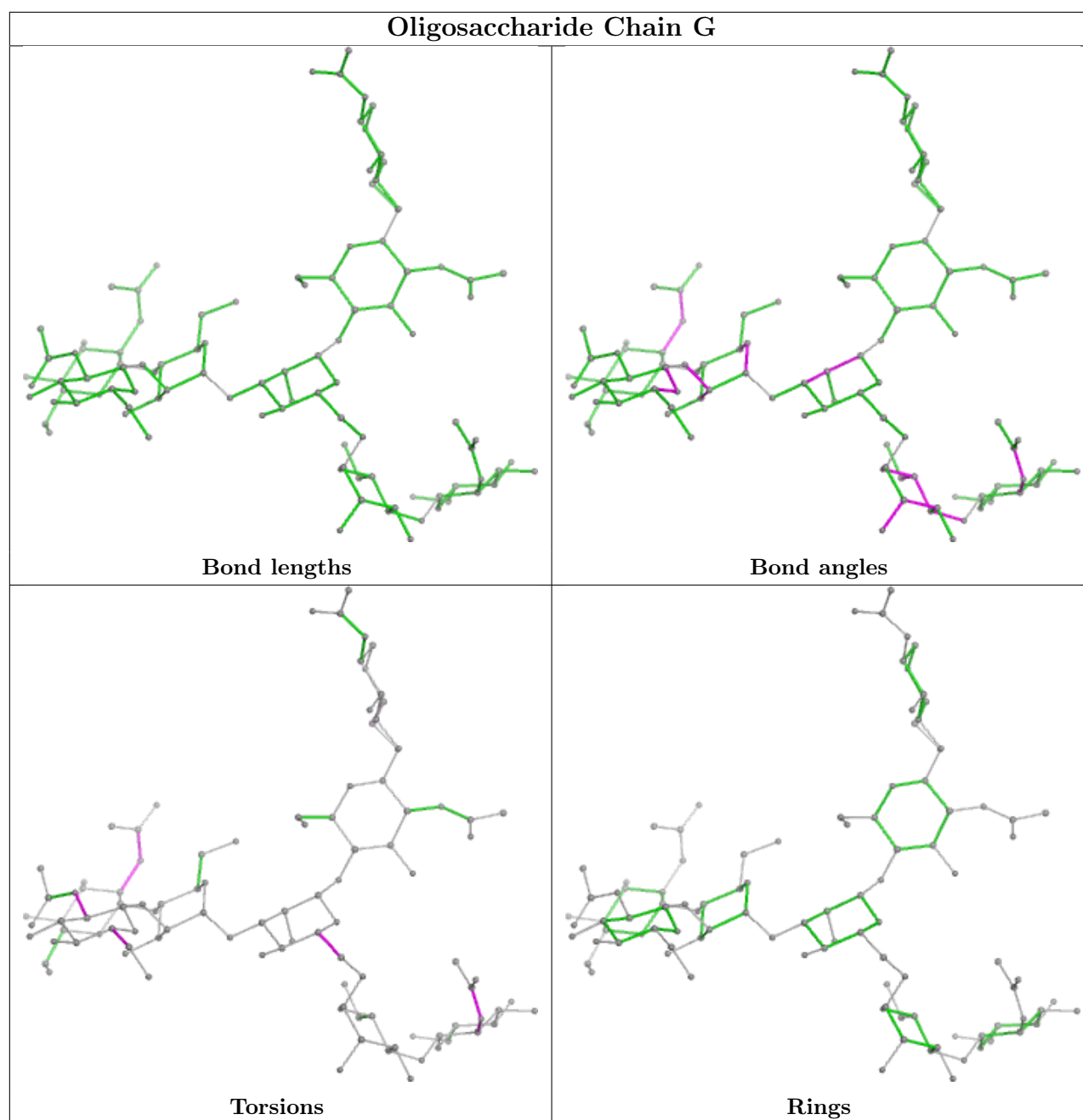


## Oligosaccharide Chain F









## 5.6 Ligand geometry [i](#)

2 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	A	601	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	B	601	1	14,14,15	0.21	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	B	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	O5-C5-C6-O6
5	B	601	NAG	O5-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
5	B	601	NAG	C4-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.

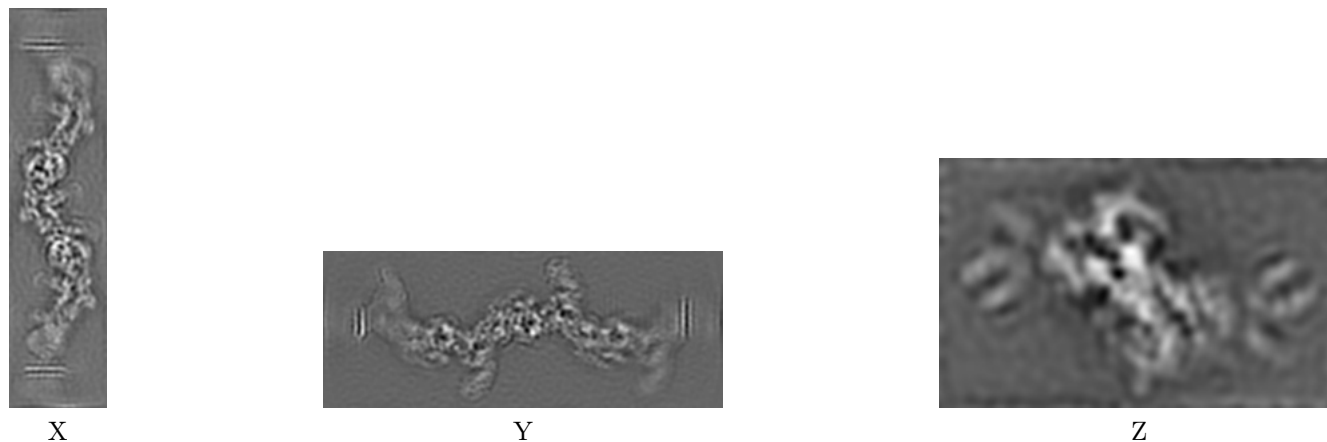
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10554. These allow visual inspection of the internal detail of the map and identification of artifacts.

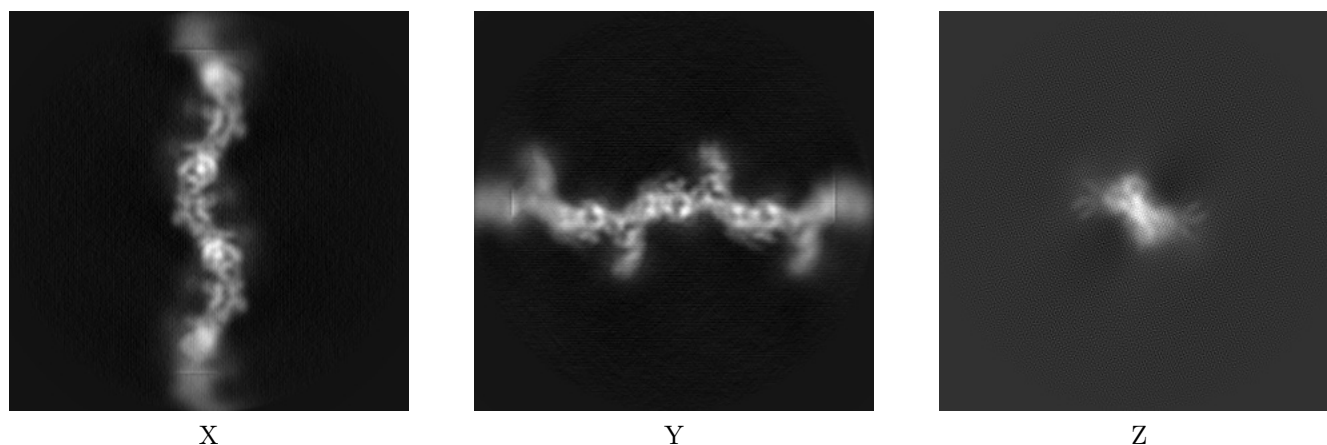
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



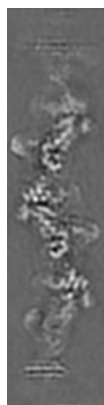
#### 6.1.2 Raw map



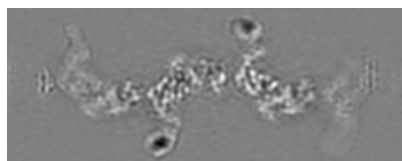
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

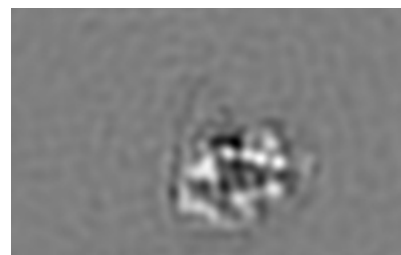
### 6.2.1 Primary map



X Index:  
67

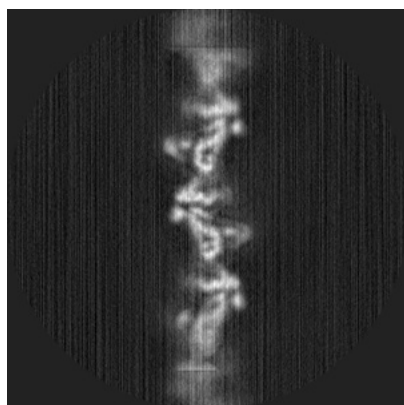


Y Index: 42

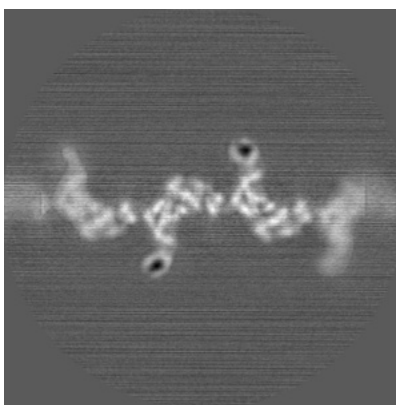


Z Index: 174

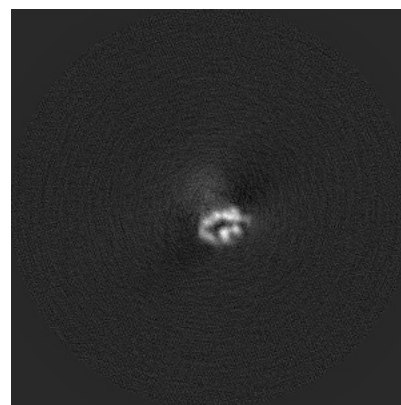
### 6.2.2 Raw map



X Index: 175



Y Index: 175

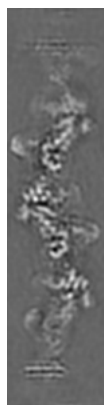


Z Index: 175

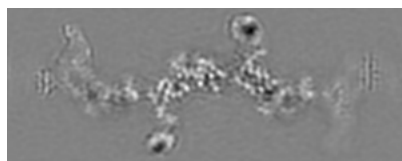
The images above show central slices of the map in three orthogonal directions.

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

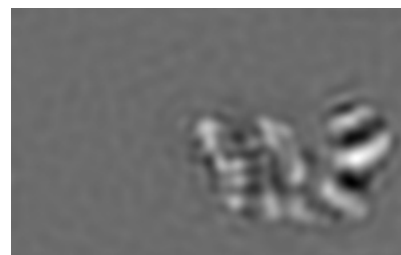
### 6.3.1 Primary map



X Index:  
67

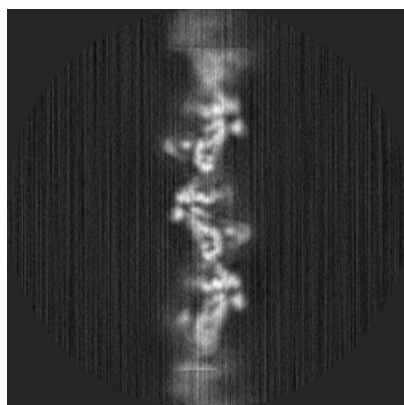


Y Index: 39

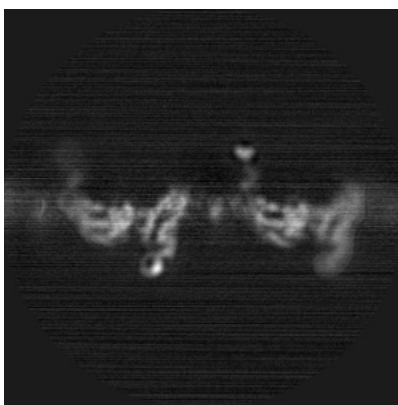


Z Index: 210

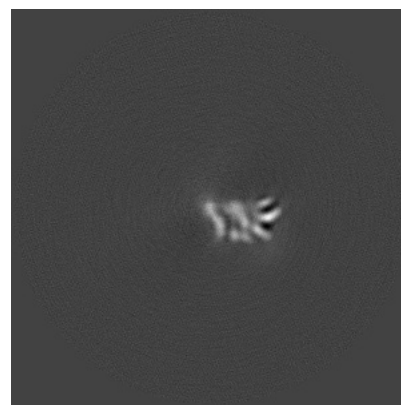
### 6.3.2 Raw map



X Index: 174



Y Index: 181

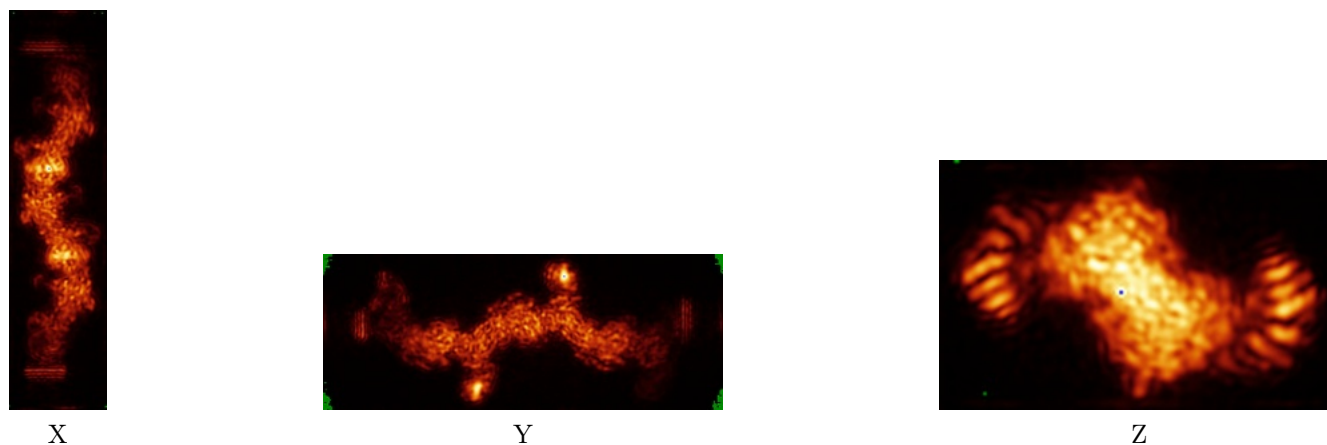


Z Index: 211

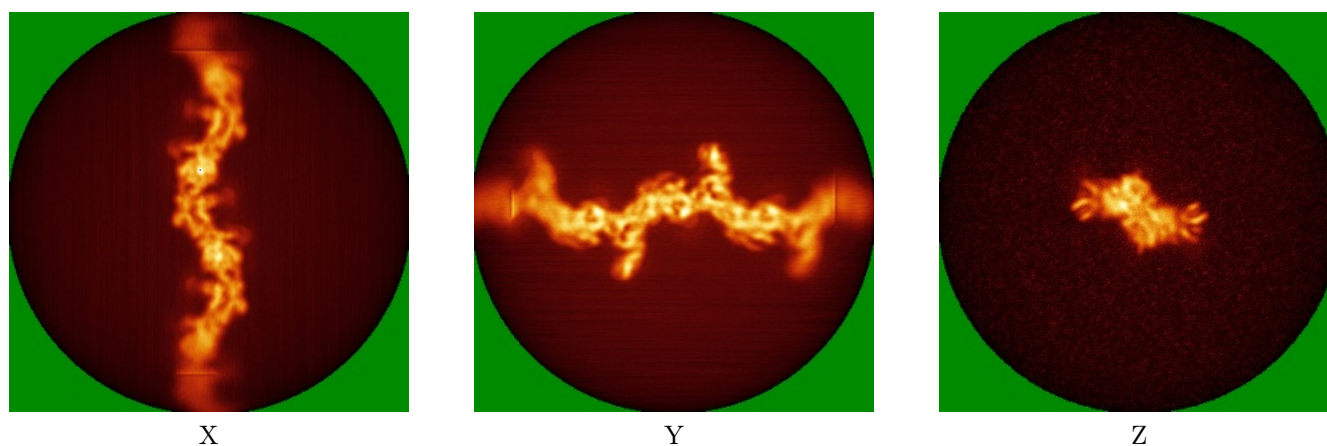
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. 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](#)

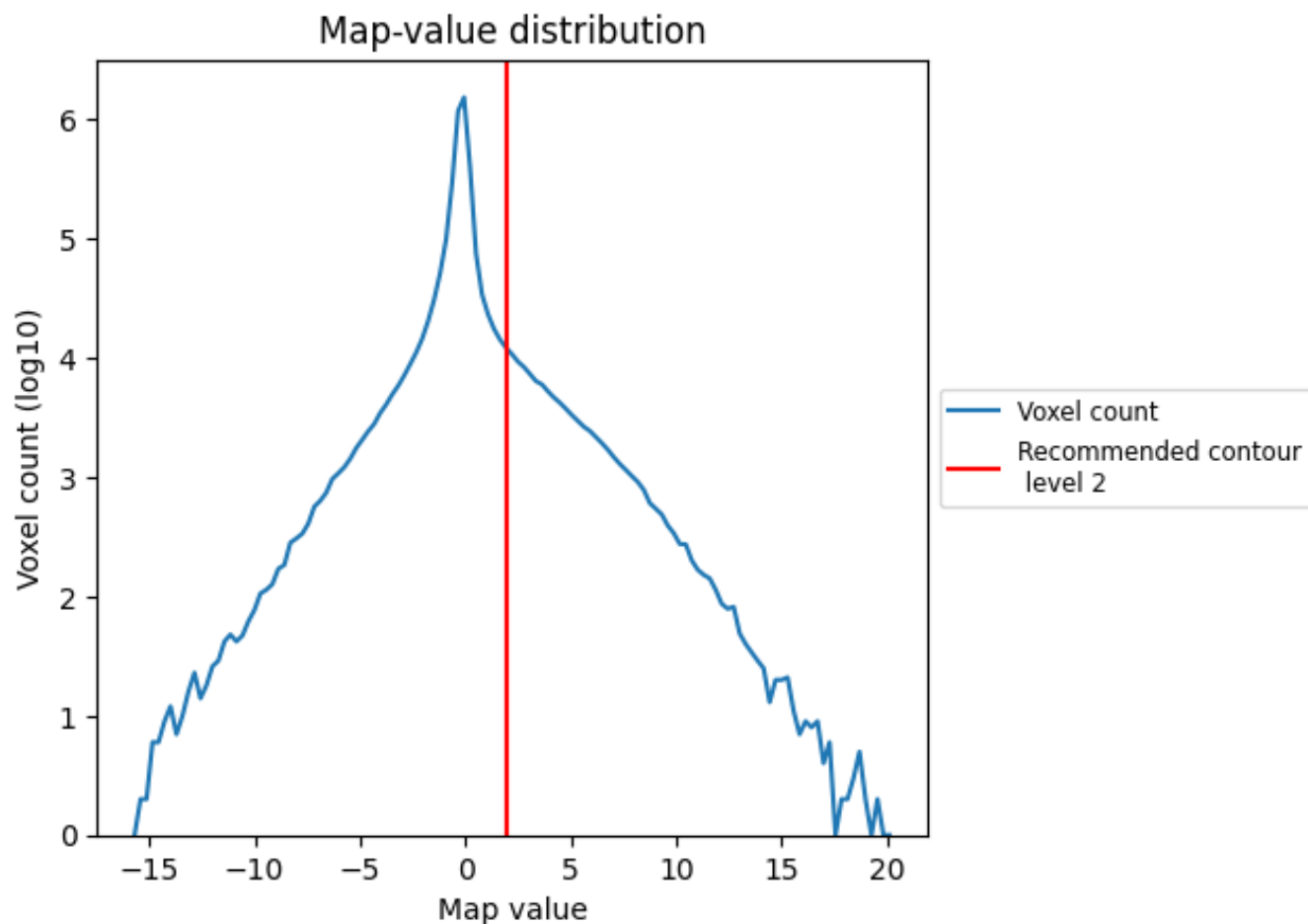
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

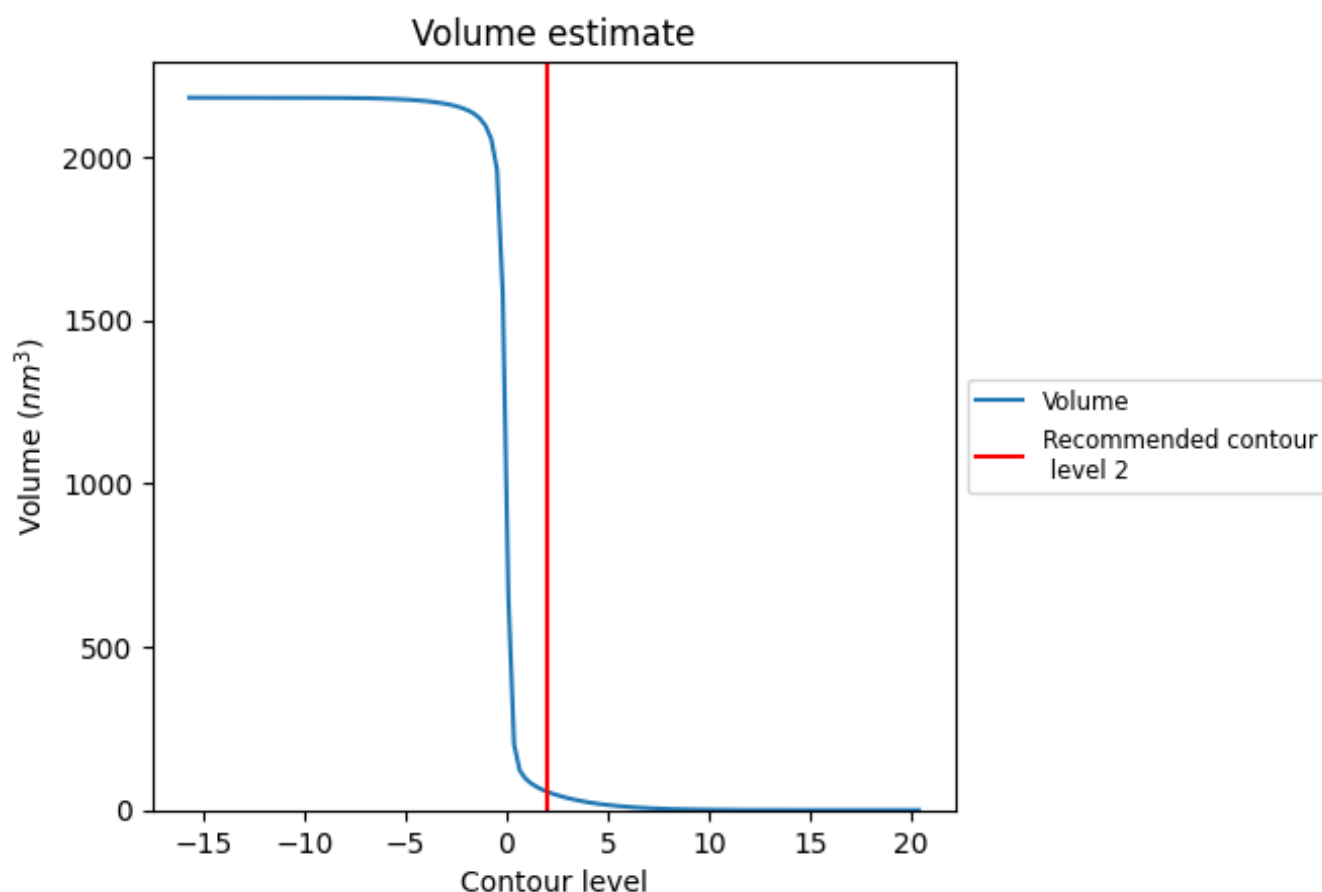
This section contains the results of statistical analysis of the map.

### 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 57 nm<sup>3</sup>; this corresponds to an approximate mass of 51 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 8 Fourier-Shell correlation ⓘ

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

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

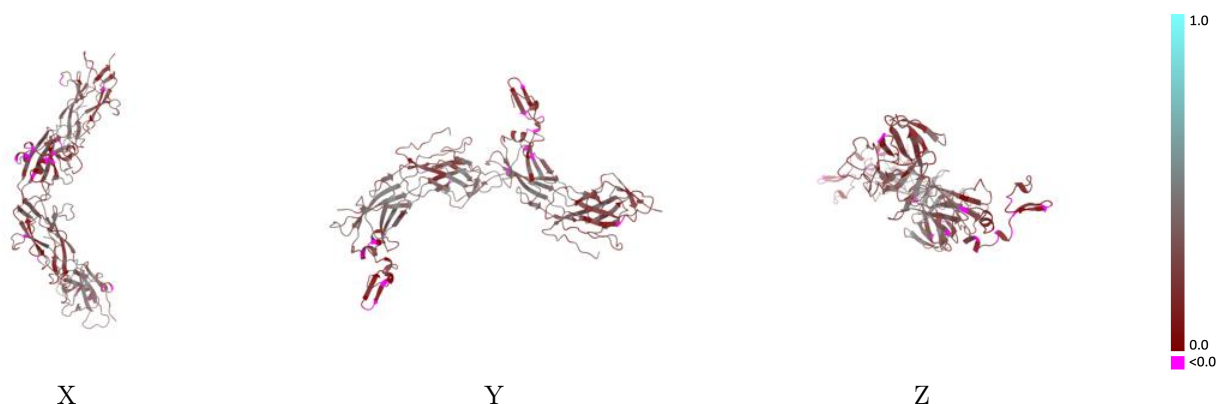
This section contains information regarding the fit between EMDB map EMD-10554 and PDB model 6TQL. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



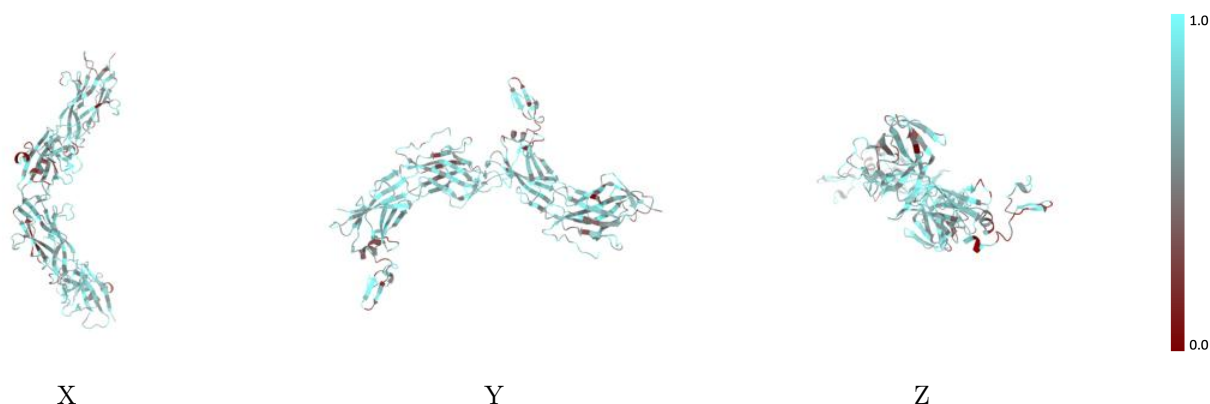
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



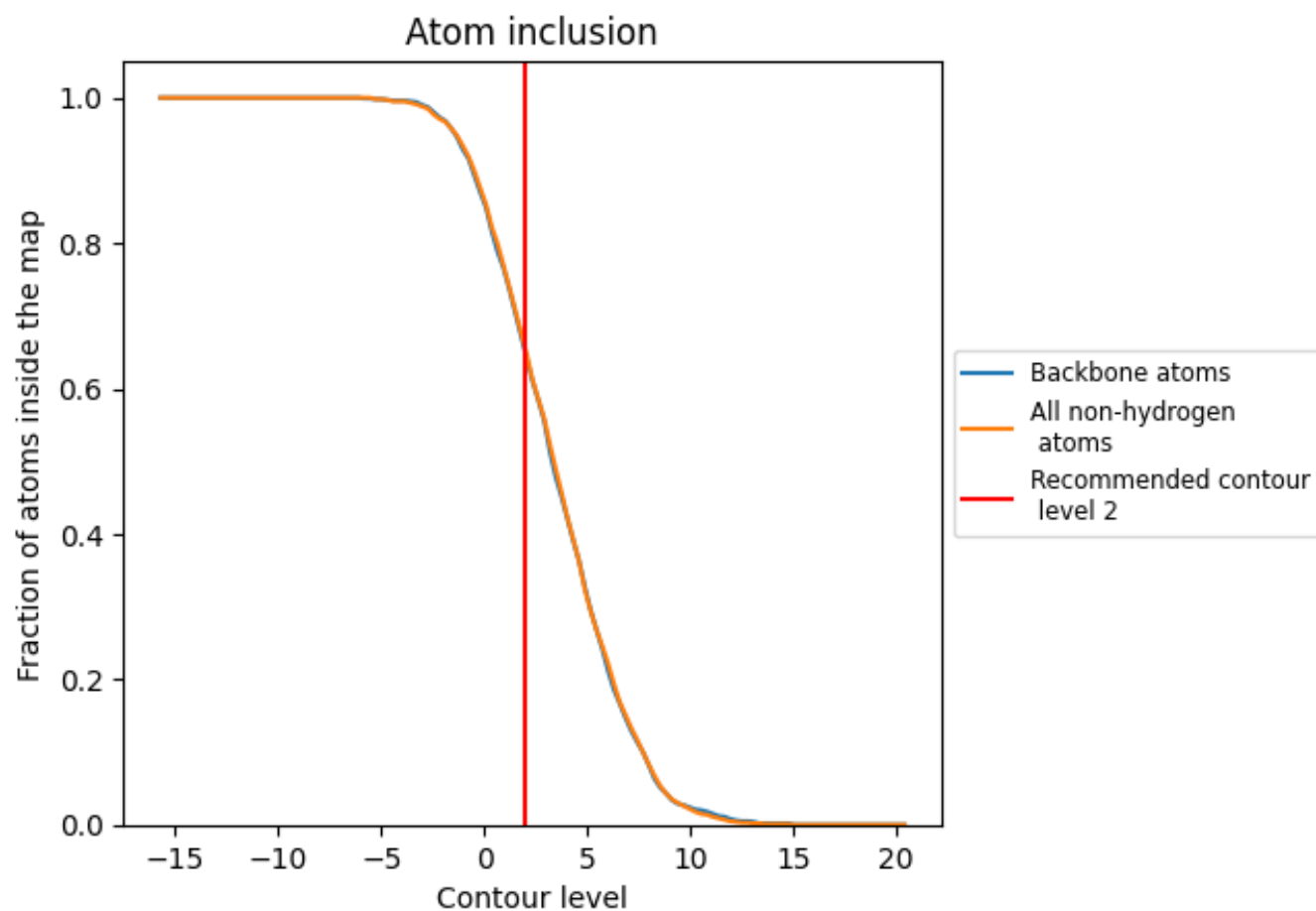
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6530	<div><div></div></div> 0.2890
A	<div><div></div></div> 0.6570	<div><div></div></div> 0.2950
B	<div><div></div></div> 0.6720	<div><div></div></div> 0.2930
C	<div><div></div></div> 0.6280	<div><div></div></div> 0.2610
D	<div><div></div></div> 0.9290	<div><div></div></div> 0.3060
E	<div><div></div></div> 0.7110	<div><div></div></div> 0.3580
F	<div><div></div></div> 0.8570	<div><div></div></div> 0.3540
G	<div><div></div></div> 0.7570	<div><div></div></div> 0.3480

1.0

0.0

<0.0