



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:08 PM UTC

PDB ID : 8HTT / pdb\_00008htt  
EMDB ID : EMD-35017  
Title : Cryo-EM structure of human TMEM87A, gluconate-bound  
Authors : Han, A.; Kim, H.M.  
Deposited on : 2022-12-21  
Resolution : 3.60 Å (reported)

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:

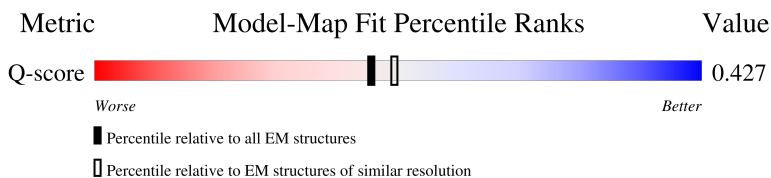
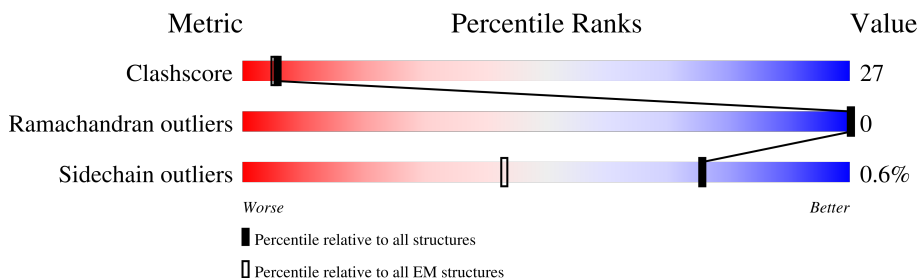
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

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

The reported resolution of this entry is 3.60 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	12797 ( 3.10 - 4.10 )

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	864	<p>24% 20% 55%</p>
2	A	2	100%
2	C	2	100%
3	D	3	<p>33% 33% 67%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	GCO	B	901	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3303 atoms, of which 11 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 Transmembrane protein 87A,EGFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	389	3184	2121	511	535	17	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	556	LEU	-	linker	UNP Q8NBN3
B	557	LYS	-	linker	UNP Q8NBN3
B	558	GLU	-	linker	UNP Q8NBN3
B	559	ASN	-	linker	UNP Q8NBN3
B	560	LEU	-	linker	UNP Q8NBN3
B	561	TYR	-	linker	UNP Q8NBN3
B	562	PHE	-	linker	UNP Q8NBN3
B	563	GLN	-	linker	UNP Q8NBN3
B	564	GLY	-	linker	UNP Q8NBN3
B	565	GLY	-	linker	UNP Q8NBN3
B	566	THR	-	linker	UNP Q8NBN3
B	567	LEU	-	linker	UNP Q8NBN3
B	568	GLU	-	linker	UNP Q8NBN3
B	569	VAL	-	linker	UNP Q8NBN3
B	570	LEU	-	linker	UNP Q8NBN3
B	571	PHE	-	linker	UNP Q8NBN3
B	572	GLN	-	linker	UNP Q8NBN3
B	573	GLY	-	linker	UNP Q8NBN3
B	574	PRO	-	linker	UNP Q8NBN3
B	575	ASN	-	linker	UNP Q8NBN3
B	576	PRO	-	linker	UNP Q8NBN3
B	577	ALA	-	linker	UNP Q8NBN3
B	578	PHE	-	linker	UNP Q8NBN3
B	579	LEU	-	linker	UNP Q8NBN3
B	580	TYR	-	linker	UNP Q8NBN3
B	581	LYS	-	linker	UNP Q8NBN3
B	582	VAL	-	linker	UNP Q8NBN3
B	583	VAL	-	linker	UNP Q8NBN3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	584	ASP	-	linker	UNP Q8NBN3
B	585	PRO	-	linker	UNP Q8NBN3
B	586	VAL	-	linker	UNP Q8NBN3
B	770	GLN	HIS	conflict	UNP A0A6M5E0N3
B	825	GLU	-	expression tag	UNP A0A6M5E0N3
B	826	PHE	-	expression tag	UNP A0A6M5E0N3
B	827	LEU	-	expression tag	UNP A0A6M5E0N3
B	828	VAL	-	expression tag	UNP A0A6M5E0N3
B	829	PRO	-	expression tag	UNP A0A6M5E0N3
B	830	ARG	-	expression tag	UNP A0A6M5E0N3
B	831	GLY	-	expression tag	UNP A0A6M5E0N3
B	832	SER	-	expression tag	UNP A0A6M5E0N3
B	833	SER	-	expression tag	UNP A0A6M5E0N3
B	834	ARG	-	expression tag	UNP A0A6M5E0N3
B	835	SER	-	expression tag	UNP A0A6M5E0N3
B	836	ALA	-	expression tag	UNP A0A6M5E0N3
B	837	TRP	-	expression tag	UNP A0A6M5E0N3
B	838	SER	-	expression tag	UNP A0A6M5E0N3
B	839	HIS	-	expression tag	UNP A0A6M5E0N3
B	840	PRO	-	expression tag	UNP A0A6M5E0N3
B	841	GLN	-	expression tag	UNP A0A6M5E0N3
B	842	PHE	-	expression tag	UNP A0A6M5E0N3
B	843	GLU	-	expression tag	UNP A0A6M5E0N3
B	844	LYS	-	expression tag	UNP A0A6M5E0N3
B	845	GLY	-	expression tag	UNP A0A6M5E0N3
B	846	GLY	-	expression tag	UNP A0A6M5E0N3
B	847	GLY	-	expression tag	UNP A0A6M5E0N3
B	848	SER	-	expression tag	UNP A0A6M5E0N3
B	849	GLY	-	expression tag	UNP A0A6M5E0N3
B	850	GLY	-	expression tag	UNP A0A6M5E0N3
B	851	GLY	-	expression tag	UNP A0A6M5E0N3
B	852	SER	-	expression tag	UNP A0A6M5E0N3
B	853	GLY	-	expression tag	UNP A0A6M5E0N3
B	854	GLY	-	expression tag	UNP A0A6M5E0N3
B	855	SER	-	expression tag	UNP A0A6M5E0N3
B	856	ALA	-	expression tag	UNP A0A6M5E0N3
B	857	TRP	-	expression tag	UNP A0A6M5E0N3
B	858	SER	-	expression tag	UNP A0A6M5E0N3
B	859	HIS	-	expression tag	UNP A0A6M5E0N3
B	860	PRO	-	expression tag	UNP A0A6M5E0N3
B	861	GLN	-	expression tag	UNP A0A6M5E0N3
B	862	PHE	-	expression tag	UNP A0A6M5E0N3

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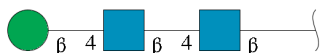
Chain	Residue	Modelled	Actual	Comment	Reference
B	863	GLU	-	expression tag	UNP A0A6M5E0N3
B	864	LYS	-	expression tag	UNP A0A6M5E0N3

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



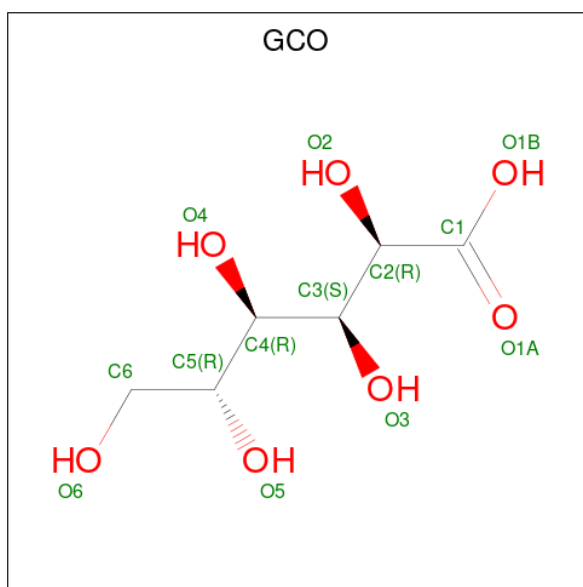
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	2	28	16	2	10	0	0
2	C	2	28	16	2	10	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	3	39	22	2	15	0	0

- Molecule 4 is D-gluconic acid (CCD ID: GCO) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	B	1	24	6	11	7	0





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	201915	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; PatchCTF in Cryosparc was used	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	68.15	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	58900	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.515	Depositor
Minimum map value	-0.291	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.101	Depositor
Map size ( $\text{\AA}$ )	271.68, 271.68, 271.68	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.849, 0.849, 0.849	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, GCO, 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	B	0.32	4/3269 (0.1%)	0.40	1/4434 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	PRO	C-N	-8.14	1.23	1.33
1	B	128	CYS	C-N	7.81	1.44	1.33
1	B	382	LEU	C-N	-6.14	1.25	1.33
1	B	129	SER	C-N	-5.58	1.26	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	VAL	O-C-N	7.34	129.00	121.87

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3184	0	3261	176	0
2	A	28	0	25	2	0
2	C	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	39	0	34	2	0
4	B	13	11	11	0	0
All	All	3292	11	3356	180	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 27.

All (180) 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:87:ALA:HB3	1:B:181:PRO:HB2	1.65	0.79
1:B:42:TRP:HB3	1:B:44:ILE:HD11	1.66	0.77
3:D:1:NAG:O3	3:D:2:NAG:H2	1.86	0.76
1:B:47:PRO:HG2	1:B:205:LEU:H	1.51	0.76
1:B:301:SER:OG	1:B:305:ARG:NH1	2.20	0.75
1:B:270:MET:HE3	1:B:270:MET:HA	1.69	0.75
1:B:98:ALA:HA	1:B:101:VAL:HG23	1.70	0.73
1:B:465:ASN:O	1:B:468:ARG:NH1	2.22	0.72
1:B:276:PHE:CE1	1:B:297:ALA:HB1	2.25	0.71
1:B:382:LEU:O	1:B:385:THR:HG22	1.91	0.71
1:B:272:GLU:O	1:B:275:VAL:HG12	1.91	0.71
1:B:72:GLU:HG3	1:B:73:PRO:HD2	1.73	0.70
1:B:41:LYS:HG2	1:B:211:GLU:HG3	1.73	0.70
1:B:72:GLU:CG	1:B:73:PRO:HD2	2.20	0.70
1:B:70:ASP:OD1	1:B:207:THR:HB	1.91	0.70
1:B:82:TRP:CE2	1:B:121:SER:HB3	2.27	0.70
1:B:389:LEU:HD22	1:B:394:ASN:HB3	1.74	0.69
1:B:350:LEU:HD11	1:B:360:ALA:HA	1.74	0.69
1:B:70:ASP:HA	1:B:130:GLU:OE2	1.92	0.69
1:B:77:SER:HA	1:B:126:GLN:O	1.91	0.69
1:B:82:TRP:NE1	1:B:121:SER:HB3	2.07	0.69
1:B:132:PHE:HE2	1:B:135:GLN:HG2	1.58	0.69
1:B:97:LYS:HB2	1:B:100:GLU:OE2	1.93	0.69
1:B:237:TYR:HB3	1:B:270:MET:SD	2.33	0.68
1:B:78:LEU:HD21	1:B:206:PHE:HE2	1.58	0.68
1:B:46:ILE:CG1	1:B:47:PRO:HD3	2.24	0.68
1:B:72:GLU:CD	1:B:73:PRO:HD2	2.19	0.68
1:B:46:ILE:CD1	1:B:206:PHE:HB2	2.24	0.68
1:B:435:TRP:O	1:B:438:LEU:HD13	1.94	0.67
1:B:46:ILE:HD11	1:B:206:PHE:HB2	1.77	0.67
1:B:280:PHE:O	1:B:283:ILE:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ALA:O	1:B:416:ILE:HG22	1.96	0.66
1:B:458:VAL:O	1:B:461:ARG:HG3	1.94	0.66
1:B:76:LEU:O	1:B:127:ASN:HA	1.96	0.65
1:B:46:ILE:HG13	1:B:47:PRO:HD3	1.78	0.65
1:B:254:ASP:C	1:B:255:LEU:HD12	2.21	0.65
1:B:425:LYS:NZ	1:B:434:ASP:OD2	2.28	0.65
1:B:358:ASP:O	1:B:362:LEU:HD13	1.97	0.65
1:B:125:PHE:HD2	1:B:129:SER:HB2	1.62	0.65
1:B:416:ILE:O	1:B:419:ILE:HG22	1.98	0.63
1:B:124:LEU:HD11	2:A:1:NAG:O7	1.98	0.63
1:B:131:LEU:O	1:B:131:LEU:HG	1.98	0.63
1:B:251:TYR:CE2	1:B:463:SER:HA	2.34	0.62
1:B:87:ALA:CB	1:B:181:PRO:HB2	2.28	0.62
1:B:42:TRP:HB3	1:B:44:ILE:CD1	2.29	0.62
1:B:233:MET:HA	1:B:236:VAL:HG12	1.79	0.62
1:B:417:VAL:O	1:B:420:ILE:HG22	1.99	0.62
1:B:340:TYR:HD1	1:B:370:LEU:HD23	1.64	0.62
1:B:221:LEU:HD23	1:B:222:GLU:N	2.15	0.61
1:B:63:THR:H	1:B:176:THR:HB	1.66	0.60
1:B:234:CYS:SG	1:B:273:LYS:HB3	2.42	0.60
1:B:311:LEU:O	1:B:314:ILE:HG22	2.01	0.60
1:B:226:LEU:HD23	1:B:280:PHE:HZ	1.65	0.60
1:B:328:VAL:HG23	1:B:328:VAL:O	2.01	0.60
1:B:235:ILE:O	1:B:239:LEU:HD23	2.02	0.59
1:B:387:LYS:O	1:B:391:LEU:HD23	2.03	0.59
1:B:72:GLU:HG3	1:B:73:PRO:CD	2.32	0.59
1:B:435:TRP:HA	1:B:438:LEU:HD11	1.83	0.59
1:B:295:ILE:HD12	1:B:349:VAL:HG23	1.84	0.59
1:B:261:TRP:HB2	1:B:311:LEU:HD11	1.83	0.59
1:B:276:PHE:HE1	1:B:297:ALA:HB1	1.66	0.58
1:B:324:PRO:HG2	1:B:326:LEU:CD2	2.33	0.58
1:B:261:TRP:CB	1:B:311:LEU:HD11	2.34	0.58
1:B:77:SER:OG	1:B:191:SER:HB3	2.04	0.58
1:B:132:PHE:CE2	1:B:135:GLN:HG2	2.38	0.58
1:B:304:LYS:HD3	1:B:449:PHE:CE2	2.38	0.58
1:B:230:PHE:CD2	1:B:276:PHE:HB3	2.39	0.58
1:B:266:ILE:HD11	1:B:457:MET:HE1	1.86	0.58
1:B:368:ALA:O	1:B:372:THR:HG23	2.04	0.57
1:B:176:THR:HG23	1:B:182:TYR:CE2	2.39	0.57
1:B:313:ILE:HD13	1:B:378:ILE:HG12	1.85	0.57
1:B:91:ASN:OD1	1:B:92:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:PHE:CE1	1:B:184:PHE:HB3	2.39	0.57
1:B:435:TRP:HA	1:B:438:LEU:CD1	2.35	0.57
1:B:273:LYS:NZ	1:B:446:ARG:HD3	2.20	0.56
1:B:176:THR:HG23	1:B:182:TYR:HE2	1.71	0.56
1:B:209:THR:HG22	1:B:211:GLU:OE1	2.06	0.56
1:B:46:ILE:HG13	1:B:47:PRO:CD	2.36	0.56
1:B:374:LEU:O	1:B:378:ILE:HG13	2.06	0.55
1:B:273:LYS:HZ1	1:B:446:ARG:HD3	1.72	0.55
1:B:270:MET:HE3	1:B:270:MET:CA	2.36	0.55
1:B:56:GLY:CA	1:B:183:ILE:HD13	2.37	0.55
1:B:91:ASN:ND2	1:B:431:CYS:HB3	2.22	0.54
1:B:226:LEU:HD23	1:B:280:PHE:CZ	2.42	0.54
1:B:233:MET:O	1:B:236:VAL:HG12	2.06	0.54
1:B:76:LEU:HD12	1:B:78:LEU:HD12	1.90	0.54
1:B:465:ASN:ND2	1:B:468:ARG:HD3	2.23	0.54
1:B:465:ASN:OD1	1:B:467:GLN:NE2	2.41	0.54
1:B:316:SER:HB3	1:B:382:LEU:HD21	1.90	0.53
1:B:406:ASN:O	1:B:409:ILE:HG22	2.08	0.53
1:B:419:ILE:O	1:B:423:THR:HG23	2.07	0.53
1:B:77:SER:C	1:B:78:LEU:HD12	2.34	0.52
1:B:319:TYR:CE1	1:B:325:ARG:HA	2.45	0.52
1:B:270:MET:HA	1:B:270:MET:CE	2.36	0.51
1:B:222:GLU:O	1:B:222:GLU:HG2	2.11	0.50
1:B:105:LEU:HD11	1:B:185:ILE:HG21	1.93	0.50
1:B:257:ARG:HE	1:B:325:ARG:HH12	1.58	0.50
1:B:324:PRO:HG2	1:B:326:LEU:HD21	1.94	0.50
1:B:97:LYS:HA	1:B:97:LYS:HE2	1.94	0.50
2:C:1:NAG:O3	2:C:2:NAG:O5	2.26	0.49
1:B:96:PHE:O	1:B:97:LYS:HE2	2.12	0.49
1:B:78:LEU:HD21	1:B:206:PHE:CE2	2.44	0.49
1:B:105:LEU:HD11	1:B:185:ILE:HD13	1.94	0.49
1:B:131:LEU:H	1:B:131:LEU:HD23	1.77	0.49
1:B:47:PRO:HG2	1:B:205:LEU:N	2.24	0.49
1:B:365:ILE:N	1:B:366:PRO:HD2	2.28	0.48
1:B:179:ASP:N	1:B:179:ASP:OD1	2.45	0.48
1:B:305:ARG:O	1:B:309:ARG:HG2	2.14	0.48
2:A:1:NAG:H82	2:A:1:NAG:O3	2.13	0.48
1:B:217:GLU:N	1:B:217:GLU:OE2	2.46	0.48
1:B:307:LEU:HA	1:B:310:THR:HG22	1.96	0.48
1:B:330:LEU:HB2	1:B:334:VAL:HB	1.95	0.48
1:B:97:LYS:HB2	1:B:100:GLU:CD	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLY:HA3	1:B:183:ILE:HD13	1.96	0.47
1:B:312:VAL:O	1:B:315:VAL:HG12	2.13	0.47
1:B:50:LYS:HA	1:B:50:LYS:HE2	1.97	0.47
1:B:92:GLU:HA	1:B:95:ASN:OD1	2.15	0.47
1:B:471:PHE:HE2	1:B:473:PRO:HB3	1.79	0.47
1:B:316:SER:CB	1:B:382:LEU:HD21	2.44	0.47
1:B:59:LEU:HD23	1:B:220:THR:OG1	2.14	0.46
1:B:190:ILE:O	1:B:190:ILE:HG13	2.15	0.46
1:B:279:GLU:HG2	1:B:290:VAL:CG2	2.45	0.46
1:B:100:GLU:N	1:B:100:GLU:OE1	2.45	0.46
1:B:309:ARG:O	1:B:313:ILE:HG12	2.16	0.46
1:B:86:SER:HA	1:B:182:TYR:CD1	2.50	0.46
1:B:43:HIS:C	1:B:44:ILE:HD12	2.42	0.45
1:B:279:GLU:HG2	1:B:290:VAL:HG23	1.99	0.45
1:B:57:LYS:HG2	1:B:58:ILE:H	1.81	0.45
1:B:438:LEU:HD12	1:B:438:LEU:N	2.32	0.45
1:B:86:SER:HA	1:B:182:TYR:HD1	1.81	0.45
1:B:465:ASN:HB3	1:B:468:ARG:NH1	2.32	0.45
1:B:45:PRO:HB3	1:B:204:ASN:HD21	1.82	0.44
1:B:66:PHE:C	1:B:67:LEU:HD12	2.42	0.44
1:B:262:ILE:O	1:B:266:ILE:HG12	2.17	0.44
1:B:294:LEU:HB3	1:B:352:VAL:HG11	1.99	0.44
1:B:319:TYR:CZ	1:B:325:ARG:HB3	2.53	0.44
1:B:349:VAL:HG13	1:B:350:LEU:N	2.32	0.44
1:B:424:MET:O	1:B:424:MET:HG3	2.18	0.44
1:B:471:PHE:HD2	1:B:473:PRO:HD3	1.81	0.44
1:B:46:ILE:HG12	1:B:47:PRO:HD3	1.99	0.44
1:B:238:VAL:O	1:B:242:VAL:HG23	2.16	0.44
1:B:52:TYR:CE1	1:B:187:HIS:HB2	2.52	0.44
1:B:357:THR:O	1:B:357:THR:HG22	2.18	0.44
1:B:61:ARG:HD2	1:B:62:ASN:N	2.33	0.44
1:B:110:GLU:O	1:B:111:LYS:HB2	2.17	0.44
1:B:257:ARG:HH21	1:B:325:ARG:NH1	2.16	0.44
1:B:411:ALA:HB2	1:B:452:ILE:CD1	2.48	0.43
1:B:58:ILE:HG12	1:B:221:LEU:HD22	2.00	0.43
3:D:2:NAG:O4	3:D:2:NAG:O6	2.34	0.43
1:B:46:ILE:N	1:B:47:PRO:CD	2.82	0.43
1:B:58:ILE:CD1	1:B:221:LEU:HD22	2.49	0.43
1:B:82:TRP:CZ3	1:B:174:LEU:HD12	2.54	0.43
1:B:252:TRP:CE2	1:B:253:ARG:HD2	2.54	0.43
1:B:254:ASP:O	1:B:255:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLN:NE2	1:B:462:PRO:HD3	2.34	0.43
1:B:276:PHE:HE1	1:B:297:ALA:CB	2.31	0.42
1:B:358:ASP:O	1:B:358:ASP:OD1	2.36	0.42
1:B:319:TYR:OH	1:B:325:ARG:HB3	2.19	0.42
1:B:176:THR:CG2	1:B:182:TYR:HE2	2.33	0.42
1:B:339:LEU:HD12	1:B:339:LEU:C	2.44	0.42
1:B:76:LEU:HD12	1:B:78:LEU:CD1	2.47	0.42
1:B:233:MET:CA	1:B:236:VAL:HG12	2.48	0.42
1:B:400:LEU:HD13	1:B:469:PHE:CE1	2.54	0.42
1:B:424:MET:O	1:B:428:ILE:HG21	2.19	0.42
1:B:41:LYS:HG2	1:B:211:GLU:CG	2.47	0.42
1:B:98:ALA:HA	1:B:101:VAL:CG2	2.47	0.42
1:B:224:TYR:N	1:B:225:PRO:HD2	2.34	0.42
1:B:472:SER:O	1:B:472:SER:OG	2.32	0.41
1:B:233:MET:HA	1:B:236:VAL:CG1	2.48	0.41
1:B:397:LYS:HE2	1:B:468:ARG:O	2.20	0.41
1:B:411:ALA:HB2	1:B:452:ILE:HD12	2.02	0.41
1:B:471:PHE:CE2	1:B:473:PRO:HB3	2.55	0.41
1:B:307:LEU:O	1:B:310:THR:HG22	2.21	0.41
1:B:396:VAL:HG11	1:B:468:ARG:HD2	2.02	0.41
1:B:319:TYR:O	1:B:321:ILE:HD12	2.21	0.41
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.84	0.40
1:B:389:LEU:HD23	1:B:389:LEU:HA	1.90	0.40
1:B:253:ARG:NE	1:B:253:ARG:HA	2.37	0.40
1:B:252:TRP:HA	1:B:255:LEU:HD11	2.03	0.40
1:B:404:PHE:CE1	1:B:456:ILE:HD12	2.57	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	383/864 (44%)	360 (94%)	23 (6%)	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	B	345/752 (46%)	343 (99%)	2 (1%)	78	79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	350	LEU
1	B	352	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	B	406	ASN
1	B	466	ASN

### 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

7 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	A	1	2,1	14,14,15	0.22	0	17,19,21	0.53	0
2	NAG	A	2	2	14,14,15	0.25	0	17,19,21	0.66	1 (5%)
2	NAG	C	1	2,1	14,14,15	0.20	0	17,19,21	0.41	0
2	NAG	C	2	2	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	D	1	3,1	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
3	NAG	D	2	3	14,14,15	0.52	0	17,19,21	0.67	1 (5%)
3	BMA	D	3	3	11,11,12	0.53	0	15,15,17	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	A	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	2.30	115.27	112.19
3	D	1	NAG	C1-O5-C5	2.22	115.16	112.19
2	A	2	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

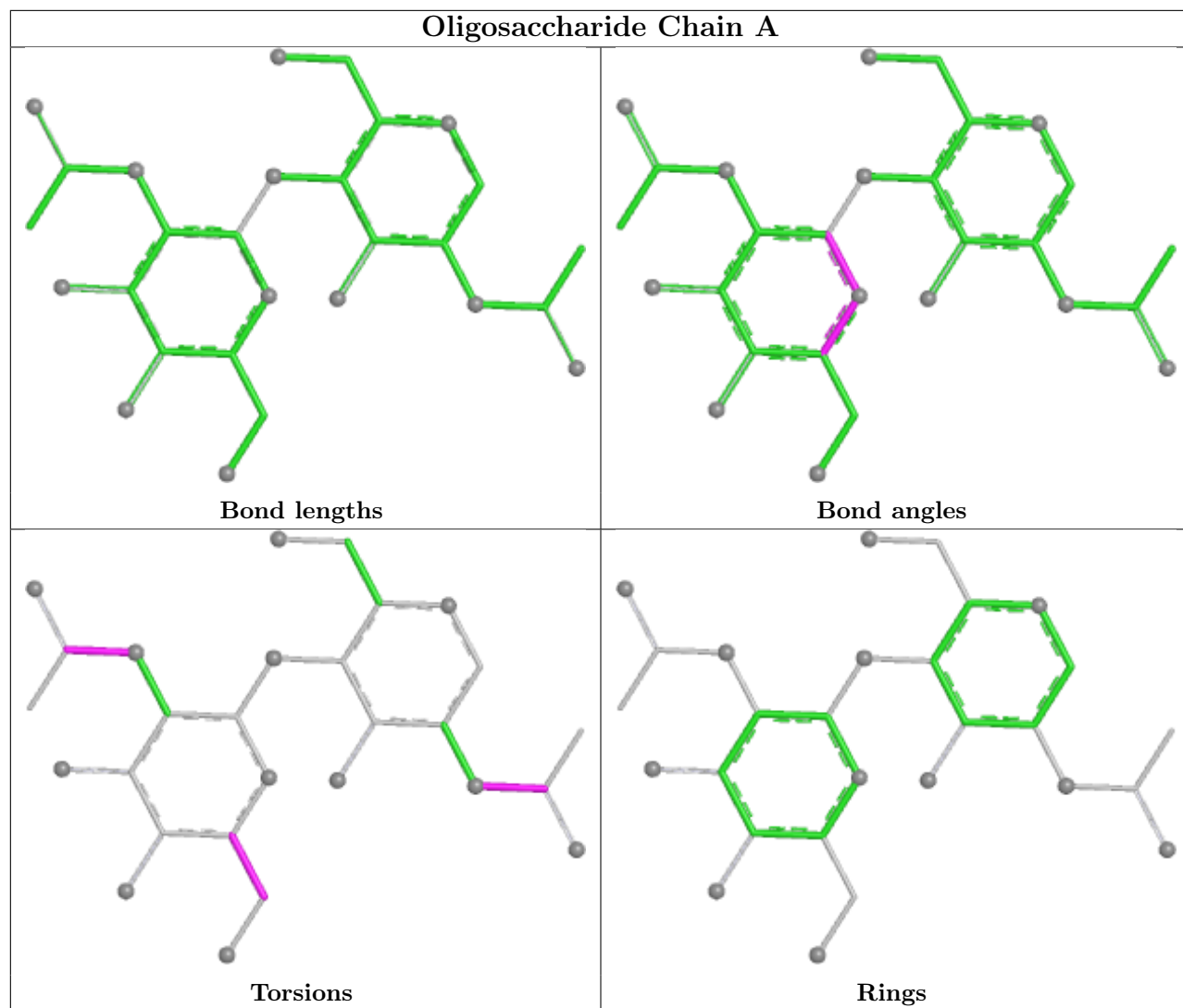
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	A	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
2	A	2	NAG	C8-C7-N2-C2
2	A	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C1-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C3-C2-N2-C7

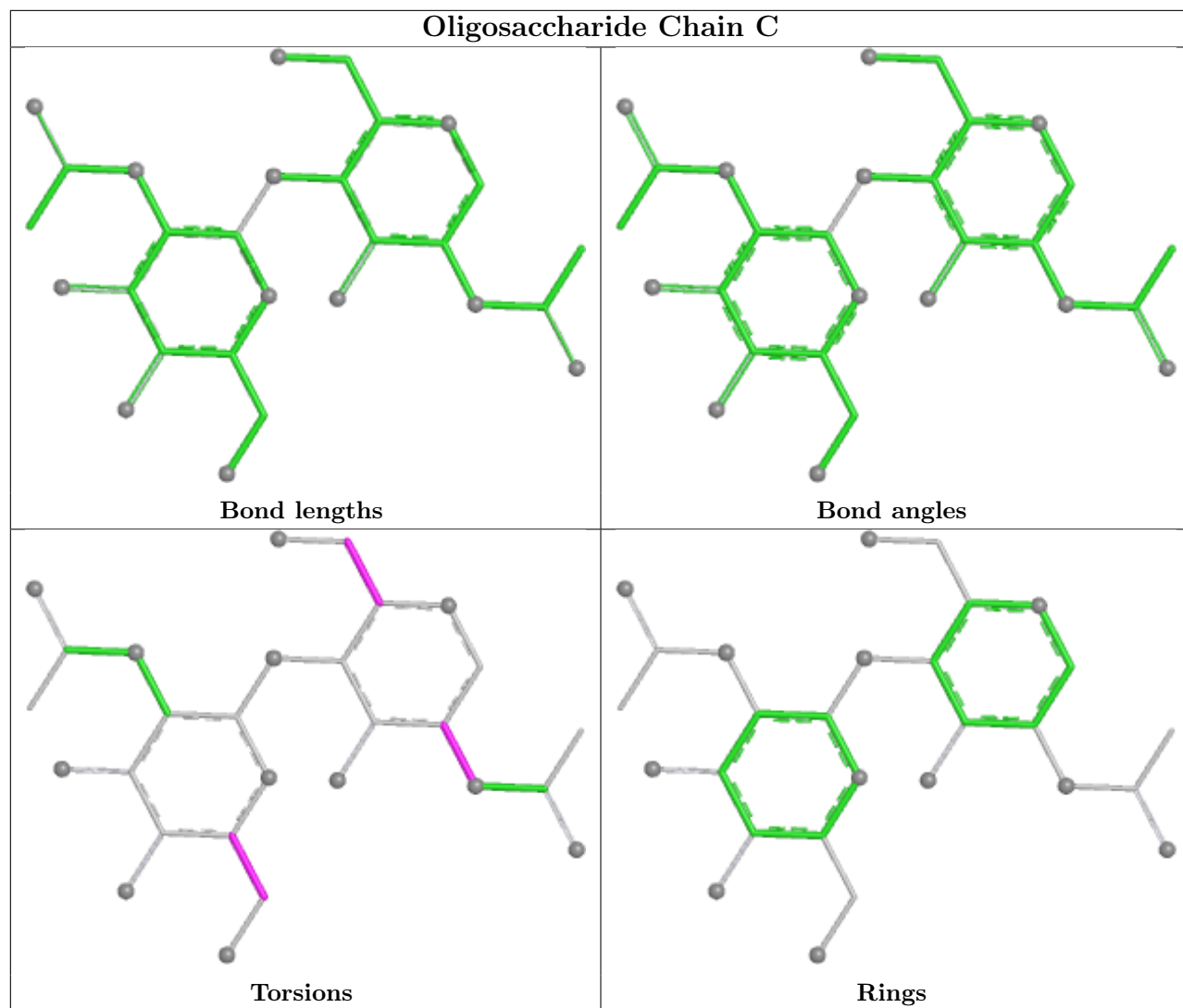
There are no ring outliers.

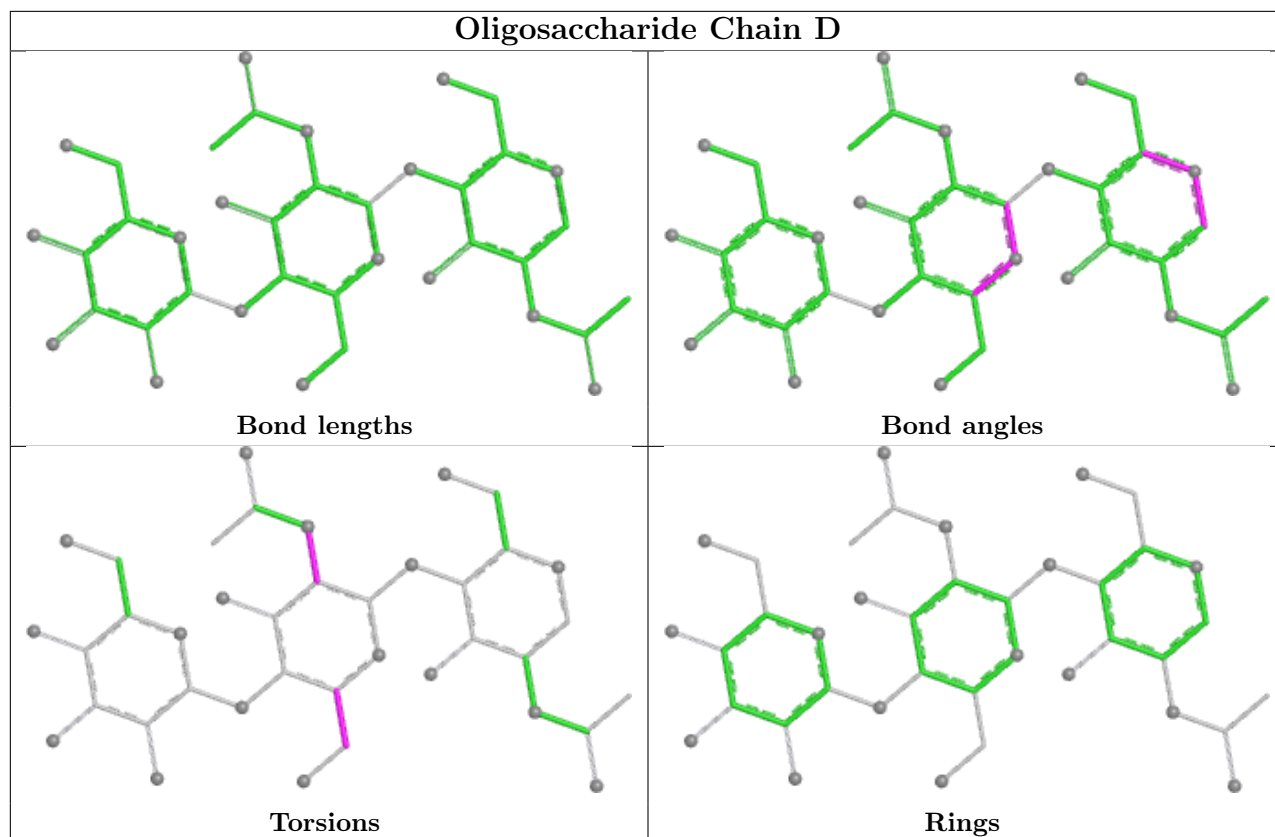
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
2	C	1	NAG	1	0
2	C	2	NAG	1	0
3	D	2	NAG	2	0
2	A	1	NAG	2	0

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







## 5.6 Ligand geometry [i](#)

1 ligand is 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$
4	GCO	B	901	-	12,12,12	0.86	0	15,16,16	2.22	5 (33%)

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
4	GCO	B	901	-	1/1/5/5	8/18/18/18	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	GCO	O5-C5-C6	4.62	119.52	109.03
4	B	901	GCO	O5-C5-C4	4.33	119.38	109.25
4	B	901	GCO	C6-C5-C4	3.65	119.60	112.17
4	B	901	GCO	O1B-C1-C2	2.43	120.08	113.31
4	B	901	GCO	C4-C3-C2	-2.41	109.36	113.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	901	GCO	C5

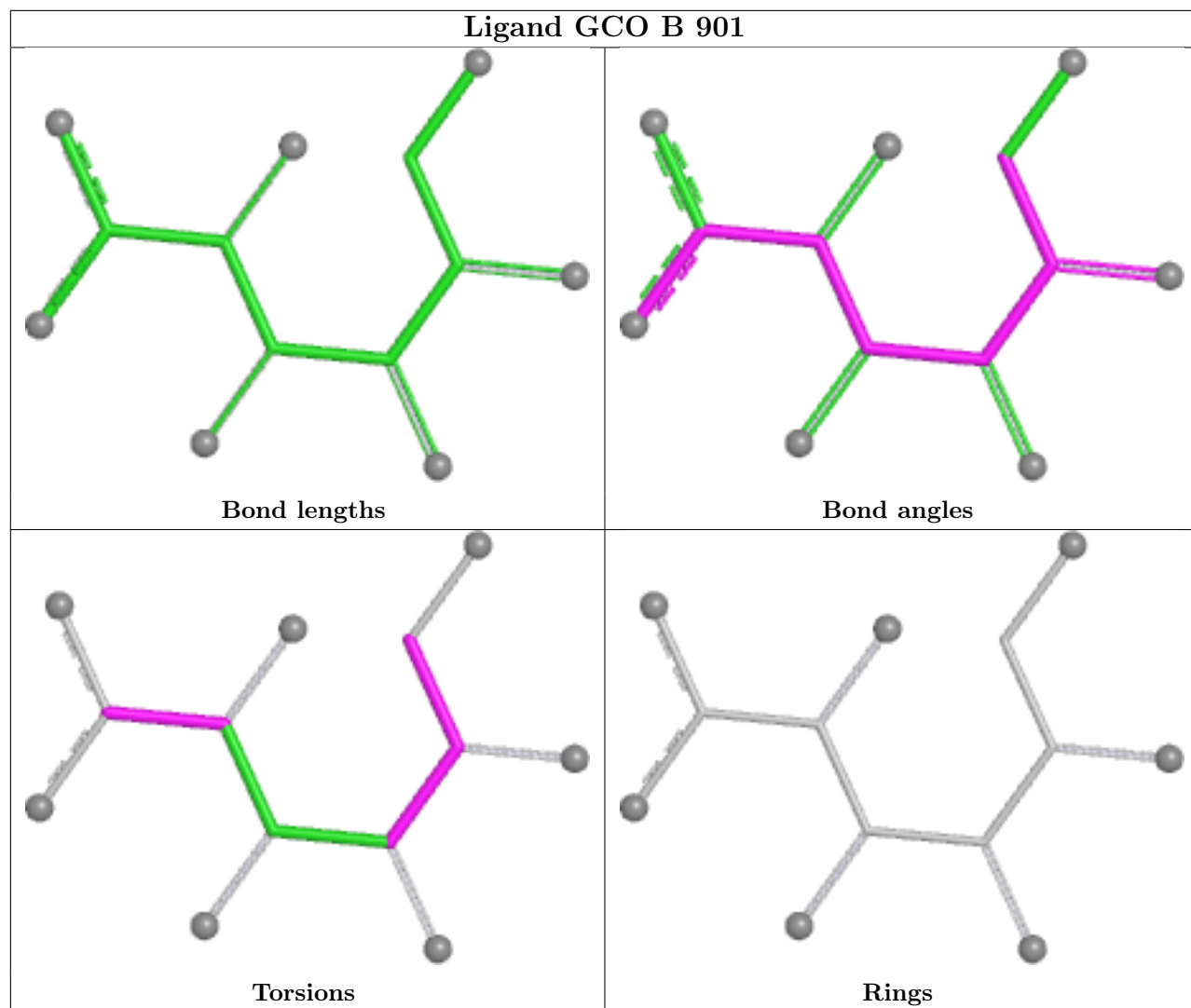
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	GCO	C3-C4-C5-O5
4	B	901	GCO	O4-C4-C5-O5
4	B	901	GCO	O5-C5-C6-O6
4	B	901	GCO	O1A-C1-C2-O2
4	B	901	GCO	O1B-C1-C2-O2
4	B	901	GCO	O4-C4-C5-C6
4	B	901	GCO	C3-C4-C5-C6
4	B	901	GCO	C4-C5-C6-O6

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

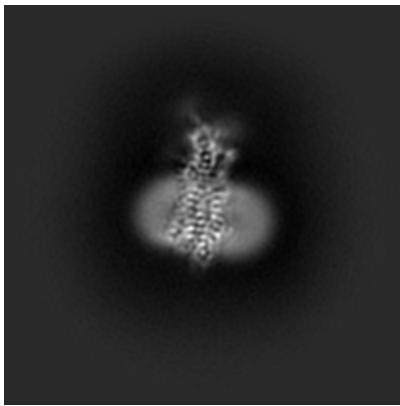
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35017. These allow visual inspection of the internal detail of the map and identification of artifacts.

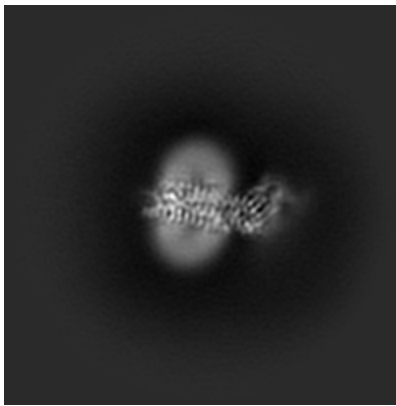
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

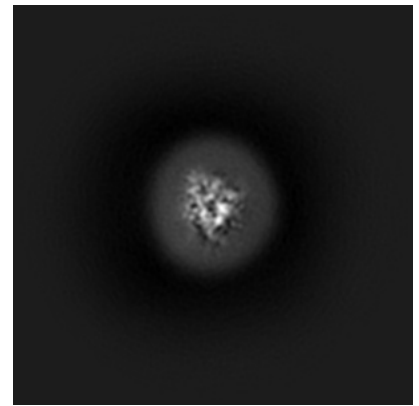
#### 6.1.1 Primary map



X

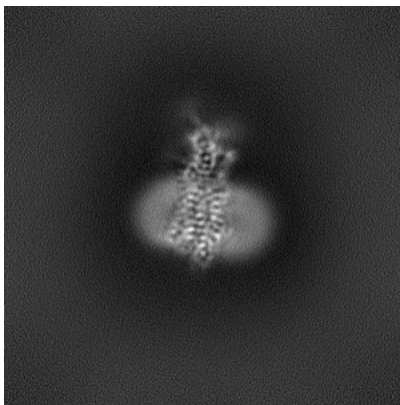


Y

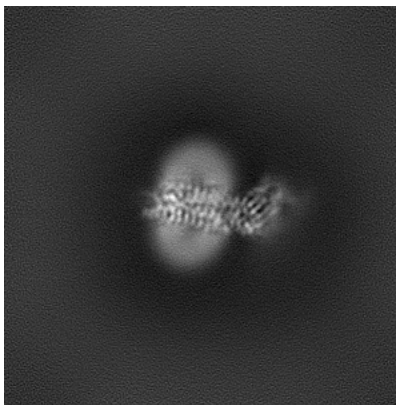


Z

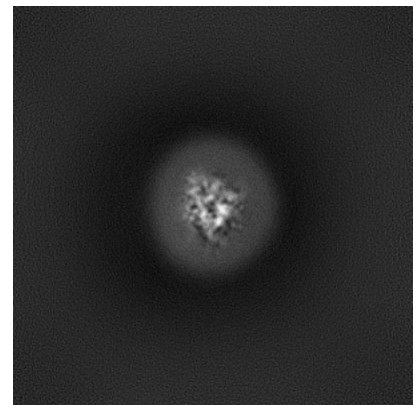
#### 6.1.2 Raw map



X



Y

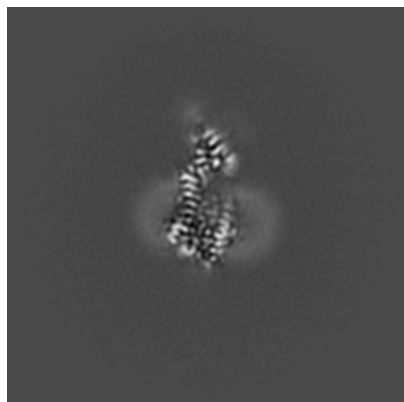


Z

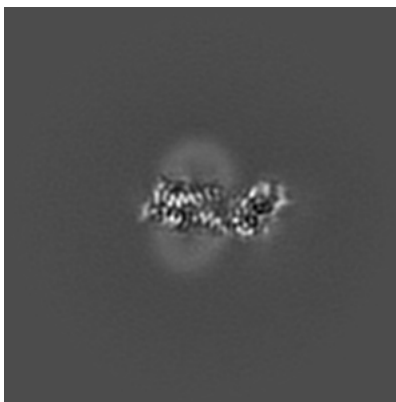
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

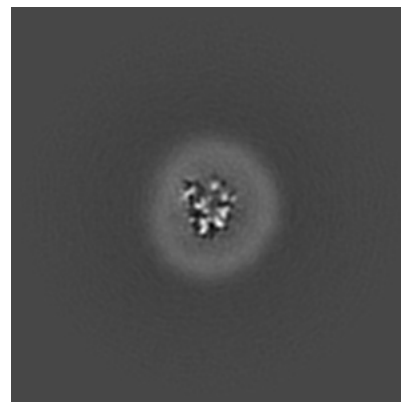
### 6.2.1 Primary map



X Index: 160

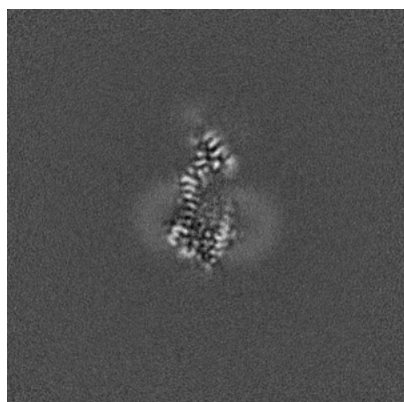


Y Index: 160

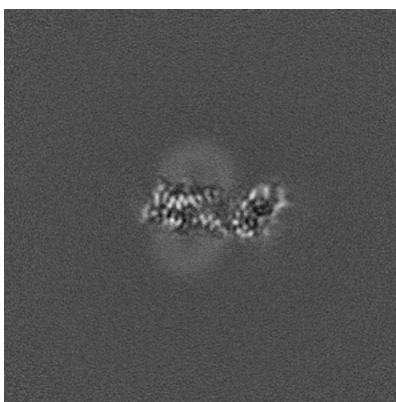


Z Index: 160

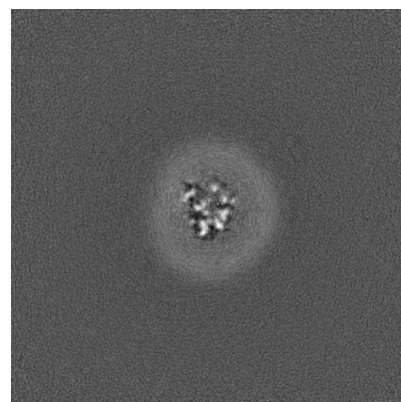
### 6.2.2 Raw map



X Index: 160



Y Index: 160

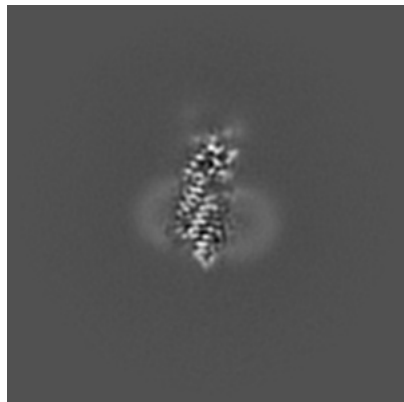


Z Index: 160

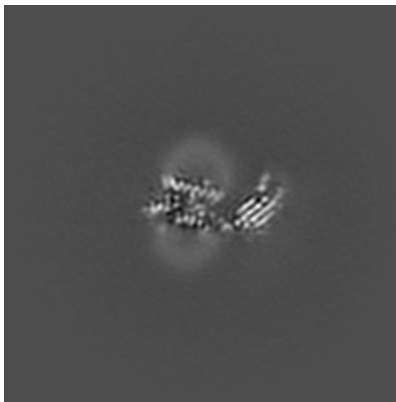
The images above show central slices of the map in three orthogonal directions.

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

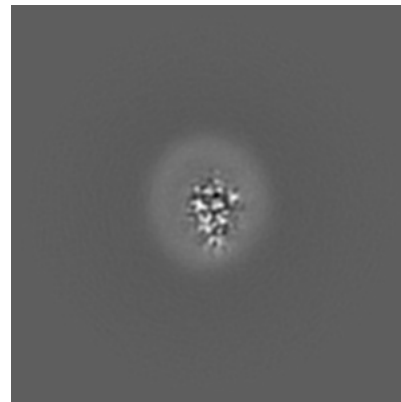
### 6.3.1 Primary map



X Index: 152

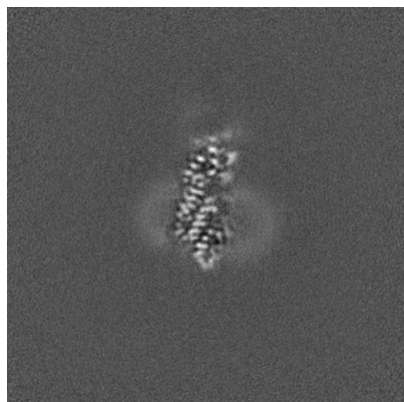


Y Index: 166

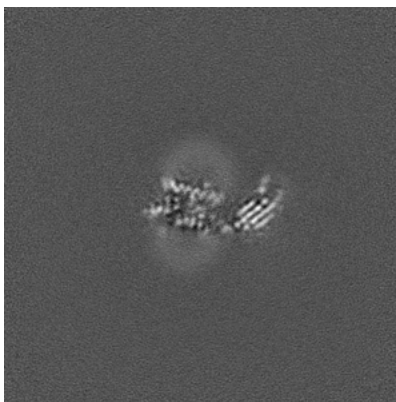


Z Index: 134

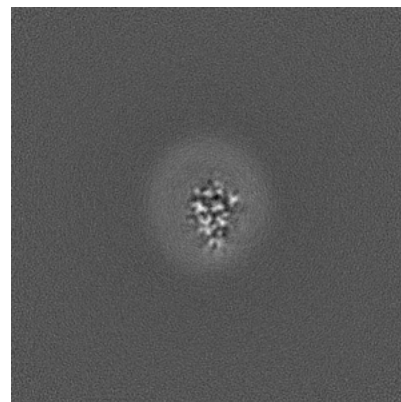
### 6.3.2 Raw map



X Index: 153



Y Index: 166



Z Index: 134

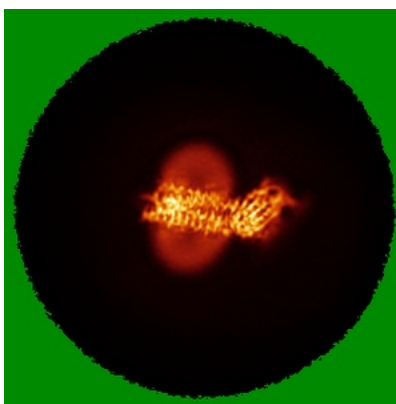
The images above show the largest variance slices of the map in three orthogonal directions.

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

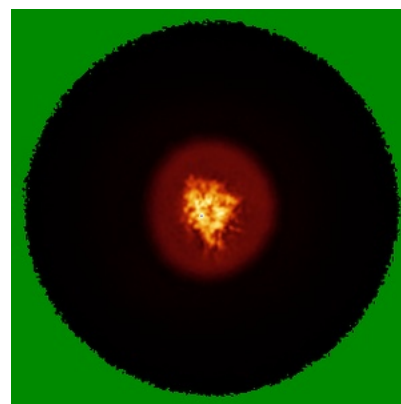
### 6.4.1 Primary map



X

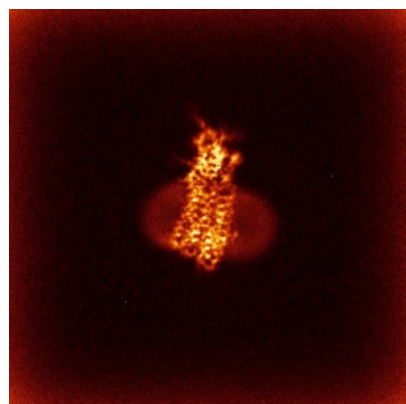


Y

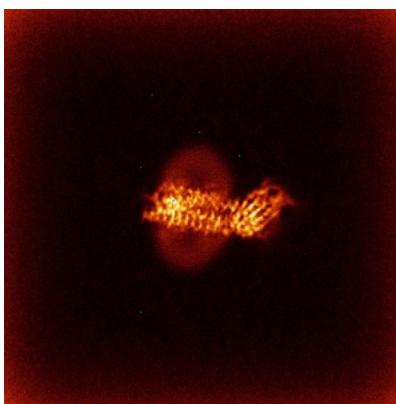


Z

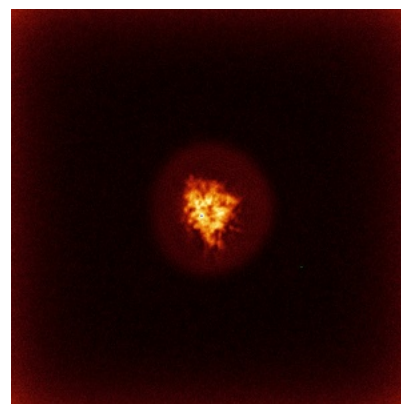
### 6.4.2 Raw map



X



Y

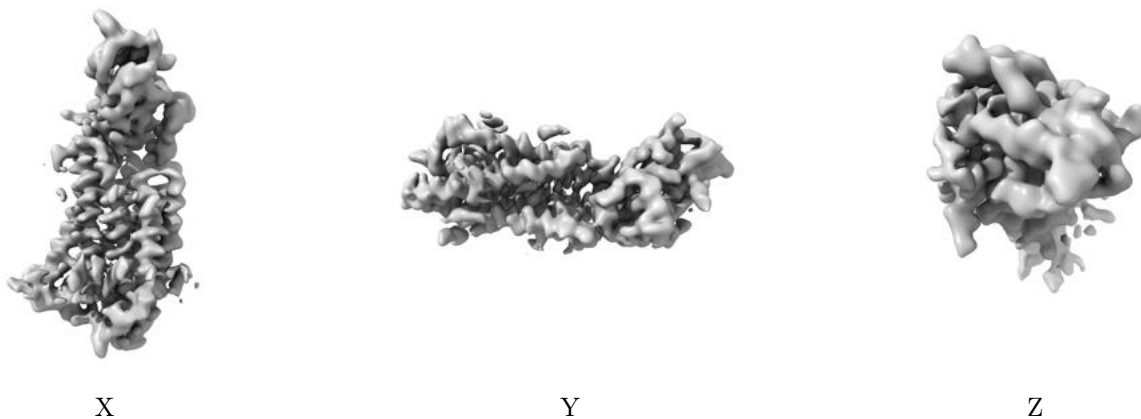


Z

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.

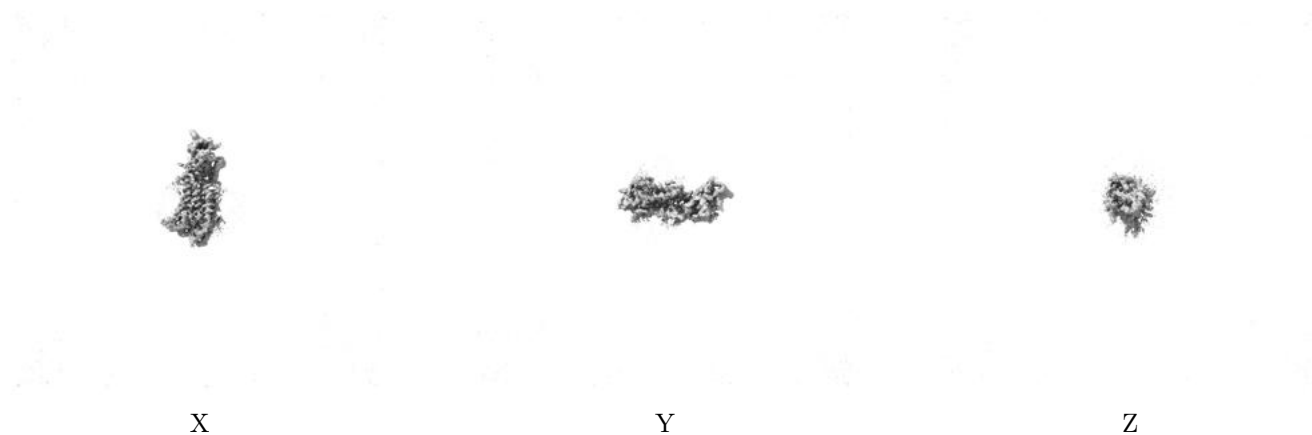
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.101. 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.

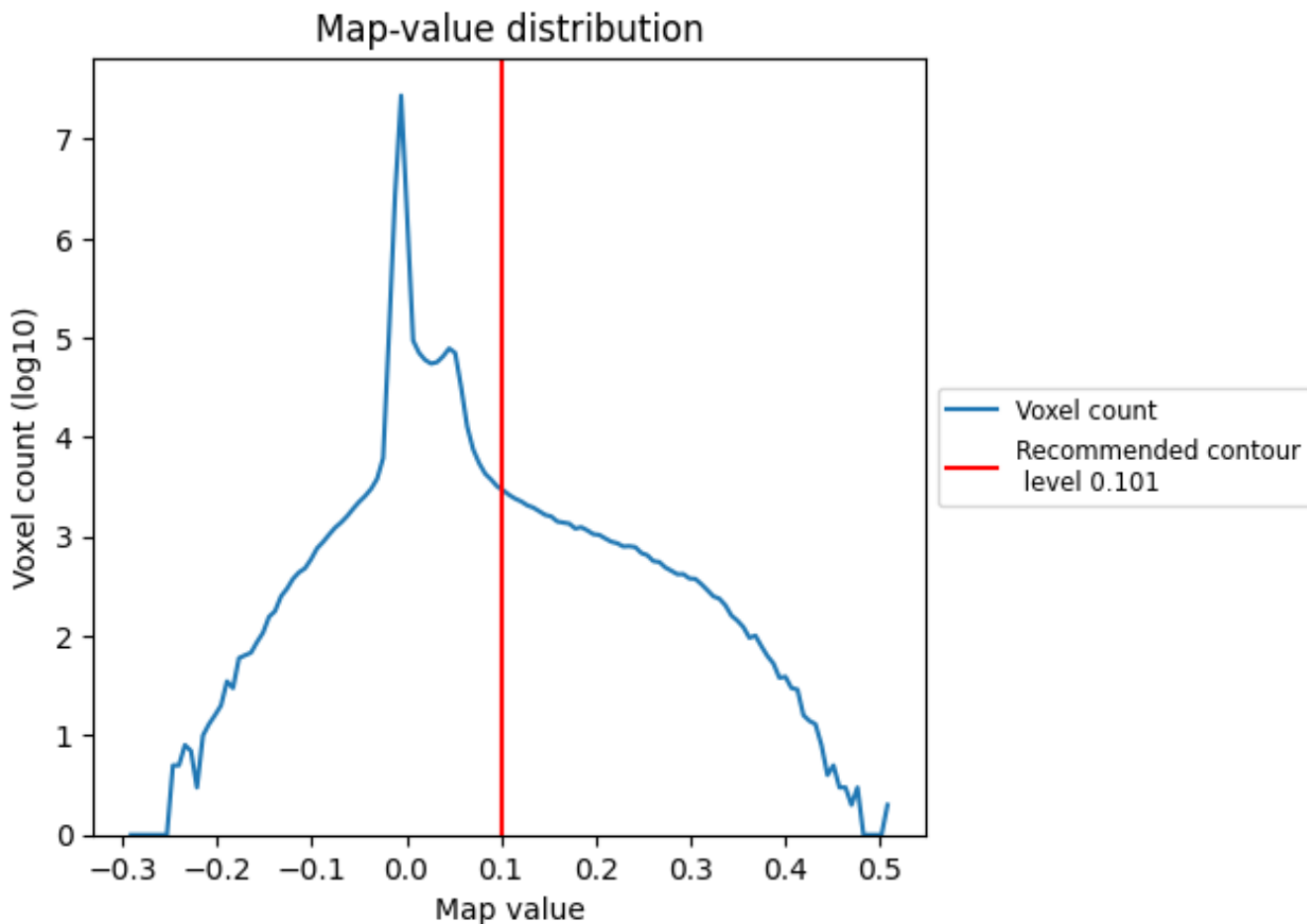
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

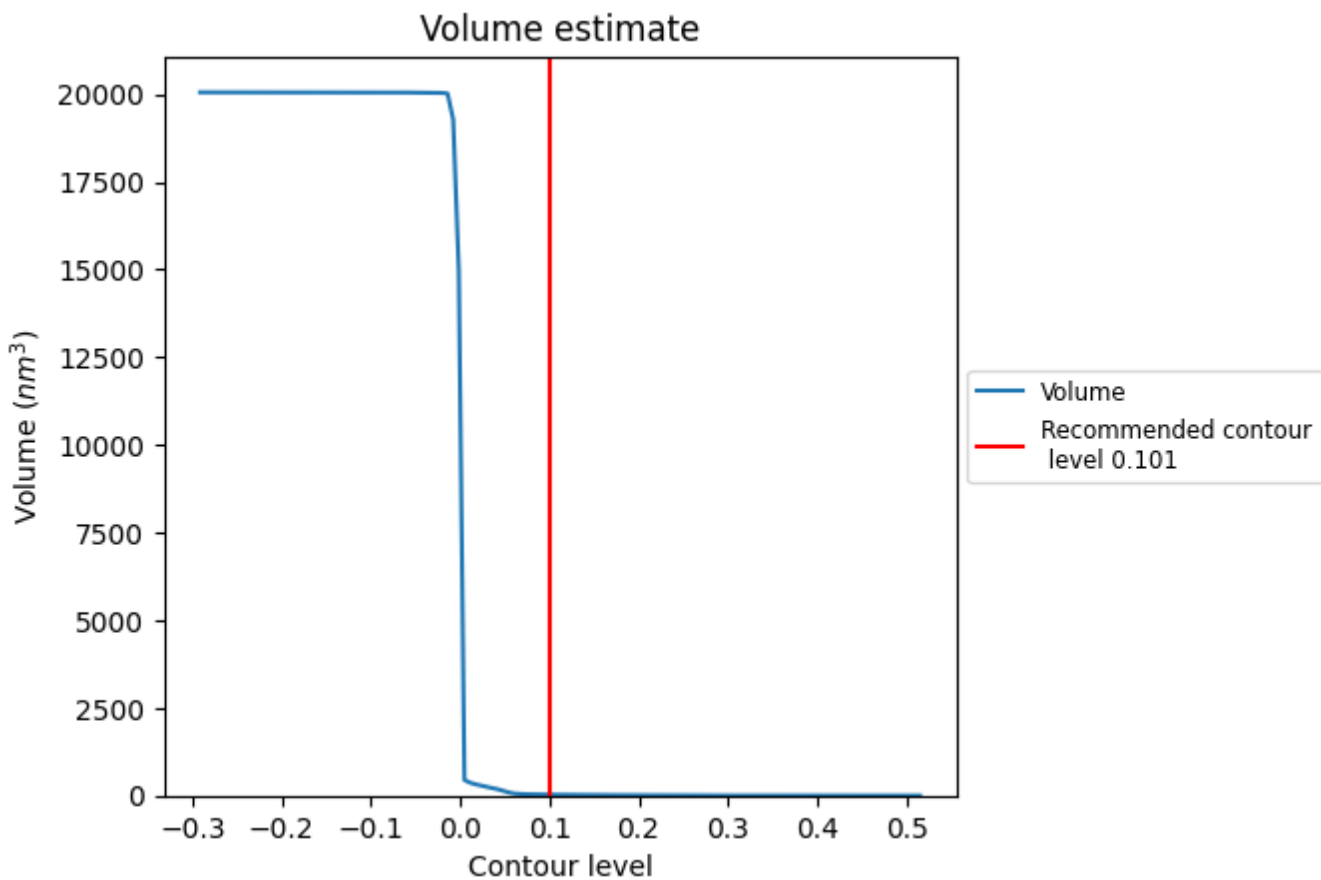
This section contains the results of statistical analysis of the map.

### 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.

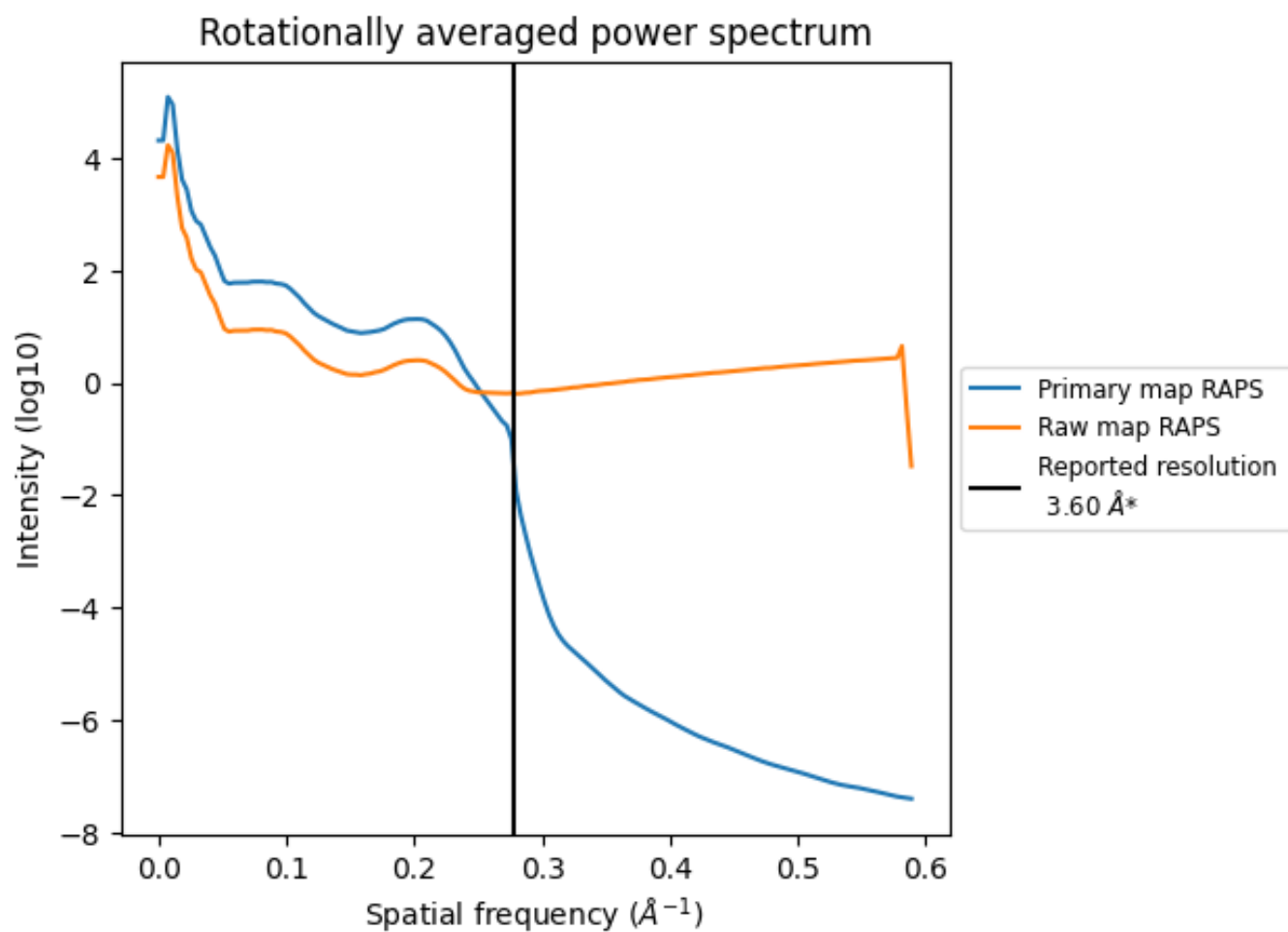
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 26 nm<sup>3</sup>; this corresponds to an approximate mass of 23 kDa.

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

### 7.3 Rotationally averaged power spectrum i

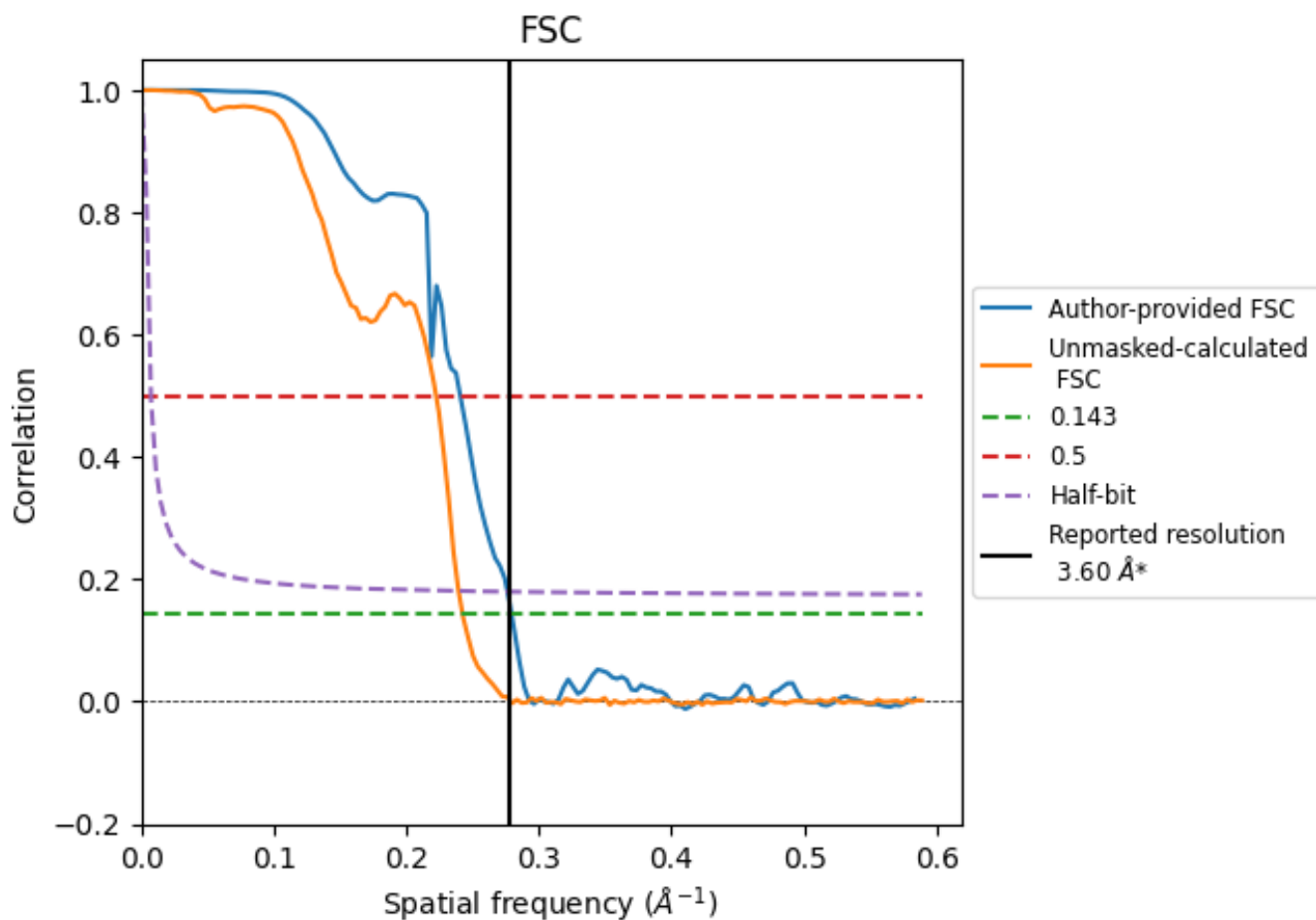


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

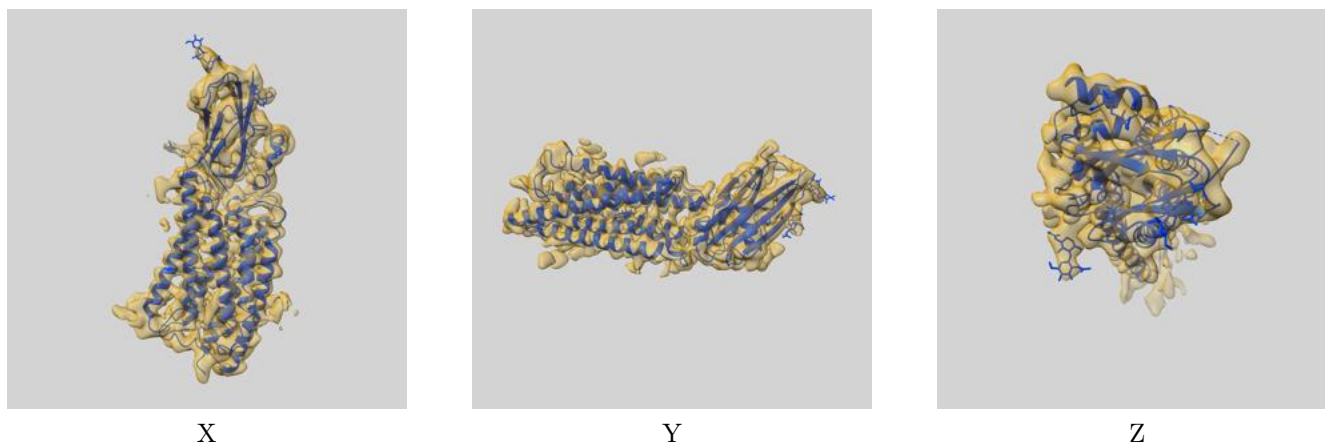
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.16	3.62
Unmasked-calculated*	4.13	4.50	4.18

\*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 4.13 differs from the reported value 3.6 by more than 10 %

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

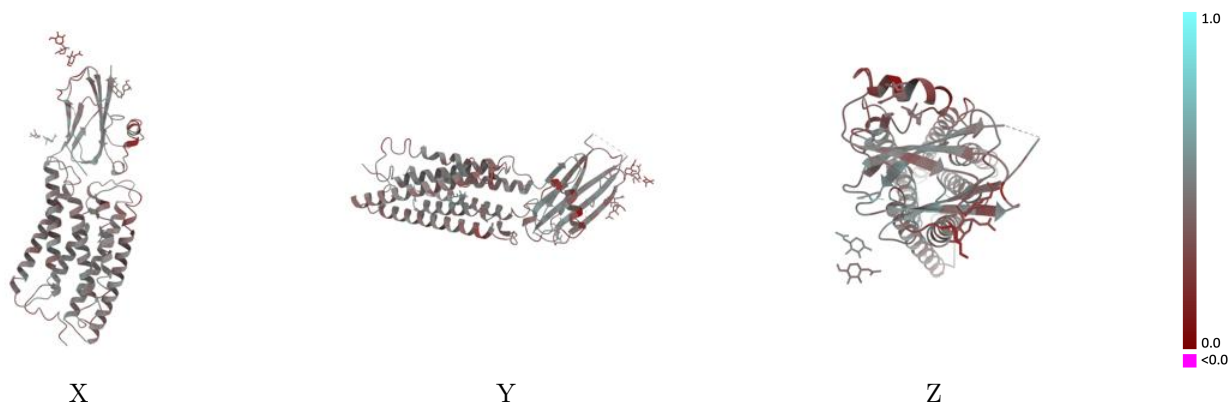
This section contains information regarding the fit between EMDB map EMD-35017 and PDB model 8HTT. Per-residue inclusion information can be found in section 3 on page 8.

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



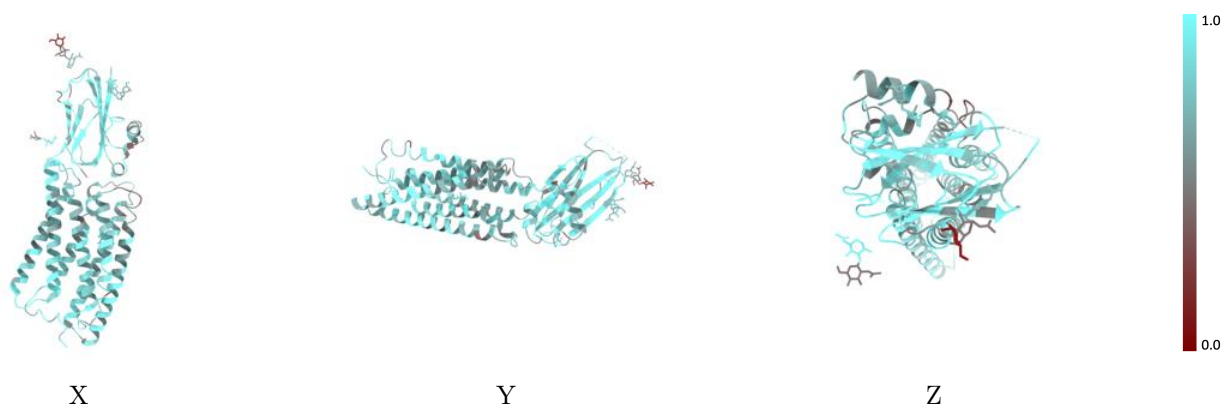
The images above show the 3D surface view of the map at the recommended contour level 0.101 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



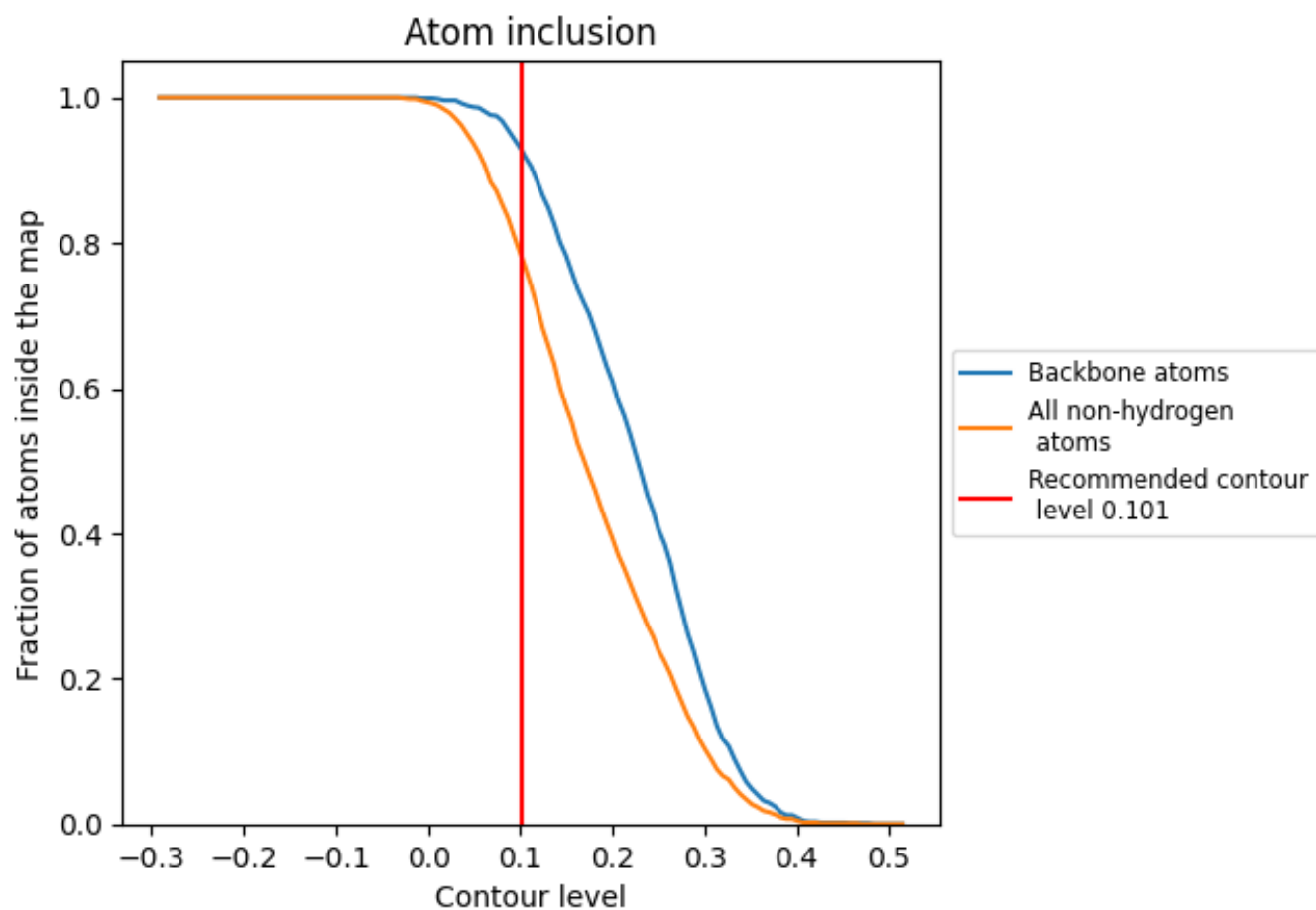
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.101).











## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7830	 0.4270
A	 0.6790	 0.3780
B	 0.7890	 0.4290
C	 0.6790	 0.4650
D	 0.4100	 0.2340

