



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:47 PM UTC

PDB ID : 9QNR / pdb_00009qnr
EMDB ID : EMD-53249
Title : Cryo-EM structure of TTYH3 in GDN after incubation with ApoE, map2
Authors : Sukalskaia, A.; Pugnetti, A.; Dutzler, R.; Plochberger, B.; Weber, F.; Karner, A.
Deposited on : 2025-03-25
Resolution : 2.91 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

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>.

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

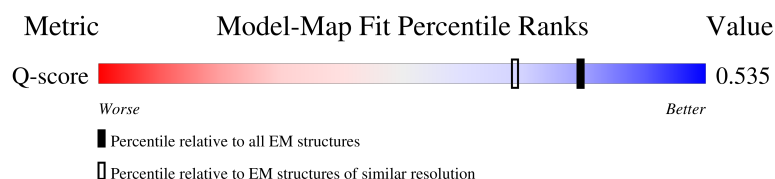
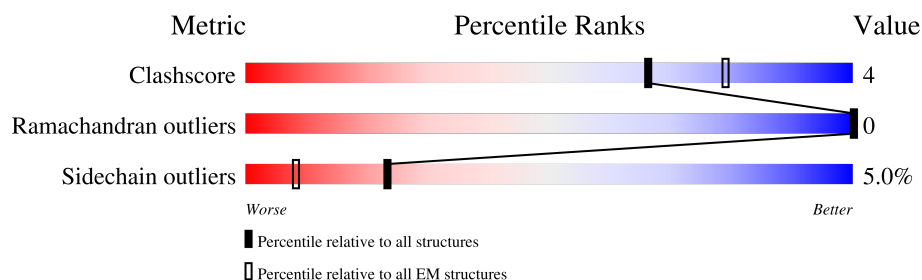
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.91 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	12972 (2.41 - 3.41)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	588	
1	B	588	
2	C	2	
2	D	2	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6222 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 Protein tweety homolog 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	392	Total	C	N	O	S	0	0
			3055	1987	502	553	13		
1	B	392	Total	C	N	O	S	0	0
			3055	1987	502	553	13		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q9C0H2
A	1	SER	-	expression tag	UNP Q9C0H2
A	524	ALA	-	expression tag	UNP Q9C0H2
A	525	LEU	-	expression tag	UNP Q9C0H2
A	526	GLU	-	expression tag	UNP Q9C0H2
A	527	VAL	-	expression tag	UNP Q9C0H2
A	528	LEU	-	expression tag	UNP Q9C0H2
A	529	PHE	-	expression tag	UNP Q9C0H2
A	530	GLN	-	expression tag	UNP Q9C0H2
A	531	GLY	-	expression tag	UNP Q9C0H2
A	532	PRO	-	expression tag	UNP Q9C0H2
A	533	GLN	-	expression tag	UNP Q9C0H2
A	534	GLY	-	expression tag	UNP Q9C0H2
A	535	THR	-	expression tag	UNP Q9C0H2
A	536	GLU	-	expression tag	UNP Q9C0H2
A	537	GLN	-	expression tag	UNP Q9C0H2
A	538	LYS	-	expression tag	UNP Q9C0H2
A	539	LEU	-	expression tag	UNP Q9C0H2
A	540	ILE	-	expression tag	UNP Q9C0H2
A	541	SER	-	expression tag	UNP Q9C0H2
A	542	GLU	-	expression tag	UNP Q9C0H2
A	543	GLU	-	expression tag	UNP Q9C0H2
A	544	ASP	-	expression tag	UNP Q9C0H2
A	545	LEU	-	expression tag	UNP Q9C0H2
A	546	ARG	-	expression tag	UNP Q9C0H2
A	547	GLY	-	expression tag	UNP Q9C0H2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ALA	-	expression tag	UNP Q9C0H2
A	549	SER	-	expression tag	UNP Q9C0H2
A	550	MET	-	expression tag	UNP Q9C0H2
A	551	ASP	-	expression tag	UNP Q9C0H2
A	552	GLU	-	expression tag	UNP Q9C0H2
A	553	LYS	-	expression tag	UNP Q9C0H2
A	554	THR	-	expression tag	UNP Q9C0H2
A	555	THR	-	expression tag	UNP Q9C0H2
A	556	GLY	-	expression tag	UNP Q9C0H2
A	557	TRP	-	expression tag	UNP Q9C0H2
A	558	ARG	-	expression tag	UNP Q9C0H2
A	559	GLY	-	expression tag	UNP Q9C0H2
A	560	GLY	-	expression tag	UNP Q9C0H2
A	561	HIS	-	expression tag	UNP Q9C0H2
A	562	VAL	-	expression tag	UNP Q9C0H2
A	563	VAL	-	expression tag	UNP Q9C0H2
A	564	GLU	-	expression tag	UNP Q9C0H2
A	565	GLY	-	expression tag	UNP Q9C0H2
A	566	LEU	-	expression tag	UNP Q9C0H2
A	567	ALA	-	expression tag	UNP Q9C0H2
A	568	GLY	-	expression tag	UNP Q9C0H2
A	569	GLU	-	expression tag	UNP Q9C0H2
A	570	LEU	-	expression tag	UNP Q9C0H2
A	571	GLU	-	expression tag	UNP Q9C0H2
A	572	GLN	-	expression tag	UNP Q9C0H2
A	573	LEU	-	expression tag	UNP Q9C0H2
A	574	ARG	-	expression tag	UNP Q9C0H2
A	575	ALA	-	expression tag	UNP Q9C0H2
A	576	ARG	-	expression tag	UNP Q9C0H2
A	577	LEU	-	expression tag	UNP Q9C0H2
A	578	GLU	-	expression tag	UNP Q9C0H2
A	579	HIS	-	expression tag	UNP Q9C0H2
A	580	HIS	-	expression tag	UNP Q9C0H2
A	581	PRO	-	expression tag	UNP Q9C0H2
A	582	GLN	-	expression tag	UNP Q9C0H2
A	583	GLY	-	expression tag	UNP Q9C0H2
A	584	GLN	-	expression tag	UNP Q9C0H2
A	585	ARG	-	expression tag	UNP Q9C0H2
A	586	GLU	-	expression tag	UNP Q9C0H2
A	587	PRO	-	expression tag	UNP Q9C0H2
B	0	MET	-	initiating methionine	UNP Q9C0H2
B	1	SER	-	expression tag	UNP Q9C0H2

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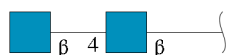
Chain	Residue	Modelled	Actual	Comment	Reference
B	524	ALA	-	expression tag	UNP Q9C0H2
B	525	LEU	-	expression tag	UNP Q9C0H2
B	526	GLU	-	expression tag	UNP Q9C0H2
B	527	VAL	-	expression tag	UNP Q9C0H2
B	528	LEU	-	expression tag	UNP Q9C0H2
B	529	PHE	-	expression tag	UNP Q9C0H2
B	530	GLN	-	expression tag	UNP Q9C0H2
B	531	GLY	-	expression tag	UNP Q9C0H2
B	532	PRO	-	expression tag	UNP Q9C0H2
B	533	GLN	-	expression tag	UNP Q9C0H2
B	534	GLY	-	expression tag	UNP Q9C0H2
B	535	THR	-	expression tag	UNP Q9C0H2
B	536	GLU	-	expression tag	UNP Q9C0H2
B	537	GLN	-	expression tag	UNP Q9C0H2
B	538	LYS	-	expression tag	UNP Q9C0H2
B	539	LEU	-	expression tag	UNP Q9C0H2
B	540	ILE	-	expression tag	UNP Q9C0H2
B	541	SER	-	expression tag	UNP Q9C0H2
B	542	GLU	-	expression tag	UNP Q9C0H2
B	543	GLU	-	expression tag	UNP Q9C0H2
B	544	ASP	-	expression tag	UNP Q9C0H2
B	545	LEU	-	expression tag	UNP Q9C0H2
B	546	ARG	-	expression tag	UNP Q9C0H2
B	547	GLY	-	expression tag	UNP Q9C0H2
B	548	ALA	-	expression tag	UNP Q9C0H2
B	549	SER	-	expression tag	UNP Q9C0H2
B	550	MET	-	expression tag	UNP Q9C0H2
B	551	ASP	-	expression tag	UNP Q9C0H2
B	552	GLU	-	expression tag	UNP Q9C0H2
B	553	LYS	-	expression tag	UNP Q9C0H2
B	554	THR	-	expression tag	UNP Q9C0H2
B	555	THR	-	expression tag	UNP Q9C0H2
B	556	GLY	-	expression tag	UNP Q9C0H2
B	557	TRP	-	expression tag	UNP Q9C0H2
B	558	ARG	-	expression tag	UNP Q9C0H2
B	559	GLY	-	expression tag	UNP Q9C0H2
B	560	GLY	-	expression tag	UNP Q9C0H2
B	561	HIS	-	expression tag	UNP Q9C0H2
B	562	VAL	-	expression tag	UNP Q9C0H2
B	563	VAL	-	expression tag	UNP Q9C0H2
B	564	GLU	-	expression tag	UNP Q9C0H2
B	565	GLY	-	expression tag	UNP Q9C0H2

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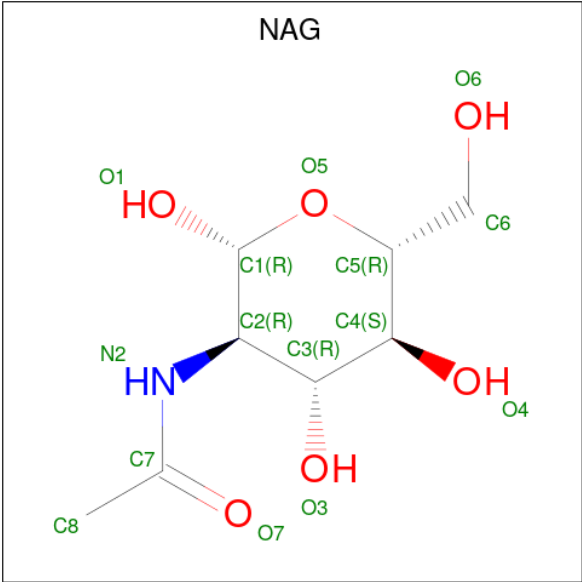
Chain	Residue	Modelled	Actual	Comment	Reference
B	566	LEU	-	expression tag	UNP Q9C0H2
B	567	ALA	-	expression tag	UNP Q9C0H2
B	568	GLY	-	expression tag	UNP Q9C0H2
B	569	GLU	-	expression tag	UNP Q9C0H2
B	570	LEU	-	expression tag	UNP Q9C0H2
B	571	GLU	-	expression tag	UNP Q9C0H2
B	572	GLN	-	expression tag	UNP Q9C0H2
B	573	LEU	-	expression tag	UNP Q9C0H2
B	574	ARG	-	expression tag	UNP Q9C0H2
B	575	ALA	-	expression tag	UNP Q9C0H2
B	576	ARG	-	expression tag	UNP Q9C0H2
B	577	LEU	-	expression tag	UNP Q9C0H2
B	578	GLU	-	expression tag	UNP Q9C0H2
B	579	HIS	-	expression tag	UNP Q9C0H2
B	580	HIS	-	expression tag	UNP Q9C0H2
B	581	PRO	-	expression tag	UNP Q9C0H2
B	582	GLN	-	expression tag	UNP Q9C0H2
B	583	GLY	-	expression tag	UNP Q9C0H2
B	584	GLN	-	expression tag	UNP Q9C0H2
B	585	ARG	-	expression tag	UNP Q9C0H2
B	586	GLU	-	expression tag	UNP Q9C0H2
B	587	PRO	-	expression tag	UNP Q9C0H2

- 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	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

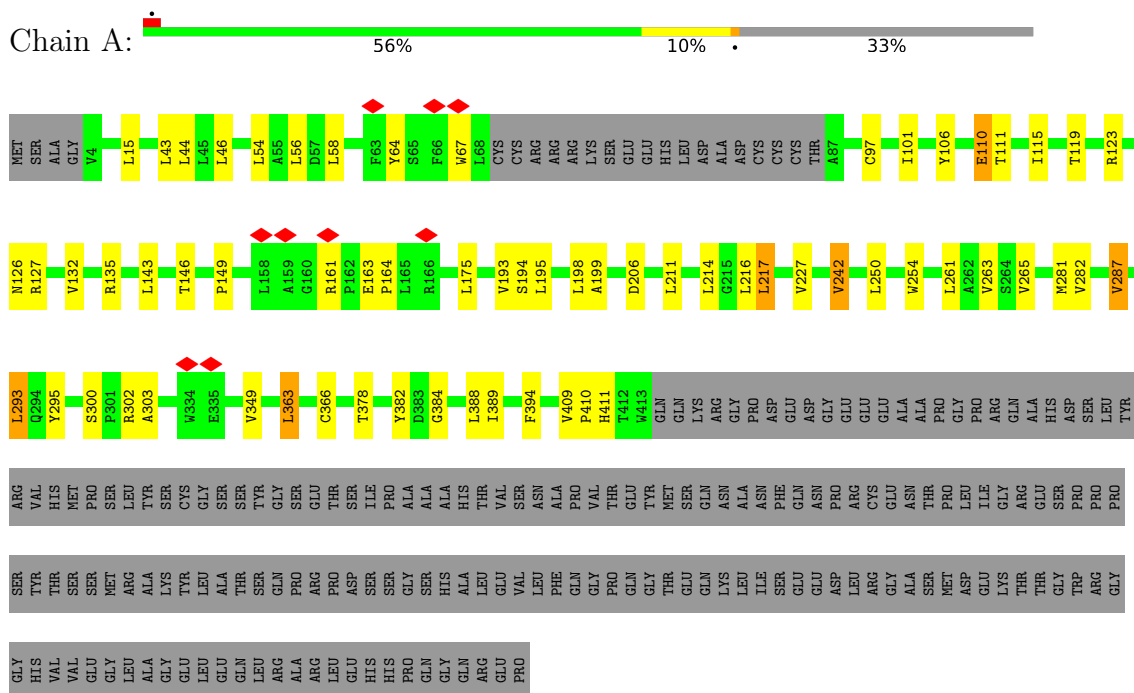


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	A	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0

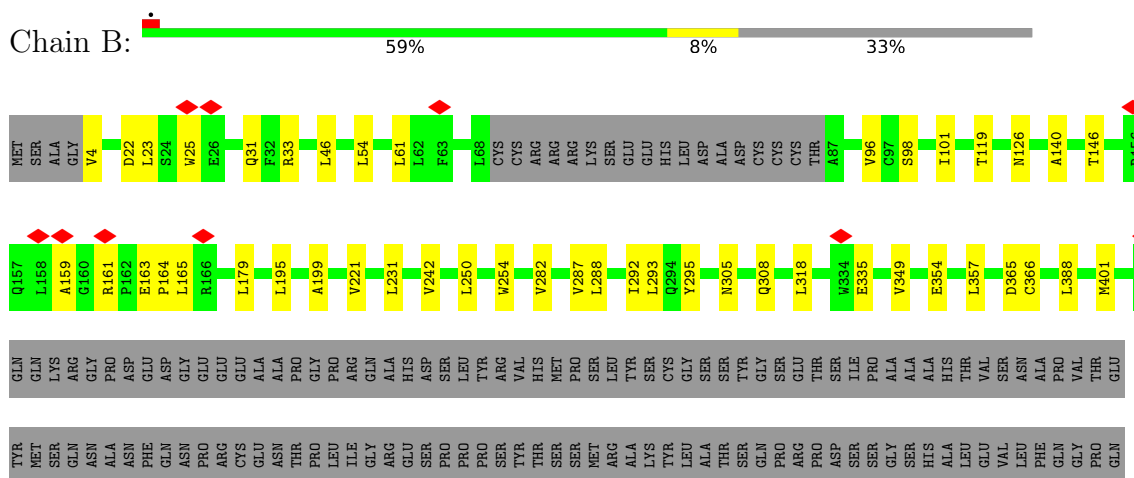
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein tweety homolog 3



• Molecule 1: Protein tweety homolog 3



GLY
THR
GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ARG
GLY
ALA
SER
MET
ASP
GLU
LYS
THR
THR
GLY
TRP
ARG
GLY
GLY
HIS
VAL
VAL
GLU
GLY
LEU
ALA
GLY
GLU
LEU
GLU
GLN
LEU
ARG
ALA
ARG
LEU
GLU
HIS
HIS
PRO
GLN
GLY
GLN
ARG
GLU
PRO

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



AG1
AG2

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



AG1
AG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	547367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.286	Depositor
Minimum map value	-1.940	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	286.44, 286.44, 286.44	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.302, 1.302, 1.302	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

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	0.15	0/3129	0.29	0/4282
1	B	0.16	0/3129	0.30	1/4282 (0.0%)
All	All	0.16	0/6258	0.30	1/8564 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	TRP	CB-CA-C	-5.89	109.77	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3055	0	3054	29	0
1	B	3055	0	3054	20	0
2	C	28	0	25	2	0
2	D	28	0	25	0	0
3	A	28	0	26	0	0
3	B	28	0	26	1	0
All	All	6222	0	6210	49	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 (49) 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:119:THR:HG23	1:A:199:ALA:HB1	1.65	0.78
1:A:15:LEU:HD11	1:A:389:ILE:HD11	1.71	0.73
1:B:119:THR:HG23	1:B:199:ALA:HB1	1.74	0.70
1:A:101:ILE:HG23	1:A:217:LEU:HD12	1.73	0.69
1:B:161:ARG:HH22	1:B:335:GLU:HG2	1.58	0.68
1:B:305:ASN:HB3	1:B:308:GLN:HB2	1.82	0.62
1:A:378:THR:O	1:A:382:TYR:HB2	2.07	0.55
1:A:146:THR:HB	1:A:349:VAL:HG21	1.89	0.54
1:A:300:SER:HB2	1:A:303:ALA:HB2	1.89	0.53
1:A:263:VAL:HG13	1:A:388:LEU:HD13	1.92	0.52
1:B:159:ALA:HA	1:B:165:LEU:HD22	1.91	0.52
1:B:287:VAL:HG12	1:B:288:LEU:HG	1.92	0.52
1:A:126:ASN:HD22	2:C:1:NAG:H83	1.73	0.52
1:A:295:TYR:CZ	1:A:366:CYS:HB3	2.46	0.51
1:A:46:LEU:HD13	1:A:265:VAL:HG21	1.93	0.51
1:A:143:LEU:HA	1:A:146:THR:HG22	1.93	0.50
1:B:140:ALA:HA	1:B:179:LEU:HD21	1.93	0.49
1:A:132:VAL:HG22	1:A:363:LEU:HB3	1.95	0.48
1:B:318:LEU:HD21	1:B:354:GLU:HB2	1.94	0.48
1:B:146:THR:HB	1:B:349:VAL:HG21	1.96	0.48
1:B:126:ASN:HB2	1:B:195:LEU:HB2	1.94	0.48
1:A:227:VAL:HB	1:A:242:VAL:HG21	1.96	0.47
1:A:193:VAL:HG21	1:A:287:VAL:HB	1.96	0.47
1:B:163:GLU:HB2	1:B:164:PRO:HD3	1.96	0.47
1:A:97:CYS:O	1:A:101:ILE:HG12	2.15	0.46
1:A:54:LEU:HB2	1:A:254:TRP:HB3	1.96	0.46
1:A:146:THR:C	1:A:149:PRO:HD2	2.41	0.46
1:A:194:SER:HA	2:C:1:NAG:H82	1.97	0.46
1:B:96:VAL:HG11	1:B:401:MET:HE3	1.98	0.46
1:B:140:ALA:HB1	3:B:601:NAG:O7	2.16	0.44
1:A:115:ILE:HG21	1:A:206:ASP:HB2	1.98	0.44
1:A:111:THR:HA	1:A:384:GLY:HA2	2.00	0.44
1:B:295:TYR:CZ	1:B:366:CYS:HB3	2.53	0.43
1:B:98:SER:O	1:B:101:ILE:HG12	2.18	0.43
1:B:318:LEU:HD22	1:B:357:LEU:HD12	2.01	0.43
1:A:161:ARG:HB3	1:A:164:PRO:HG2	2.00	0.42
1:B:54:LEU:HB2	1:B:254:TRP:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TYR:HA	1:A:67:TRP:HD1	1.83	0.42
1:A:409:VAL:N	1:A:410:PRO:HD2	2.33	0.42
1:B:161:ARG:HB3	1:B:164:PRO:HD2	2.01	0.42
1:A:282:VAL:HG21	1:A:293:LEU:HD13	2.01	0.42
1:B:101:ILE:HD12	1:B:221:VAL:HG22	2.02	0.41
1:A:106:TYR:CZ	1:A:110:GLU:HG3	2.56	0.41
1:B:31:GLN:O	1:B:33:ARG:HG2	2.19	0.41
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.94	0.41
1:A:163:GLU:HB2	1:A:164:PRO:HD3	2.02	0.41
1:B:282:VAL:HG21	1:B:293:LEU:HD13	2.03	0.41
1:A:123:ARG:O	1:A:127:ARG:HG2	2.20	0.40
1:A:282:VAL:HG21	1:A:293:LEU:HD22	2.03	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	388/588 (66%)	378 (97%)	10 (3%)	0	100	100
1	B	388/588 (66%)	383 (99%)	5 (1%)	0	100	100
All	All	776/1176 (66%)	761 (98%)	15 (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	328/491 (67%)	306 (93%)	22 (7%)	15	41
1	B	328/491 (67%)	317 (97%)	11 (3%)	32	65
All	All	656/982 (67%)	623 (95%)	33 (5%)	23	52

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	44	LEU
1	A	56	LEU
1	A	110	GLU
1	A	135	ARG
1	A	175	LEU
1	A	195	LEU
1	A	198	LEU
1	A	211	LEU
1	A	214	LEU
1	A	216	LEU
1	A	217	LEU
1	A	242	VAL
1	A	250	LEU
1	A	261	LEU
1	A	281	MET
1	A	287	VAL
1	A	293	LEU
1	A	302	ARG
1	A	363	LEU
1	A	394	PHE
1	A	411	HIS
1	B	4	VAL
1	B	22	ASP
1	B	23	LEU
1	B	46	LEU
1	B	61	LEU
1	B	231	LEU
1	B	242	VAL
1	B	250	LEU
1	B	292	ILE
1	B	365	ASP
1	B	388	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	B	41	GLN
1	B	172	GLN
1	B	305	ASN
1	B	411	HIS

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 ⓘ

4 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	0.78	0	17,19,21	1.10	1 (5%)
2	NAG	C	2	2	14,14,15	0.75	0	17,19,21	0.86	0
2	NAG	D	1	2,1	14,14,15	0.74	0	17,19,21	0.80	0
2	NAG	D	2	2	14,14,15	0.73	0	17,19,21	0.88	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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	3.11	127.06	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

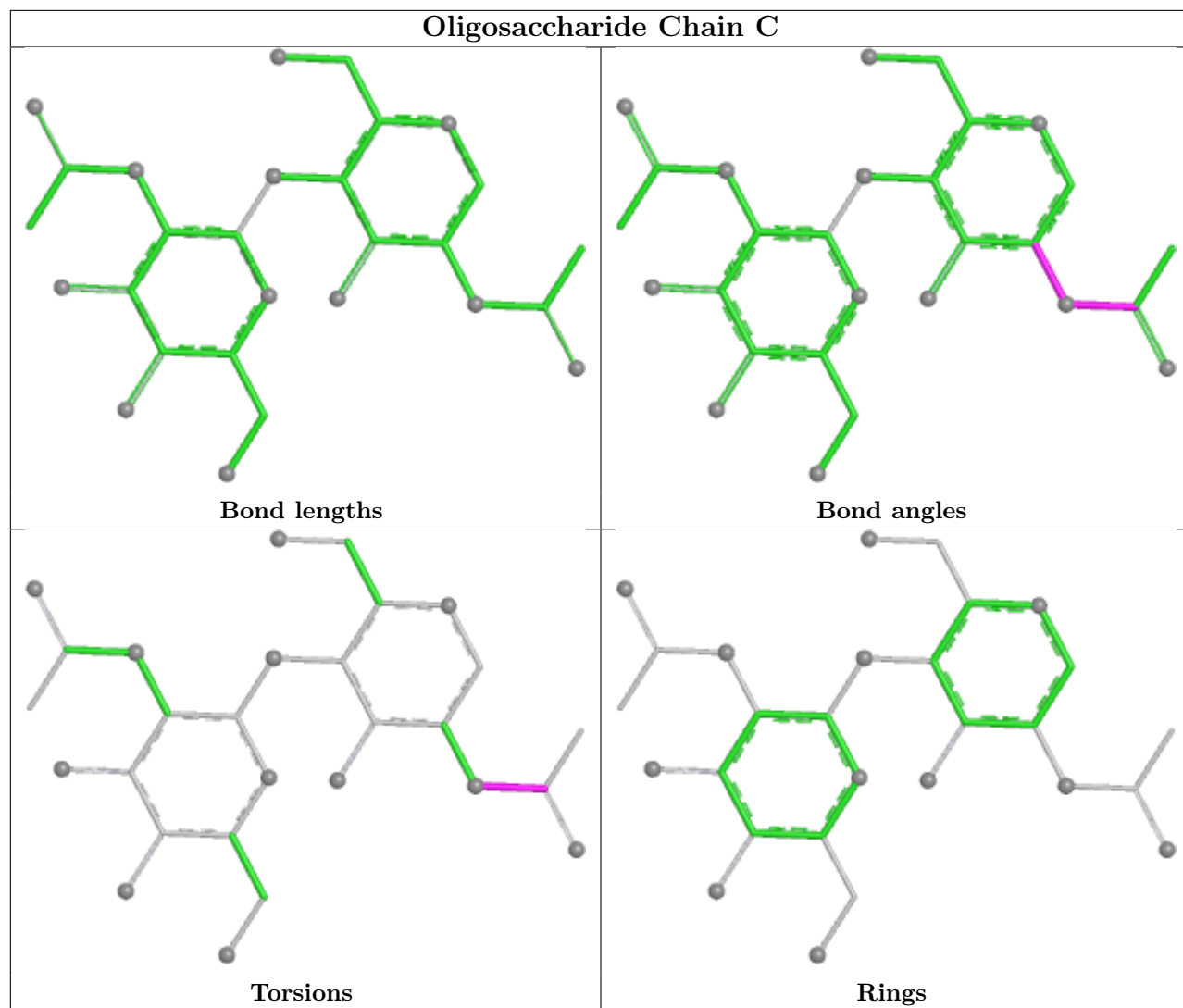
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

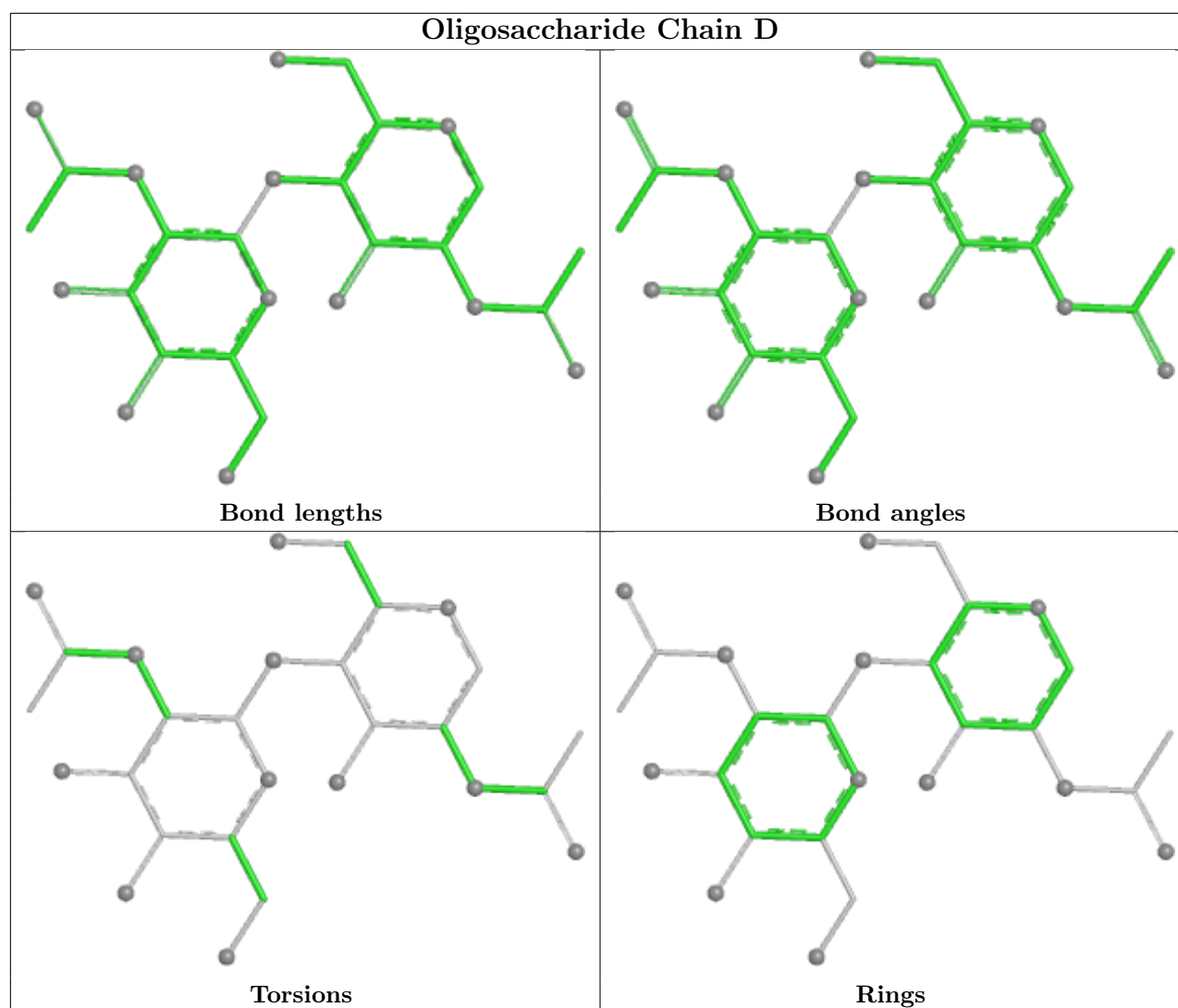
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	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](#)

4 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	$\# Z > 2$
3	NAG	B	602	1	14,14,15	0.77	0	17,19,21	1.03	1 (5%)
3	NAG	A	601	1	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	B	601	1	14,14,15	0.71	0	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	602	1	14,14,15	0.67	0	17,19,21	1.48	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	3/6/23/26	0/1/1/1
3	NAG	A	602	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAG	C2-N2-C7	3.43	127.49	122.90
3	B	602	NAG	C1-O5-C5	2.46	115.48	112.19
3	A	602	NAG	O5-C1-C2	-2.44	107.52	111.29
3	A	602	NAG	C1-O5-C5	2.32	115.29	112.19
3	B	601	NAG	O5-C1-C2	-2.32	107.71	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAG	C8-C7-N2-C2
3	A	601	NAG	O7-C7-N2-C2
3	B	601	NAG	C8-C7-N2-C2
3	B	601	NAG	O7-C7-N2-C2
3	A	602	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	A	602	NAG	C3-C2-N2-C7
3	A	602	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	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.

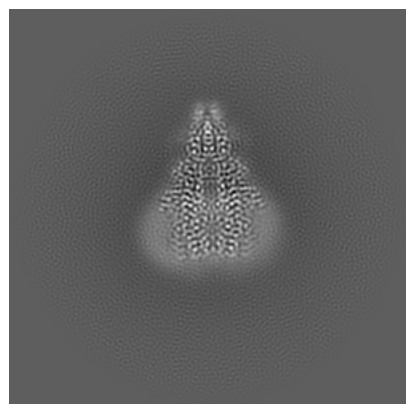
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53249. These allow visual inspection of the internal detail of the map and identification of artifacts.

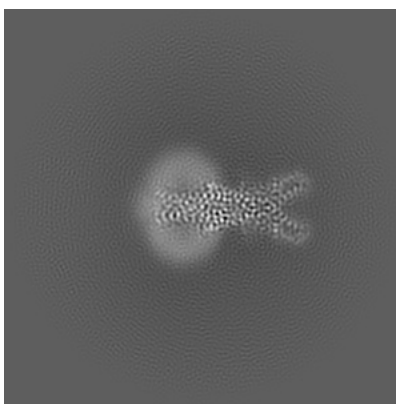
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

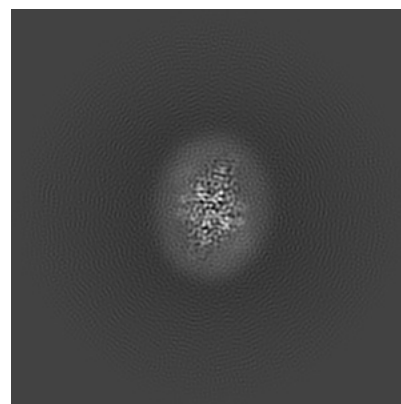
6.1.1 Primary map



X

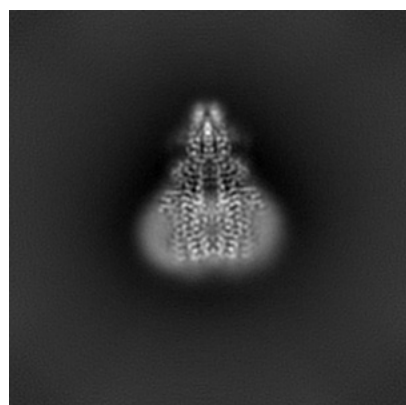


Y

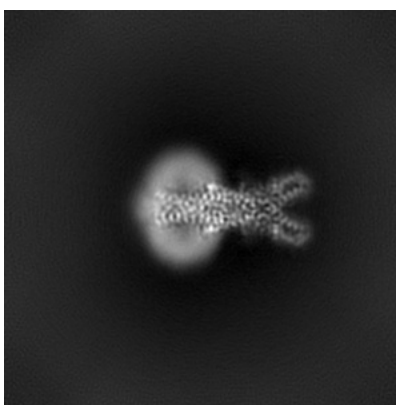


Z

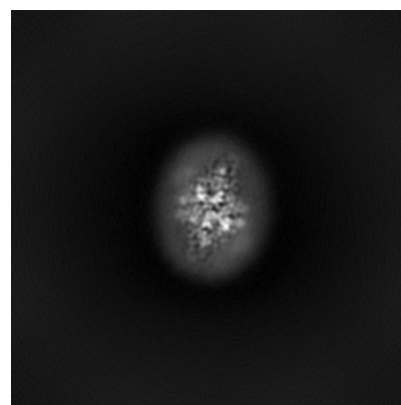
6.1.2 Raw map



X



Y

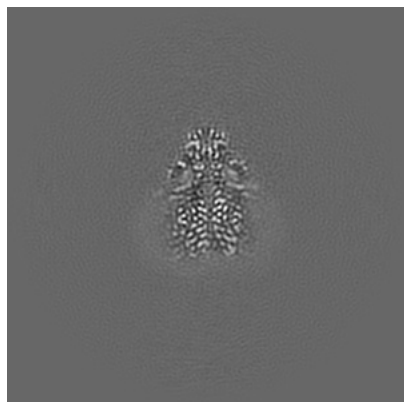


Z

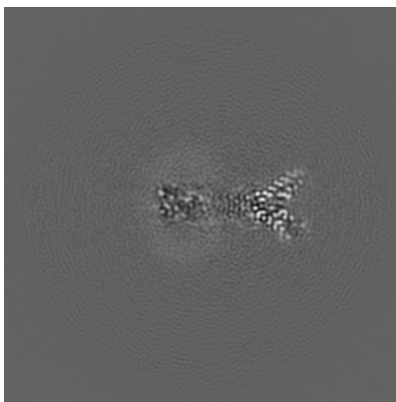
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

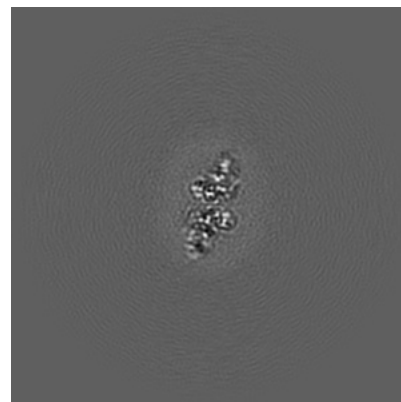
6.2.1 Primary map



X Index: 110

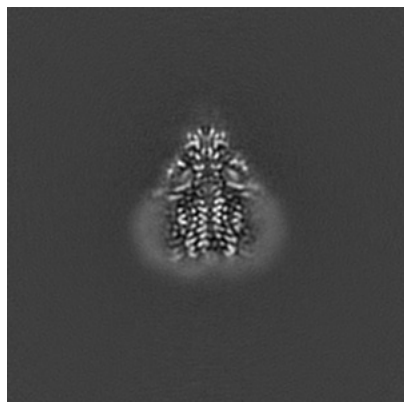


Y Index: 110

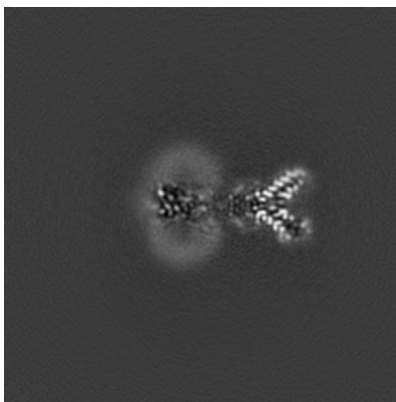


Z Index: 110

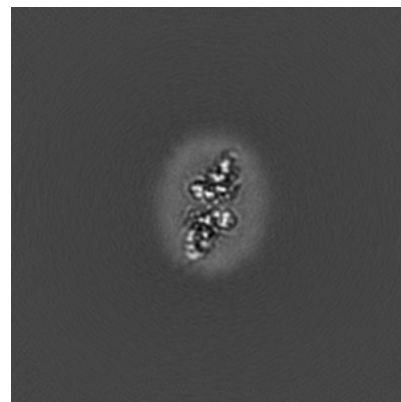
6.2.2 Raw map



X Index: 110



Y Index: 110

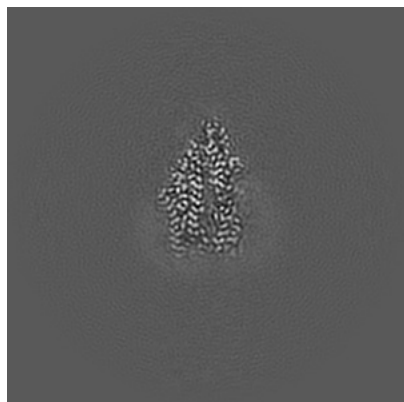


Z Index: 110

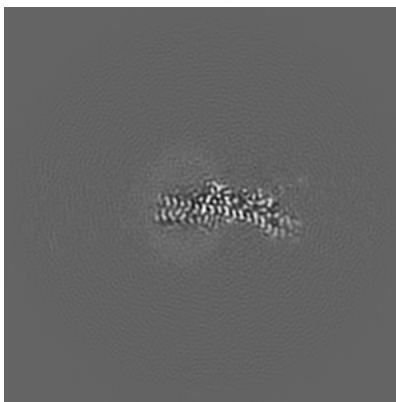
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

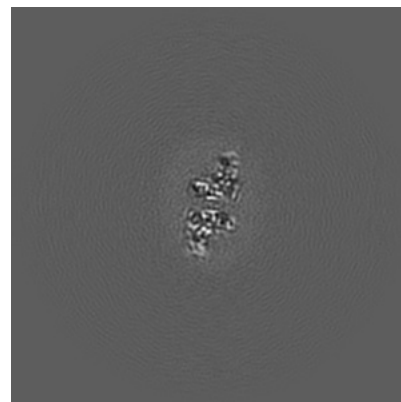
6.3.1 Primary map



X Index: 106

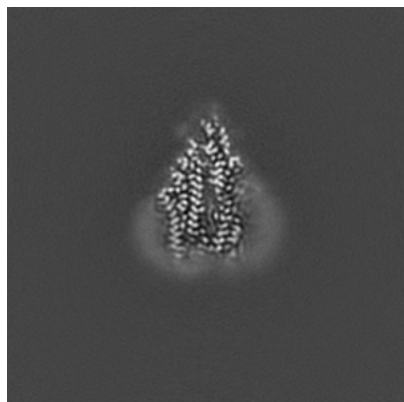


Y Index: 117

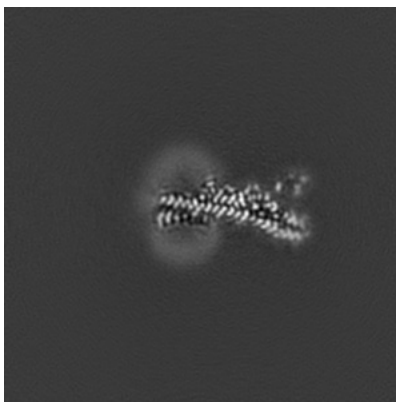


Z Index: 112

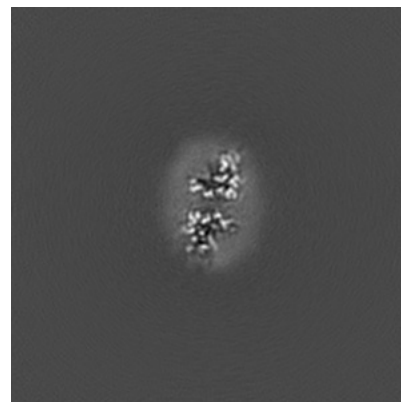
6.3.2 Raw map



X Index: 106



Y Index: 115

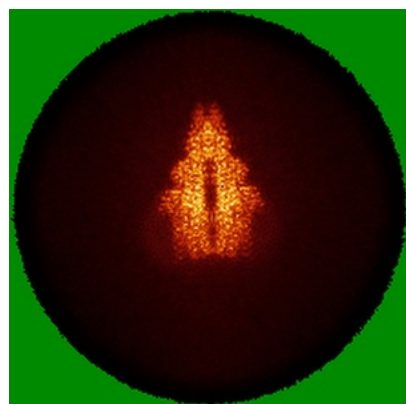


Z Index: 114

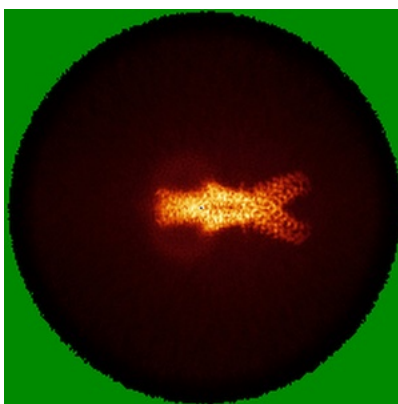
The images above show the largest variance slices of the map in three orthogonal directions.

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

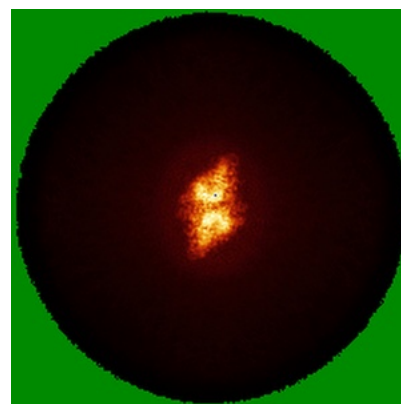
6.4.1 Primary map



X

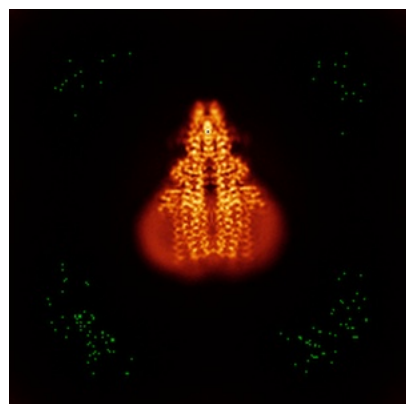


Y

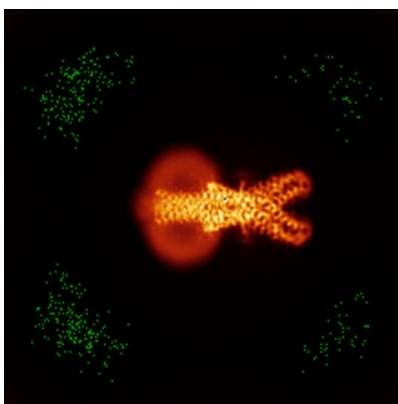


Z

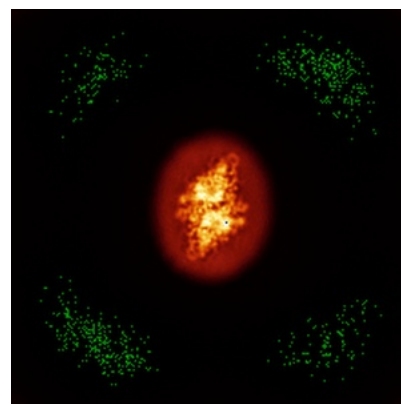
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

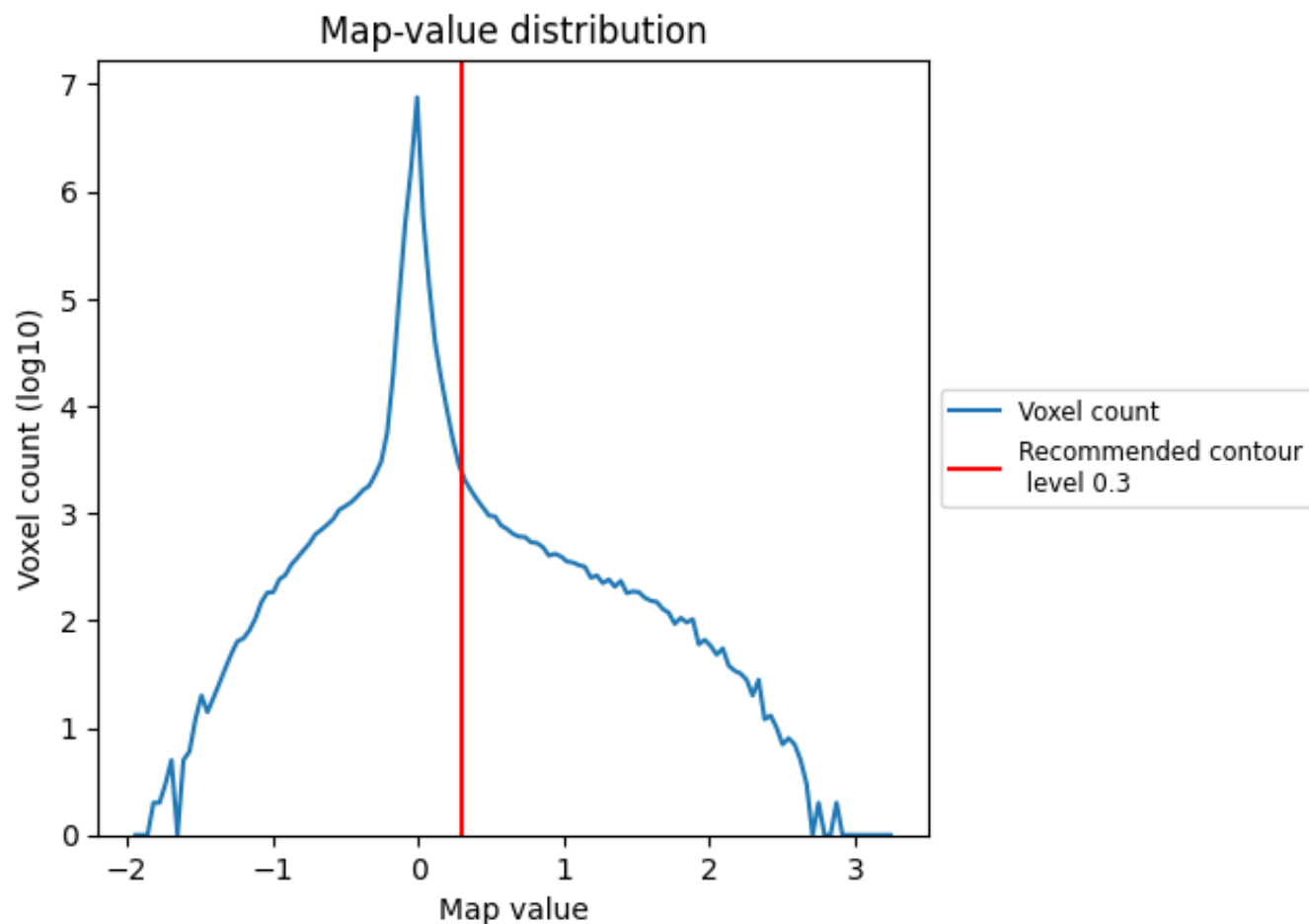
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

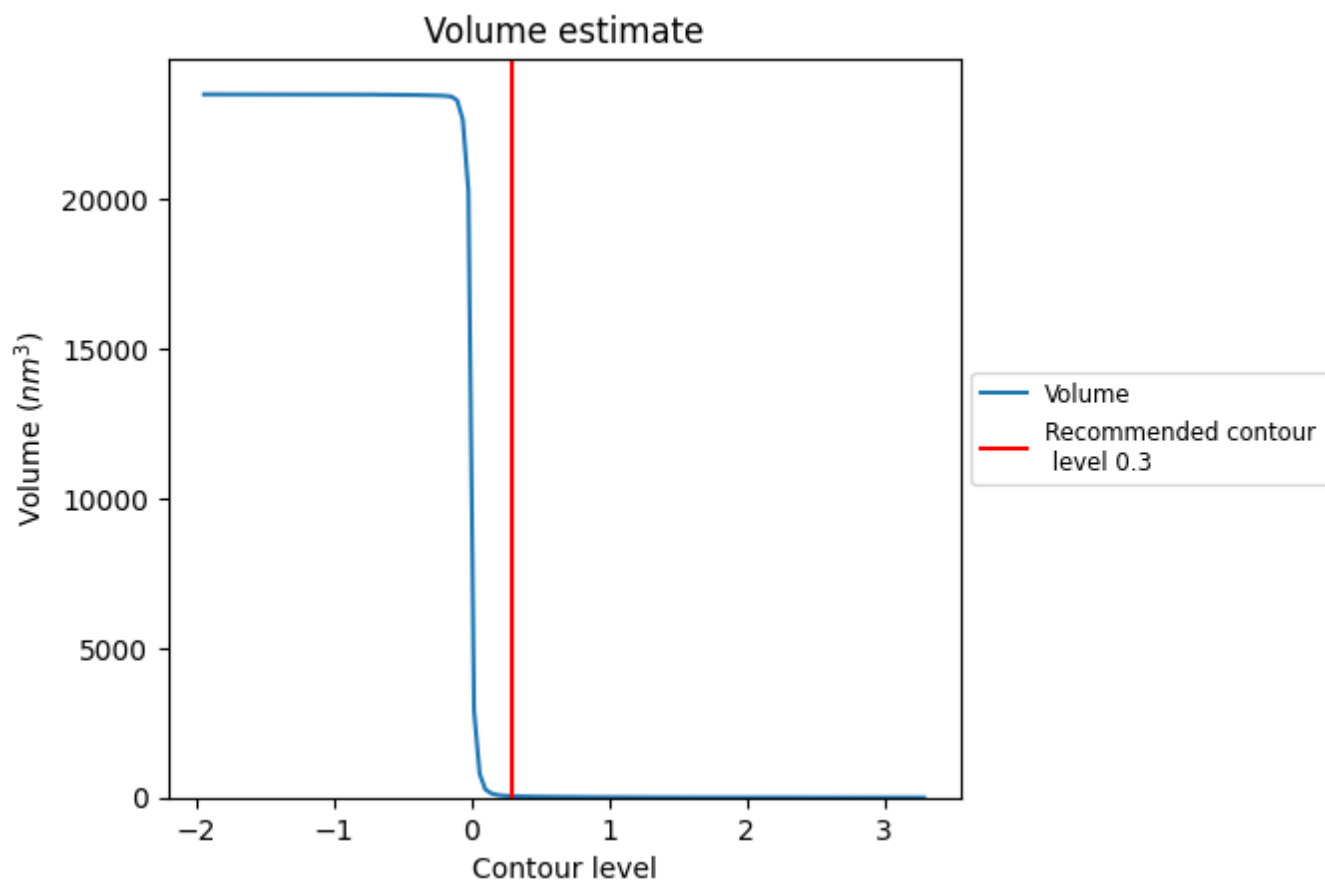
This section contains the results of statistical analysis of the map.

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.

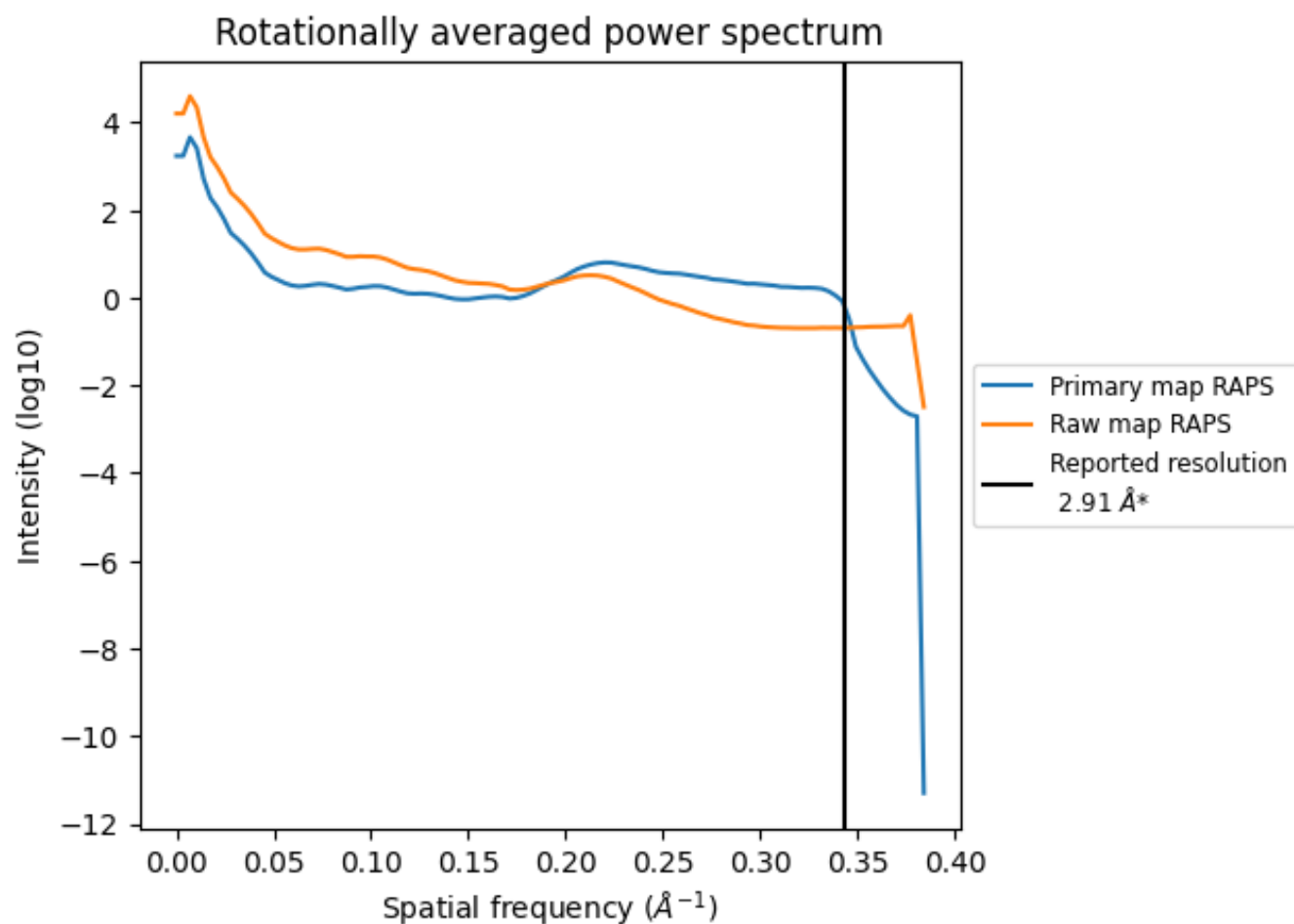
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 41 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 ⓘ

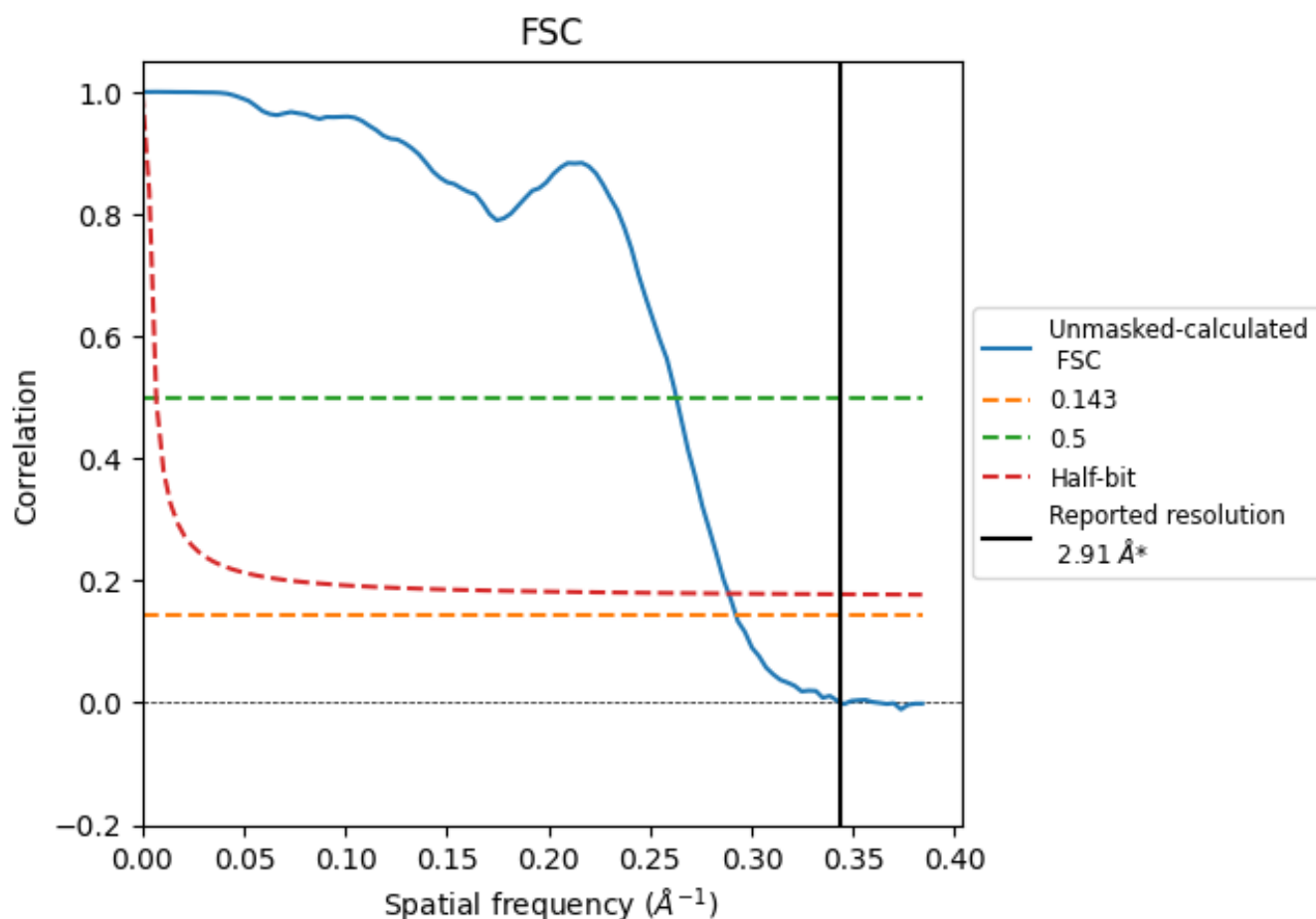


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.344 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

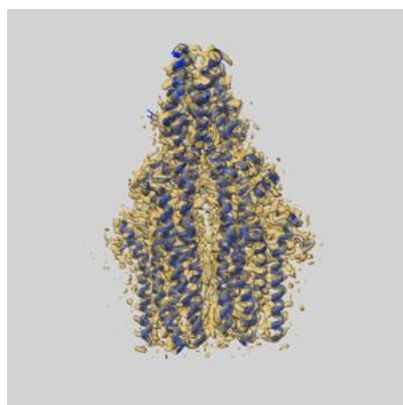
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.42	3.80	3.46

*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 3.42 differs from the reported value 2.91 by more than 10 %

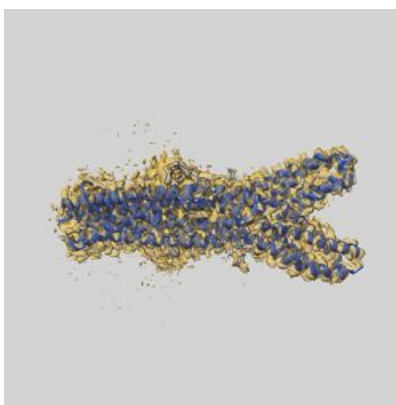
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53249 and PDB model 9QNR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

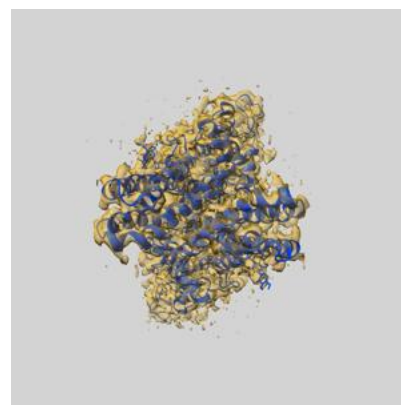
9.1 Map-model overlay [i](#)



X



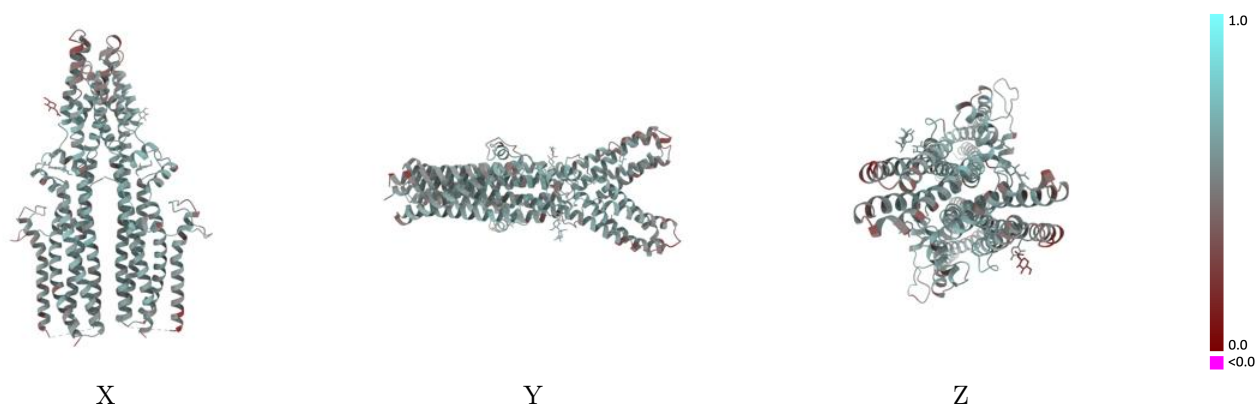
Y



Z

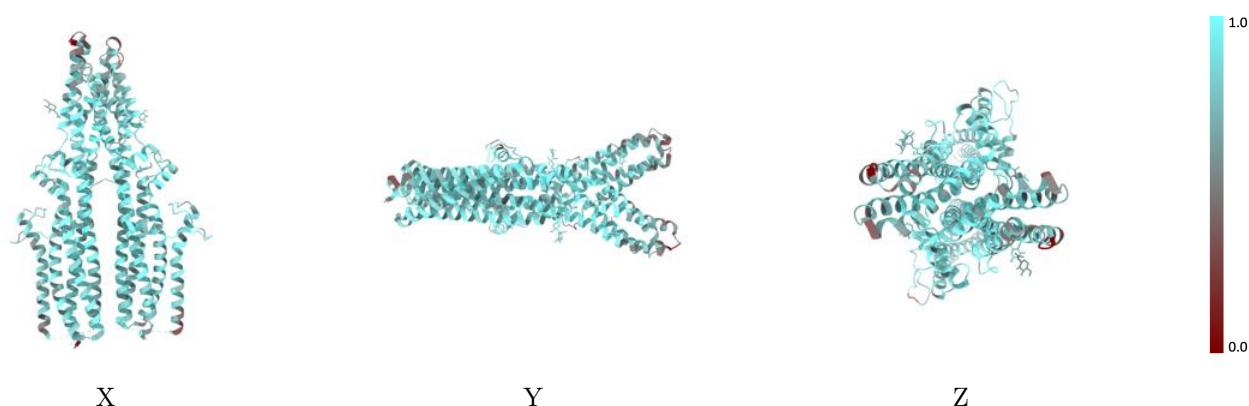
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



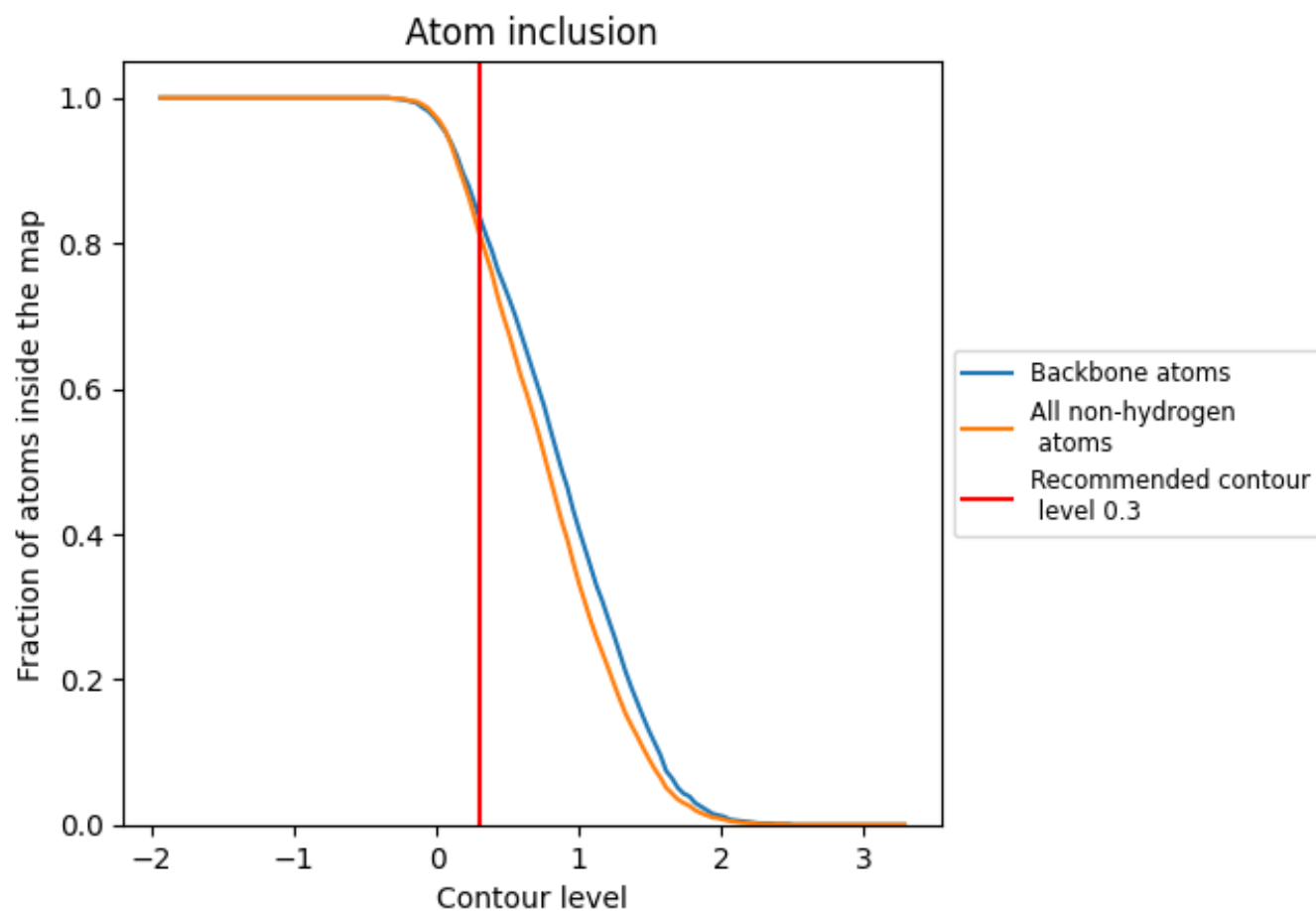
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8120	0.5350
A	0.8130	0.5380
B	0.8100	0.5320
C	0.7860	0.5850
D	0.8570	0.5500

