



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 11:23 AM JST

PDB ID : 8HXK
EMDB ID : EMD-35079
Title : BANAL-20-236 S1 in complex with R. Affinis ACE2
Authors : Wang, X.; Xu, G.
Deposited on : 2023-01-04
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary 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.dev113
Mogul : 1.8.5 (274361), 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

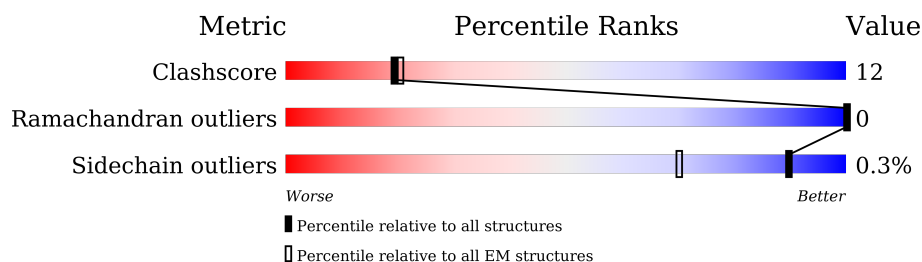
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	662	
2	B	1282	
3	C	2	
3	D	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10340 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	597	Total	C	N	O	S	0	0
			4894	3125	817	922	30		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP A0A7D7J6S6
A	-2	GLU	-	expression tag	UNP A0A7D7J6S6
A	-1	THR	-	expression tag	UNP A0A7D7J6S6
A	0	ASP	-	expression tag	UNP A0A7D7J6S6
A	1	THR	-	expression tag	UNP A0A7D7J6S6
A	2	LEU	-	expression tag	UNP A0A7D7J6S6
A	3	LEU	-	expression tag	UNP A0A7D7J6S6
A	4	LEU	-	expression tag	UNP A0A7D7J6S6
A	5	TRP	-	expression tag	UNP A0A7D7J6S6
A	6	VAL	-	expression tag	UNP A0A7D7J6S6
A	10	TRP	SER	conflict	UNP A0A7D7J6S6
A	11	VAL	LEU	conflict	UNP A0A7D7J6S6
A	12	PRO	VAL	conflict	UNP A0A7D7J6S6
A	13	GLY	ALA	conflict	UNP A0A7D7J6S6
A	14	SER	VAL	conflict	UNP A0A7D7J6S6
A	16	GLY	ALA	conflict	UNP A0A7D7J6S6
A	17	LYS	ALA	conflict	UNP A0A7D7J6S6
A	18	LEU	GLN	conflict	UNP A0A7D7J6S6
A	616	SER	-	expression tag	UNP A0A7D7J6S6
A	617	ARG	-	expression tag	UNP A0A7D7J6S6
A	618	GLY	-	expression tag	UNP A0A7D7J6S6
A	619	SER	-	expression tag	UNP A0A7D7J6S6
A	620	GLY	-	expression tag	UNP A0A7D7J6S6
A	621	LEU	-	expression tag	UNP A0A7D7J6S6
A	622	GLU	-	expression tag	UNP A0A7D7J6S6
A	623	VAL	-	expression tag	UNP A0A7D7J6S6
A	624	LEU	-	expression tag	UNP A0A7D7J6S6
A	625	PHE	-	expression tag	UNP A0A7D7J6S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	626	GLN	-	expression tag	UNP A0A7D7J6S6
A	627	GLY	-	expression tag	UNP A0A7D7J6S6
A	628	PRO	-	expression tag	UNP A0A7D7J6S6
A	629	GLY	-	expression tag	UNP A0A7D7J6S6
A	630	SER	-	expression tag	UNP A0A7D7J6S6
A	631	TRP	-	expression tag	UNP A0A7D7J6S6
A	632	SER	-	expression tag	UNP A0A7D7J6S6
A	633	HIS	-	expression tag	UNP A0A7D7J6S6
A	634	PRO	-	expression tag	UNP A0A7D7J6S6
A	635	GLN	-	expression tag	UNP A0A7D7J6S6
A	636	PHE	-	expression tag	UNP A0A7D7J6S6
A	637	GLU	-	expression tag	UNP A0A7D7J6S6
A	638	LYS	-	expression tag	UNP A0A7D7J6S6
A	639	GLY	-	expression tag	UNP A0A7D7J6S6
A	640	GLY	-	expression tag	UNP A0A7D7J6S6
A	641	GLY	-	expression tag	UNP A0A7D7J6S6
A	642	SER	-	expression tag	UNP A0A7D7J6S6
A	643	GLY	-	expression tag	UNP A0A7D7J6S6
A	644	GLY	-	expression tag	UNP A0A7D7J6S6
A	645	GLY	-	expression tag	UNP A0A7D7J6S6
A	646	SER	-	expression tag	UNP A0A7D7J6S6
A	647	GLY	-	expression tag	UNP A0A7D7J6S6
A	648	GLY	-	expression tag	UNP A0A7D7J6S6
A	649	SER	-	expression tag	UNP A0A7D7J6S6
A	650	ALA	-	expression tag	UNP A0A7D7J6S6
A	651	TRP	-	expression tag	UNP A0A7D7J6S6
A	652	SER	-	expression tag	UNP A0A7D7J6S6
A	653	HIS	-	expression tag	UNP A0A7D7J6S6
A	654	PRO	-	expression tag	UNP A0A7D7J6S6
A	655	GLN	-	expression tag	UNP A0A7D7J6S6
A	656	PHE	-	expression tag	UNP A0A7D7J6S6
A	657	GLU	-	expression tag	UNP A0A7D7J6S6
A	658	LYS	-	expression tag	UNP A0A7D7J6S6

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	676	Total	C	N	O	S	0	0
			5320	3399	883	1014	24		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	CYS	HIS	conflict	UNP A0A7D6P0R3
B	11	SER	LEU	conflict	UNP A0A7D6P0R3
B	24	THR	ALA	conflict	UNP A0A7D6P0R3
B	34	HIS	GLN	conflict	UNP A0A7D6P0R3
B	48	SER	THR	conflict	UNP A0A7D6P0R3
B	63	ILE	VAL	conflict	UNP A0A7D6P0R3
B	74	GLY	SER	conflict	UNP A0A7D6P0R3
B	83	ILE	VAL	conflict	UNP A0A7D6P0R3
B	145	PHE	TYR	conflict	UNP A0A7D6P0R3
B	173	PRO	SER	conflict	UNP A0A7D6P0R3
B	179	SER	ALA	conflict	UNP A0A7D6P0R3
B	207	SER	THR	conflict	UNP A0A7D6P0R3
B	217	SER	ILE	conflict	UNP A0A7D6P0R3
B	228	LEU	ILE	conflict	UNP A0A7D6P0R3
B	236	ARG	LYS	conflict	UNP A0A7D6P0R3
B	274	LYS	ASN	conflict	UNP A0A7D6P0R3
B	288	SER	ALA	conflict	UNP A0A7D6P0R3
B	302	PHE	LEU	conflict	UNP A0A7D6P0R3
B	320	ASP	GLU	conflict	UNP A0A7D6P0R3
B	413	LYS	ARG	conflict	UNP A0A7D6P0R3
B	489	LYS	GLN	conflict	UNP A0A7D6P0R3
B	525	LYS	GLN	conflict	UNP A0A7D6P0R3
B	530	ILE	VAL	conflict	UNP A0A7D6P0R3
B	552	ASN	SER	conflict	UNP A0A7D6P0R3
B	600	ALA	THR	conflict	UNP A0A7D6P0R3
B	630	ARG	SER	conflict	UNP A0A7D6P0R3
B	680	ALA	SER	conflict	UNP A0A7D6P0R3
B	683	SER	ALA	conflict	UNP A0A7D6P0R3
B	700	SER	ALA	conflict	UNP A0A7D6P0R3
B	739	THR	ILE	conflict	UNP A0A7D6P0R3
B	785	GLN	PRO	conflict	UNP A0A7D6P0R3
B	978	PRO	LYS	conflict	UNP A0A7D6P0R3
B	979	PRO	VAL	conflict	UNP A0A7D6P0R3
B	1062	ALA	SER	conflict	UNP A0A7D6P0R3
B	1070	ALA	THR	conflict	UNP A0A7D6P0R3
B	1076	ASP	GLU	conflict	UNP A0A7D6P0R3
B	1117	ASN	SER	conflict	UNP A0A7D6P0R3
B	1194	GLN	GLU	conflict	UNP A0A7D6P0R3
B	1201	LEU	-	expression tag	UNP A0A7D6P0R3
B	1202	GLU	-	expression tag	UNP A0A7D6P0R3
B	1203	GLY	-	expression tag	UNP A0A7D6P0R3
B	1204	SER	-	expression tag	UNP A0A7D6P0R3
B	1205	GLY	-	expression tag	UNP A0A7D6P0R3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1206	TYR	-	expression tag	UNP A0A7D6P0R3
B	1207	ILE	-	expression tag	UNP A0A7D6P0R3
B	1208	PRO	-	expression tag	UNP A0A7D6P0R3
B	1209	GLU	-	expression tag	UNP A0A7D6P0R3
B	1210	ALA	-	expression tag	UNP A0A7D6P0R3
B	1211	PRO	-	expression tag	UNP A0A7D6P0R3
B	1212	ARG	-	expression tag	UNP A0A7D6P0R3
B	1213	ASP	-	expression tag	UNP A0A7D6P0R3
B	1214	GLY	-	expression tag	UNP A0A7D6P0R3
B	1215	GLN	-	expression tag	UNP A0A7D6P0R3
B	1216	ALA	-	expression tag	UNP A0A7D6P0R3
B	1217	TYR	-	expression tag	UNP A0A7D6P0R3
B	1218	VAL	-	expression tag	UNP A0A7D6P0R3
B	1219	ARG	-	expression tag	UNP A0A7D6P0R3
B	1220	LYS	-	expression tag	UNP A0A7D6P0R3
B	1221	ASP	-	expression tag	UNP A0A7D6P0R3
B	1222	GLY	-	expression tag	UNP A0A7D6P0R3
B	1223	GLU	-	expression tag	UNP A0A7D6P0R3
B	1224	TRP	-	expression tag	UNP A0A7D6P0R3
B	1225	VAL	-	expression tag	UNP A0A7D6P0R3
B	1226	LEU	-	expression tag	UNP A0A7D6P0R3
B	1227	LEU	-	expression tag	UNP A0A7D6P0R3
B	1228	SER	-	expression tag	UNP A0A7D6P0R3
B	1229	THR	-	expression tag	UNP A0A7D6P0R3
B	1230	PHE	-	expression tag	UNP A0A7D6P0R3
B	1231	LEU	-	expression tag	UNP A0A7D6P0R3
B	1232	GLY	-	expression tag	UNP A0A7D6P0R3
B	1233	ARG	-	expression tag	UNP A0A7D6P0R3
B	1234	SER	-	expression tag	UNP A0A7D6P0R3
B	1235	LEU	-	expression tag	UNP A0A7D6P0R3
B	1236	GLU	-	expression tag	UNP A0A7D6P0R3
B	1237	VAL	-	expression tag	UNP A0A7D6P0R3
B	1238	LEU	-	expression tag	UNP A0A7D6P0R3
B	1239	PHE	-	expression tag	UNP A0A7D6P0R3
B	1240	GLN	-	expression tag	UNP A0A7D6P0R3
B	1241	GLY	-	expression tag	UNP A0A7D6P0R3
B	1242	PRO	-	expression tag	UNP A0A7D6P0R3
B	1243	GLY	-	expression tag	UNP A0A7D6P0R3
B	1244	HIS	-	expression tag	UNP A0A7D6P0R3
B	1245	HIS	-	expression tag	UNP A0A7D6P0R3
B	1246	HIS	-	expression tag	UNP A0A7D6P0R3
B	1247	HIS	-	expression tag	UNP A0A7D6P0R3

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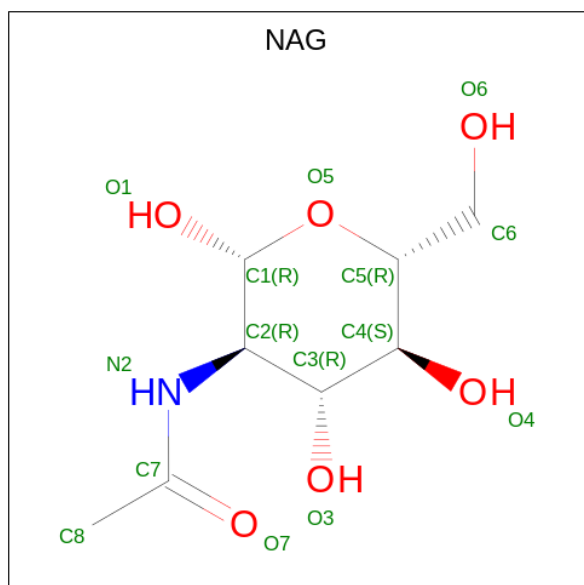
Chain	Residue	Modelled	Actual	Comment	Reference
B	1248	HIS	-	expression tag	UNP A0A7D6P0R3
B	1249	HIS	-	expression tag	UNP A0A7D6P0R3
B	1250	HIS	-	expression tag	UNP A0A7D6P0R3
B	1251	HIS	-	expression tag	UNP A0A7D6P0R3
B	1252	SER	-	expression tag	UNP A0A7D6P0R3
B	1253	ALA	-	expression tag	UNP A0A7D6P0R3
B	1254	TRP	-	expression tag	UNP A0A7D6P0R3
B	1255	SER	-	expression tag	UNP A0A7D6P0R3
B	1256	HIS	-	expression tag	UNP A0A7D6P0R3
B	1257	PRO	-	expression tag	UNP A0A7D6P0R3
B	1258	GLN	-	expression tag	UNP A0A7D6P0R3
B	1259	PHE	-	expression tag	UNP A0A7D6P0R3
B	1260	GLU	-	expression tag	UNP A0A7D6P0R3
B	1261	LYS	-	expression tag	UNP A0A7D6P0R3
B	1262	GLY	-	expression tag	UNP A0A7D6P0R3
B	1263	GLY	-	expression tag	UNP A0A7D6P0R3
B	1264	GLY	-	expression tag	UNP A0A7D6P0R3
B	1265	SER	-	expression tag	UNP A0A7D6P0R3
B	1266	GLY	-	expression tag	UNP A0A7D6P0R3
B	1267	GLY	-	expression tag	UNP A0A7D6P0R3
B	1268	GLY	-	expression tag	UNP A0A7D6P0R3
B	1269	GLY	-	expression tag	UNP A0A7D6P0R3
B	1270	SER	-	expression tag	UNP A0A7D6P0R3
B	1271	GLY	-	expression tag	UNP A0A7D6P0R3
B	1272	GLY	-	expression tag	UNP A0A7D6P0R3
B	1273	SER	-	expression tag	UNP A0A7D6P0R3
B	1274	ALA	-	expression tag	UNP A0A7D6P0R3
B	1275	TRP	-	expression tag	UNP A0A7D6P0R3
B	1276	SER	-	expression tag	UNP A0A7D6P0R3
B	1277	HIS	-	expression tag	UNP A0A7D6P0R3
B	1278	PRO	-	expression tag	UNP A0A7D6P0R3
B	1279	GLN	-	expression tag	UNP A0A7D6P0R3
B	1280	PHE	-	expression tag	UNP A0A7D6P0R3
B	1281	GLU	-	expression tag	UNP A0A7D6P0R3
B	1282	LYS	-	expression tag	UNP A0A7D6P0R3

- Molecule 3 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
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

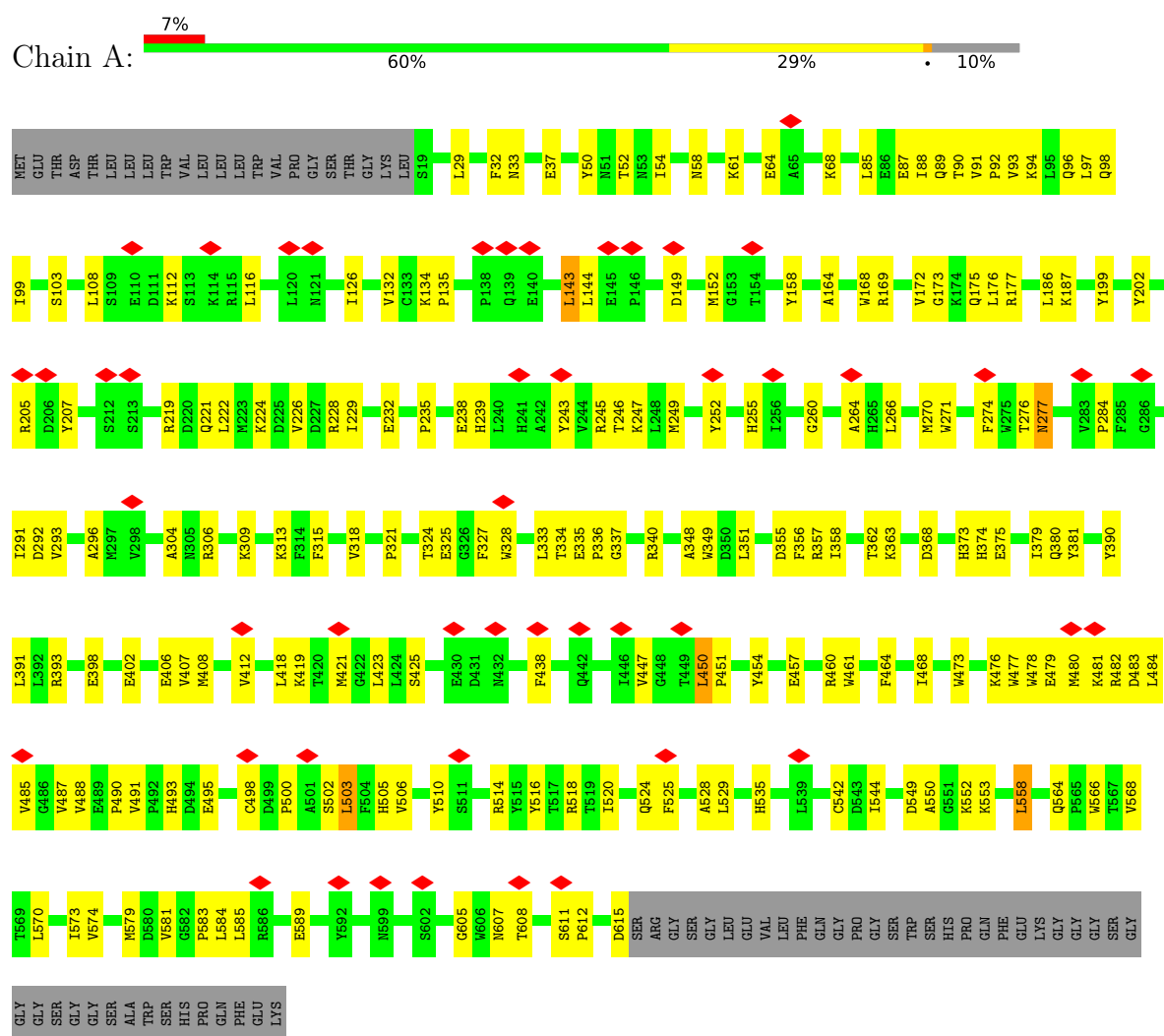


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

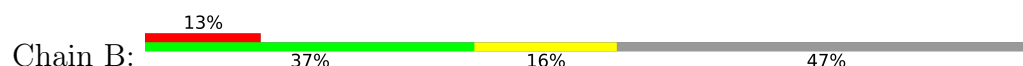
3 Residue-property plots

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

• Molecule 1: Angiotensin-converting enzyme



• Molecule 2: Spike glycoprotein





LEU
GLY
ARG
SER
LEU
GLU
VAL
LEU
PHE
GLN
GLY
PRO
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS
GLY
GLY
GLY
SER
GLY
GLY
GLY
GLY
GLY
GLY
GLY
GLY
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

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

Chain C:

100%

NAG1
NAG2

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

Chain D:

50%

50%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.028	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0102	Depositor
Map size (\AA)	262.87997, 262.87997, 262.87997	wwPDB
Map dimensions	248, 248, 248	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/5036	0.63	4/6835 (0.1%)
2	B	0.30	0/5459	0.62	1/7441 (0.0%)
All	All	0.30	0/10495	0.63	5/14276 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	85	ASP	CB-CG-OD1	8.60	126.04	118.30
1	A	450	LEU	CA-CB-CG	6.91	131.20	115.30
1	A	143	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	558	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	503	LEU	CA-CB-CG	5.43	127.78	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	387	CYS	Peptide

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	4894	0	4663	126	0
2	B	5320	0	5120	124	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	56	0	52	1	0
4	B	14	0	13	0	0
All	All	10340	0	9898	250	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 12.

The worst 5 of 250 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)
2:B:357:CYS:O	2:B:520:VAL:HA	1.72	0.88
2:B:628:THR:O	2:B:632:TYR:HB2	1.73	0.88
1:A:90:THR:HG22	1:A:92:PRO:HD2	1.75	0.69
2:B:100:ILE:HG22	2:B:101:VAL:HG13	1.76	0.68
2:B:667:CYS:HA	2:B:689:MET:HG3	1.76	0.67

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	595/662 (90%)	567 (95%)	28 (5%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	674/1282 (53%)	586 (87%)	88 (13%)	0	100	100
All	All	1269/1944 (65%)	1153 (91%)	116 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	532/582 (91%)	530 (100%)	2 (0%)	89	91
2	B	593/1106 (54%)	592 (100%)	1 (0%)	92	94
All	All	1125/1688 (67%)	1122 (100%)	3 (0%)	90	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	ARG
1	A	277	ASN
2	B	194	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.47	0	17,19,21	0.58	0
3	NAG	C	2	3	14,14,15	0.55	0	17,19,21	0.42	0
3	NAG	D	1	3,2	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	D	2	3	14,14,15	1.21	2 (14%)	17,19,21	0.80	1 (5%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C1	3.54	1.49	1.43
3	D	2	NAG	C1-C2	2.78	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	2	NAG	C2-N2-C7	2.31	126.19	122.90

There are no chirality outliers.

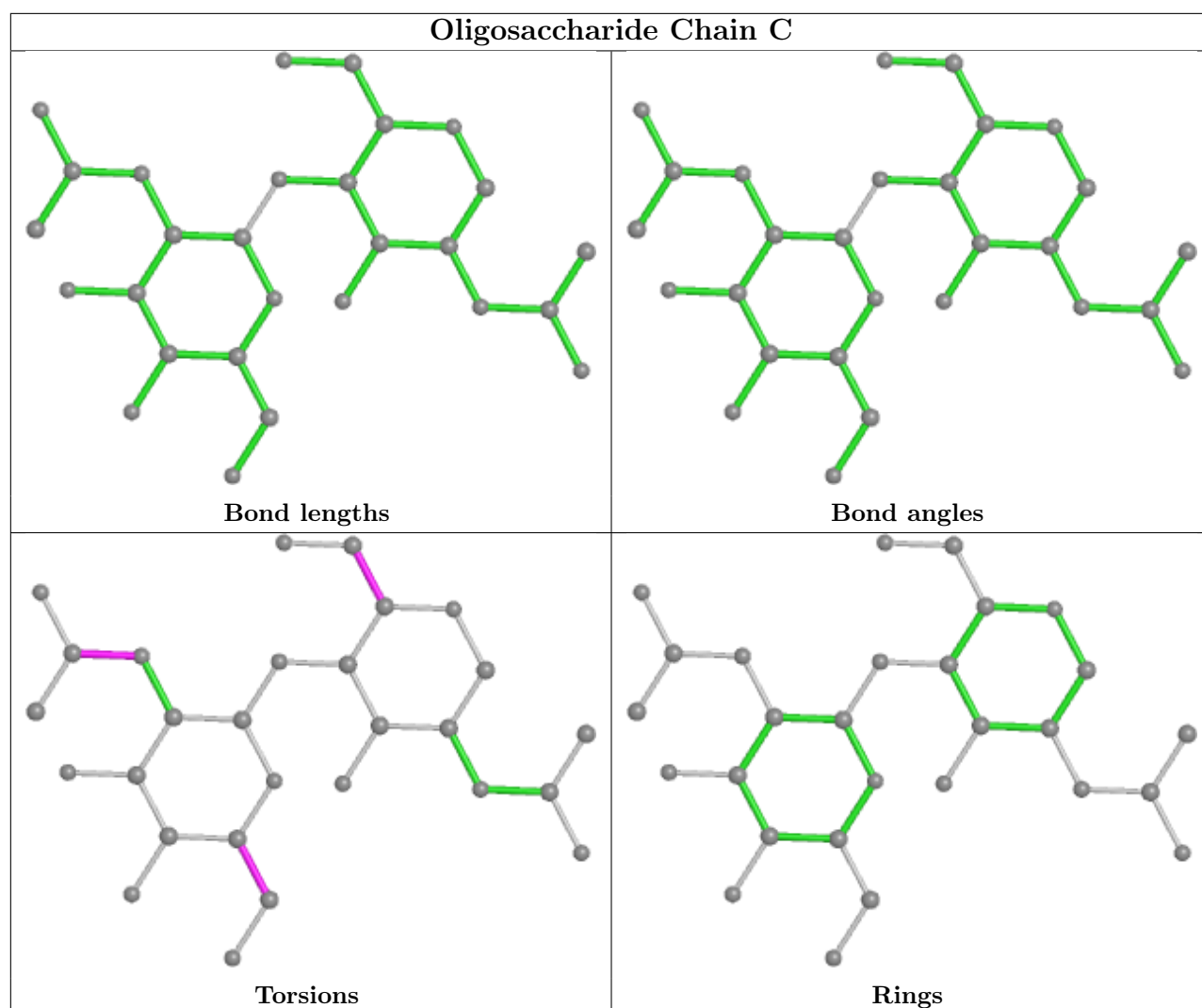
5 of 7 torsion outliers are listed below:

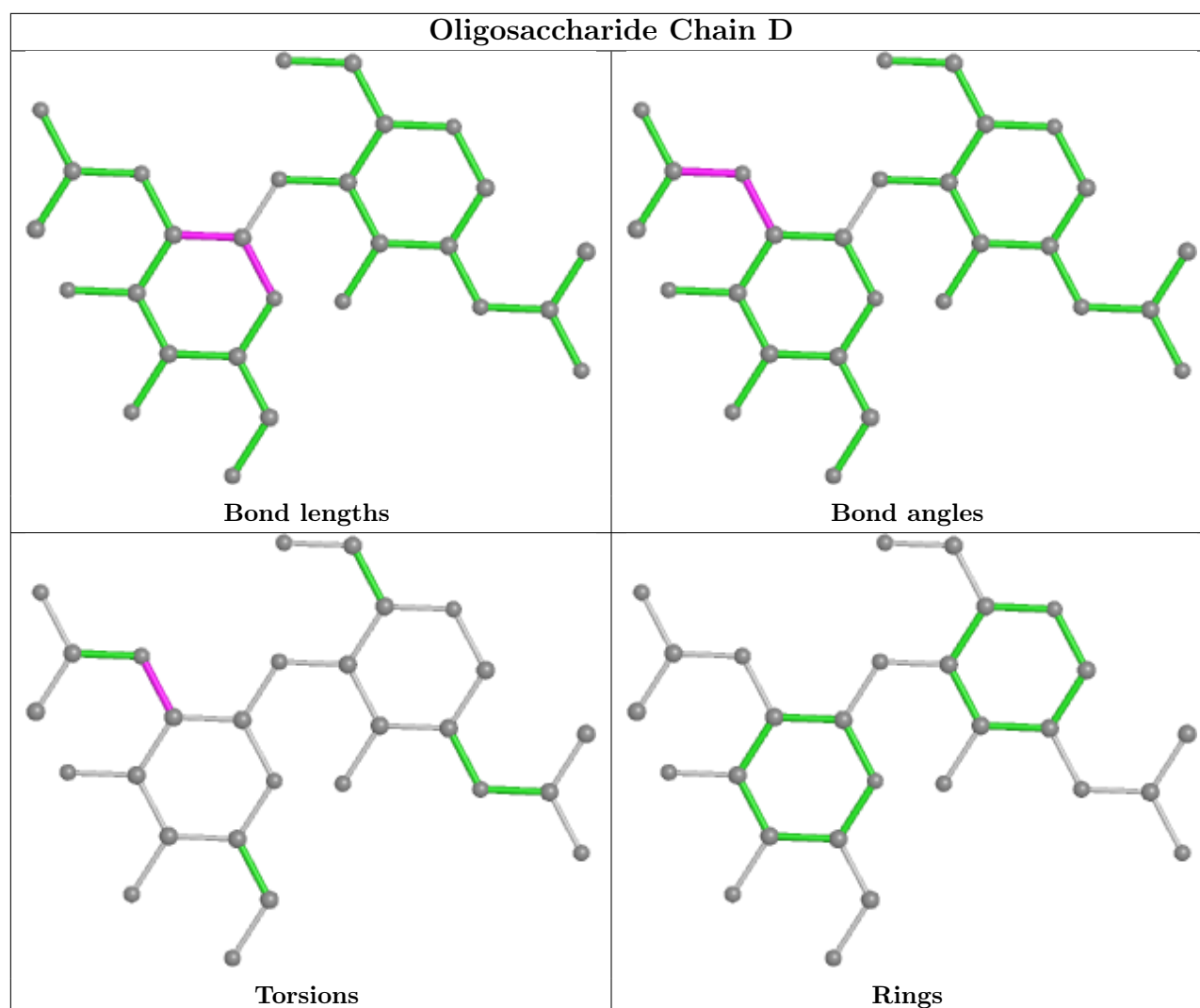
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	NAG	B	1301	2	14,14,15	0.46	0	17,19,21	0.42	0
4	NAG	A	702	1	14,14,15	0.58	0	17,19,21	0.51	0
4	NAG	A	701	1	14,14,15	0.26	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	703	1	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
4	NAG	A	704	1	14,14,15	0.30	0	17,19,21	0.66	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
4	NAG	B	1301	2	-	2/6/23/26	0/1/1/1
4	NAG	A	702	1	-	0/6/23/26	0/1/1/1
4	NAG	A	701	1	-	2/6/23/26	0/1/1/1
4	NAG	A	703	1	-	3/6/23/26	0/1/1/1
4	NAG	A	704	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	NAG	C2-N2-C7	2.39	126.31	122.90
4	A	704	NAG	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	NAG	O5-C5-C6-O6
4	A	701	NAG	C8-C7-N2-C2
4	A	701	NAG	O7-C7-N2-C2
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	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.

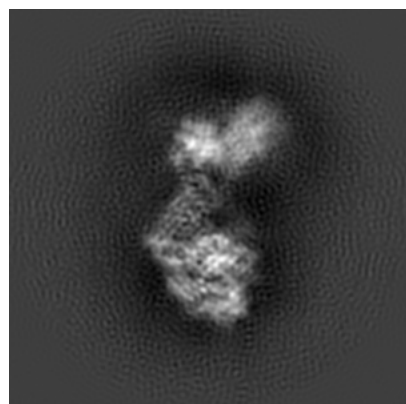
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35079. These allow visual inspection of the internal detail of the map and identification of artifacts.

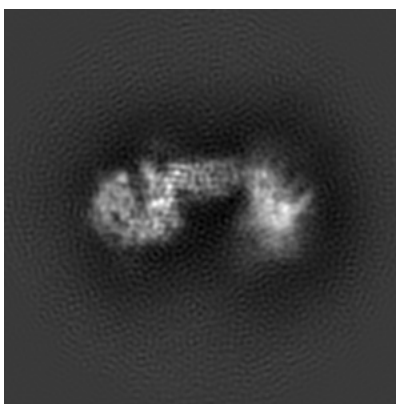
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

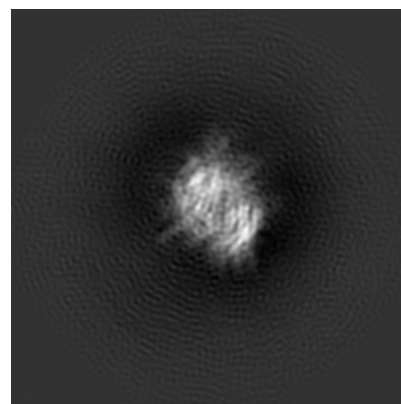
6.1.1 Primary map



X

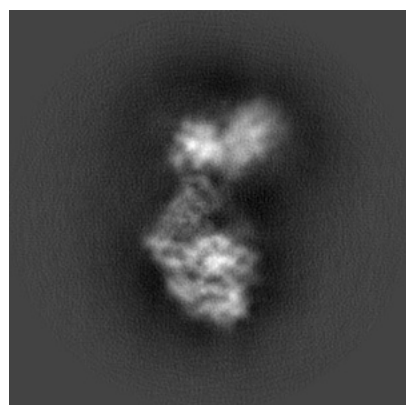


Y

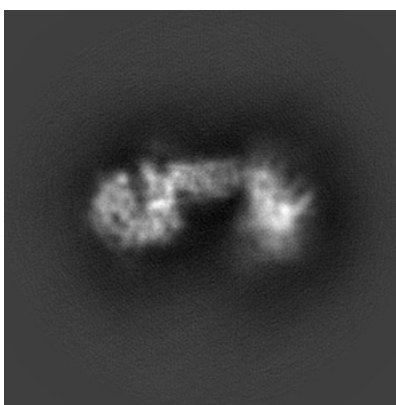


Z

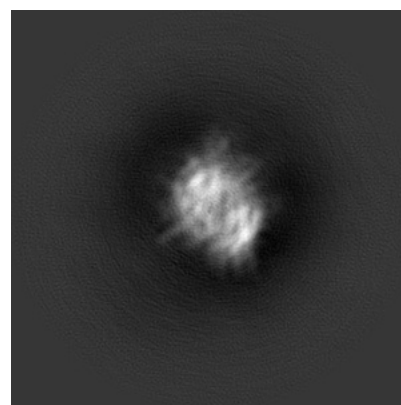
6.1.2 Raw map



X



Y

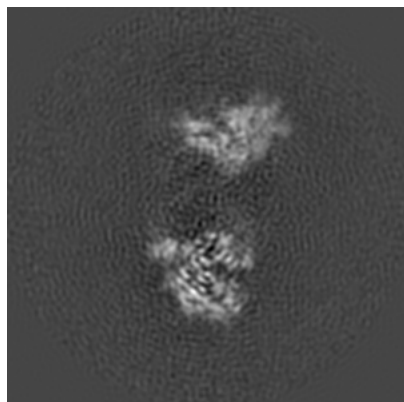


Z

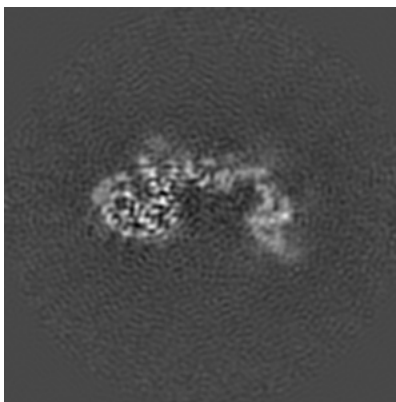
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

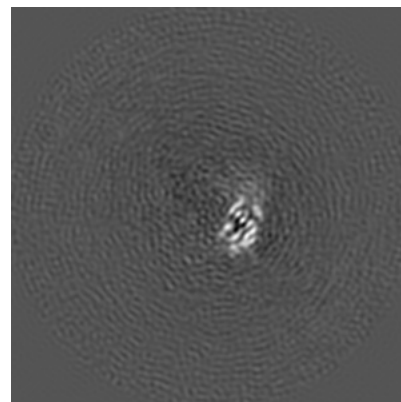
6.2.1 Primary map



X Index: 124

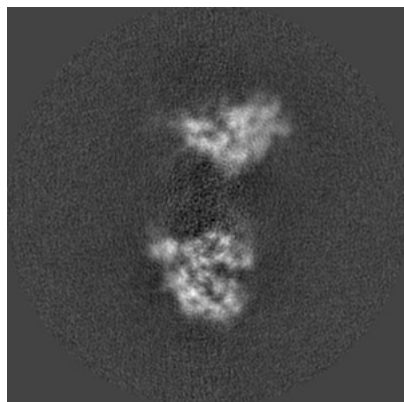


Y Index: 124

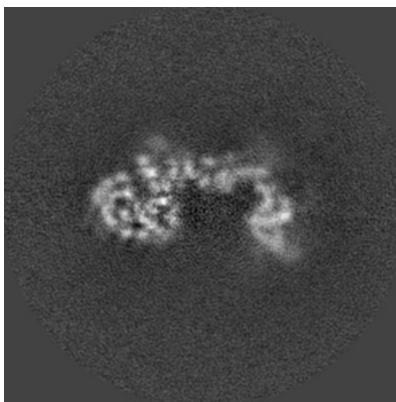


Z Index: 124

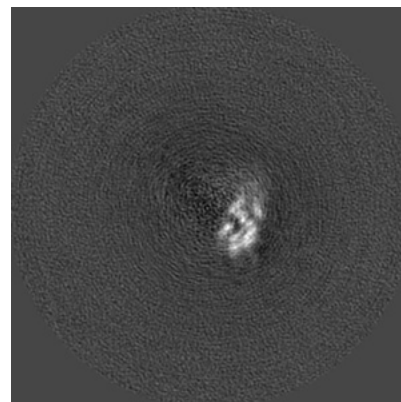
6.2.2 Raw map



X Index: 124



Y Index: 124

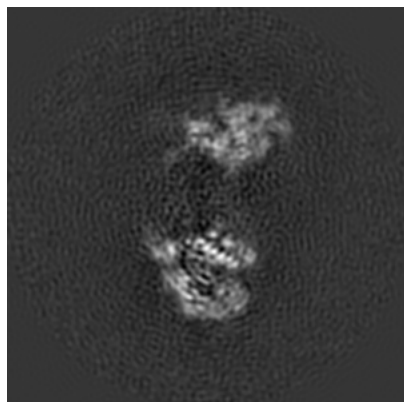


Z Index: 124

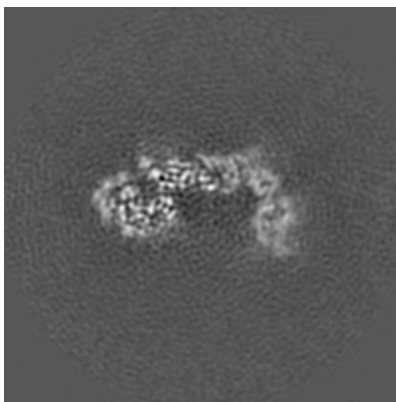
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

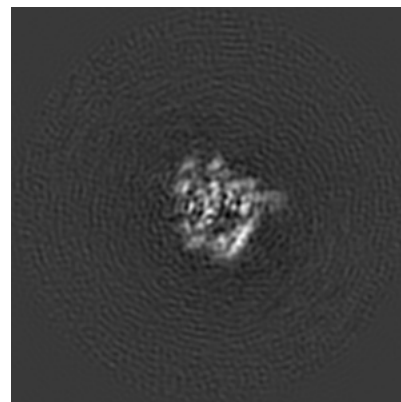
6.3.1 Primary map



X Index: 126

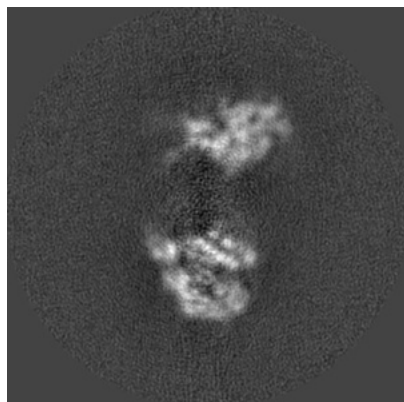


Y Index: 120

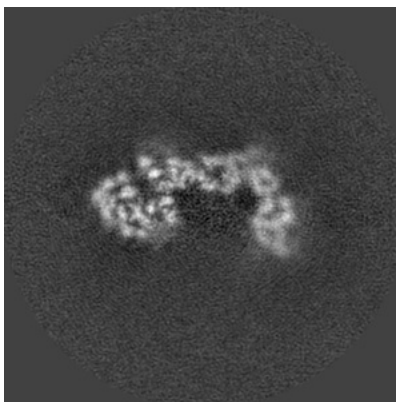


Z Index: 91

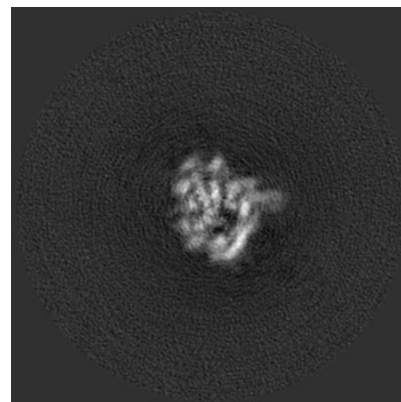
6.3.2 Raw map



X Index: 126



Y Index: 121

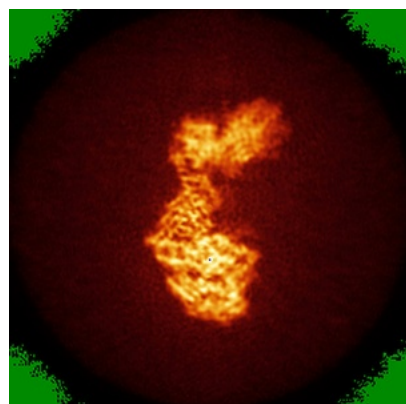


Z Index: 92

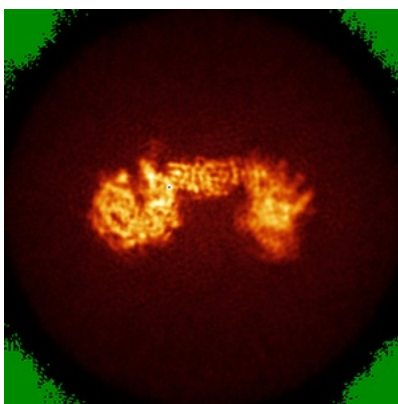
The images above show the largest variance slices of the map in three orthogonal directions.

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

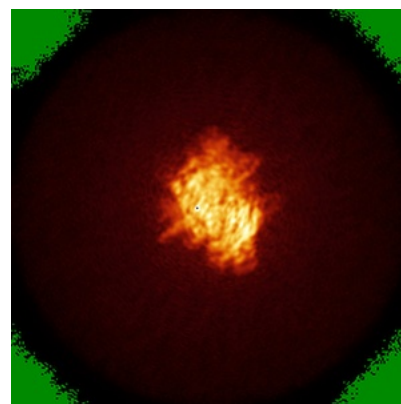
6.4.1 Primary map



X

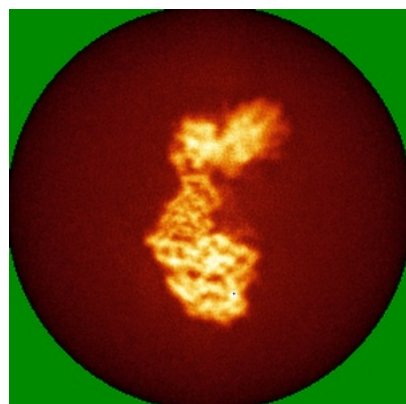


Y

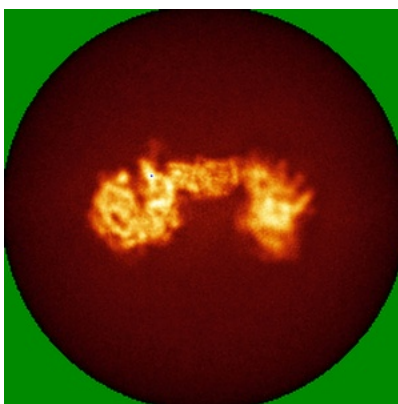


Z

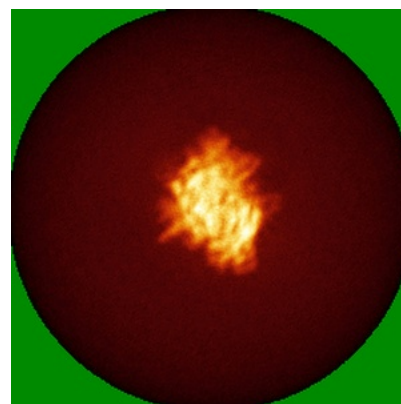
6.4.2 Raw map



X



Y

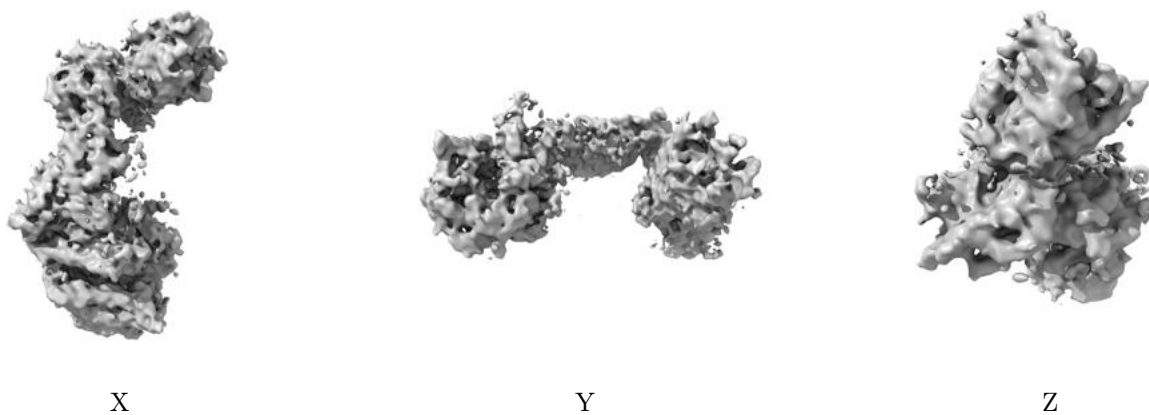


Z

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.

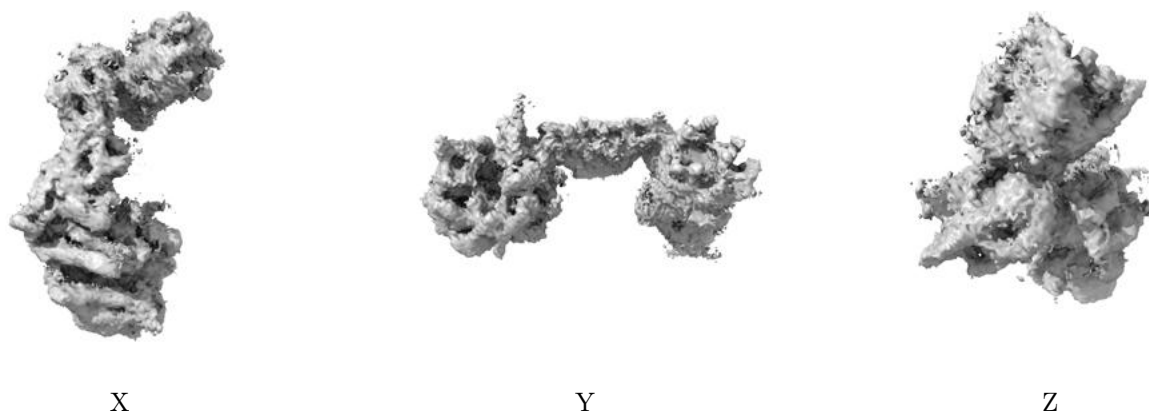
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0102. 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.

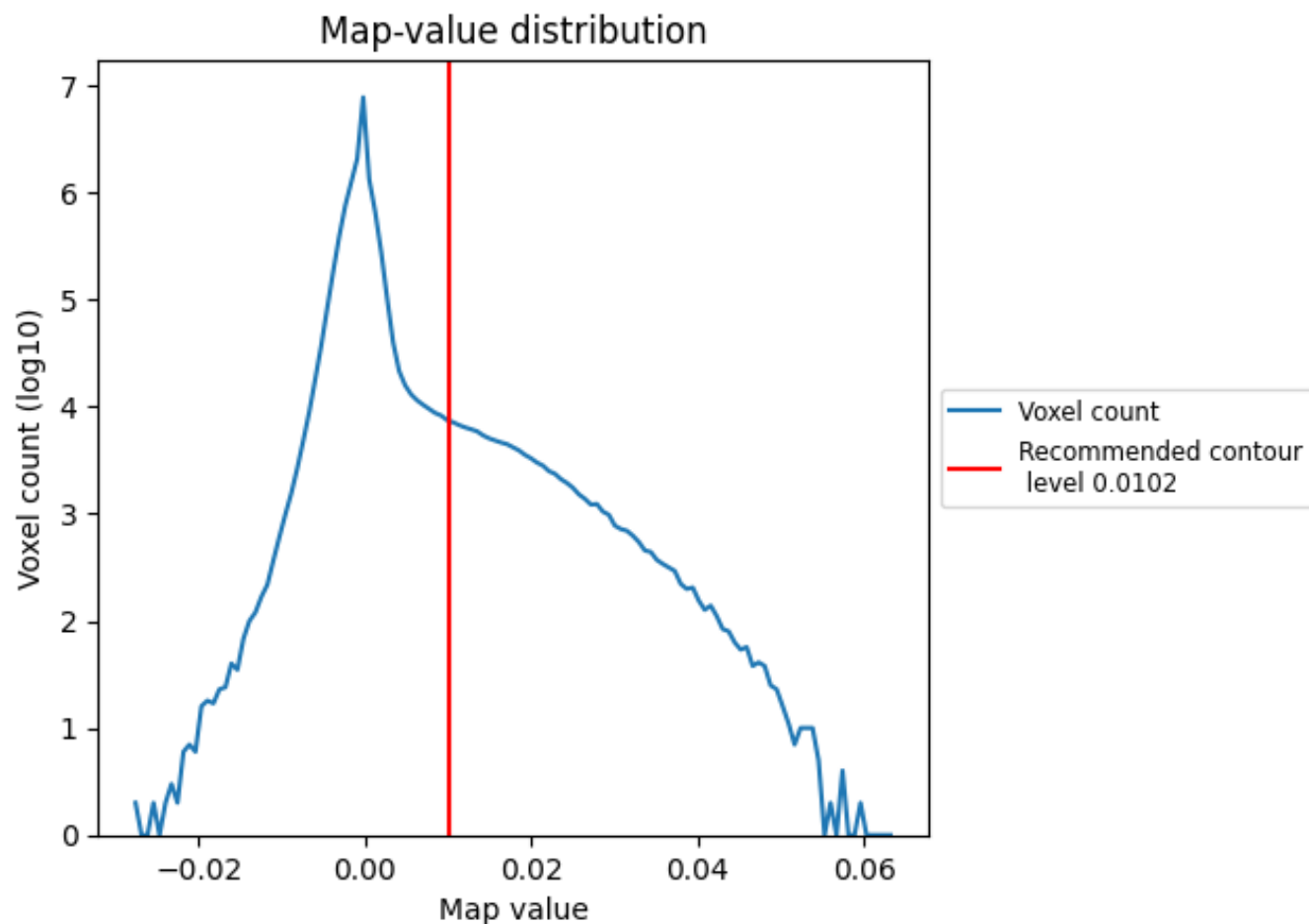
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

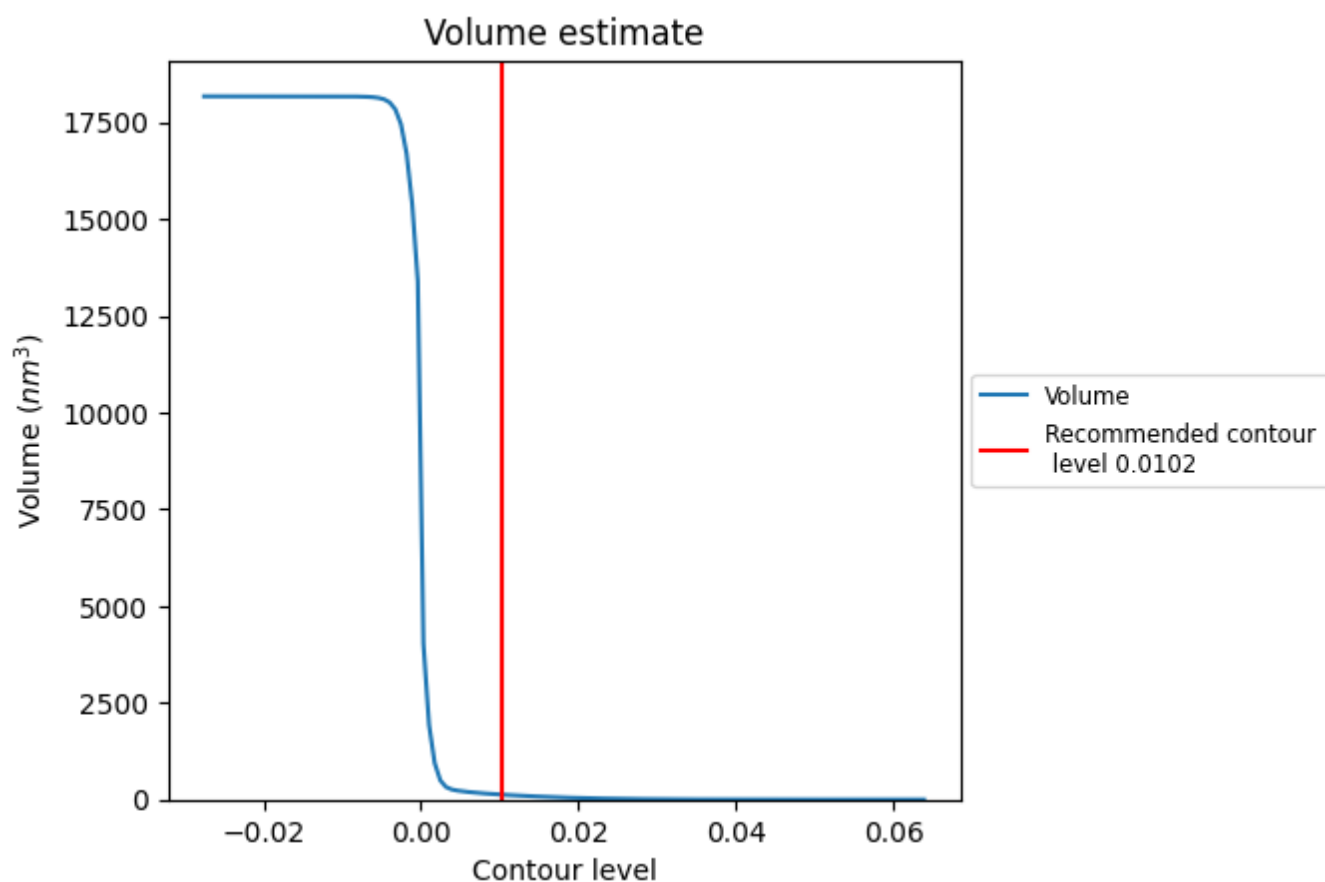
This section contains the results of statistical analysis of the map.

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.

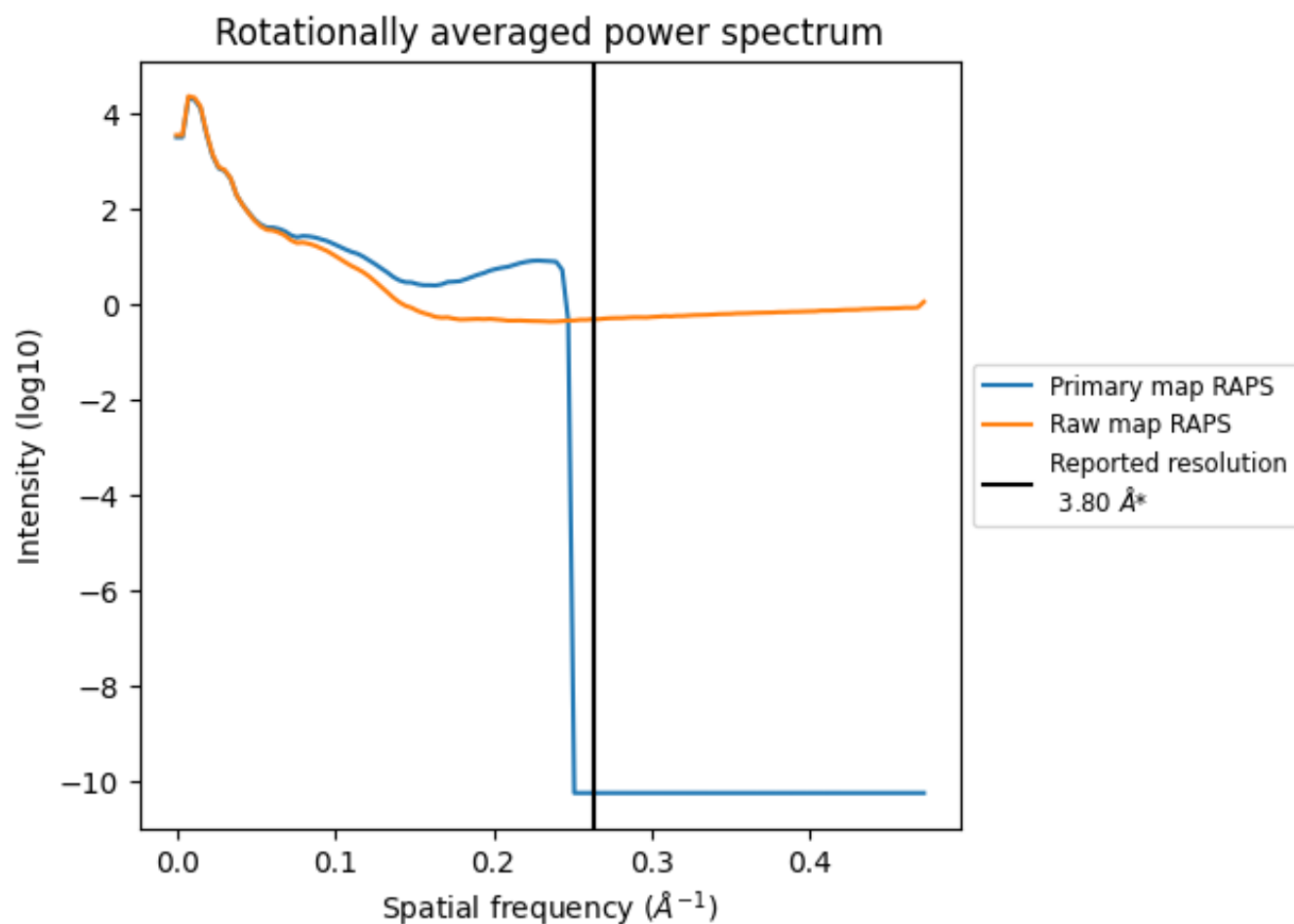
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 115 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 ⓘ

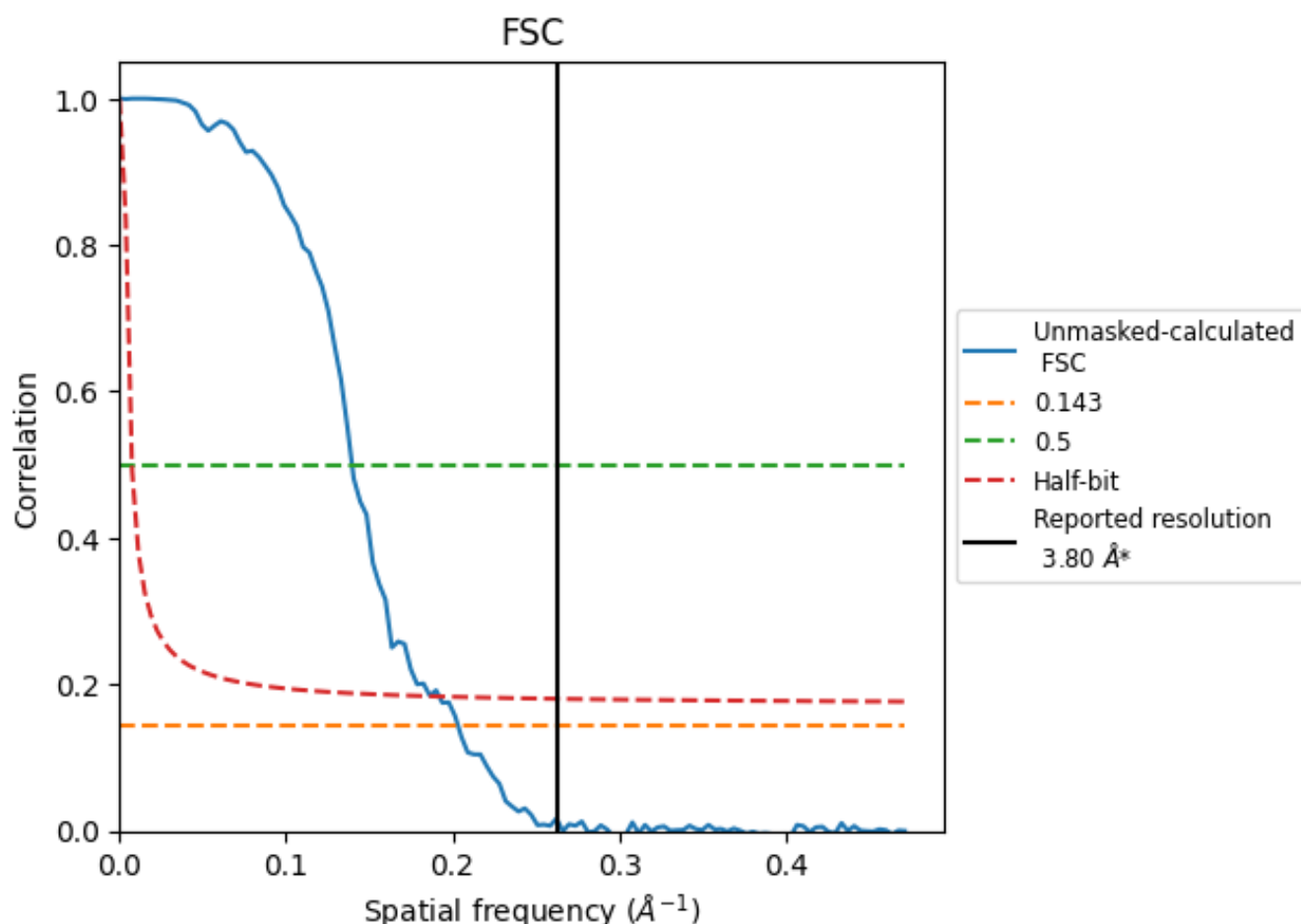


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

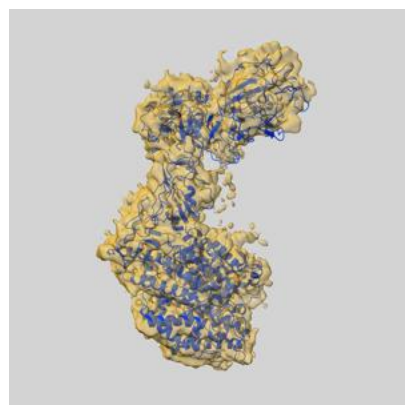
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.92	7.16	5.21

*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 4.92 differs from the reported value 3.8 by more than 10 %

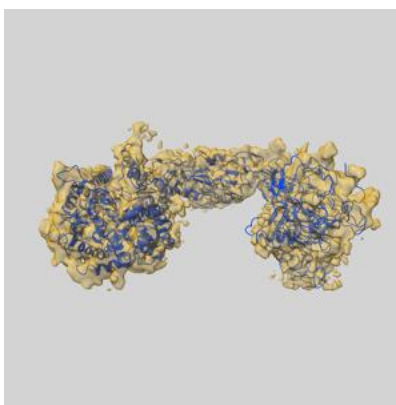
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35079 and PDB model 8HXK. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

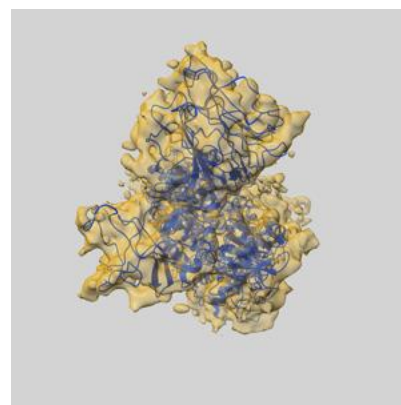
9.1 Map-model overlay [i](#)



X



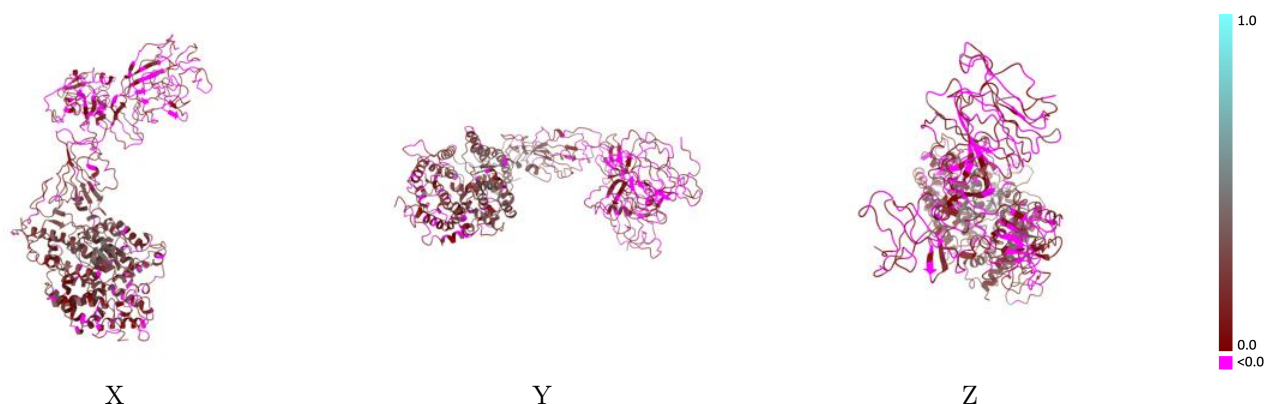
Y



Z

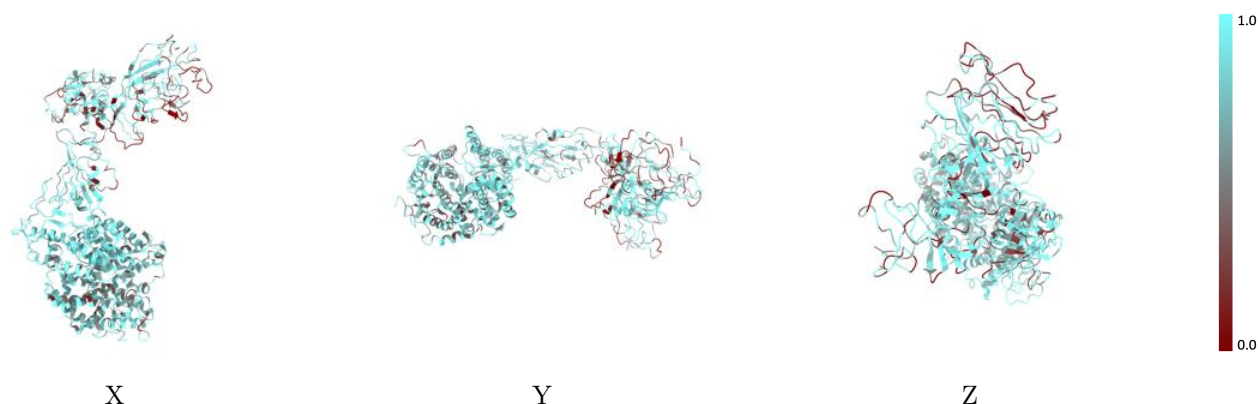
The images above show the 3D surface view of the map at the recommended contour level 0.0102 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



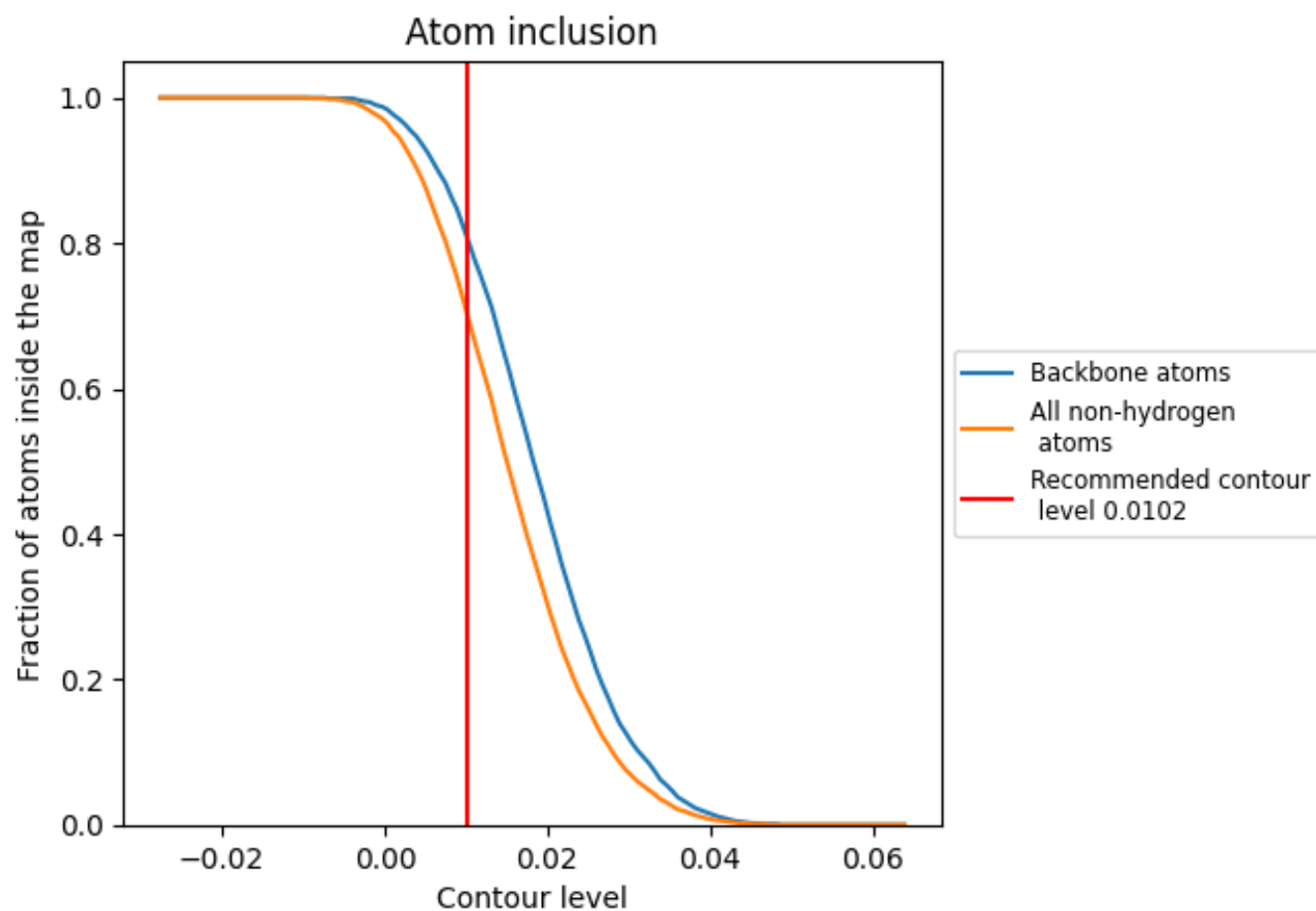
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0102).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 70% 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 (0.0102) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6990	<div></div> 0.1190
A	<div></div> 0.7670	<div></div> 0.1820
B	<div></div> 0.6370	<div></div> 0.0600
C	<div></div> 0.6430	<div></div> 0.1140
D	<div></div> 0.5710	<div></div> 0.2630

