



# wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 06:04 AM UTC

PDB ID : 9DKK / pdb\_00009dkk  
EMDB ID : EMD-46960  
Title : Designed miniproteins potently inhibit and protect against MERS-CoV. MERS-CoV S in complex with miniprotein cb3\_GGGSGGGS\_SB175, linker 7 (Local refinement of two RBDs and 2 miniproteins)  
Authors : Tortorici, M.A.; Seattle Structural Genomics Center for Infectious Disease (SSGCID); Veesler, D.  
Deposited on : 2024-09-09  
Resolution : 3.30 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](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>.

---

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

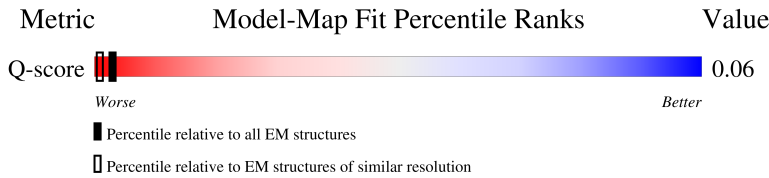
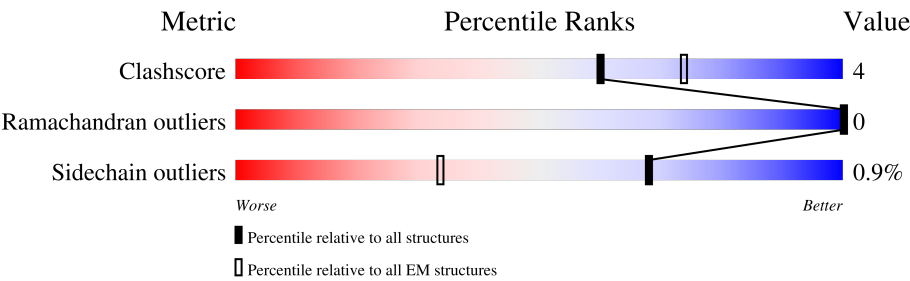
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.30 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	15087 ( 2.80 - 3.80 )

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

Mol	Chain	Length	Quality of chain
1	A	1366	<div><div>10% 12% 85%</div></div>
1	B	1366	<div><div>11% 14% 85%</div></div>
2	C	144	<div><div>31% 35% 61%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	144	<div><div></div><div>26%</div><div>34%</div><div>66%</div></div>
3	E	2	<div><div></div><div>100%</div><div>50%</div><div>50%</div></div>
3	F	2	<div><div></div><div>100%</div><div>100%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3782 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 Spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	205	Total	C	N	O	S	0	0
			1492	972	248	261	11		
1	A	205	Total	C	N	O	S	0	0
			1498	978	247	262	11		

- Molecule 2 is a protein called Miniprotein cb3\_GGGSGGGS\_SB175.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	49	Total	C	N	O	0	0
			309	205	51	53		
2	C	56	Total	C	N	O	0	0
			399	258	70	71		

- 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	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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





L411	T412	K413	L414	L415	S416	L417	F418	S419	V420	N421	D422	F423	T424	C425	S426	Q427	I428	A431	A432	I433	A434	S435	M436	L441	I442	L443	D444	Y445	F446	S447	Y448	P449	L450	S451	M452	K453	S454	D455	L456	S457	V458	S459	S460	A461	I464	S465	Q466	F467	N468	Y469	K470	Q471	S472	F473	S474	M475																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
P476	T477	C478	L479	I480	L481	A482	T483	V484	P485	H486	N487	L488	T489	T490	I491	T492	K493	P494	L495	K496	Y497	S498	Y499	I500	N501	K502	C503	S504	R505	L506	L507	S508	D509	D510	R511	T512	E513	V514	P515	Q516	L517	V518	N519	A520	N521	Q522	Y523	S524	P525	C526	V527	S528	I529	V530	P531	V534	V535	E536																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
D637	G538	D639	Y540	Y541	R542	K543	Q544	L545	S546	P547	L548	E549	G550	W553	L554	S557	G558	S559	T560	V561	A562	M563	T564	E565	Q566	I573	T574	V575	Q576	Y577	GLY	THR	T581	N582	S583	V584	C585	P586	K587	L588	GLU	PHE	ALA	ASN	ASP	THR	LYS	ILE	ALA	SER	GLN	LEU	GLY	CYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
VAL	GLU	TYR	SER	LEU	TYR	ALA	SER	GLY	PHE	VAL	ALA	ASN	CYS	HIS	THR	GLN	MET	ARG	GLN	GLN	PHE	ARG	ALA	ASP	VAL	GLY	GLY	LEU	ARG	VAL	GLY	ASP	THR	ASN	THR	TYR	PRO	GLY	ARG	VAL	GLY	ASN	VAL	GLY	THR	GLY	ASN	THR	GLY	THR	GLY	ASN	THR	GLY	VAL	GLY	ASN	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GLY	THR	GLY	VAL	GL

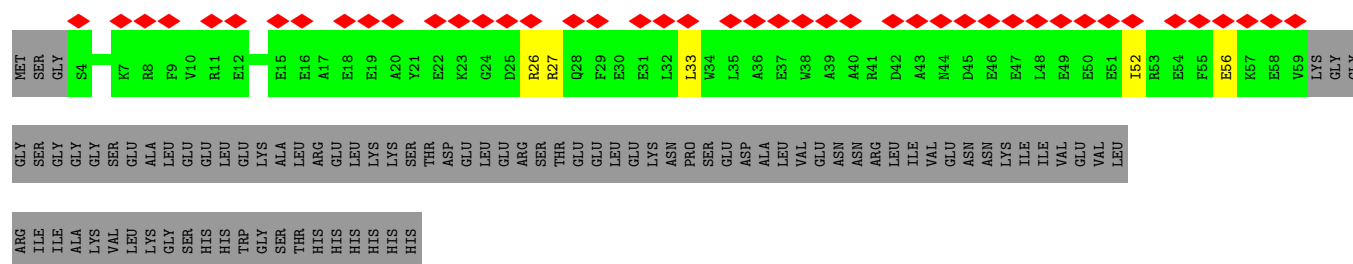
● Molecule 2: Miniprotein cb3\_GGSGGGS\_SB175



MET	SER	GLY	SER	P5	V6	K7	R8	F9	V10	R11	L14	E15	E16	A17	E18	E19	A20	Y21	E22	K23	GLY	ASP	R26	R27	Q28	F29	E30	E31	L32	L33	A36	E37	W38	A39	A40	R41	D42	A43	ASN	ASP	E46	E47	L48	E49	E50	E51	I52	R53	E54	F55	E56	K57	GLU	VAL	LYS	GLY	GLY
-----	-----	-----	-----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



- Molecule 2: Miniprotein cb3 GGGSGGGS SB175



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169944	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.242	Depositor
Minimum map value	-2.502	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.519	Depositor
Map size (Å)	512.0, 512.0, 512.0	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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	0.39	0/1536	0.55	1/2106 (0.0%)
1	B	0.32	0/1528	0.41	0/2098
2	C	0.35	0/407	0.51	0/557
2	D	0.07	0/314	0.16	0/432
All	All	0.34	0/3785	0.47	1/5193 (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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	490	THR	N-CA-C	-5.13	105.03	113.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	505	ARG	Sidechain

## 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	1498	0	1350	20	0
1	B	1492	0	1352	10	0
2	C	399	0	328	4	0
2	D	309	0	221	0	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
All	All	3782	0	3327	32	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.

The worst 5 of 32 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:465:SER:O	2:C:27:ARG:NH2	2.35	0.58
1:B:456:LEU:HD23	1:B:481:LEU:HD11	1.87	0.56
1:A:408:ASN:HA	1:A:585:CYS:O	2.05	0.56
1:A:496:LYS:NZ	1:A:535:TRP:O	2.32	0.54
1:B:545:LEU:HD11	1:B:554:LEU:HB2	1.91	0.53

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	201/1366 (15%)	192 (96%)	9 (4%)	0	100	100
1	B	201/1366 (15%)	194 (96%)	7 (4%)	0	100	100
2	C	54/144 (38%)	54 (100%)	0	0	100	100
2	D	43/144 (30%)	43 (100%)	0	0	100	100
All	All	499/3020 (16%)	483 (97%)	16 (3%)	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	140/1174 (12%)	138 (99%)	2 (1%)	59	73
1	B	140/1174 (12%)	139 (99%)	1 (1%)	76	80
2	C	28/124 (23%)	28 (100%)	0	100	100
2	D	15/124 (12%)	15 (100%)	0	100	100
All	All	323/2596 (12%)	320 (99%)	3 (1%)	68	78

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

Mol	Chain	Res	Type
1	B	458	VAL
1	A	491	ILE
1	A	507	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	427	GLN
1	B	436	ASN
1	A	486	HIS
1	A	522	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	E	1	3,1	14,14,15	0.38	0	17,19,21	0.55	0
3	NAG	E	2	3	14,14,15	0.38	0	17,19,21	0.49	0
3	NAG	F	1	3,1	14,14,15	0.39	0	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.38	0	17,19,21	0.45	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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

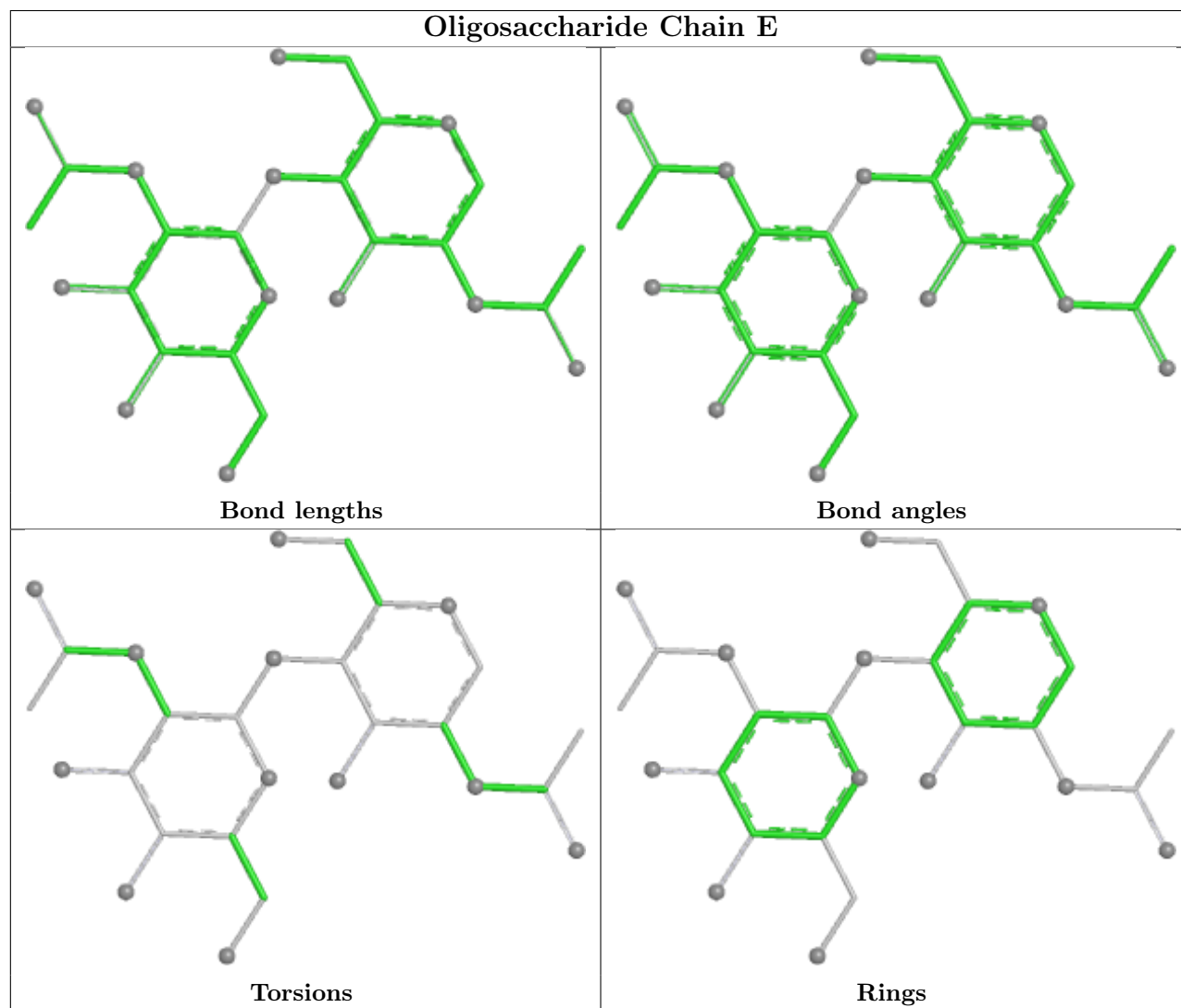
There are no torsion outliers.

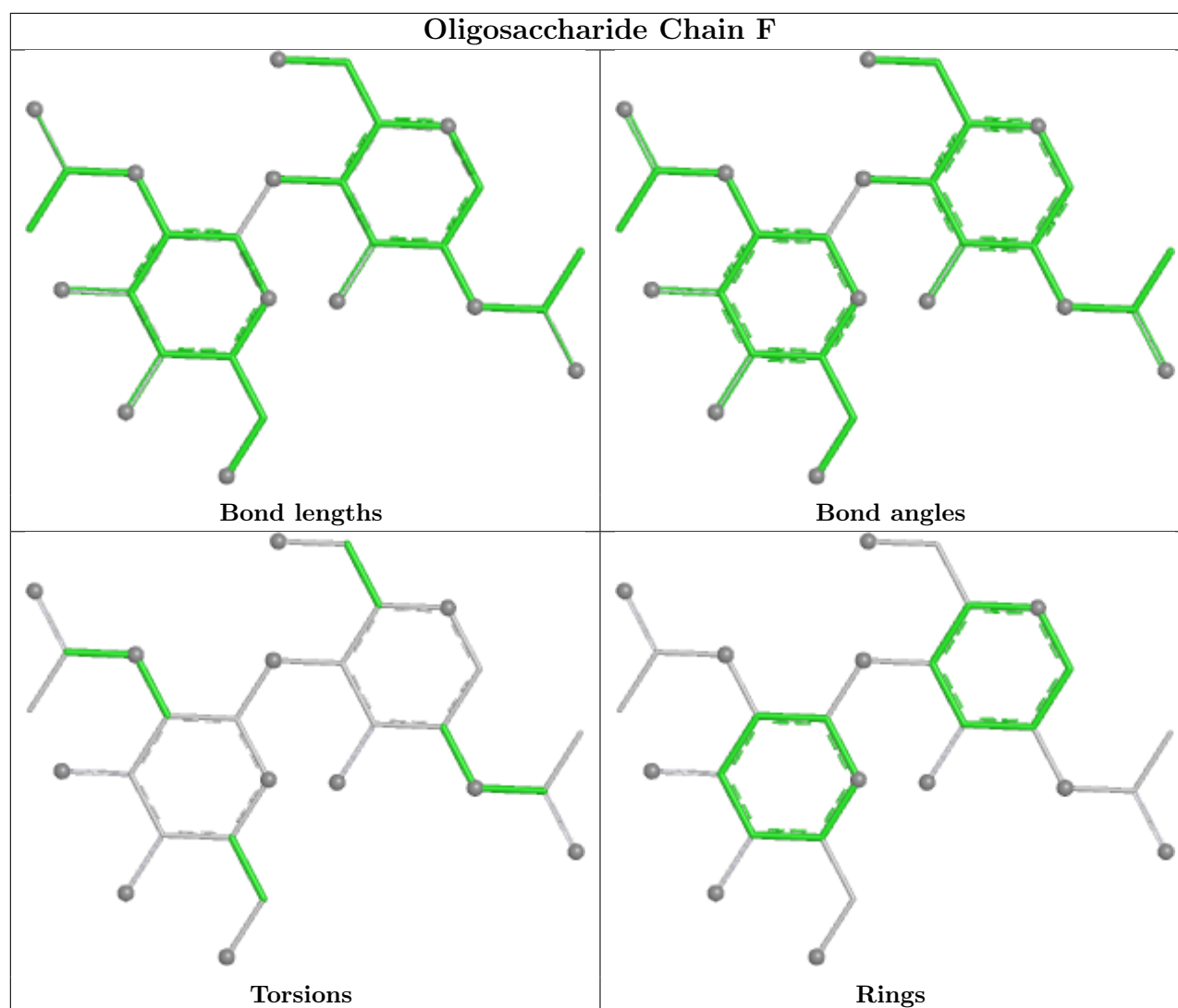
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0

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





## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	1401	1	14,14,15	0.71	0	17,19,21	0.85	0
4	NAG	A	1401	1	14,14,15	0.74	0	17,19,21	0.71	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
4	NAG	B	1401	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

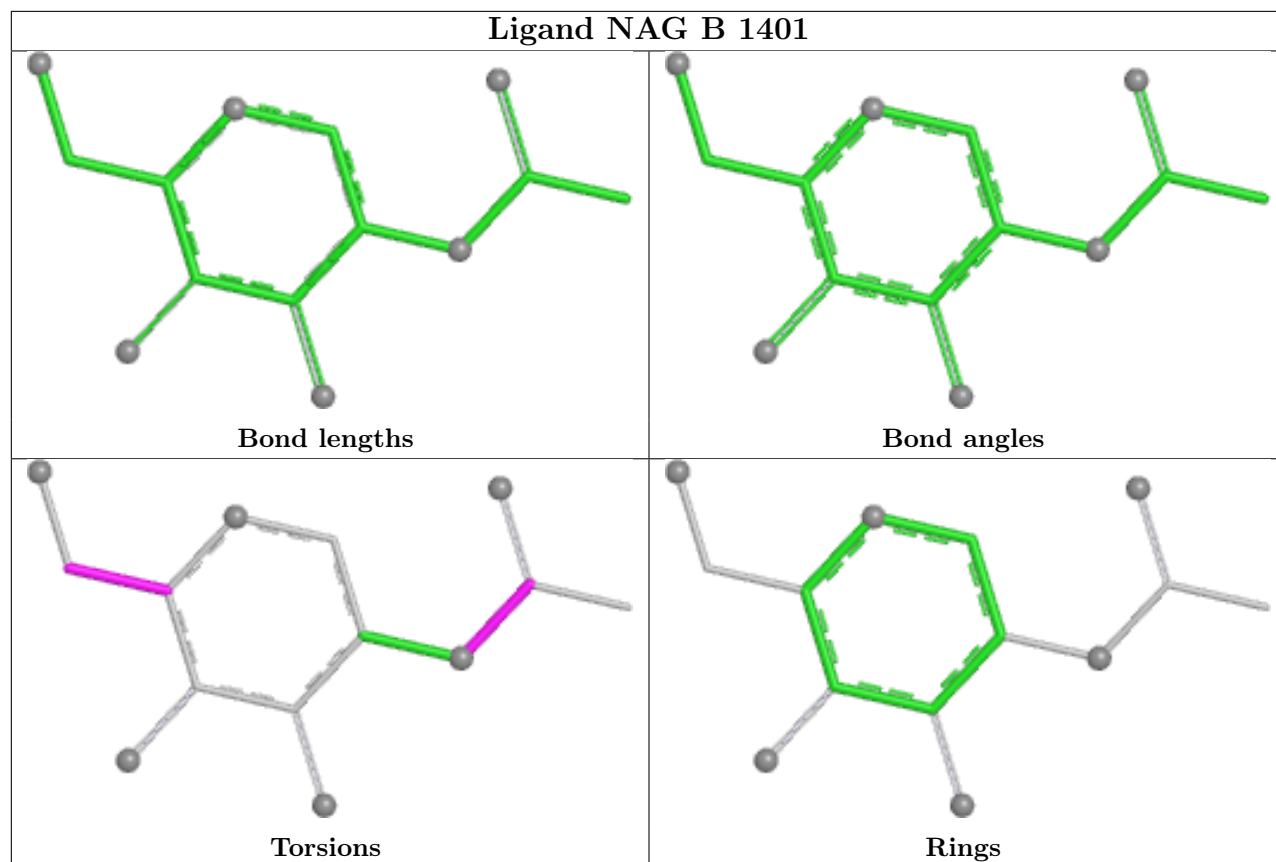
Mol	Chain	Res	Type	Atoms
4	B	1401	NAG	C8-C7-N2-C2
4	B	1401	NAG	O7-C7-N2-C2
4	B	1401	NAG	O5-C5-C6-O6

There are no ring outliers.

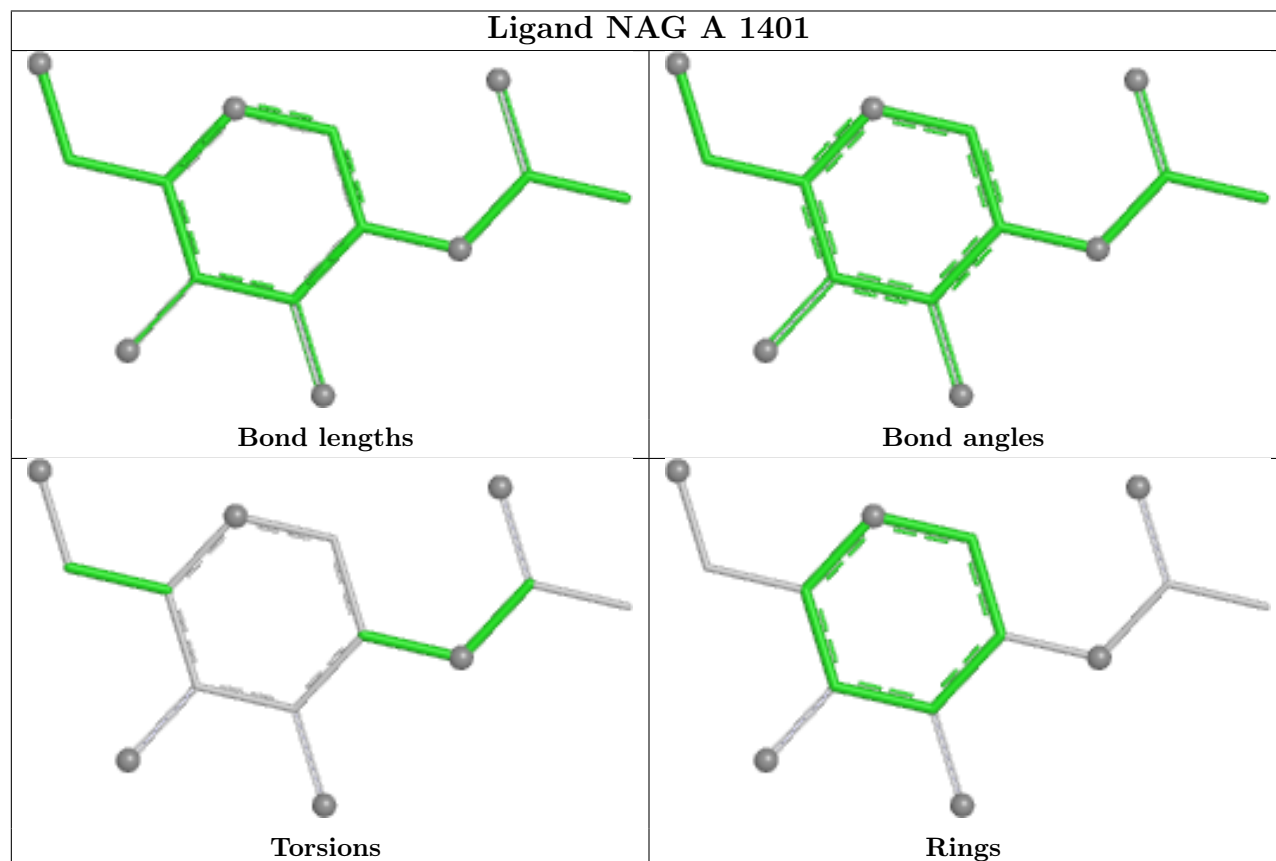
No monomer is involved in short contacts.

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.

## Ligand NAG B 1401



## Ligand NAG A 1401



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

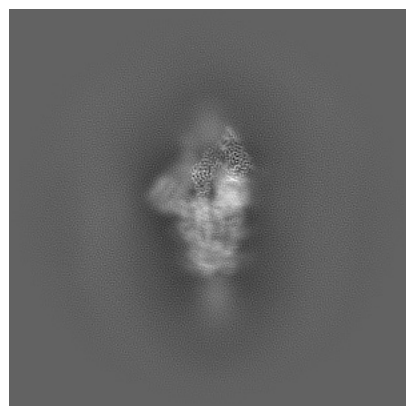
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46960. These allow visual inspection of the internal detail of the map and identification of artifacts.

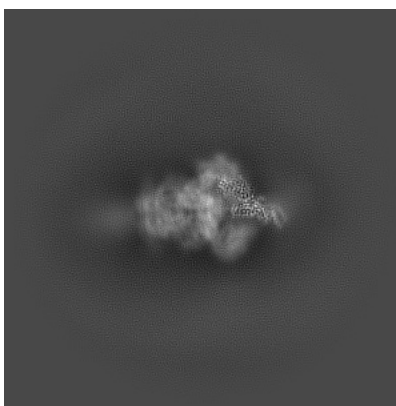
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

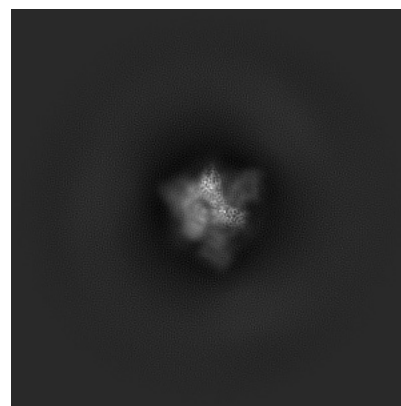
#### 6.1.1 Primary map



X

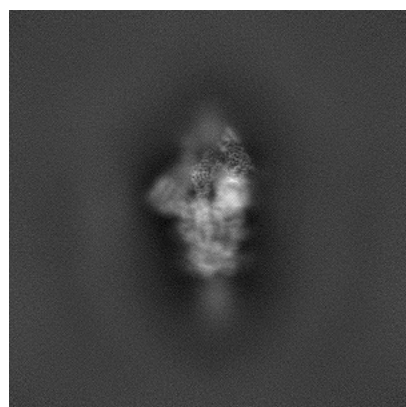


Y

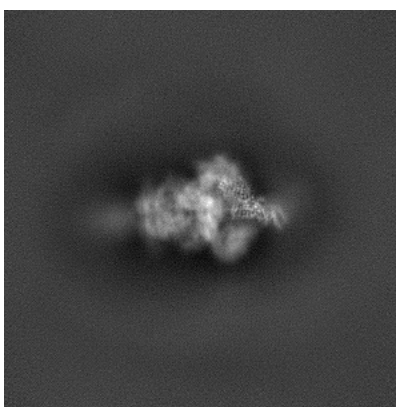


Z

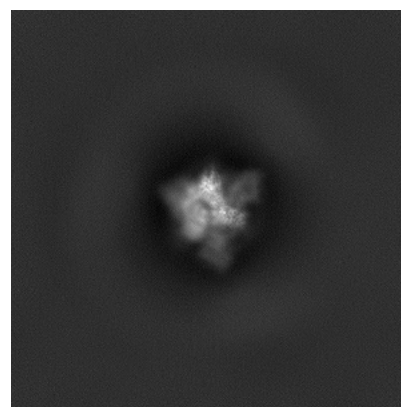
#### 6.1.2 Raw map



X



Y



Z

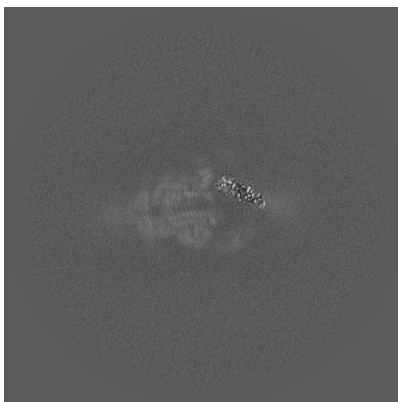
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

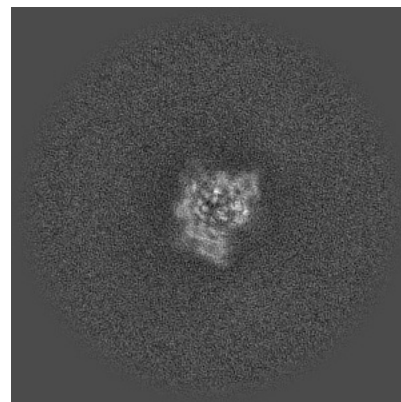
### 6.2.1 Primary map



X Index: 256



Y Index: 256

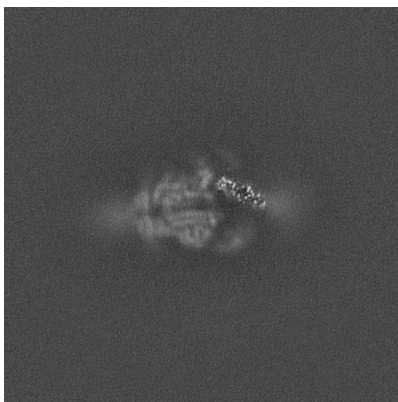


Z Index: 256

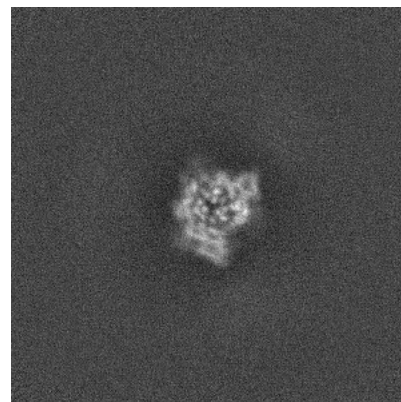
### 6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

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

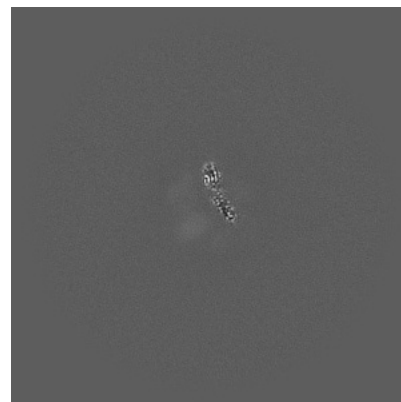
### 6.3.1 Primary map



X Index: 257



Y Index: 248



Z Index: 311

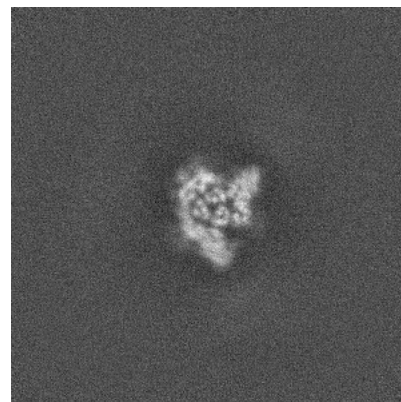
### 6.3.2 Raw map



X Index: 257



Y Index: 282



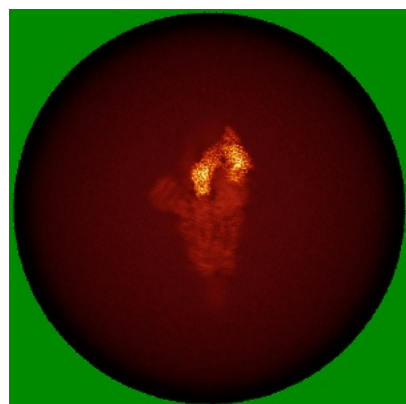
Z Index: 262

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

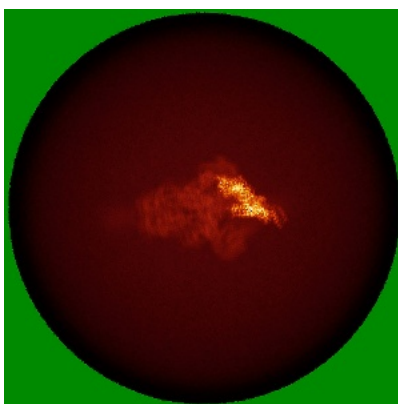


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

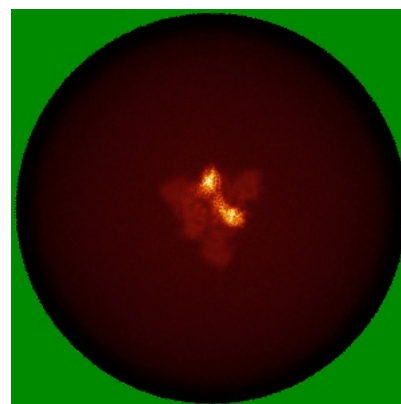
### 6.4.1 Primary map



X

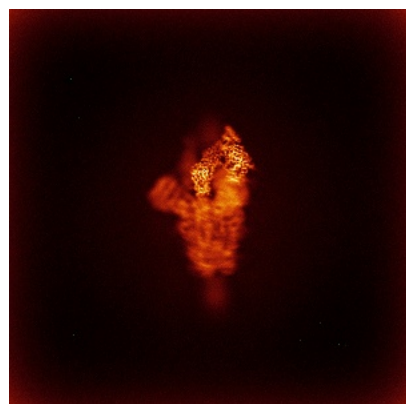


Y

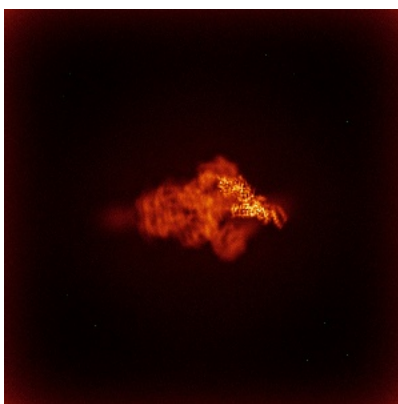


Z

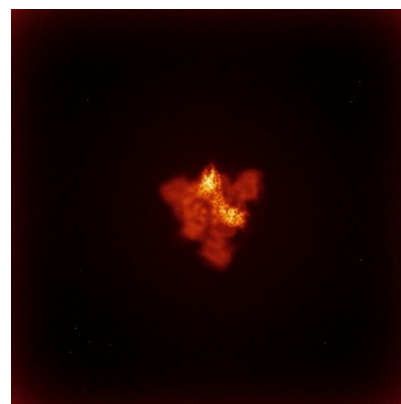
### 6.4.2 Raw map



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.

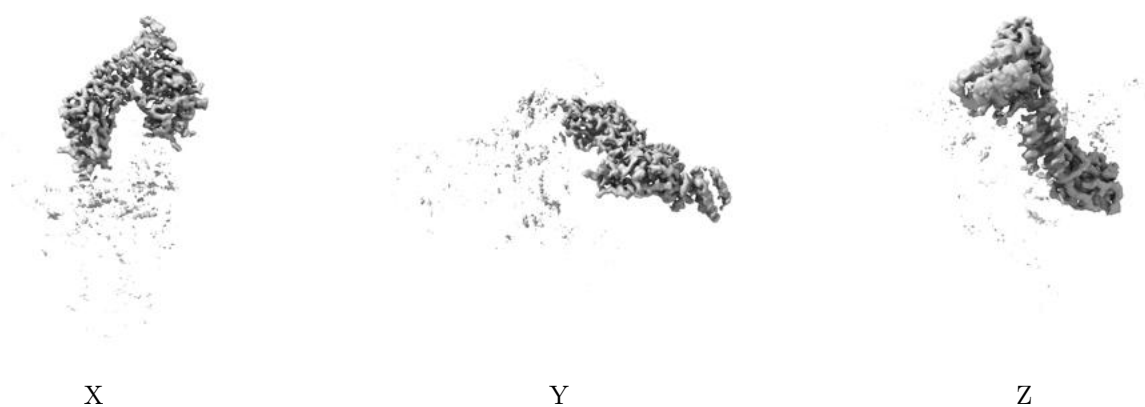
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.519. 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](#)

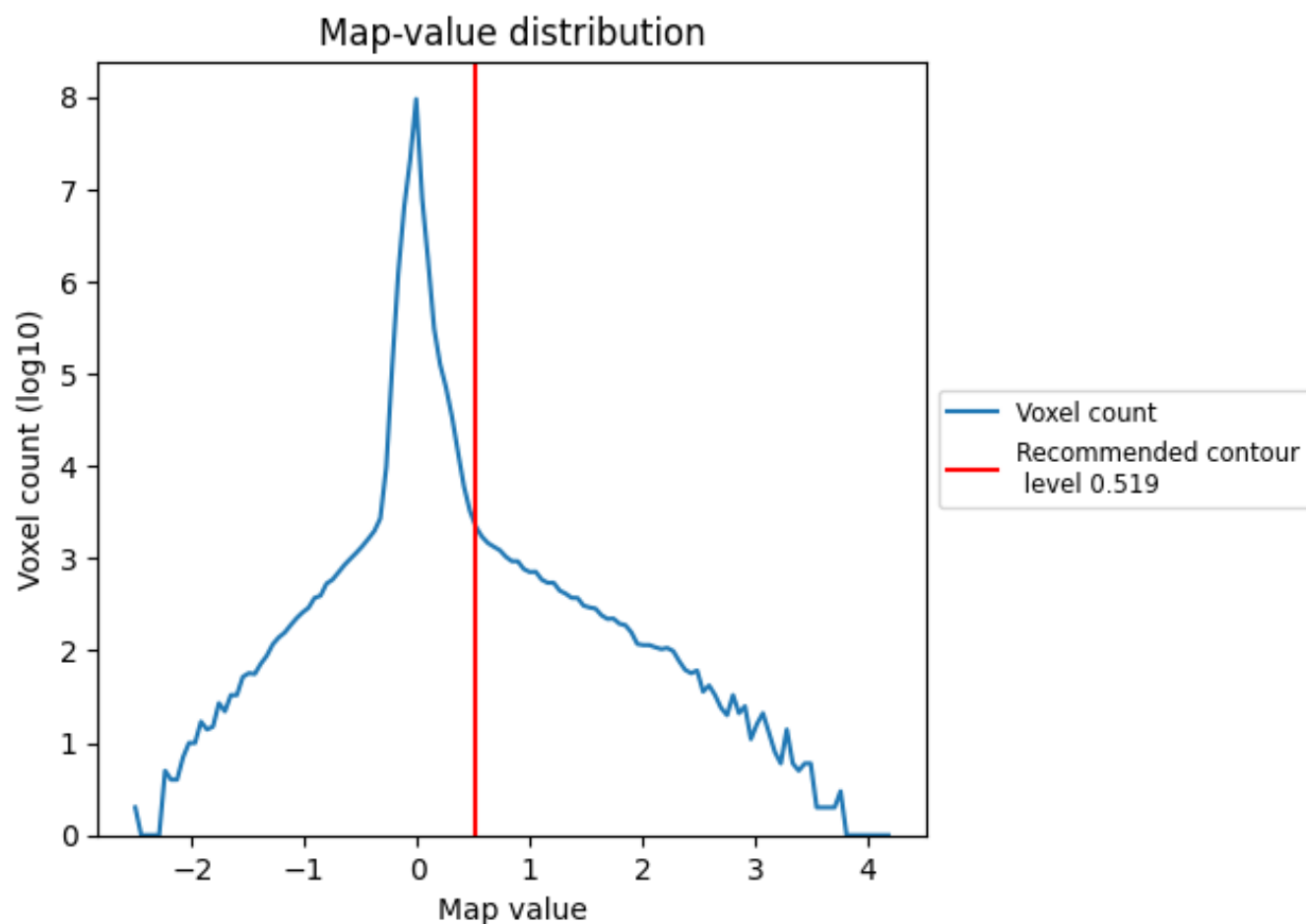
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

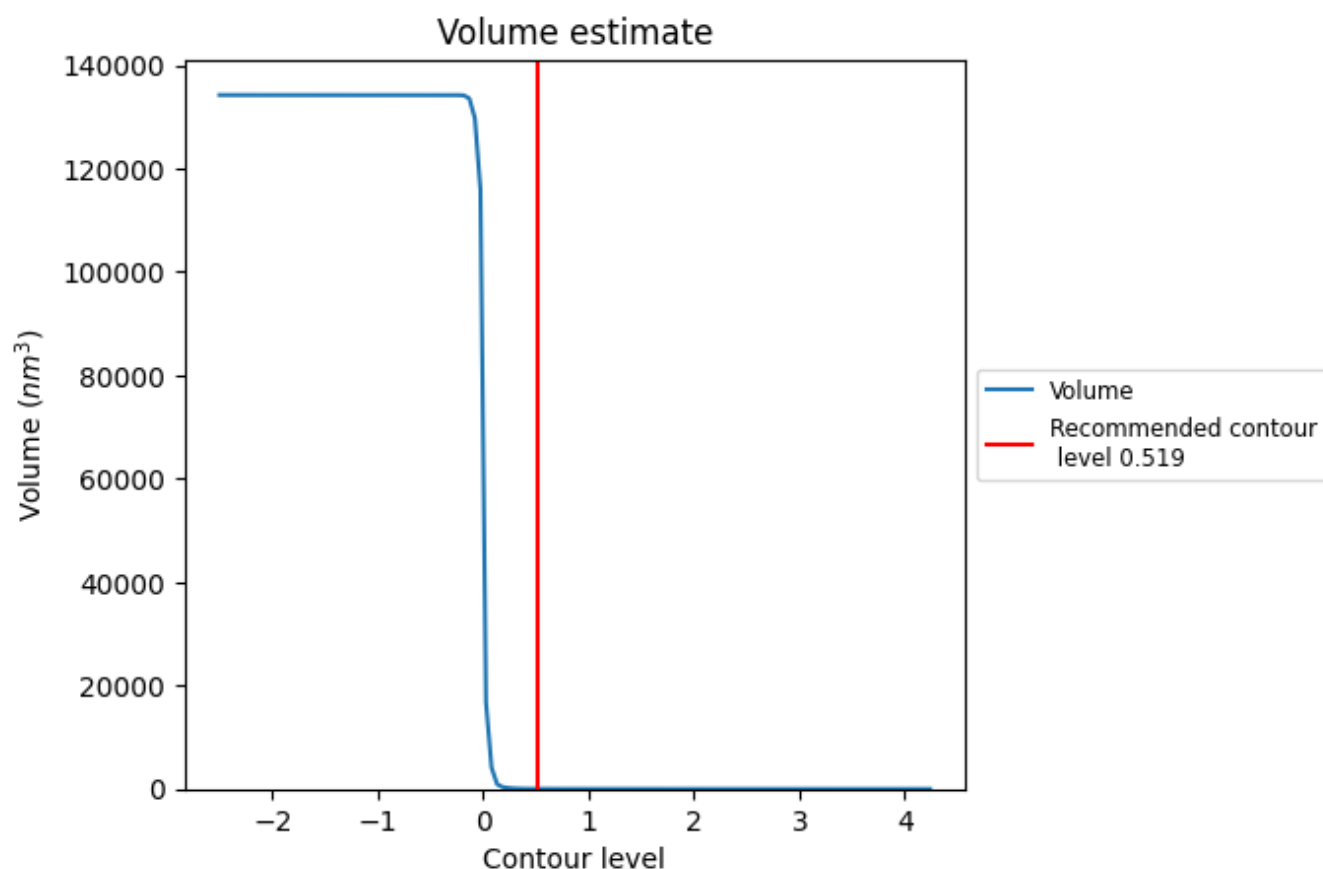
This section contains the results of statistical analysis of the map.

### 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.

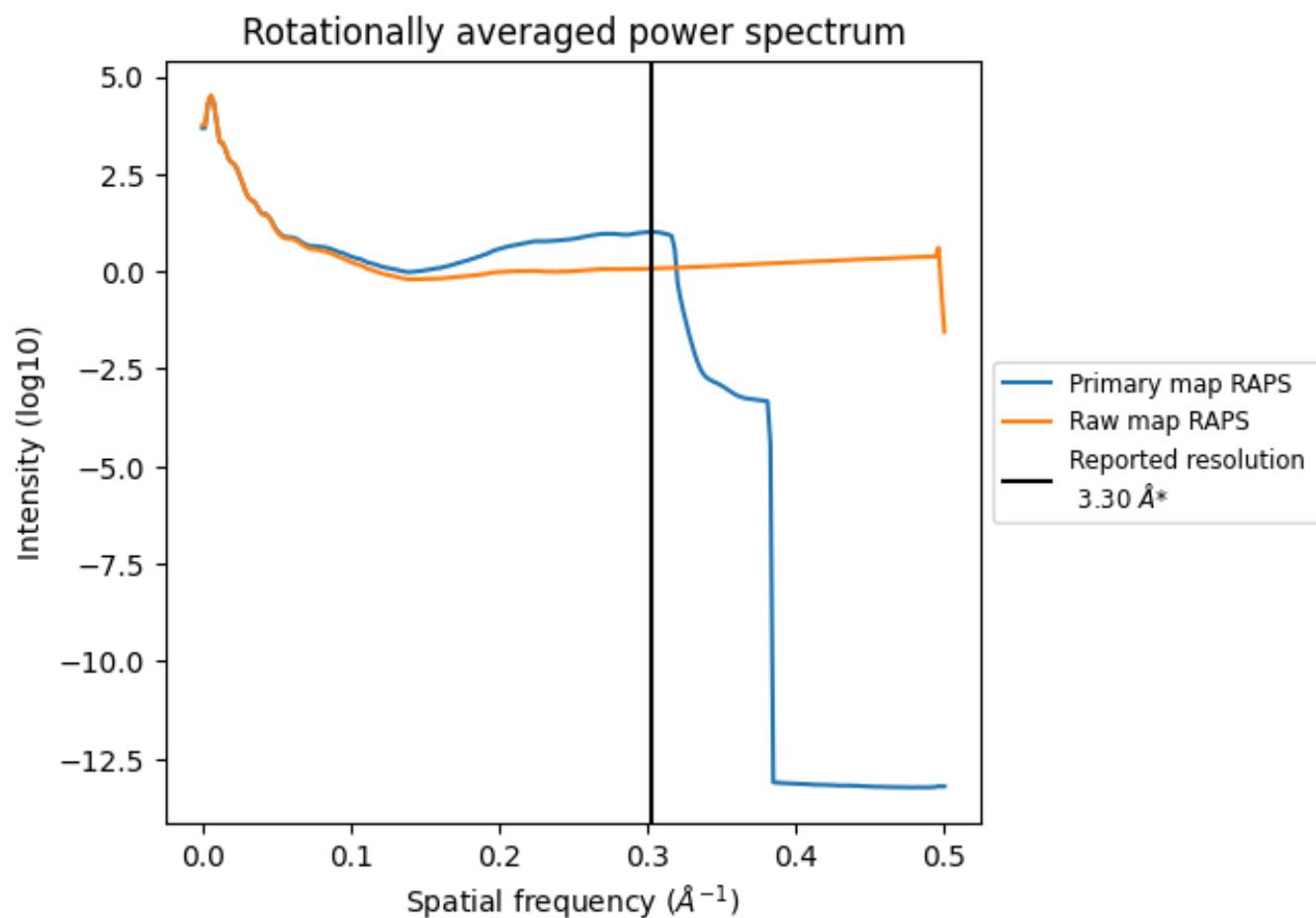
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 20  $\text{nm}^3$ ; this corresponds to an approximate mass of 18 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 ⓘ

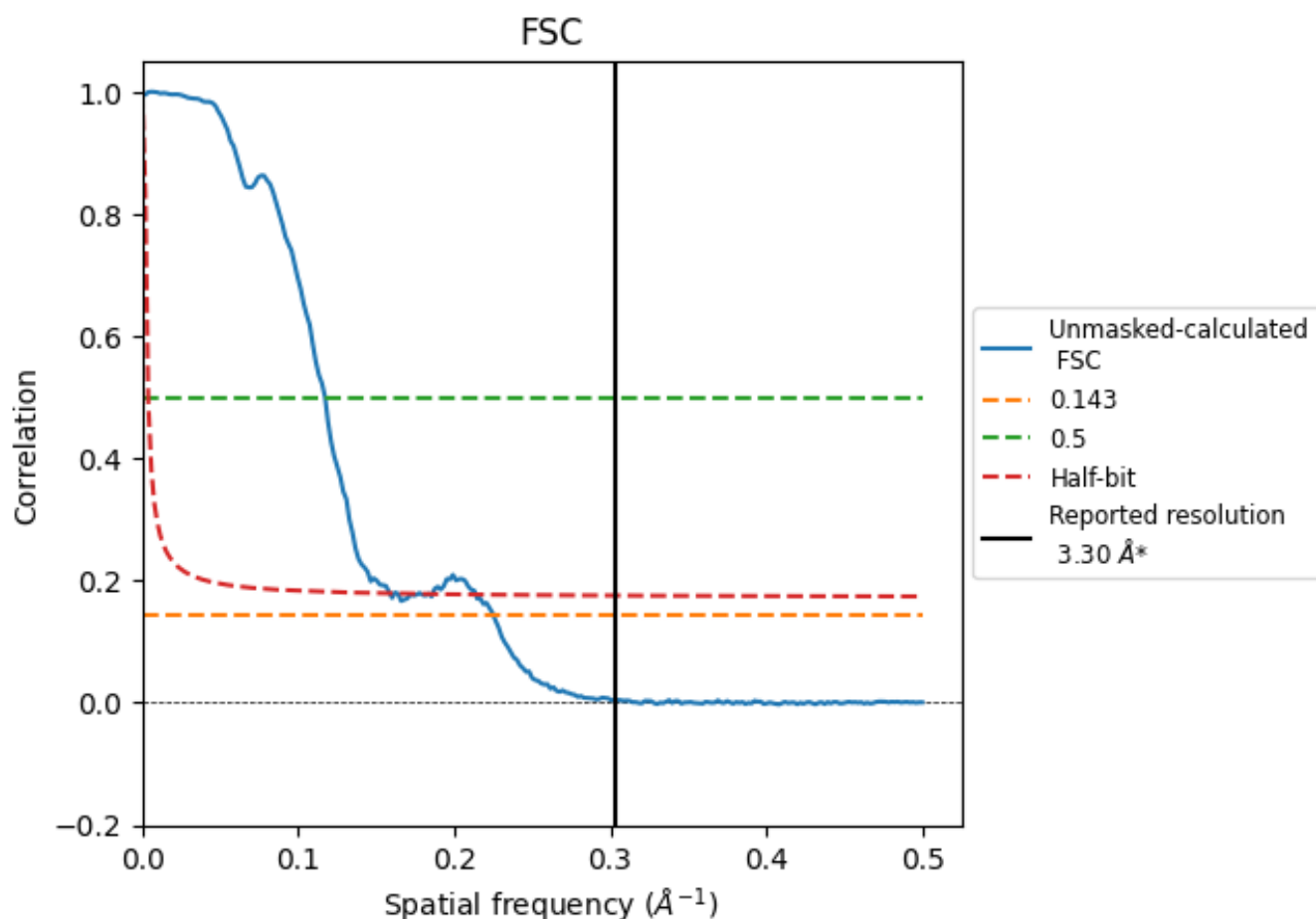


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

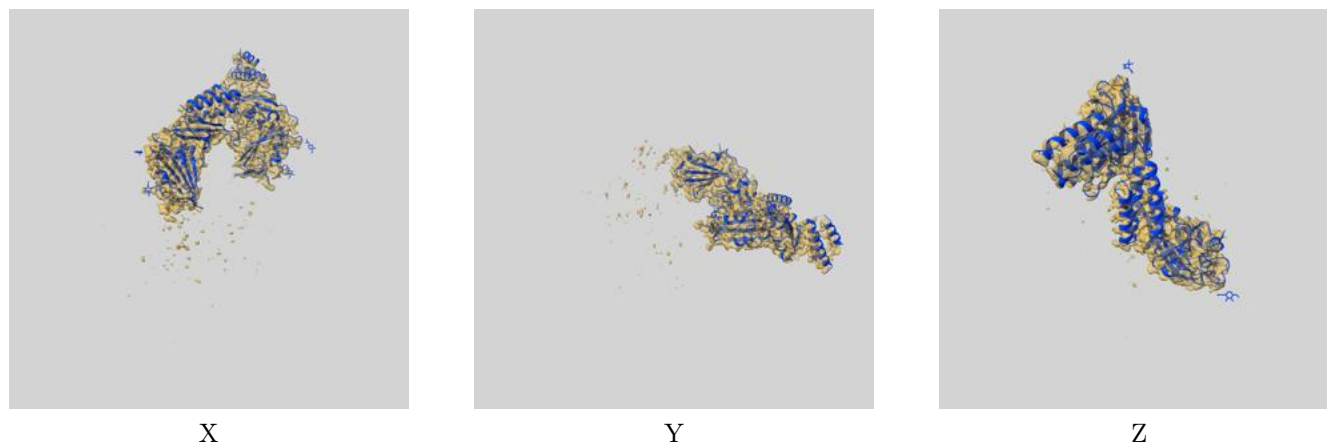
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	8.53	6.30

\*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 4.44 differs from the reported value 3.3 by more than 10 %

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

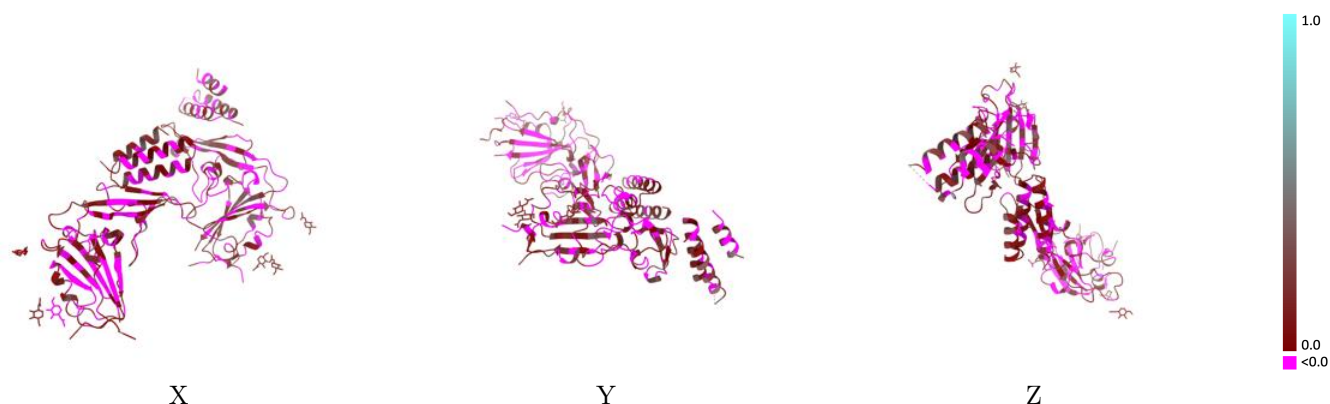
This section contains information regarding the fit between EMDB map EMD-46960 and PDB model 9DKK. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



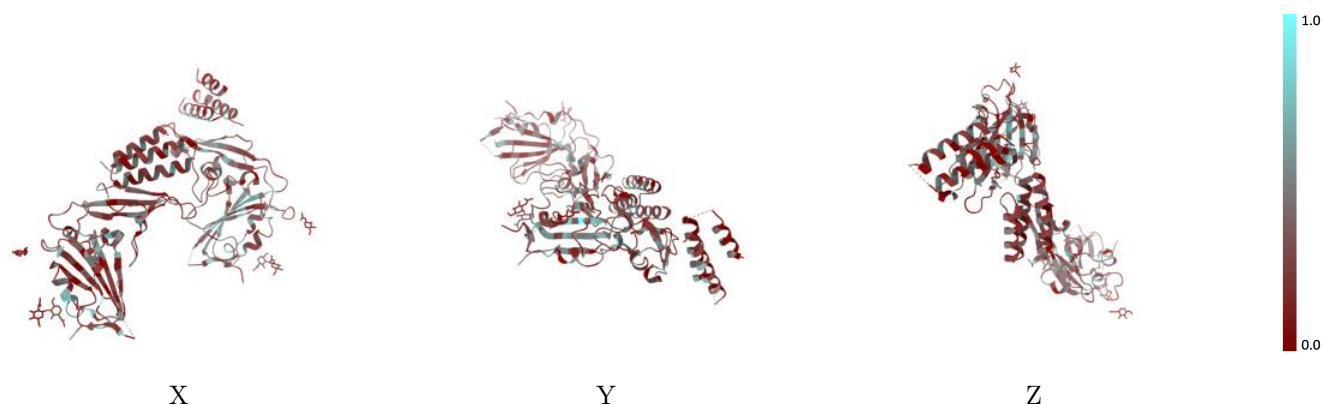
The images above show the 3D surface view of the map at the recommended contour level 0.519 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



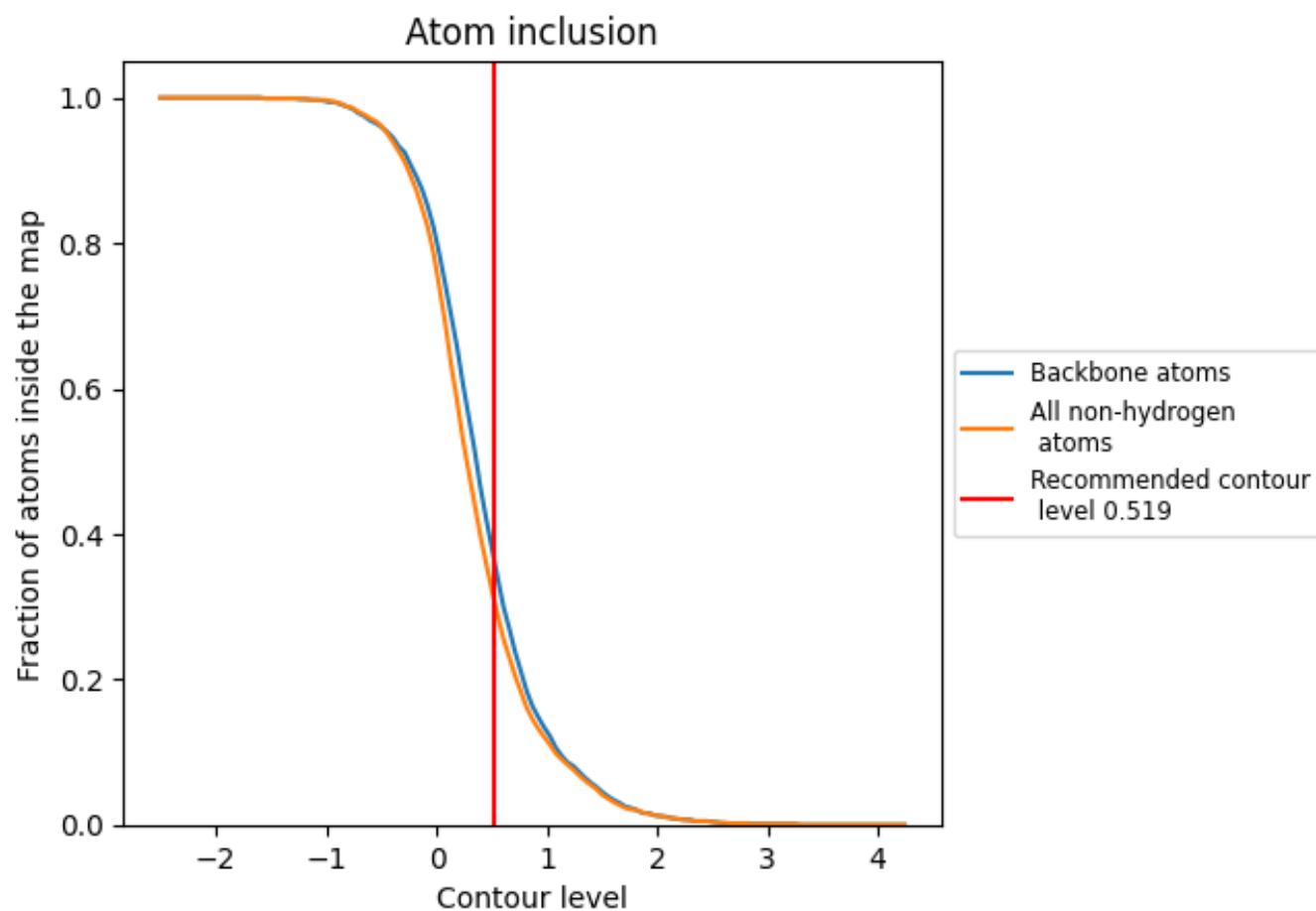
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.519).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 31% 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 (0.519) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.3100	<div><div></div></div> 0.0600
A	<div><div></div></div> 0.3410	<div><div></div></div> 0.0640
B	<div><div></div></div> 0.2980	<div><div></div></div> 0.0410
C	<div><div></div></div> 0.2920	<div><div></div></div> 0.0750
D	<div><div></div></div> 0.2670	<div><div></div></div> 0.1070
E	<div><div></div></div> 0.2500	<div><div></div></div> 0.1630
F	<div><div></div></div> 0.1070	<div><div></div></div> 0.0190

1.0

0.0

<0.0