



Full wwPDB EM Validation Report ⓘ

May 23, 2026 – 05:15 PM EDT

PDB ID : 9Z3K / pdb_00009z3k
EMDB ID : EMD-73787
Title : SARS-CoV-2 S2 trimer stabilized in the early fusion intermediate conformation by circular permutation and clamping by gp41 (E-FICs-v1)
Authors : McCallum, M.; Seattle Structural Genomics Center for Infectious Disease (SS-GCID); Veesler, D.
Deposited on : 2025-11-07
Resolution : 3.30 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

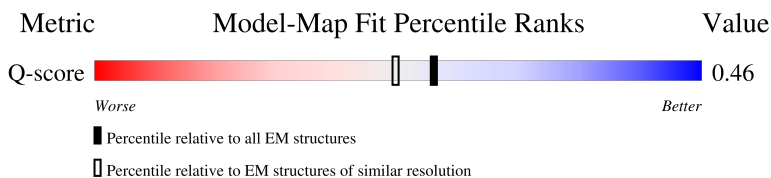
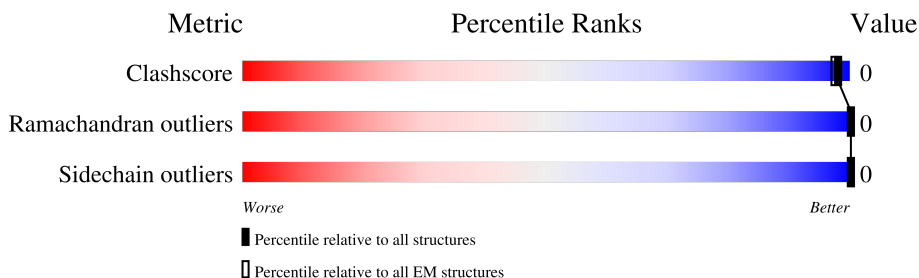
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 ≥ 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	608	 64% 34%
1	B	608	 64% 34%
1	C	608	 64% 34%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8448 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	A	404	Total	C	N	O	S	0	0
			2732	1747	496	480	9		
1	B	404	Total	C	N	O	S	0	0
			2732	1747	496	480	9		
1	C	404	Total	C	N	O	S	0	0
			2732	1747	496	480	9		

There are 513 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	735	MET	-	expression tag	UNP Q12306
A	736	THR	-	expression tag	UNP Q12306
A	737	ARG	-	expression tag	UNP Q12306
A	738	LEU	-	expression tag	UNP Q12306
A	739	THR	-	expression tag	UNP Q12306
A	740	VAL	-	expression tag	UNP Q12306
A	741	LEU	-	expression tag	UNP Q12306
A	742	ALA	-	expression tag	UNP Q12306
A	743	LEU	-	expression tag	UNP Q12306
A	744	LEU	-	expression tag	UNP Q12306
A	745	ALA	-	expression tag	UNP Q12306
A	746	GLY	-	expression tag	UNP Q12306
A	747	LEU	-	expression tag	UNP Q12306
A	748	LEU	-	expression tag	UNP Q12306
A	749	ALA	-	expression tag	UNP Q12306
A	750	SER	-	expression tag	UNP Q12306
A	751	SER	-	expression tag	UNP Q12306
A	752	ARG	-	expression tag	UNP Q12306
A	753	ALA	-	expression tag	UNP Q12306
A	754	SER	-	expression tag	UNP Q12306
A	849	ASN	-	linker	UNP Q12306
A	850	ASP	-	linker	UNP Q12306
A	851	ASP	-	linker	UNP Q12306
A	852	ASP	-	linker	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
A	853	ASP	-	linker	UNP Q12306
A	854	LYS	-	linker	UNP Q12306
A	855	THR	-	linker	UNP Q12306
A	856	GLY	-	linker	UNP Q12306
A	857	THR	-	linker	UNP Q12306
A	858	GLY	-	linker	UNP Q12306
A	859	SER	-	linker	UNP Q12306
A	860	THR	-	linker	UNP Q12306
A	861	VAL	-	linker	UNP Q12306
A	862	GLN	-	linker	UNP Q12306
A	863	VAL	-	linker	UNP Q12306
A	864	ARG	-	linker	UNP Q12306
A	865	LYS	-	linker	UNP Q12306
A	866	LEU	-	linker	UNP Q12306
A	867	LEU	-	linker	UNP Q12306
A	868	SER	-	linker	UNP Q12306
A	869	GLY	-	linker	UNP Q12306
A	870	ILE	-	linker	UNP Q12306
A	871	VAL	-	linker	UNP Q12306
A	872	GLN	-	linker	UNP Q12306
A	873	GLN	-	linker	UNP Q12306
A	874	GLN	-	linker	UNP Q12306
A	875	SER	-	linker	UNP Q12306
A	876	ASN	-	linker	UNP Q12306
A	877	LEU	-	linker	UNP Q12306
A	878	LEU	-	linker	UNP Q12306
A	879	ARG	-	linker	UNP Q12306
A	880	ALA	-	linker	UNP Q12306
A	881	ILE	-	linker	UNP Q12306
A	882	GLU	-	linker	UNP Q12306
A	883	ALA	-	linker	UNP Q12306
A	884	GLN	-	linker	UNP Q12306
A	885	GLN	-	linker	UNP Q12306
A	886	HIS	-	linker	UNP Q12306
A	887	LEU	-	linker	UNP Q12306
A	888	LEU	-	linker	UNP Q12306
A	889	LYS	-	linker	UNP Q12306
A	890	LEU	-	linker	UNP Q12306
A	891	THR	-	linker	UNP Q12306
A	892	VAL	-	linker	UNP Q12306
A	893	TRP	-	linker	UNP Q12306
A	894	GLY	-	linker	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
A	895	ILE	-	linker	UNP Q12306
A	896	LYS	-	linker	UNP Q12306
A	897	GLN	-	linker	UNP Q12306
A	898	LEU	-	linker	UNP Q12306
A	899	GLN	-	linker	UNP Q12306
A	900	ALA	-	linker	UNP Q12306
A	901	GLN	-	linker	UNP Q12306
A	902	VAL	-	linker	UNP Q12306
A	903	GLU	-	linker	UNP Q12306
A	904	GLU	-	linker	UNP Q12306
A	905	ARG	-	linker	UNP Q12306
A	906	ILE	-	linker	UNP Q12306
A	907	ASN	-	linker	UNP Q12306
A	908	ALA	-	linker	UNP Q12306
A	909	ILE	-	linker	UNP Q12306
A	910	GLU	-	linker	UNP Q12306
A	911	THR	-	linker	UNP Q12306
A	912	ALA	-	linker	UNP Q12306
A	913	ILE	-	linker	UNP Q12306
A	985	ALA	ASP	conflict	UNP P0DTC2
A	1132	THR	-	linker	UNP P0DTC2
A	1829	PRO	-	expression tag	UNP P0DTC2
A	1830	ASP	-	expression tag	UNP P0DTC2
A	1831	PRO	-	expression tag	UNP P0DTC2
A	1832	GLY	-	expression tag	UNP P0DTC2
A	1833	SER	-	expression tag	UNP P0DTC2
A	1834	ASN	-	expression tag	UNP P0DTC2
A	1835	GLU	-	expression tag	UNP P0DTC2
A	1836	GLU	-	expression tag	UNP P0DTC2
A	1837	TRP	-	expression tag	UNP P0DTC2
A	1838	LEU	-	expression tag	UNP P0DTC2
A	1839	GLN	-	expression tag	UNP P0DTC2
A	1840	TRP	-	expression tag	UNP P0DTC2
A	1841	ASP	-	expression tag	UNP P0DTC2
A	1842	LYS	-	expression tag	UNP P0DTC2
A	1843	GLU	-	expression tag	UNP P0DTC2
A	1844	ILE	-	expression tag	UNP P0DTC2
A	1845	SER	-	expression tag	UNP P0DTC2
A	1846	ASN	-	expression tag	UNP P0DTC2
A	1847	TYR	-	expression tag	UNP P0DTC2
A	1848	THR	-	expression tag	UNP P0DTC2
A	1849	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1850	ILE	-	expression tag	UNP P0DTC2
A	1851	ILE	-	expression tag	UNP P0DTC2
A	1852	TYR	-	expression tag	UNP P0DTC2
A	1853	GLU	-	expression tag	UNP P0DTC2
A	1854	LEU	-	expression tag	UNP P0DTC2
A	1855	ILE	-	expression tag	UNP P0DTC2
A	1856	GLU	-	expression tag	UNP P0DTC2
A	1857	GLU	-	expression tag	UNP P0DTC2
A	1858	SER	-	expression tag	UNP P0DTC2
A	1859	GLN	-	expression tag	UNP P0DTC2
A	1860	LYS	-	expression tag	UNP P0DTC2
A	1861	GLN	-	expression tag	UNP P0DTC2
A	1862	GLN	-	expression tag	UNP P0DTC2
A	1863	GLU	-	expression tag	UNP P0DTC2
A	1864	LYS	-	expression tag	UNP P0DTC2
A	1865	ASN	-	expression tag	UNP P0DTC2
A	1133	GLU	-	expression tag	UNP P0DTC2
A	1134	GLN	-	expression tag	UNP P0DTC2
A	1135	GLU	-	expression tag	UNP P0DTC2
A	1136	LEU	-	expression tag	UNP P0DTC2
A	1137	LEU	-	expression tag	UNP P0DTC2
A	1138	GLU	-	expression tag	UNP P0DTC2
A	1139	LEU	-	expression tag	UNP P0DTC2
A	1140	ASP	-	expression tag	UNP P0DTC2
A	1141	LYS	-	expression tag	UNP P0DTC2
A	1142	SER	-	expression tag	UNP P0DTC2
A	1143	SER	-	expression tag	UNP P0DTC2
A	1144	GLY	-	expression tag	UNP P0DTC2
A	1145	GLY	-	expression tag	UNP P0DTC2
A	1146	THR	-	expression tag	UNP P0DTC2
A	1147	ASP	-	expression tag	UNP P0DTC2
A	1148	ASP	-	expression tag	UNP P0DTC2
A	1149	ASP	-	expression tag	UNP P0DTC2
A	1150	ASP	-	expression tag	UNP P0DTC2
A	1151	LYS	-	expression tag	UNP P0DTC2
A	1152	THR	-	expression tag	UNP P0DTC2
A	1153	GLY	-	expression tag	UNP P0DTC2
A	1154	SER	-	expression tag	UNP P0DTC2
A	1155	LEU	-	expression tag	UNP P0DTC2
A	1156	ASN	-	expression tag	UNP P0DTC2
A	1157	ASP	-	expression tag	UNP P0DTC2
A	1158	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1159	PHE	-	expression tag	UNP P0DTC2
A	1160	GLU	-	expression tag	UNP P0DTC2
A	1161	ALA	-	expression tag	UNP P0DTC2
A	1162	GLN	-	expression tag	UNP P0DTC2
A	1163	LYS	-	expression tag	UNP P0DTC2
A	1164	ILE	-	expression tag	UNP P0DTC2
A	1165	GLU	-	expression tag	UNP P0DTC2
A	1166	TRP	-	expression tag	UNP P0DTC2
A	1167	HIS	-	expression tag	UNP P0DTC2
A	1168	GLU	-	expression tag	UNP P0DTC2
A	1169	GLN	-	expression tag	UNP P0DTC2
A	1170	GLY	-	expression tag	UNP P0DTC2
A	1171	SER	-	expression tag	UNP P0DTC2
A	1172	HIS	-	expression tag	UNP P0DTC2
A	1173	HIS	-	expression tag	UNP P0DTC2
A	1174	HIS	-	expression tag	UNP P0DTC2
A	1175	HIS	-	expression tag	UNP P0DTC2
A	1176	HIS	-	expression tag	UNP P0DTC2
A	1177	HIS	-	expression tag	UNP P0DTC2
A	1178	HIS	-	expression tag	UNP P0DTC2
A	1179	HIS	-	expression tag	UNP P0DTC2
B	735	MET	-	expression tag	UNP Q12306
B	736	THR	-	expression tag	UNP Q12306
B	737	ARG	-	expression tag	UNP Q12306
B	738	LEU	-	expression tag	UNP Q12306
B	739	THR	-	expression tag	UNP Q12306
B	740	VAL	-	expression tag	UNP Q12306
B	741	LEU	-	expression tag	UNP Q12306
B	742	ALA	-	expression tag	UNP Q12306
B	743	LEU	-	expression tag	UNP Q12306
B	744	LEU	-	expression tag	UNP Q12306
B	745	ALA	-	expression tag	UNP Q12306
B	746	GLY	-	expression tag	UNP Q12306
B	747	LEU	-	expression tag	UNP Q12306
B	748	LEU	-	expression tag	UNP Q12306
B	749	ALA	-	expression tag	UNP Q12306
B	750	SER	-	expression tag	UNP Q12306
B	751	SER	-	expression tag	UNP Q12306
B	752	ARG	-	expression tag	UNP Q12306
B	753	ALA	-	expression tag	UNP Q12306
B	754	SER	-	expression tag	UNP Q12306
B	849	ASN	-	linker	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
B	850	ASP	-	linker	UNP Q12306
B	851	ASP	-	linker	UNP Q12306
B	852	ASP	-	linker	UNP Q12306
B	853	ASP	-	linker	UNP Q12306
B	854	LYS	-	linker	UNP Q12306
B	855	THR	-	linker	UNP Q12306
B	856	GLY	-	linker	UNP Q12306
B	857	THR	-	linker	UNP Q12306
B	858	GLY	-	linker	UNP Q12306
B	859	SER	-	linker	UNP Q12306
B	860	THR	-	linker	UNP Q12306
B	861	VAL	-	linker	UNP Q12306
B	862	GLN	-	linker	UNP Q12306
B	863	VAL	-	linker	UNP Q12306
B	864	ARG	-	linker	UNP Q12306
B	865	LYS	-	linker	UNP Q12306
B	866	LEU	-	linker	UNP Q12306
B	867	LEU	-	linker	UNP Q12306
B	868	SER	-	linker	UNP Q12306
B	869	GLY	-	linker	UNP Q12306
B	870	ILE	-	linker	UNP Q12306
B	871	VAL	-	linker	UNP Q12306
B	872	GLN	-	linker	UNP Q12306
B	873	GLN	-	linker	UNP Q12306
B	874	GLN	-	linker	UNP Q12306
B	875	SER	-	linker	UNP Q12306
B	876	ASN	-	linker	UNP Q12306
B	877	LEU	-	linker	UNP Q12306
B	878	LEU	-	linker	UNP Q12306
B	879	ARG	-	linker	UNP Q12306
B	880	ALA	-	linker	UNP Q12306
B	881	ILE	-	linker	UNP Q12306
B	882	GLU	-	linker	UNP Q12306
B	883	ALA	-	linker	UNP Q12306
B	884	GLN	-	linker	UNP Q12306
B	885	GLN	-	linker	UNP Q12306
B	886	HIS	-	linker	UNP Q12306
B	887	LEU	-	linker	UNP Q12306
B	888	LEU	-	linker	UNP Q12306
B	889	LYS	-	linker	UNP Q12306
B	890	LEU	-	linker	UNP Q12306
B	891	THR	-	linker	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
B	892	VAL	-	linker	UNP Q12306
B	893	TRP	-	linker	UNP Q12306
B	894	GLY	-	linker	UNP Q12306
B	895	ILE	-	linker	UNP Q12306
B	896	LYS	-	linker	UNP Q12306
B	897	GLN	-	linker	UNP Q12306
B	898	LEU	-	linker	UNP Q12306
B	899	GLN	-	linker	UNP Q12306
B	900	ALA	-	linker	UNP Q12306
B	901	GLN	-	linker	UNP Q12306
B	902	VAL	-	linker	UNP Q12306
B	903	GLU	-	linker	UNP Q12306
B	904	GLU	-	linker	UNP Q12306
B	905	ARG	-	linker	UNP Q12306
B	906	ILE	-	linker	UNP Q12306
B	907	ASN	-	linker	UNP Q12306
B	908	ALA	-	linker	UNP Q12306
B	909	ILE	-	linker	UNP Q12306
B	910	GLU	-	linker	UNP Q12306
B	911	THR	-	linker	UNP Q12306
B	912	ALA	-	linker	UNP Q12306
B	913	ILE	-	linker	UNP Q12306
B	985	ALA	ASP	conflict	UNP P0DTC2
B	1132	THR	-	linker	UNP P0DTC2
B	1829	PRO	-	expression tag	UNP P0DTC2
B	1830	ASP	-	expression tag	UNP P0DTC2
B	1831	PRO	-	expression tag	UNP P0DTC2
B	1832	GLY	-	expression tag	UNP P0DTC2
B	1833	SER	-	expression tag	UNP P0DTC2
B	1834	ASN	-	expression tag	UNP P0DTC2
B	1835	GLU	-	expression tag	UNP P0DTC2
B	1836	GLU	-	expression tag	UNP P0DTC2
B	1837	TRP	-	expression tag	UNP P0DTC2
B	1838	LEU	-	expression tag	UNP P0DTC2
B	1839	GLN	-	expression tag	UNP P0DTC2
B	1840	TRP	-	expression tag	UNP P0DTC2
B	1841	ASP	-	expression tag	UNP P0DTC2
B	1842	LYS	-	expression tag	UNP P0DTC2
B	1843	GLU	-	expression tag	UNP P0DTC2
B	1844	ILE	-	expression tag	UNP P0DTC2
B	1845	SER	-	expression tag	UNP P0DTC2
B	1846	ASN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1847	TYR	-	expression tag	UNP P0DTC2
B	1848	THR	-	expression tag	UNP P0DTC2
B	1849	HIS	-	expression tag	UNP P0DTC2
B	1850	ILE	-	expression tag	UNP P0DTC2
B	1851	ILE	-	expression tag	UNP P0DTC2
B	1852	TYR	-	expression tag	UNP P0DTC2
B	1853	GLU	-	expression tag	UNP P0DTC2
B	1854	LEU	-	expression tag	UNP P0DTC2
B	1855	ILE	-	expression tag	UNP P0DTC2
B	1856	GLU	-	expression tag	UNP P0DTC2
B	1857	GLU	-	expression tag	UNP P0DTC2
B	1858	SER	-	expression tag	UNP P0DTC2
B	1859	GLN	-	expression tag	UNP P0DTC2
B	1860	LYS	-	expression tag	UNP P0DTC2
B	1861	GLN	-	expression tag	UNP P0DTC2
B	1862	GLN	-	expression tag	UNP P0DTC2
B	1863	GLU	-	expression tag	UNP P0DTC2
B	1864	LYS	-	expression tag	UNP P0DTC2
B	1865	ASN	-	expression tag	UNP P0DTC2
B	1133	GLU	-	expression tag	UNP P0DTC2
B	1134	GLN	-	expression tag	UNP P0DTC2
B	1135	GLU	-	expression tag	UNP P0DTC2
B	1136	LEU	-	expression tag	UNP P0DTC2
B	1137	LEU	-	expression tag	UNP P0DTC2
B	1138	GLU	-	expression tag	UNP P0DTC2
B	1139	LEU	-	expression tag	UNP P0DTC2
B	1140	ASP	-	expression tag	UNP P0DTC2
B	1141	LYS	-	expression tag	UNP P0DTC2
B	1142	SER	-	expression tag	UNP P0DTC2
B	1143	SER	-	expression tag	UNP P0DTC2
B	1144	GLY	-	expression tag	UNP P0DTC2
B	1145	GLY	-	expression tag	UNP P0DTC2
B	1146	THR	-	expression tag	UNP P0DTC2
B	1147	ASP	-	expression tag	UNP P0DTC2
B	1148	ASP	-	expression tag	UNP P0DTC2
B	1149	ASP	-	expression tag	UNP P0DTC2
B	1150	ASP	-	expression tag	UNP P0DTC2
B	1151	LYS	-	expression tag	UNP P0DTC2
B	1152	THR	-	expression tag	UNP P0DTC2
B	1153	GLY	-	expression tag	UNP P0DTC2
B	1154	SER	-	expression tag	UNP P0DTC2
B	1155	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1156	ASN	-	expression tag	UNP P0DTC2
B	1157	ASP	-	expression tag	UNP P0DTC2
B	1158	ILE	-	expression tag	UNP P0DTC2
B	1159	PHE	-	expression tag	UNP P0DTC2
B	1160	GLU	-	expression tag	UNP P0DTC2
B	1161	ALA	-	expression tag	UNP P0DTC2
B	1162	GLN	-	expression tag	UNP P0DTC2
B	1163	LYS	-	expression tag	UNP P0DTC2
B	1164	ILE	-	expression tag	UNP P0DTC2
B	1165	GLU	-	expression tag	UNP P0DTC2
B	1166	TRP	-	expression tag	UNP P0DTC2
B	1167	HIS	-	expression tag	UNP P0DTC2
B	1168	GLU	-	expression tag	UNP P0DTC2
B	1169	GLN	-	expression tag	UNP P0DTC2
B	1170	GLY	-	expression tag	UNP P0DTC2
B	1171	SER	-	expression tag	UNP P0DTC2
B	1172	HIS	-	expression tag	UNP P0DTC2
B	1173	HIS	-	expression tag	UNP P0DTC2
B	1174	HIS	-	expression tag	UNP P0DTC2
B	1175	HIS	-	expression tag	UNP P0DTC2
B	1176	HIS	-	expression tag	UNP P0DTC2
B	1177	HIS	-	expression tag	UNP P0DTC2
B	1178	HIS	-	expression tag	UNP P0DTC2
B	1179	HIS	-	expression tag	UNP P0DTC2
C	735	MET	-	expression tag	UNP Q12306
C	736	THR	-	expression tag	UNP Q12306
C	737	ARG	-	expression tag	UNP Q12306
C	738	LEU	-	expression tag	UNP Q12306
C	739	THR	-	expression tag	UNP Q12306
C	740	VAL	-	expression tag	UNP Q12306
C	741	LEU	-	expression tag	UNP Q12306
C	742	ALA	-	expression tag	UNP Q12306
C	743	LEU	-	expression tag	UNP Q12306
C	744	LEU	-	expression tag	UNP Q12306
C	745	ALA	-	expression tag	UNP Q12306
C	746	GLY	-	expression tag	UNP Q12306
C	747	LEU	-	expression tag	UNP Q12306
C	748	LEU	-	expression tag	UNP Q12306
C	749	ALA	-	expression tag	UNP Q12306
C	750	SER	-	expression tag	UNP Q12306
C	751	SER	-	expression tag	UNP Q12306
C	752	ARG	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
C	753	ALA	-	expression tag	UNP Q12306
C	754	SER	-	expression tag	UNP Q12306
C	849	ASN	-	linker	UNP Q12306
C	850	ASP	-	linker	UNP Q12306
C	851	ASP	-	linker	UNP Q12306
C	852	ASP	-	linker	UNP Q12306
C	853	ASP	-	linker	UNP Q12306
C	854	LYS	-	linker	UNP Q12306
C	855	THR	-	linker	UNP Q12306
C	856	GLY	-	linker	UNP Q12306
C	857	THR	-	linker	UNP Q12306
C	858	GLY	-	linker	UNP Q12306
C	859	SER	-	linker	UNP Q12306
C	860	THR	-	linker	UNP Q12306
C	861	VAL	-	linker	UNP Q12306
C	862	GLN	-	linker	UNP Q12306
C	863	VAL	-	linker	UNP Q12306
C	864	ARG	-	linker	UNP Q12306
C	865	LYS	-	linker	UNP Q12306
C	866	LEU	-	linker	UNP Q12306
C	867	LEU	-	linker	UNP Q12306
C	868	SER	-	linker	UNP Q12306
C	869	GLY	-	linker	UNP Q12306
C	870	ILE	-	linker	UNP Q12306
C	871	VAL	-	linker	UNP Q12306
C	872	GLN	-	linker	UNP Q12306
C	873	GLN	-	linker	UNP Q12306
C	874	GLN	-	linker	UNP Q12306
C	875	SER	-	linker	UNP Q12306
C	876	ASN	-	linker	UNP Q12306
C	877	LEU	-	linker	UNP Q12306
C	878	LEU	-	linker	UNP Q12306
C	879	ARG	-	linker	UNP Q12306
C	880	ALA	-	linker	UNP Q12306
C	881	ILE	-	linker	UNP Q12306
C	882	GLU	-	linker	UNP Q12306
C	883	ALA	-	linker	UNP Q12306
C	884	GLN	-	linker	UNP Q12306
C	885	GLN	-	linker	UNP Q12306
C	886	HIS	-	linker	UNP Q12306
C	887	LEU	-	linker	UNP Q12306
C	888	LEU	-	linker	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
C	889	LYS	-	linker	UNP Q12306
C	890	LEU	-	linker	UNP Q12306
C	891	THR	-	linker	UNP Q12306
C	892	VAL	-	linker	UNP Q12306
C	893	TRP	-	linker	UNP Q12306
C	894	GLY	-	linker	UNP Q12306
C	895	ILE	-	linker	UNP Q12306
C	896	LYS	-	linker	UNP Q12306
C	897	GLN	-	linker	UNP Q12306
C	898	LEU	-	linker	UNP Q12306
C	899	GLN	-	linker	UNP Q12306
C	900	ALA	-	linker	UNP Q12306
C	901	GLN	-	linker	UNP Q12306
C	902	VAL	-	linker	UNP Q12306
C	903	GLU	-	linker	UNP Q12306
C	904	GLU	-	linker	UNP Q12306
C	905	ARG	-	linker	UNP Q12306
C	906	ILE	-	linker	UNP Q12306
C	907	ASN	-	linker	UNP Q12306
C	908	ALA	-	linker	UNP Q12306
C	909	ILE	-	linker	UNP Q12306
C	910	GLU	-	linker	UNP Q12306
C	911	THR	-	linker	UNP Q12306
C	912	ALA	-	linker	UNP Q12306
C	913	ILE	-	linker	UNP Q12306
C	985	ALA	ASP	conflict	UNP P0DTC2
C	1132	THR	-	linker	UNP P0DTC2
C	1829	PRO	-	expression tag	UNP P0DTC2
C	1830	ASP	-	expression tag	UNP P0DTC2
C	1831	PRO	-	expression tag	UNP P0DTC2
C	1832	GLY	-	expression tag	UNP P0DTC2
C	1833	SER	-	expression tag	UNP P0DTC2
C	1834	ASN	-	expression tag	UNP P0DTC2
C	1835	GLU	-	expression tag	UNP P0DTC2
C	1836	GLU	-	expression tag	UNP P0DTC2
C	1837	TRP	-	expression tag	UNP P0DTC2
C	1838	LEU	-	expression tag	UNP P0DTC2
C	1839	GLN	-	expression tag	UNP P0DTC2
C	1840	TRP	-	expression tag	UNP P0DTC2
C	1841	ASP	-	expression tag	UNP P0DTC2
C	1842	LYS	-	expression tag	UNP P0DTC2
C	1843	GLU	-	expression tag	UNP P0DTC2

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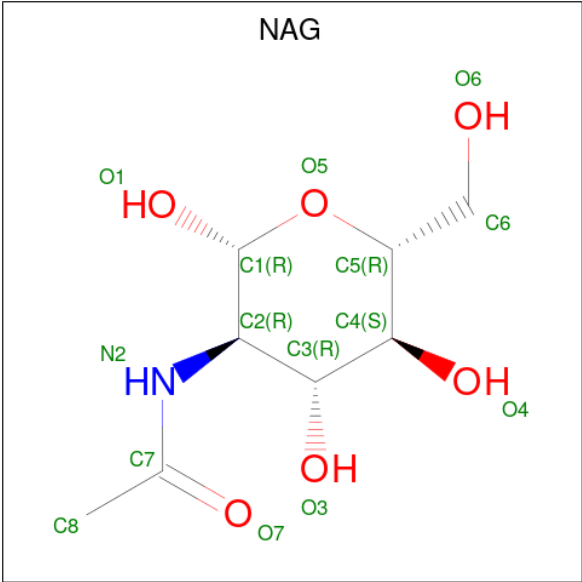
Chain	Residue	Modelled	Actual	Comment	Reference
C	1844	ILE	-	expression tag	UNP P0DTC2
C	1845	SER	-	expression tag	UNP P0DTC2
C	1846	ASN	-	expression tag	UNP P0DTC2
C	1847	TYR	-	expression tag	UNP P0DTC2
C	1848	THR	-	expression tag	UNP P0DTC2
C	1849	HIS	-	expression tag	UNP P0DTC2
C	1850	ILE	-	expression tag	UNP P0DTC2
C	1851	ILE	-	expression tag	UNP P0DTC2
C	1852	TYR	-	expression tag	UNP P0DTC2
C	1853	GLU	-	expression tag	UNP P0DTC2
C	1854	LEU	-	expression tag	UNP P0DTC2
C	1855	ILE	-	expression tag	UNP P0DTC2
C	1856	GLU	-	expression tag	UNP P0DTC2
C	1857	GLU	-	expression tag	UNP P0DTC2
C	1858	SER	-	expression tag	UNP P0DTC2
C	1859	GLN	-	expression tag	UNP P0DTC2
C	1860	LYS	-	expression tag	UNP P0DTC2
C	1861	GLN	-	expression tag	UNP P0DTC2
C	1862	GLN	-	expression tag	UNP P0DTC2
C	1863	GLU	-	expression tag	UNP P0DTC2
C	1864	LYS	-	expression tag	UNP P0DTC2
C	1865	ASN	-	expression tag	UNP P0DTC2
C	1133	GLU	-	expression tag	UNP P0DTC2
C	1134	GLN	-	expression tag	UNP P0DTC2
C	1135	GLU	-	expression tag	UNP P0DTC2
C	1136	LEU	-	expression tag	UNP P0DTC2
C	1137	LEU	-	expression tag	UNP P0DTC2
C	1138	GLU	-	expression tag	UNP P0DTC2
C	1139	LEU	-	expression tag	UNP P0DTC2
C	1140	ASP	-	expression tag	UNP P0DTC2
C	1141	LYS	-	expression tag	UNP P0DTC2
C	1142	SER	-	expression tag	UNP P0DTC2
C	1143	SER	-	expression tag	UNP P0DTC2
C	1144	GLY	-	expression tag	UNP P0DTC2
C	1145	GLY	-	expression tag	UNP P0DTC2
C	1146	THR	-	expression tag	UNP P0DTC2
C	1147	ASP	-	expression tag	UNP P0DTC2
C	1148	ASP	-	expression tag	UNP P0DTC2
C	1149	ASP	-	expression tag	UNP P0DTC2
C	1150	ASP	-	expression tag	UNP P0DTC2
C	1151	LYS	-	expression tag	UNP P0DTC2
C	1152	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1153	GLY	-	expression tag	UNP P0DTC2
C	1154	SER	-	expression tag	UNP P0DTC2
C	1155	LEU	-	expression tag	UNP P0DTC2
C	1156	ASN	-	expression tag	UNP P0DTC2
C	1157	ASP	-	expression tag	UNP P0DTC2
C	1158	ILE	-	expression tag	UNP P0DTC2
C	1159	PHE	-	expression tag	UNP P0DTC2
C	1160	GLU	-	expression tag	UNP P0DTC2
C	1161	ALA	-	expression tag	UNP P0DTC2
C	1162	GLN	-	expression tag	UNP P0DTC2
C	1163	LYS	-	expression tag	UNP P0DTC2
C	1164	ILE	-	expression tag	UNP P0DTC2
C	1165	GLU	-	expression tag	UNP P0DTC2
C	1166	TRP	-	expression tag	UNP P0DTC2
C	1167	HIS	-	expression tag	UNP P0DTC2
C	1168	GLU	-	expression tag	UNP P0DTC2
C	1169	GLN	-	expression tag	UNP P0DTC2
C	1170	GLY	-	expression tag	UNP P0DTC2
C	1171	SER	-	expression tag	UNP P0DTC2
C	1172	HIS	-	expression tag	UNP P0DTC2
C	1173	HIS	-	expression tag	UNP P0DTC2
C	1174	HIS	-	expression tag	UNP P0DTC2
C	1175	HIS	-	expression tag	UNP P0DTC2
C	1176	HIS	-	expression tag	UNP P0DTC2
C	1177	HIS	-	expression tag	UNP P0DTC2
C	1178	HIS	-	expression tag	UNP P0DTC2
C	1179	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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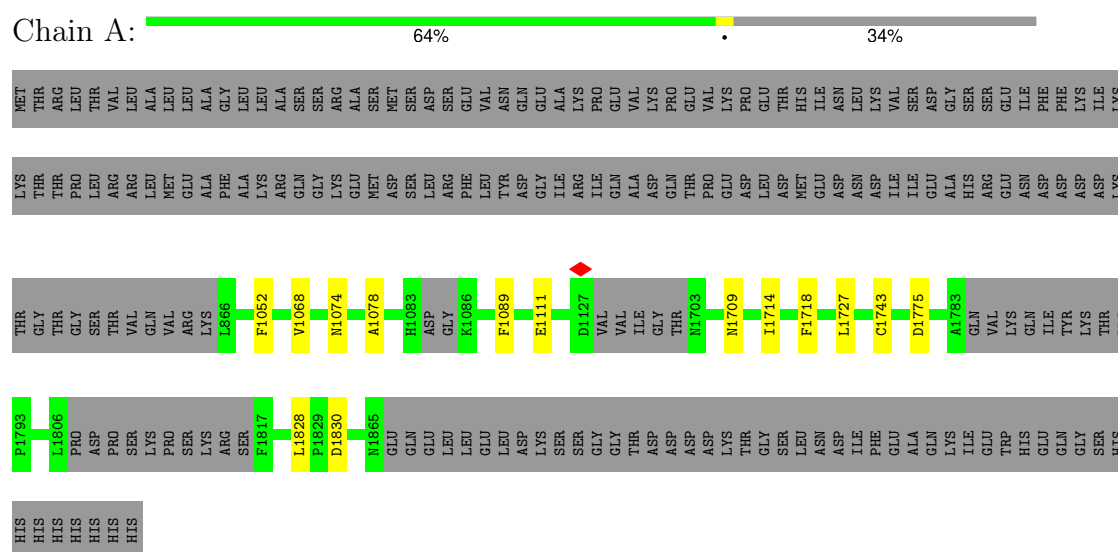
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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	

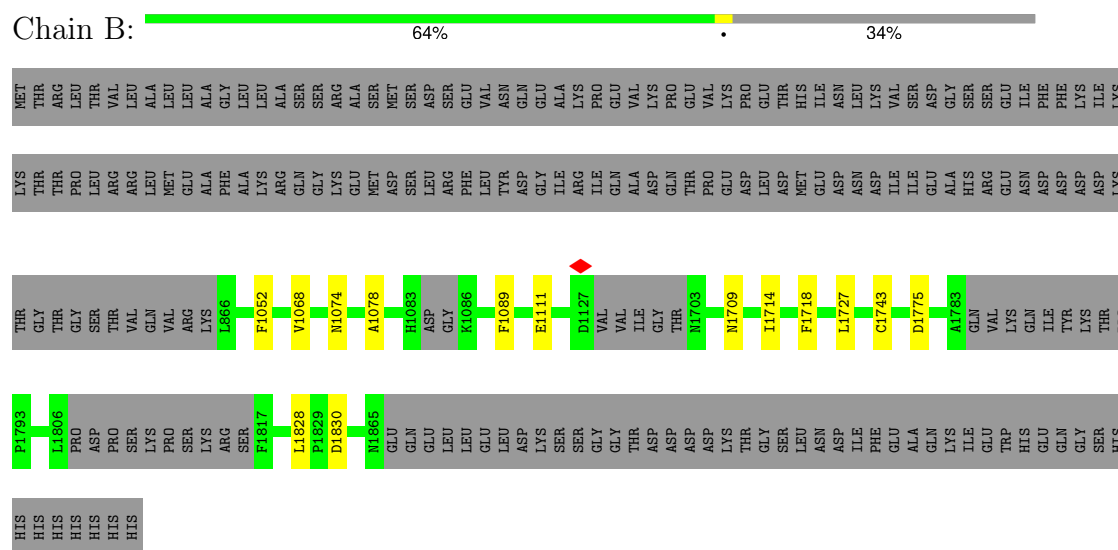
3 Residue-property plots

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: SPIKE PROTEIN



• Molecule 1: SPIKE PROTEIN



• Molecule 1: SPIKE PROTEIN

Response	Percentage
Yes, it is a crisis	64%
No, it is not a crisis	34%

HIS	F1793	THR	LYS	MET
HIS	L1906	GLY	THR	THR
HIS	PRO	GLY	PRO	LEU
HIS	ASP	SER	LEU	THR
HIS	PRO	THR	ARG	VAL
HIS	SER	VAL	ARG	LEU
	LYS	GLN	MET	ALA
	PRO	VAL	LEU	LEU
	SER	ARG	GLU	LEU
	LYS	LYS	ALA	ALA
	ARG	L866	PHE	GLY
	SER	F1052	ALA	LEU
	F1817	LYS	LYS	LEU
	L1928	ARG	ALA	ALA
	P1829	V1068	GLN	SER
	D1830	N1074	SER	SER
	N1865	LYS	LYS	ARG
	GLU	A1078	GLU	ALA
	GLN	THR	GLU	ALA
	GLU	H1083	MET	SER
	LEU	ASP	ASP	MET
	LEU	GLY	LEU	SER
	LEU	K1086	ARG	ASP
	GLU	F1089	PHE	ASP
	LEU	LYS	LEU	SER
	ASP	F1089	TYR	ASN
	LYS	E1111	GLN	GLN
	SER	LYS	GLY	GLU
	SER	D1127	ILE	ALA
	SER	VAL	ARG	LYS
	GLY	VAL	ILE	PRO
	GLY	ILE	GLN	GLU
	THR	GLY	ALA	VAL
	ASP	THR	ASP	LYS
	ASP	N1703	GLN	PRO
	ASP	THR	THR	VAL
	LYS	N1709	GLU	LYS
	THR	LYS	ASP	PRO
	GLY	I1714	LEU	GLU
	SER	THR	ASP	THR
	LEU	F1718	MET	HIS
	ASN	GLN	ILE	GLU
	ASP	ASP	ASP	ASN
	ILE	L1727	ASN	LEU
	PHE	C1743	ASP	LYS
	GLU	D1775	ILE	VAL
	ALA	LYS	GLU	VAL
	LYS	A1783	ALA	GLY
	ILE	GLN	HIS	SER
	GLU	VAL	ARG	SER
	TRP	LYS	GLU	GLU
	HIS	GLN	ASN	ILE
	GLU	ILE	ASP	PHE
	GLN	TYR	ASP	PHE
	GLY	LYS	ASP	LYS
	SER	THR	ASP	ILE
	HIS	THR	LYS	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114104	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.374	Depositor
Minimum map value	-1.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	530.56, 530.56, 530.56	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.829, 0.829, 0.829	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	0.72	3/2778 (0.1%)	0.83	16/3803 (0.4%)
1	B	0.72	3/2778 (0.1%)	0.83	16/3803 (0.4%)
1	C	0.72	3/2778 (0.1%)	0.83	16/3803 (0.4%)
All	All	0.72	9/8334 (0.1%)	0.83	48/11409 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1709	ASN	C-O	-5.45	1.17	1.23
1	A	1709	ASN	C-O	-5.40	1.17	1.23
1	B	1709	ASN	C-O	-5.37	1.17	1.23
1	C	1074	ASN	CA-CB	-5.25	1.46	1.53
1	A	1074	ASN	CA-CB	-5.23	1.46	1.53
1	B	1074	ASN	CA-CB	-5.17	1.46	1.53
1	B	1743	CYS	N-CA	5.13	1.52	1.46
1	A	1743	CYS	N-CA	5.11	1.52	1.46
1	C	1743	CYS	N-CA	5.10	1.52	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1828	LEU	CA-C-N	6.94	126.86	119.85
1	C	1828	LEU	C-N-CA	6.94	126.86	119.85
1	B	1828	LEU	CA-C-N	6.92	126.84	119.85
1	B	1828	LEU	C-N-CA	6.92	126.84	119.85
1	A	1828	LEU	CA-C-N	6.91	126.82	119.85
1	A	1828	LEU	C-N-CA	6.91	126.82	119.85
1	C	1111	GLU	CA-C-N	6.86	127.23	119.83
1	C	1111	GLU	C-N-CA	6.86	127.23	119.83
1	A	1111	GLU	CA-C-N	6.84	127.22	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1111	GLU	C-N-CA	6.84	127.22	119.83
1	B	1111	GLU	CA-C-N	6.81	127.18	119.83
1	B	1111	GLU	C-N-CA	6.81	127.18	119.83
1	C	1830	ASP	CA-C-N	6.55	127.07	119.47
1	C	1830	ASP	C-N-CA	6.55	127.07	119.47
1	A	1830	ASP	CA-C-N	6.53	127.04	119.47
1	A	1830	ASP	C-N-CA	6.53	127.04	119.47
1	B	1830	ASP	CA-C-N	6.52	127.03	119.47
1	B	1830	ASP	C-N-CA	6.52	127.03	119.47
1	B	1078	ALA	CA-C-N	6.46	126.22	119.05
1	B	1078	ALA	C-N-CA	6.46	126.22	119.05
1	A	1078	ALA	CA-C-N	6.43	126.19	119.05
1	A	1078	ALA	C-N-CA	6.43	126.19	119.05
1	C	1078	ALA	CA-C-N	6.43	126.19	119.05
1	C	1078	ALA	C-N-CA	6.43	126.19	119.05
1	B	1714	ILE	CA-C-N	6.26	126.28	119.90
1	B	1714	ILE	C-N-CA	6.26	126.28	119.90
1	A	1714	ILE	CA-C-N	6.25	126.28	119.90
1	A	1714	ILE	C-N-CA	6.25	126.28	119.90
1	C	1714	ILE	CA-C-N	6.24	126.26	119.90
1	C	1714	ILE	C-N-CA	6.24	126.26	119.90
1	C	1052	PHE	CA-C-N	6.07	125.98	119.85
1	C	1052	PHE	C-N-CA	6.07	125.98	119.85
1	A	1052	PHE	CA-C-N	6.03	125.94	119.85
1	A	1052	PHE	C-N-CA	6.03	125.94	119.85
1	B	1052	PHE	CA-C-N	5.99	125.90	119.85
1	B	1052	PHE	C-N-CA	5.99	125.90	119.85
1	B	1727	LEU	CA-C-N	5.60	126.04	119.99
1	B	1727	LEU	C-N-CA	5.60	126.04	119.99
1	C	1727	LEU	CA-C-N	5.59	126.03	119.99
1	C	1727	LEU	C-N-CA	5.59	126.03	119.99
1	A	1727	LEU	CA-C-N	5.59	126.03	119.99
1	A	1727	LEU	C-N-CA	5.59	126.03	119.99
1	B	1068	VAL	CA-C-N	5.32	125.62	119.93
1	B	1068	VAL	C-N-CA	5.32	125.62	119.93
1	C	1068	VAL	CA-C-N	5.30	125.61	119.93
1	C	1068	VAL	C-N-CA	5.30	125.61	119.93
1	A	1068	VAL	CA-C-N	5.29	125.59	119.93
1	A	1068	VAL	C-N-CA	5.29	125.59	119.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2732	0	2261	3	0
1	B	2732	0	2261	3	0
1	C	2732	0	2261	3	0
2	A	84	0	78	0	0
2	B	84	0	78	0	0
2	C	84	0	78	0	0
All	All	8448	0	7017	6	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 0.

All (6) 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:1718:PHE:HB2	1:B:1089:PHE:HZ	1.80	0.47
1:B:1718:PHE:HB2	1:C:1089:PHE:HZ	1.80	0.47
1:A:1089:PHE:HZ	1:C:1718:PHE:HB2	1.80	0.46
1:A:1775:ASP:OD1	1:A:1775:ASP:C	2.62	0.43
1:C:1775:ASP:OD1	1:C:1775:ASP:C	2.62	0.42
1:B:1775:ASP:C	1:B:1775:ASP:OD1	2.62	0.41

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	394/608 (65%)	388 (98%)	6 (2%)	0	100	100
1	B	394/608 (65%)	388 (98%)	6 (2%)	0	100	100
1	C	394/608 (65%)	388 (98%)	6 (2%)	0	100	100
All	All	1182/1824 (65%)	1164 (98%)	18 (2%)	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	197/537 (37%)	197 (100%)	0	100	100
1	B	197/537 (37%)	197 (100%)	0	100	100
1	C	197/537 (37%)	197 (100%)	0	100	100
All	All	591/1611 (37%)	591 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1002	GLN
1	A	1005	GLN
1	A	1011	GLN
1	B	1002	GLN
1	B	1005	GLN
1	B	1011	GLN
1	C	1002	GLN
1	C	1005	GLN
1	C	1011	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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
2	NAG	B	1403	1	14,14,15	1.17	1 (7%)	17,19,21	1.07	2 (11%)
2	NAG	C	1404	1	14,14,15	0.95	1 (7%)	17,19,21	1.04	2 (11%)
2	NAG	A	1403	1	14,14,15	1.17	1 (7%)	17,19,21	1.07	2 (11%)
2	NAG	A	1401	1	14,14,15	0.96	2 (14%)	17,19,21	1.09	2 (11%)
2	NAG	B	1401	1	14,14,15	0.96	2 (14%)	17,19,21	1.09	2 (11%)
2	NAG	B	1404	1	14,14,15	0.95	1 (7%)	17,19,21	1.04	2 (11%)
2	NAG	A	1402	1	14,14,15	0.94	1 (7%)	17,19,21	1.03	2 (11%)
2	NAG	A	1405	1	14,14,15	1.09	2 (14%)	17,19,21	1.02	2 (11%)
2	NAG	A	1406	1	14,14,15	0.95	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	B	1405	1	14,14,15	1.09	2 (14%)	17,19,21	1.02	2 (11%)
2	NAG	C	1406	1	14,14,15	0.96	2 (14%)	17,19,21	1.02	1 (5%)
2	NAG	B	1402	1	14,14,15	0.93	1 (7%)	17,19,21	1.03	2 (11%)
2	NAG	C	1403	1	14,14,15	1.18	1 (7%)	17,19,21	1.08	2 (11%)
2	NAG	C	1401	1	14,14,15	0.97	2 (14%)	17,19,21	1.09	2 (11%)
2	NAG	C	1402	1	14,14,15	0.94	1 (7%)	17,19,21	1.03	2 (11%)
2	NAG	C	1405	1	14,14,15	1.09	2 (14%)	17,19,21	1.02	2 (11%)
2	NAG	A	1404	1	14,14,15	0.95	1 (7%)	17,19,21	1.05	2 (11%)
2	NAG	B	1406	1	14,14,15	0.95	2 (14%)	17,19,21	1.02	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1406	1	-	0/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1403	NAG	C1-C2	3.43	1.57	1.52
2	A	1403	NAG	C1-C2	3.38	1.56	1.52
2	B	1403	NAG	C1-C2	3.36	1.56	1.52
2	C	1405	NAG	C1-C2	2.90	1.56	1.52
2	B	1405	NAG	C1-C2	2.87	1.56	1.52
2	A	1405	NAG	C1-C2	2.86	1.56	1.52
2	B	1404	NAG	C1-C2	2.40	1.55	1.52
2	A	1404	NAG	C1-C2	2.40	1.55	1.52
2	C	1404	NAG	C1-C2	2.38	1.55	1.52
2	C	1402	NAG	C1-C2	2.14	1.55	1.52
2	C	1405	NAG	O5-C5	2.13	1.47	1.43
2	A	1402	NAG	C1-C2	2.13	1.55	1.52
2	B	1402	NAG	C1-C2	2.12	1.55	1.52
2	A	1405	NAG	O5-C5	2.10	1.47	1.43
2	C	1401	NAG	C1-C2	2.09	1.55	1.52
2	B	1405	NAG	O5-C5	2.08	1.47	1.43
2	B	1401	NAG	C1-C2	2.07	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1401	NAG	O5-C5	2.07	1.47	1.43
2	B	1406	NAG	O5-C5	2.05	1.47	1.43
2	A	1401	NAG	O5-C5	2.04	1.47	1.43
2	A	1406	NAG	O5-C5	2.04	1.47	1.43
2	C	1406	NAG	O5-C5	2.03	1.47	1.43
2	B	1401	NAG	O5-C5	2.03	1.47	1.43
2	A	1401	NAG	C1-C2	2.03	1.55	1.52
2	C	1406	NAG	C1-C2	2.03	1.55	1.52
2	B	1406	NAG	C1-C2	2.02	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1401	NAG	C8-C7-N2	2.66	120.53	116.12
2	A	1401	NAG	C8-C7-N2	2.65	120.52	116.12
2	B	1401	NAG	C8-C7-N2	2.65	120.51	116.12
2	C	1406	NAG	C8-C7-N2	2.48	120.23	116.12
2	C	1403	NAG	C2-N2-C7	-2.47	119.59	122.90
2	A	1403	NAG	C2-N2-C7	-2.47	119.59	122.90
2	A	1406	NAG	C8-C7-N2	2.46	120.20	116.12
2	B	1406	NAG	C8-C7-N2	2.46	120.20	116.12
2	B	1403	NAG	C2-N2-C7	-2.46	119.60	122.90
2	C	1402	NAG	C8-C7-N2	2.35	120.01	116.12
2	A	1404	NAG	C8-C7-N2	2.33	119.99	116.12
2	C	1405	NAG	C8-C7-N2	2.33	119.98	116.12
2	B	1402	NAG	C8-C7-N2	2.33	119.98	116.12
2	C	1404	NAG	C8-C7-N2	2.33	119.98	116.12
2	A	1402	NAG	C8-C7-N2	2.32	119.97	116.12
2	B	1404	NAG	C8-C7-N2	2.32	119.97	116.12
2	A	1405	NAG	C8-C7-N2	2.32	119.96	116.12
2	B	1405	NAG	C8-C7-N2	2.32	119.96	116.12
2	C	1403	NAG	C8-C7-N2	2.27	119.88	116.12
2	A	1403	NAG	C8-C7-N2	2.26	119.87	116.12
2	B	1403	NAG	C8-C7-N2	2.26	119.86	116.12
2	B	1404	NAG	C2-N2-C7	-2.25	119.89	122.90
2	A	1404	NAG	C2-N2-C7	-2.23	119.91	122.90
2	C	1404	NAG	C2-N2-C7	-2.21	119.94	122.90
2	B	1401	NAG	C2-N2-C7	-2.21	119.94	122.90
2	A	1405	NAG	C2-N2-C7	-2.19	119.96	122.90
2	C	1405	NAG	C2-N2-C7	-2.19	119.97	122.90
2	B	1405	NAG	C2-N2-C7	-2.18	119.98	122.90
2	A	1401	NAG	C2-N2-C7	-2.17	119.99	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1401	NAG	C2-N2-C7	-2.17	119.99	122.90
2	B	1402	NAG	C2-N2-C7	-2.13	120.05	122.90
2	A	1402	NAG	C2-N2-C7	-2.11	120.07	122.90
2	C	1402	NAG	C2-N2-C7	-2.11	120.08	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

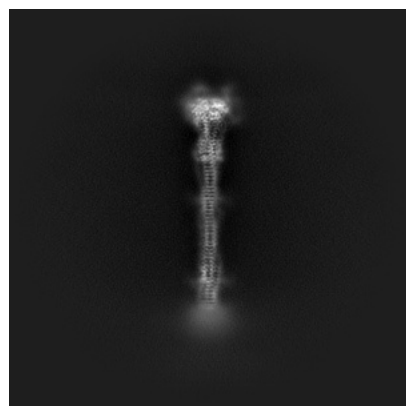
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73787. These allow visual inspection of the internal detail of the map and identification of artifacts.

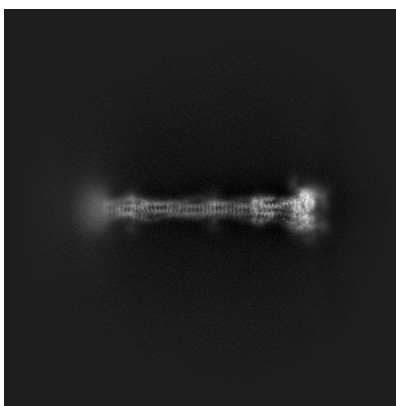
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

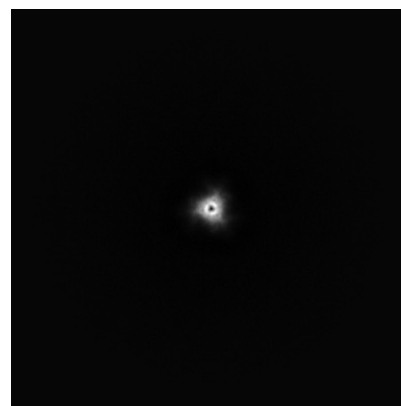
6.1.1 Primary map



X



Y

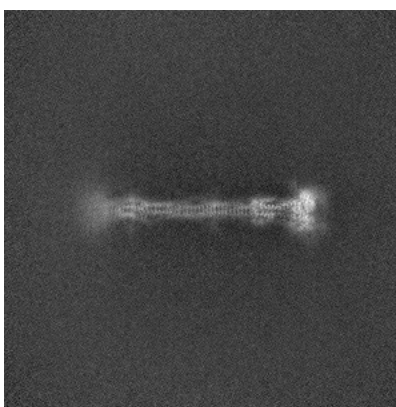


Z

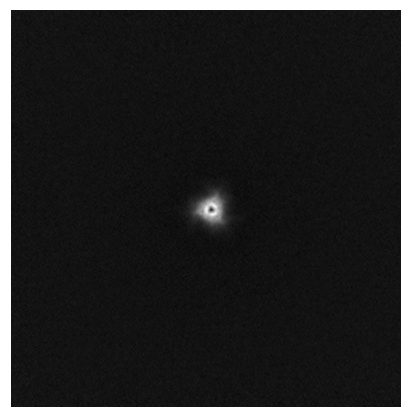
6.1.2 Raw map



X



Y



Z

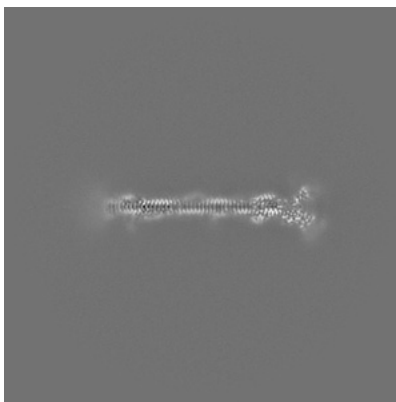
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

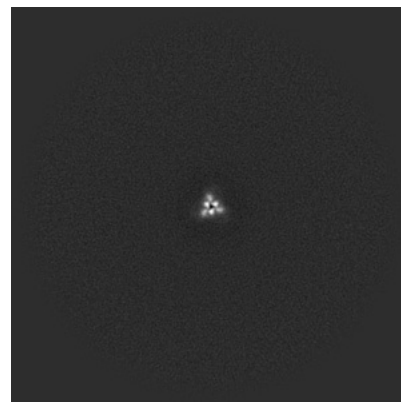
6.2.1 Primary map



X Index: 320



Y Index: 320

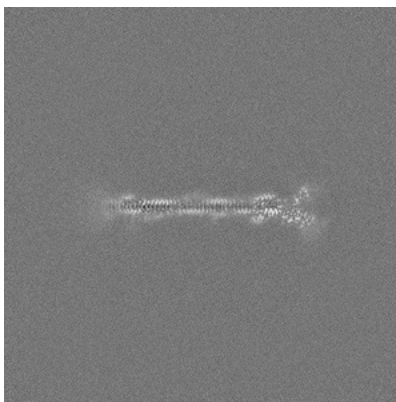


Z Index: 320

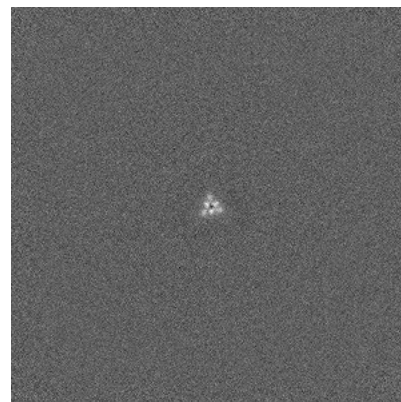
6.2.2 Raw map



X Index: 320



Y Index: 320

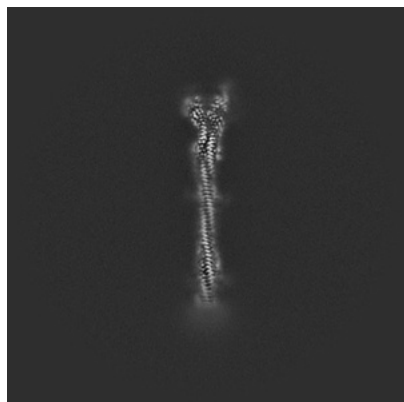


Z Index: 320

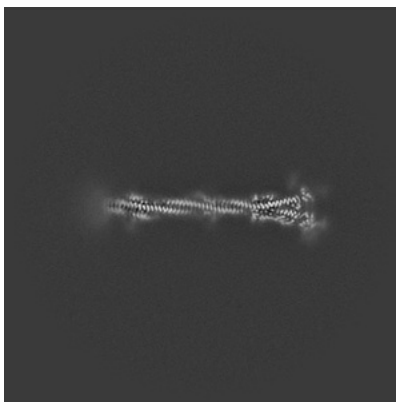
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

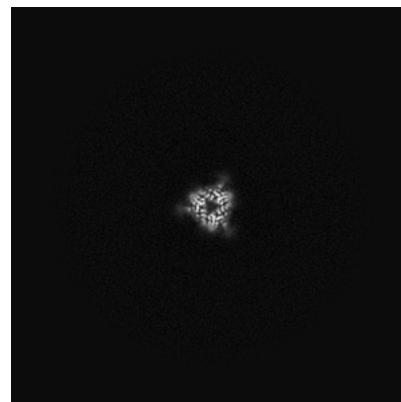
6.3.1 Primary map



X Index: 326



Y Index: 314

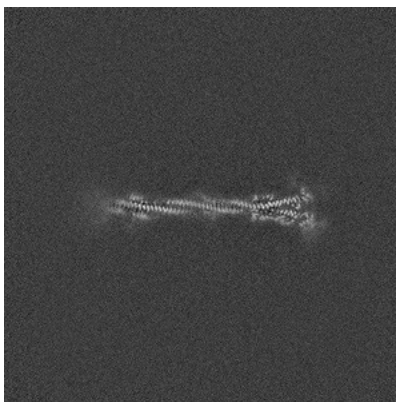


Z Index: 484

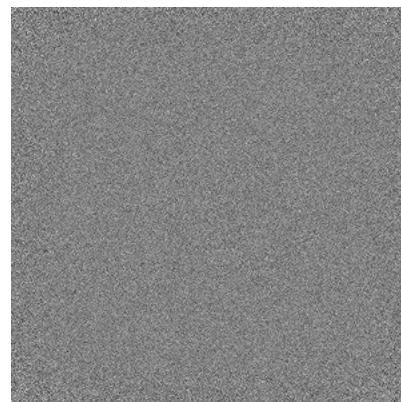
6.3.2 Raw map



X Index: 326



Y Index: 314

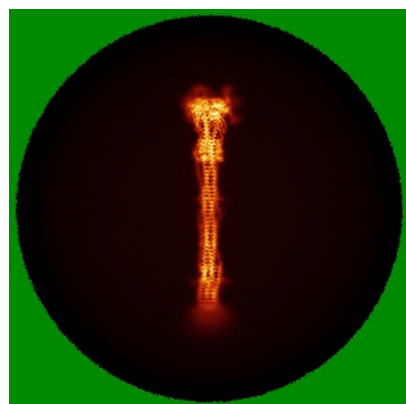


Z Index: 0

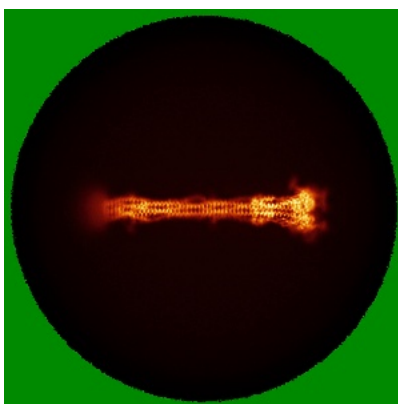
The images above show the largest variance slices of the map in three orthogonal directions.

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

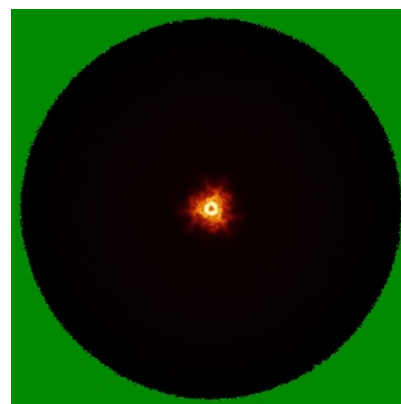
6.4.1 Primary map



X

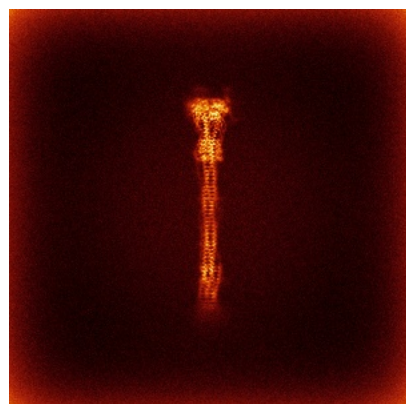


Y

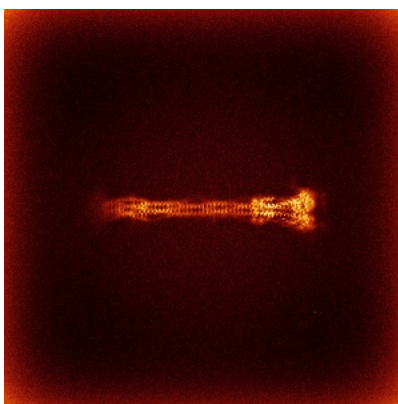


Z

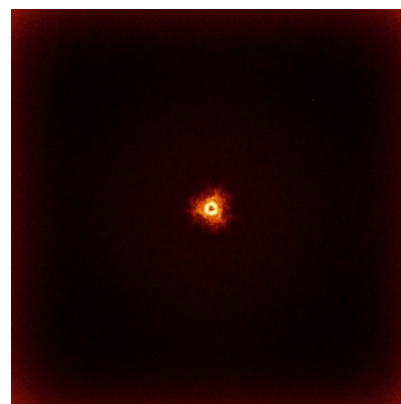
6.4.2 Raw map



X



Y

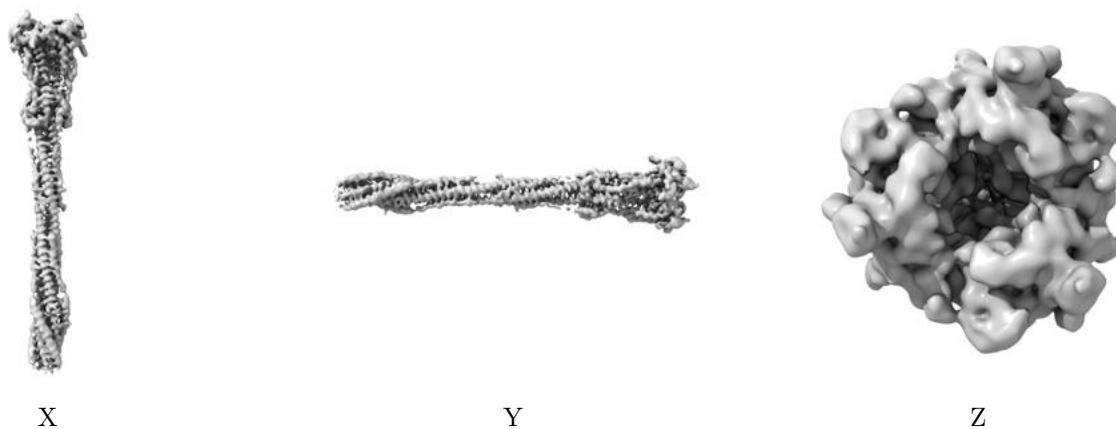


Z

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.

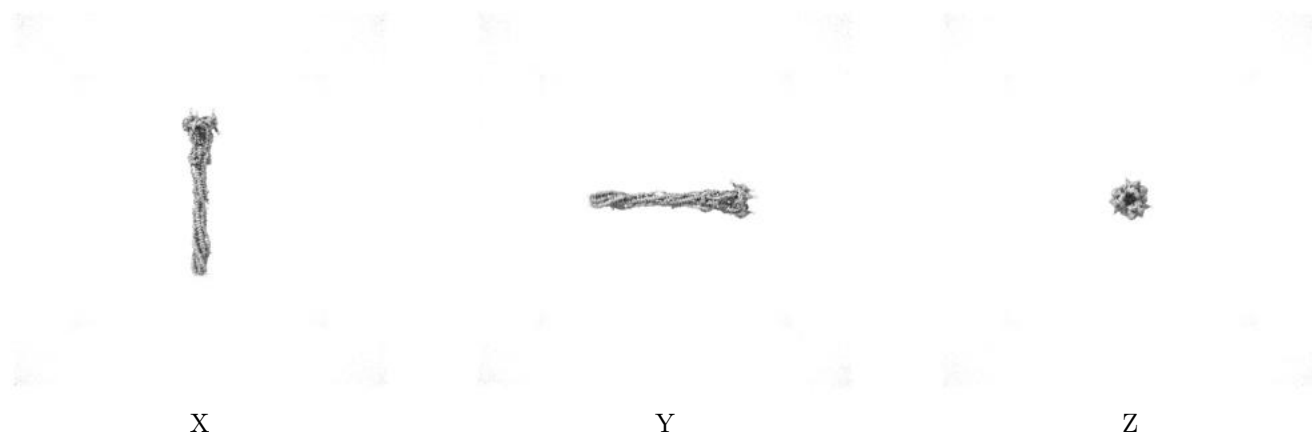
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

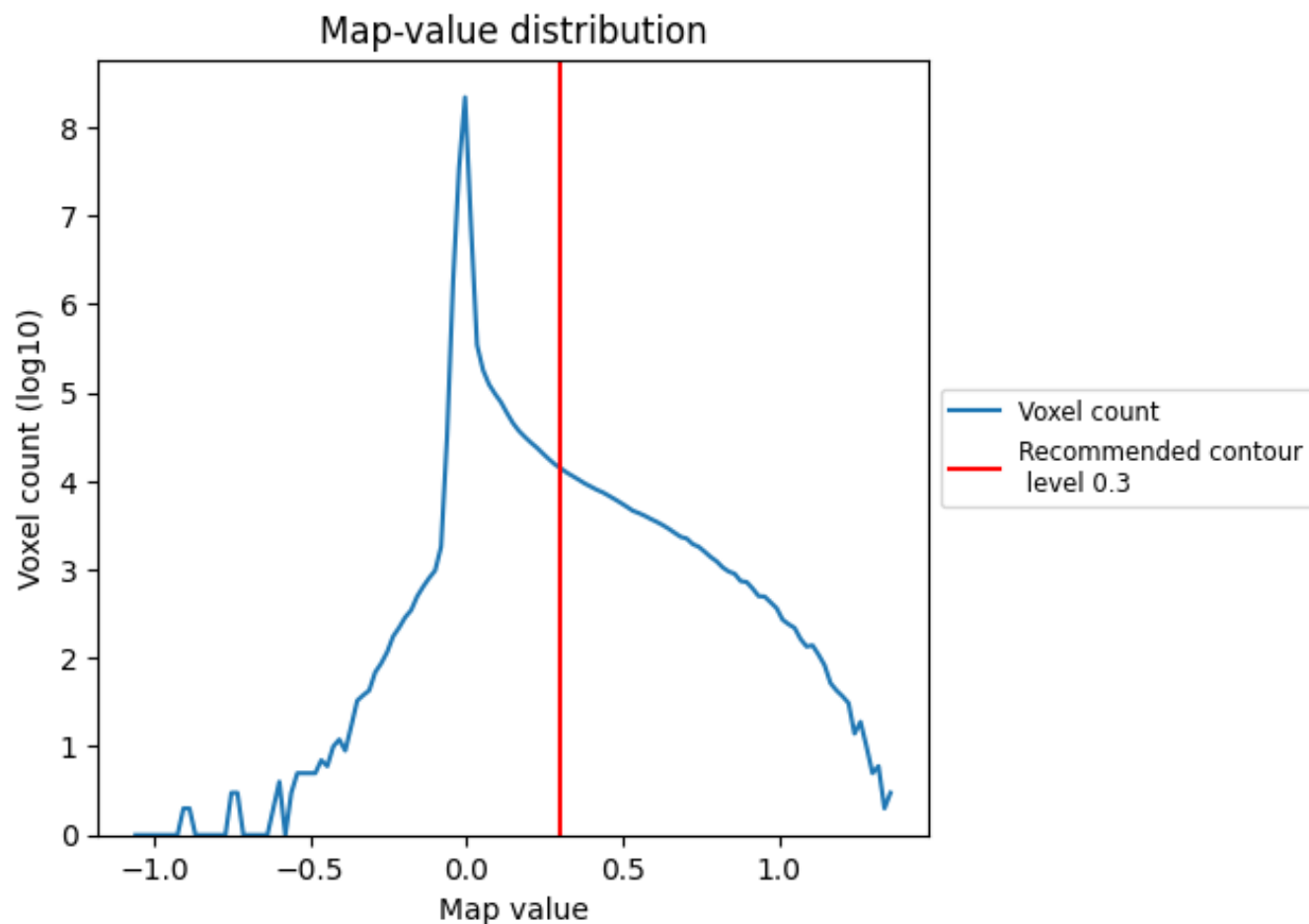
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

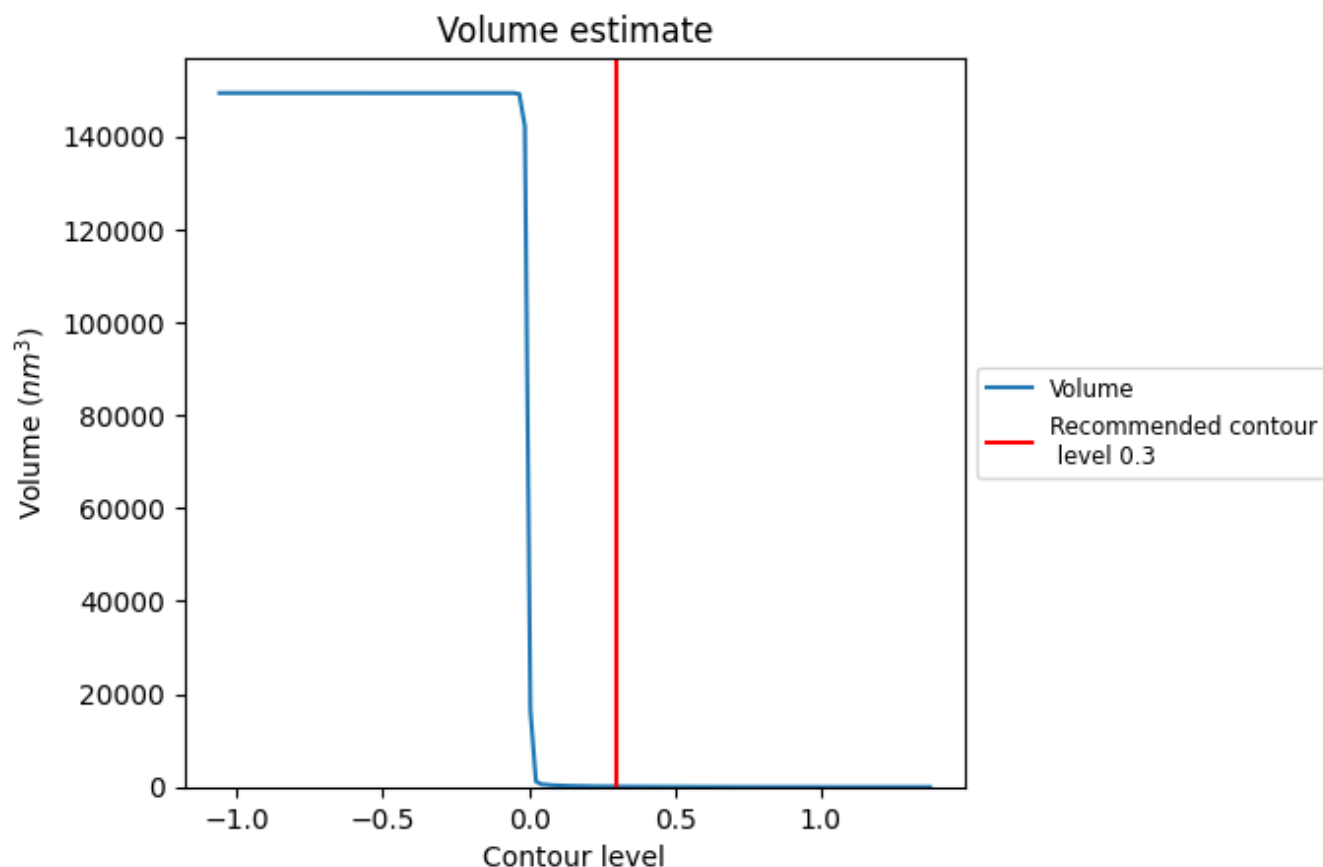
This section contains the results of statistical analysis of the map.

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.

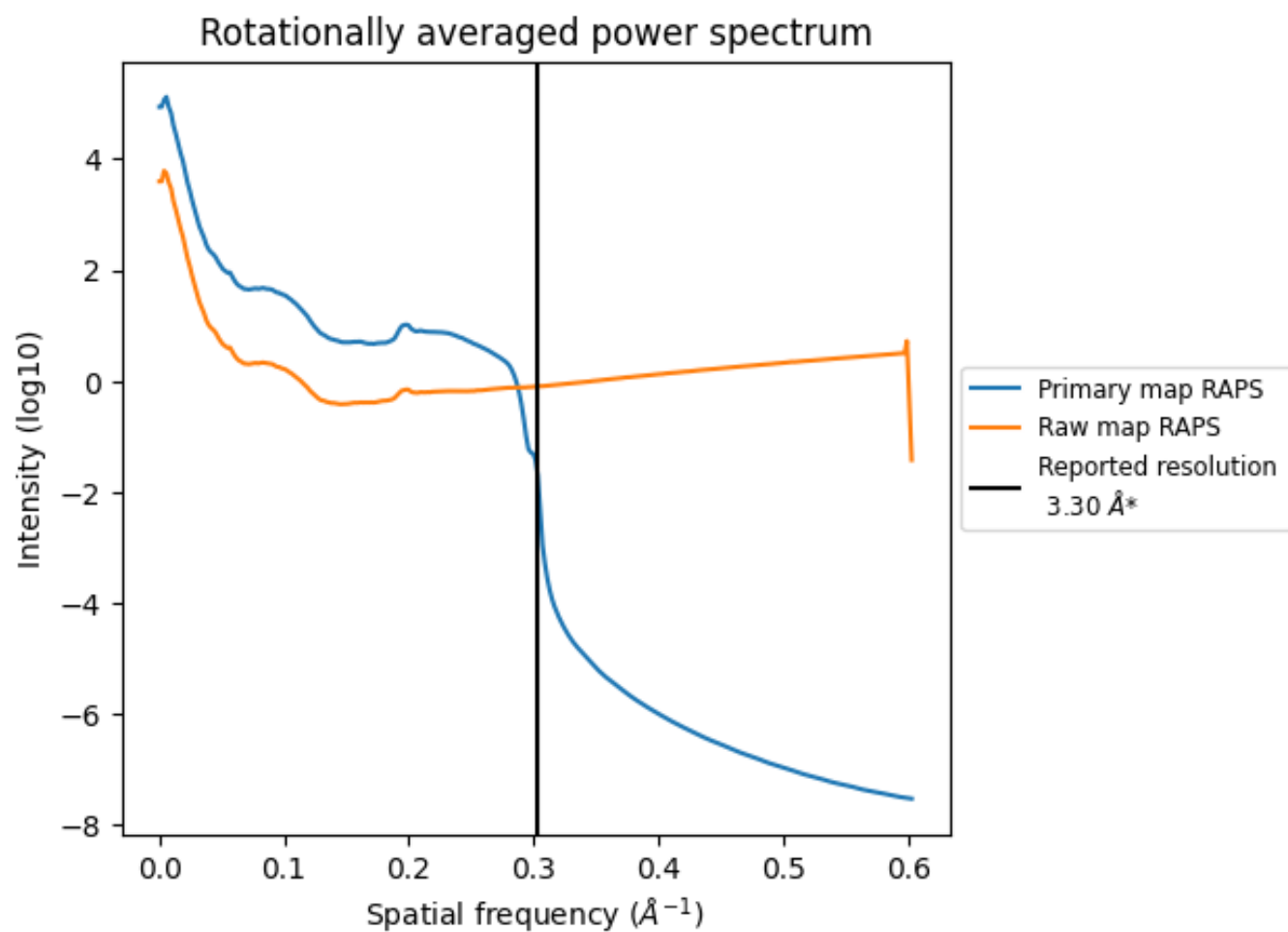
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm^3 ; this corresponds to an approximate mass of 80 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 ⓘ

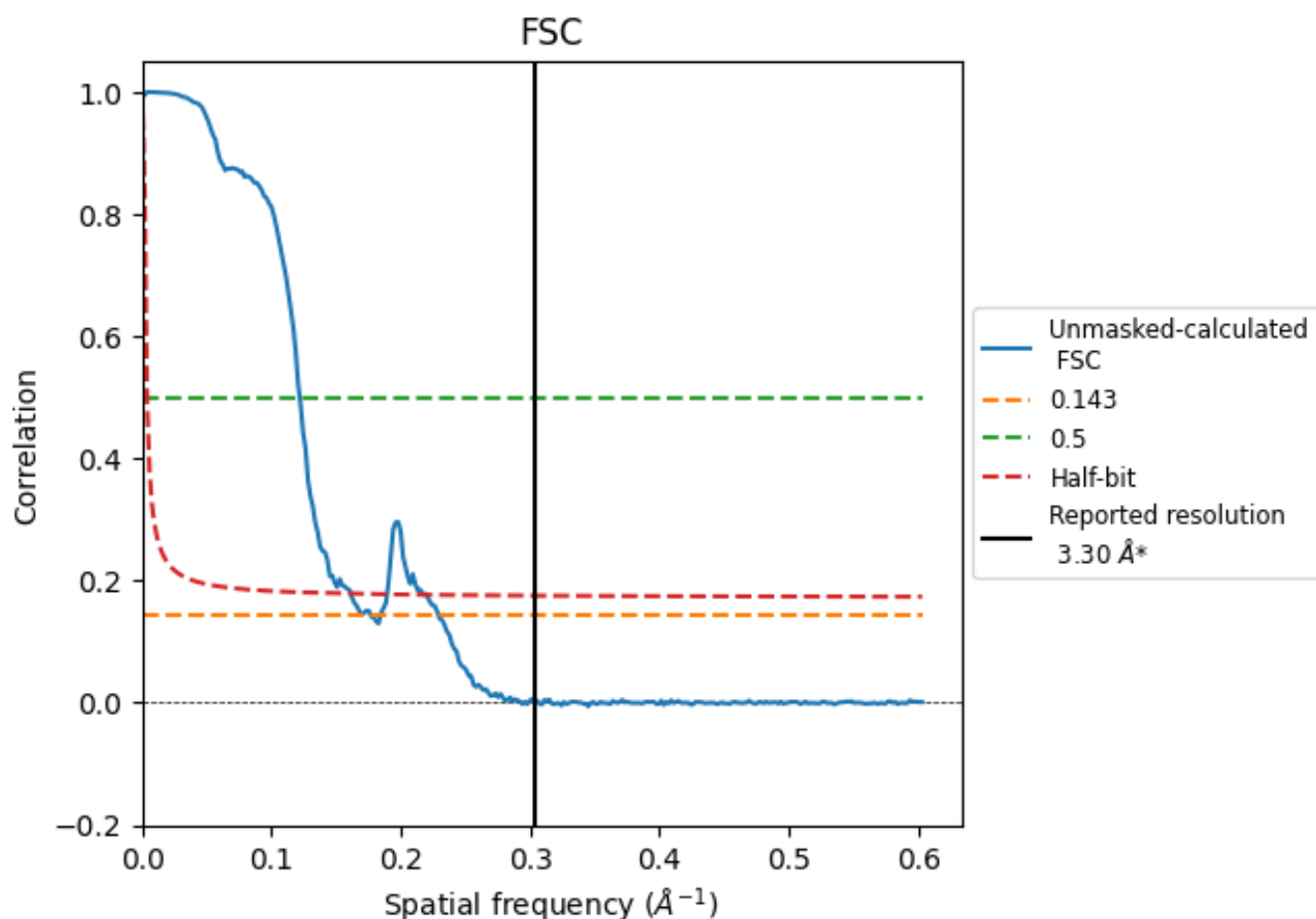


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

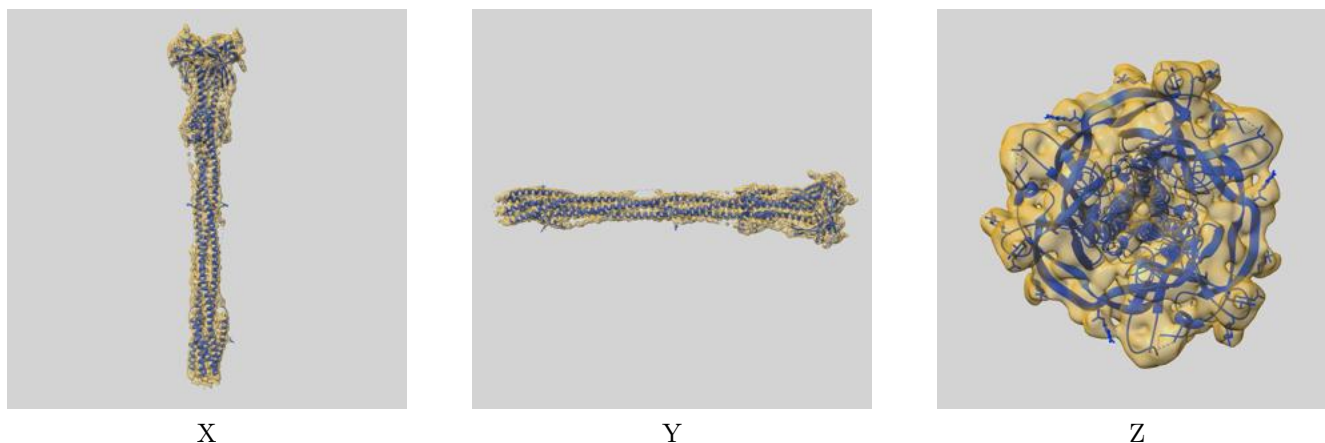
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.66	8.21	6.20

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

9 Map-model fit [i](#)

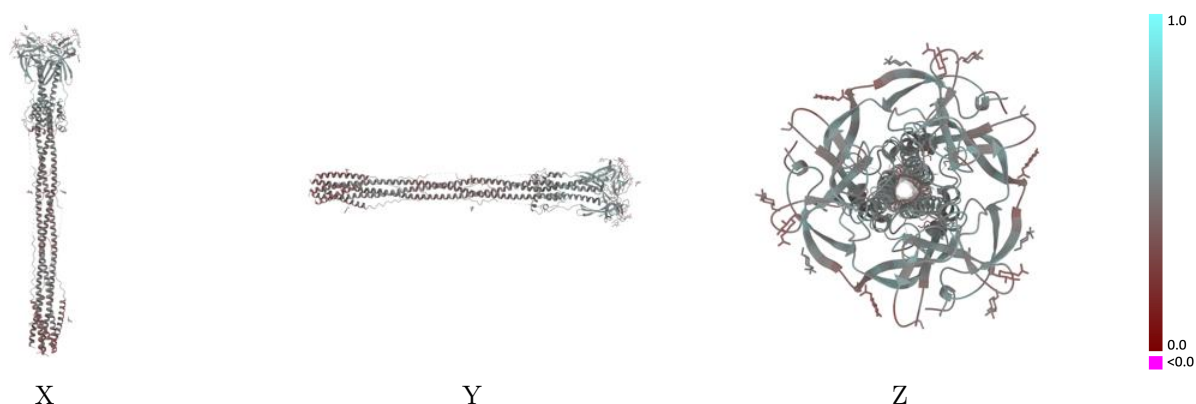
This section contains information regarding the fit between EMDB map EMD-73787 and PDB model 9Z3K. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



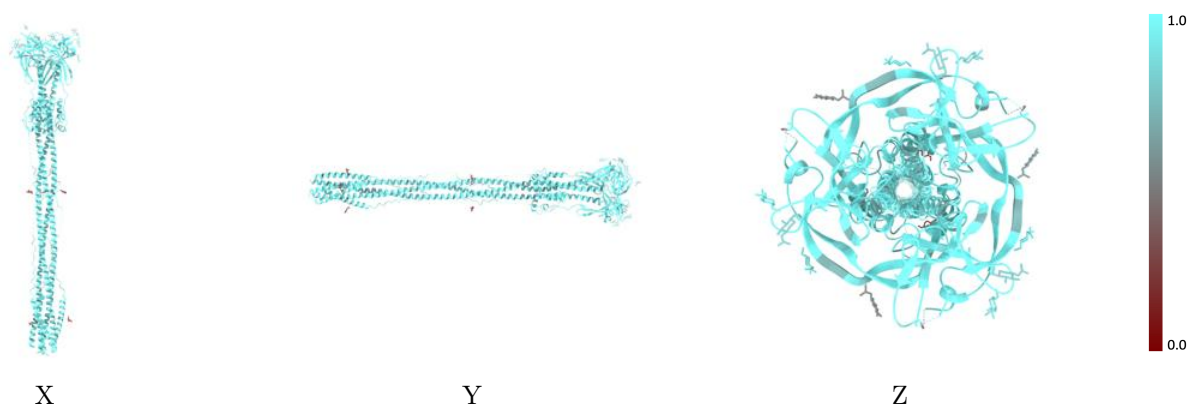
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



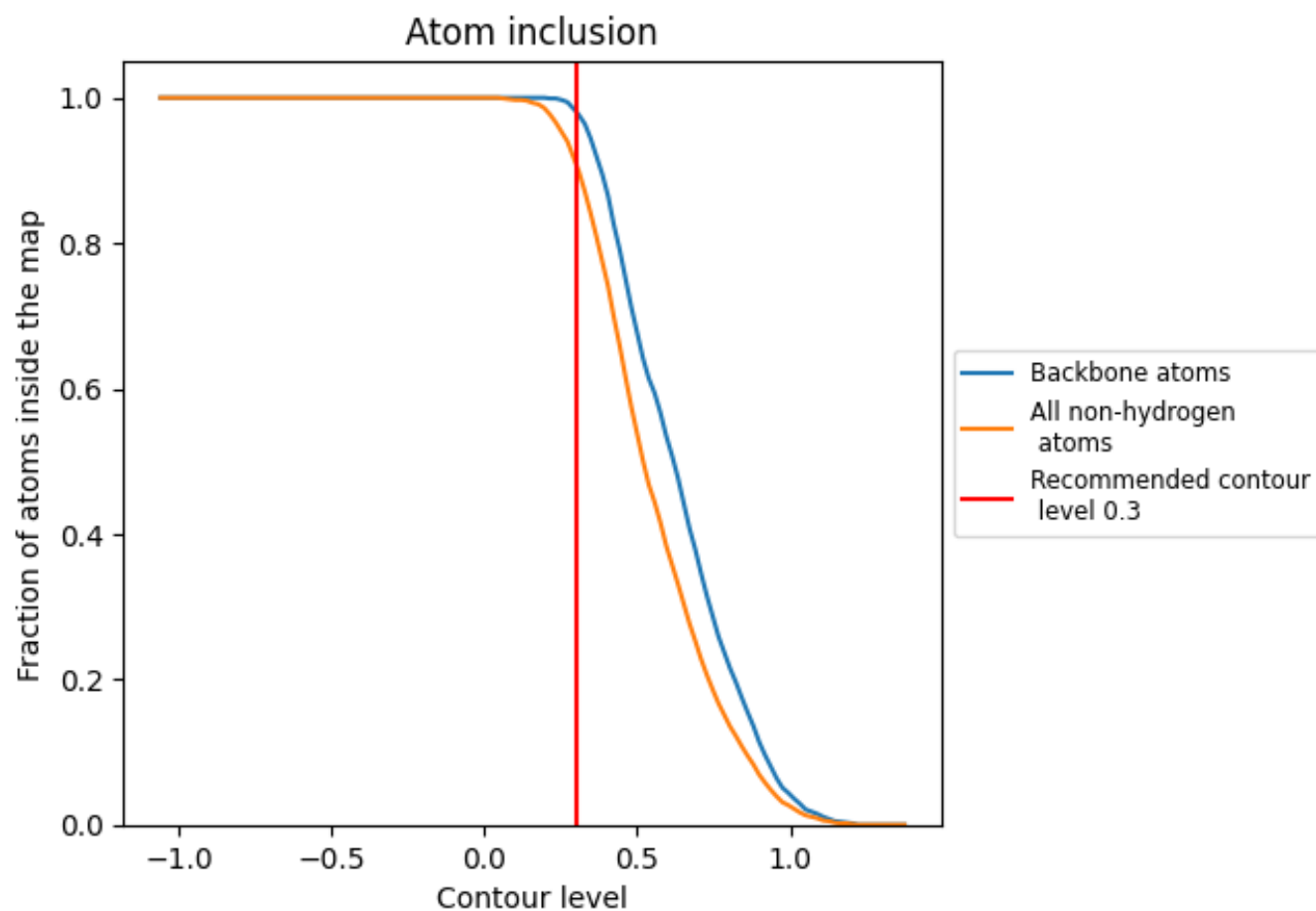
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 98% of all backbone atoms, 91% 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	0.9080	0.4600
A	0.9100	0.4610
B	0.9070	0.4600
C	0.9080	0.4600

