



## wwPDB EM Validation Summary Report ⓘ

Mar 4, 2024 – 09:51 PM EST

PDB ID : 8UCQ  
EMDB ID : EMD-42135  
Title : CryoEM structure of Sec7 autoinhibited conformation  
Authors : Brownfield, B.A.; Fromme, J.C.  
Deposited on : 2023-09-27  
Resolution : 3.70 Å (reported)  
Based on initial model : .

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>.

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

EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

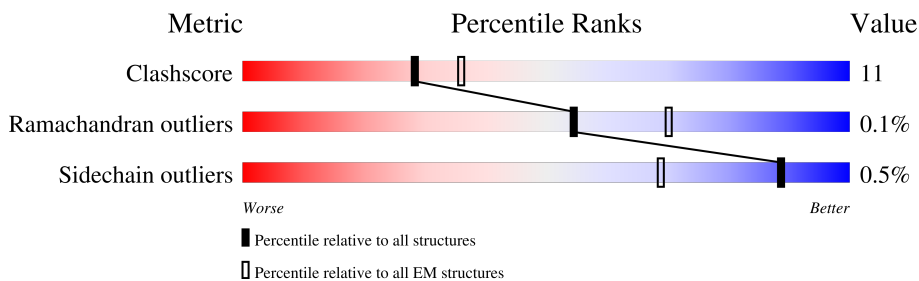
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1937	
1	B	1937	

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 19766 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 SEC7 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1232	9883	6351	1682	1793	57	0	0
1	A	1232	9883	6351	1682	1793	57	0	0

There are 306 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	MET	-	initiating methionine	UNP A0A3S5CXE1
B	-26	GLU	-	expression tag	UNP A0A3S5CXE1
B	-25	GLN	-	expression tag	UNP A0A3S5CXE1
B	-24	LYS	-	expression tag	UNP A0A3S5CXE1
B	-23	LEU	-	expression tag	UNP A0A3S5CXE1
B	-22	ILE	-	expression tag	UNP A0A3S5CXE1
B	-21	SER	-	expression tag	UNP A0A3S5CXE1
B	-20	GLU	-	expression tag	UNP A0A3S5CXE1
B	-19	GLU	-	expression tag	UNP A0A3S5CXE1
B	-18	ASP	-	expression tag	UNP A0A3S5CXE1
B	-17	LEU	-	expression tag	UNP A0A3S5CXE1
B	-16	ASN	-	expression tag	UNP A0A3S5CXE1
B	-15	SER	-	expression tag	UNP A0A3S5CXE1
B	-14	ALA	-	expression tag	UNP A0A3S5CXE1
B	-13	VAL	-	expression tag	UNP A0A3S5CXE1
B	-12	ASP	-	expression tag	UNP A0A3S5CXE1
B	-11	HIS	-	expression tag	UNP A0A3S5CXE1
B	-10	HIS	-	expression tag	UNP A0A3S5CXE1
B	-9	HIS	-	expression tag	UNP A0A3S5CXE1
B	-8	HIS	-	expression tag	UNP A0A3S5CXE1
B	-7	HIS	-	expression tag	UNP A0A3S5CXE1
B	-6	HIS	-	expression tag	UNP A0A3S5CXE1
B	-5	ARG	-	expression tag	UNP A0A3S5CXE1
B	-4	ILE	-	expression tag	UNP A0A3S5CXE1
B	-3	PRO	-	expression tag	UNP A0A3S5CXE1
B	-2	GLY	-	expression tag	UNP A0A3S5CXE1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	LEU	-	expression tag	UNP A0A3S5CXE1
B	0	ILE	-	expression tag	UNP A0A3S5CXE1
B	1	ASN	-	expression tag	UNP A0A3S5CXE1
B	88	THR	SER	conflict	UNP A0A3S5CXE1
B	1787	LEU	-	expression tag	UNP A0A3S5CXE1
B	1788	VAL	-	expression tag	UNP A0A3S5CXE1
B	1789	VAL	-	expression tag	UNP A0A3S5CXE1
B	1790	GLU	-	expression tag	UNP A0A3S5CXE1
B	1791	LEU	-	expression tag	UNP A0A3S5CXE1
B	1792	LEU	-	expression tag	UNP A0A3S5CXE1
B	1793	GLY	-	expression tag	UNP A0A3S5CXE1
B	1794	LYS	-	expression tag	UNP A0A3S5CXE1
B	1795	ASP	-	expression tag	UNP A0A3S5CXE1
B	1796	LEU	-	expression tag	UNP A0A3S5CXE1
B	1797	GLY	-	expression tag	UNP A0A3S5CXE1
B	1798	GLN	-	expression tag	UNP A0A3S5CXE1
B	1799	ASP	-	expression tag	UNP A0A3S5CXE1
B	1800	LEU	-	expression tag	UNP A0A3S5CXE1
B	1801	ARG	-	expression tag	UNP A0A3S5CXE1
B	1802	ALA	-	expression tag	UNP A0A3S5CXE1
B	1803	ALA	-	expression tag	UNP A0A3S5CXE1
B	1804	LEU	-	expression tag	UNP A0A3S5CXE1
B	1805	LEU	-	expression tag	UNP A0A3S5CXE1
B	1806	LEU	-	expression tag	UNP A0A3S5CXE1
B	1807	VAL	-	expression tag	UNP A0A3S5CXE1
B	1808	LEU	-	expression tag	UNP A0A3S5CXE1
B	1809	ARG	-	expression tag	UNP A0A3S5CXE1
B	1810	ARG	-	expression tag	UNP A0A3S5CXE1
B	1811	VAL	-	expression tag	UNP A0A3S5CXE1
B	1812	GLY	-	expression tag	UNP A0A3S5CXE1
B	1813	GLU	-	expression tag	UNP A0A3S5CXE1
B	1814	VAL	-	expression tag	UNP A0A3S5CXE1
B	1815	GLY	-	expression tag	UNP A0A3S5CXE1
B	1816	LEU	-	expression tag	UNP A0A3S5CXE1
B	1817	GLY	-	expression tag	UNP A0A3S5CXE1
B	1818	ILE	-	expression tag	UNP A0A3S5CXE1
B	1819	GLU	-	expression tag	UNP A0A3S5CXE1
B	1820	GLY	-	expression tag	UNP A0A3S5CXE1
B	1821	MET	-	expression tag	UNP A0A3S5CXE1
B	1822	GLY	-	expression tag	UNP A0A3S5CXE1
B	1823	SER	-	expression tag	UNP A0A3S5CXE1
B	1824	GLY	-	expression tag	UNP A0A3S5CXE1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1825	GLY	-	expression tag	UNP A0A3S5CXE1
B	1826	ALA	-	expression tag	UNP A0A3S5CXE1
B	1827	ALA	-	expression tag	UNP A0A3S5CXE1
B	1828	ALA	-	expression tag	UNP A0A3S5CXE1
B	1829	ALA	-	expression tag	UNP A0A3S5CXE1
B	1830	ALA	-	expression tag	UNP A0A3S5CXE1
B	1831	ALA	-	expression tag	UNP A0A3S5CXE1
B	1832	ALA	-	expression tag	UNP A0A3S5CXE1
B	1833	GLY	-	expression tag	UNP A0A3S5CXE1
B	1834	ALA	-	expression tag	UNP A0A3S5CXE1
B	1835	ALA	-	expression tag	UNP A0A3S5CXE1
B	1836	ALA	-	expression tag	UNP A0A3S5CXE1
B	1837	ALA	-	expression tag	UNP A0A3S5CXE1
B	1838	SER	-	expression tag	UNP A0A3S5CXE1
B	1839	SER	-	expression tag	UNP A0A3S5CXE1
B	1840	GLY	-	expression tag	UNP A0A3S5CXE1
B	1841	GLN	-	expression tag	UNP A0A3S5CXE1
B	1842	GLY	-	expression tag	UNP A0A3S5CXE1
B	1843	ASN	-	expression tag	UNP A0A3S5CXE1
B	1844	GLY	-	expression tag	UNP A0A3S5CXE1
B	1845	ASN	-	expression tag	UNP A0A3S5CXE1
B	1846	GLY	-	expression tag	UNP A0A3S5CXE1
B	1847	ALA	-	expression tag	UNP A0A3S5CXE1
B	1848	ALA	-	expression tag	UNP A0A3S5CXE1
B	1849	ALA	-	expression tag	UNP A0A3S5CXE1
B	1850	ALA	-	expression tag	UNP A0A3S5CXE1
B	1851	ALA	-	expression tag	UNP A0A3S5CXE1
B	1852	ALA	-	expression tag	UNP A0A3S5CXE1
B	1853	ASP	-	expression tag	UNP A0A3S5CXE1
B	1854	SER	-	expression tag	UNP A0A3S5CXE1
B	1855	GLU	-	expression tag	UNP A0A3S5CXE1
B	1856	ARG	-	expression tag	UNP A0A3S5CXE1
B	1857	ARG	-	expression tag	UNP A0A3S5CXE1
B	1858	SER	-	expression tag	UNP A0A3S5CXE1
B	1859	SER	-	expression tag	UNP A0A3S5CXE1
B	1860	VAL	-	expression tag	UNP A0A3S5CXE1
B	1861	LEU	-	expression tag	UNP A0A3S5CXE1
B	1862	SER	-	expression tag	UNP A0A3S5CXE1
B	1863	VAL	-	expression tag	UNP A0A3S5CXE1
B	1864	PRO	-	expression tag	UNP A0A3S5CXE1
B	1865	SER	-	expression tag	UNP A0A3S5CXE1
B	1866	GLY	-	expression tag	UNP A0A3S5CXE1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1867	PRO	-	expression tag	UNP A0A3S5CXE1
B	1868	ARG	-	expression tag	UNP A0A3S5CXE1
B	1869	HIS	-	expression tag	UNP A0A3S5CXE1
B	1870	THR	-	expression tag	UNP A0A3S5CXE1
B	1871	PRO	-	expression tag	UNP A0A3S5CXE1
B	1872	SER	-	expression tag	UNP A0A3S5CXE1
B	1873	MET	-	expression tag	UNP A0A3S5CXE1
B	1874	ASP	-	expression tag	UNP A0A3S5CXE1
B	1875	SER	-	expression tag	UNP A0A3S5CXE1
B	1876	LEU	-	expression tag	UNP A0A3S5CXE1
B	1877	ASN	-	expression tag	UNP A0A3S5CXE1
B	1878	ASP	-	expression tag	UNP A0A3S5CXE1
B	1879	ASP	-	expression tag	UNP A0A3S5CXE1
B	1880	PRO	-	expression tag	UNP A0A3S5CXE1
B	1881	SER	-	expression tag	UNP A0A3S5CXE1
B	1882	ARG	-	expression tag	UNP A0A3S5CXE1
B	1883	GLN	-	expression tag	UNP A0A3S5CXE1
B	1884	VAL	-	expression tag	UNP A0A3S5CXE1
B	1885	MET	-	expression tag	UNP A0A3S5CXE1
B	1886	GLY	-	expression tag	UNP A0A3S5CXE1
B	1887	LYS	-	expression tag	UNP A0A3S5CXE1
B	1888	ALA	-	expression tag	UNP A0A3S5CXE1
B	1889	GLU	-	expression tag	UNP A0A3S5CXE1
B	1890	GLN	-	expression tag	UNP A0A3S5CXE1
B	1891	LYS	-	expression tag	UNP A0A3S5CXE1
B	1892	LEU	-	expression tag	UNP A0A3S5CXE1
B	1893	ILE	-	expression tag	UNP A0A3S5CXE1
B	1894	SER	-	expression tag	UNP A0A3S5CXE1
B	1895	GLU	-	expression tag	UNP A0A3S5CXE1
B	1896	GLU	-	expression tag	UNP A0A3S5CXE1
B	1897	ASP	-	expression tag	UNP A0A3S5CXE1
B	1898	LEU	-	expression tag	UNP A0A3S5CXE1
B	1899	ASN	-	expression tag	UNP A0A3S5CXE1
B	1900	SER	-	expression tag	UNP A0A3S5CXE1
B	1901	ALA	-	expression tag	UNP A0A3S5CXE1
B	1902	VAL	-	expression tag	UNP A0A3S5CXE1
B	1903	ASP	-	expression tag	UNP A0A3S5CXE1
B	1904	HIS	-	expression tag	UNP A0A3S5CXE1
B	1905	HIS	-	expression tag	UNP A0A3S5CXE1
B	1906	HIS	-	expression tag	UNP A0A3S5CXE1
B	1907	HIS	-	expression tag	UNP A0A3S5CXE1
B	1908	HIS	-	expression tag	UNP A0A3S5CXE1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1909	HIS	-	expression tag	UNP A0A3S5CXE1
A	-27	MET	-	initiating methionine	UNP A0A3S5CXE1
A	-26	GLU	-	expression tag	UNP A0A3S5CXE1
A	-25	GLN	-	expression tag	UNP A0A3S5CXE1
A	-24	LYS	-	expression tag	UNP A0A3S5CXE1
A	-23	LEU	-	expression tag	UNP A0A3S5CXE1
A	-22	ILE	-	expression tag	UNP A0A3S5CXE1
A	-21	SER	-	expression tag	UNP A0A3S5CXE1
A	-20	GLU	-	expression tag	UNP A0A3S5CXE1
A	-19	GLU	-	expression tag	UNP A0A3S5CXE1
A	-18	ASP	-	expression tag	UNP A0A3S5CXE1
A	-17	LEU	-	expression tag	UNP A0A3S5CXE1
A	-16	ASN	-	expression tag	UNP A0A3S5CXE1
A	-15	SER	-	expression tag	UNP A0A3S5CXE1
A	-14	ALA	-	expression tag	UNP A0A3S5CXE1
A	-13	VAL	-	expression tag	UNP A0A3S5CXE1
A	-12	ASP	-	expression tag	UNP A0A3S5CXE1
A	-11	HIS	-	expression tag	UNP A0A3S5CXE1
A	-10	HIS	-	expression tag	UNP A0A3S5CXE1
A	-9	HIS	-	expression tag	UNP A0A3S5CXE1
A	-8	HIS	-	expression tag	UNP A0A3S5CXE1
A	-7	HIS	-	expression tag	UNP A0A3S5CXE1
A	-6	HIS	-	expression tag	UNP A0A3S5CXE1
A	-5	ARG	-	expression tag	UNP A0A3S5CXE1
A	-4	ILE	-	expression tag	UNP A0A3S5CXE1
A	-3	PRO	-	expression tag	UNP A0A3S5CXE1
A	-2	GLY	-	expression tag	UNP A0A3S5CXE1
A	-1	LEU	-	expression tag	UNP A0A3S5CXE1
A	0	ILE	-	expression tag	UNP A0A3S5CXE1
A	1	ASN	-	expression tag	UNP A0A3S5CXE1
A	88	THR	SER	conflict	UNP A0A3S5CXE1
A	1787	LEU	-	expression tag	UNP A0A3S5CXE1
A	1788	VAL	-	expression tag	UNP A0A3S5CXE1
A	1789	VAL	-	expression tag	UNP A0A3S5CXE1
A	1790	GLU	-	expression tag	UNP A0A3S5CXE1
A	1791	LEU	-	expression tag	UNP A0A3S5CXE1
A	1792	LEU	-	expression tag	UNP A0A3S5CXE1
A	1793	GLY	-	expression tag	UNP A0A3S5CXE1
A	1794	LYS	-	expression tag	UNP A0A3S5CXE1
A	1795	ASP	-	expression tag	UNP A0A3S5CXE1
A	1796	LEU	-	expression tag	UNP A0A3S5CXE1
A	1797	GLY	-	expression tag	UNP A0A3S5CXE1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1798	GLN	-	expression tag	UNP A0A3S5CXE1
A	1799	ASP	-	expression tag	UNP A0A3S5CXE1
A	1800	LEU	-	expression tag	UNP A0A3S5CXE1
A	1801	ARG	-	expression tag	UNP A0A3S5CXE1
A	1802	ALA	-	expression tag	UNP A0A3S5CXE1
A	1803	ALA	-	expression tag	UNP A0A3S5CXE1
A	1804	LEU	-	expression tag	UNP A0A3S5CXE1
A	1805	LEU	-	expression tag	UNP A0A3S5CXE1
A	1806	LEU	-	expression tag	UNP A0A3S5CXE1
A	1807	VAL	-	expression tag	UNP A0A3S5CXE1
A	1808	LEU	-	expression tag	UNP A0A3S5CXE1
A	1809	ARG	-	expression tag	UNP A0A3S5CXE1
A	1810	ARG	-	expression tag	UNP A0A3S5CXE1
A	1811	VAL	-	expression tag	UNP A0A3S5CXE1
A	1812	GLY	-	expression tag	UNP A0A3S5CXE1
A	1813	GLU	-	expression tag	UNP A0A3S5CXE1
A	1814	VAL	-	expression tag	UNP A0A3S5CXE1
A	1815	GLY	-	expression tag	UNP A0A3S5CXE1
A	1816	LEU	-	expression tag	UNP A0A3S5CXE1
A	1817	GLY	-	expression tag	UNP A0A3S5CXE1
A	1818	ILE	-	expression tag	UNP A0A3S5CXE1
A	1819	GLU	-	expression tag	UNP A0A3S5CXE1
A	1820	GLY	-	expression tag	UNP A0A3S5CXE1
A	1821	MET	-	expression tag	UNP A0A3S5CXE1
A	1822	GLY	-	expression tag	UNP A0A3S5CXE1
A	1823	SER	-	expression tag	UNP A0A3S5CXE1
A	1824	GLY	-	expression tag	UNP A0A3S5CXE1
A	1825	GLY	-	expression tag	UNP A0A3S5CXE1
A	1826	ALA	-	expression tag	UNP A0A3S5CXE1
A	1827	ALA	-	expression tag	UNP A0A3S5CXE1
A	1828	ALA	-	expression tag	UNP A0A3S5CXE1
A	1829	ALA	-	expression tag	UNP A0A3S5CXE1
A	1830	ALA	-	expression tag	UNP A0A3S5CXE1
A	1831	ALA	-	expression tag	UNP A0A3S5CXE1
A	1832	ALA	-	expression tag	UNP A0A3S5CXE1
A	1833	GLY	-	expression tag	UNP A0A3S5CXE1
A	1834	ALA	-	expression tag	UNP A0A3S5CXE1
A	1835	ALA	-	expression tag	UNP A0A3S5CXE1
A	1836	ALA	-	expression tag	UNP A0A3S5CXE1
A	1837	ALA	-	expression tag	UNP A0A3S5CXE1
A	1838	SER	-	expression tag	UNP A0A3S5CXE1
A	1839	SER	-	expression tag	UNP A0A3S5CXE1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1840	GLY	-	expression tag	UNP A0A3S5CXE1
A	1841	GLN	-	expression tag	UNP A0A3S5CXE1
A	1842	GLY	-	expression tag	UNP A0A3S5CXE1
A	1843	ASN	-	expression tag	UNP A0A3S5CXE1
A	1844	GLY	-	expression tag	UNP A0A3S5CXE1
A	1845	ASN	-	expression tag	UNP A0A3S5CXE1
A	1846	GLY	-	expression tag	UNP A0A3S5CXE1
A	1847	ALA	-	expression tag	UNP A0A3S5CXE1
A	1848	ALA	-	expression tag	UNP A0A3S5CXE1
A	1849	ALA	-	expression tag	UNP A0A3S5CXE1
A	1850	ALA	-	expression tag	UNP A0A3S5CXE1
A	1851	ALA	-	expression tag	UNP A0A3S5CXE1
A	1852	ALA	-	expression tag	UNP A0A3S5CXE1
A	1853	ASP	-	expression tag	UNP A0A3S5CXE1
A	1854	SER	-	expression tag	UNP A0A3S5CXE1
A	1855	GLU	-	expression tag	UNP A0A3S5CXE1
A	1856	ARG	-	expression tag	UNP A0A3S5CXE1
A	1857	ARG	-	expression tag	UNP A0A3S5CXE1
A	1858	SER	-	expression tag	UNP A0A3S5CXE1
A	1859	SER	-	expression tag	UNP A0A3S5CXE1
A	1860	VAL	-	expression tag	UNP A0A3S5CXE1
A	1861	LEU	-	expression tag	UNP A0A3S5CXE1
A	1862	SER	-	expression tag	UNP A0A3S5CXE1
A	1863	VAL	-	expression tag	UNP A0A3S5CXE1
A	1864	PRO	-	expression tag	UNP A0A3S5CXE1
A	1865	SER	-	expression tag	UNP A0A3S5CXE1
A	1866	GLY	-	expression tag	UNP A0A3S5CXE1
A	1867	PRO	-	expression tag	UNP A0A3S5CXE1
A	1868	ARG	-	expression tag	UNP A0A3S5CXE1
A	1869	HIS	-	expression tag	UNP A0A3S5CXE1
A	1870	THR	-	expression tag	UNP A0A3S5CXE1
A	1871	PRO	-	expression tag	UNP A0A3S5CXE1
A	1872	SER	-	expression tag	UNP A0A3S5CXE1
A	1873	MET	-	expression tag	UNP A0A3S5CXE1
A	1874	ASP	-	expression tag	UNP A0A3S5CXE1
A	1875	SER	-	expression tag	UNP A0A3S5CXE1
A	1876	LEU	-	expression tag	UNP A0A3S5CXE1
A	1877	ASN	-	expression tag	UNP A0A3S5CXE1
A	1878	ASP	-	expression tag	UNP A0A3S5CXE1
A	1879	ASP	-	expression tag	UNP A0A3S5CXE1
A	1880	PRO	-	expression tag	UNP A0A3S5CXE1
A	1881	SER	-	expression tag	UNP A0A3S5CXE1

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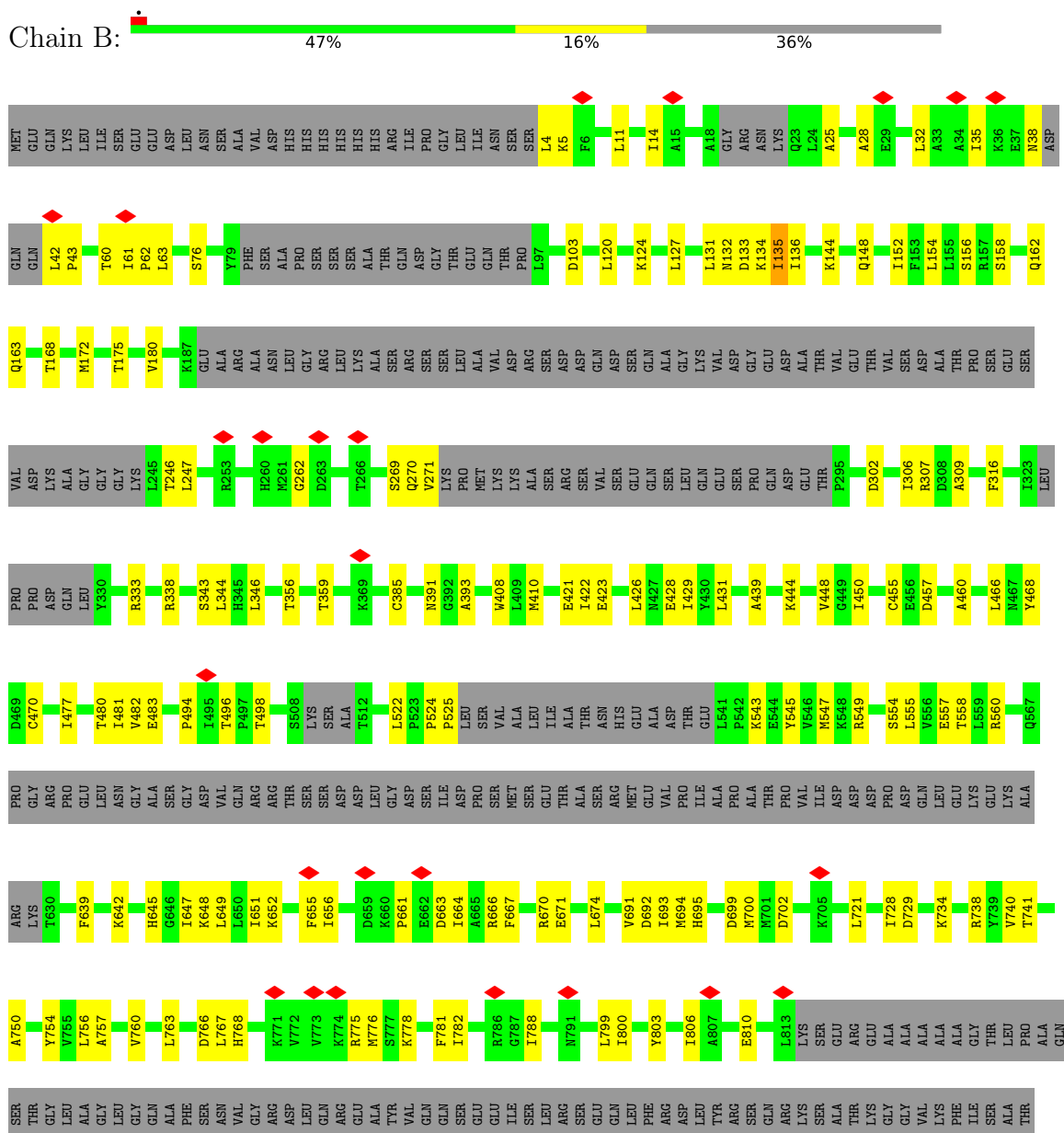
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1882	ARG	-	expression tag	UNP A0A3S5CXE1
A	1883	GLN	-	expression tag	UNP A0A3S5CXE1
A	1884	VAL	-	expression tag	UNP A0A3S5CXE1
A	1885	MET	-	expression tag	UNP A0A3S5CXE1
A	1886	GLY	-	expression tag	UNP A0A3S5CXE1
A	1887	LYS	-	expression tag	UNP A0A3S5CXE1
A	1888	ALA	-	expression tag	UNP A0A3S5CXE1
A	1889	GLU	-	expression tag	UNP A0A3S5CXE1
A	1890	GLN	-	expression tag	UNP A0A3S5CXE1
A	1891	LYS	-	expression tag	UNP A0A3S5CXE1
A	1892	LEU	-	expression tag	UNP A0A3S5CXE1
A	1893	ILE	-	expression tag	UNP A0A3S5CXE1
A	1894	SER	-	expression tag	UNP A0A3S5CXE1
A	1895	GLU	-	expression tag	UNP A0A3S5CXE1
A	1896	GLU	-	expression tag	UNP A0A3S5CXE1
A	1897	ASP	-	expression tag	UNP A0A3S5CXE1
A	1898	LEU	-	expression tag	UNP A0A3S5CXE1
A	1899	ASN	-	expression tag	UNP A0A3S5CXE1
A	1900	SER	-	expression tag	UNP A0A3S5CXE1
A	1901	ALA	-	expression tag	UNP A0A3S5CXE1
A	1902	VAL	-	expression tag	UNP A0A3S5CXE1
A	1903	ASP	-	expression tag	UNP A0A3S5CXE1
A	1904	HIS	-	expression tag	UNP A0A3S5CXE1
A	1905	HIS	-	expression tag	UNP A0A3S5CXE1
A	1906	HIS	-	expression tag	UNP A0A3S5CXE1
A	1907	HIS	-	expression tag	UNP A0A3S5CXE1
A	1908	HIS	-	expression tag	UNP A0A3S5CXE1
A	1909	HIS	-	expression tag	UNP A0A3S5CXE1

### 3 Residue-property plots

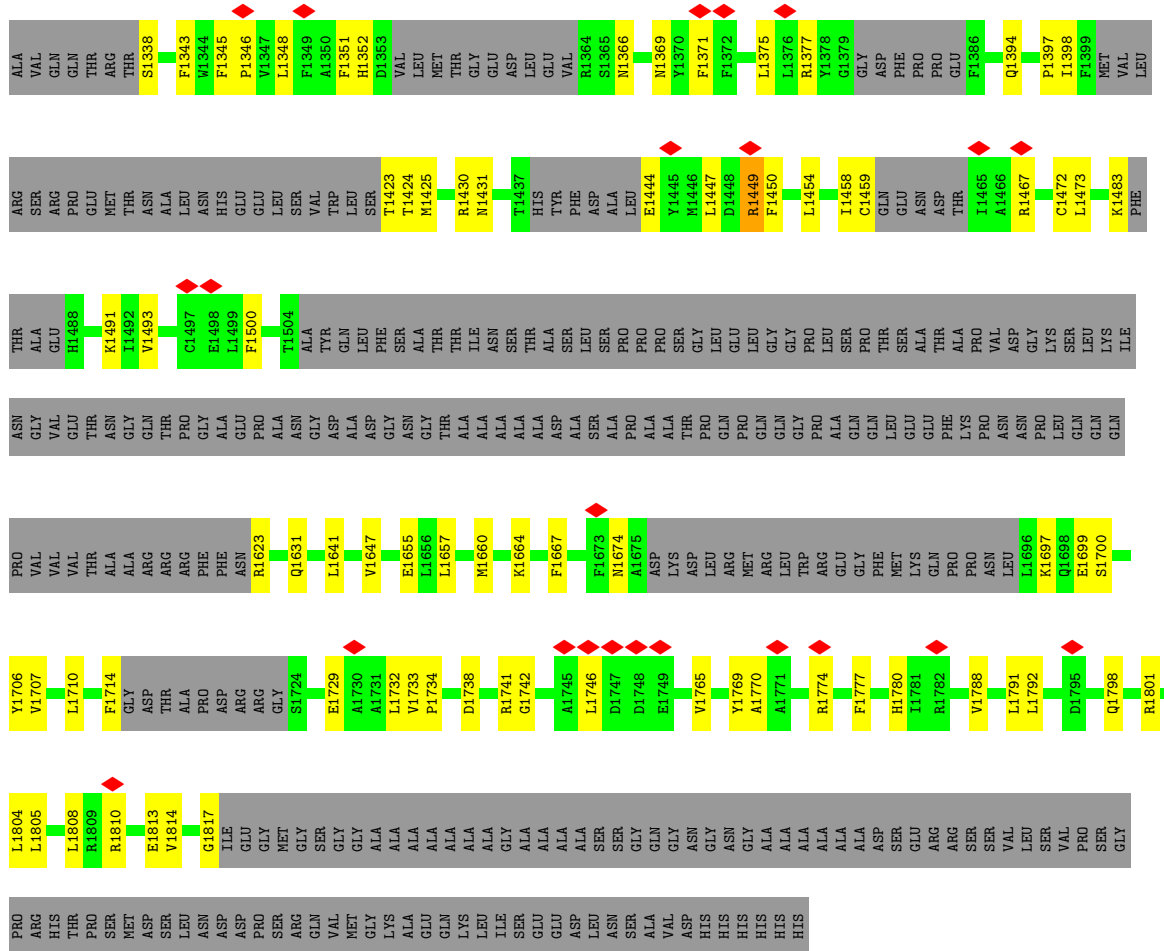
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: SEC7 domain-containing protein











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196888	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55.6	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	63000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	195.124	Depositor
Minimum map value	-93.830	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.374	Depositor
Recommended contour level	41.0	Depositor
Map size (Å)	848.11053, 848.11053, 848.11053	wwPDB
Map dimensions	487, 487, 487	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7415, 1.7415, 1.7415	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.25	0/10050	0.47	1/13560 (0.0%)
1	B	0.27	0/10050	0.49	0/13560
All	All	0.26	0/20100	0.48	1/27120 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9883	0	10037	202	0
1	B	9883	0	10037	220	0
All	All	19766	0	20074	419	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 11.

The worst 5 of 419 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:ILE:HD12	1:B:656:ILE:HG21	1.67	0.77
1:B:1351:PHE:HB3	1:B:1371:PHE:HB2	1.71	0.73
1:A:1351:PHE:HB3	1:A:1371:PHE:HB2	1.71	0.73
1:B:156:SER:HB3	1:B:162:GLN:HG3	1.71	0.72
1:B:1493:VAL:HG21	1:B:1655:GLU:HB3	1.70	0.72

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	1178/1937 (61%)	1139 (97%)	38 (3%)	1 (0%)	51	83
1	B	1178/1937 (61%)	1133 (96%)	44 (4%)	1 (0%)	51	83
All	All	2356/3874 (61%)	2272 (96%)	82 (4%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	ILE
1	A	135	ILE

#### 5.3.2 Protein sidechains [i](#)

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

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

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1089/1657 (66%)	1083 (99%)	6 (1%)	86	93
1	B	1089/1657 (66%)	1085 (100%)	4 (0%)	91	95
All	All	2178/3314 (66%)	2168 (100%)	10 (0%)	89	94

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1467	ARG
1	A	1623	ARG
1	A	1774	ARG
1	B	1774	ARG
1	A	1181	LYS

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

Mol	Chain	Res	Type
1	A	132	ASN
1	A	166	GLN
1	A	391	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

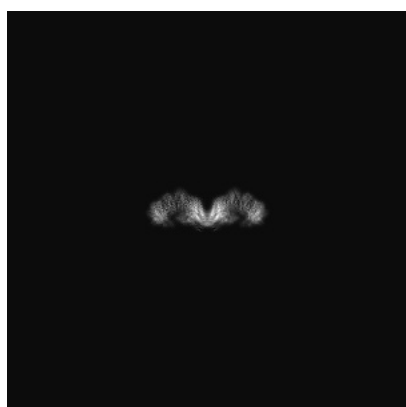
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42135. These allow visual inspection of the internal detail of the map and identification of artifacts.

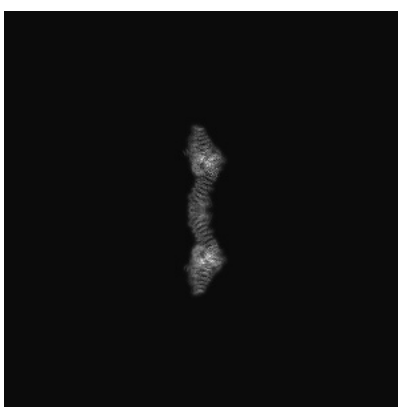
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

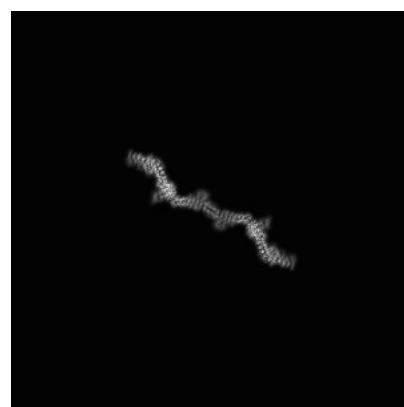
#### 6.1.1 Primary map



X



Y

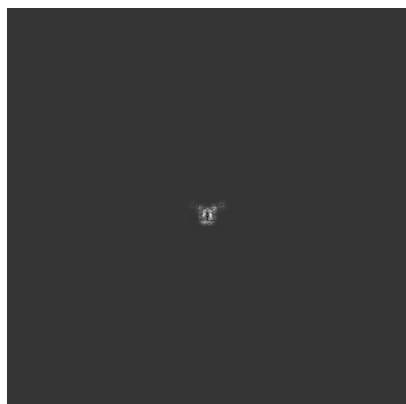


Z

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

### 6.2 Central slices [i](#)

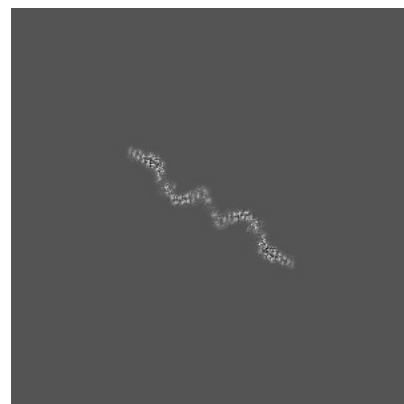
#### 6.2.1 Primary map



X Index: 243



Y Index: 243



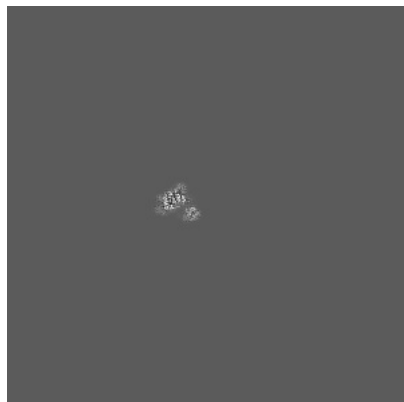
Z Index: 243



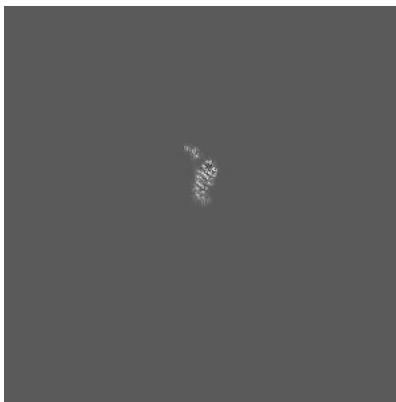
The images above show central slices of the map in three orthogonal directions.

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

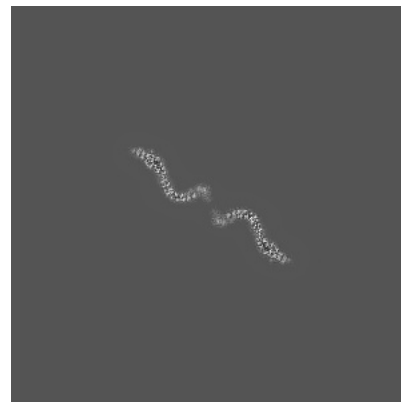
### 6.3.1 Primary map



X Index: 305



Y Index: 231

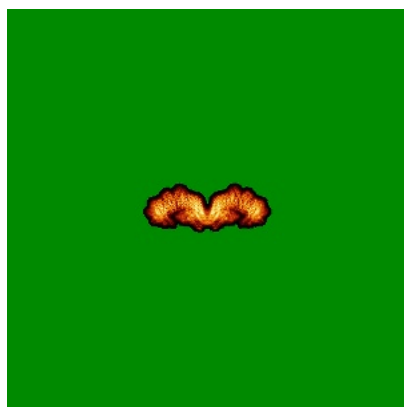


Z Index: 246

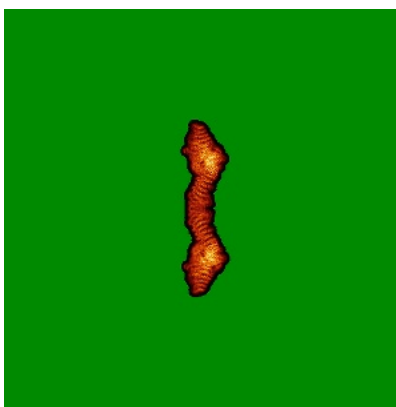
The images above show the largest variance slices of the map in three orthogonal directions.

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

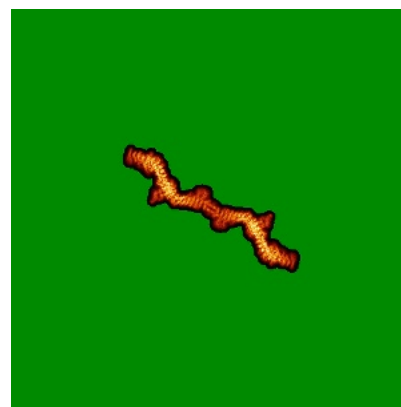
### 6.4.1 Primary map



X



Y

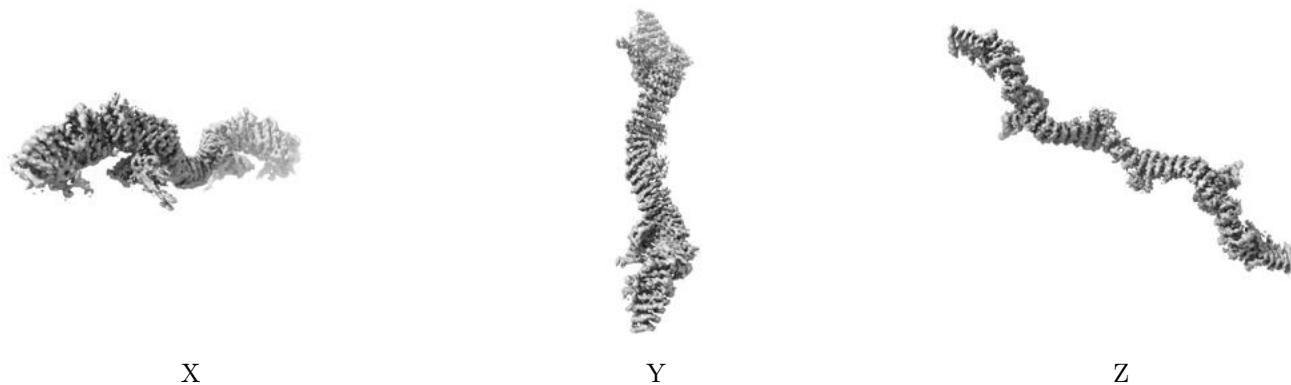


Z

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 41.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

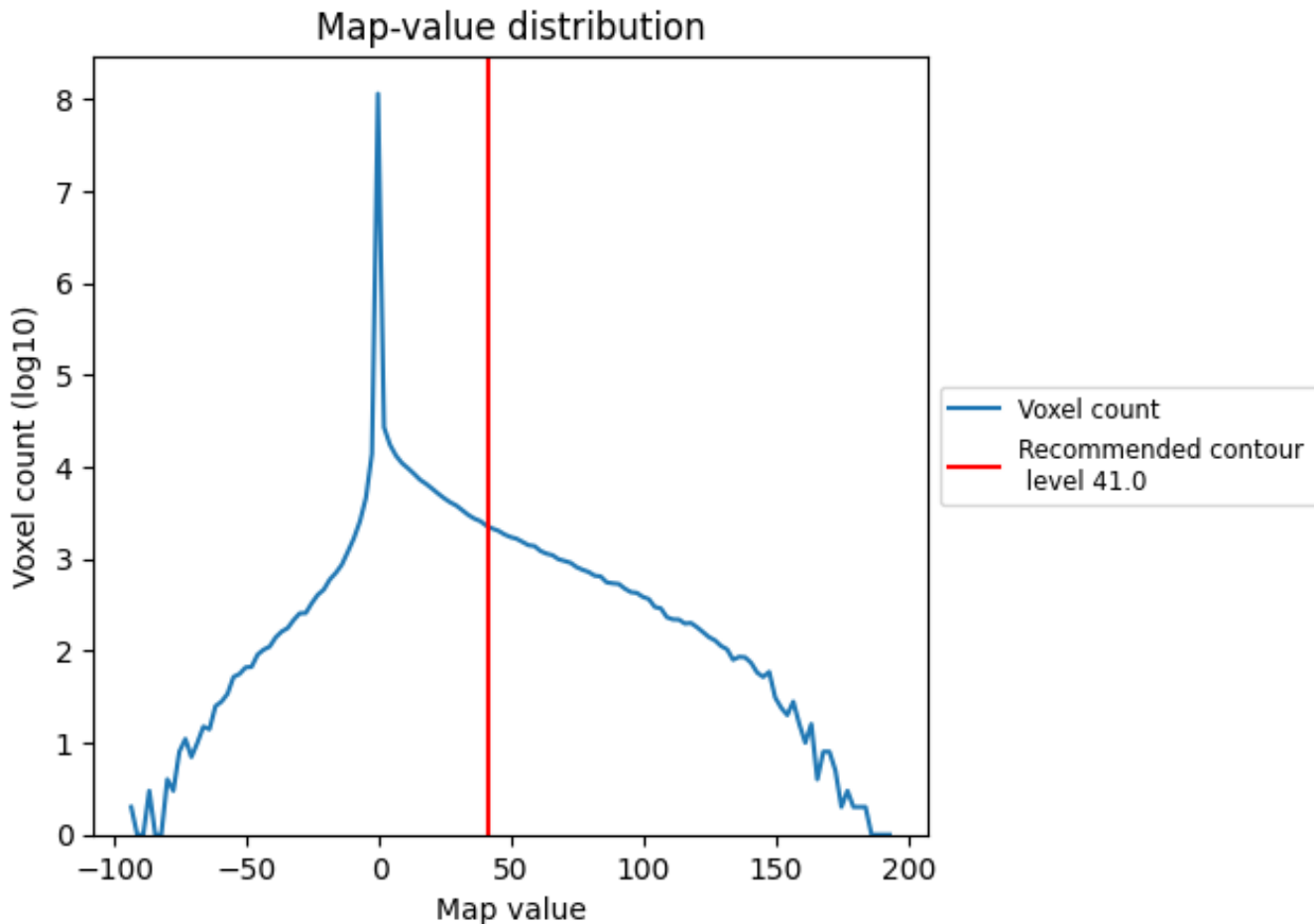
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

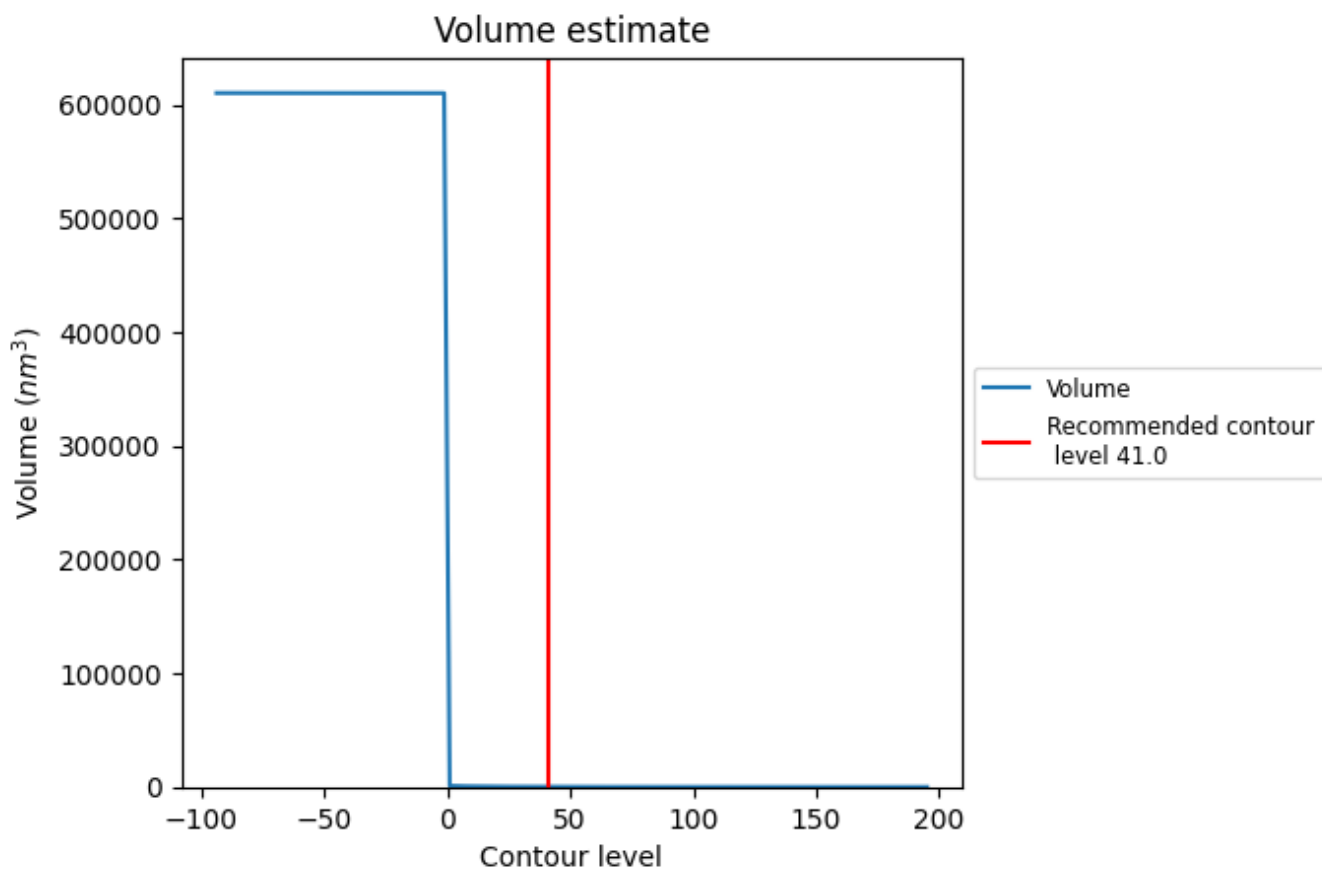
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

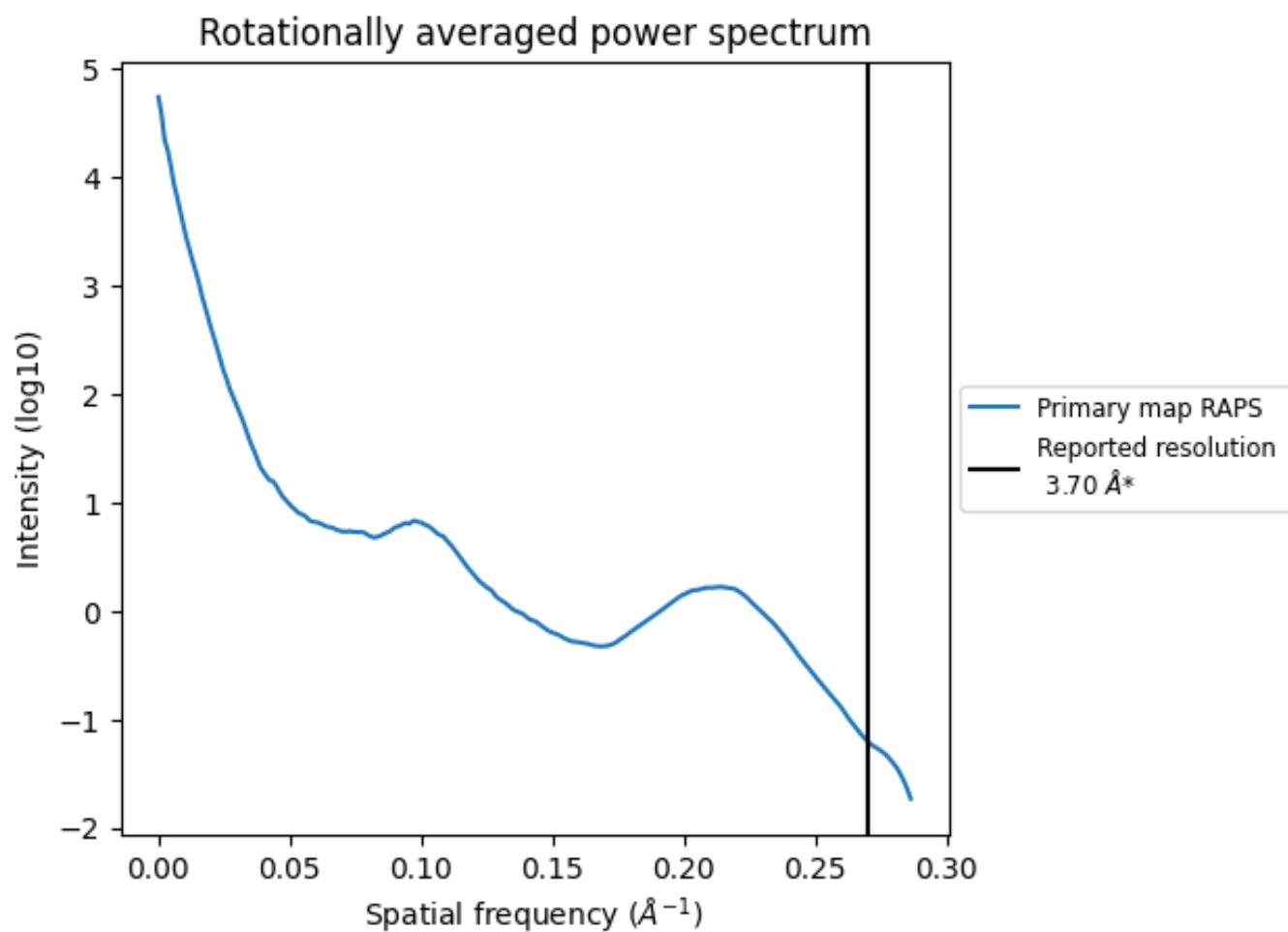
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 170 nm<sup>3</sup>; this corresponds to an approximate mass of 154 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

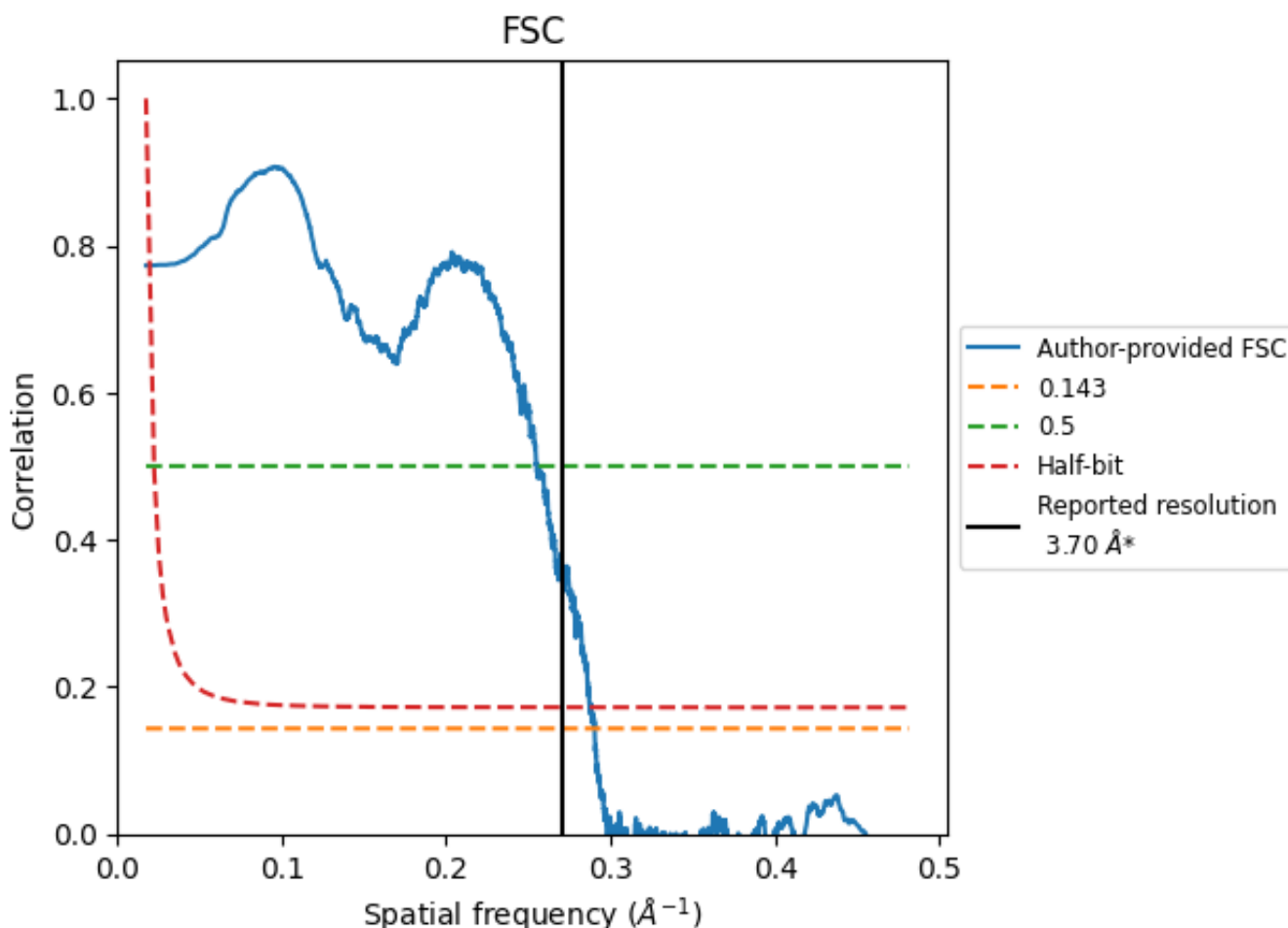


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

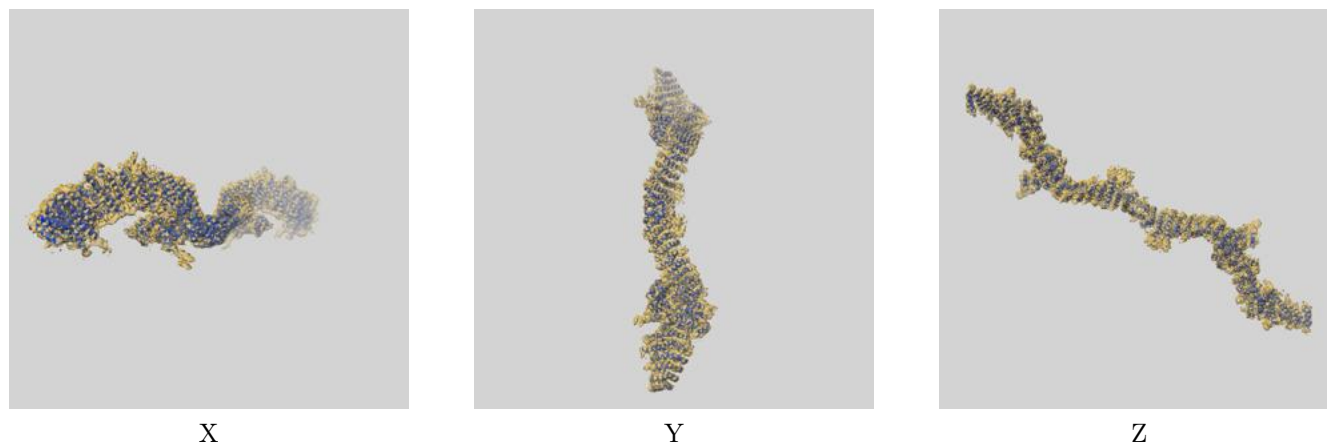
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.44	3.92	3.48
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

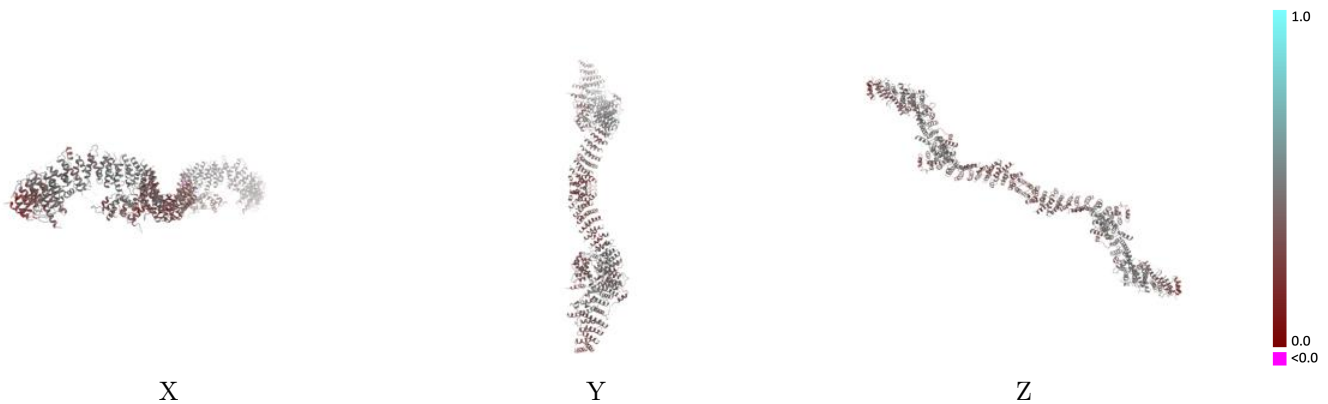
This section contains information regarding the fit between EMDB map EMD-42135 and PDB model 8UCQ. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



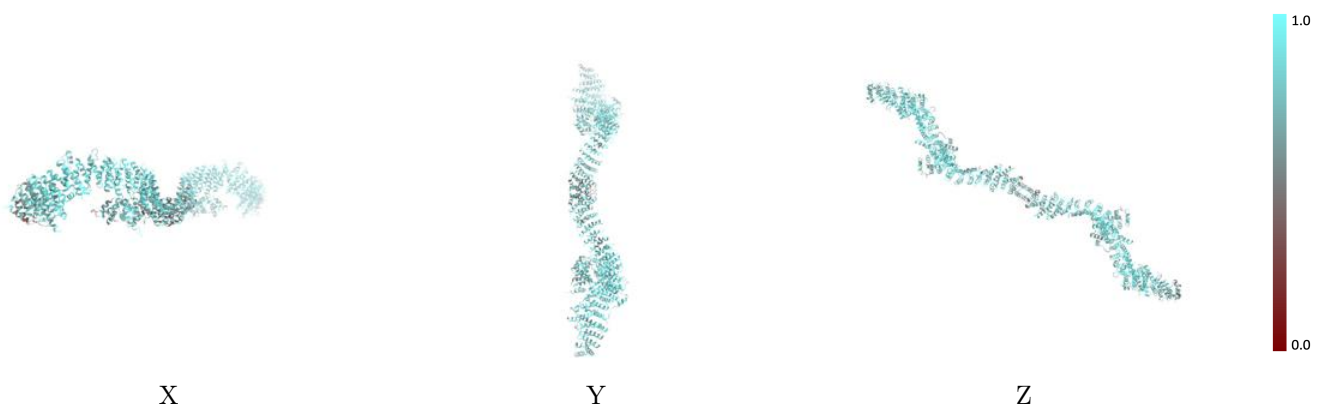
The images above show the 3D surface view of the map at the recommended contour level 41.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



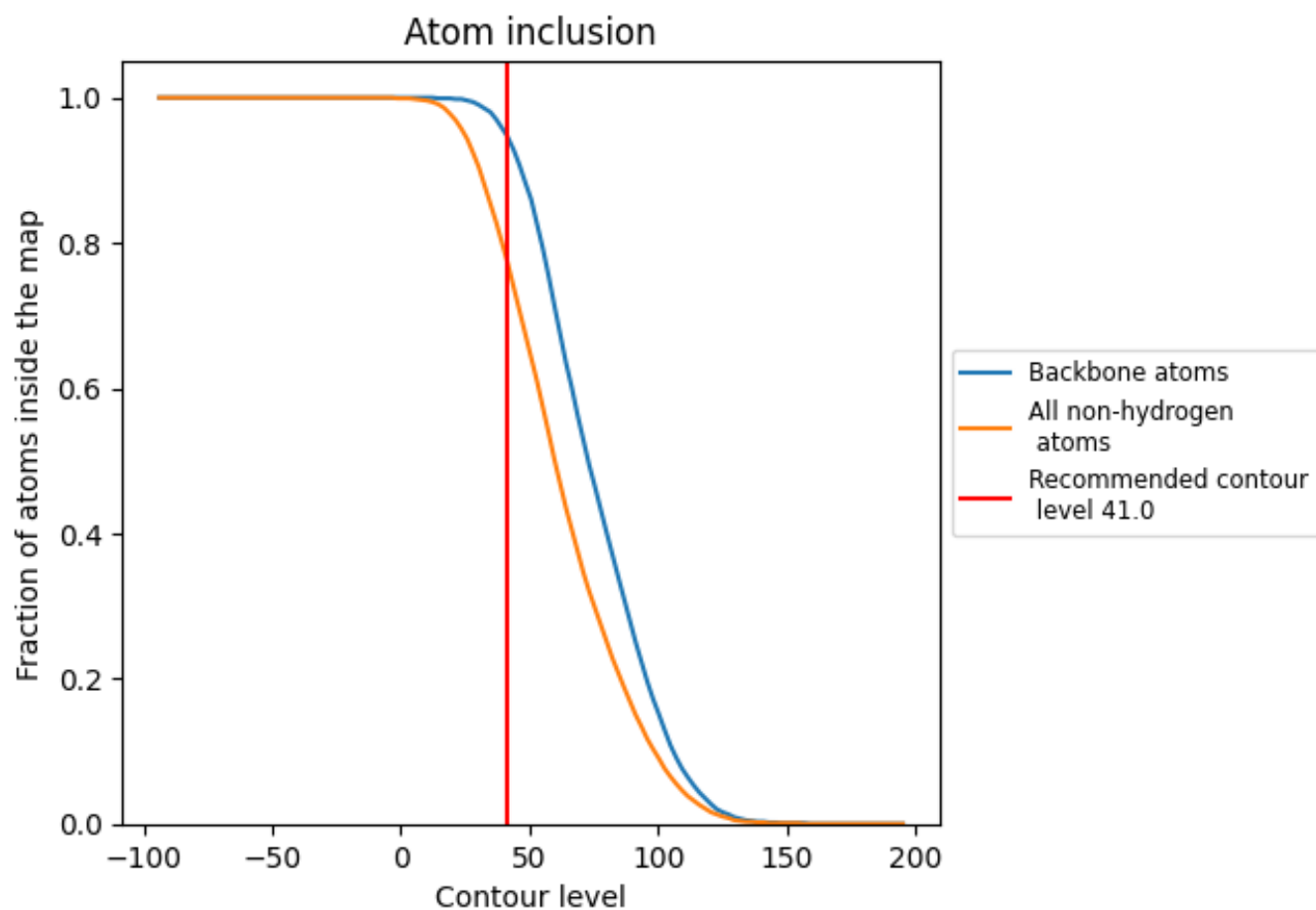
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (41.0).







## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (41.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7780	 0.4040
A	 0.7860	 0.3950
B	 0.7710	 0.4120

