



wwPDB EM Validation Summary Report ⓘ

May 19, 2024 – 09:42 am BST

PDB ID : 6YEW
EMDB ID : EMD-10796
Title : Morganella morganii TcdA4 in complex with porcine mucosa heparin
Authors : Roderer, D.; Broecker, F.; Sitsel, O.; Kaplonek, P.; Leidreiter, F.; Seeberger, P.H.; Raunser, S.
Deposited on : 2020-03-25
Resolution : 3.20 Å(reported)
Based on initial model : 6RW9

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92
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) : 2.36.2

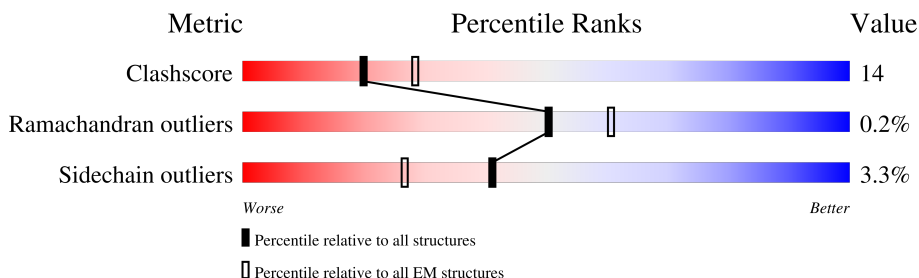
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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 ≥ 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	2469	
1	B	2469	
1	C	2469	
1	D	2469	
1	E	2469	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 88700 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.

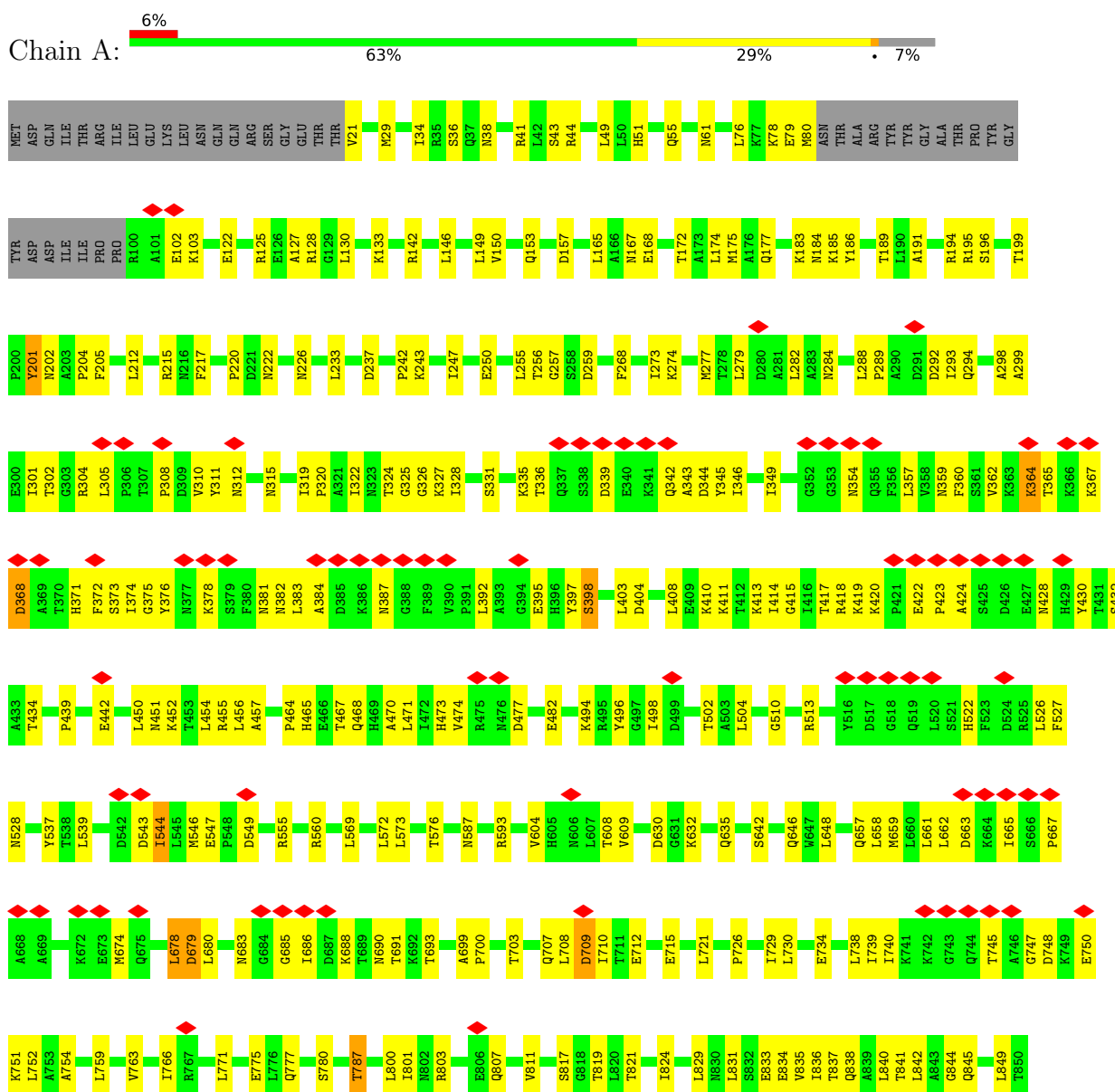
- Molecule 1 is a protein called Insecticidal toxin protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0
1	B	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0
1	C	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0
1	D	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0
1	E	2285	Total 17740	C 11194	N 3070	O 3415	S 61	0	0

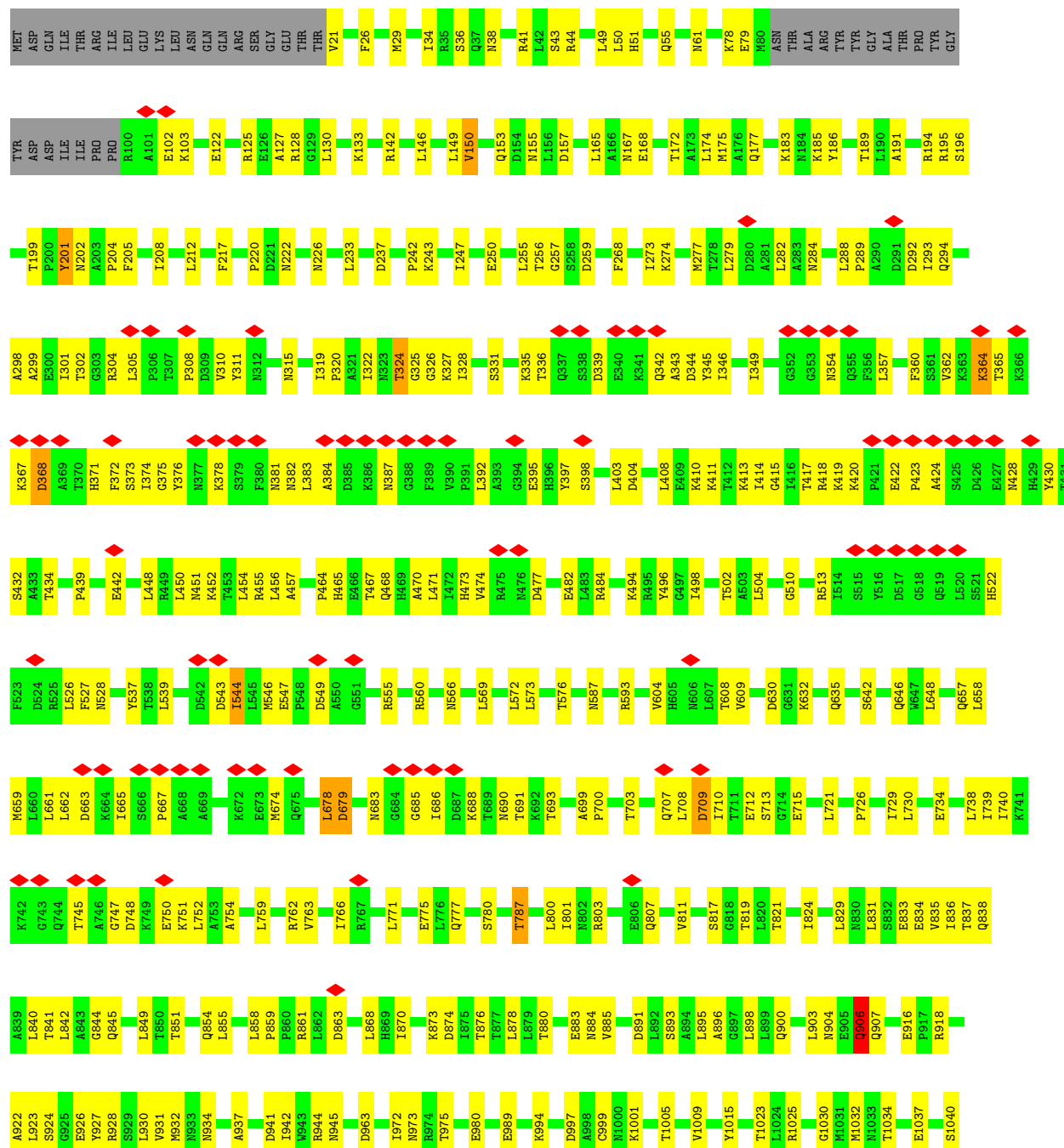
3 Residue-property plots

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

- Molecule 1: Insecticidal toxin protein

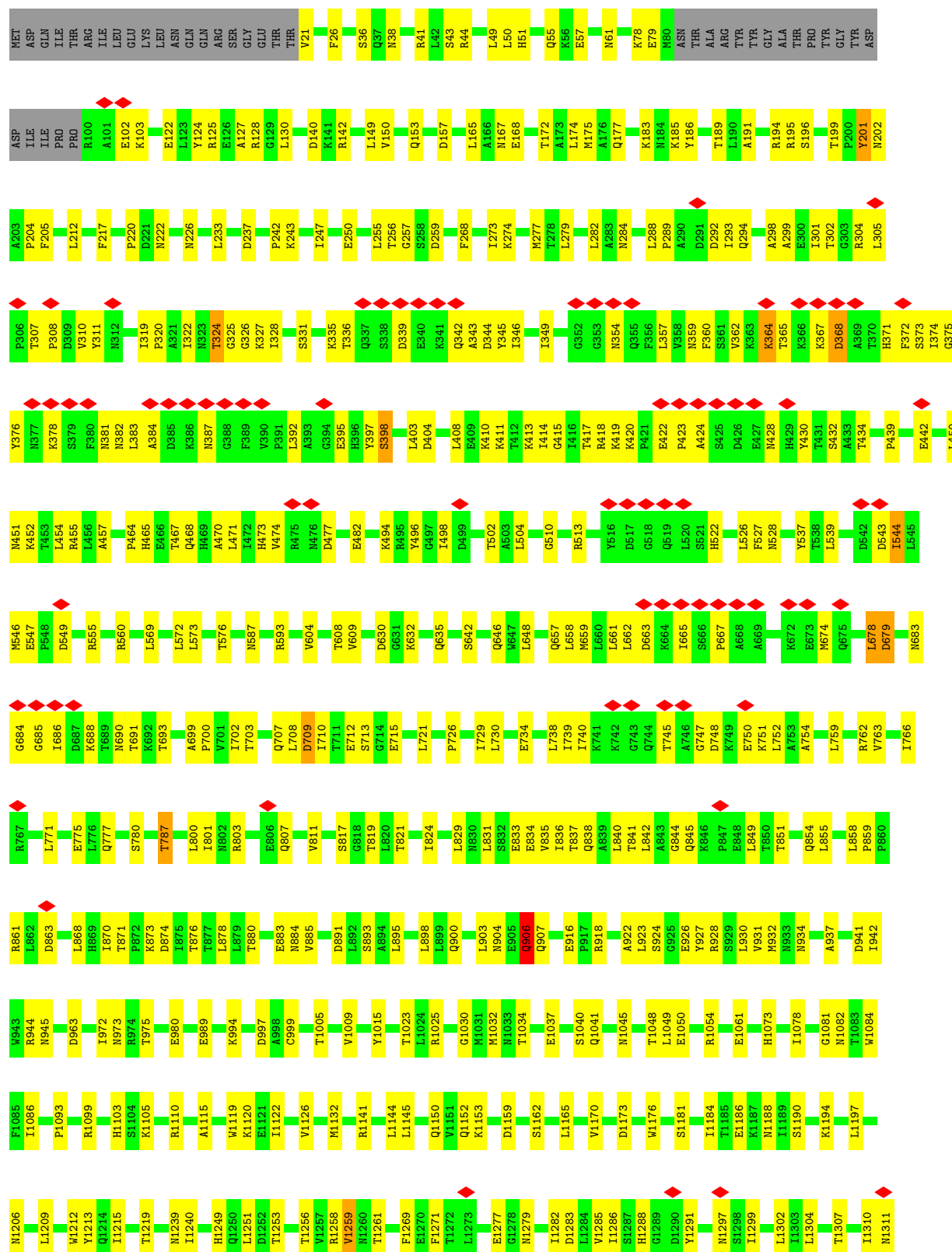


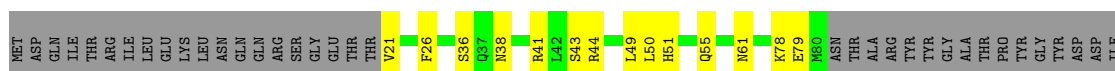




C2400	G2406	H2407	G2408	G2410	G2411	G2412	G2413	G2414	L2417	L2418	F2419	G2424	F2427	T2430	D2433	D2434	N2436	S2437	L2438	T2439	L2440	S2441	F2442	G2447	E2448	K2449	K2450	P2451	L2452	L2453	L2454	L2455	S2456	L2457	L2458	L2459	L2460	T2468	G2469																																				
T2308	D2309	N2310	T2311	T2312	T2317	A2318	G2325	D2326	S2327	N2328	L2329	P2330	ALA	SER	THR	GLY	SER	LEU	MET	T2338	A2339	D2340	N2341	Q2342	L2343	H2344	A2345	A2346	F2347	Y2358	R2366	R2367	I2368	K2369	Q2370	I2371	T2374	L2375	P2376	A2377	L2378	V2379	Q2383	T2388	F2389	R2390	Y2391	N2394	S2395	L2396																									
I2168	Q2174	V2180	T2183	E2186	R2189	E2190	E2204	R2208	R2209	F2210	Y2216	L2223	R2229	D2232	R2237	C2238	A2100	A2101	A2102	M2105	V2114	S2117	R2118	W2119	P2123	S2131	L2132	D2142	S2145	Q2146	S2147	E2148	R2152	E2156	K2161	S2166	E2167	I2168	Q2174	V2180	T2183	E2186	R2189	E2190	E2204	R2208	R2209	F2210	Y2216	L2223	R2229	D2232	R2237	C2238	A2100	A2101	A2102	M2105	V2114	S2117	R2118	W2119	P2123	S2131	L2132	D2142	S2145	Q2146	S2147	E2148	R2152	E2156	K2161	S2166	E2167
D1833	K1834	Y1836	D1842	T1843	M1849	Y1850	Y1851	L1866	F1866	S1867	E1871	L1875	D1880	K1881	T1882	Q1883	A1884	K1885	Q1886	F1887	H1888	D1889	E1890	I1891	R1895	G1898	L1899	L1900	P1901	D1902	V1903	ARG	THR	P1915	Q1916	Y1924	Y1925	Q1926	M1927	L1928	E1929	M1930	R1931	I1941	D1942	G1943																													
T1713	F1714	A1715	G1716	L1717	A1718	V1722	T1723	G1724	Q1727	E1730	P1731	M1732	S1735	W1743	E1744	Y1748	T1749	P1750	V1753	R1756	L1757	E1760	F1763	N1767	A1777	A1781	W1784	R1785	V1786	R1787	P1788	E1791	D1798	D1801	K1823	D1826	L1827	R1831	G1832																																				
R1621	A1622	F1623	T1624	L1625	Y1626	Y1627	S1628	N1629	D1630	G1633	S1634	K1635	Y1640	S1641	L1644	S1645	V1646	M1649	V1652	K1653	L1654	P1661	GLY	LYS	ASN	ALA	VAL	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																																
G1506	A1507	I1508	N1509	M1510	N1511	L1512	K1521	I1516	K1517	V1518	K1521	A1528	T1529	T1530	Y1532	K1533	L1534	V1535	T1536	K1537	K1538	V1542	Q1543	K1544	V1545	S1547	W1560	D1561	R1566	T1572	T1591	Q1592	Y1593	E1596	P1597	L1607	K1610	P1611	Y1612	D1613	K1614	N1615	H1617	N1620																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
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ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
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ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
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ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
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ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU	THR	LEU	GLU	GLU	ASP	LYS	TYR	THR	ILE	SER	THR	GLY	LYS	LYS	LEU	GLY	THR	LEU	LEU	GLY	LYS	ASP	ARG	LEU	VAL	GLN	GLN	ALA	GLN	Q1674	Y1678	L1679	N1680	Q1690	I1691	R1695	N1699	S1708	V1709	M1710	T1711	G1712																															
ASP	ARG	LEU																																																																									

• Molecule 1: Insecticidal toxin protein









F2442	R2366	E2273	E2156	E2010	A1906	P1788	Q1690	L1607	R1489
G2447	R2367	S2274	E2161	E2013	T1910	E1791	I1691	K1610	E1490
E2448	K2368	L2275	K2161	D2013	P1915	D1798	R1695	Y1611	T1491
K2449	Q2370	L2277	S2166	L2020	Q1916	D1801	R1699	D1613	L1492
Q2450	I2371	E2283	E2167	Q2024	Y1924	Y1816	D1706	K1614	S1500
K2451	Q2374	Q2284	I2168	E2027	Y1925	K1823	K1707	N1615	I1501
F2452	L2375	L2287	E2176	Q2036	Q1926	D1826	S1708	T1616	T1502
L2453	P2376	L2287	V2180	Q2037	M1927	L1827	V1709	H1617	I1503
L2454	A2377	E2294	R2181	Q2038	L1928	D1831	M1710	N1620	G1506
S2455	L2378	L2295	E2188	A2039	E1929	G1832	G1712	R1621	A1507
L2456	V2379	V2296	T2183	L2040	R1931	D1833	T1713	A1622	D1508
L2457	Q2383	V2300	E2186	E2042	I1941	G1834	F1714	F1623	I1509
T2458	R2386	L2302	M2187	E2046	D1942	K1834	A1715	Y1626	N1510
D2459	I2388	E2295	Q2188	E2049	G1943	A1835	G1716	Y1628	M1511
L2460	F2389	V2296	R2189	L2049	P1944	Y1836	L1717	N1629	L1512
L2461	R2390	E2296	E2190	Q2058	P1945	D1842	A1718	D1630	I1516
T2462	Y2391	Q2198	Q2198	L2049	L1946	T1843	V1722	A1631	K1517
R2465	N2394	E2204	E2204	Q2059	L1948	E1846	G1724	T1632	V1518
C2468	S2395	F2205	F2205	R2060	P1949	M1849	Q1727	G1633	K1521
C2469	L2396	R2208	R2209	L2067	V1950	Y1851	E1730	S1634	A1528
	C2400	F2210	F2210	E2075	A1952	Y1885	P1731	Y1640	T1529
	I2403	Y2216	Y2216	R2078	P1954	F1866	M1732	S1641	T1530
A2404	A2404	R2222	R2222	L2079	P1955	S1867	E1744	L1644	T1531
L2405	S2406	R2223	R2223	L2082	D1956	L1875	W1743	S1645	K1533
S2406	H2407	L2226	L2226	Q2083	P1957	D1880	E1748	V1646	L1534
H2407	G2408	I2226	I2226	L2084	A1958	K1881	T1749	N1649	Y1536
G2408	I2409	R2229	R2229	S2085	A1959	T1882	P1750	K1537	K1538
I2409	R2410	D2232	D2232	L2093	L1960	Q1883	V1753	V1542	V1542
R2410	D2411	R2237	R2237	D2097	S1962	A1884	R1756	K1653	Q1543
D2412	D2412	C2238	C2238	A2100	A1963	K1885	L1757	K1544	K1544
G2413	G2413	E2242	E2242	N2108	A1964	Q1886	E1760	V1546	V1546
L2414	L2414	T2249	T2249	V2114	A1965	H1888	L1763	I1546	S1547
F2415	F2415	D2251	D2251	S2131	A1966	E1890	M1767	W1560	W1560
R2416	R2416	Y2256	Y2256	L2132	S1968	T1891	A1777	D1561	D1561
D2417	L2417	I2257	I2257	A2141	K1972	R1895	A1781	R1566	R1566
L2417	L2417	K2258	K2258	S2145	S1976	G1898	A1781	T1572	T1572
N2420	N2420	S2259	S2259	Q2146	P1980	L1899	A1781	I1576	I1576
W2424	W2424	G2260	G2260	S2147	A1981	P1901	W1784	T1591	T1591
I2430	I2430	A2261	A2261	E2148	M1982	D1902	R1785	K1592	K1592
D2433	D2433	M2270	M2270	R2152	R1992	V1903	V1786	Y1593	Y1593
D2434	D2434				S1993	ARG	R1787	E1596	E1596
D2435	D2435				L1994	THR		P1597	P1597
N2436	N2436				M1999				
N2437	N2437				Q2000				
S2437	S2437				F2001				
L2438	L2438								
T2439	T2439								
L2440	L2440								
S2441	S2441								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	182506	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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	0.53	0/18078	0.54	1/24569 (0.0%)
1	B	0.53	0/18078	0.54	1/24569 (0.0%)
1	C	0.53	0/18078	0.54	1/24569 (0.0%)
1	D	0.53	0/18078	0.54	1/24569 (0.0%)
1	E	0.53	0/18078	0.54	1/24569 (0.0%)
All	All	0.53	0/90390	0.54	5/122845 (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	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	10

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	906	GLN	CA-CB-CG	7.66	130.26	113.40
1	C	906	GLN	CA-CB-CG	7.66	130.25	113.40
1	B	906	GLN	CA-CB-CG	7.66	130.25	113.40
1	A	906	GLN	CA-CB-CG	7.65	130.22	113.40
1	D	906	GLN	CA-CB-CG	7.64	130.21	113.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1560	TRP	Peptide
1	A	1722	VAL	Peptide
1	B	1560	TRP	Peptide
1	B	1722	VAL	Peptide
1	C	1560	TRP	Peptide

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	17740	0	17523	523	0
1	B	17740	0	17523	504	0
1	C	17740	0	17523	510	0
1	D	17740	0	17523	532	0
1	E	17740	0	17523	550	0
All	All	88700	0	87615	2432	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 14.

The worst 5 of 2432 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:D:325:GLY:HA2	1:E:1865:ILE:HD11	1.38	1.04
1:B:1713:THR:HG22	1:B:1715:ALA:H	1.38	0.89
1:C:1713:THR:HG22	1:C:1715:ALA:H	1.38	0.87
1:A:1713:THR:HG22	1:A:1715:ALA:H	1.38	0.87
1:E:1713:THR:HG22	1:E:1715:ALA:H	1.37	0.86

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	2273/2469 (92%)	2101 (92%)	168 (7%)	4 (0%)	47	79
1	B	2273/2469 (92%)	2101 (92%)	168 (7%)	4 (0%)	47	79
1	C	2273/2469 (92%)	2101 (92%)	168 (7%)	4 (0%)	47	79
1	D	2273/2469 (92%)	2100 (92%)	169 (7%)	4 (0%)	47	79
1	E	2273/2469 (92%)	2101 (92%)	168 (7%)	4 (0%)	47	79
All	All	11365/12345 (92%)	10504 (92%)	841 (7%)	20 (0%)	50	79

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1723	THR
1	A	1724	GLY
1	B	1723	THR
1	B	1724	GLY
1	C	1723	THR

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	1886/2101 (90%)	1823 (97%)	63 (3%)	38	71
1	B	1886/2101 (90%)	1823 (97%)	63 (3%)	38	71
1	C	1886/2101 (90%)	1823 (97%)	63 (3%)	38	71
1	D	1886/2101 (90%)	1823 (97%)	63 (3%)	38	71
1	E	1886/2101 (90%)	1823 (97%)	63 (3%)	38	71
All	All	9430/10505 (90%)	9115 (97%)	315 (3%)	41	71

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1948	LEU
1	E	1591	THR
1	D	2097	ASP
1	E	442	GLU
1	E	2093	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1227	HIS
1	E	1028	GLN
1	D	1620	ASN
1	E	38	ASN
1	E	1617	HIS

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.

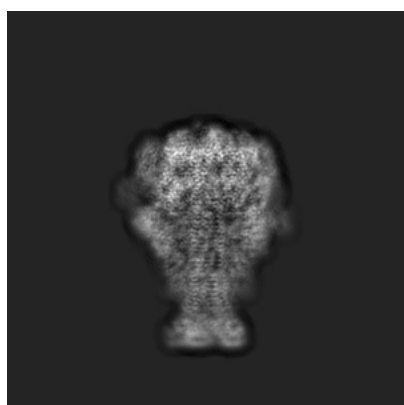
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10796. These allow visual inspection of the internal detail of the map and identification of artifacts.

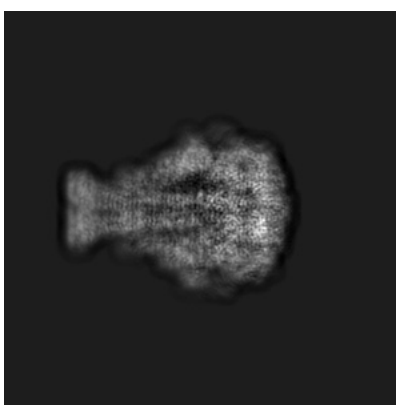
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

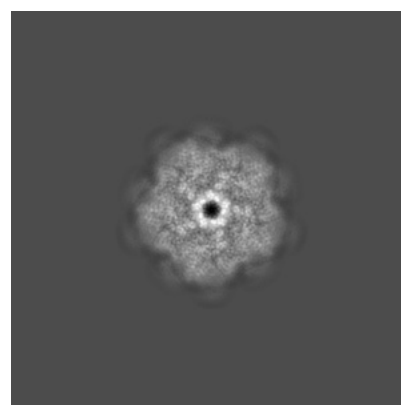
6.1.1 Primary map



X



Y

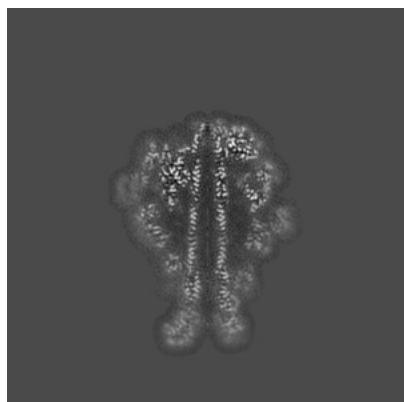


Z

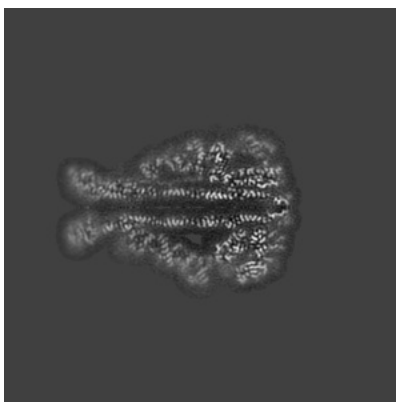
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

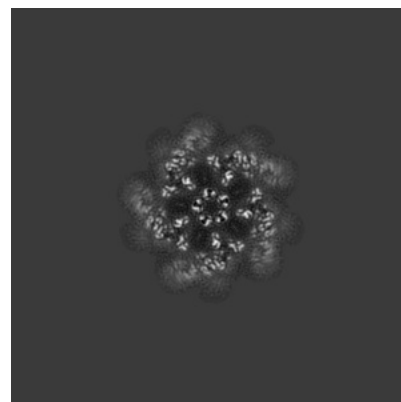
6.2.1 Primary map



X Index: 192



Y Index: 192

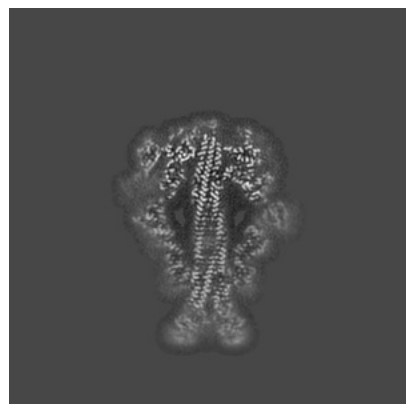


Z Index: 192

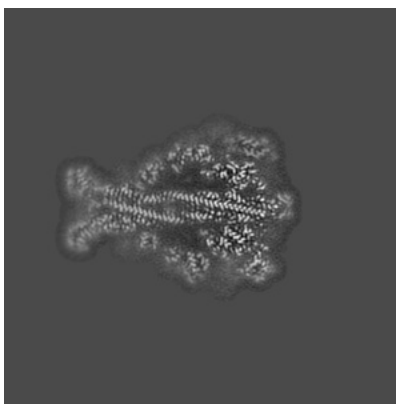
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

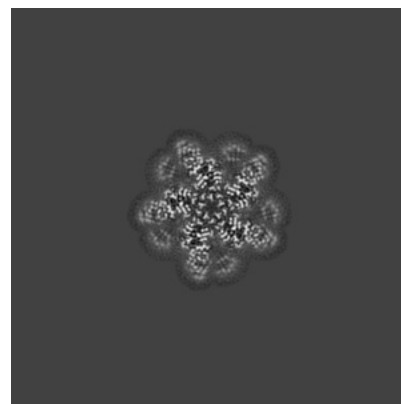
6.3.1 Primary map



X Index: 182



Y Index: 182

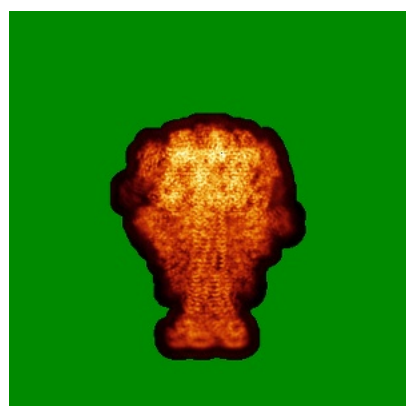


Z Index: 246

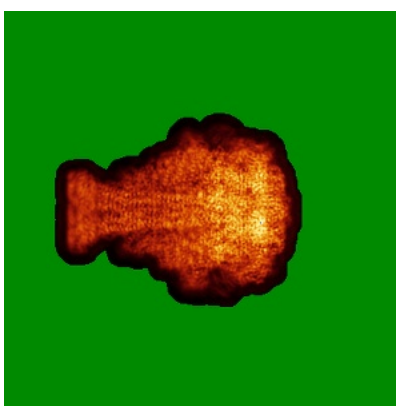
The images above show the largest variance slices of the map in three orthogonal directions.

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

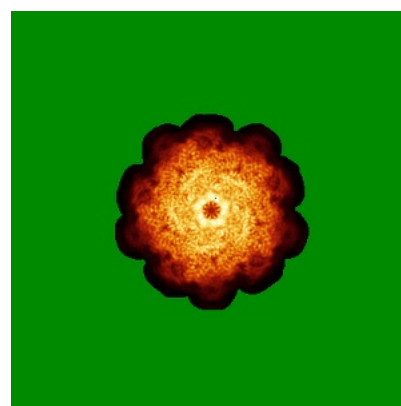
6.4.1 Primary map



X



Y

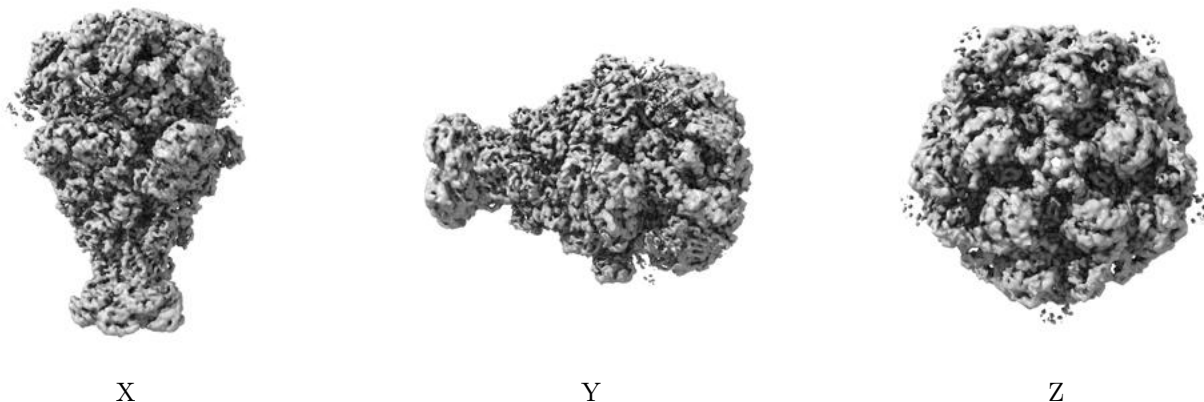


Z

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

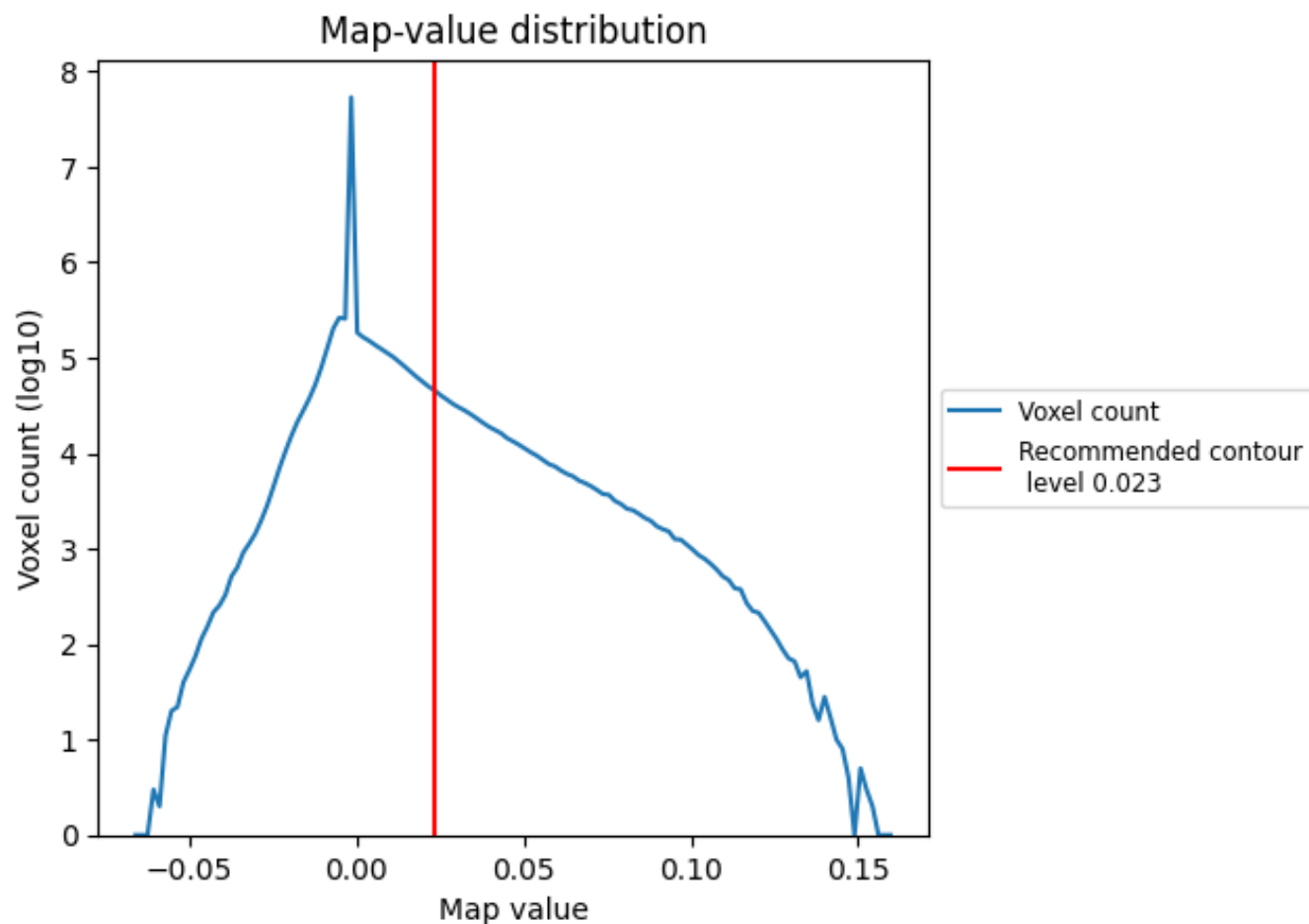
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

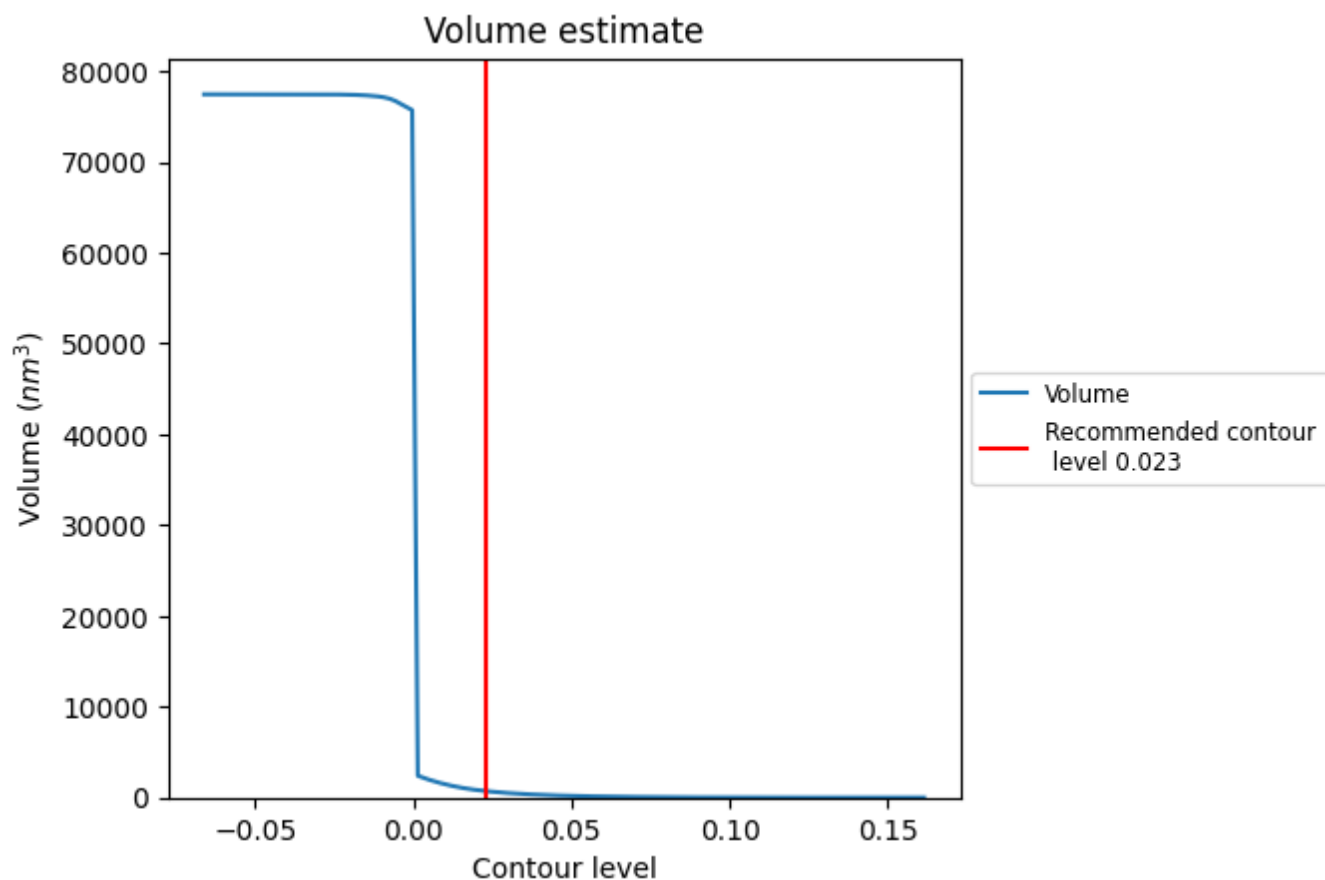
This section contains the results of statistical analysis of the map.

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.

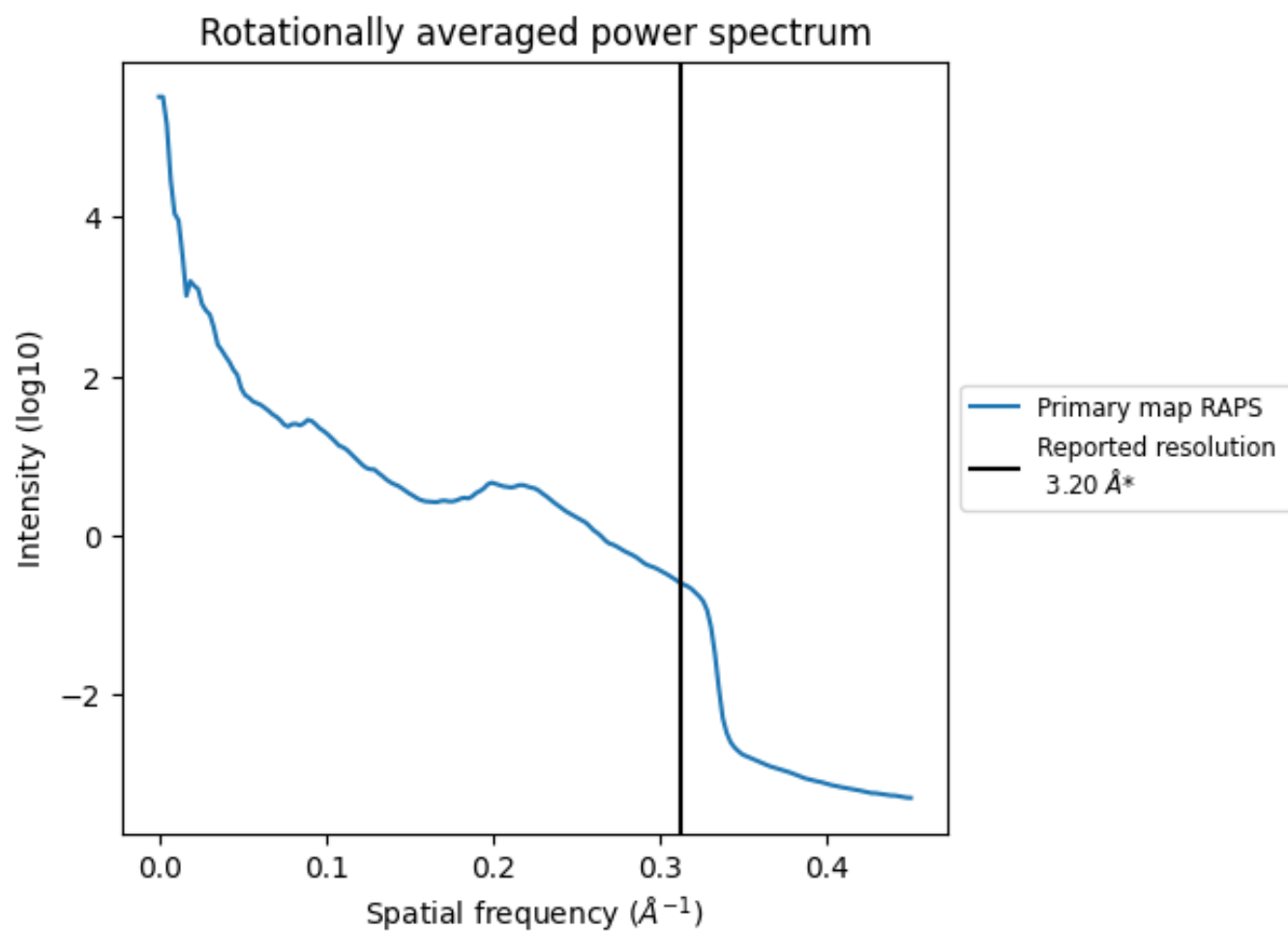
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 712 nm³; this corresponds to an approximate mass of 643 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 0.312 Å⁻¹

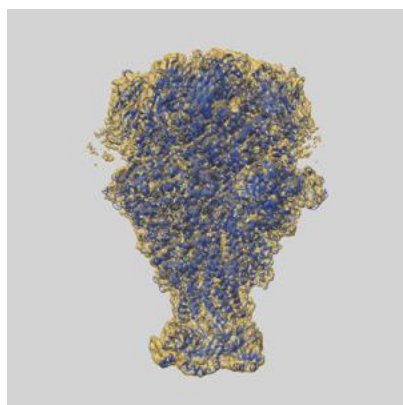
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

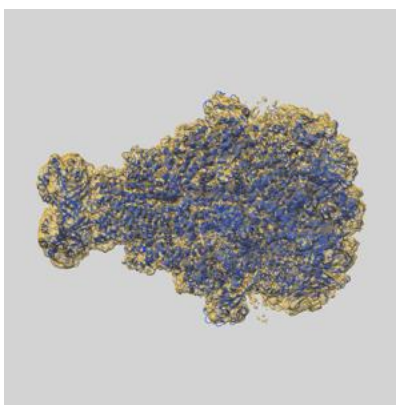
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10796 and PDB model 6YEW. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

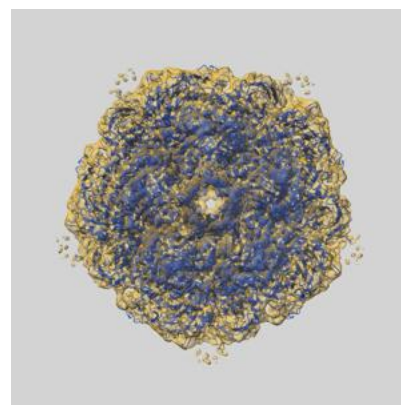
9.1 Map-model overlay [i](#)



X



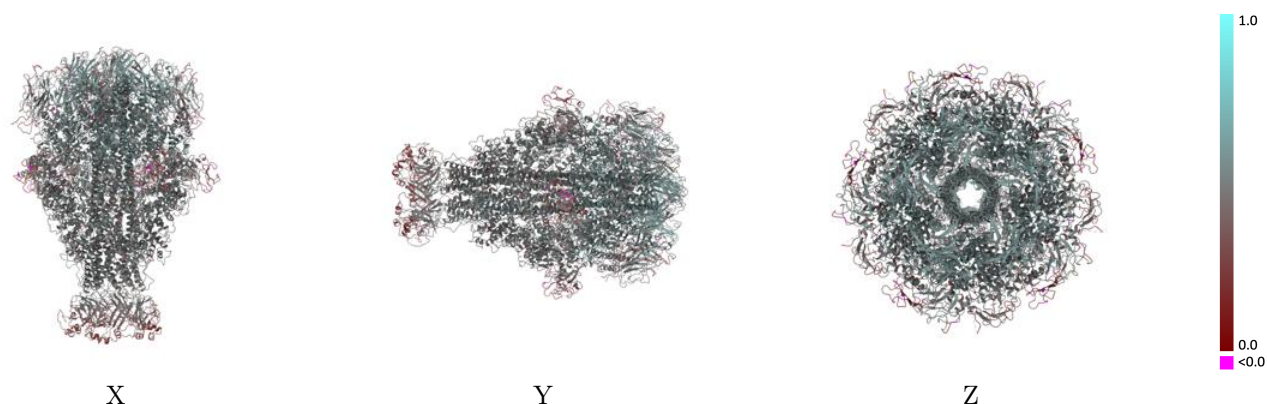
Y



Z

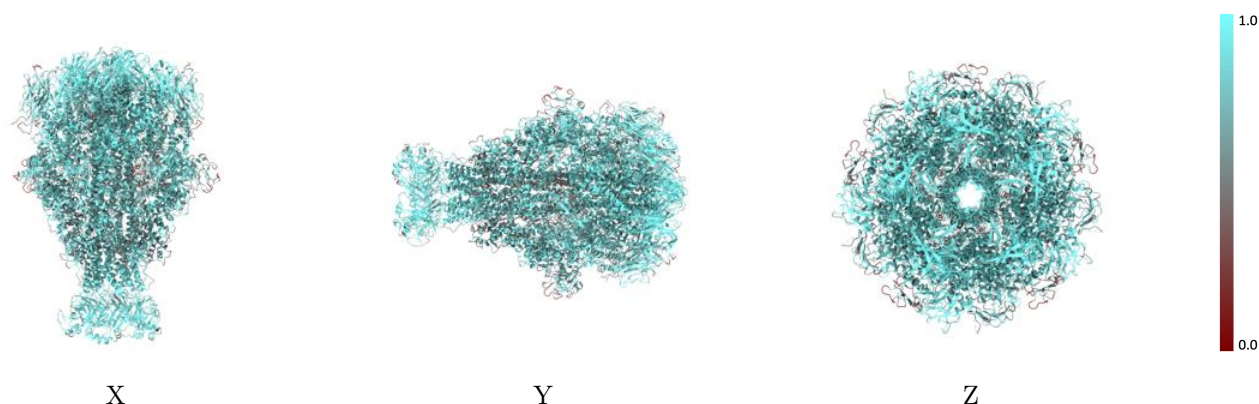
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



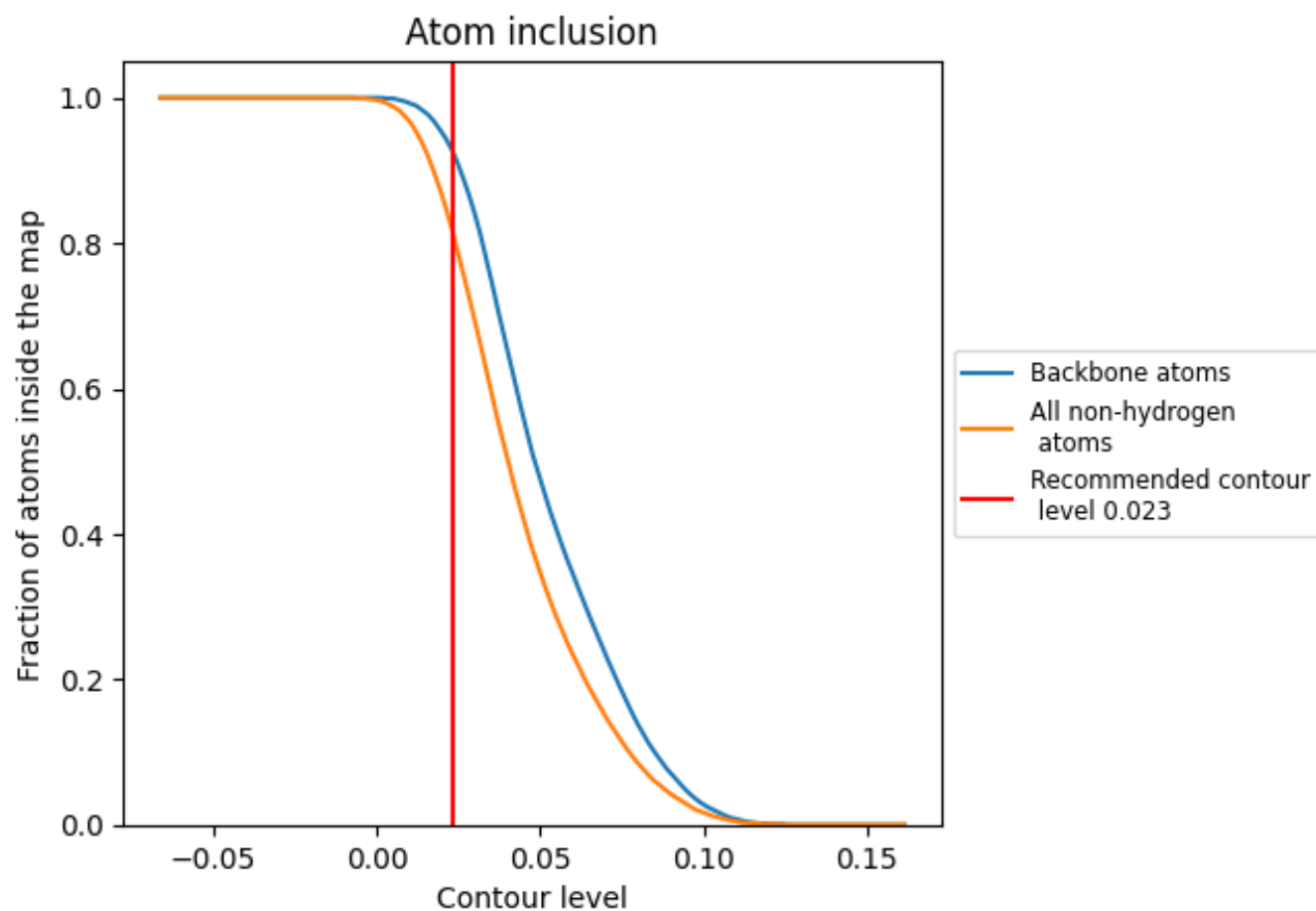
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 82% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8200	<div></div> 0.4780
A	<div></div> 0.8230	<div></div> 0.4800
B	<div></div> 0.8240	<div></div> 0.4810
C	<div></div> 0.8240	<div></div> 0.4810
D	<div></div> 0.8210	<div></div> 0.4790
E	<div></div> 0.8110	<div></div> 0.4710

