



wwPDB EM Validation Summary Report ⓘ

Aug 30, 2026 – 12:31 AM JST

PDB ID : 9VM7 / pdb_00009vm7
EMDB ID : EMD-65179
Title : Structure of DOCK6 tetramer complexed with Rac1
Authors : Kukimoto-Niino, M.; Katsura, K.; Ishizuka-Katsura, Y.; Yonemochi, M.;
Hanada, K.; Shirouzu, M.
Deposited on : 2025-06-27
Resolution : 6.85 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
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) : 2.50

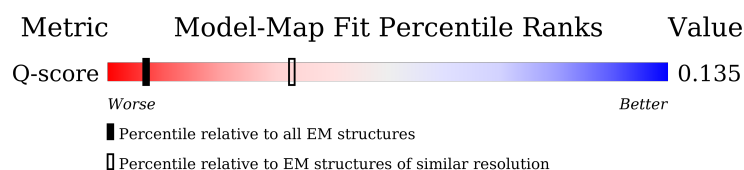
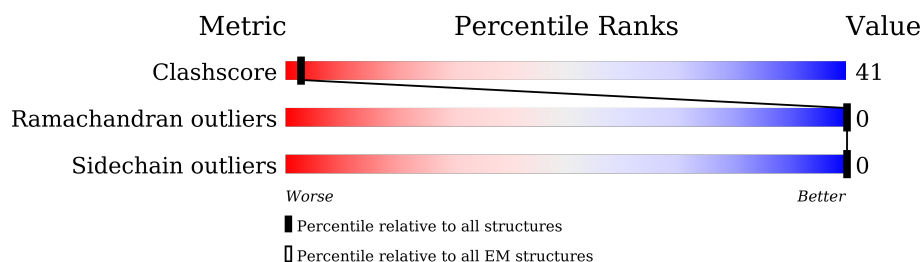
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.85 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.



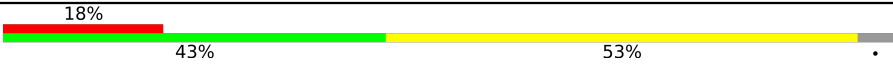
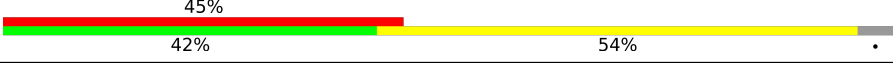
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	459 (6.35 - 7.30)

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	2053	9% 32% 50% 18%
1	C	2053	9% 32% 50% 18%
1	E	2053	8% 32% 50% 18%
1	G	2053	7% 32% 50% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	184	 18% 43% 53% .
2	D	184	 15% 42% 54% .
2	F	184	 45% 42% 54% .
2	H	184	 47% 40% 57% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 59424 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 Dedicator of cytokinesis protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1688	Total	C	N	O	S	0	0
			13471	8606	2331	2475	59		
1	C	1688	Total	C	N	O	S	0	0
			13471	8606	2331	2475	59		
1	E	1688	Total	C	N	O	S	0	0
			13471	8606	2331	2475	59		
1	G	1688	Total	C	N	O	S	0	0
			13471	8606	2331	2475	59		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q96HP0
A	-4	GLY	-	expression tag	UNP Q96HP0
A	-3	SER	-	expression tag	UNP Q96HP0
A	-2	GLY	-	expression tag	UNP Q96HP0
A	-1	GLY	-	expression tag	UNP Q96HP0
A	0	SER	-	expression tag	UNP Q96HP0
C	-5	GLY	-	expression tag	UNP Q96HP0
C	-4	GLY	-	expression tag	UNP Q96HP0
C	-3	SER	-	expression tag	UNP Q96HP0
C	-2	GLY	-	expression tag	UNP Q96HP0
C	-1	GLY	-	expression tag	UNP Q96HP0
C	0	SER	-	expression tag	UNP Q96HP0
E	-5	GLY	-	expression tag	UNP Q96HP0
E	-4	GLY	-	expression tag	UNP Q96HP0
E	-3	SER	-	expression tag	UNP Q96HP0
E	-2	GLY	-	expression tag	UNP Q96HP0
E	-1	GLY	-	expression tag	UNP Q96HP0
E	0	SER	-	expression tag	UNP Q96HP0
G	-5	GLY	-	expression tag	UNP Q96HP0
G	-4	GLY	-	expression tag	UNP Q96HP0
G	-3	SER	-	expression tag	UNP Q96HP0
G	-2	GLY	-	expression tag	UNP Q96HP0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q96HP0
G	0	SER	-	expression tag	UNP Q96HP0

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
2	D	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
2	F	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		
2	H	177	Total	C	N	O	S	0	0
			1385	890	228	259	8		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLY	-	expression tag	UNP P63000
B	-5	SER	-	expression tag	UNP P63000
B	-4	SER	-	expression tag	UNP P63000
B	-3	GLY	-	expression tag	UNP P63000
B	-2	SER	-	expression tag	UNP P63000
B	-1	SER	-	expression tag	UNP P63000
B	0	GLY	-	expression tag	UNP P63000
B	15	ALA	GLY	engineered mutation	UNP P63000
D	-6	GLY	-	expression tag	UNP P63000
D	-5	SER	-	expression tag	UNP P63000
D	-4	SER	-	expression tag	UNP P63000
D	-3	GLY	-	expression tag	UNP P63000
D	-2	SER	-	expression tag	UNP P63000
D	-1	SER	-	expression tag	UNP P63000
D	0	GLY	-	expression tag	UNP P63000
D	15	ALA	GLY	engineered mutation	UNP P63000
F	-6	GLY	-	expression tag	UNP P63000
F	-5	SER	-	expression tag	UNP P63000
F	-4	SER	-	expression tag	UNP P63000
F	-3	GLY	-	expression tag	UNP P63000
F	-2	SER	-	expression tag	UNP P63000
F	-1	SER	-	expression tag	UNP P63000
F	0	GLY	-	expression tag	UNP P63000
F	15	ALA	GLY	engineered mutation	UNP P63000

Continued on next page...

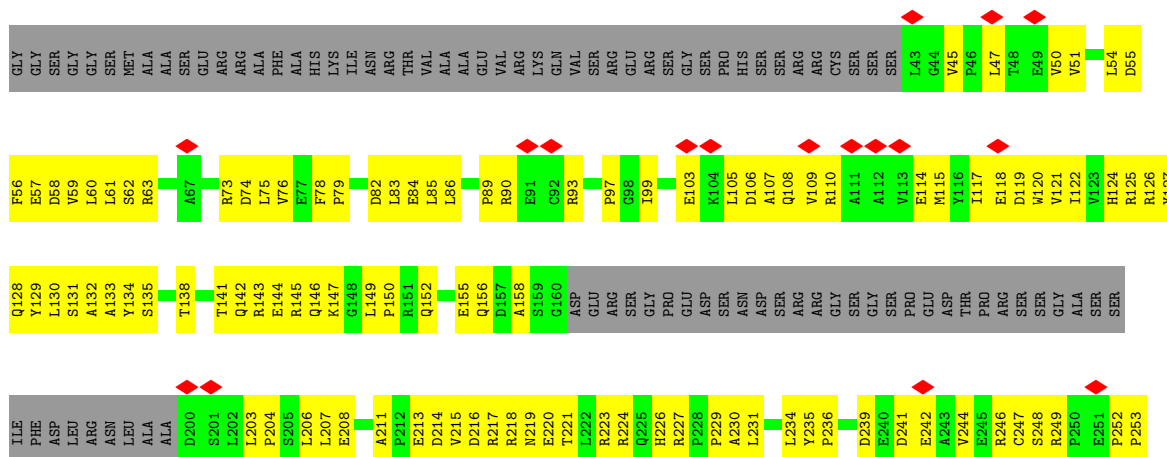
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-6	GLY	-	expression tag	UNP P63000
H	-5	SER	-	expression tag	UNP P63000
H	-4	SER	-	expression tag	UNP P63000
H	-3	GLY	-	expression tag	UNP P63000
H	-2	SER	-	expression tag	UNP P63000
H	-1	SER	-	expression tag	UNP P63000
H	0	GLY	-	expression tag	UNP P63000
H	15	ALA	GLY	engineered mutation	UNP P63000





Chain C:

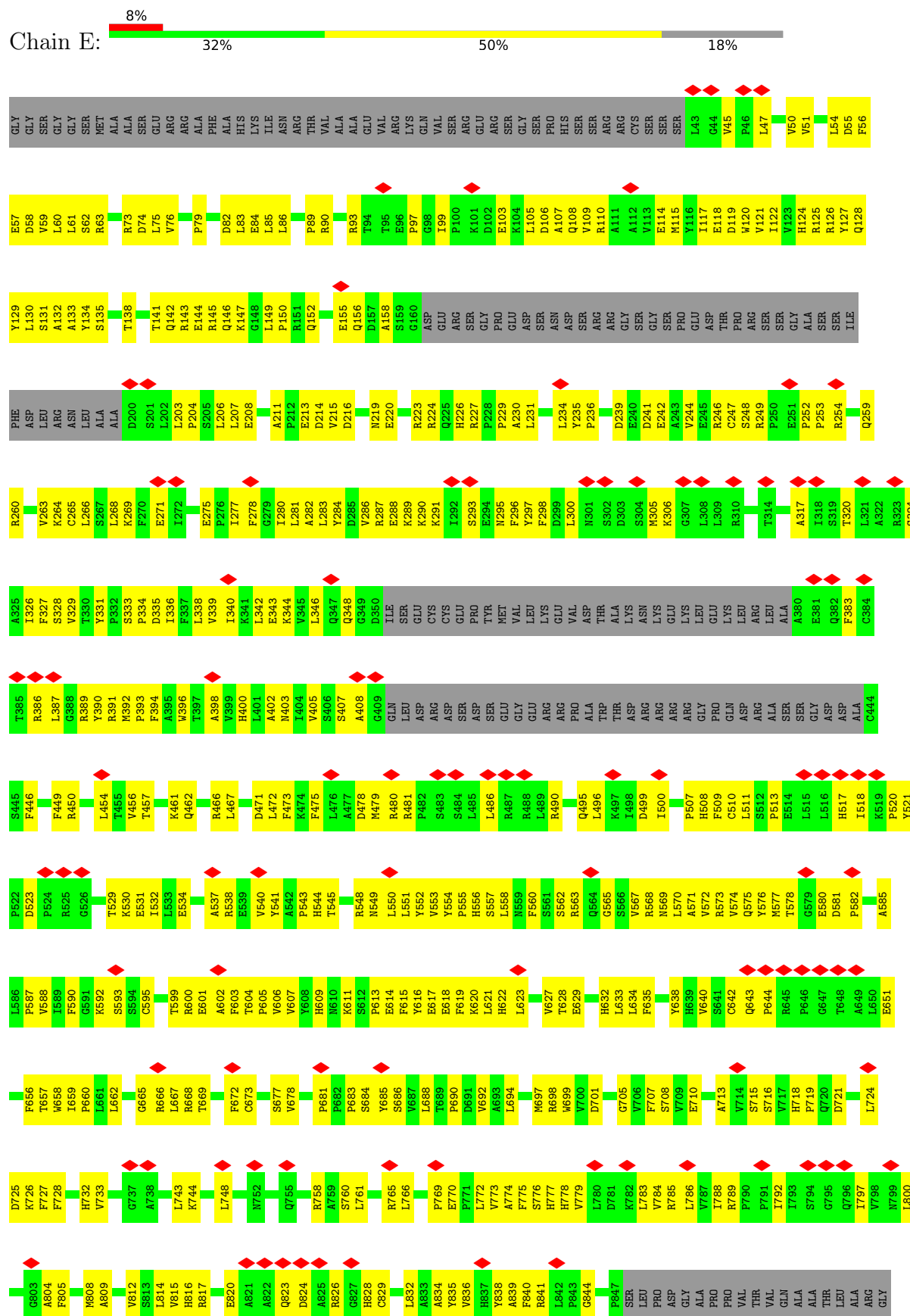






● Molecule 1: Dedicator of cytokinesis protein 6

Chain E:





SER	L1899	D1836	K1772	L1899	D1836	L1699	Y1700
LEU	T1900	R1837	E1773	T1900	R1837	LEU	Y1700
ASN	P1901	V1838	P1774	P1901	V1838	ASN	
ARG	E1902	T1839	S1775	E1902	T1839	K1968	
ALA	V1903	I1840	I1776	V1903	I1840	L1970	
SER		F1841	T1777		F1841	R1971	
PHE		D1842			D1842	F1974	
ARG	L1906	R1843		L1906	R1843		
LYS	E1907	M1844	I1782	E1907	M1844	K1979	
ALA	D1908	Y1845	S1783	D1908	Y1845		
ASP	M1909	G1846	H1784	M1909	G1846	E1982	
LEU	Q1910	L1847	R1786	Q1910	L1847	D1983	
	K1911	R1848	E1787	K1911	R1848	E1984	
	K1912	T1849	E1788	K1912	T1849	L1985	
	T1913	F1850	F1789	T1913	F1850	E1986	
	R1914	L1851	E1790	R1914	L1851	K1987	
		F1852	T1791		F1852	N1988	
	F1918	C1853	E1792	F1918	C1853		
	A1919	T1854	R1793	A1919	T1854		
	T1920	P1855	F1794	T1920	P1855		
	E1921	F1856	G1795	E1921	F1856	L1991	
	Q1922	T1857		Q1922	T1857	I1992	
	D1923			D1923			
	P1924	L1862	D1797	P1924	L1862	K1997	
	D1925	H1863	V1798	D1925	H1863	E1998	
	D1926	G1864	H1799	D1926	G1864	Y1999	
	A1927	E1865	E1800	A1927	E1865	H2000	
	K1928	L1866	L1801	K1928	L1866	R2001	
	M1929	P1867	K1802	M1929	P1867	E2002	
	L1930	E1868	K1803	L1930	E1868	L2003	
	Q1931	Q1869	D1804	Q1931	Q1869	E2004	
	M1932	H1870	S1805	M1932	H1870	R2005	
	V1933	K1871	S1806	V1933	K1871	H2006	
	L1934	R1872	P1807	L1934	R1872	Y2007	
	Q1935	L1873	V1808	Q1935	L1873	C2008	
	G1936	T1874	D1809	G1936	T1874	R2009	
	S1937	L1875	K1810	S1937	L1875	L2010	
	V1938	L1876	S1811	V1938	L1876	R2011	
	G1939	S1877	K1812	G1939	S1877	E2012	
	P1940	T1878	L1813	P1940	T1878	A2013	
	T1941	D1879	D1814	T1941	D1879	L2014	
	V1942	H1880		V1942	H1880	Q2015	
	N1943	A1881	K1817	N1943	A1881	P2016	
	L1947	F1882	A1818	L1947	F1882	L2018	
	E1948	Y1884	Y1819	E1948	Y1884	T2019	
		T1885	I1820		T1885	GLN	
		K1886	Q1821		K1886	ARG	
	Q1951	T1887	I1822	Q1951	T1887	LEU	
	V1952	R1888	T1823	V1952	R1888	PRO	
	F1953	L1889	E1824	F1953	L1889	GLN	
	L1954	R1890	E1825	L1954	R1890	LEU	
	A1955	V1891	E1826	A1955	V1891	MET	
		C1892	P1827		C1892	ALA	
	E1959	H1893	Y1828	E1959	H1893	PRO	
	D1960	E1894	T1829	D1960	E1894	THR	
	P1961	E1895	D1830	P1961	E1895	PRO	
	K1962	E1896	T1831	K1962	E1896	PRO	
	L1963	T1897	E1832	L1963	T1897	GLY	
	F1964	V1898	E1833	F1964	V1898	LEU	
			L1834			ARG	
			K1835			ASN	

• Molecule 1: Dedicator of cytokinesis protein 6

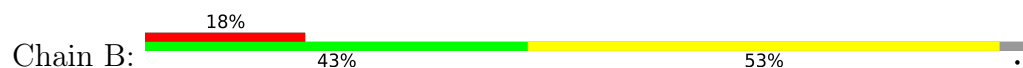


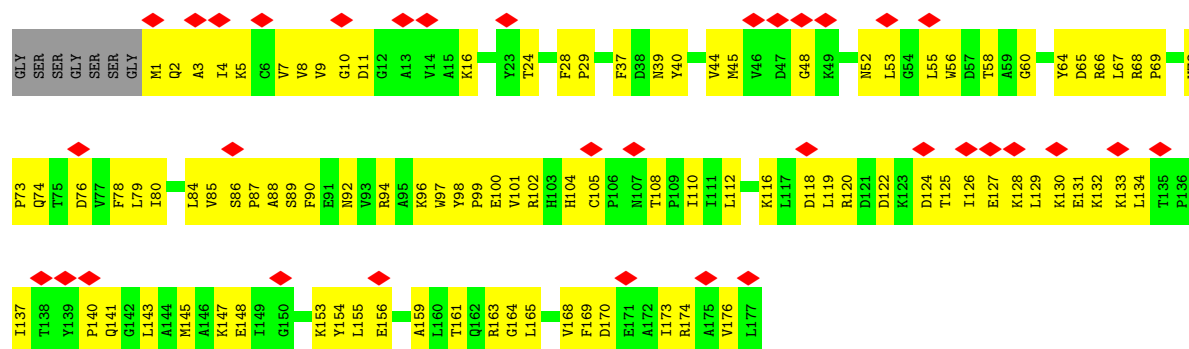
GLY GLY SER GLY GLY MET ALA ALA SER GLU ARG ARG ALA PHE HIS LYS ILE ASN ARG THR VAL ALA GLU VAL ARG GLN VAL SER ARG GLU SER GLY PRO HIS SER SER ARG ARG CYS SER SER L43 G44 V45 P46 L47 V50 V51 L54 D55 F56	E57 D58 V59 L60 L61 S62 R63 A67 E68 P69 R73 D74 L75 V76 P79 D82 L83 E84 L85 L86 P89 R90 E91 C92 R93 P97 G98 I99 E103 K104 L105 D106 A107 Q108 V109 R110 A111 A112 V113 E114 M115 Y116 I117 E118 D119 W120 I121 I122 V123 H124 R125 R126 Y127	Q128 Y129 L130 S131 A132 A133 A134 S135 T138 T141 Q142 R143 E144 Q145 Q146 K147 G148 L149 P150 R151 Q152 E155 Q156 D157 A158 C160 ASP GLU ARG SER GLY PRO GLU ASP SER ASN ASP SER ARG ARG GLY SER GLY SER PRO GLU ASP D200 S201 L202 L203 P204 S205 L206 L207 E208 A211 P212 E213 D214 V215 D216 N219 E220 R223 R224 Q225 H226 R227 P228 P229 A230 L231 L234 Y235 P236 D239 E240 D241 E242 A243 E245 R246 C247 S248 R249 P250 E251 P252 P253 R254	Q259 R260 I261 L262 V263 K264 C265 L266 S267 L268 K269 F270 E271 I272 E273 L274 E275 P276 L277 F278 G279 L280 L281 A282 L283 Y284 D285 V286 R287 E288 K289 Q290 K291 L292 S293 E294 N295 F296 Y297 F298 D299 L300 N301 S302 D303 S304 M305 K306 R310 G313 T314 A317 L318 S319 T320 L321 A322	R323 S324 A325 L326 F327 S328 V329 T330 Y331 P332 S333 P334 D335 I336 F337 L338 V339 I340 K341 L342 E343 K344 V345 L346 Q347 Q348 G349 D350 ILE SER GLU CYS CYS GLU PRO TYR MET VAL GLY LEU GLY ARG ARG PRO ALA TRP ASP ASN ARG ARG ARG ARG GLY PRO GLN ASP ARG ALA SER SER GLY ASP	F383 C384 T385 R386 L387 G388 R389 Y390 R391 K392 P393 F394 A395 V396 T397 A398 V399 H400 L401 A402 M403 L404 V405 S406 S407 A408 G409 GLN LEU ASP ASP ASP SER ASP SER SER GLU GLY GLY ARG ARG PRO ALA TRP ASP ASN ARG ARG ARG ARG GLY PRO GLN ASP ARG ALA SER SER GLY ASP
---	--	---	--	--	---

V1257	L1258	W1259	V1260	L1261	K1262	N1263	T1264	E1265	P1266	A1267	L1268	L1269	Q1270	R1271	W1272	A1273	T1274	D1275	L1276	T1277	L1278	P1279	Q1280	L1281	G1282	R1283	L1284	L1285	D1286	L1287	L1288	Y1289	G1290	C1291	L1292	A1293	A1294	E1295	F1296	Y1297	K1298	G1299	A1302	F1303	R1304	E1305	I1306	N1307	SER	LEU	THR	PHE	LYS	LYS	SER	LEU	ASP	MET
A1128	F1129	L1130	L1131	L1131	H1132	K1133	K1134	A1135	A1136	T1137	A1138	V1139	L1142	L1143	L1143	H1146	D1149	P1150	R1151	Y1152	A1153	E1154	A1155	T1156	V1157	K1158	A1159	R1160	V1161	A1162	E1163	L1164	Y1165	L1166	P1167	L1168	L1169	I1170	SER	I1171	A1172	R1173	D1174	T1175	L1176	P1177	R1178	L1179	F1182	A1183	E1184	GLY	PRO	GLY	GLN	ARG	A1255	C1256
ARG	LEU	ALA	SER	MET	LEU	ASP	ASP	THR	GLU	GLY	GLU	GLY	ASP	ILE	ALA	ALA	THR	ILE	ASN	PRO	SER	VAL	ALA	MET	ALA	ILE	ALA	GLY	GLY	PRO	LEU	ALA	PRO	GLY	ARG	ALA	ILE	SER	GLN	PRO	THR	ALA	SER	ALA	GLY	C1243	E1248	S1249	S1250	PRO	GLY	GLN	ARG	A1255	C1256			
A998	F999	L1000	L1001	S1002	D1003	L1004	W1005	SER	PRO	SER	LEU	V1007	L1008	D1009	VAL	SER	GLN	SER	THR	PHE	SER	SER	Q1087	D1090	P1091	K1092	V1093	T1094	S1095	M1096	L1099	S1100	G1101	P1102	L1103	R1104	Q1105	Q1106	H1107	F1108	L1109	A1110	G1111	L1112	L1113	L1114	T1115	E1116	L1117	A1120	L1121	E1122	E1124					
A926	I927	L928	Q929	H930	A931	W932	F933	F934	F935	Q936	L937	W938	W939	X940	S941	N942	H945	L946	L947	Q950	R951	T954	P955	R956	K957	L958	R959	G962	R963	F964	L965	T968	V972	V975	G976	L977	E978	V979	I980	V983	H984	L989	A990	E991	H992	L993	H994	A995	L997									
ARG	GLY	SER	GLY	ARG	PRO	ALA	SER	LEU	TVR	LEU	ALA	ARG	SER	LYS	ILE	SER	SER	ASN	PRO	ASP	LEU	ALA	VAL	VAL	ALA	PRO	GLY	VAL	D897	E898	V899	R901	I902	L903	K906	L907	L908	H909	E910	E911	L912	A913	L914	Q915	W916	V917	V918	S919	S920	S921	A922	V923	R924	E925				
A998	F999	L1000	L1001	S1002	D1003	L1004	W1005	SER	PRO	SER	LEU	V1007	L1008	D1009	VAL	SER	GLN	SER	THR	PHE	SER	SER	Q1087	D1090	P1091	K1092	V1093	T1094	S1095	M1096	L1099	S1100	G1101	P1102	L1103	R1104	Q1105	Q1106	H1107	F1108	L1109	A1110	G1111	L1112	L1113	L1114	T1115	E1116	L1117	A1120	L1121	E1122	E1124					
A1128	F1129	L1130	L1131	H1132	K1133	K1134	A1135	A1136	T1137	A1138	V1139	L1142	L1143	L1143	H1146	D1149	P1150	R1151	Y1152	A1153	E1154	A1155	T1156	V1157	K1158	A1159	R1160	V1161	A1162	E1163	L1164	Y1165	L1166	P1167	L1168	L1169	I1170	SER	I1171	A1172	R1173	D1174	T1175	L1176	P1177	R1178	L1179	F1182	A1183	E1184	GLY	PRO	GLY	GLN	ARG	A1255	C1256	
ARG	LEU	ALA	SER	MET	LEU	ASP	ASP	THR	GLU	GLY	GLU	GLY	ASP	ILE	ALA	ALA	THR	ILE	ASN	PRO	SER	VAL	ALA	MET	ALA	ILE	ALA	GLY	GLY	PRO	LEU	ALA	PRO	GLY	ARG	ALA	ILE	SER	GLN	PRO	THR	ALA	SER	ALA	GLY	C1243	E1248	S1249	S1250	PRO	GLY	GLN	ARG	A1255	C1256			
Y1257	P522	S523	P524	R525	T529	K530	E531	I532	L533	E534	A537	R538	E539	V540	P541	A542	P543	H544	T545	R548	N549	L550	L551	Y552	V553	Y554	P555	H556	S557	F560	S561	S562	R563	Q564	S566	V567	R568	N569	L570	A571	V572	R573	V574	Q575	Y576	M577	T578	G579	E580	S583	Q584	A585	L586					
P587	V588	I589	F590	G591	K592	S593	S594	C595	S596	T599	R600	E601	A602	F603	T604	P605	V606	V607	Y608	H609	N610	K611	S612	P613	F614	F615	Y616	E617	E618	F619	K620	L621	H622	L623	P624	A625	C626	T628	E629	M630	H631	H632	L633	L634	F635	Y638	H639	V640	S641	C642	Q643	P644	R645	P646	G647	T648		
A649	L650	E651	F656	L657	W658	P659	P660	L661	L662	R666	L667	R668	T669	F672	C673	S677	V678	P681	P682	P683	S684	Y685	S686	V687	L688	T689	P690	H691	V692	A693	L694	P695	G696	M697	R698	D701	G702	H703	K704	G705	V706	F707	V708	V709	E710	A713	S715	S716	V717	H718	P719							
Q720	D721	L724	D725	K726	F727	F728	H732	V733	G737	P740	L743	K744	L748	Q755	E756	L757	R758	A759	S760	L761	R765	L766	P769	E770	V773	A774	F775	S776	H777	V778	V779	L780	L783	V784	R785	L786	V787	I788	R789	P790	P791	I792	I793	S794	I797	V798	N799											
L800	G801	R802	G803	A804	F805	M808	A809	V812	S813	L814	V815	H816	R817	E820	A821	A822	Q823	D824	A825	G827	L832	A833	A834	Y835	V836	H837	Y838	A839	F840	R841	L842	P843	G844	P847	SER	LEU	PRO	ASP	GLY	ALA	PRO	VAL	THR	VAL	GLN	ALA	ALA	THR	LEU	ALA								

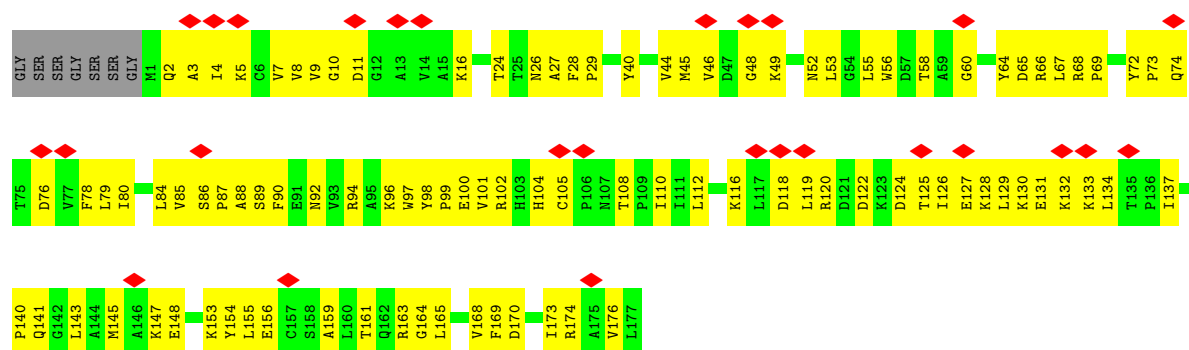
ALA	LYS	V1380	L1443	V1514	L1578	V1695	P1712	S1763	N1844	D1908	K1979
SER	ALA	E1381	E1446	G1515	I1579	S1646	I1713	H1784	Y1845	M1909	E1982
PHE	ARG	G1382	K1446	T1516	D1580	F1647	L1714	L1765	G1846	Q1910	D1983
ARG	LEU	N1383	F1447	T1517	L1581	Q1648	E1715	L1766	L1847	K1911	A1984
LYS	GLU	L1384	E1453	Q1518	M1582	N1649	R1718	E1767	R1848	T1912	L1985
ASP	GLU	A1385	E1454	N1519	Y1583	I1650	D1719	F1768	F1850	R1914	R1986
LEU	ALA	T1386	C1459	F1520	R1584	S1651	Y1720	F1769	L1851	T1920	K1987
	ILE	S1389	E1521	S1522	I1585	N1652	K1721	T1790	C1852	Q1921	N1988
	LEU	L1390	E1523	E1524	R1587	N1653	L1722	T1791	C1853	Q1922	K1989
	THR	V1391	L1462	H1524	G1588	V1654	L1723	E1792	L1854	F1855	A1990
	ILE	V1392	C1463	L1525	Y1589	E1656	V1726	F1794	P1856	D1923	L1991
	GLY	L1393	L1464	L1526	Q1590	E1657	H1727	G1795	T1857	P1924	I1992
	ALA	D1394	R1465	R1527	G1591	S1658	G1728	D1796	A1862	P1925	G1993
	ARG	L1395	L1466	S1528	P1592	D1662	Q1731	V1798	H1863	A1927	P1994
	GLN	L1396	L1467	L1529	P1593	D1663	E1732	V1799	G1864	M1929	D1995
	GLU	E1397	R1468	K1530	R1596	L1664	A1733	E1800	E1865	L1930	Q1996
	MET	I1398	H1469	T1531	L1597	L1665	I1737	I1801	L1866	Q1931	K1997
	VAL	I1399	C1470	I1532	T1598	S1666	H1738	I1802	P1867	M1932	E1998
	ARG	Q1401	R1473	L1533	W1599	P1667	H1739	K1803	E1868	V1933	Y1999
	ARG	T1402	S1475	Y1535	L1600	D1668	Q1740	D1804	Q1869	L1934	H2000
	SER	L1403	T1476	E1536	Q1601	E1669	S1741	S1805	H1870	Q1935	R2001
	GLU	S1406	T1477	E1537	M1602	G1670	E1745	N1806	K1871	S1936	E2002
	ARG	E1407	R1478	E1538	M1603	G1671	R1746	V1808	K1872	S1937	L2003
	PRO	A1408	T1479	E1539	K1606	K1676	R1747	D1809	L1873	V1938	E2004
	GLY	A1410	S1482	M1540	H1607	K1677	F1748	K1810	T1874	G1939	R2005
	ASN	S1411	E1483	B1543	L1610	F1678	G1749	S1811	L1875	P1940	N2006
	PRO	V1412	S1484	F1547	H1613	T1679	L1750	K1812	L1876	T1941	Y2007
	GLU	L1413	E1485	A1549	A1614	E1680	Y1751	L1813	S1877	N1942	C2008
	ASN	G1414	Y1486	Q1550	E1615	G1682	F1752	D1814	T1878	Q1944	L2010
	VAL	V1415	L1487	Q1551	E1616	L1683	R1753	K1817	H1880	G1945	R2011
	ARG	A1416	L1488	Q1552	A1617	V1684	F1756	I1819	A1881	F1946	E2012
	TRP	L1417	M1489	L1554	C1619	G1685	G1758	I1820	F1882	E1948	A2013
	ARG	K1418	L1490	D1553	Q1618	L1686	F1757	Q1821	Y1884	Q1951	L2014
	LYS	V1419	Q1491	F1555	C1619	L1687	I1757	I1822	I1885	F1952	Q2015
	SER	V1420	M1492	M1555	M1620	E1688	G1761	T1823	K1886	F1953	P2016
	VAL	L1421	T1495	F1556	H1621	Q1689	L1764	Y1824	T1897	L1954	L2017
	THR	S1423	G1496	L1557	V1621	A1690	D1765	V1825	R1888	A1955	L2018
	HIS	L1424	H1497	L1558	H1622	Y1693	E1766	E1826	I1889	E1956	T2019
	TRP	G1425	N1498	H1559	L1626	F1694	Q1767	P1827	R1890	V1891	GLN
	LYS	S1426	F1499	M1560	V1627	T1695	E1770	Y1828	H1893	C1892	ARG
	GLN	A1427	A1500	K1563	A1628	M1696	I1771	F1829	L1894	H1894	LEU
	SER	Q1428	R1501	T1563	E1629	Y1700	K1772	D1830	E1895	E1895	PRO
	ASP	A1430	V1502	D1564	L1633	G1697	E1773	T1831	L1896	T1897	ALA
	ARG	L1431	K1503	T1565	L1634	G1698	P1774	Y1832	L1897	V1898	PRO
		F1432	M1504	K1566	E1635	L1699	S1775	K1835	L1898	L1899	THR
		L1433	Q1505	M1568	D1636	Y1703	I1776	D1836	T1900	P1901	PRO
		Q1434	V1506	K1569	H1637	N1704	T1777	E1837	E1902	L1963	PRO
		H1435	T1507	H1571	H1638	E1705	K1778	L1838	E1903	F1964	GLY
		G1436	S1508	Q1570	R1639	V1706	L1779	T1839	E1906	L1965	LEU
		L1437	L1510	Q1572	H1637	Y1707	A1780	Y1840	I1907	H1966	ARG
		A1438	E1512	P1574	H1638	K1708	I1781	D1841	I1908	H1967	ASN
		T1439	S1513	E1573	L1640	N1709	I1782	R1842	E1909	P1968	SER
		Q1440	L1513	P1575	C1644	L1710		R1843		L1970	LEU
										R1971	ASN
										F1974	ARG

• Molecule 2: Ras-related C3 botulinum toxin substrate 1

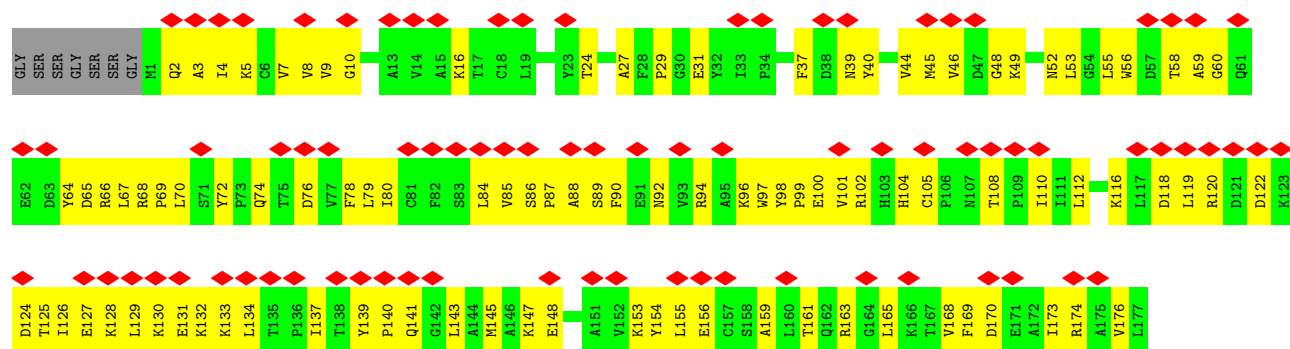




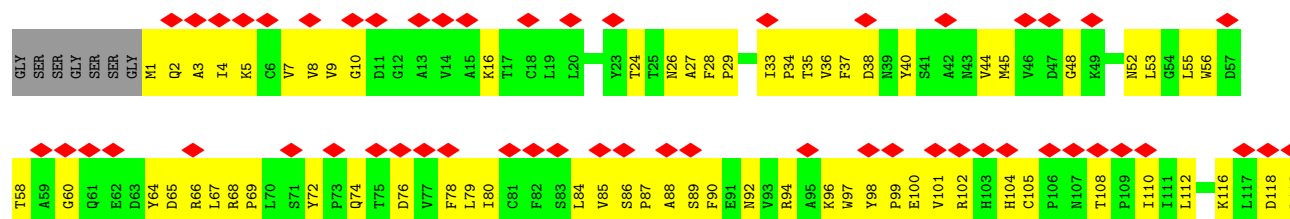
• Molecule 2: Ras-related C3 botulinum toxin substrate 1



• Molecule 2: Ras-related C3 botulinum toxin substrate 1



• Molecule 2: Ras-related C3 botulinum toxin substrate 1



R120	D121	D122	K123	D124	T125	I126	E127	K128	L129	K130	E131	K132	K133	L134	T135	P136	I137	T138	Y139	P140	Q141	G142	L143	A144	M145	M146	K147	E148	I149	G150	A151	V152	K153	Y154	L155	E156	C157	S158	A159	L160	T161	Q162	R163	G164	L165	K166	T167	V168	F169	D170	E171	A172	I173	R174	A175	V176	L177
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	112745	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 ($e^-/\text{\AA}^2$)	49.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.095	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	452.2, 452.2, 452.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	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	0.30	0/13787	0.58	1/18706 (0.0%)
1	C	0.30	0/13787	0.58	1/18706 (0.0%)
1	E	0.30	0/13787	0.58	1/18706 (0.0%)
1	G	0.30	0/13787	0.58	1/18706 (0.0%)
2	B	0.24	0/1415	0.56	0/1924
2	D	0.24	0/1415	0.56	0/1924
2	F	0.24	0/1415	0.56	0/1924
2	H	0.24	0/1415	0.56	0/1924
All	All	0.29	0/60808	0.58	4/82520 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1620	MET	CB-CG-SD	-5.18	97.16	112.70
1	E	1620	MET	CB-CG-SD	-5.18	97.17	112.70
1	A	1620	MET	CB-CG-SD	-5.17	97.19	112.70
1	G	1620	MET	CB-CG-SD	-5.17	97.21	112.70

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	13471	0	13448	1129	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	13471	0	13448	1131	0
1	E	13471	0	13448	1123	0
1	G	13471	0	13448	1129	0
2	B	1385	0	1407	110	0
2	D	1385	0	1407	100	0
2	F	1385	0	1407	121	0
2	H	1385	0	1407	111	0
All	All	59424	0	59420	4847	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 41.

The worst 5 of 4847 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:1731:GLN:HG2	1:C:1731:GLN:HG2	1.38	1.04
1:E:1932:MET:HE2	2:F:56:TRP:HA	1.41	1.02
1:A:1731:GLN:CG	1:C:1731:GLN:HG2	1.91	0.99
1:E:1720:TYR:HB3	1:G:1738:MET:HE2	1.47	0.97
1:E:1756:PHE:O	1:E:1766:GLU:HA	1.65	0.96

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	1672/2053 (81%)	1542 (92%)	130 (8%)	0	100	100
1	C	1672/2053 (81%)	1543 (92%)	129 (8%)	0	100	100
1	E	1672/2053 (81%)	1542 (92%)	130 (8%)	0	100	100
1	G	1672/2053 (81%)	1541 (92%)	131 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
2	D	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
2	F	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
2	H	175/184 (95%)	165 (94%)	10 (6%)	0	100	100
All	All	7388/8948 (83%)	6828 (92%)	560 (8%)	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	1476/1773 (83%)	1476 (100%)	0	100	100
1	C	1476/1773 (83%)	1476 (100%)	0	100	100
1	E	1476/1773 (83%)	1476 (100%)	0	100	100
1	G	1476/1773 (83%)	1476 (100%)	0	100	100
2	B	153/157 (98%)	153 (100%)	0	100	100
2	D	153/157 (98%)	153 (100%)	0	100	100
2	F	153/157 (98%)	153 (100%)	0	100	100
2	H	153/157 (98%)	153 (100%)	0	100	100
All	All	6516/7720 (84%)	6516 (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. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	108	GLN
1	G	1590	GLN
1	G	219	ASN
1	G	778	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	104	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 oligosaccharides 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.

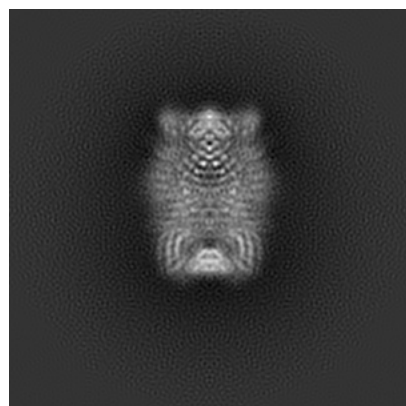
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65179. These allow visual inspection of the internal detail of the map and identification of artifacts.

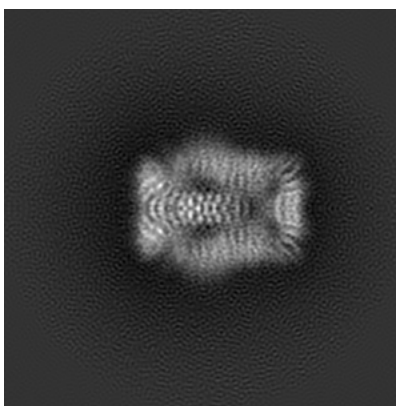
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

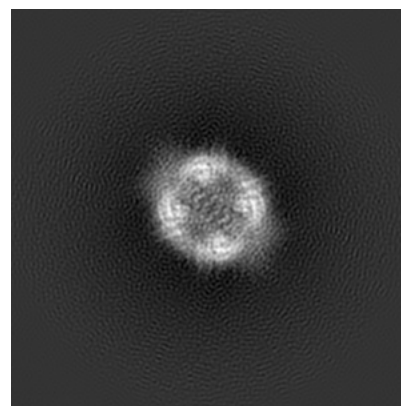
6.1.1 Primary map



X

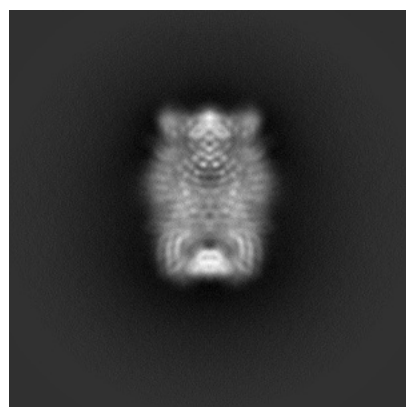


Y

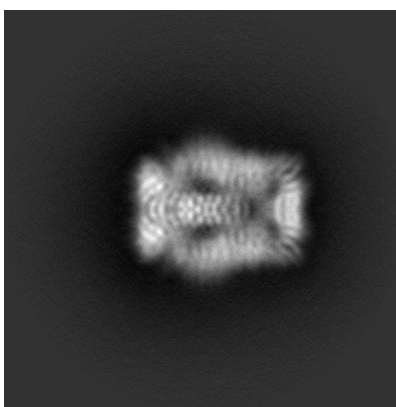


Z

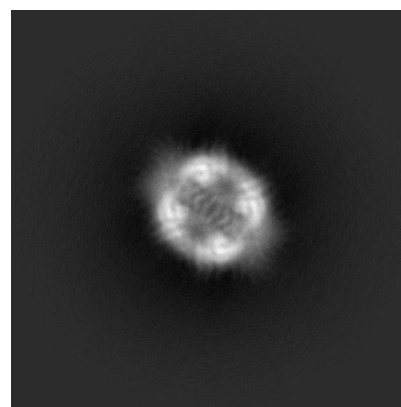
6.1.2 Raw map



X



Y



Z

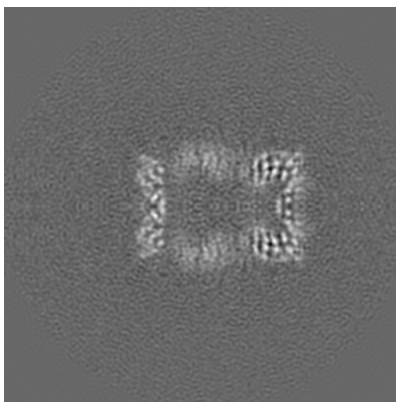
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

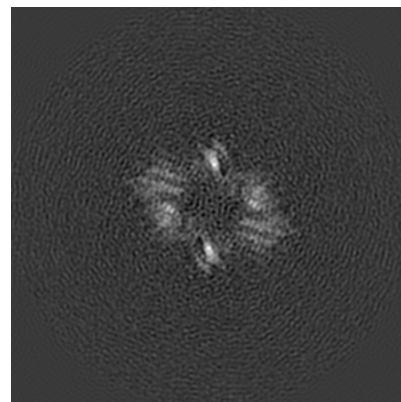
6.2.1 Primary map



X Index: 170

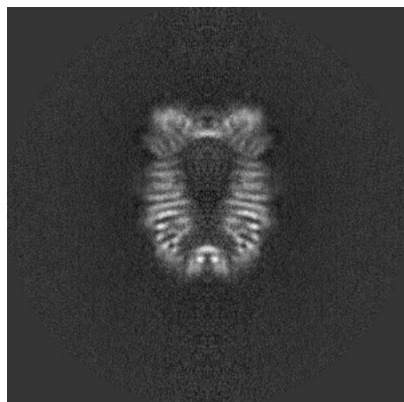


Y Index: 170

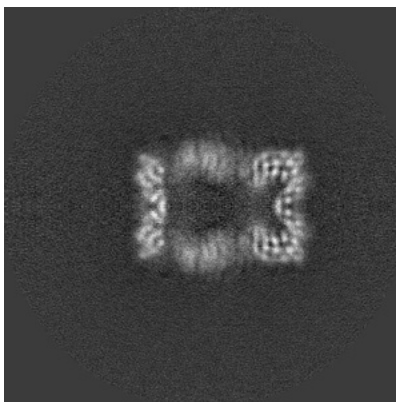


Z Index: 170

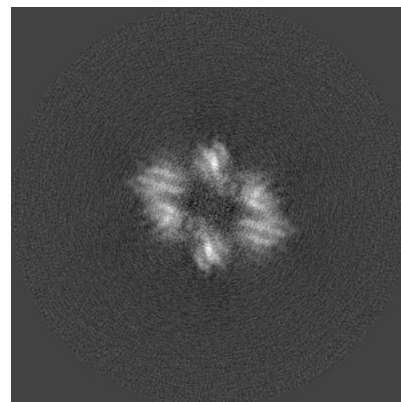
6.2.2 Raw map



X Index: 170



Y Index: 170



Z Index: 170

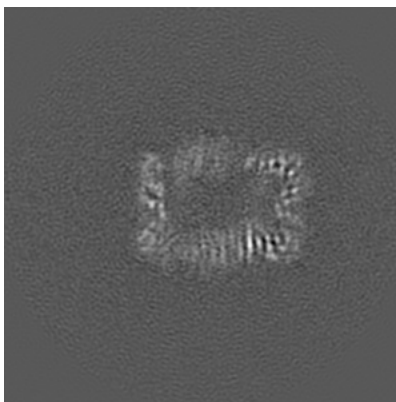
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

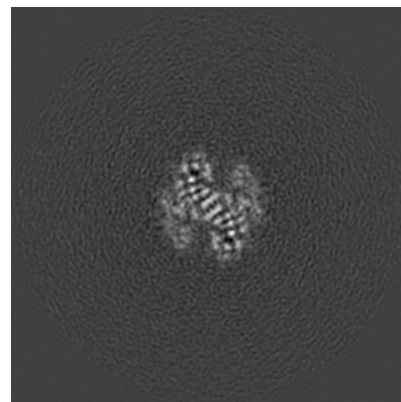
6.3.1 Primary map



X Index: 174

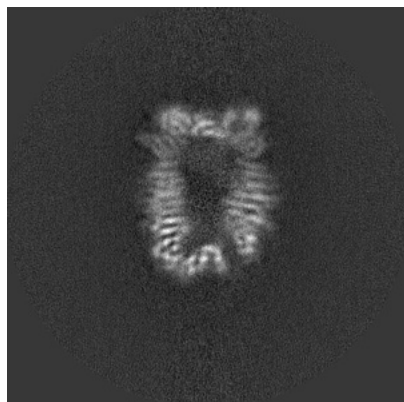


Y Index: 165

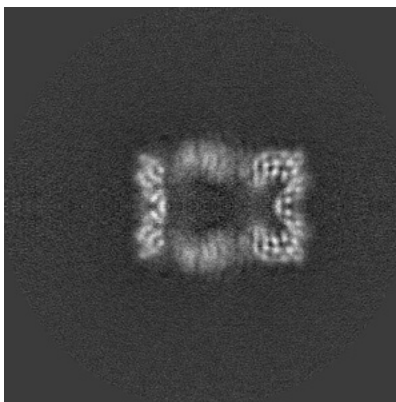


Z Index: 126

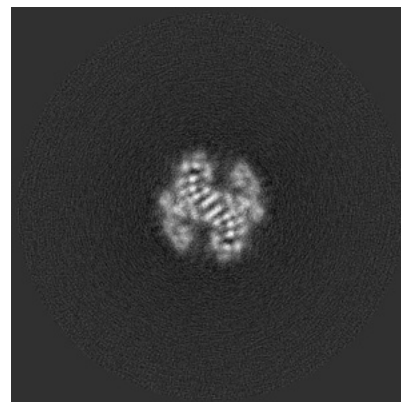
6.3.2 Raw map



X Index: 174



Y Index: 170

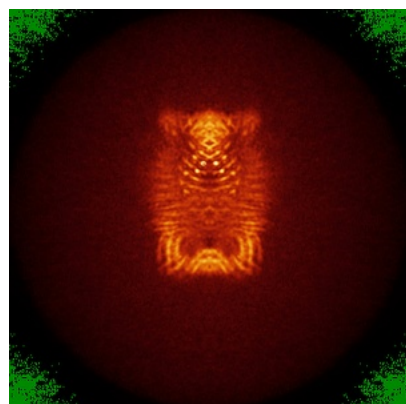


Z Index: 125

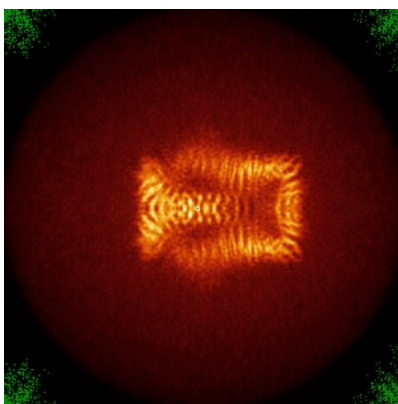
The images above show the largest variance slices of the map in three orthogonal directions.

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

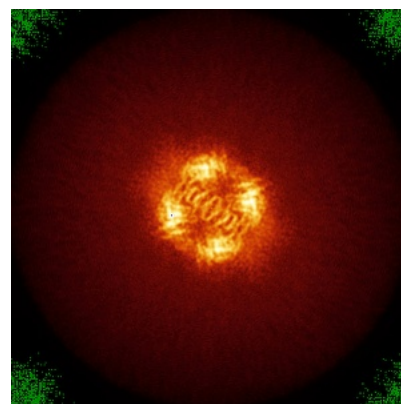
6.4.1 Primary map



X

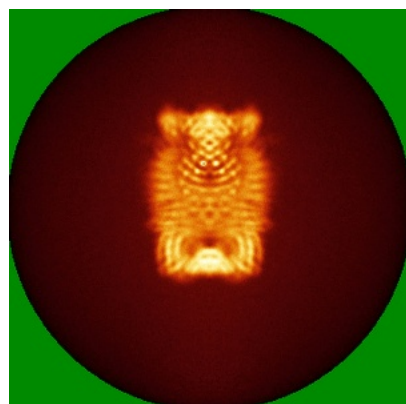


Y

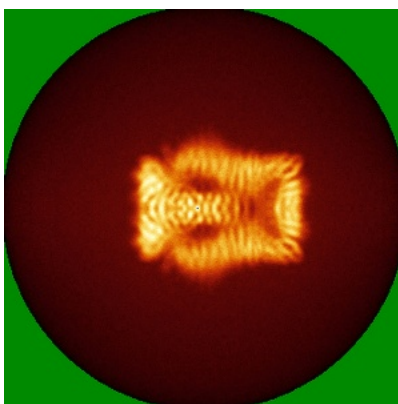


Z

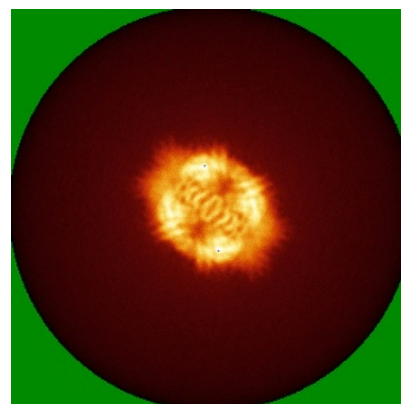
6.4.2 Raw map



X



Y

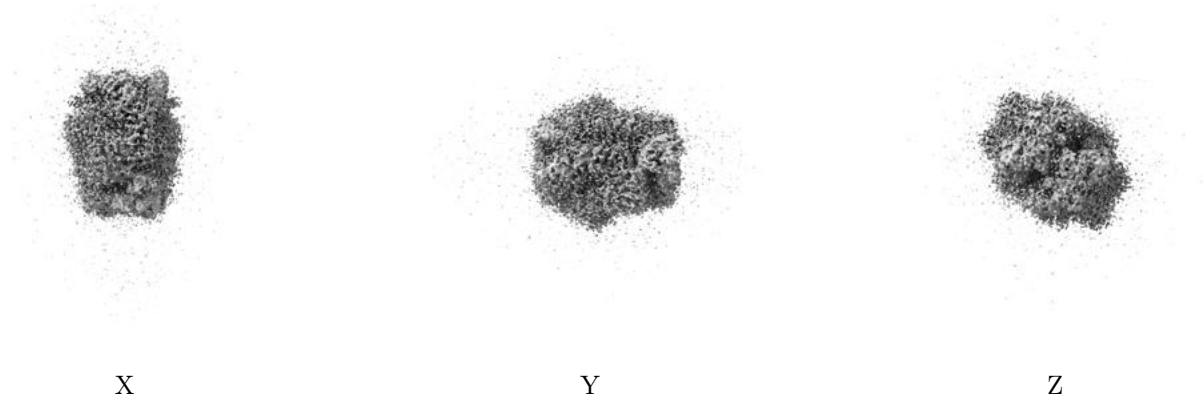


Z

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.

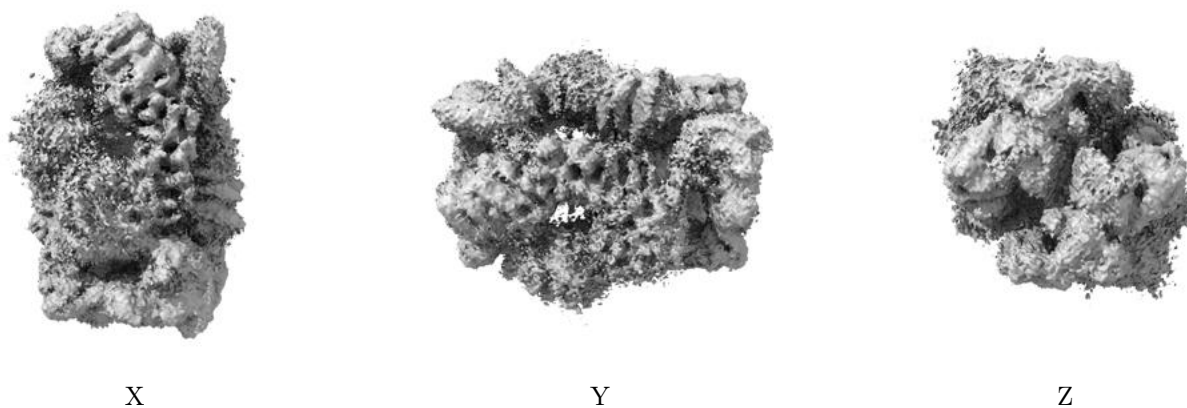
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

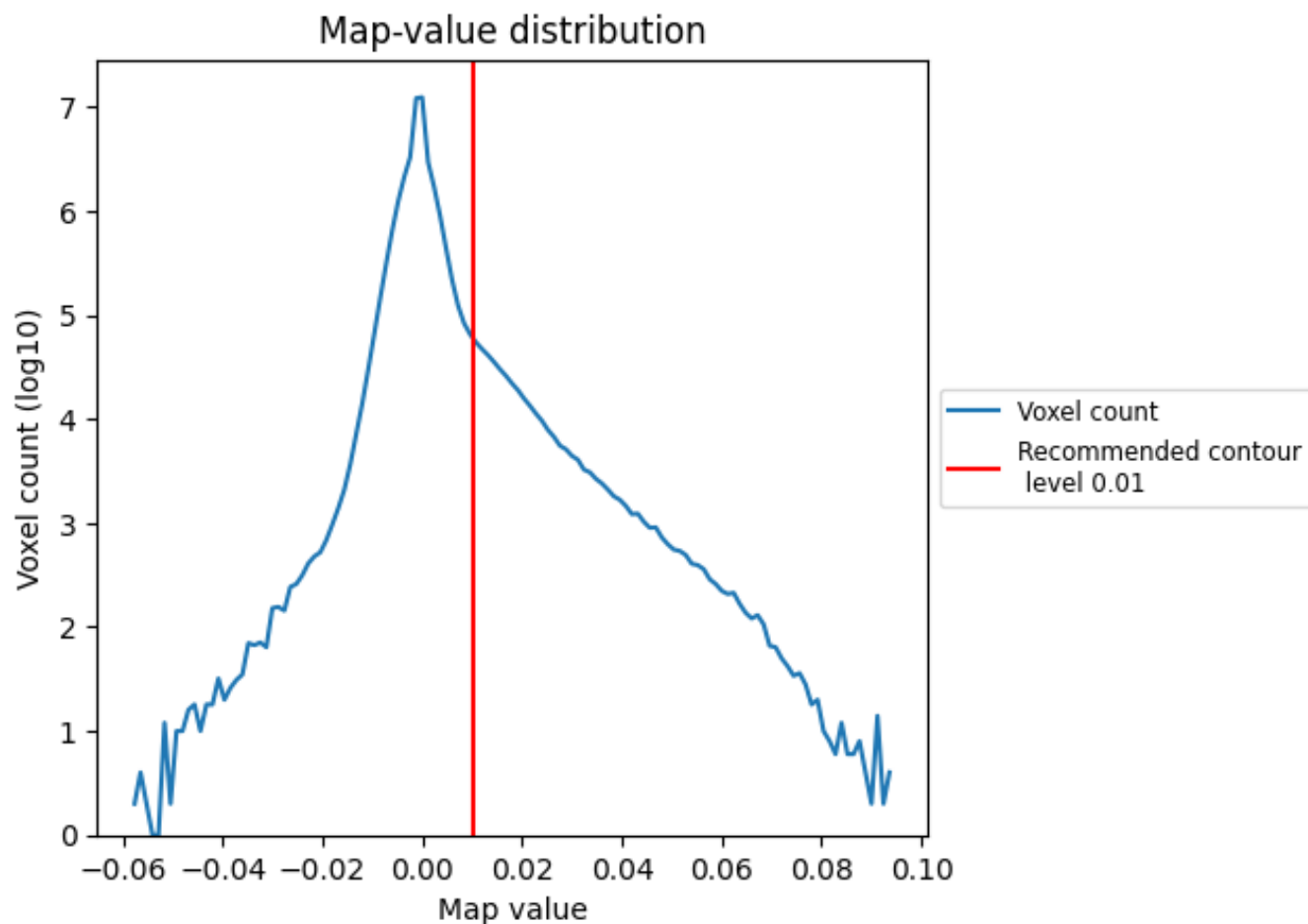
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

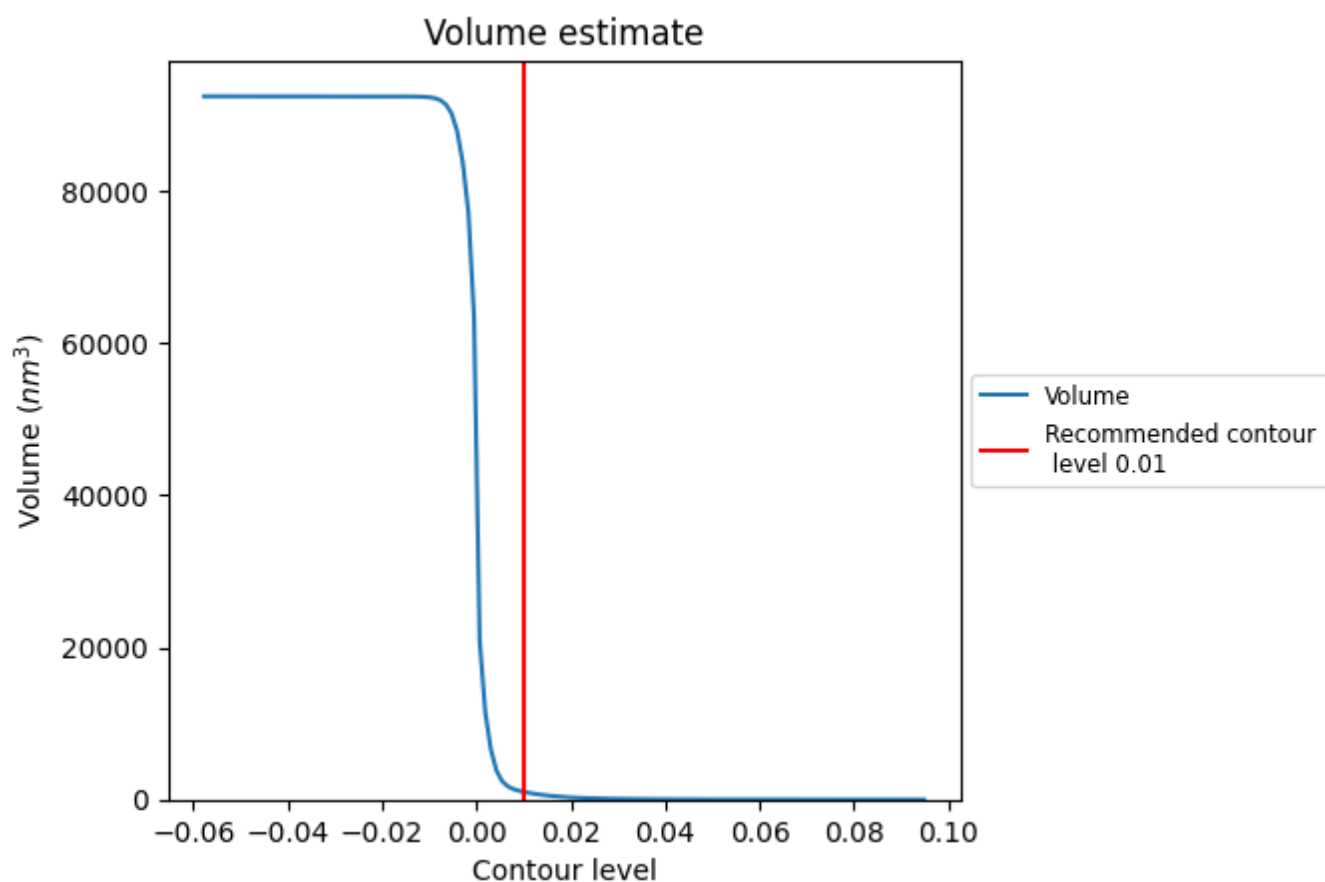
This section contains the results of statistical analysis of the map.

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.

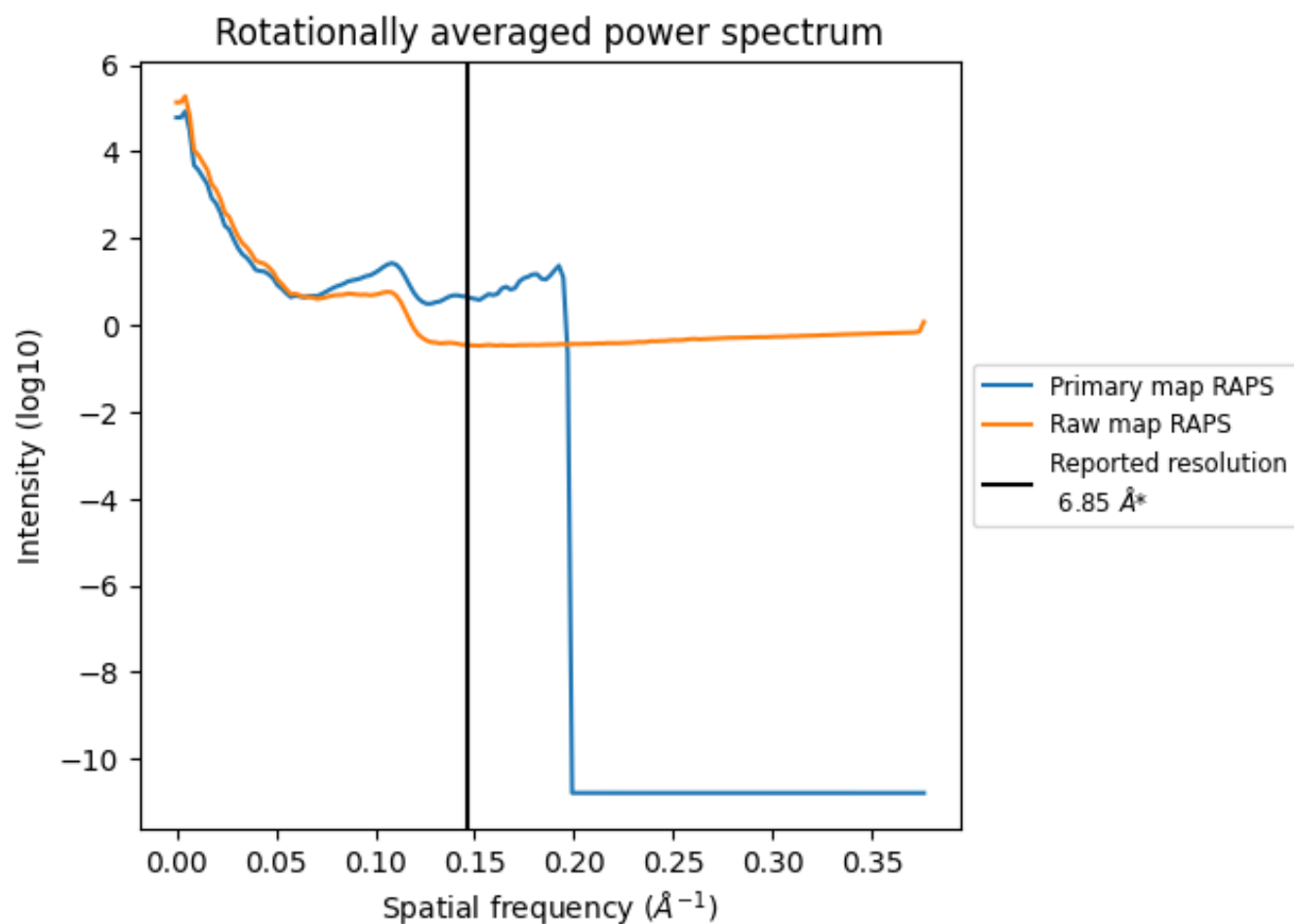
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1014 nm³; this corresponds to an approximate mass of 916 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 ⓘ

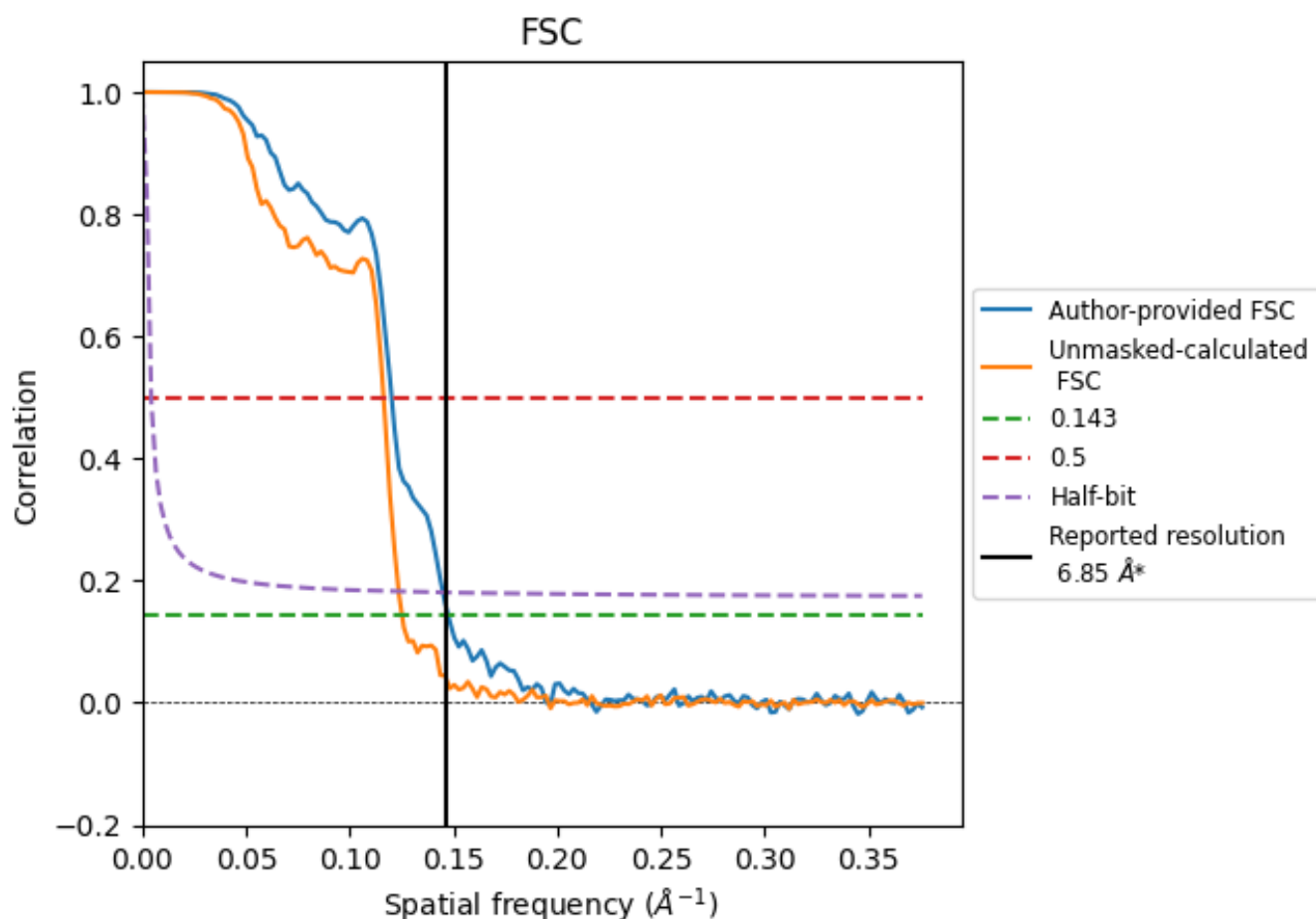


*Reported resolution corresponds to spatial frequency of 0.146 $\text{\AA}^{-1}$

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 0.146 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

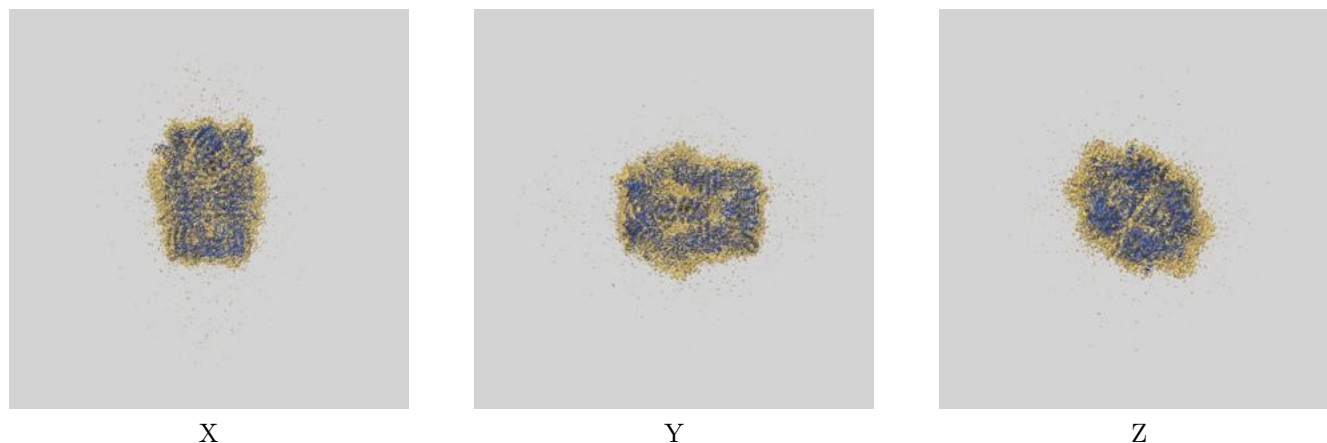
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.85	-	-
Author-provided FSC curve	6.78	8.32	6.90
Unmasked-calculated*	7.99	8.60	8.08

*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 7.99 differs from the reported value 6.85 by more than 10 %

9 Map-model fit [i](#)

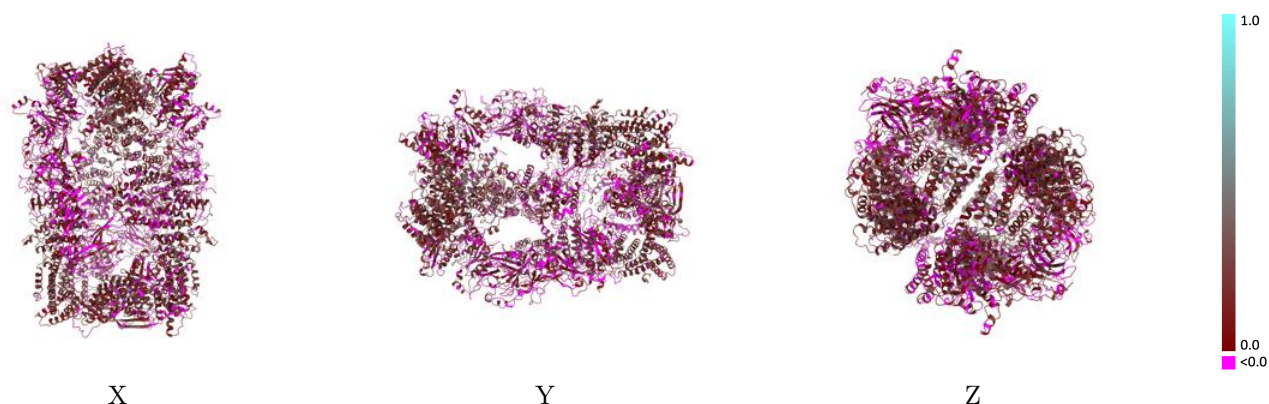
This section contains information regarding the fit between EMDB map EMD-65179 and PDB model 9VM7. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



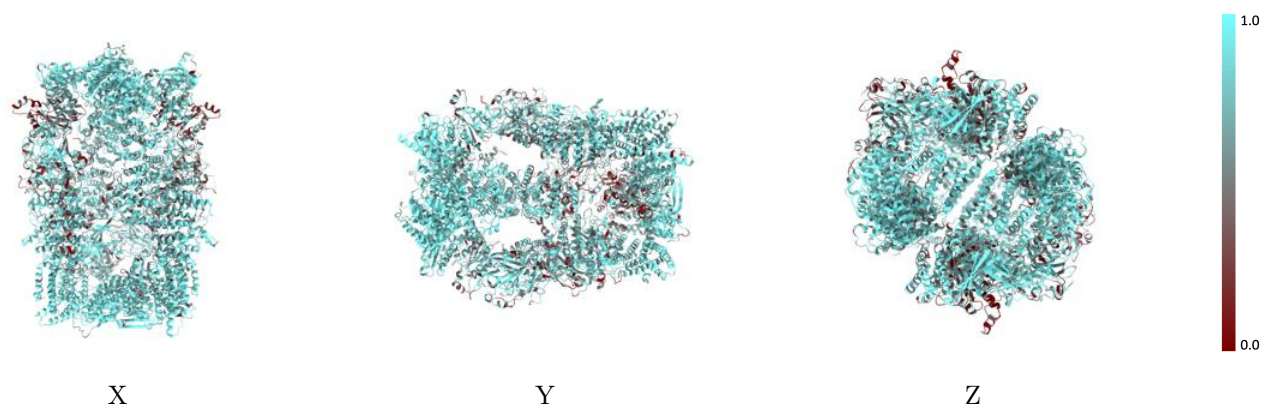
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



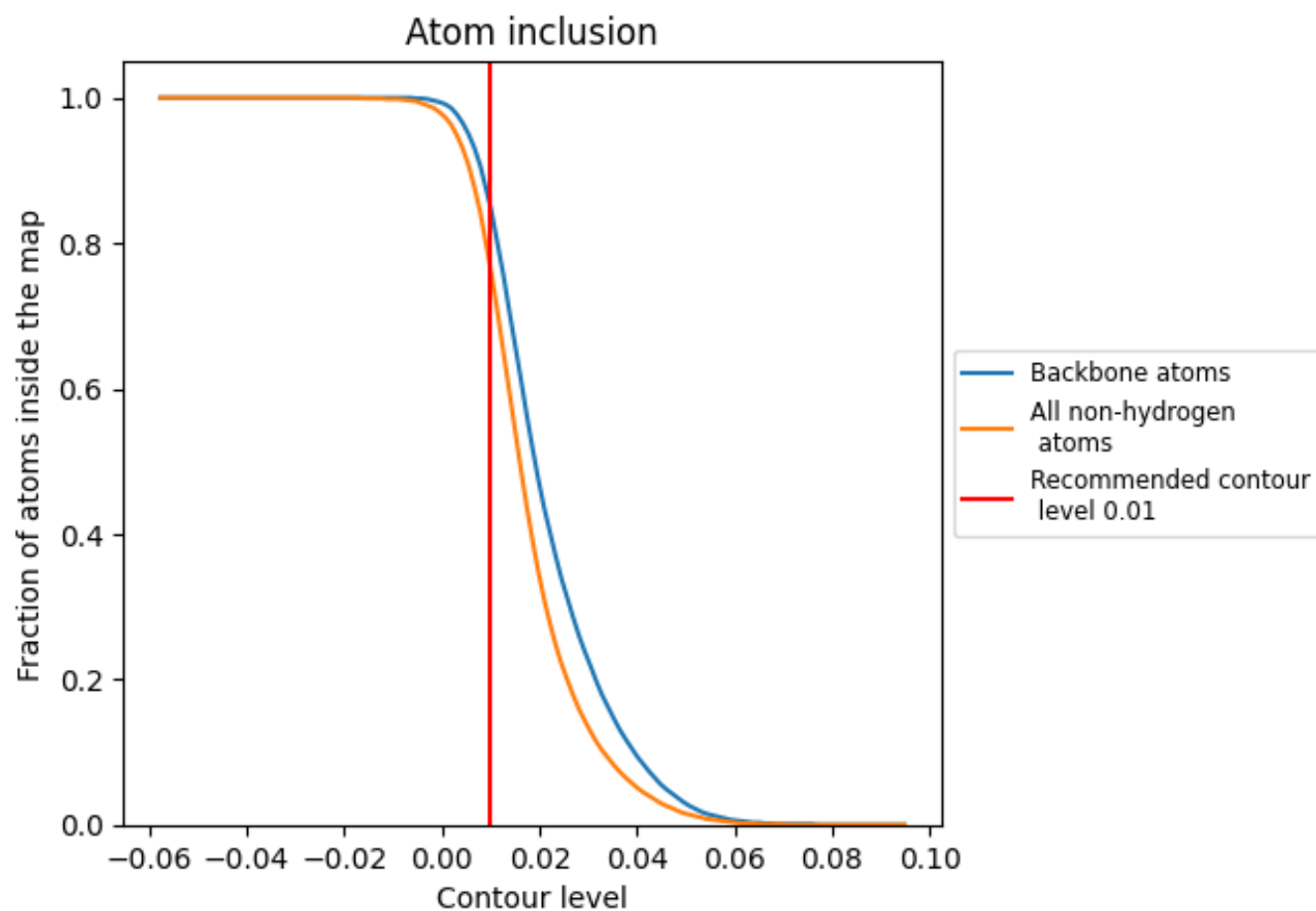
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.1350
A	0.7800	0.1280
B	0.6890	0.1220
C	0.7890	0.1420
D	0.7290	0.1330
E	0.7740	0.1320
F	0.4560	0.0830
G	0.7940	0.1520
H	0.4390	0.0770

