



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 12:51 PM JST

PDB ID : 6L54
EMDB ID : EMD-0837
Title : Structure of SMG189
Authors : Xu, Y.; Qi, Y.
Deposited on : 2019-10-22
Resolution : 3.43 Å(reported)

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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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

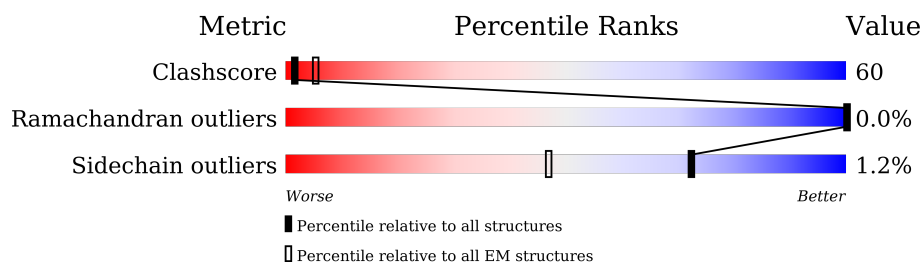
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 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	3661	 5% 19% 33% 48%
2	B	991	 13% 26% 61%
3	C	520	 19% 39% 41%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	C	601	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20387 atoms, of which 857 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 Serine/threonine-protein kinase SMG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1911	Total	C	N	O	S	0	0
			13859	8742	2364	2681	72		

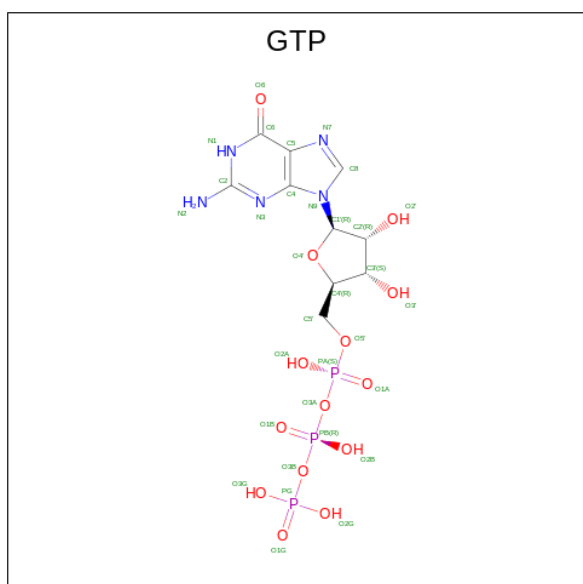
- Molecule 2 is a protein called Protein SMG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	389	Total	C	H	N	O	S	0	0
			3551	2036	393	548	554	20		

- Molecule 3 is a protein called Protein SMG9.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	308	Total	C	H	N	O	S	0	0
			2944	1591	464	423	449	17		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	

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.

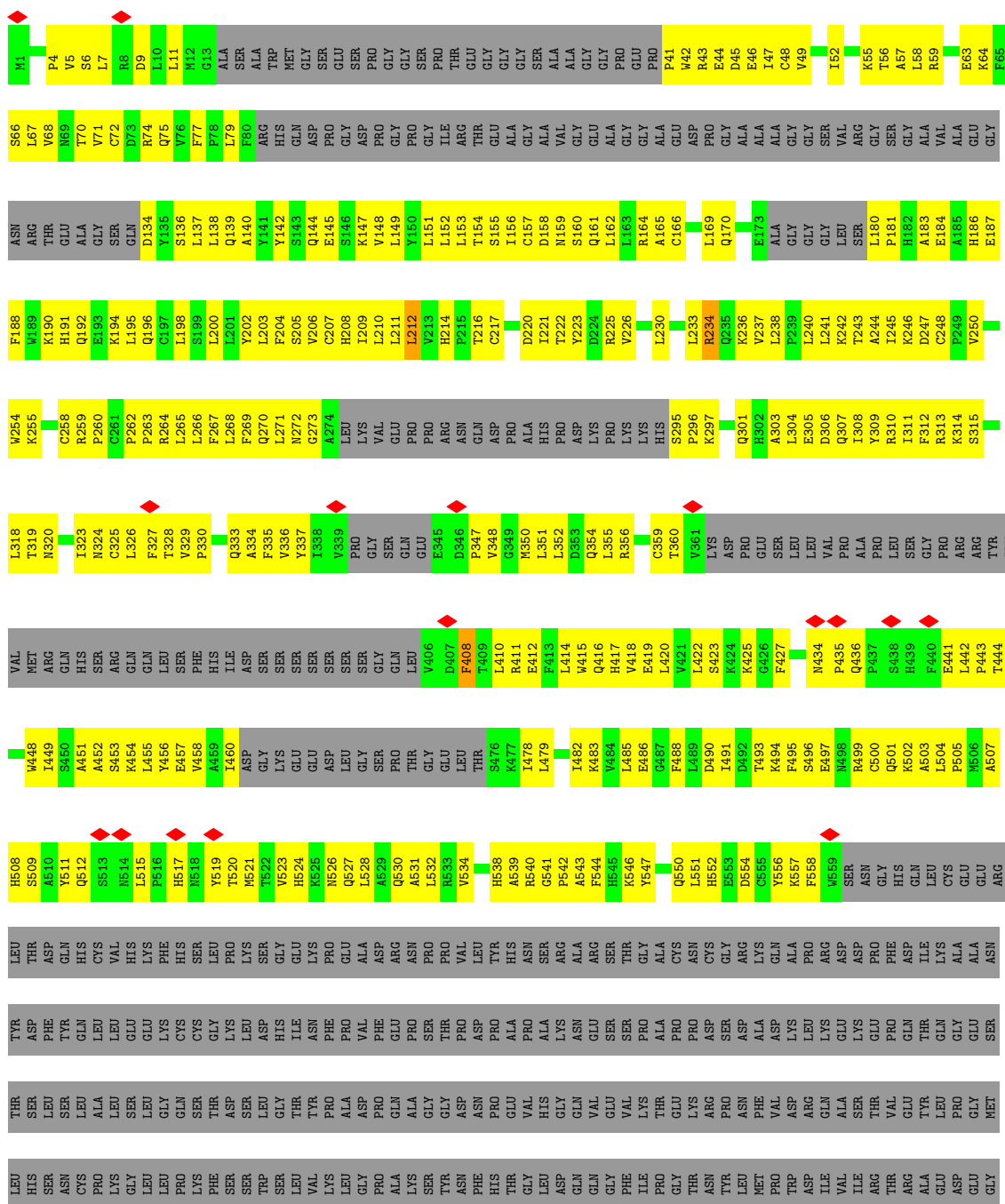
• Molecule 1: Serine/threonine-protein kinase SMG1



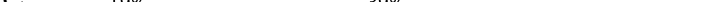
T1427	L1360	L1294	SER	G1101	M1035	ASP	T900	L826	G763	THR	P636	G570
A1428	E1361	R1295	LEU	K1102	R1036	ASN	P901	V829	A766	THR	T637	E571
ALA	L1368	S1296	SER	M1103	V1037	D970	P902	L830	N767	ALA	M572	M572
PHE	L1369	S1297	LEU	L1104	G1038	G974	N904	S831	T768	THR	V638	T573
ALA	T1370	V1298	PHE	I1107	L1039	N975	N905	N832	L769	LYS	F639	C574
ARG	L1300	G1299	SER	M1108	L1040	N976	N906	N832	V770	LYS	L642	A575
ASP	A1303	L1300	PRO	S1109	P1044	G977	K907	T836	E771	HIS	N645	L576
LYS	CYS	THR	THR	Q1112	A1045	R978	T908	E837	D772	PHE	N646	N577
CYS	ASP	THR	ASP	Q1113	A1045	R979	D909	I838	N773	SER	L646	N578
GLY	SER	THR	SER	A1114	V1048	R980	D910	I839	N774	ILE	M647	L579
VAL	PRO	PRO	PRO	E1115	R1049	N981	N911	Q839	ILE	ILE	I648	L580
THR	VAL	VAL	VAL	G1116	R1049	L982	V911	Q840	ILE	LEU	V649	H581
GLN	ILE	ILE	ILE	R1117	F1052	L983	Q914	E840	ILE	LEU	S582	S582
GLU	M1184	L1185	GLN	K1120	P1053	Q985	N918	L843	CYS	CYS	H650	GLN
LEU	Y1185	L1186	LEU	S1122	L1054	L987	E919	L845	LEU	GLN	D652	LEU
LEU	L1186	L1186	LEU	W1123	LEU	E988	A920	R946	ALA	ALA	P653	PRO
PRO	K1189	L1189	THR	E1124	THR	N989	Q922	K851	SER	SER	V655	GLU
GLY	A1190	L1190	GLY	Y1125	GLY	E991	T924	A852	HIS	HIS	H656	ALA
GLN	G1191	L1191	GLY	Y1125	GLY	E992	V925	P853	ALA	ALA	P657	CYS
ASN	E1192	L1192	ASN	L1129	GLY	L993	L926	T856	LEU	LEU	A659	ILE
ILE	I1195	L1195	ILE	C1136	THR	M934	L926	F857	SER	LYS	I660	LYS
ASN	S1196	L1196	ASN	A1131	LEU	Y995	T931	H858	SER	HIS	A663	HIS
ARG	L1197	L1197	ARG	T1132	LEU	Y998	P932	P859	LEU	GLU	V664	GLU
LEU	A1198	L1198	LEU	W1133	SER	E999	L933	Q860	PRO	LEU	L665	A596
ALA	D1199	L1199	ALA	C1138	GLN	A1002	G934	D861	ASP	ASP	T667	F597
GLY	V1203	L1203	GLY	I1139	ASN	A1002	Q937	F862	LEU	LEU	L668	F602
SER	Q1204	L1204	SER	S1140	GLY	ASN	D938	S863	LEU	LEU	H671	N603
LYS	E1205	L1205	LYS	P1141	E1070	ALA	T939	D864	GLN	GLN	C672	D605
GLY	W1206	L1206	GLY	ASP	E1071	LEU	Q941	V865	ARG	ARG	T673	N606
ILE	Q1207	L1207	ILE	LYS	T1072	THR	Q941	I866	CYS	CYS	A607	A607
ASP	W1208	L1208	ASP	SER	T1073	SER	T942	S867	VAL	VAL	R674	K608
MET	A1209	L1209	MET	VAL	M1074	PRO	I943	F868	ASP	ASP	H675	F609
LYS	H1211	L1211	LYS	THR	M1075	P1009	I943	L869	LEU	LEU	D676	V610
LEU	D1212	L1212	LEU	THR	V1076	A1010	T946	L870	C802	C802	H677	V611
LEU	L1213	L1213	LEU	LEU	V1077	V1011	T947	H875	R803	R803	PHE	I612
PRO	K1214	L1214	PRO	ALA	E1078	F1015	R948	S949	V804	V804	ILE	F613
ASN	L1215	L1215	ASN	ASN	E1079	F1016	LEU	N881	Q805	Q805	SER	D614
SER	THR	THR	SER	GLY	C1081	Y1017	ALA	N882	L806	L806	SER	L615
SER	SER	SER	SER	ARG	E1082	T1018	ALA	L883	H808	H808	LEU	L618
PRO	THR	THR	PRO	ASN	L1083	N1019	HIS	E884	S809	S809	SER	T619
LEU	SER	SER	LEU	ALA	H1084	Q1021	THR	L885	G810	G810	SER	T620
LEU	SER	SER	LEU	ALA	C1085	T1022	ASN	F887	T811	T811	PRO	I621
LEU	SER	SER	LEU	PRO	P1086	D1025	PRO	Y888	R814	R814	SER	G622
ASN	ASN	ASN	ASN	PRO	A1087	W1026	ASP	S889	F817	F817	PHE	A624
LYS	LYS	LYS	LYS	LYS	A1088	Q891	GLN	C890	LEU	LEU	ASP	K625
LYS	SER	SER	LYS	HIS	I1089	L1027	ASP	Q891	PRO	PRO	GLY	L628
ALA	ASP	ASP	ALA	SER	Q1090	T1028	VAL	R892	L820	L820	ALA	I629
ASP	ALA	ALA	ASP	LEU	G1091	R1029	SER	L893	L821	L821	HIS	G630
PHE	THR	THR	PHE	ASN	I1092	I1030	GLN	D894	L822	L822	VAL	I629
ASN	ASN	ASN	ASN	GLY	I1092	I1031	TRP	K895	S823	S823	ILE	G630
TYR	ILE	ILE	TYR	GLU	W1095	S1033	THR	R896	I824	I824	SER	A633
ILE	LYS	LYS	ILE	ARG	S1096	S1033	THR	D897	S824	S824	THR	L634
LYS	LYS	LYS	LYS	ARG	V1100	I1034	ALA	Q898	P825	P825	VAL	S635

A2297	E2309	W2310	W2311	E2312	T2313	T2314	Q2315	Q2316	W2317	R2319	S2320	T2321	A2322	W2323	M2324	S2325	W2326	W2327	T2330	I2331	G2332	L2333	G2334	D2335	R2336	H2337	L2338	D2339	W2340	W2341	L2342	L2343	D2344	M2345	T2346	G2347	E2349	W2350	H2351	L2352	T2353	D2354	W2355	W2356	W2357	C2358									
ASP	T2245	V2246	R2247	R2248	R2249	S2250	E2251	L2252	Y2253	Y2254	S2255	S2256	L2257	A2260	LEU	LYS	THR	VAL	GLY	LEU	SER	LEU	ASP	VAL	SER	R2272	R2273	D2274	D2275	P2276	L2277	H2278	W2279	M2280	K2281	A2282	V2283	L2284	E2285	E2286	L2287	M2288	E2289	P2292	W2293	L2294	W2295	K2296	ALA	GLN					
M2167	Q2168	F2169	L2170	S2171	L2172	W2173	M2174	T2175	M2176	F2177	A2178	T2179	I2180	M2181	Q2182	Q2183	E2184	T2185	P2186	R2187	F2188	R2191	H2192	Y2193	S2194	W2195	T2196	P2197	S2202	G2203	L2204	L2205	Q2206	W2207	W2208	D2209	G2210	A2211	T2212	L2213	L2214	F2215	G2216	L2217	W2218	R2219	R2220	W2221	Q2222	Q2223	R2224	L2228	K2232	ALA	GLN
T2103	N2104	T2105	E2106	T2107	A2108	L2109	W2113	SER	ALA	ARG	ASP	THR	W2119	T2120	T2121	H2122	S2123	V2124	G2125	G2126	T2127	T2128	T2129	L2130	L2131	P2132	T2133	K2134	T2135	K2136	T2137	K2138	K2139	L2140	L2141	G2144	S2145	ASP	GLY	LYS	S2149	P2151	Y2152	L2153	F2154	K2155	E2158	D2159	L2160	H2161	L2162	D2163	E2164	R2165	T2166
THR	PRO	HIS	E2037	K2038	W2039	F2040	D2041	N2042	W2043	Y2044	D2045	A2047	I2048	E2053	K2054	K2056	T2057	P2058	L2059	ASN	PRO	ALA	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	S2077	L2078	K2084	R2085	A2086	S2087	Y2088	I2089	L2092	E2093	E2094	I2095	S2096	P2097	W2098	L2099	A2100	M2102			
L1955	V1958	T1959	L1960	L1961	E1964	L1971	Q1972	Q1973	H1974	M1975	V1976	L1977	L1978	I1981	Q1982	L1983	L1984	E1985	D1986	E1987	V1988	L1989	R1990	V1991	GLN	ASN	ASN	GLN	ASN	M1926	Q1927	D1928	C1929	Y1930	I1933	V1934	D1935	S1938	S1939	P1942	T1943	M1944	V1945	L1946	Q1947	V1948	Q1949	M1950	L1951	R2025	V1952	A1953	E1954		
GLU	GLU	LEU	LEU	VAL	SER	CYS	GLU	GLY	GLY	SER	PRO	PRO	ALA	GLN	ASP	SER	ASN	LYS	ASP	GLU	LYS	GLY	LEU	ASN	GLN	ASP	GLN	ALA	M1926	Q1927	D1928	C1929	Y1930	I1933	V1934	D1935	S1938	S1939	P1942	T1943	M1944	V1945	L1946	Q1947	V1948	Q1949	M1950	L1951	R2025	V1952	A1953	E1954			
K1756	L1757	G1760	ILE	PRO	LEU	ASP	GLU	ASP	ASP	PRO	ARG	LEU	HIS	SER	HIS	ARG	VAL	GLN	THR	ASP	ASP	M1784	V1785	V1786	M1787	A1788	T1789	L1790	R1791	L1792	L1793	R1794	L1795	L1796	V1797	E1802	L1803	L1807	E1808	H1809	E1812	T1813	P1815	T1816	A1817	P1818	W1819	R1820	G1821	I1822					
I1823	P1824	Q1825	L1826	F1827	H1832	P1833	E1834	V1835	W1836	R1837	L1838	I1841	C1842	N1843	L1844	L1845	V1848	A1849	L1855	I1856	L1857	Y1858	P1859	A1860	I1861	V1862	G1863	T1864	I1865	S1866	SER	SER	GLN	SER	ALA	ASN	PHE	THR	ILE	PRO	THR	LEU	GLY	ASN	ILE	GLN									
THR	LEU	GLN	ILE	THR	GLU	SER	GLU	ASN	GLU	ASP	PRO	ARG	LEU	HIS	SER	HIS	ARG	VAL	GLN	THR	ASP	ASP	M1784	V1785	V1786	M1787	A1788	T1789	L1790	R1791	L1792	L1793	R1794	L1795	L1796	V1797	E1802	L1803	L1807	E1808	H1809	E1812	T1813	P1815	T1816	A1817	P1818	W1819	R1820	G1821	I1822				
S1624	W1625	Y1626	R1627	W1628	G1630	R1631	V1632	W1633	W1634	D1635	L1636	A1637	Q1638	G1640	L1645	R1648	E1649	K1650	S1651	E1652	Q1653	Q1654	N1655	L1656	L1657	P1658	D1659	T1660	I1661	T1662	E1663	E1664	K1665	E1667	R1668	I1669	I1672	L1673	G1674	Q1675	A1676	V1677	CYS	ARG	PRO	ALA	GLY	ILE	GLN	ASP	GLU	ASP	ILE		
GLY	LEU	SER	LEU	SER	LYS	ASN	ILE	ASN	THR	LEU	ILE	GLU	LEU	PRO	SER	VAL	ASN	THR	MET	GLU	GLU	TYR	P1582	S1586	E1587	S1588	T1589	V1590	H1591	I1592	G1593	E1596	P1597	D1598	F1599	I1600	L1604	Y1605	H1606	L1607	S1608	S1609	V1610	Q1611	A1612	PRO	GLU	ALA	VAL	A1616	W1619	L1622	A1623		
T1488	K1489	T1493	H1499	A1500	M1501	E1502	M1503	L1504	A1508	I1509	S1510	F1511	C1512	K1513	S1514	V1515	E1518	Y1519	A1520	W1521	A1522	K1523	S1524	I1525	L1526	T1527	V1528	L1529	K1530	W1531	T1532	Q1533	A1534	E1535	W1536	K1537	E1538	T1539	SER	GLY	GLN	LYS	GLN	VAL	T1577	ARG	ALA	GLN	HIS	GLN	ASN	PHE	THR		





- Molecule 3: Protein SMG9

Chain C:  19% 39% 41%

L512	Y515	L518	L519	ALA
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	420000	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	48.493	Depositor
Minimum map value	-23.751	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP

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	0.23	0/14051	0.39	1/19153 (0.0%)
2	B	0.23	0/3231	0.38	0/4367
3	C	0.24	0/2539	0.41	2/3440 (0.1%)
All	All	0.23	0/19821	0.39	3/26960 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3627	PRO	N-CA-CB	5.64	110.06	103.30
3	C	325	PHE	C-N-CA	5.33	135.04	121.70
3	C	399	HIS	C-N-CA	5.19	134.67	121.70

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	13859	0	13122	1769	0
2	B	3158	393	3174	331	0
3	C	2480	464	2469	302	0
4	C	32	0	11	9	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19530	857	18776	2308	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 60.

The worst 5 of 2308 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:1502:GLU:HA	1:A:1503:MET:HB2	1.30	1.09
2:B:198:LEU:HD11	2:B:483:LYS:HE2	1.36	1.06
1:A:649:VAL:HG11	1:A:667:THR:HB	1.40	1.04
1:A:820:LEU:HD22	1:A:886:LEU:HB2	1.35	1.03
3:C:406:LEU:HB2	3:C:422:LEU:HA	1.40	1.03

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	1853/3661 (51%)	1684 (91%)	168 (9%)	1 (0%)	51	83
2	B	373/991 (38%)	345 (92%)	28 (8%)	0	100	100
3	C	300/520 (58%)	274 (91%)	26 (9%)	0	100	100
All	All	2526/5172 (49%)	2303 (91%)	222 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1086	PRO

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1398/3224 (43%)	1379 (99%)	19 (1%)	67	85
2	B	351/847 (41%)	348 (99%)	3 (1%)	78	90
3	C	279/450 (62%)	277 (99%)	2 (1%)	84	93
All	All	2028/4521 (45%)	2004 (99%)	24 (1%)	72	87

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1989	LYS
1	A	2279	VAL
1	A	2253	TYR
1	A	2374	ARG
1	A	773	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1825	GLN
3	C	463	HIS
2	B	139	GLN
3	C	412	ASN
3	C	284	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	C	601	5	26,34,34	1.13	2 (7%)	32,54,54	1.65	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	C	601	5	-	5/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	GTP	C5-C6	-4.01	1.39	1.47
4	C	601	GTP	C2-N3	2.21	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	GTP	PA-O3A-PB	-4.26	118.21	132.83
4	C	601	GTP	PB-O3B-PG	-3.54	120.67	132.83
4	C	601	GTP	C5-C6-N1	3.18	119.58	113.95
4	C	601	GTP	C8-N7-C5	2.98	108.66	102.99
4	C	601	GTP	C3'-C2'-C1'	2.86	105.29	100.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

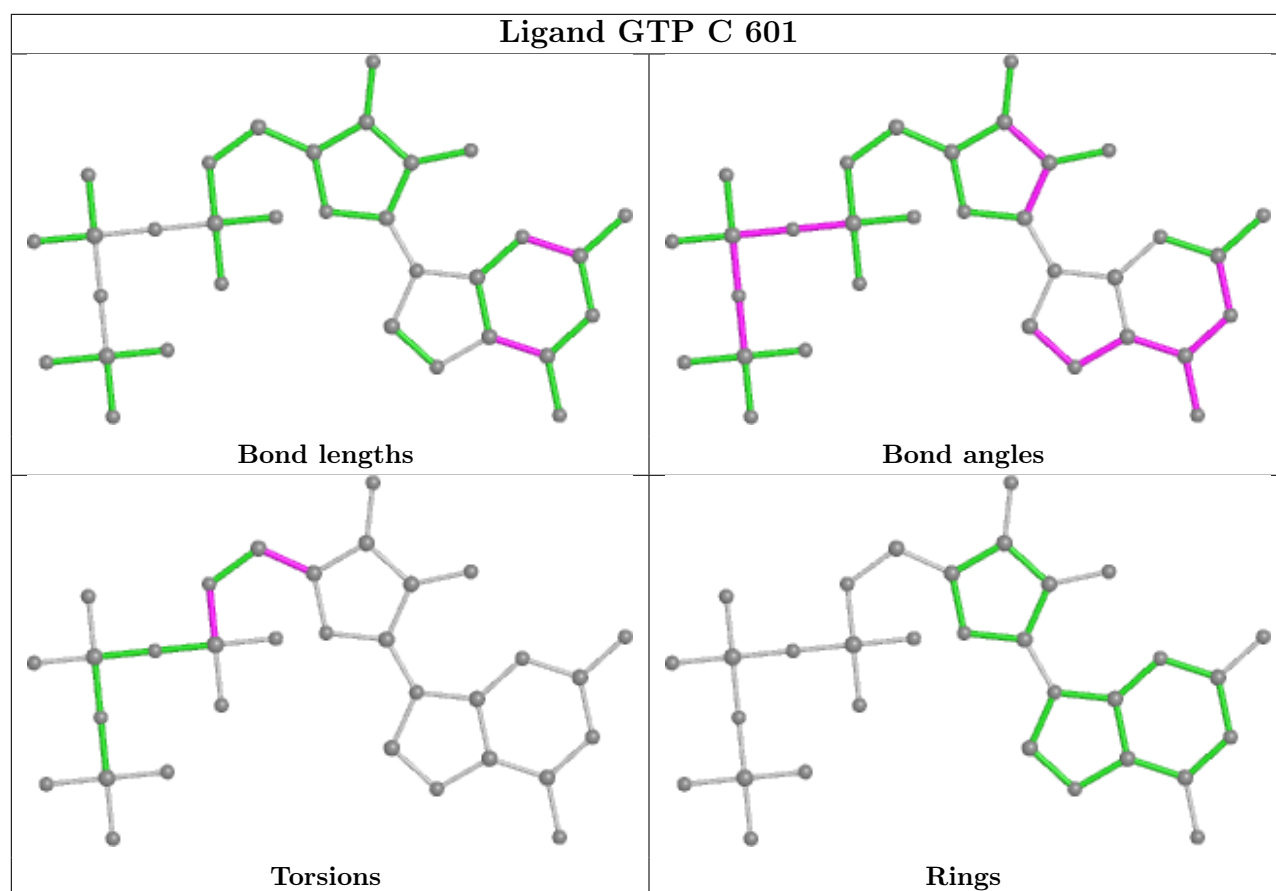
Mol	Chain	Res	Type	Atoms
4	C	601	GTP	C5'-O5'-PA-O3A
4	C	601	GTP	C3'-C4'-C5'-O5'
4	C	601	GTP	O4'-C4'-C5'-O5'
4	C	601	GTP	C5'-O5'-PA-O1A
4	C	601	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	GTP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

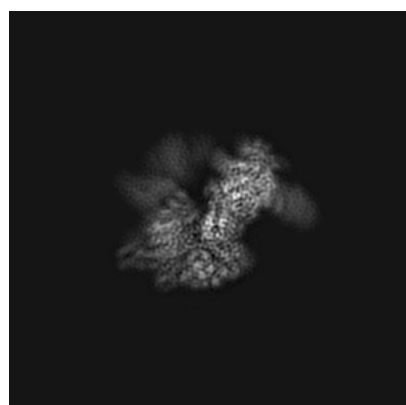
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0837. These allow visual inspection of the internal detail of the map and identification of artifacts.

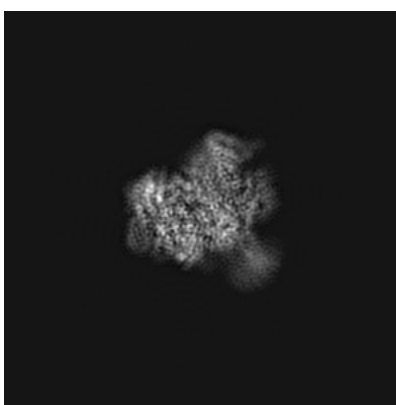
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

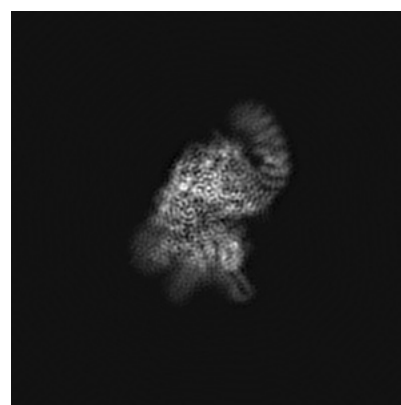
6.1.1 Primary map



X



Y

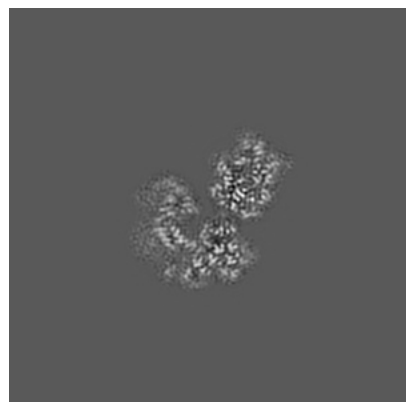


Z

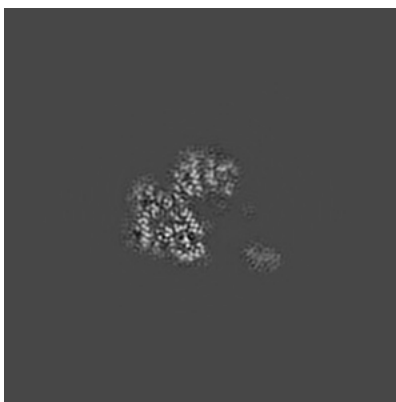
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

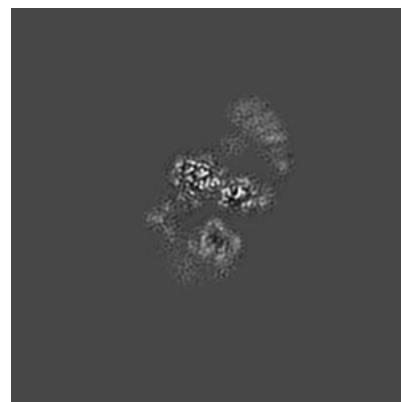
6.2.1 Primary map



X Index: 160



Y Index: 160

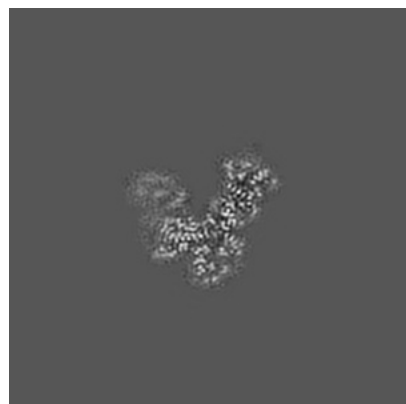


Z Index: 160

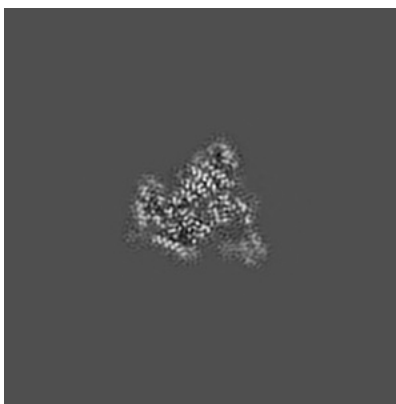
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

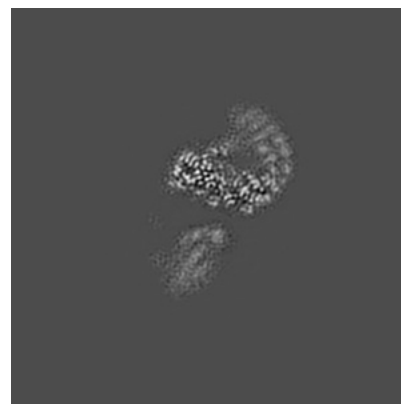
6.3.1 Primary map



X Index: 147



Y Index: 172



Z Index: 171

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

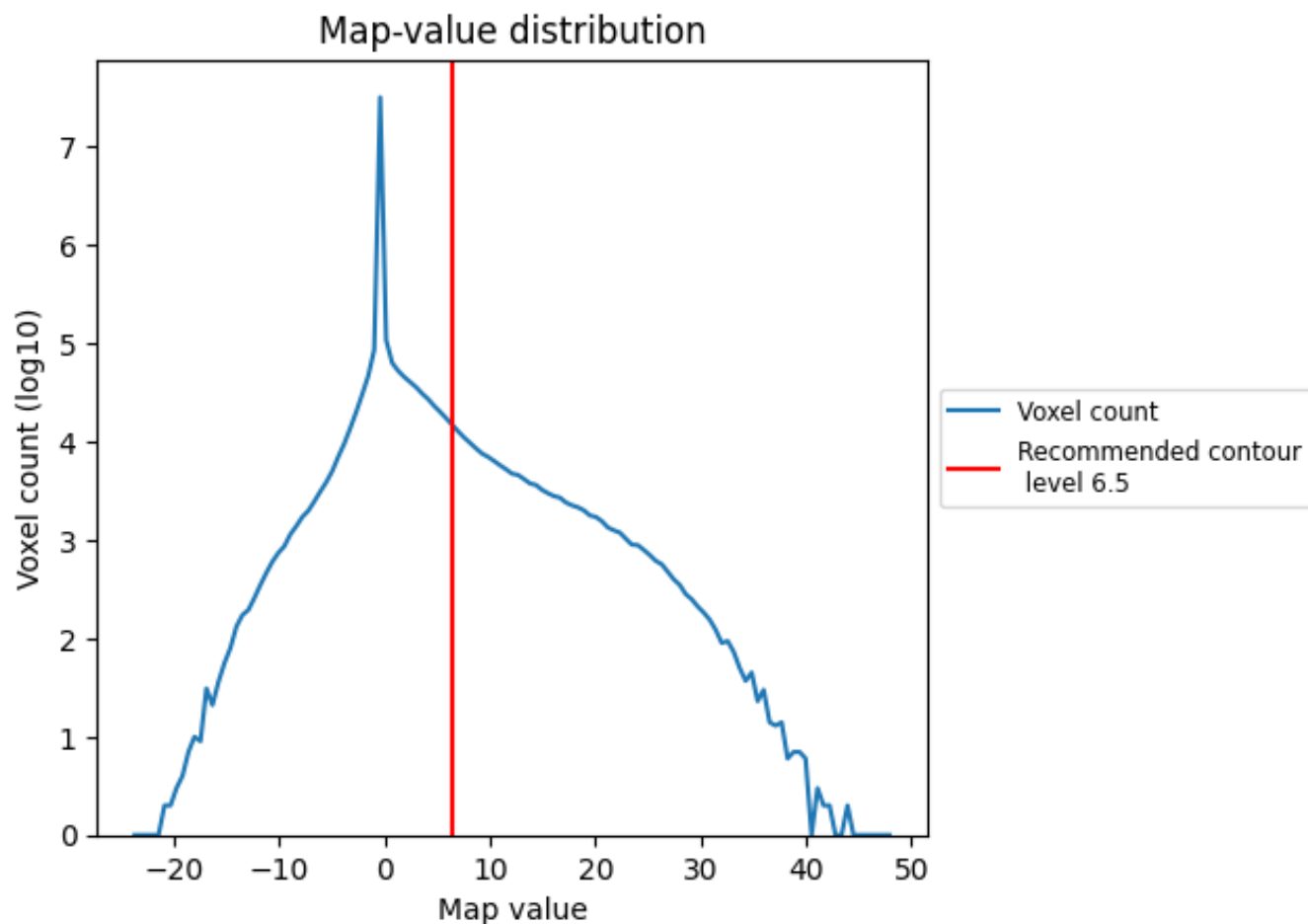
6.5 Mask visualisation

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

7 Map analysis [i](#)

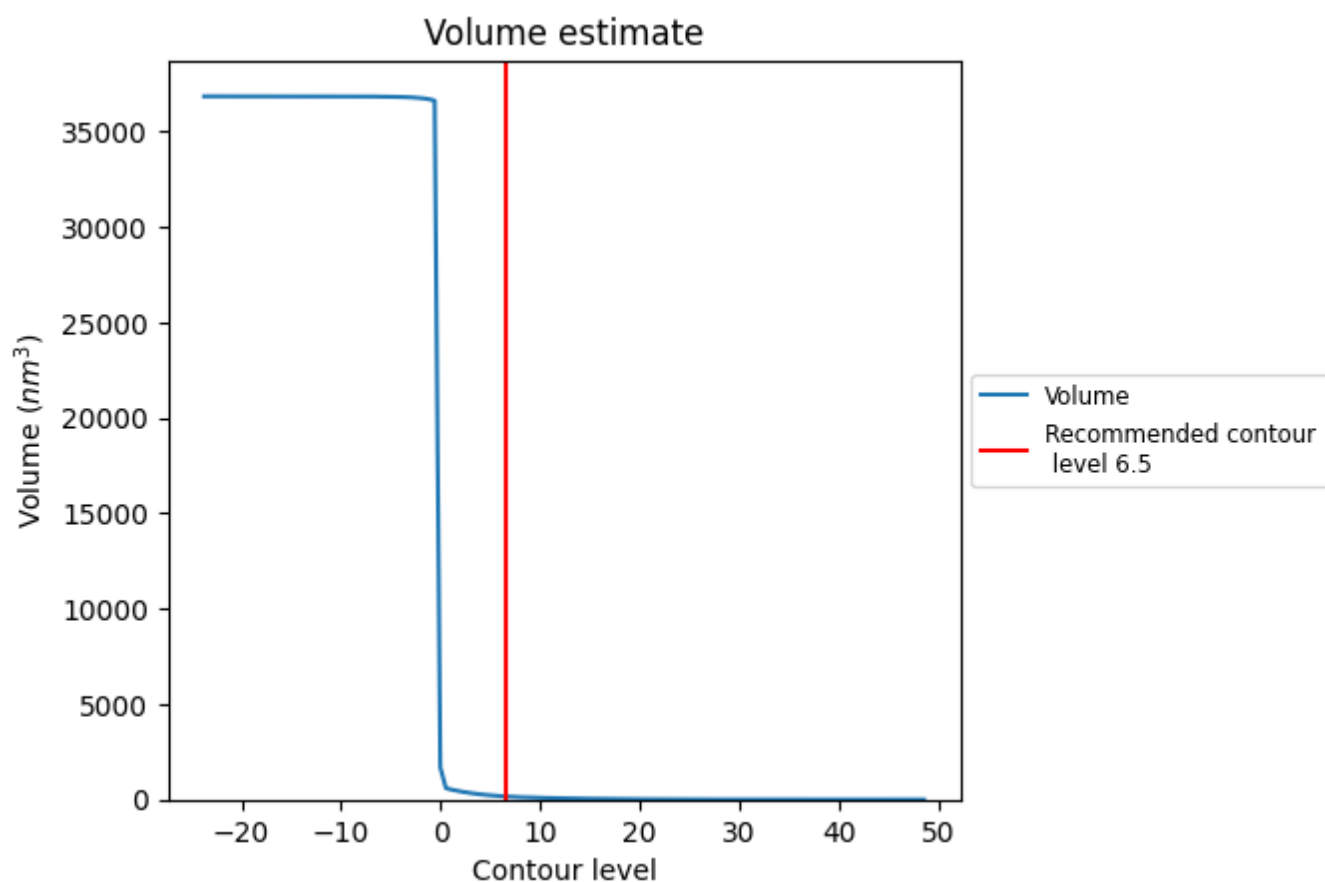
This section contains the results of statistical analysis of the map.

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.

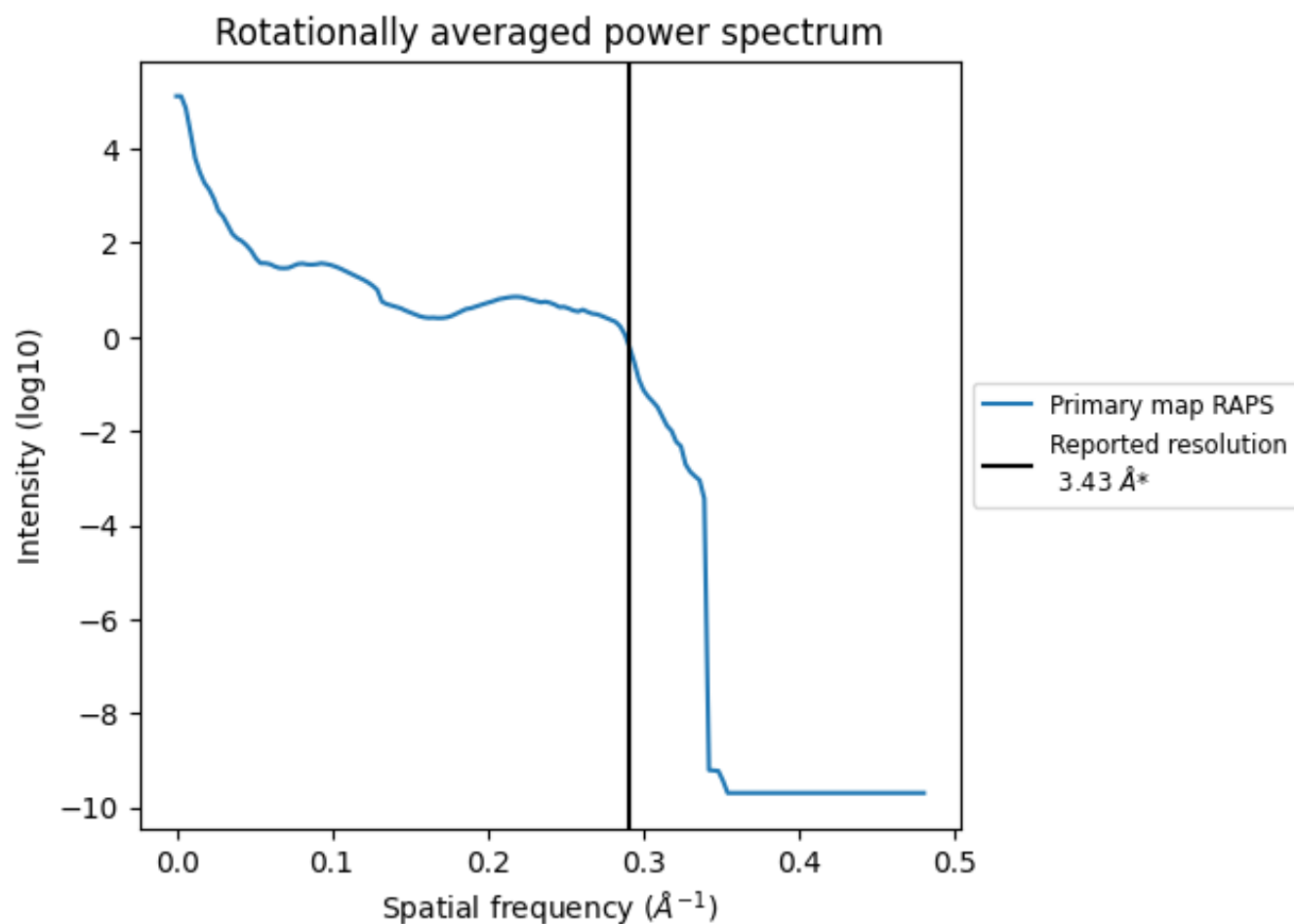
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 163 nm^3 ; this corresponds to an approximate mass of 148 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 0.292 Å⁻¹

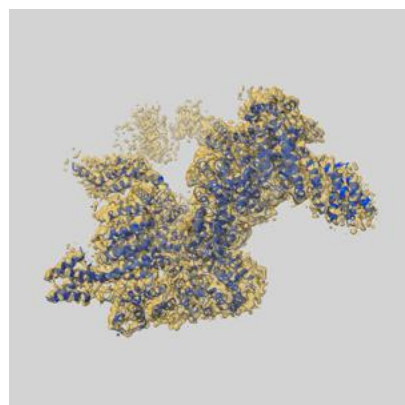
8 Fourier-Shell correlation

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

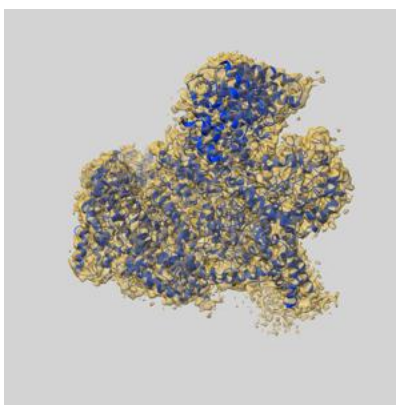
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0837 and PDB model 6L54. Per-residue inclusion information can be found in section 3 on page 5.

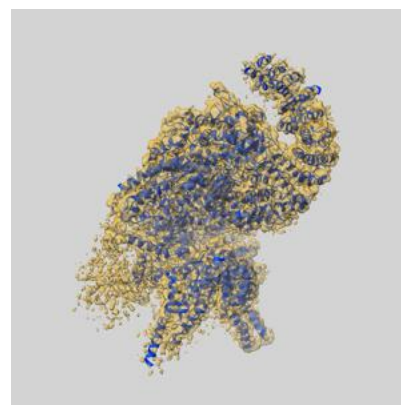
9.1 Map-model overlay [i](#)



X



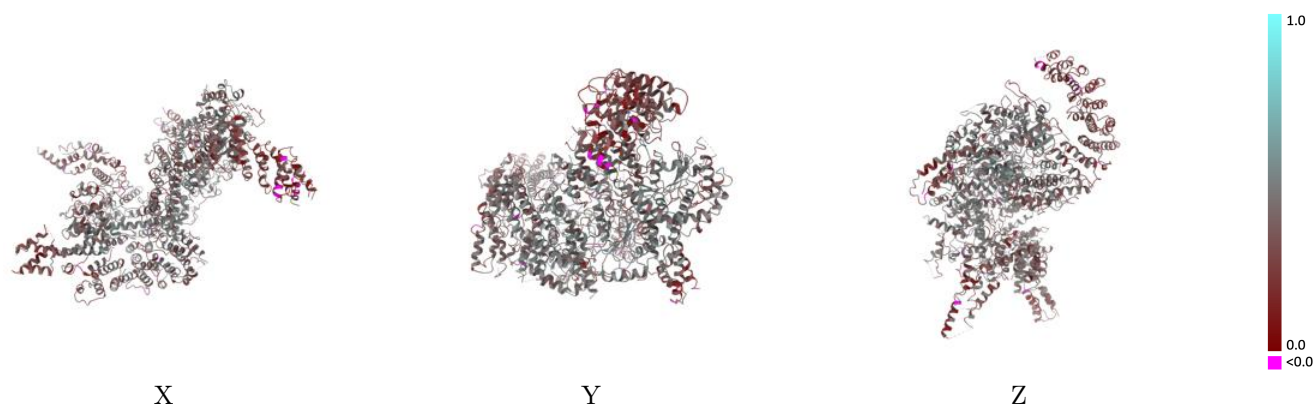
Y



Z

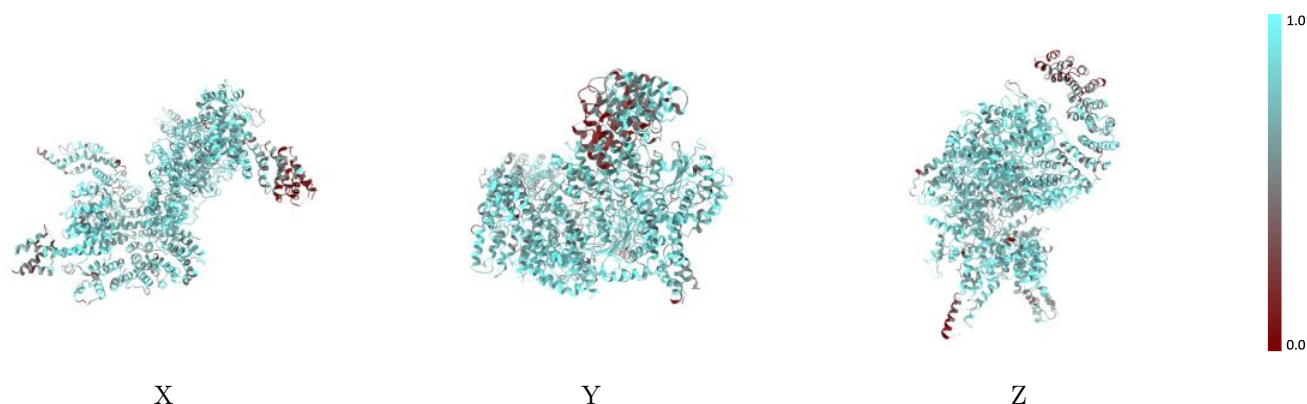
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



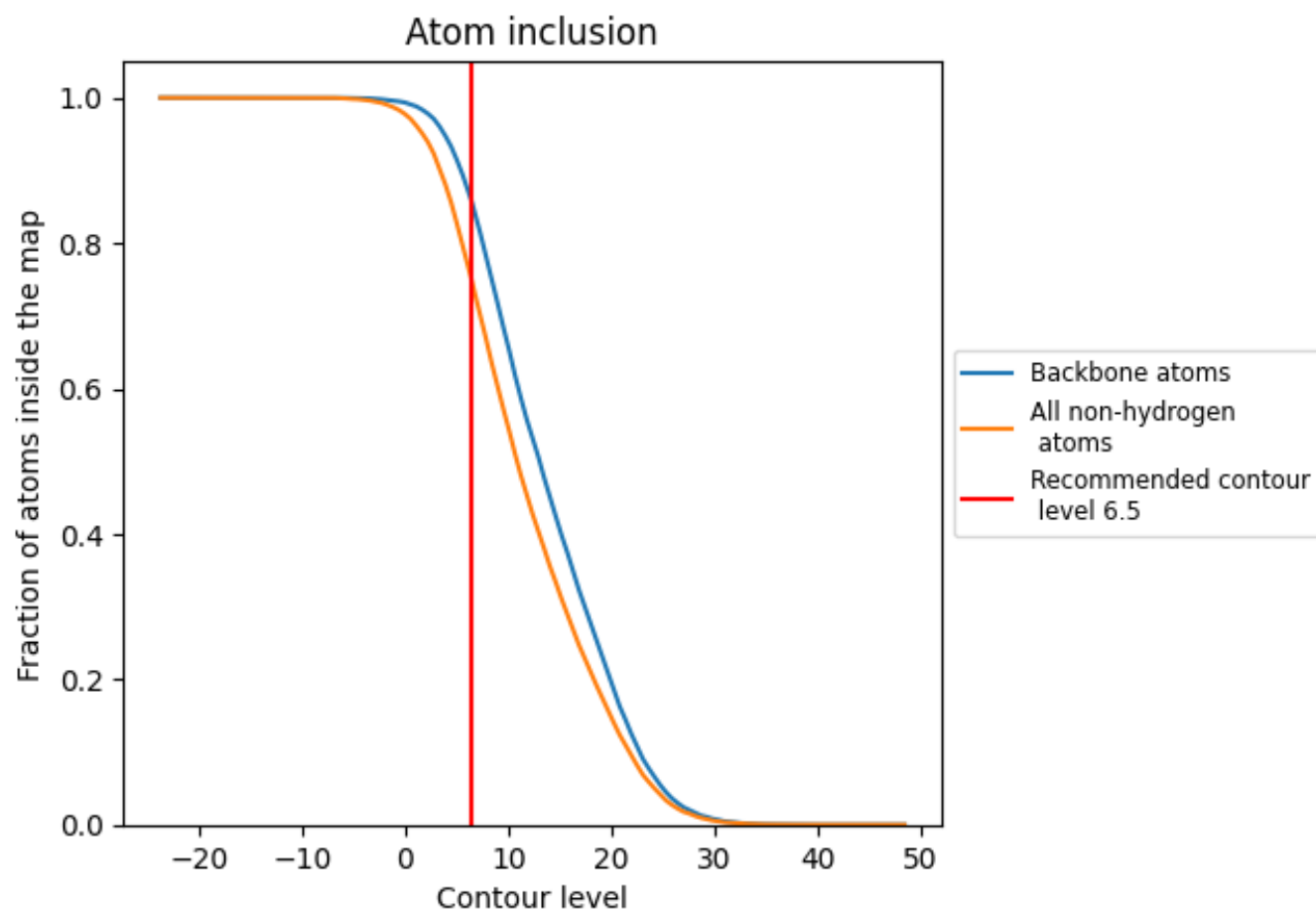
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 75% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7471	<div></div> 0.3840
A	<div></div> 0.7330	<div></div> 0.3640
B	<div></div> 0.7737	<div></div> 0.4080
C	<div></div> 0.8350	<div></div> 0.4640

