



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:13 AM UTC

PDB ID : 9I1J / pdb_00009i1j
EMDB ID : EMD-52571
Title : Cryo-EM structure of mouse RNF213:UBE2L3 transthiolation intermediate, chemically stabilized, and ATPgS
Authors : Grabarczyk, D.B.; Ahel, J.; Clausen, T.
Deposited on : 2025-01-16
Resolution : 3.80 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

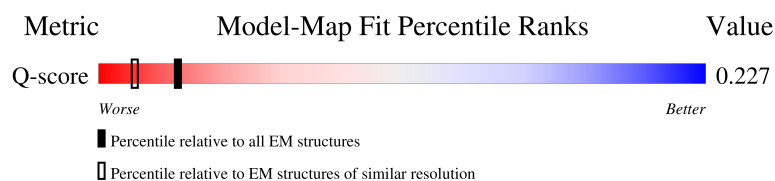
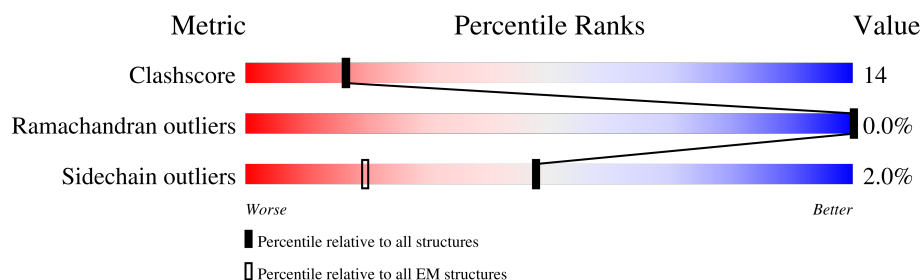
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	4836	
2	B	166	

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
6	ADP	A	5205	-	-	X	-
6	ADP	A	5206	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36793 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 E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4423	Total	C	N	O	S	0	0
			35465	22611	6087	6556	211		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	MET	-	initiating methionine	UNP E9Q555
A	327	ALA	-	expression tag	UNP E9Q555
A	328	SER	-	expression tag	UNP E9Q555
A	329	TRP	-	expression tag	UNP E9Q555
A	330	SER	-	expression tag	UNP E9Q555
A	331	HIS	-	expression tag	UNP E9Q555
A	332	PRO	-	expression tag	UNP E9Q555
A	333	GLN	-	expression tag	UNP E9Q555
A	334	PHE	-	expression tag	UNP E9Q555
A	335	GLU	-	expression tag	UNP E9Q555
A	336	LYS	-	expression tag	UNP E9Q555
A	337	GLY	-	expression tag	UNP E9Q555
A	338	SER	-	expression tag	UNP E9Q555
A	?	-	VAL	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	?	-	ASN	deletion	UNP E9Q555
A	?	-	ARG	deletion	UNP E9Q555
A	5149	GLY	-	expression tag	UNP E9Q555
A	5150	GLY	-	expression tag	UNP E9Q555
A	5151	GLY	-	expression tag	UNP E9Q555
A	5152	HIS	-	expression tag	UNP E9Q555
A	5153	HIS	-	expression tag	UNP E9Q555
A	5154	HIS	-	expression tag	UNP E9Q555
A	5155	HIS	-	expression tag	UNP E9Q555
A	5156	HIS	-	expression tag	UNP E9Q555
A	5157	HIS	-	expression tag	UNP E9Q555
A	5158	HIS	-	expression tag	UNP E9Q555
A	5159	HIS	-	expression tag	UNP E9Q555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

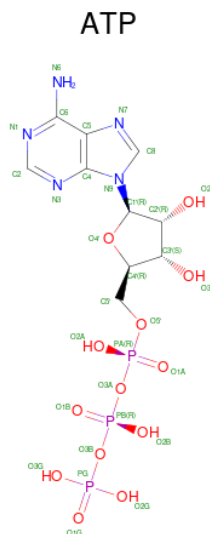
- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	153	Total	C	N	O	S	0	0
			1240	792	214	230	4		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLY	-	expression tag	UNP P68036
B	-10	TRP	-	expression tag	UNP P68036
B	-9	SER	-	expression tag	UNP P68036
B	-8	HIS	-	expression tag	UNP P68036
B	-7	PRO	-	expression tag	UNP P68036
B	-6	GLN	-	expression tag	UNP P68036
B	-5	PHE	-	expression tag	UNP P68036
B	-4	GLU	-	expression tag	UNP P68036
B	-3	LYS	-	expression tag	UNP P68036
B	-2	PRO	-	expression tag	UNP P68036
B	-1	GLY	-	expression tag	UNP P68036
B	0	SER	-	expression tag	UNP P68036
B	17	SER	CYS	conflict	UNP P68036
B	137	SER	CYS	conflict	UNP P68036

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
5	A	2	Total Zn 2 2	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

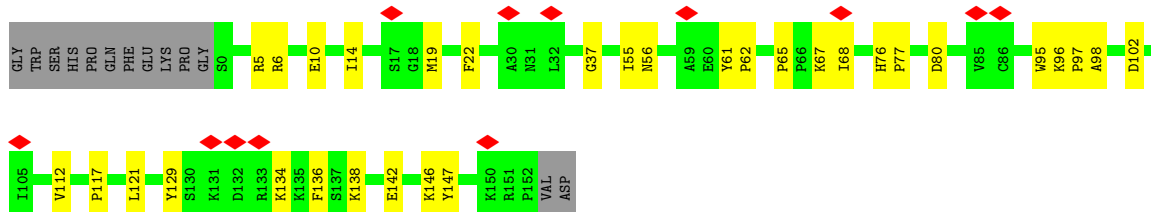
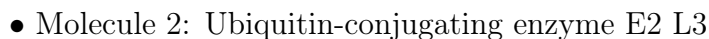


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

HIS	G2027	G1945	R1841	A1753	K1856	V1576	H1489	A1385	Q1314	LEU	V1148	G1081
THR	I2028	L1946	R1842	F1754	R1857	M1580	G1490	R1386	A1315	ASP	Q1149	Q1082
ASP	P2029	C1947	C1943	L1755	L1663	M1582	S1491	T1388	Q1387	LYS	V1150	L1083
	L2032	G1949	L1844	D1760	M1664	Q1581	V1492	E1389	V1316	ASP	D1151	E1084
	F2033	L1855	S1855	L1761	F1665	R1582	E1493	L1390	S1317	PRO	F1152	L1085
		L1856	L1856	L1762	T1667	L1583	L1494	V1391		ARG		
		L1857	L1857	L1763	Q1670	I1588	S1495	A1397	K1320	E1229	H1159	
		L1858	L1858	L1764	L1671	L1590	L1497	L1398	V1321	V1232	S1160	E1088
		L1859	L1859	L1765	Q1675	L1591	L1498	L1404	Q1324	S1233	Q1161	H1089
		L1860	L1860	L1766	T1675	L1592	L1499	L1404	V1325	P1235	L1163	F1093
		L1861	L1861	L1767	S1675	M1595	L1499	G1416	R1326	E1236	S1164	L1094
		L1862	L1862	L1768	L1678	M1596	L1499	E1417	R1327	V1237	N1185	
		L1863	L1863	L1769	L1678	M1597	L1499	L1420	A1328	L1241	E1170	W1097
		L1864	L1864	L1770	L1678	M1598	L1499	I1420	L1329	L1241	N1098	N1098
		L1865	L1865	L1771	L1678	F1598	L1499	D1423	G1330	N1248	L1099	N1099
		L1866	L1866	L1772	L1678	F1599	L1499	F1428	V1331	F1249	A1171	N1100
		L1867	L1867	L1773	L1678	T1600	L1499	V1432	T1332	L1262	L1175	R1101
		L1868	L1868	L1774	L1678	L1600	L1499	Y1435	S1336	K1260	ASN	R1102
		L1869	L1869	L1775	L1678	L1600	L1499	L1439	V1337	I1261	ASN	R1103
		L1870	L1870	L1776	L1678	L1600	L1499	M1442	L1338	LEU	PRO	LEU
		L1871	L1871	L1777	L1678	L1600	L1499	R1445	M1339	PRO	PRO	PRO
		L1872	L1872	L1778	L1678	L1600	L1499	L1445	E1265	SER	ASN	GLN
		L1873	L1873	L1779	L1678	L1600	L1499	L1445	V1266	SER	GLU	GLU
		L1874	L1874	L1780	L1678	L1600	L1499	L1445	D1267	LYS	LYS	LYS
		L1875	L1875	L1781	L1678	L1600	L1499	L1445	E1267	ALA	ALA	ALA
		L1876	L1876	L1782	L1678	L1600	L1499	L1445	I1269	CYS	D1112	D1112
		L1877	L1877	L1783	L1678	L1600	L1499	L1445	F1270		L1117	L1117
		L1878	L1878	L1784	L1678	L1600	L1499	L1445	V1273		K1118	K1118
		L1879	L1879	L1785	L1678	L1600	L1499	L1445	E1274		R1119	R1119
		L1880	L1880	L1786	L1678	L1600	L1499	L1445	I1193		L1120	L1120
		L1881	L1881	L1787	L1678	L1600	L1499	L1445	D1275		D1123	D1123
		L1882	L1882	L1788	L1678	L1600	L1499	L1445	K1276		L1124	L1124
		L1883	L1883	L1789	L1678	L1600	L1499	L1445	M1196		L1125	L1125
		L1884	L1884	L1790	L1678	L1600	L1499	L1445	F1126		F1126	F1126
		L1885	L1885	L1791	L1678	L1600	L1499	L1445	L1127		L1127	L1127
		L1886	L1886	L1792	L1678	L1600	L1499	L1445	K1128		K1128	K1128
		L1887	L1887	L1793	L1678	L1600	L1499	L1445	Q1129		Q1129	Q1129
		L1888	L1888	L1794	L1678	L1600	L1499	L1445	E1130		E1130	E1130
		L1889	L1889	L1795	L1678	L1600	L1499	L1445	K1131		K1131	K1131
		L1890	L1890	L1796	L1678	L1600	L1499	L1445	S1202		S1202	S1202
		L1891	L1891	L1797	L1678	L1600	L1499	L1445	L1284		L1284	L1284
		L1892	L1892	L1798	L1678	L1600	L1499	L1445	K1204		K1204	K1204
		L1893	L1893	L1799	L1678	L1600	L1499	L1445	D1205		D1205	D1205
		L1894	L1894	L1800	L1678	L1600	L1499	L1445	S1206		S1206	S1206
		L1895	L1895	L1801	L1678	L1600	L1499	L1445	H1207		H1207	H1207
		L1896	L1896	L1802	L1678	L1600	L1499	L1445	I1208		I1208	I1208
		L1897	L1897	L1803	L1678	L1600	L1499	L1445	Q1209		Q1209	Q1209
		L1898	L1898	L1804	L1678	L1600	L1499	L1445	R1139		R1139	R1139
		L1899	L1899	L1805	L1678	L1600	L1499	L1445	D1211		D1211	D1211
		L1900	L1900	L1806	L1678	L1600	L1499	L1445	F1212		F1212	F1212
		L1901	L1901	L1807	L1678	L1600	L1499	L1445	E1215		E1215	E1215
		L1902	L1902	L1808	L1678	L1600	L1499	L1445	E1218		E1218	E1218
		L1903	L1903	L1809	L1678	L1600	L1499	L1445	W1221		W1221	W1221
		L1904	L1904	L1810	L1678	L1600	L1499	L1445	THR		THR	THR
		L1905	L1905	L1811	L1678	L1600	L1499	L1445				
		L1906	L1906	L1812	L1678	L1600	L1499	L1445				
		L1907	L1907	L1813	L1678	L1600	L1499	L1445				
		L1908	L1908	L1814	L1678	L1600	L1499	L1445				
		L1909	L1909	L1815	L1678	L1600	L1499	L1445				
		L1910	L1910	L1816	L1678	L1600	L1499	L1445				
		L1911	L1911	L1817	L1678	L1600	L1499	L1445				
		L1912	L1912	L1818	L1678	L1600	L1499	L1445				
		L1913	L1913	L1819	L1678	L1600	L1499	L1445				
		L1914	L1914	L1820	L1678	L1600	L1499	L1445				
		L1915	L1915	L1821	L1678	L1600	L1499	L1445				
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		L1919	L1919	L1825	L1678	L1600	L1499	L1445				
		L1920	L1920	L1826	L1678	L1600	L1499	L1445				
		L1921	L1921	L1827	L1678	L1600	L1499	L1445				
		L1922	L1922	L1828	L1678	L1600	L1499	L1445				
		L1923	L1923	L1829	L1678	L1600	L1499	L1445				
		L1924	L1924	L1830	L1678	L1600	L1499	L1445				
		L1925	L1925	L1831	L1678	L1600	L1499	L1445				
		L1926	L1926	L1832	L1678	L1600	L1499	L1445				
		L1927	L1927	L1833	L1678	L1600	L1499	L1445				
		L1928	L1928	L1834	L1678	L1600	L1499	L1445				
		L1929	L1929	L1835	L1678	L1600	L1499	L1445				
		L1930	L1930	L1836	L1678	L1600	L1499	L1445				
		L1931	L1931	L1837	L1678	L1600	L1499	L1445				
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		L1933	L1933	L1839	L1678	L1600	L1499	L1445				
		L1934	L1934	L1840	L1678	L1600	L1499	L1445				
		L1935	L1935	L1841	L1678	L1600	L1499	L1445				
		L1936	L1936	L1842	L1678	L1600	L1499	L1445				
		L1937	L1937	L1843	L1678	L1600	L1499	L1445				
		L1938	L1938	L1844	L1678	L1600	L1499	L1445				
		L1939	L1939	L1845	L1678	L1600	L1499	L1445				
		L1940	L1940	L1846	L1678	L1600	L1499	L1445				
		L1941	L1941	L1847	L1678	L1600	L1499	L1445				
		L1942	L1942	L1848	L1678	L1600	L1499	L1445				
		L1943	L1943	L1849	L1678	L1600	L1499	L1445				
		L1944	L1944	L1850	L1678	L1600	L1499	L1445				
		L1945	L1945	L1851	L1678	L1600	L1499	L1445				
		L1946	L1946	L1852	L1678	L1600	L1499	L1445				
		L1947	L1947	L1853	L1678	L1600	L1499	L1445				
		L1948	L1948	L1854	L1678	L1600	L1499	L1445				
		L1949	L1949	L1855	L1678	L1600	L1499	L1445				
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		L1951	L1951	L1857	L1678	L1600	L1499	L1445				
		L1952	L1952	L1858	L1678	L1600	L1499	L1445				
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		L1954	L1954	L1860	L1678	L1600	L1499	L1445				
		L1955	L1955	L1861	L1678	L1600	L1499	L1445				
		L1956	L1956	L1862	L1678	L1600	L1499	L1445				
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		L1958	L1958	L1864	L1678	L1600	L1499	L1445				
		L1959	L1959	L1865	L1678	L1600	L1499	L1445				
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		L1961	L1961	L1867	L1678	L1600	L1499	L1445				
		L1962	L1962	L1868	L1678	L1600	L1499	L1445				
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		L1964	L1964	L1870	L1678	L1600	L1499	L1445				
		L1965	L1965	L1871	L1678	L1600	L1499	L1445				
		L1966	L1966	L1872	L1678	L1600	L1499	L1445				
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		L1968	L1968	L1874	L1678	L1600	L1499	L1445				
		L1969	L1969	L1875	L1678	L1600	L1499	L1445				
		L1970	L1970	L1876	L1678	L1600	L1499	L1445				
		L1971	L1971	L1877	L1678	L1600	L1499	L1445				
		L1972	L1972	L1878	L1678	L1600	L1499	L1445				

Q3260	A3261	H3262	L3263	R3264	K3265	T3266	H3267	H3268	E3269	C3185	C3270	S3187	A3186	V3188	V3189	L3190	C3191	S3192	V3193	E3194	R3195	L3196	D3288	V3291	S3294	R3297	G3298	K3302	V3305	L3306	V3311	D3312	T3313	E3314	F3317	L3318	V3321	K3332	V3335	L3349	K3354	A3357	I3358	I3361	T3367							
D3163	Q3164	F3165	V3176	F3177	I3178	G3179	Q3085	K3086	V3087	V3088	D3089	L3090	G3091	L3092	H3095	R3096	V3097	K3098	H3102	L3107	E3112	V3115	V3116	F3120	P3121	V3122	P3123	L3124	I3125	K3130	H3131	V3132	L3133	D3134	M3135	V3138	W3142	Q3143	K3144	S3145	I3146	V3147	L3150	F3157	A3158	D3159	V3160	K3161	A3162			
Q2981	N2982	I2983	C2984	P2985	G2986	P2987	Q2988	A2989	S2990	S2991	R2992	G2993	L2994	D2995	G2996	A2997	Y3001	L3002	L3003	V3004	L3005	K2922	M2923	V2924	F2925	A3011	L3012	Q3013	L3014	L3015	Q3016	Q3017	L3018	F3019	F3020	Q3023	G3030	S3031	P3034	Q3035	I3046	V3049	M3053	M3058	L3061	L3062						
I2872	E2876	C2877	L2878	C2879	L2884	V2885	Q2886	D2887	K2888	L2889	R2890	Y2900	L2914	R2915	D2916	Y2917	Y2918	S2919	L2920	I2921	K2922	M2923	V2924	F2925	K2932	L2935	I2940	T2941	L2945	R2946	N2947	F2948	S2949	L2957	F2960	T2961	A2967	R2968	Y2969	K2970	E2971	E2972	V2973	V2976	E2977	L2978						
C2786	Q2791	S2800	V2801	V2802	V2803	L2804	V2807	G2808	L2809	A2810	S2813	P2814	K2815	L2816	P2817	L2818	K2819	T2820	L2821	H2822	P2823	L2824	L2825	L2830	E2831	Y2837	K2838	L2839	V2840	G2841	F2842	S2846	H2847	N2848	A2849	L2850	A2853	K2854	N2855	R2857	G2858	L2859	V2860	V2861	P2866	L2867	K2868					
L2709	K2710	V2713	M2716	I2720	E2721	I2724	F2725	L2726	F2727	L2728	V2729	G2730	K2731	P2732	Q2733	K2736	S2737	L2738	L2739	K2740	V2743	A2744	D2745	A2746	M2747	Q2748	Q2749	Q2750	A2751	A2752	F2753	F2757	R2758	C2759	L2760	K2763	Q2762	V2763	H2764	L2765	V2766	C2770	T2775	P2776	L2780	S2781	T2782	F2783				
H2613	D2614	L2615	S2616	L2619	L2620	K2621	K2625	F2626	L2627	H2635	V2642	L2643	K2644	S2645	L2646	V2647	M2648	L2650	G2651	V2652	C2653	Y2654	H2655	E2659	E2660	K2661	Y2664	R2665	L2668	F2672	P2673	K2674	P2675	V2676	S2679	E2685	V2686	V2689	Q2690	L2694	P2698	I2703	A2704									
L2537	P2538	L2539	L2540	Q2541	D2542	F2543	G2544	Q2545	L2546	N2547	K2552	L2553	Y2554	Q2556	Q2557	L2558	V2559	Q2560	D2564	S2565	S2567	V2568	N2569	T2573	C2574	V2575	L2576	D2578	V2579	L2580	S2581	F2586	R2590	E2591	N2592	E2593	F2596	V2597	S2598	L2599	R2600	D2601	V2602	E2603	R2604	C2605	V2606	W2611	F2612			
G2343	I2344	P2350	E2355	L2356	T2357	L2362	K2363	L2364	L2365	E2368	M2369	R2370	F2371	P2376	V2377	I2378	M2380	G2381	E2382	T2383	G2384	C2385	K2386	K2387	T2388	R2389	L2390	I2391	K2392	L2397	M2407	H2413	G2414	G2415	P2418	I2421	Y2422	V2425	K2426	R2430	T2431	A2432	Q2438	D2442								
H2264	P2265	Y2266	F2267	F2268	F2269	N2270	H2273	M2274	T2275	M2276	T2277	F2278	I2279	K2280	F2281	Y2290	A2293	K2300	V2301	I2302	K2303	K2304	K2305	K2306	M2307	T2308	K2309	E2310	L2311	F2312	D2313	G2314	L2315	R2316	Q2317	Q2318	R2319	V2320	P2321	F2322	N2328	L2329	P2330	R2331	Y2332	L2333	K2334	L2335	L2338	C2339	A2340	L2342
S2193	I2194	K2197	S2198	A2199	F2200	T2201	Q2202	D2203	T2204	L2205	F2208	V2212	V2213	T2214	F2215	M2216	L2218	M2219	F2223	A2224	T2225	T2226	T2227	LEU	HIS	THR	SER	ASP	GLN	SER	PRO	GLY	ARG	GLN	SER	VAL	THR	ILE	GLY	GLU	VAL	E2247	E2248	L2249	L2250	A2251	L2255	R2256	K2257	E2260		





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31607	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0047	Depositor
Map size (Å)	379.96, 379.96, 379.96	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18, 1.18, 1.18	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: ATP, MG, ZN, ADP

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	0.15	0/36204	0.41	4/48982 (0.0%)
2	B	0.16	0/1271	0.40	0/1719
All	All	0.15	0/37475	0.41	4/50701 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4604	VAL	N-CA-C	-5.66	106.97	112.29
1	A	748	GLU	CA-C-N	-5.57	113.41	122.65
1	A	748	GLU	C-N-CA	-5.57	113.41	122.65
1	A	3711	GLN	CA-CB-CG	5.27	124.64	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4165	GLU	Peptide
1	A	641	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35465	0	35592	1019	0
2	B	1240	0	1240	25	0
3	A	31	0	12	6	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	54	0	24	28	0
All	All	36793	0	36868	1037	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 1037 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:2704:ALA:HB3	6:A:5206:ADP:N6	1.45	1.31
1:A:2704:ALA:CB	6:A:5206:ADP:HN61	1.65	1.09
1:A:2922:LYS:NZ	6:A:5206:ADP:H1'	1.85	0.92
1:A:717:MET:HE1	1:A:749:ASN:HD21	1.40	0.86
1:A:2757:PHE:HA	1:A:2760:LEU:HD12	1.57	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	4393/4836 (91%)	4059 (92%)	332 (8%)	2 (0%)	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	151/166 (91%)	150 (99%)	1 (1%)	0	100	100
All	All	4544/5002 (91%)	4209 (93%)	333 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3122	VAL
1	A	4166	PRO

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	3968/4342 (91%)	3887 (98%)	81 (2%)	48	65
2	B	135/148 (91%)	135 (100%)	0	100	100
All	All	4103/4490 (91%)	4022 (98%)	81 (2%)	48	65

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3579	THR
1	A	4752	ILE
1	A	3678	THR
1	A	4262	GLN
1	A	4965	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2981	GLN
1	A	3673	GLN
1	A	3016	GLN
1	A	3541	ASN
1	A	3777	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
3	ATP	A	5201	-	32,33,33	0.30	0	48,52,52	0.39	0
6	ADP	A	5205	-	28,29,29	1.45	4 (14%)	43,45,45	1.70	9 (20%)
6	ADP	A	5206	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)

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
3	ATP	A	5201	-	-	6/22/38/38	0/3/3/3
6	ADP	A	5205	-	-	7/16/32/32	0/3/3/3
6	ADP	A	5206	-	-	6/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	5205	ADP	C5-C4	4.89	1.47	1.39
6	A	5206	ADP	C5-C4	4.75	1.47	1.39
6	A	5206	ADP	C5-C6	2.74	1.48	1.41
6	A	5205	ADP	C5-C6	2.68	1.48	1.41
6	A	5206	ADP	C8-N7	2.38	1.36	1.31

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5206	ADP	C5-C4-N3	-5.88	118.63	126.72
6	A	5205	ADP	C5-C4-N3	-5.22	119.53	126.72
6	A	5206	ADP	N3-C4-N9	4.54	134.90	127.17
6	A	5205	ADP	N3-C4-N9	4.00	133.97	127.17
6	A	5206	ADP	C2-N3-C4	3.70	120.87	111.83

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5201	ATP	C5'-O5'-PA-O1A
3	A	5201	ATP	C5'-O5'-PA-O3A
3	A	5201	ATP	O4'-C4'-C5'-O5'
6	A	5205	ADP	C5'-O5'-PA-O1A
6	A	5205	ADP	C5'-O5'-PA-O2A

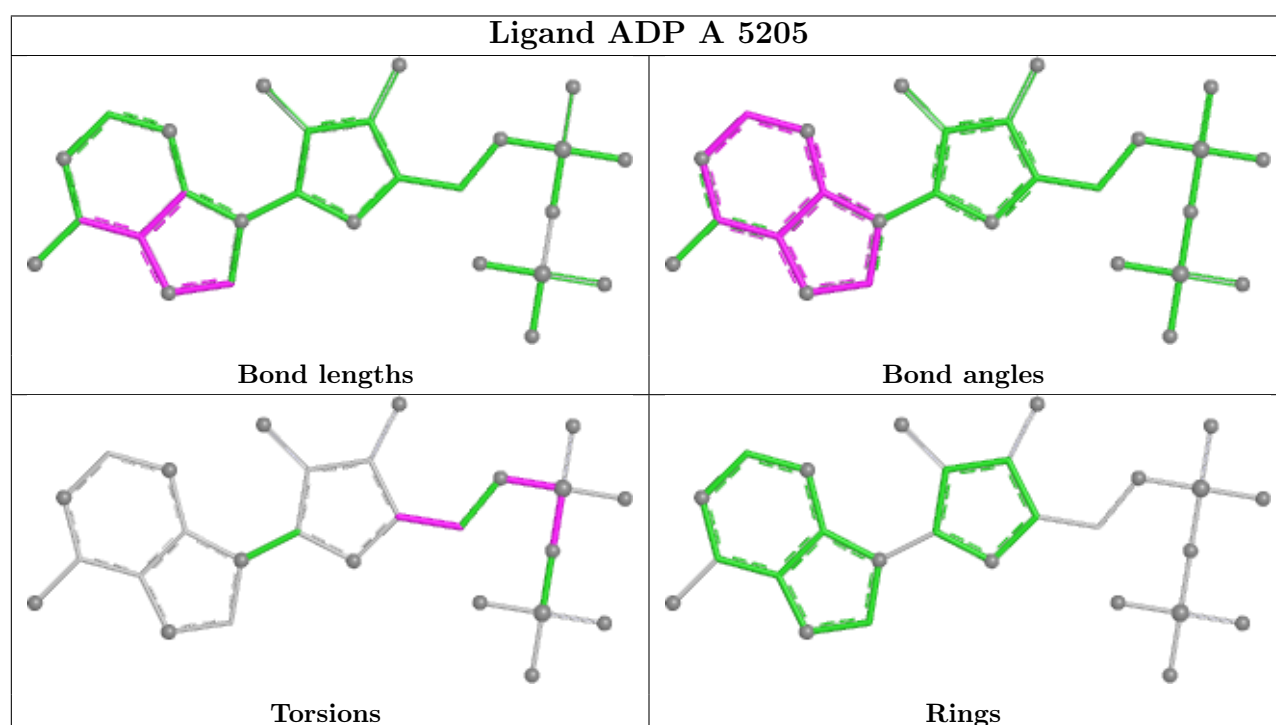
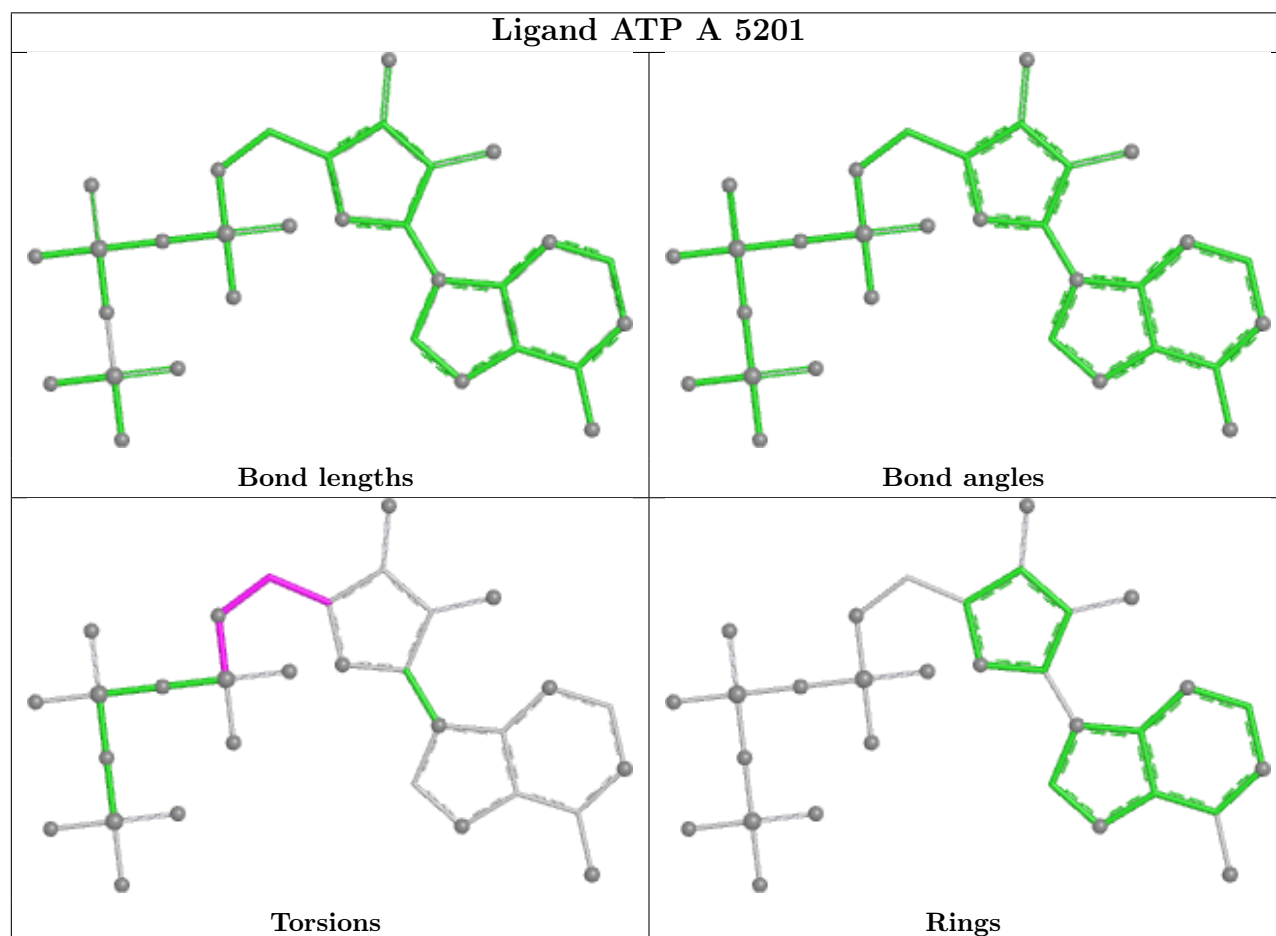
There are no ring outliers.

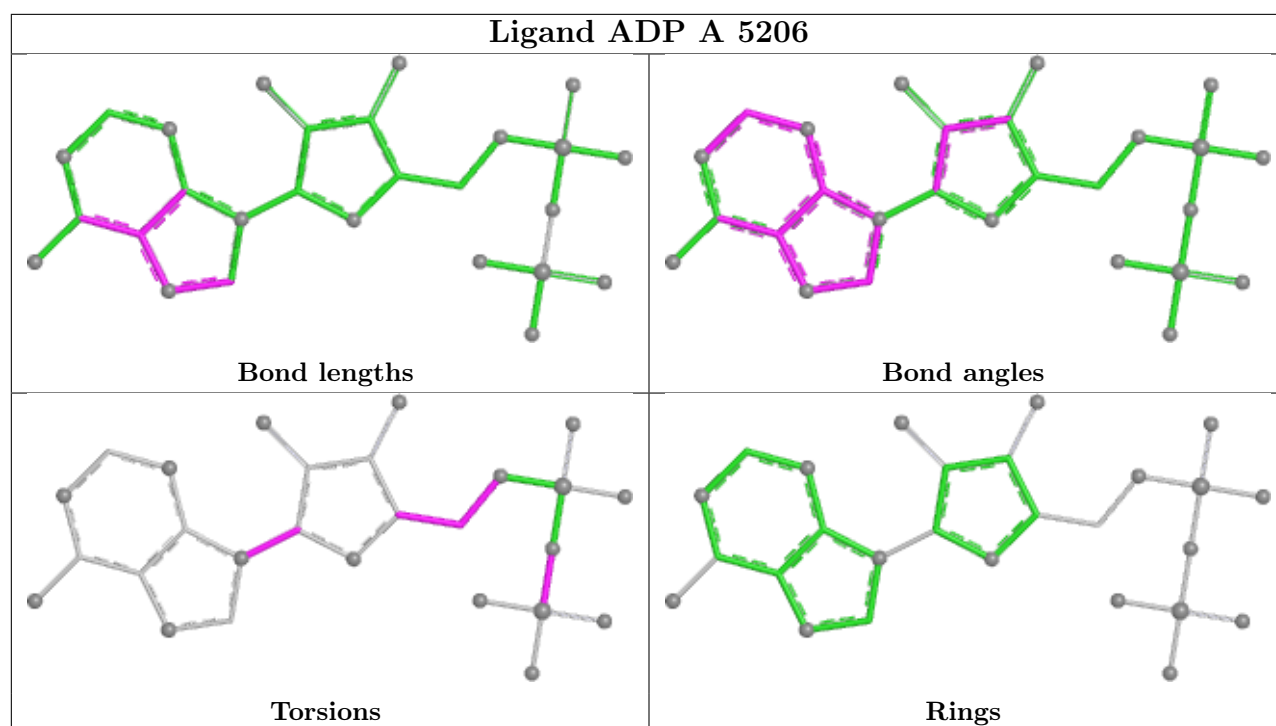
3 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5201	ATP	6	0
6	A	5205	ADP	19	0
6	A	5206	ADP	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.

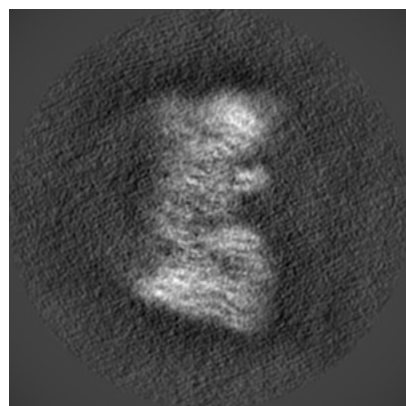
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52571. These allow visual inspection of the internal detail of the map and identification of artifacts.

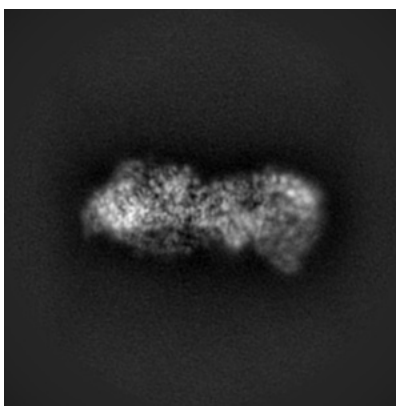
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

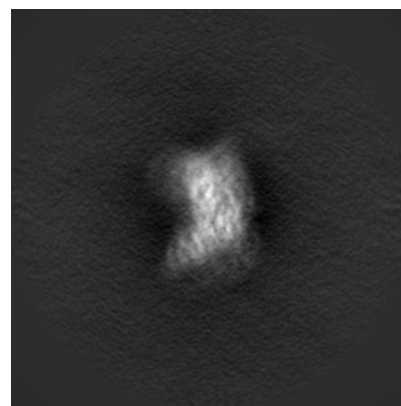
6.1.1 Primary map



X

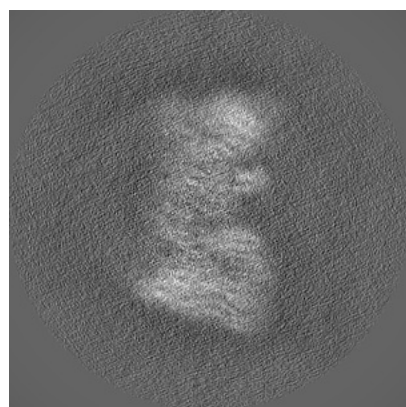


Y

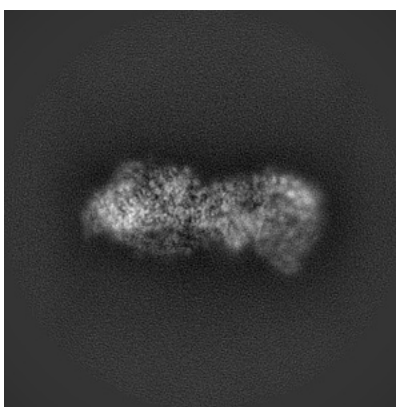


Z

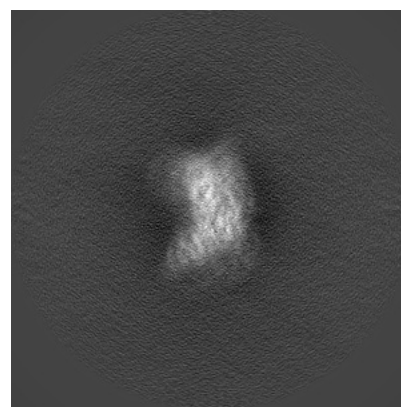
6.1.2 Raw map



X



Y

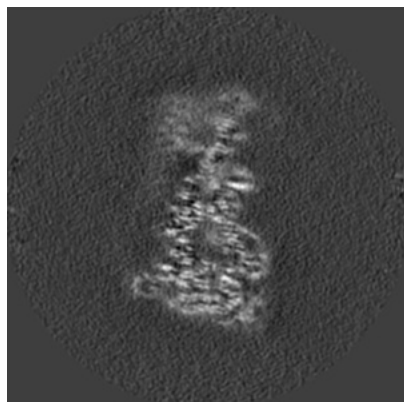


Z

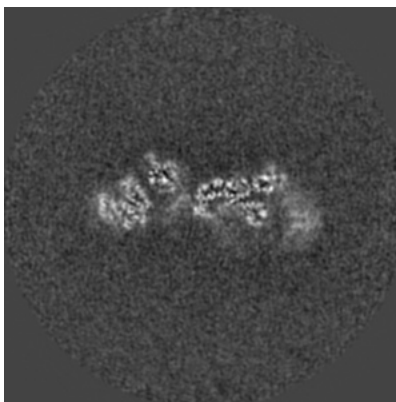
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

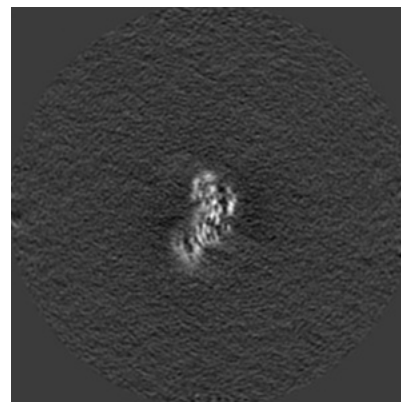
6.2.1 Primary map



X Index: 161

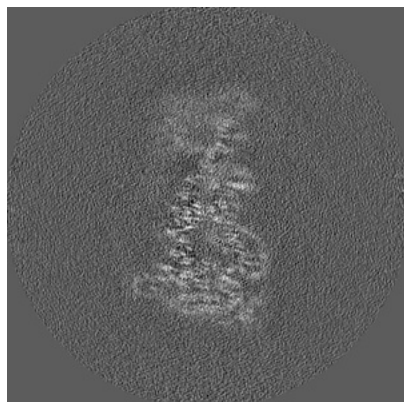


Y Index: 161

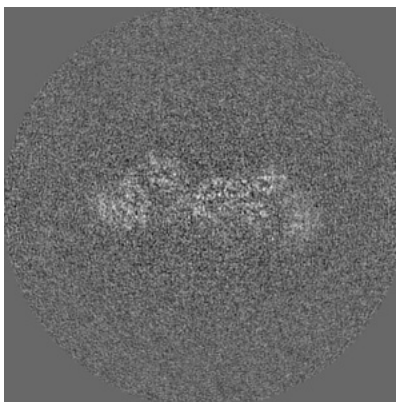


Z Index: 161

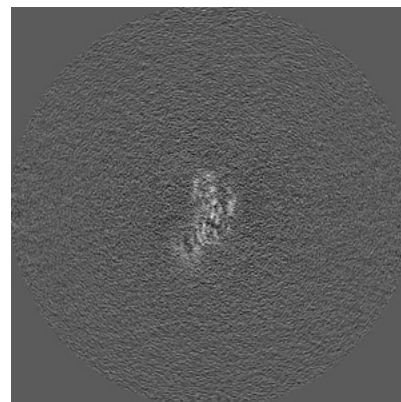
6.2.2 Raw map



X Index: 161



Y Index: 161

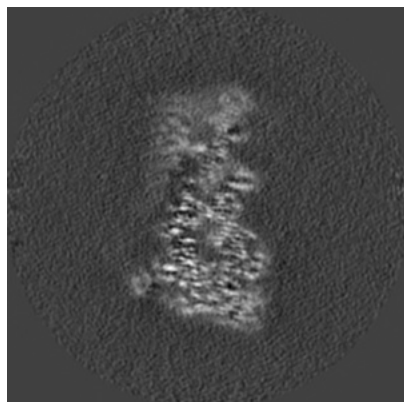


Z Index: 161

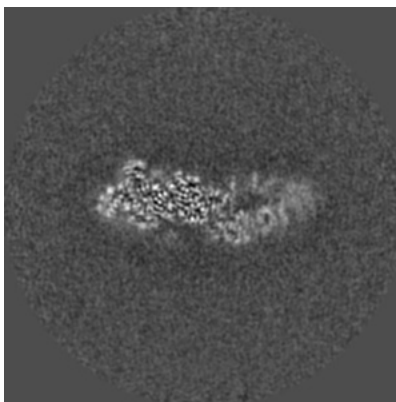
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

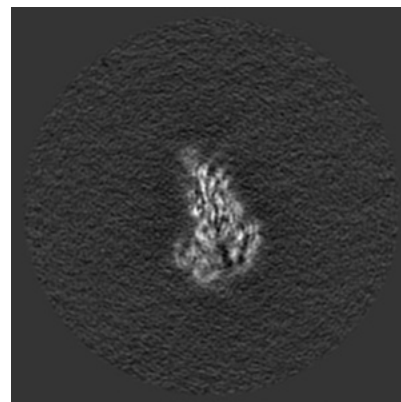
6.3.1 Primary map



X Index: 159

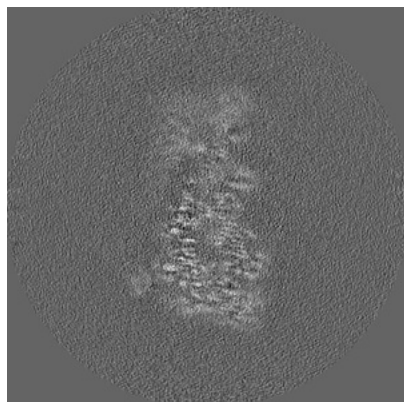


Y Index: 142

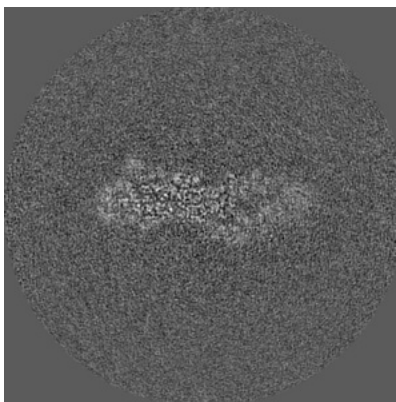


Z Index: 101

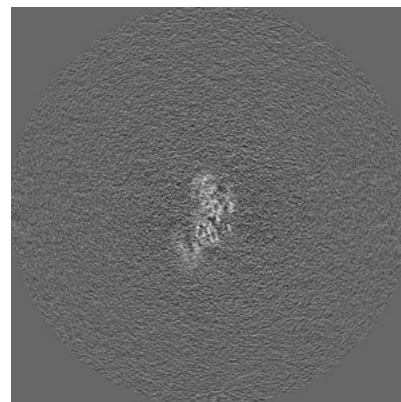
6.3.2 Raw map



X Index: 159



Y Index: 145

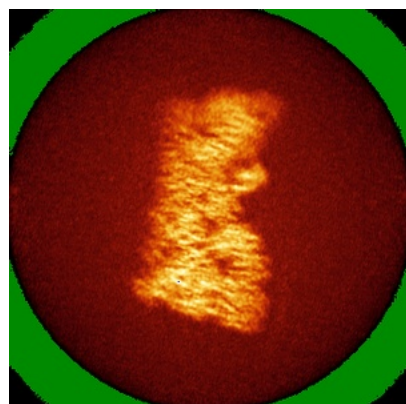


Z Index: 160

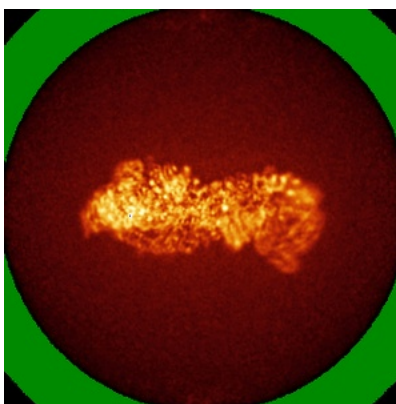
The images above show the largest variance slices of the map in three orthogonal directions.

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

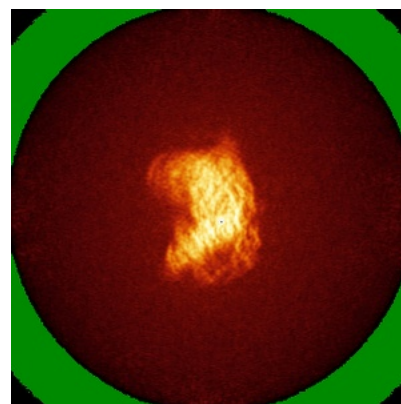
6.4.1 Primary map



X

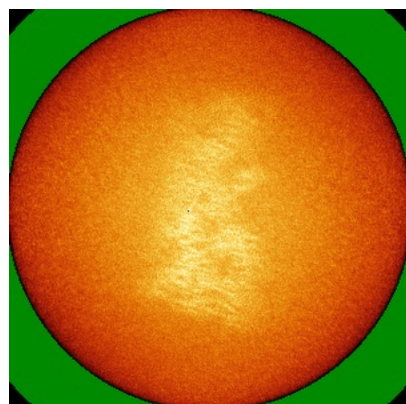


Y

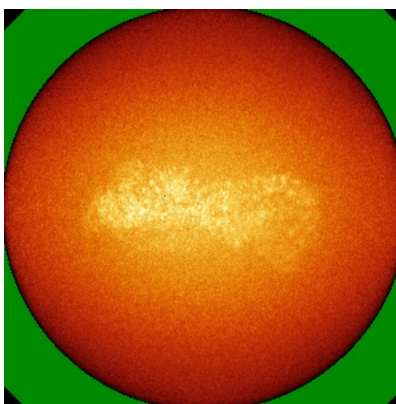


Z

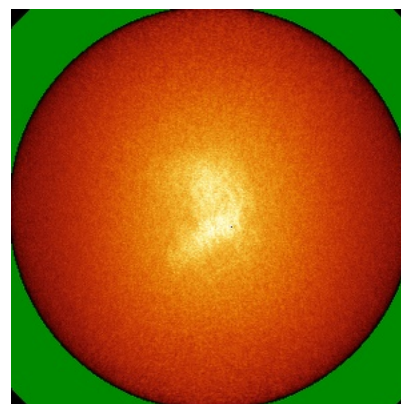
6.4.2 Raw map



X



Y

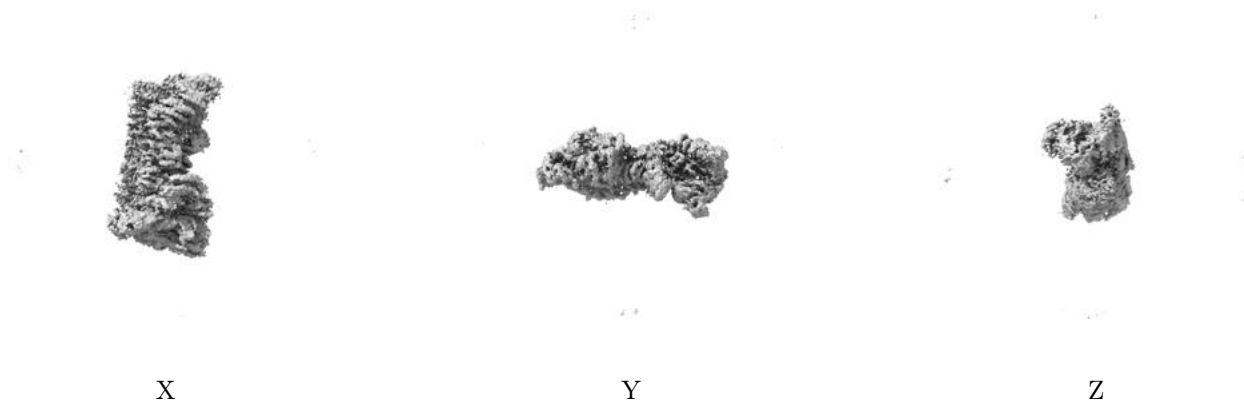


Z

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.

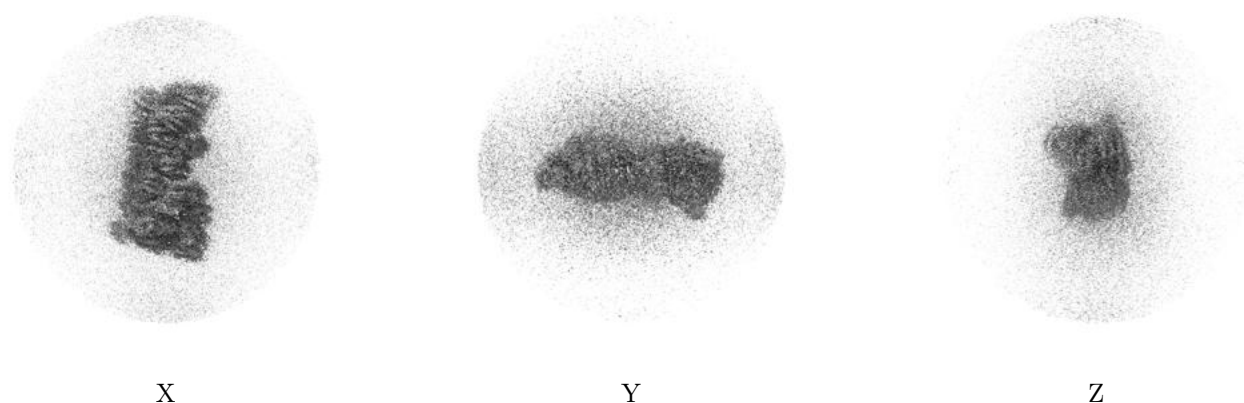
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0047. 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.

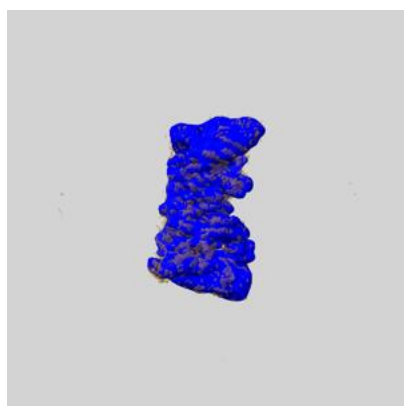
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

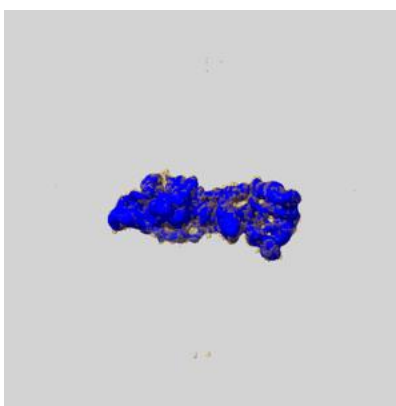
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

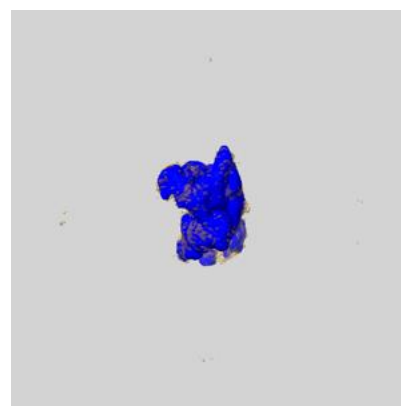
6.6.1 emd_52571_msk_1.map [i](#)



X



Y

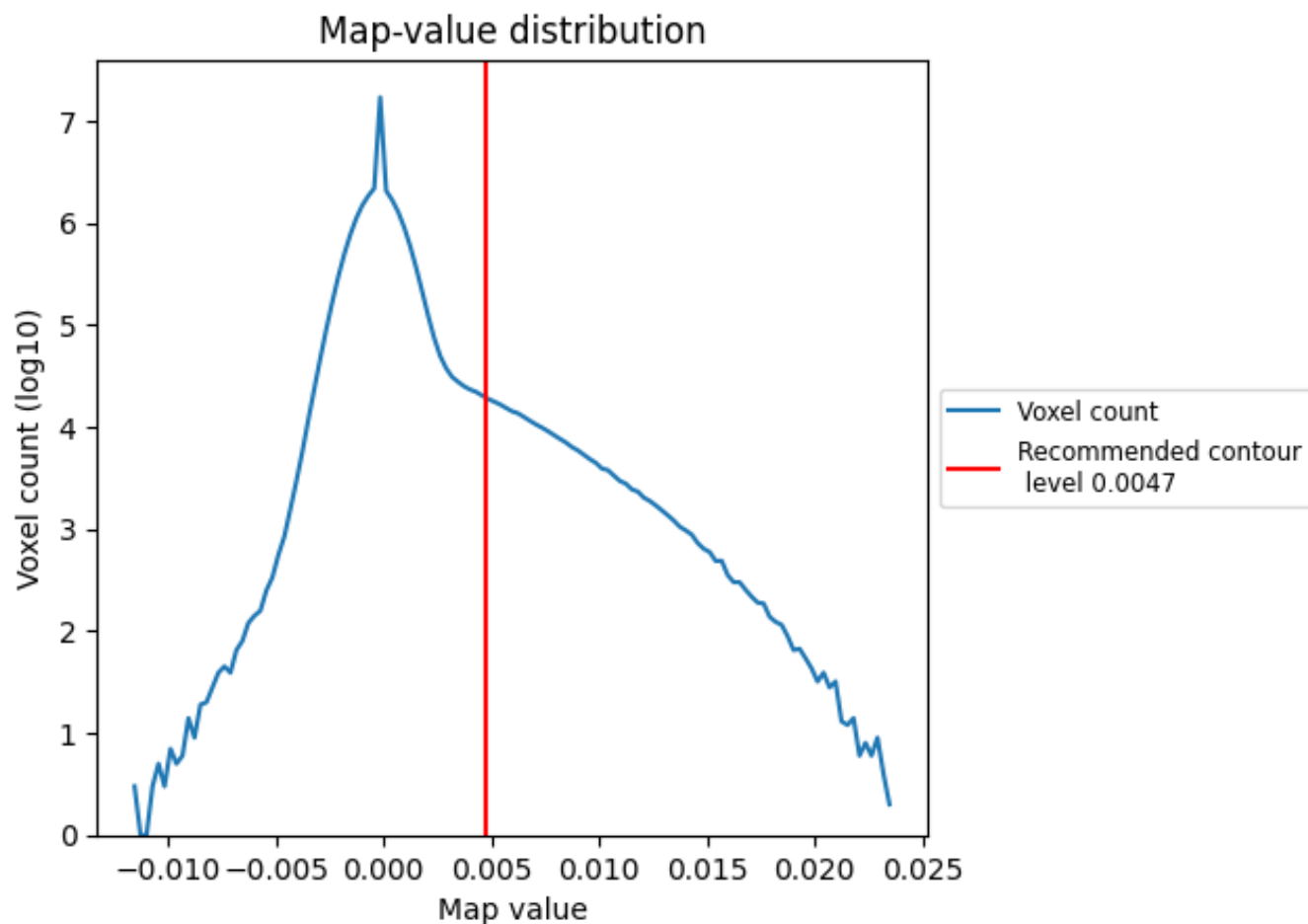


Z

7 Map analysis [i](#)

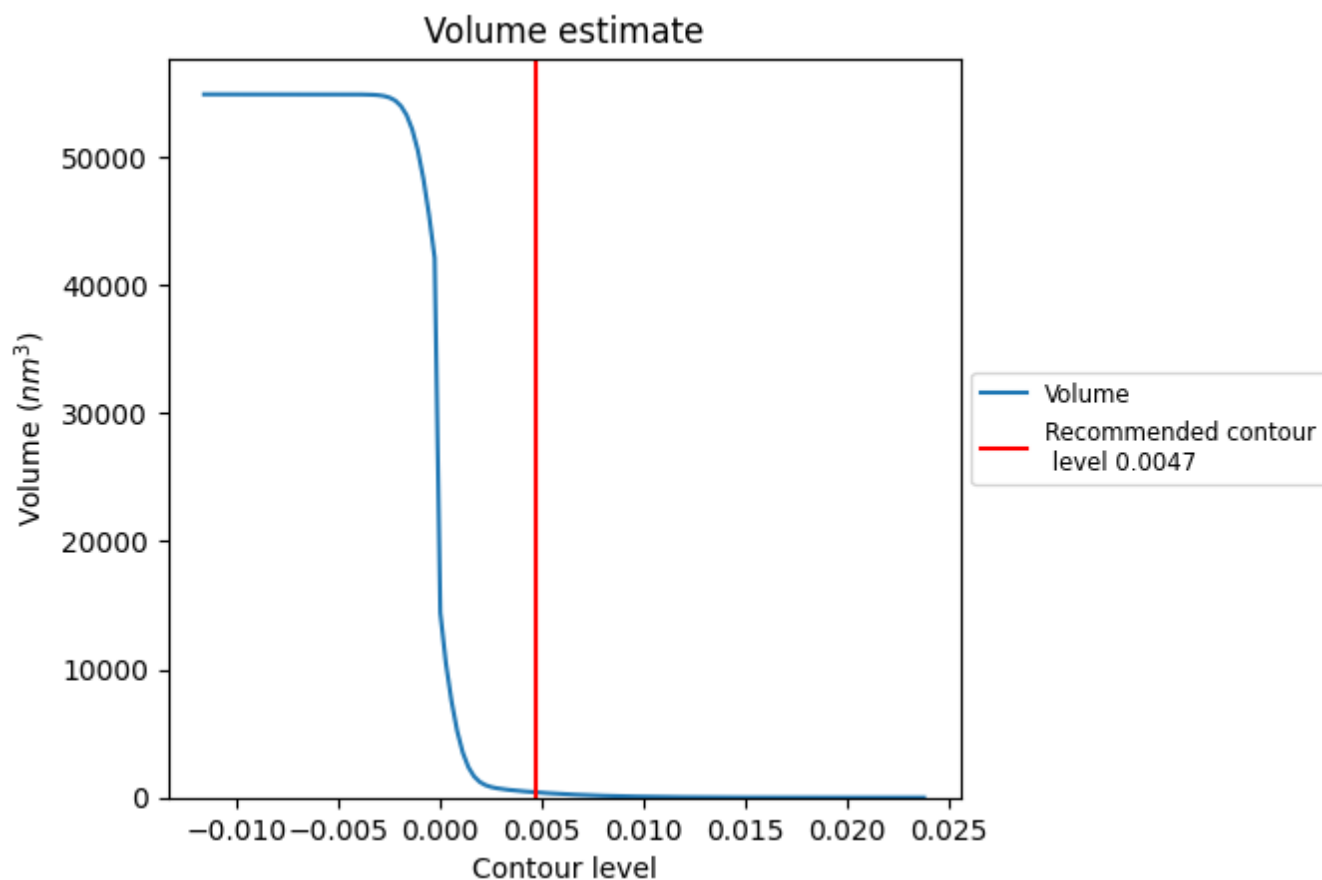
This section contains the results of statistical analysis of the map.

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.

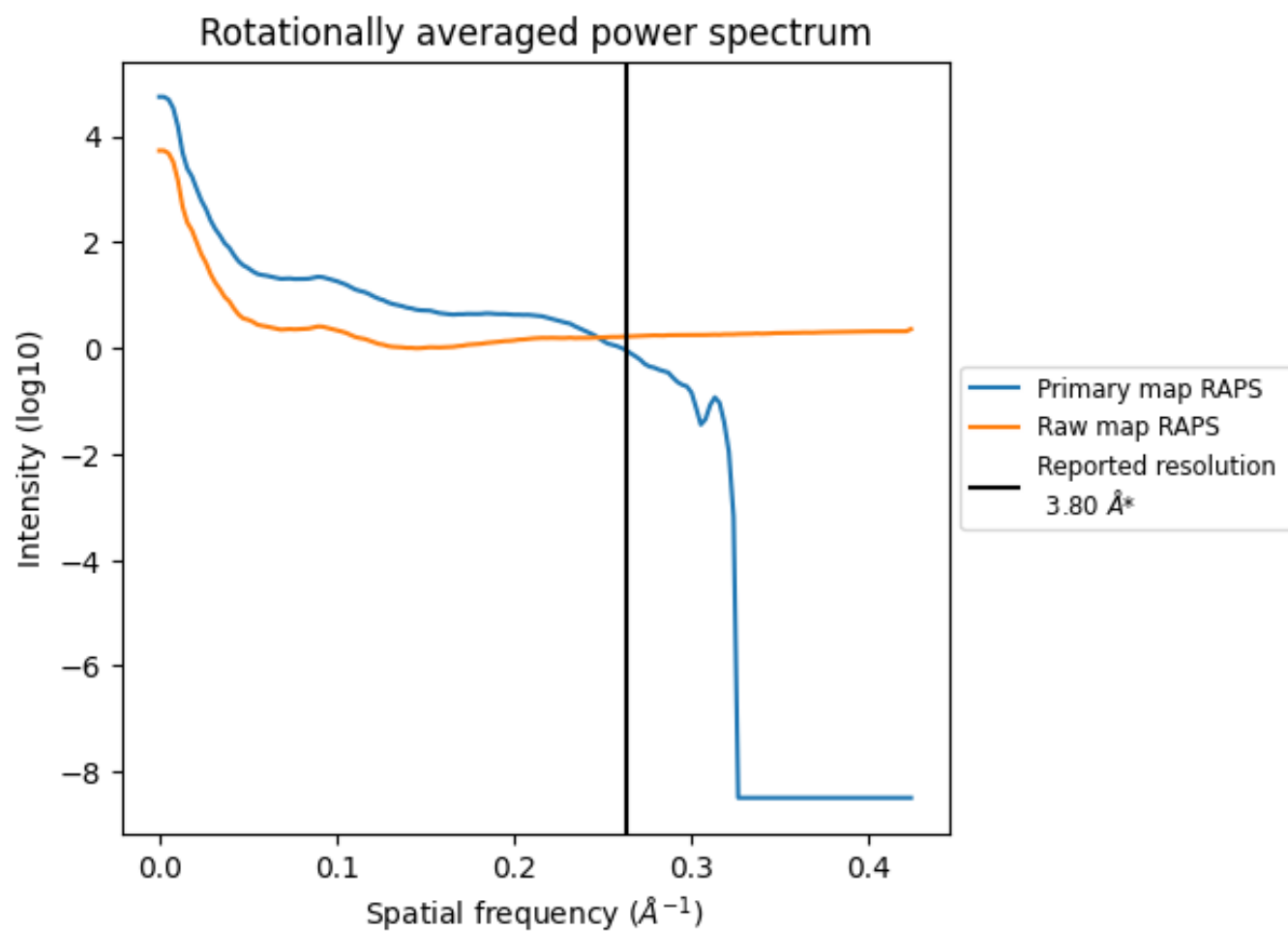
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 411 nm³; this corresponds to an approximate mass of 371 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 ⓘ

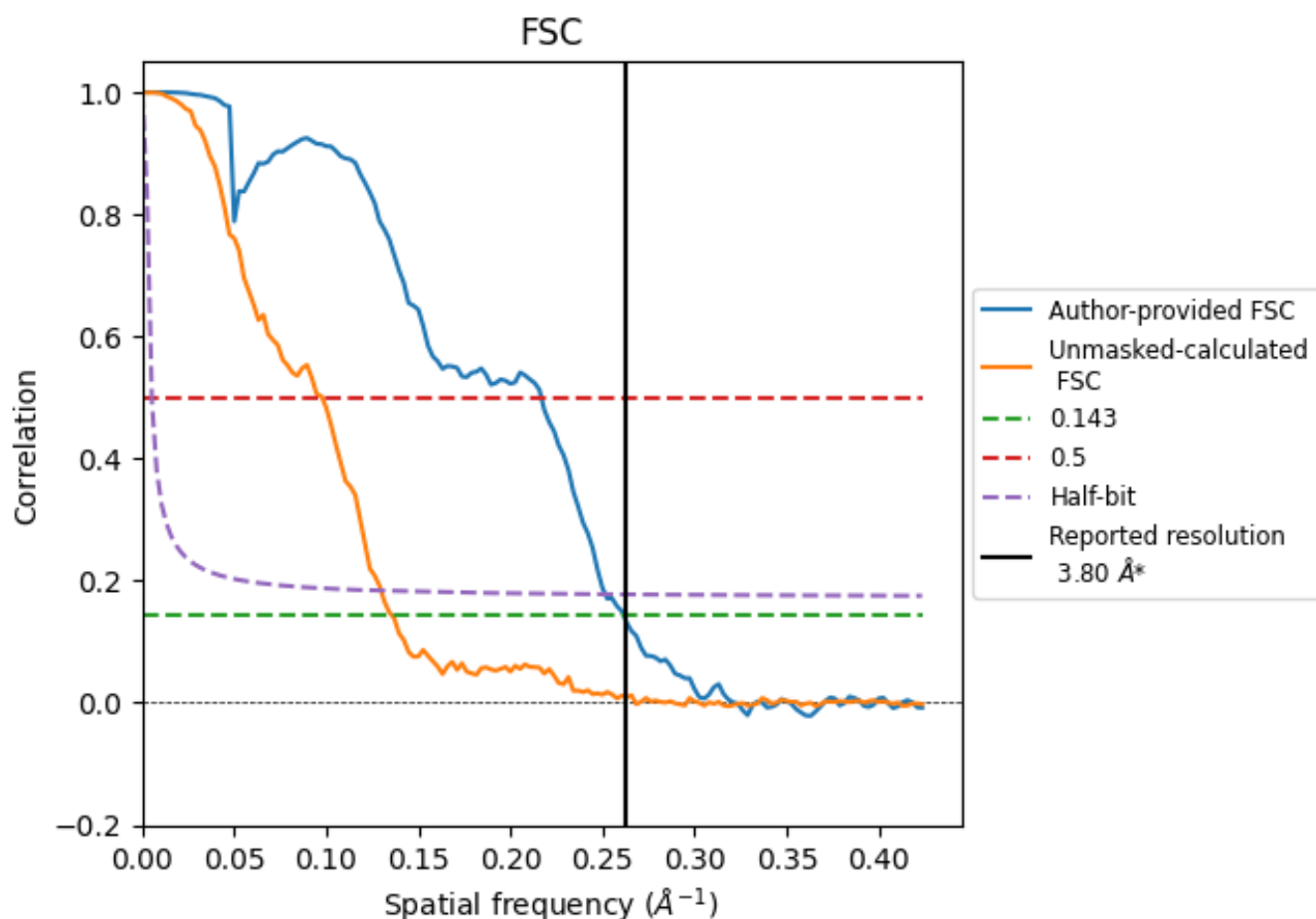


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

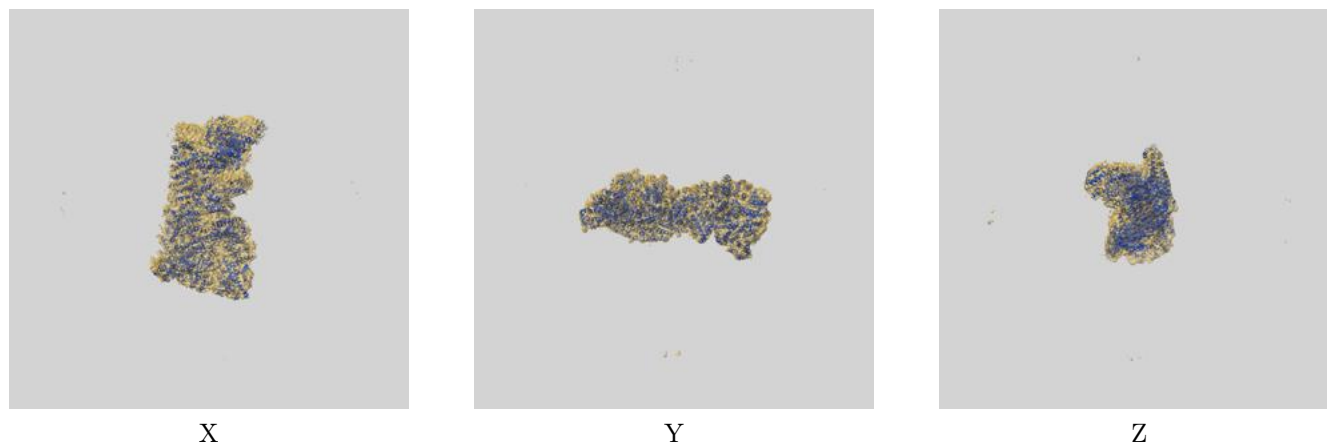
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.61	3.97
Unmasked-calculated*	7.37	10.25	7.71

*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 7.37 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

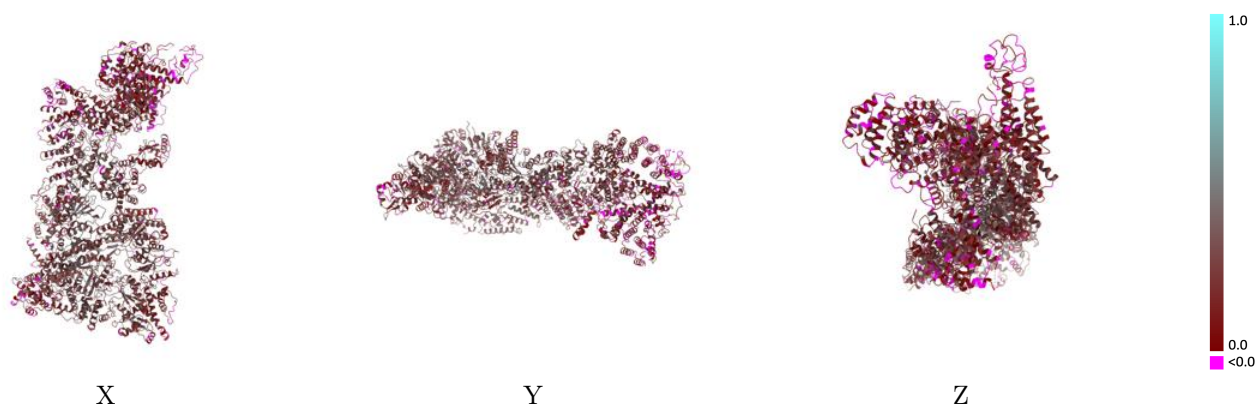
This section contains information regarding the fit between EMDB map EMD-52571 and PDB model 9I1J. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



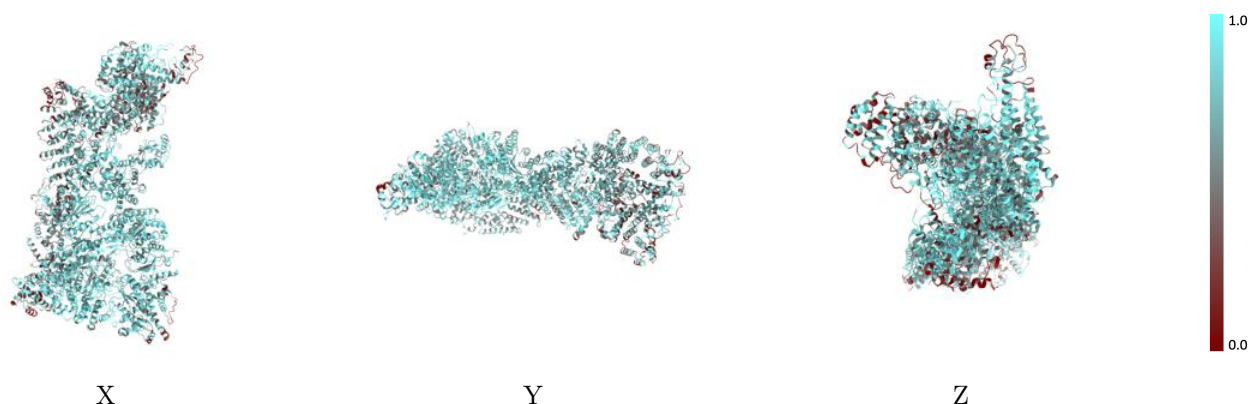
The images above show the 3D surface view of the map at the recommended contour level 0.0047 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



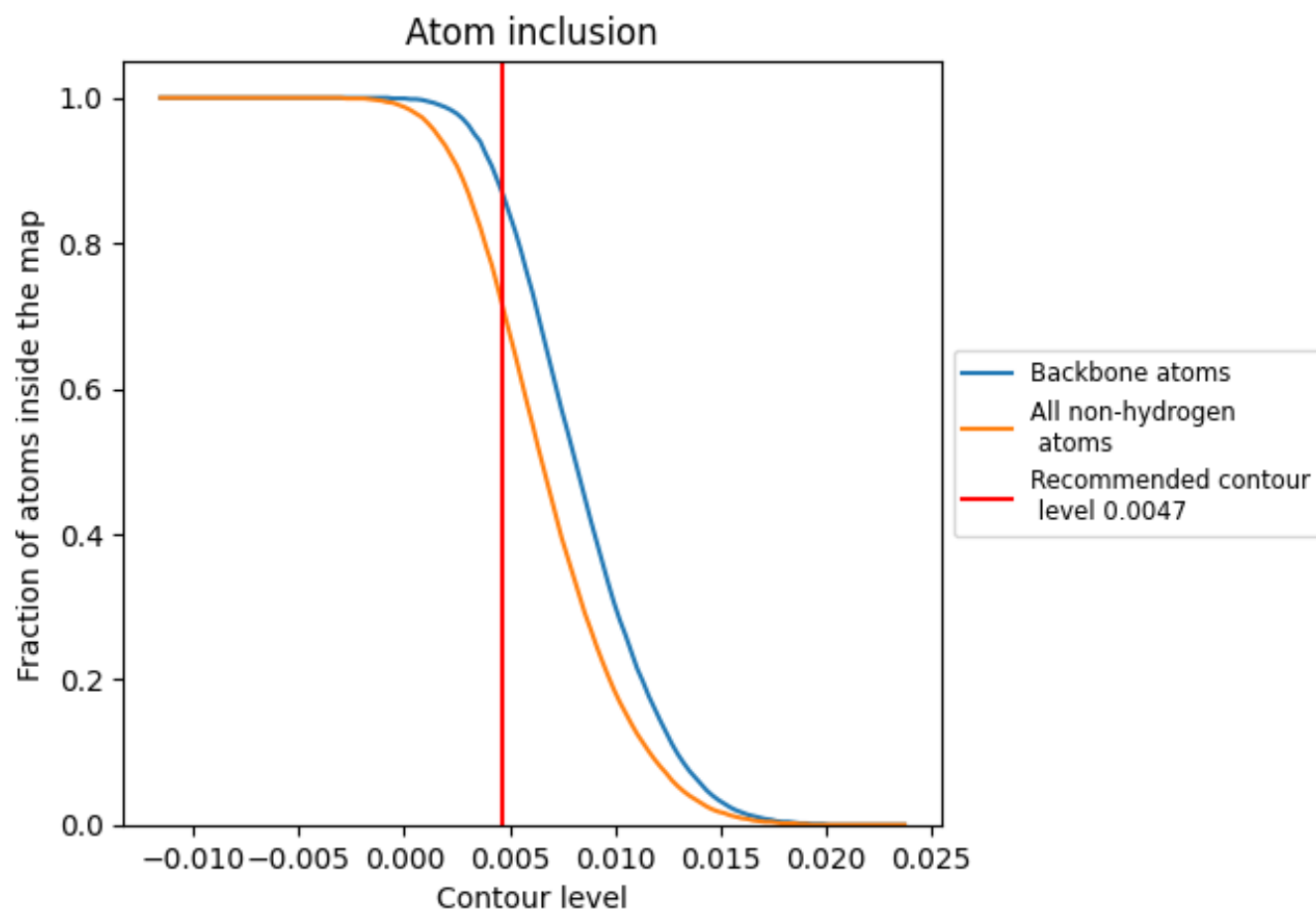
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0047).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.0047) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7100	<div></div> 0.2270
A	<div></div> 0.7080	<div></div> 0.2290
B	<div></div> 0.7800	<div></div> 0.1800

