



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:09 PM UTC

PDB ID : 7SIC / pdb_00007sic
EMDB ID : EMD-25140
Title : Human ATM Dimer
Authors : Warren, C.; Pavletich, N.P.
Deposited on : 2021-10-13
Resolution : 2.51 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

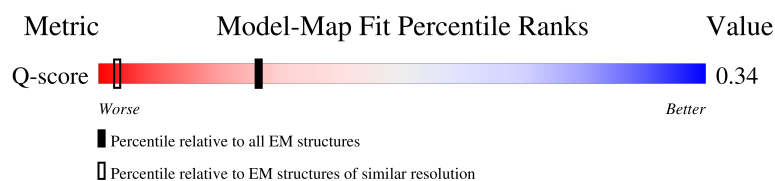
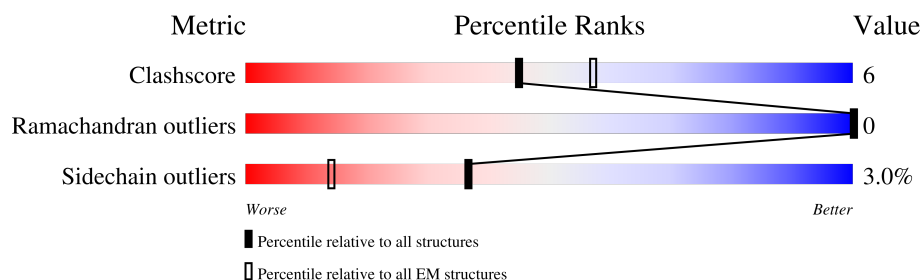
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.51 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	7159 (2.01 - 3.01)

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	3056	44% 75% 16% 9%
1	B	3056	44% 75% 15% 9%

2 Entry composition [i](#)

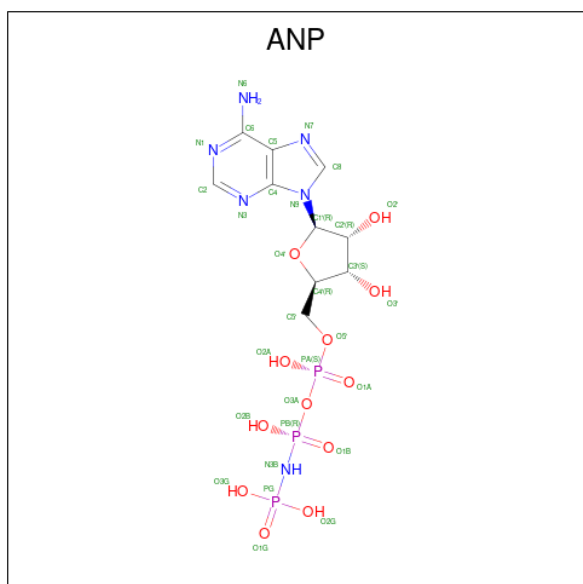
There are 3 unique types of molecules in this entry. The entry contains 44484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2773	Total	C	N	O	S	0	0
			22210	14200	3774	4083	153		
1	B	2773	Total	C	N	O	S	0	0
			22210	14200	3774	4083	153		

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

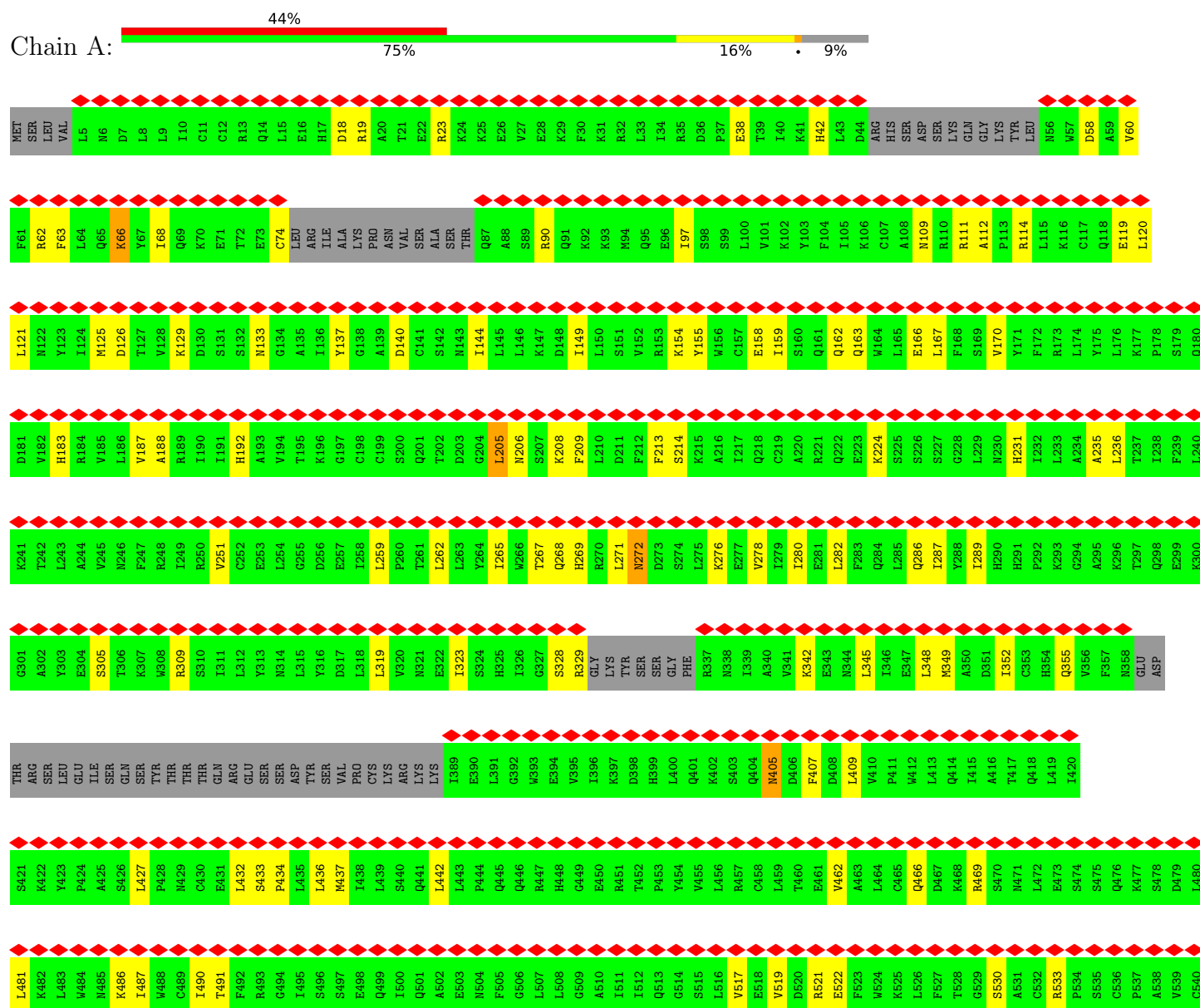
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Mg 1	0
3	B	1	Total 1	Mg 1	0

3 Residue-property plots

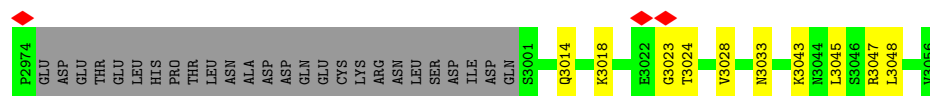
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Serine-protein kinase ATM

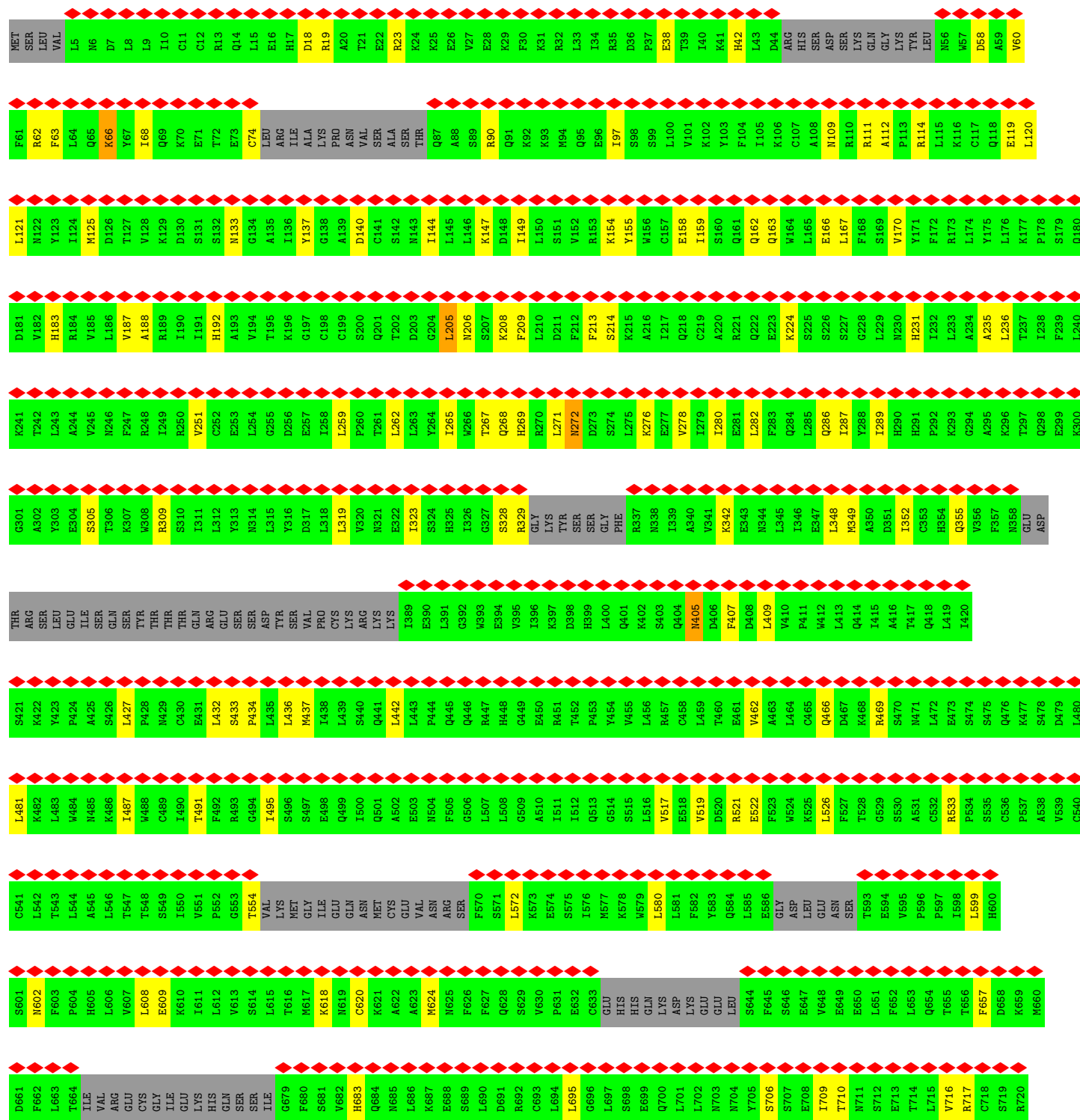
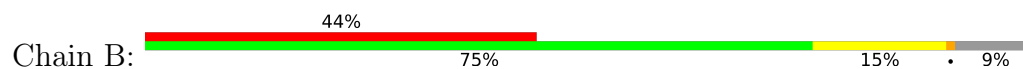


I1261	F1201	PRO	N1081	V1021	L961	L901	ASP	THR	Q781	L721	D661	S601	C541
R1262	G1202	E1142	H1082	I1022	P962	K902	THR	THR	L782	L722	F662	N602	L542
H1264	Y1203	T1143	H1083	G1023	P962	F903	GLY	GLY	L783	L723	F663	F603	T543
H1266	R1204	L1144	Q1084	A1024	E964	L904	ASN	ASN	T784	G724	T664	P604	L544
F1265	R1205	D1145	V1085	F1025	D965	C905	LEU	LEU	R785	Y725	ILE	H605	A545
D1266	L1206	E1146	R1086	W1026	V966	L906	MET	MET	C786	L726	VAL	L606	L546
E1267	E1207	I1147	M1087	W1027	L967	L907	GLU	GLU	L787	G727	GLU	V607	T547
V1268	D1208	M1148	L1088	L1028	E968	V908	GLU	GLU	S788	C728	CYS	L608	T548
K1269	F1209	K1149	A1089	T1029	E969	T909	GLN	GLN	N789	Y729	GLY	E609	S549
S1270	M1210	R1150	A1090	K1030	L970	T910	SER	SER	C790	C730	ILE	K610	I550
I1271	A1211	K1151	E1091	E1031	P971	Q912	SER	SER	T791	Y731	LYS	L611	V551
A1272	S1212	S1152	S1092	R1032	P972	Q912	MET	MET	K792	M732	HIS	L612	P552
M1273	H1213	V1153	I1093	K1033	L973	T913	LEU	LEU	K793	G733	GLN	V613	G553
Q1274	L1214	L1154	N1094	Y1034	S974	N914	PHE	PHE	S794	V734	SER	S614	T554
I1275	D1215	L1155	R1095	T1035	N975	T915	ASN	ASN	F795	I735	ILE	L615	VAL
Q1276	Y1216	T1156	L1096	F1036	V976	V916	ASP	ASP	N796	A736	G679	T616	LYS
E1277	E1217	L1157	F1097	S1037	C977	S917	TYR	TYR	K797	E737	F680	M617	GLY
D1278	V1218	I1158	Q1098	V1038	S978	F918	ASP	ASP	I798	E738	S681	K618	ILE
W1279	L1219	A1159	D1099	R1039	L979	R919	SER	SER	A799	E739	V682	N619	GLU
K1280	E1220	V1160	T1100	M1040	Y980	A920	VAL	VAL	S800	A740	H683	C620	GLN
S1281	W1221	V1161	K1101	A1041	N981	A921	SER	SER	G801	Y741	Q684	K621	ASN
L1282	L1222	L1162	ASP	L1042	R982	D922	ALA	ALA	F802	K742	L685	A622	MET
T1283	N1223	S1163	SER	V1043	D983	I923	ASN	ASN	F803	E743	L686	G623	CYS
L1284	L1224	C1164	SER	N1044	Q984	R924	GLU	GLU	L804	E744	K687	M624	VAL
D1285	Q1225	S1165	ARG	C1045	D985	R925	PRO	PRO	R805	L745	E688	N625	ASN
C1286	D1226	P1166	LEU	L1046	V986	K926	GLY	GLY	L806	F746	S689	F626	ARG
F1287	T1227	I1167	L1108	L1047	C987	L927	GLU	GLU	L807	Q747	L690	F627	SER
P1288	E1228	C1168	K1109	T1048	K988	L928	SER	SER	T808	K748	D691	Q628	GLY
K1289	Y1229	E1169	A1110	L1049	X989	M929	GLN	GLN	S809	A749	R692	S629	VAL
I1290	N1230	K1170	L1111	L1050	I990	L930			K810	K750	C693	V630	ASN
L1291	S1232	A1172	P1112	E1051	N991	I931			L812	S751	L694	P631	ARG
M1292	S1233	L1173	K1114	A1052	L992	D932			N813	L752	L695	E632	ARG
N1293	F1234	F1174	L1115	P1054	V994	S934			D814	M753	G696	C633	SER
L1294	P1235	A1175	L1116	Y1055	L995	T935			I815	Q754	L697	C633	
T1295	F1236	L1176	Q1117	S1056	H996	L936			A816	A756	S698	HIS	
Y1297	I1237	C1177	T1118	K1057	V997	E937			D817	G757	E699	GLN	
F1298	L1238	K1178	A1119	W1058	V998	P938			I818	E758	Q700	LYS	
A1299	L1239	S1179	F1120	A1059	X999	T939			C819	S759	L701	ASP	
Y1300	N1240	V1180	E1121	I1060	M1000	K940			K820	I760	L702	GLU	
E1301	Y1241	K1181	M1122	L1061	L1001	S941			S821	T761	N703	GLU	
G1302	T1242	E1182	A1123	N1062	G1002	L942			L822	L762	N704	LEU	
T1303	N1243	M1183	Y1124	V1063	Q1003	H943			A823	Y705	L705	S644	
R1304	I1244	G1184	L1125	M1064	S1004	L944			S824	S706	S706	F645	
D1305	E1245	L1185	K1126	G1065	N1005	H945			F825	K764	E708	S646	
S1306	D1246	E1186	A1127	K1066	M1006	M946			D894	K766	I709	E647	
G1307	F1247	P1187	Q1128	D1067	D1007	Y947			LYS	T767	T710	E649	
M1308	Y1248	H1188	E1129	F1068	S1008	L948			LYS	N768	N711	E650	
A1309	R1249	L1189	G1130	P1069	E1009	M949			PRO	E769	S712	L651	
Q1310	S1250	V1190	M1131	T1069	S1009	L950			PHE	E770	E713	F652	
Q1311	C1251	K1191	R1132	V1070	M1010	L951			ASP	F771	T714	L653	
R1312	Y1252	K1192	E1133	E1071	T1011	K952			ARG	R772	L715	Q654	
E1313	V1253	V1193	L1134	N1072	R1012	E953			GLY	I773	V716	T655	
T1314	V1254	L1194	M1134	F1074	D1013	L954			VAL	G774	R717	I598	
A1315	L1255	E1195	SER	T1075	A1014	L954			GLU	S775	C718	F657	
T1316	P1257	K1196	SER	Q1076	Q1015	P955			GLU	T776	S719	L659	
K1317	H1258	V1197	ALA	F1077	G1016	G956			SER	S777	D658	H600	
V1318	L1259	S1198	GLU	Q1017	Q1017	E957			MET	R777	R720		
Y1319	V1260	E1199	ASN	F1018	F1018	E958			GLU	M778			
D1320		T1200		A1079	L1019	Y959			ASP	M780			





• Molecule 1: Serine-protein kinase ATM



I1469	I1473	Q1478	R1479	P1480	A1391	Y1392	I1393	S1394	I1483	M1484	D1485	V1486	R1489	D1496	S1499	Q1503	T1504	A1505	Y1508	C1509	D1510	A1512	D1511	Y1519	G1522	T1523	L1524	L1527	V1528	Y1529	E1424	E1530	Q1425	Q1531	V1532	E1428	E1533	V1534	Q1535	Y1433	Q1537	V1538	L1539	D1540	D1548	M1549	K1550	D1551	M1552	E1553	M1554	L1555																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</
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LEU	HIS	PRO	THR	LEU	ASN	ALA	ASP	ASP	ASP	GLN	GLU	CYS	LYS	ARG	ASN	LEU	SER	LEU	ASP	ILE	GLN	S3001	Q3014	K3018	E3022	G3023	T3024	V3028	N3033	K3043	N3044	L3045	S3046	R3047	L3048	V3056															
L2859	E2860	D2861	V2862	V2863	V2864	T2865	T2866	T2867	E2868	L2869	T2874	G2875	N2879	I2883	R2891	L2892	A2893	V2896	N2897	L2898	P2899	K2700	D2703	C2704	V2705	D2708	R2719	D2720	V2727	V2731	M2734	E2744	T2745	R2746	K2749	L2750	T2751	I2752	R2763	R2792	D2795	K2810									
G2533	G2534	H2538	L2544	T2556	L2561	A2562	A2564	N2565	E2570	T2573	LYS	PRO	GLU	VAL	ALA	ARG	ARG	ARG	ARG	ILE	THR	LYS	ASN	VAL	PRO	LYS	GLN	S2591	S2592	Q2593	A2602	I2606	R2612	Q2615	M2616	L2623	L2633	D2634	A2635	K2643	D2650	L2656									
L2416	L2417	K2418	R2419	A2420	K2421	E2422	GLU	VAL	GLY	LEU	LEU	ARG	GLU	HIS	LYS	ILE	GLN	THR	ASN	R2436	Y2437	T2438	V2439	K2440	V2441	Q2442	R2443	E2444	L2445	E2446	L2447	D2448	E2449	E2457	D2458	R2459	K2460	R2461	L2474	H2480	V2483	M2509	Y2514	K2515	F2516	L2517	M2520	T2529	K2530	M2531	M2532
W2239	D2240	M2241	I2247	K2248	H2254	T2268	P2271	V2284	S2285	C2286	G2287	V2288	S2289	E2290	L2307	T2311	L2319	A2324	A2325	M2326	M2327	L2332	T2333	Y2334	T2335	Q2358	A2368	G2369	M2370	Y2371	D2372	G2373	E2374	S2375	E2378	L2379	K2383	M2384	T2401	E2402	K2406	A2415									
Q2101	W2104	W2109	D2110	H2111	C2112	THR	SER	VAL	SER	LYS	GLU	VAL	GLU	G2121	Q2133	S2141	T2142	S2146	L2147	K2148	C2159	K2160	L2163	V2166	A2178	L2188	R2191	S2192	V2193	T2194	H2195	R2196	Q2197	L2198	S2199	E2200	D2214	S2215	L2226	R2227	T2228	M2235	E2236	K2237	E2238						
A1694	S1695	Y1696	T1697	K1701	D1705	L1708	Q1709	M1710	M1714	L1715	N1720	T1721	V1734	L1737	T1745	G1746	H1747	E1751	K1754	M1755	T1756	L1761	Q1765	P1766	T1769	S1770	R1771	K1772	K1773	P1778	R1779	F1780	D1781	K1782	E1783	P1797	L1798	S1799	F1800	N1801	H1802	T1806									
K1820	C1821	E1822	I1823	L1827	T1835	D1836	F1837	Q1852	M1860	T1864	F1869	F1870	T1871	R1875	H1876	PHE	GLN	THR	THR	THR	PRO	ALA	ASN	LEU	ASP	SER	GLU	HIS	PHE	PHE	ARG	C1899	D1902	K1903	M1909	M1916	S1924	E1959	K1972	R1973											
S1974	LEU	ALA	PHE	GLU	GLY	GLN	SER	T1984	T1985	S1988	L1989	K1992	E1995	E1996	R2010	G2023	G2024	K2025	M2026	L2027	Q2028	P2029	T2030	T2031	R2032	L2033	R2034	T2048	Y2049	T2059	R2060	Q2061	T2064	G2072	L2084	D2085	Y2086	E2087	M2088	K2089	D2090	V2091	C2092	P2093	L2095						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	303604	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 ($e^-/\text{\AA}^2$)	53.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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, ANP

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	0.11	0/22624	0.30	0/30565
1	B	0.11	0/22624	0.30	0/30565
All	All	0.11	0/45248	0.30	0/61130

There are no bond length outliers.

There are no bond angle outliers.

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	22210	0	22392	292	0
1	B	22210	0	22392	286	0
2	A	31	0	13	1	0
2	B	31	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	44484	0	44810	566	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 6.

The worst 5 of 566 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1312:ARG:HG3	1:B:1312:ARG:HH11	1.31	0.95
1:A:1312:ARG:HG3	1:A:1312:ARG:HH11	1.31	0.93
1:B:2458:ASP:OD1	1:B:2461:ARG:NH2	2.23	0.71
1:B:1509:CYS:HB2	1:B:1512:ALA:HB2	1.73	0.71
1:A:1509:CYS:HB2	1:A:1512:ALA:HB2	1.73	0.71

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	2735/3056 (90%)	2687 (98%)	48 (2%)	0	100	100
1	B	2735/3056 (90%)	2687 (98%)	48 (2%)	0	100	100
All	All	5470/6112 (90%)	5374 (98%)	96 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2469/2780 (89%)	2394 (97%)	75 (3%)	36	64
1	B	2469/2780 (89%)	2394 (97%)	75 (3%)	36	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4938/5560 (89%)	4788 (97%)	150 (3%)	37 64

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1322	LEU
1	B	2674	THR
1	B	1509	CYS
1	B	1806	ILE
1	A	1575	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1951	HIS
1	B	2658	ASN
1	B	2061	GLN
1	B	2480	HIS
1	B	2742	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	ANP	A	3101	3	33,33,33	0.93	4 (12%)	45,52,52	0.54	0
2	ANP	B	3101	3	33,33,33	0.93	4 (12%)	45,52,52	0.54	0

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
2	ANP	A	3101	3	-	4/18/38/38	0/3/3/3
2	ANP	B	3101	3	-	4/18/38/38	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)
2	A	3101	ANP	PG-O1G	2.53	1.50	1.46
2	B	3101	ANP	PG-O1G	2.53	1.50	1.46
2	A	3101	ANP	PB-O3A	-2.43	1.56	1.59
2	B	3101	ANP	PB-O3A	-2.43	1.56	1.59
2	A	3101	ANP	PG-N3B	2.39	1.69	1.63

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

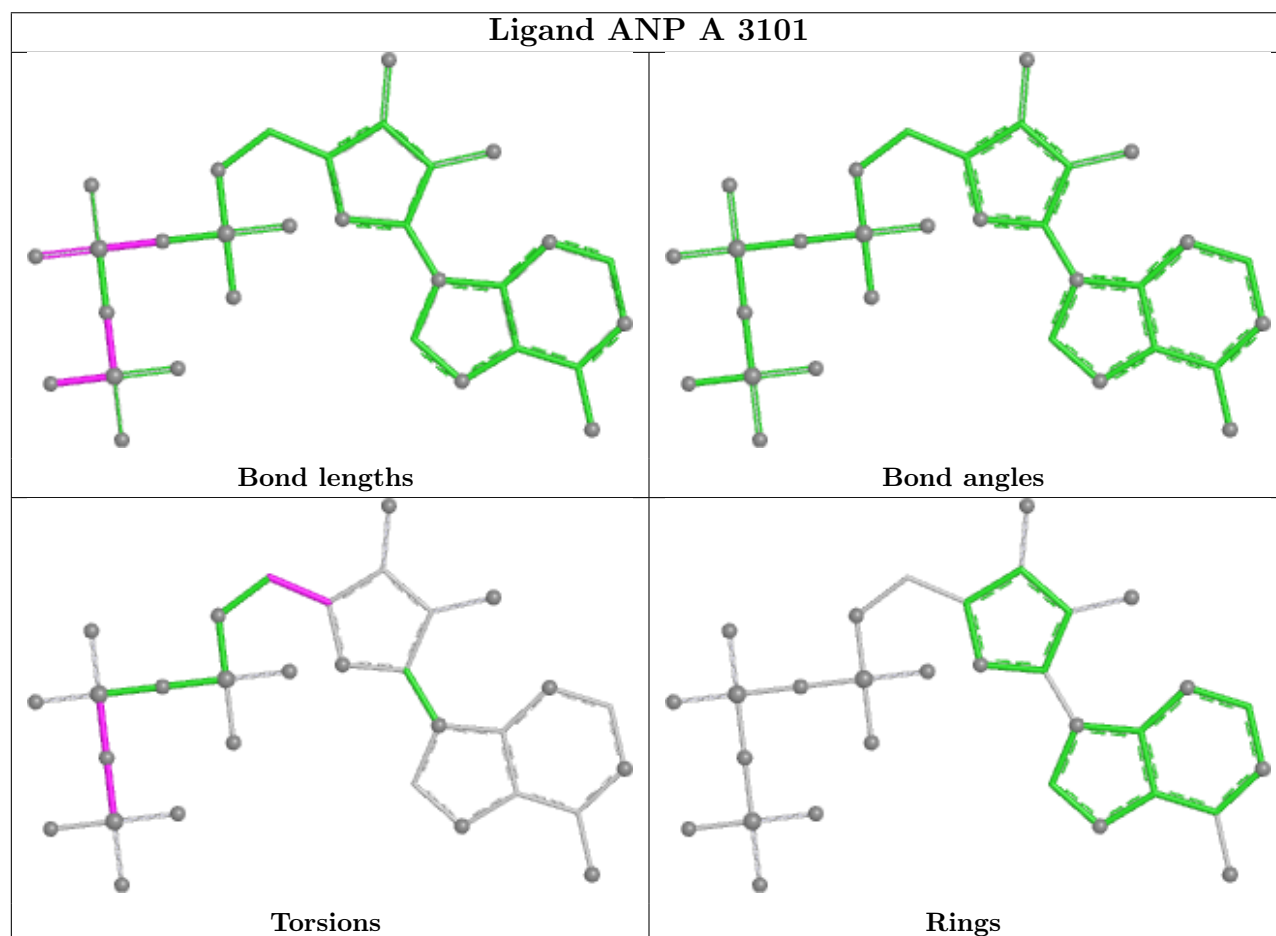
Mol	Chain	Res	Type	Atoms
2	A	3101	ANP	PB-N3B-PG-O1G
2	A	3101	ANP	PG-N3B-PB-O1B
2	B	3101	ANP	PB-N3B-PG-O1G
2	B	3101	ANP	PG-N3B-PB-O1B
2	A	3101	ANP	O4'-C4'-C5'-O5'

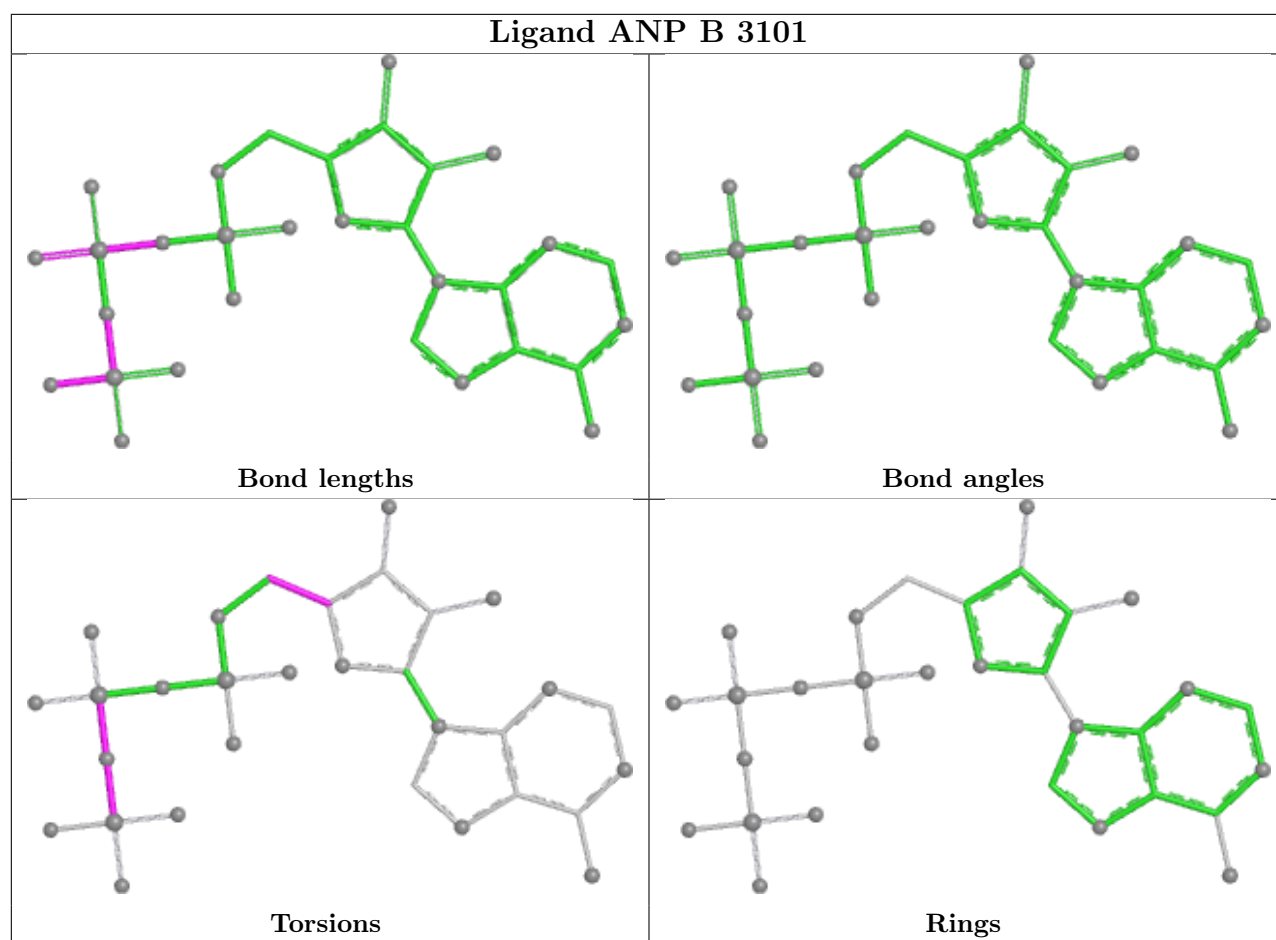
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3101	ANP	1	0
2	B	3101	ANP	1	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.

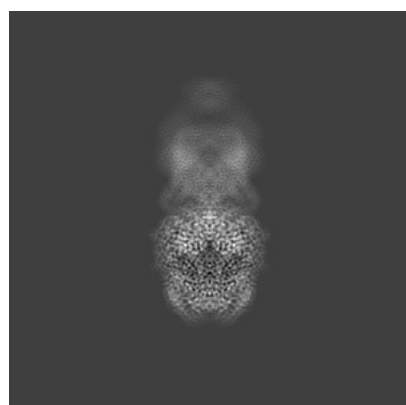
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25140. These allow visual inspection of the internal detail of the map and identification of artifacts.

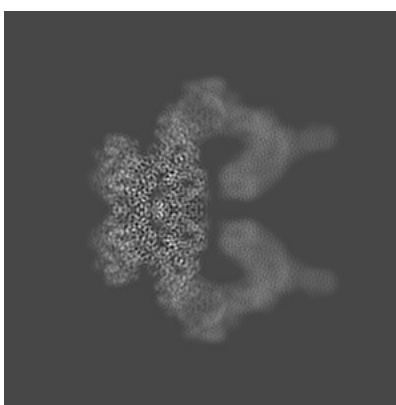
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

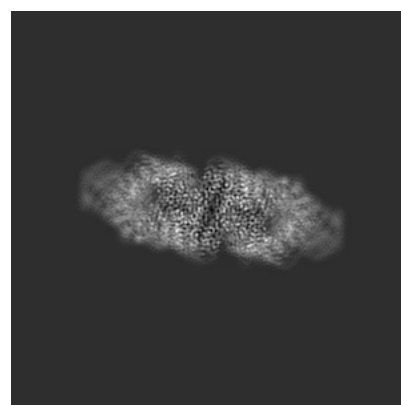
6.1.1 Primary map



X



Y

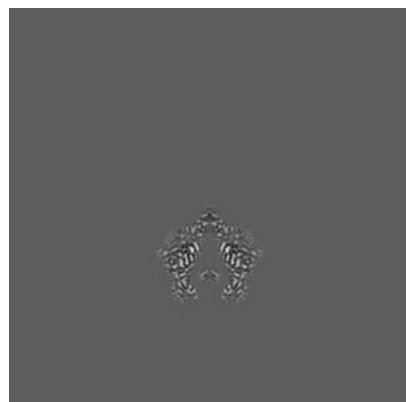


Z

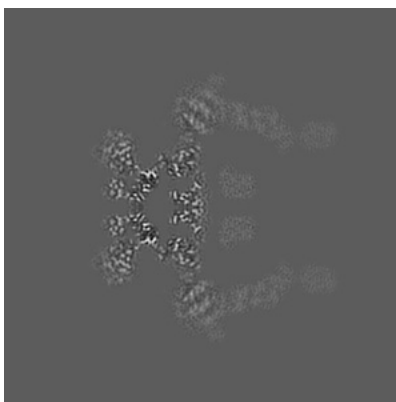
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

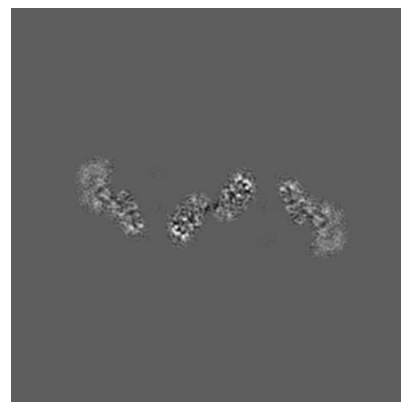
6.2.1 Primary map



X Index: 150



Y Index: 150

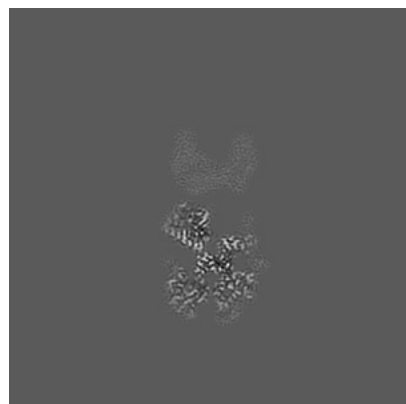


Z Index: 150

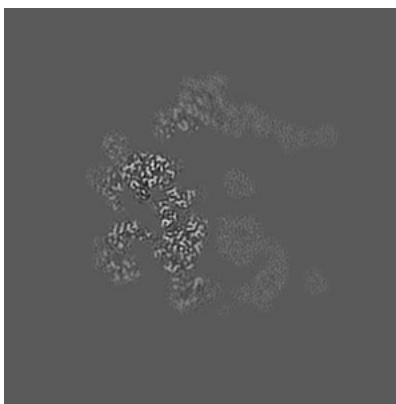
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

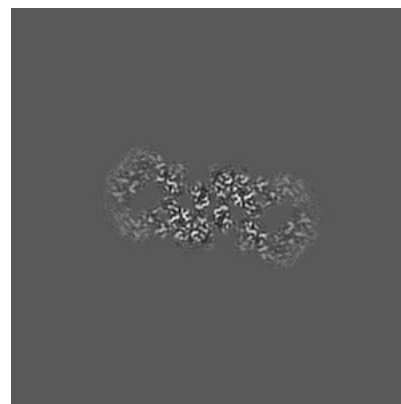
6.3.1 Primary map



X Index: 127



Y Index: 140

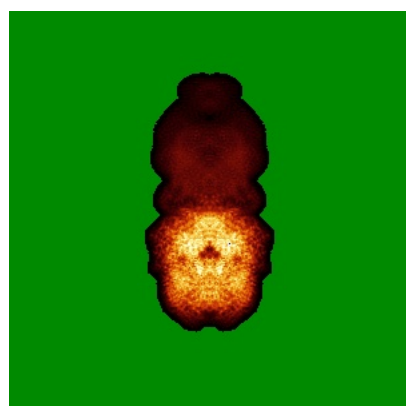


Z Index: 128

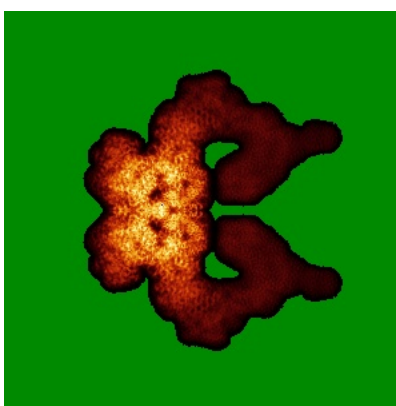
The images above show the largest variance slices of the map in three orthogonal directions.

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

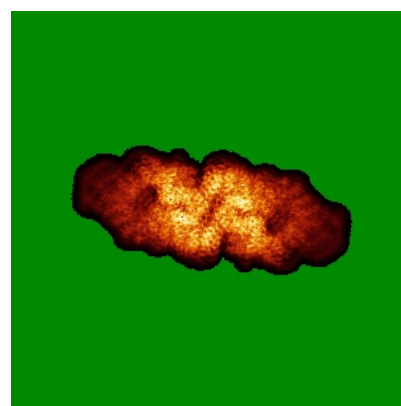
6.4.1 Primary map



X



Y

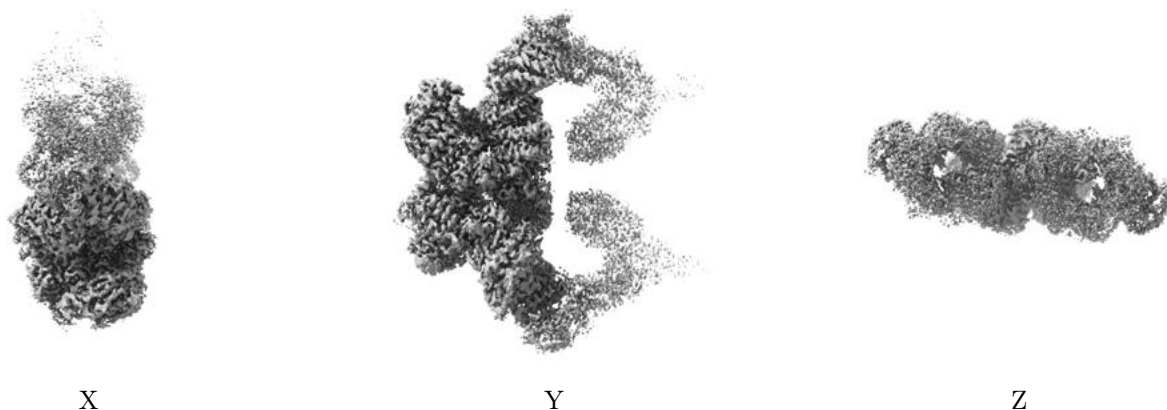


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

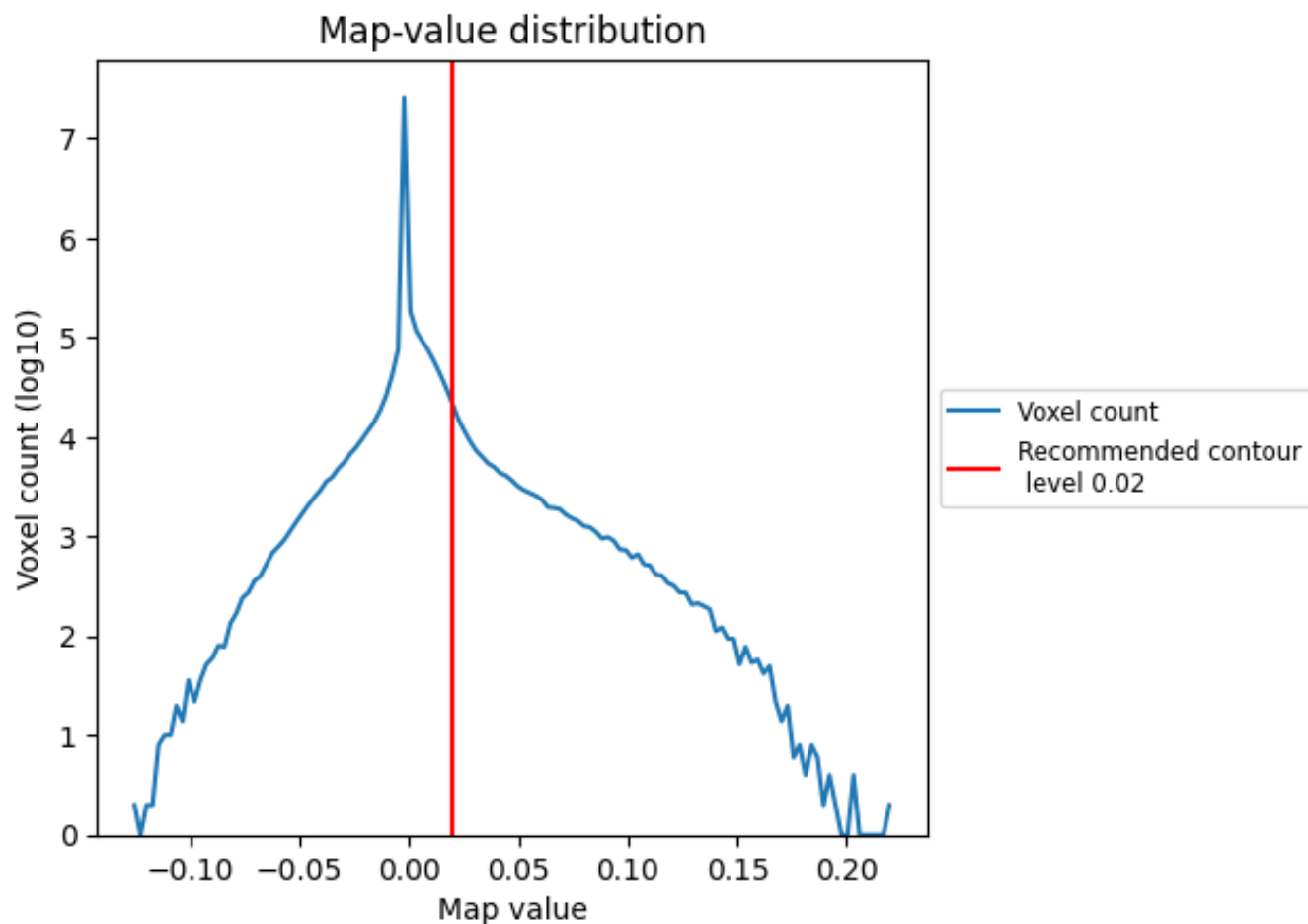
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

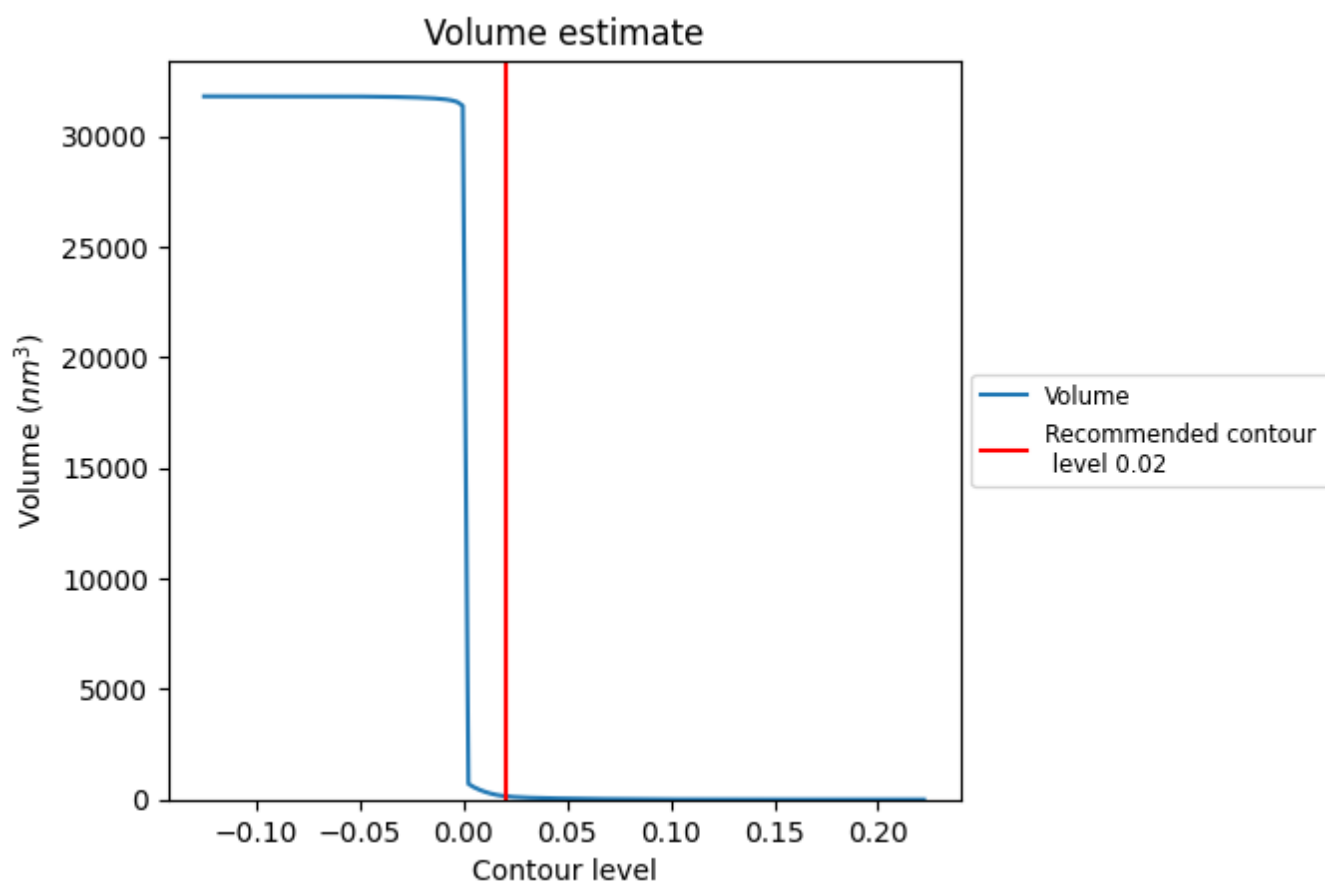
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

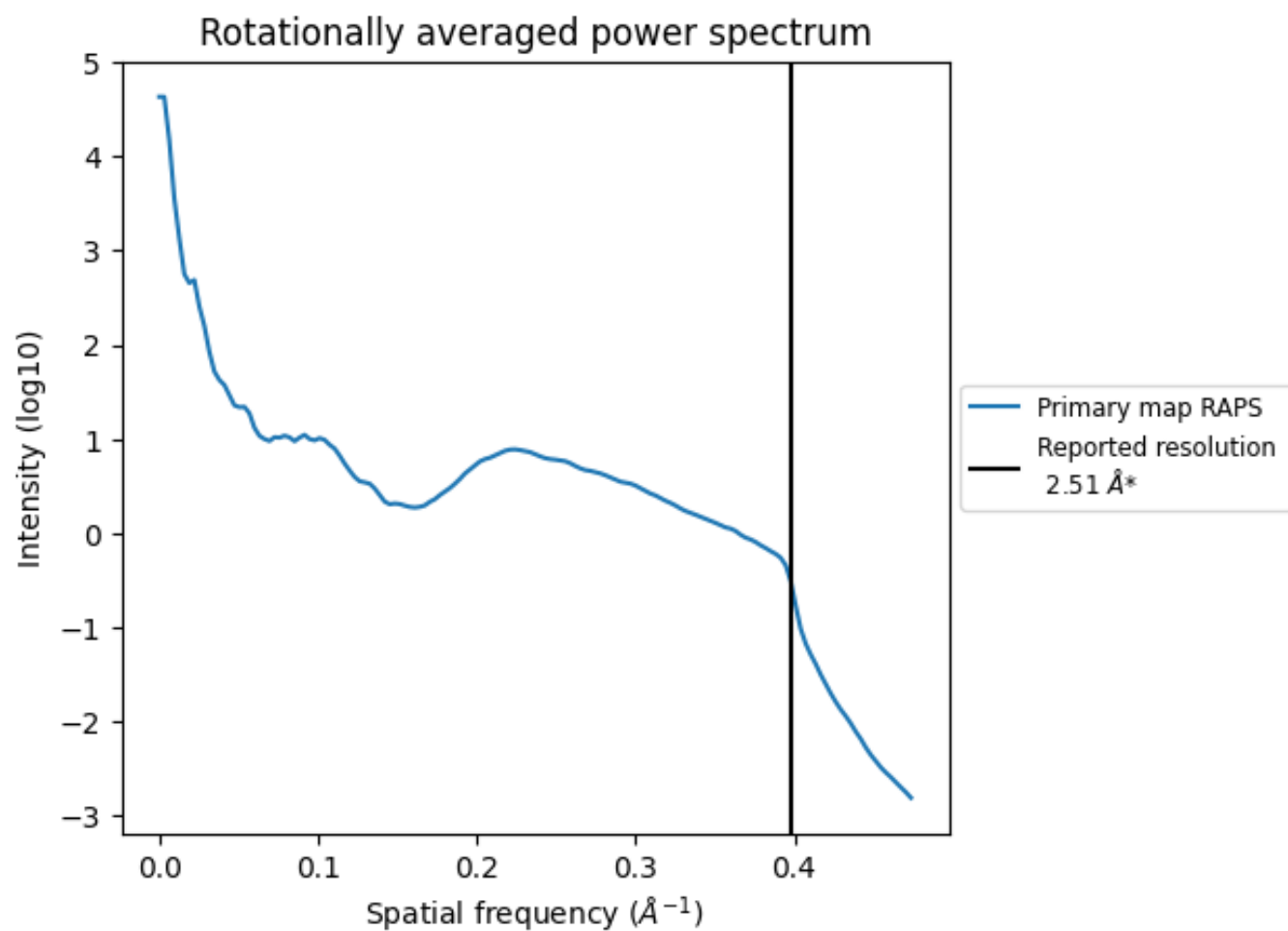
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

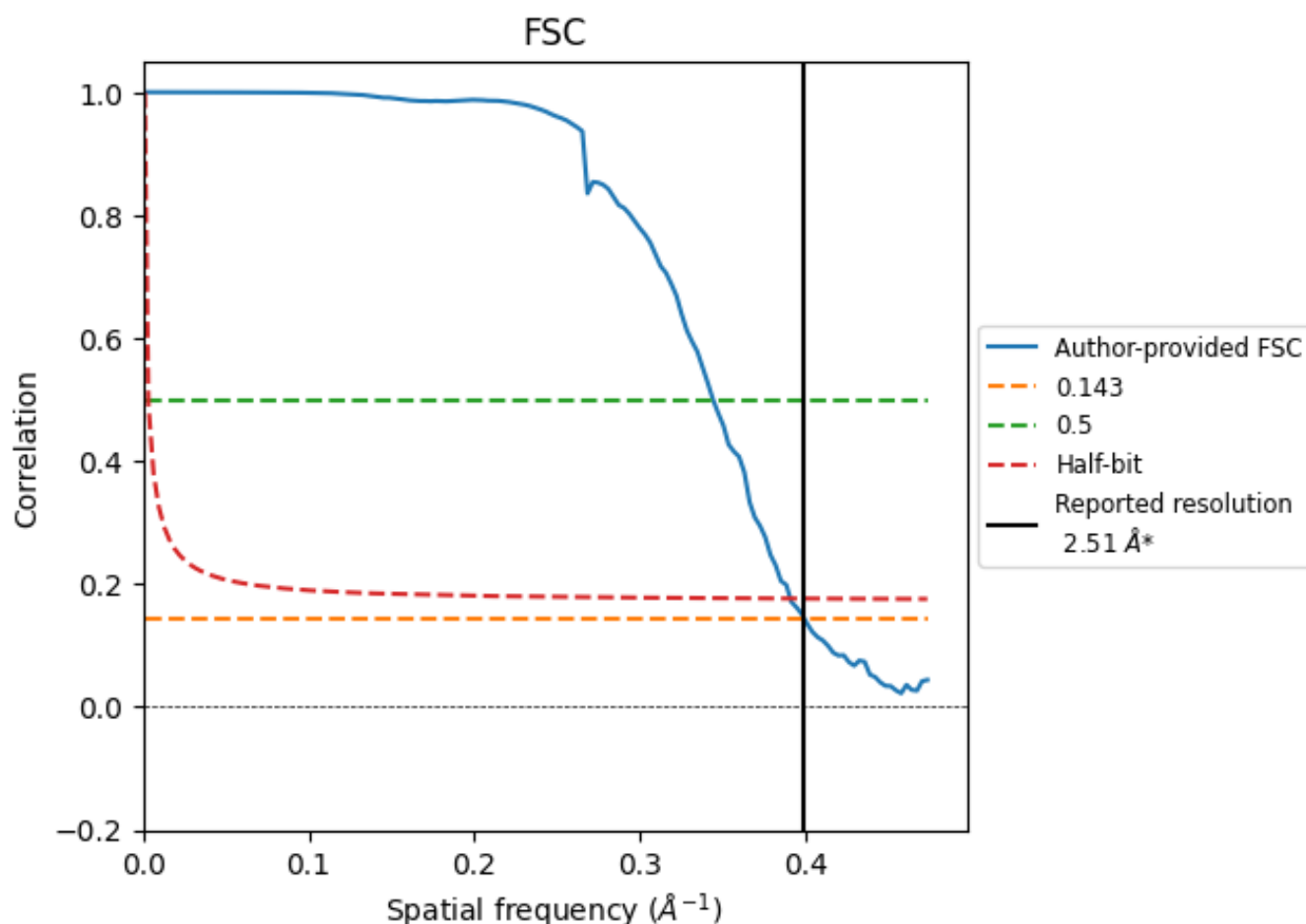


*Reported resolution corresponds to spatial frequency of 0.398 Å⁻¹

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 0.398 Å⁻¹

8.2 Resolution estimates [i](#)

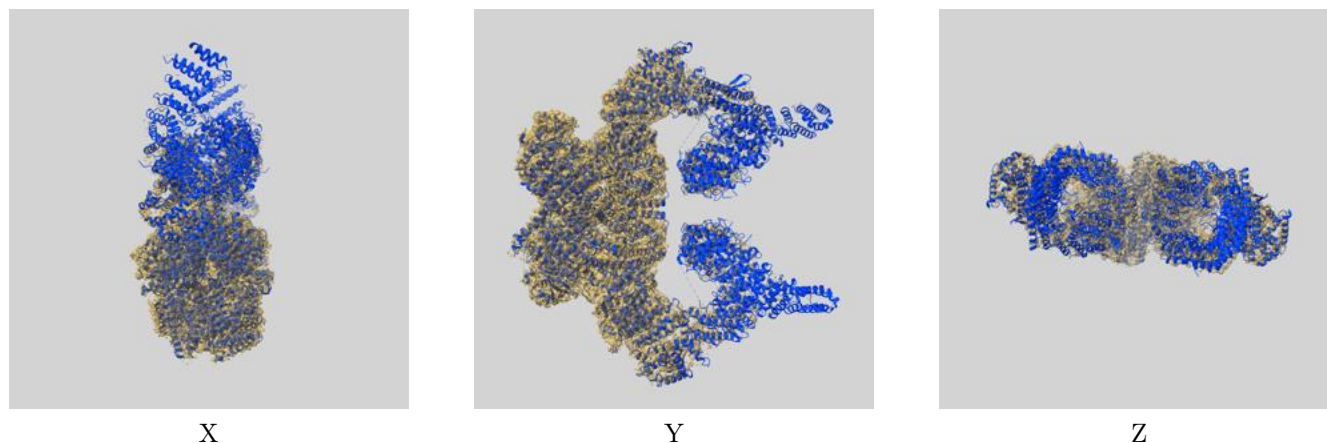
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.51	-	-
Author-provided FSC curve	2.50	2.91	2.56
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

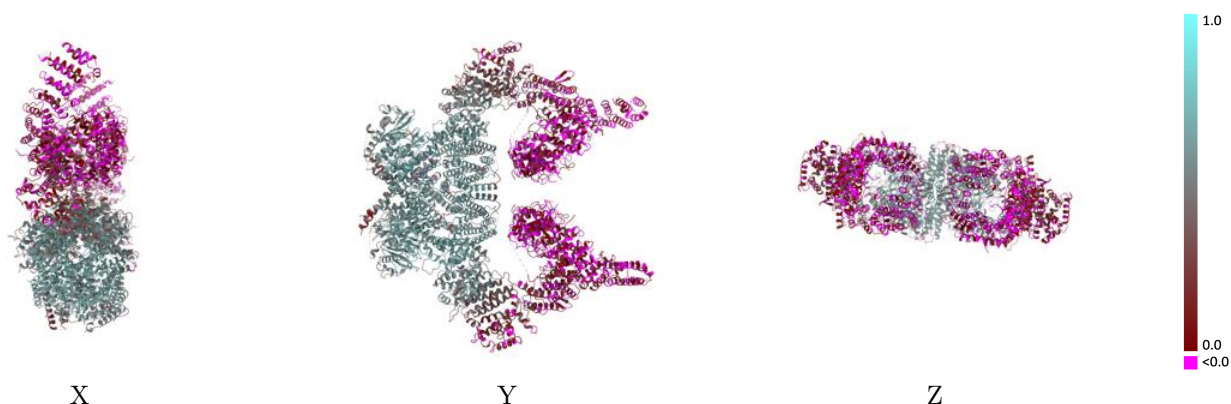
This section contains information regarding the fit between EMDB map EMD-25140 and PDB model 7SIC. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



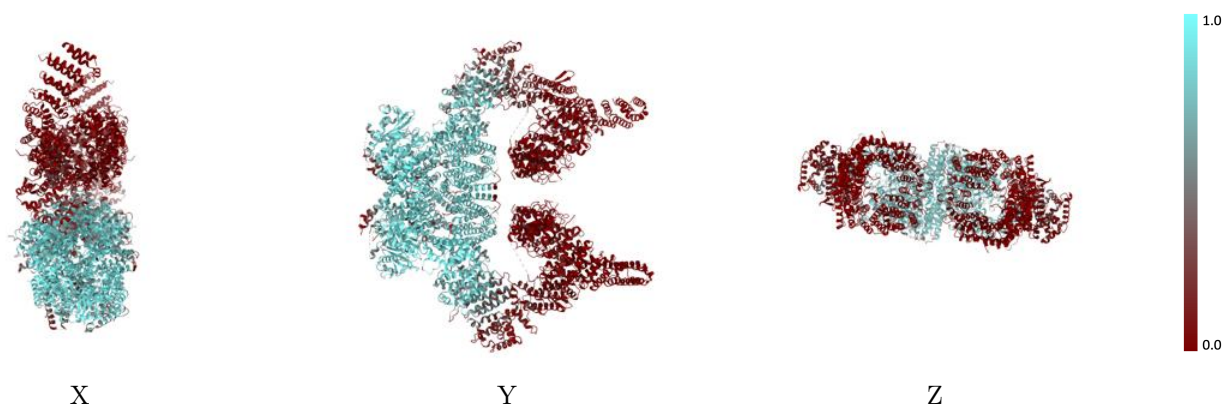
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



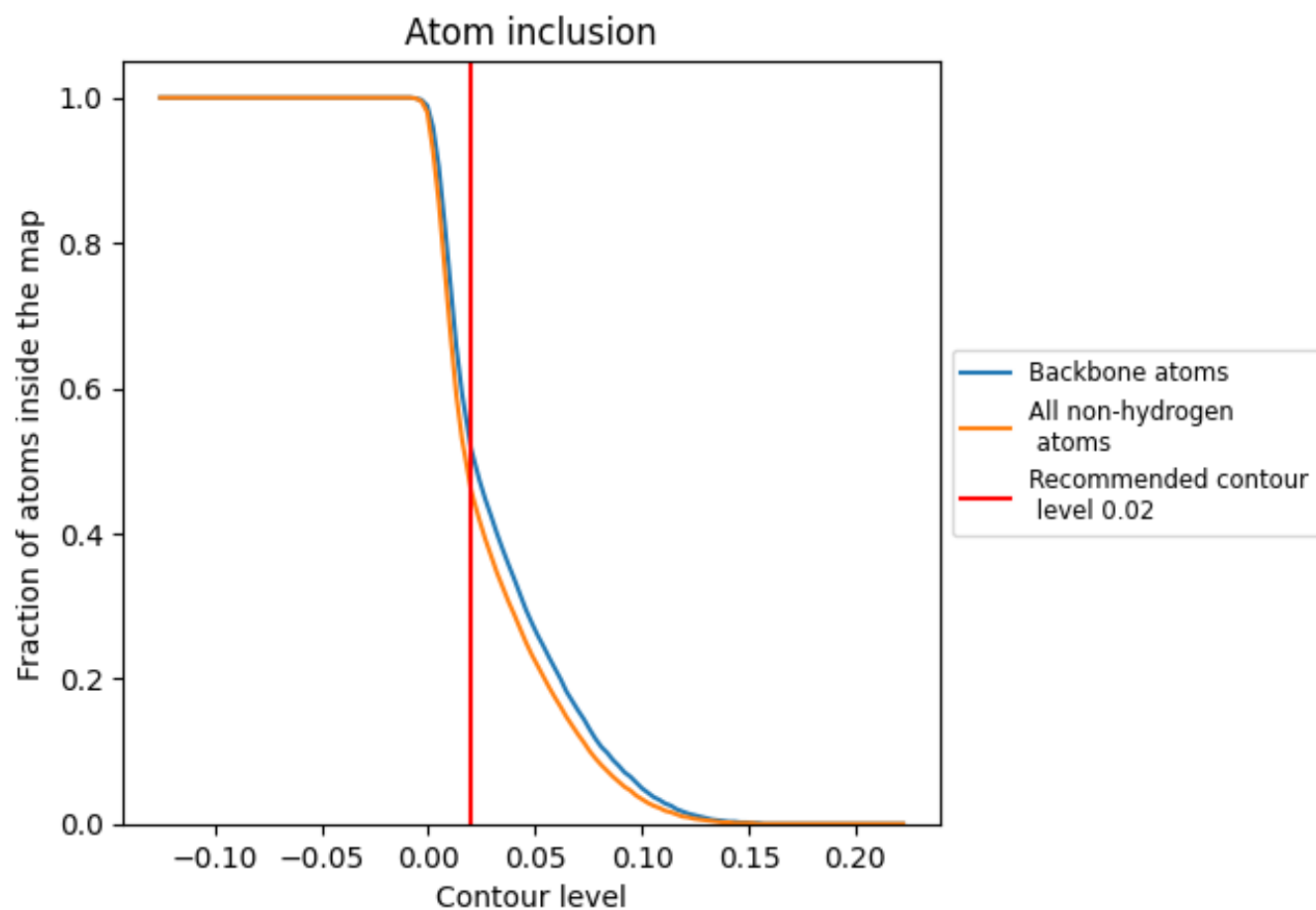
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 46% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4600	0.3400
A	0.4600	0.3400
B	0.4600	0.3400

