



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 08:03 PM UTC

PDB ID : 8OXM / pdb_00008oxm
EMDB ID : EMD-17265
Title : ATM(Q2971A) activated by oxidative stress in complex with Mg AMP-PNP and p53 peptide
Authors : Howes, A.C.; Perisic, O.; Williams, R.L.
Deposited on : 2023-05-02
Resolution : 3.30 Å(reported)
Based on initial model : 7SIC

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

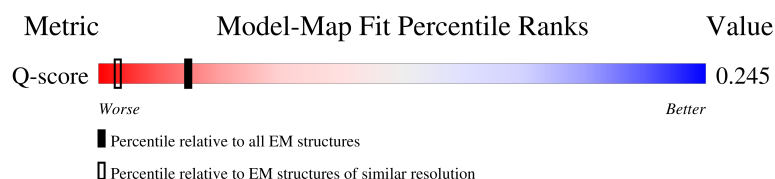
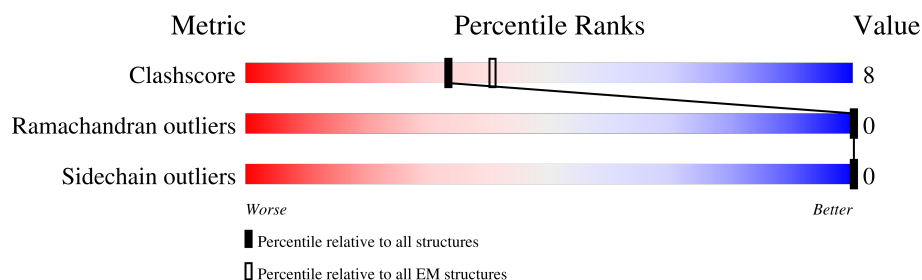
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	E	12	33% 50%8%42%
1	F	12	42% 58%42%
2	A	3184	25% 67%19%14%
2	B	3184	24% 68%18%14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 44174 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	E	7	Total	C	N	O	0	0
			53	33	8	12		
1	F	7	Total	C	N	O	0	0
			53	33	8	12		

- Molecule 2 is a protein called Serine-protein kinase ATM.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2748	Total	C	N	O	S	0	0
			22001	14066	3738	4046	151		
2	B	2748	Total	C	N	O	S	0	0
			22001	14066	3738	4046	151		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-127	MET	-	initiating methionine	UNP Q13315
A	-126	ASP	-	expression tag	UNP Q13315
A	-125	TYR	-	expression tag	UNP Q13315
A	-124	LYS	-	expression tag	UNP Q13315
A	-123	ASP	-	expression tag	UNP Q13315
A	-122	ASP	-	expression tag	UNP Q13315
A	-121	ASP	-	expression tag	UNP Q13315
A	-120	ASP	-	expression tag	UNP Q13315
A	-119	LYS	-	expression tag	UNP Q13315
A	-118	HIS	-	expression tag	UNP Q13315
A	-117	MET	-	expression tag	UNP Q13315
A	-116	GLY	-	expression tag	UNP Q13315
A	-115	VAL	-	expression tag	UNP Q13315
A	-114	GLN	-	expression tag	UNP Q13315
A	-113	VAL	-	expression tag	UNP Q13315
A	-112	GLU	-	expression tag	UNP Q13315
A	-111	THR	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-110	ILE	-	expression tag	UNP Q13315
A	-109	SER	-	expression tag	UNP Q13315
A	-108	PRO	-	expression tag	UNP Q13315
A	-107	GLY	-	expression tag	UNP Q13315
A	-106	ASP	-	expression tag	UNP Q13315
A	-105	GLY	-	expression tag	UNP Q13315
A	-104	ARG	-	expression tag	UNP Q13315
A	-103	THR	-	expression tag	UNP Q13315
A	-102	PHE	-	expression tag	UNP Q13315
A	-101	PRO	-	expression tag	UNP Q13315
A	-100	LYS	-	expression tag	UNP Q13315
A	-99	ARG	-	expression tag	UNP Q13315
A	-98	GLY	-	expression tag	UNP Q13315
A	-97	GLN	-	expression tag	UNP Q13315
A	-96	THR	-	expression tag	UNP Q13315
A	-95	CYS	-	expression tag	UNP Q13315
A	-94	VAL	-	expression tag	UNP Q13315
A	-93	VAL	-	expression tag	UNP Q13315
A	-92	HIS	-	expression tag	UNP Q13315
A	-91	TYR	-	expression tag	UNP Q13315
A	-90	THR	-	expression tag	UNP Q13315
A	-89	GLY	-	expression tag	UNP Q13315
A	-88	MET	-	expression tag	UNP Q13315
A	-87	LEU	-	expression tag	UNP Q13315
A	-86	GLU	-	expression tag	UNP Q13315
A	-85	ASP	-	expression tag	UNP Q13315
A	-84	GLY	-	expression tag	UNP Q13315
A	-83	LYS	-	expression tag	UNP Q13315
A	-82	LYS	-	expression tag	UNP Q13315
A	-81	PHE	-	expression tag	UNP Q13315
A	-80	ASP	-	expression tag	UNP Q13315
A	-79	SER	-	expression tag	UNP Q13315
A	-78	SER	-	expression tag	UNP Q13315
A	-77	ARG	-	expression tag	UNP Q13315
A	-76	ASP	-	expression tag	UNP Q13315
A	-75	ARG	-	expression tag	UNP Q13315
A	-74	ASN	-	expression tag	UNP Q13315
A	-73	LYS	-	expression tag	UNP Q13315
A	-72	PRO	-	expression tag	UNP Q13315
A	-71	PHE	-	expression tag	UNP Q13315
A	-70	LYS	-	expression tag	UNP Q13315
A	-69	PHE	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-68	MET	-	expression tag	UNP Q13315
A	-67	LEU	-	expression tag	UNP Q13315
A	-66	GLY	-	expression tag	UNP Q13315
A	-65	LYS	-	expression tag	UNP Q13315
A	-64	GLN	-	expression tag	UNP Q13315
A	-63	GLU	-	expression tag	UNP Q13315
A	-62	VAL	-	expression tag	UNP Q13315
A	-61	ILE	-	expression tag	UNP Q13315
A	-60	ARG	-	expression tag	UNP Q13315
A	-59	GLY	-	expression tag	UNP Q13315
A	-58	TRP	-	expression tag	UNP Q13315
A	-57	GLU	-	expression tag	UNP Q13315
A	-56	GLU	-	expression tag	UNP Q13315
A	-55	GLY	-	expression tag	UNP Q13315
A	-54	VAL	-	expression tag	UNP Q13315
A	-53	ALA	-	expression tag	UNP Q13315
A	-52	GLN	-	expression tag	UNP Q13315
A	-51	MET	-	expression tag	UNP Q13315
A	-50	SER	-	expression tag	UNP Q13315
A	-49	VAL	-	expression tag	UNP Q13315
A	-48	GLY	-	expression tag	UNP Q13315
A	-47	GLN	-	expression tag	UNP Q13315
A	-46	ARG	-	expression tag	UNP Q13315
A	-45	ALA	-	expression tag	UNP Q13315
A	-44	LYS	-	expression tag	UNP Q13315
A	-43	LEU	-	expression tag	UNP Q13315
A	-42	THR	-	expression tag	UNP Q13315
A	-41	ILE	-	expression tag	UNP Q13315
A	-40	SER	-	expression tag	UNP Q13315
A	-39	PRO	-	expression tag	UNP Q13315
A	-38	ASP	-	expression tag	UNP Q13315
A	-37	TYR	-	expression tag	UNP Q13315
A	-36	ALA	-	expression tag	UNP Q13315
A	-35	TYR	-	expression tag	UNP Q13315
A	-34	GLY	-	expression tag	UNP Q13315
A	-33	ALA	-	expression tag	UNP Q13315
A	-32	THR	-	expression tag	UNP Q13315
A	-31	GLY	-	expression tag	UNP Q13315
A	-30	HIS	-	expression tag	UNP Q13315
A	-29	PRO	-	expression tag	UNP Q13315
A	-28	GLY	-	expression tag	UNP Q13315
A	-27	ILE	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	ILE	-	expression tag	UNP Q13315
A	-25	PRO	-	expression tag	UNP Q13315
A	-24	PRO	-	expression tag	UNP Q13315
A	-23	HIS	-	expression tag	UNP Q13315
A	-22	ALA	-	expression tag	UNP Q13315
A	-21	THR	-	expression tag	UNP Q13315
A	-20	LEU	-	expression tag	UNP Q13315
A	-19	VAL	-	expression tag	UNP Q13315
A	-18	PHE	-	expression tag	UNP Q13315
A	-17	ASP	-	expression tag	UNP Q13315
A	-16	VAL	-	expression tag	UNP Q13315
A	-15	GLU	-	expression tag	UNP Q13315
A	-14	LEU	-	expression tag	UNP Q13315
A	-13	LEU	-	expression tag	UNP Q13315
A	-12	LYS	-	expression tag	UNP Q13315
A	-11	LEU	-	expression tag	UNP Q13315
A	-10	GLU	-	expression tag	UNP Q13315
A	-9	GLY	-	expression tag	UNP Q13315
A	-8	GLY	-	expression tag	UNP Q13315
A	-7	SER	-	expression tag	UNP Q13315
A	-6	ALA	-	expression tag	UNP Q13315
A	-5	GLY	-	expression tag	UNP Q13315
A	-4	SER	-	expression tag	UNP Q13315
A	-3	GLY	-	expression tag	UNP Q13315
A	-2	SER	-	expression tag	UNP Q13315
A	-1	ALA	-	expression tag	UNP Q13315
A	0	SER	-	expression tag	UNP Q13315
A	2971	ALA	GLN	engineered mutation	UNP Q13315
B	-127	MET	-	initiating methionine	UNP Q13315
B	-126	ASP	-	expression tag	UNP Q13315
B	-125	TYR	-	expression tag	UNP Q13315
B	-124	LYS	-	expression tag	UNP Q13315
B	-123	ASP	-	expression tag	UNP Q13315
B	-122	ASP	-	expression tag	UNP Q13315
B	-121	ASP	-	expression tag	UNP Q13315
B	-120	ASP	-	expression tag	UNP Q13315
B	-119	LYS	-	expression tag	UNP Q13315
B	-118	HIS	-	expression tag	UNP Q13315
B	-117	MET	-	expression tag	UNP Q13315
B	-116	GLY	-	expression tag	UNP Q13315
B	-115	VAL	-	expression tag	UNP Q13315
B	-114	GLN	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-113	VAL	-	expression tag	UNP Q13315
B	-112	GLU	-	expression tag	UNP Q13315
B	-111	THR	-	expression tag	UNP Q13315
B	-110	ILE	-	expression tag	UNP Q13315
B	-109	SER	-	expression tag	UNP Q13315
B	-108	PRO	-	expression tag	UNP Q13315
B	-107	GLY	-	expression tag	UNP Q13315
B	-106	ASP	-	expression tag	UNP Q13315
B	-105	GLY	-	expression tag	UNP Q13315
B	-104	ARG	-	expression tag	UNP Q13315
B	-103	THR	-	expression tag	UNP Q13315
B	-102	PHE	-	expression tag	UNP Q13315
B	-101	PRO	-	expression tag	UNP Q13315
B	-100	LYS	-	expression tag	UNP Q13315
B	-99	ARG	-	expression tag	UNP Q13315
B	-98	GLY	-	expression tag	UNP Q13315
B	-97	GLN	-	expression tag	UNP Q13315
B	-96	THR	-	expression tag	UNP Q13315
B	-95	CYS	-	expression tag	UNP Q13315
B	-94	VAL	-	expression tag	UNP Q13315
B	-93	VAL	-	expression tag	UNP Q13315
B	-92	HIS	-	expression tag	UNP Q13315
B	-91	TYR	-	expression tag	UNP Q13315
B	-90	THR	-	expression tag	UNP Q13315
B	-89	GLY	-	expression tag	UNP Q13315
B	-88	MET	-	expression tag	UNP Q13315
B	-87	LEU	-	expression tag	UNP Q13315
B	-86	GLU	-	expression tag	UNP Q13315
B	-85	ASP	-	expression tag	UNP Q13315
B	-84	GLY	-	expression tag	UNP Q13315
B	-83	LYS	-	expression tag	UNP Q13315
B	-82	LYS	-	expression tag	UNP Q13315
B	-81	PHE	-	expression tag	UNP Q13315
B	-80	ASP	-	expression tag	UNP Q13315
B	-79	SER	-	expression tag	UNP Q13315
B	-78	SER	-	expression tag	UNP Q13315
B	-77	ARG	-	expression tag	UNP Q13315
B	-76	ASP	-	expression tag	UNP Q13315
B	-75	ARG	-	expression tag	UNP Q13315
B	-74	ASN	-	expression tag	UNP Q13315
B	-73	LYS	-	expression tag	UNP Q13315
B	-72	PRO	-	expression tag	UNP Q13315

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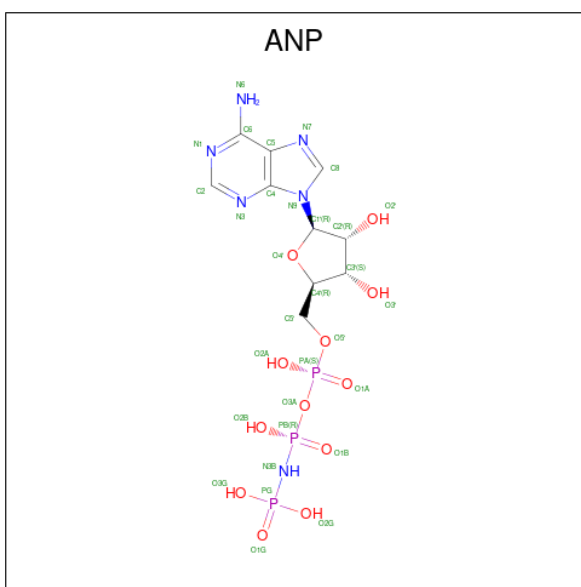
Chain	Residue	Modelled	Actual	Comment	Reference
B	-71	PHE	-	expression tag	UNP Q13315
B	-70	LYS	-	expression tag	UNP Q13315
B	-69	PHE	-	expression tag	UNP Q13315
B	-68	MET	-	expression tag	UNP Q13315
B	-67	LEU	-	expression tag	UNP Q13315
B	-66	GLY	-	expression tag	UNP Q13315
B	-65	LYS	-	expression tag	UNP Q13315
B	-64	GLN	-	expression tag	UNP Q13315
B	-63	GLU	-	expression tag	UNP Q13315
B	-62	VAL	-	expression tag	UNP Q13315
B	-61	ILE	-	expression tag	UNP Q13315
B	-60	ARG	-	expression tag	UNP Q13315
B	-59	GLY	-	expression tag	UNP Q13315
B	-58	TRP	-	expression tag	UNP Q13315
B	-57	GLU	-	expression tag	UNP Q13315
B	-56	GLU	-	expression tag	UNP Q13315
B	-55	GLY	-	expression tag	UNP Q13315
B	-54	VAL	-	expression tag	UNP Q13315
B	-53	ALA	-	expression tag	UNP Q13315
B	-52	GLN	-	expression tag	UNP Q13315
B	-51	MET	-	expression tag	UNP Q13315
B	-50	SER	-	expression tag	UNP Q13315
B	-49	VAL	-	expression tag	UNP Q13315
B	-48	GLY	-	expression tag	UNP Q13315
B	-47	GLN	-	expression tag	UNP Q13315
B	-46	ARG	-	expression tag	UNP Q13315
B	-45	ALA	-	expression tag	UNP Q13315
B	-44	LYS	-	expression tag	UNP Q13315
B	-43	LEU	-	expression tag	UNP Q13315
B	-42	THR	-	expression tag	UNP Q13315
B	-41	ILE	-	expression tag	UNP Q13315
B	-40	SER	-	expression tag	UNP Q13315
B	-39	PRO	-	expression tag	UNP Q13315
B	-38	ASP	-	expression tag	UNP Q13315
B	-37	TYR	-	expression tag	UNP Q13315
B	-36	ALA	-	expression tag	UNP Q13315
B	-35	TYR	-	expression tag	UNP Q13315
B	-34	GLY	-	expression tag	UNP Q13315
B	-33	ALA	-	expression tag	UNP Q13315
B	-32	THR	-	expression tag	UNP Q13315
B	-31	GLY	-	expression tag	UNP Q13315
B	-30	HIS	-	expression tag	UNP Q13315

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	PRO	-	expression tag	UNP Q13315
B	-28	GLY	-	expression tag	UNP Q13315
B	-27	ILE	-	expression tag	UNP Q13315
B	-26	ILE	-	expression tag	UNP Q13315
B	-25	PRO	-	expression tag	UNP Q13315
B	-24	PRO	-	expression tag	UNP Q13315
B	-23	HIS	-	expression tag	UNP Q13315
B	-22	ALA	-	expression tag	UNP Q13315
B	-21	THR	-	expression tag	UNP Q13315
B	-20	LEU	-	expression tag	UNP Q13315
B	-19	VAL	-	expression tag	UNP Q13315
B	-18	PHE	-	expression tag	UNP Q13315
B	-17	ASP	-	expression tag	UNP Q13315
B	-16	VAL	-	expression tag	UNP Q13315
B	-15	GLU	-	expression tag	UNP Q13315
B	-14	LEU	-	expression tag	UNP Q13315
B	-13	LEU	-	expression tag	UNP Q13315
B	-12	LYS	-	expression tag	UNP Q13315
B	-11	LEU	-	expression tag	UNP Q13315
B	-10	GLU	-	expression tag	UNP Q13315
B	-9	GLY	-	expression tag	UNP Q13315
B	-8	GLY	-	expression tag	UNP Q13315
B	-7	SER	-	expression tag	UNP Q13315
B	-6	ALA	-	expression tag	UNP Q13315
B	-5	GLY	-	expression tag	UNP Q13315
B	-4	SER	-	expression tag	UNP Q13315
B	-3	GLY	-	expression tag	UNP Q13315
B	-2	SER	-	expression tag	UNP Q13315
B	-1	ALA	-	expression tag	UNP Q13315
B	0	SER	-	expression tag	UNP Q13315
B	2971	ALA	GLN	engineered mutation	UNP Q13315

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

- 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 Mg 1 1	0
4	B	1	Total Mg 1 1	0

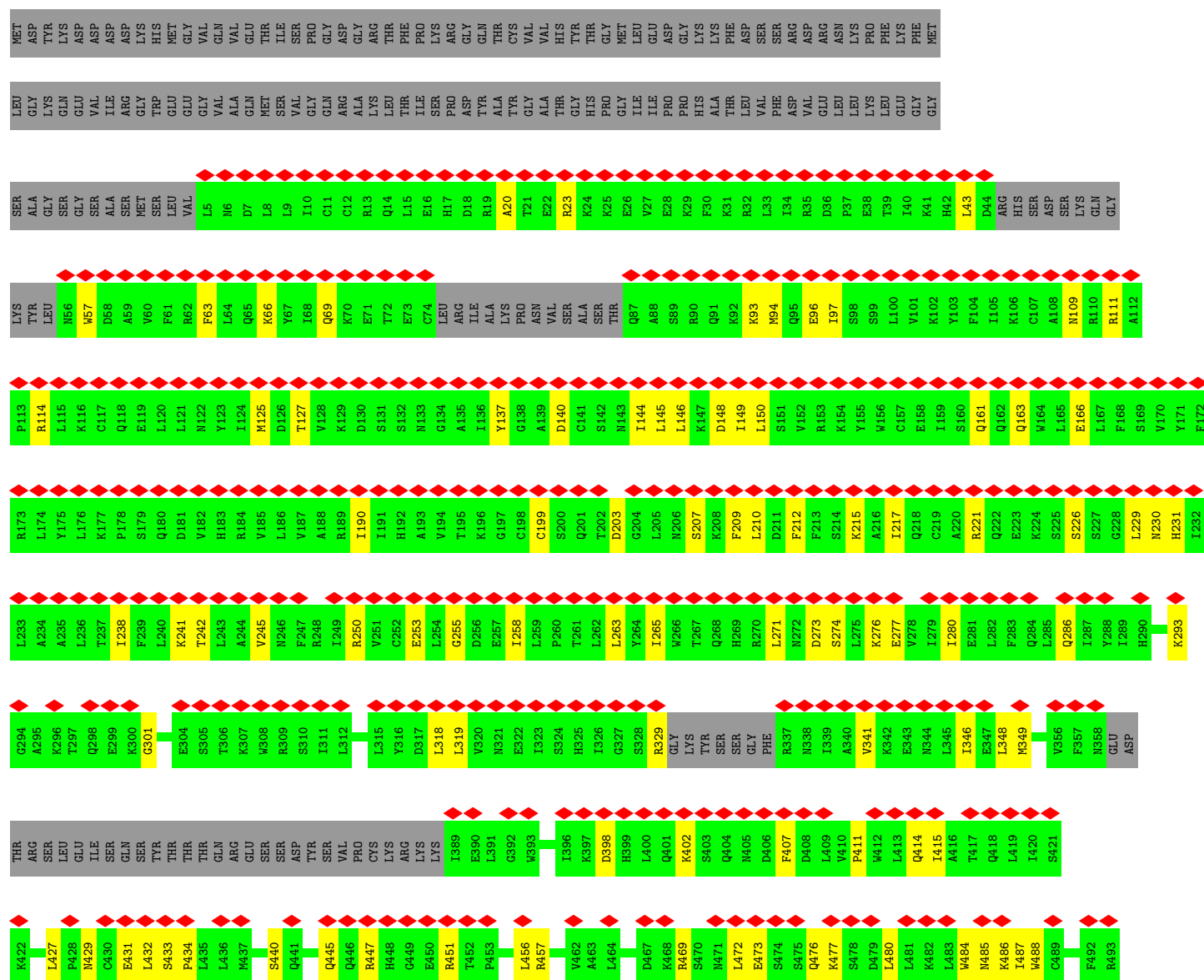
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0
5	B	1	Total Zn 1 1	0



M1071	E1072	V1073	F1074	T1075	L1078	A1079	D1080	N1081	H1082	H1083	Q1084	V1085	A1090	E1091	R1095	Q1098	T1099	L1100	K1101	GLY	ASP	SER	SER	ARG	LEU	L1108	K1109	A1110	L1111	Q1116	E1121	N1122	A1123	Q1128	E1129	G1130	M1131	R1132	E1133	M1134	SER	HIS	SER	ALA	GLU	ASN	PRO	E1142	T1143	L1144	D1145	E1146	
I1147	Y1148	N1149	L1154	T1155	T1156	L1157	I1158	A1159	L1162	S1163	P1166	E1169	K1170	L1173	F1174	A1175	L1176	C1177	K1178	S1179	V1180	K1181	E1182	N1183	G1184	L1185	L1189	V1190	K1191	K1192	V1193	L1194	D1285	C1286	F1287	P1288	K1289	I1290	L1291	V1292	N1293	L1294	Y1297	F1298	A1299	Y1300	E1301	G1302	T1303	R1304	Q1225		
D1226	T1227	E1228	F1234	T1235	F1236	I1237	L1238	L1239	N1240	Y1241	T1242	MET	V1318	Y1319	D1320	M1321	L1322	K1323	S1324	E1325	N1326	L1327	L1328	G1329	K1330	Q1331	D1332	H1334	I1337	S1338	P1341	V1344	V1345	E1346	L1347	L1348	M1349	T1350	L1351	P1354	ALA	ASN	SER	SER	ALA	GLN	SER	THR	ASP	LEU	CYS	PHE	SER
GLY	D1371	L1372	P1376	N1377	P1378	F1381	V1385	I1386	K1387	S1394	K1398	T1399	K1400	L1401	K1402	I1404	L1405	E1406	I1407	K1410	Y1415	Q1416	K1417	I1418	L1419	L1420	A1421	E1424	Q1425	A1426	H1436	R1437	I1438	L1439	K1440	I1441	Y1442	H1443	S1447	L1450	K1451	D1452	I1453	K1454	L1457	G1458							
G1459	A1460	V1464	L1465	V1468	R1479	PRO	CYS	ILE	MET	ASP	SER	VAL	SER	LEU	ARG	S1490	L1493	A1510	L1513	E1514	L1517	L1524	V1538	L1539	D1540	L1541	L1542	K1543	N1552	E1553	N1554	L1555	L1561	P1566	F1571	D1572	L1573	L1574	R1575	I1576	T1577	L1590	T1594	Q1765									
V1600	P1607	R1610	L1611	L1614	K1625	M1628	D1637	L1652	A1658	H1661	P1680	S1684	T1685	I1686	D1693	K1701	E1704	D1705	L1708	N1719	V1734	L1737	L1741	H1747	S1748	E1751	I1752	Y1753	K1754	T1757	D1758	P1759	M1760	L1761	L1764	Q1765																	
P1766	F1767	R1768	THR	SER	ARG	LYS	LYS	PHE	LEU	GLU	VAL	PRO	ARG	PHE	ASP	GLY	ASN	P1785	L1789	L1798	S1799	E1800	N1801	H1802	I1806	T1810	C1821	L1824	L1827	K1834	T1835	D1836	F1837	C1838	P1843	W1858	R1859	V1866	F1869	F1870	H1876	PHE	SER	GLN	THR								
SER	ARG	THR	THR	PRO	ALA	ASN	LEU	ASP	SER	GLU	GLU	SER	HIS	PHE	GLY	ARG	C1899	C1900	L1901	Q1906	M1909	V1912	Y1915	M1916	Q1919	K1920	R1921	A1931	F1932	W1933	L1934	D1935	L1936	N1937	Y1938	V1944	F1952	T1953	A1954	L1955	Y1961	K1964	S1974	LEU	ALA	PHE	GLU						
GLU	GLY	SER	SER	T1984	Q2002	E2007	L2008	T2009	R2010	S2011	T2012	G2013	E2014	C2021	M2041	K2044	L2051	T2065	L2068	L2077	L2081	W2091	L2095	H2099	Q2100	Q2101	W2104	R2105	C2112	THR	SER	VAL	SER	LYS	GLU	VAL	G2121	Y2129	L2147														
R2151	V2152	K2153	E2156	E2157	N2158	K2159	L2160	L2163	V2166	L2169	T2172	L2173	S2174	T2179	L2182	E2183	R2191	S2192	Q2197	E2200	T2203	D2216	F2217	L2231	E2238	R2244	L2251	T2252	K2253	V2256	E2257	T2260	P2271	L2275	F2276	D2320	A2324																
N2327	L2330	T2335	V2355	T2356	Q2357	Q2358	T2359	A2364	D2372	Q2373	E2374	D2377	R2380	N2381	G2382	L2390	R2400	L2401	Y2404	K2413	Q2414	A2415	K2421	R2431	R2443	E2444	L2445	R2459	E2468	N2472	G2477	F2485	L2492	T2513	Y2514	K2515	F2516																
L2517	P2518	L2519	N2520	Q2521	Q2522	R2526	K2530	Q2531	N2532	Q2533	G2536	E2539	T2545	T2548	N2567	T2573	PRO	GLU	VAL	ALA	ARG	K2413	Q2414	A2415	K2421	R2431	R2443	E2444	L2445	R2459	E2468	N2472	G2477	F2485	L2492	T2513	Y2514	K2515	F2516														

- Molecule 2: Serine-protein kinase ATM







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30707	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 ($e^-/\text{\AA}^2$)	39.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.537	Depositor
Minimum map value	-0.253	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	330.4, 330.4, 330.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.826, 0.826, 0.826	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: ZN, ANP, MG

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	E	0.07	0/54	0.25	0/73
1	F	0.08	0/54	0.23	0/73
2	A	0.09	0/22409	0.24	0/30274
2	B	0.09	0/22409	0.25	0/30274
All	All	0.09	0/44926	0.25	0/60694

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	E	53	0	51	1	0
1	F	53	0	51	0	0
2	A	22001	0	22171	380	0
2	B	22001	0	22171	363	0
3	A	31	0	13	1	0
3	B	31	0	13	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
All	All	44174	0	44470	735	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 8.

The worst 5 of 735 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)
2:A:902:LYS:HE3	2:A:949:MET:HE2	1.54	0.89
2:A:901:LEU:HB2	2:A:949:MET:HE1	1.67	0.77
2:B:1876:HIS:CE1	2:B:1899:CYS:SG	2.73	0.76
2:A:259:LEU:HD21	2:A:286:GLN:HE22	1.51	0.76
2:B:718:CYS:SG	2:B:748:LYS:NZ	2.59	0.76

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	E	5/12 (42%)	5 (100%)	0	0	100	100
1	F	5/12 (42%)	5 (100%)	0	0	100	100
2	A	2708/3184 (85%)	2652 (98%)	56 (2%)	0	100	100
2	B	2708/3184 (85%)	2651 (98%)	57 (2%)	0	100	100
All	All	5426/6392 (85%)	5313 (98%)	113 (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	E	7/12 (58%)	7 (100%)	0	100	100
1	F	7/12 (58%)	7 (100%)	0	100	100
2	A	2444/2883 (85%)	2444 (100%)	0	100	100
2	B	2444/2883 (85%)	2444 (100%)	0	100	100
All	All	4902/5790 (85%)	4902 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
2	B	765	ASN
2	B	1310	GLN
2	B	996	HIS
2	B	1116	GLN
2	B	1416	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 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	$\# Z > 2$
3	ANP	A	3101	4	33,33,33	0.93	4 (12%)	45,52,52	0.58	0
3	ANP	B	3101	4	33,33,33	0.93	4 (12%)	45,52,52	0.58	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
3	ANP	A	3101	4	-	6/18/38/38	0/3/3/3
3	ANP	B	3101	4	-	6/18/38/38	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)
3	B	3101	ANP	PG-O1G	2.55	1.50	1.46
3	A	3101	ANP	PG-O1G	2.55	1.50	1.46
3	B	3101	ANP	PG-N3B	2.43	1.69	1.63
3	A	3101	ANP	PG-N3B	2.43	1.69	1.63
3	B	3101	ANP	PB-O1B	2.42	1.49	1.46

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	PB-N3B-PG-O1G
3	A	3101	ANP	C5'-O5'-PA-O1A
3	A	3101	ANP	C5'-O5'-PA-O3A

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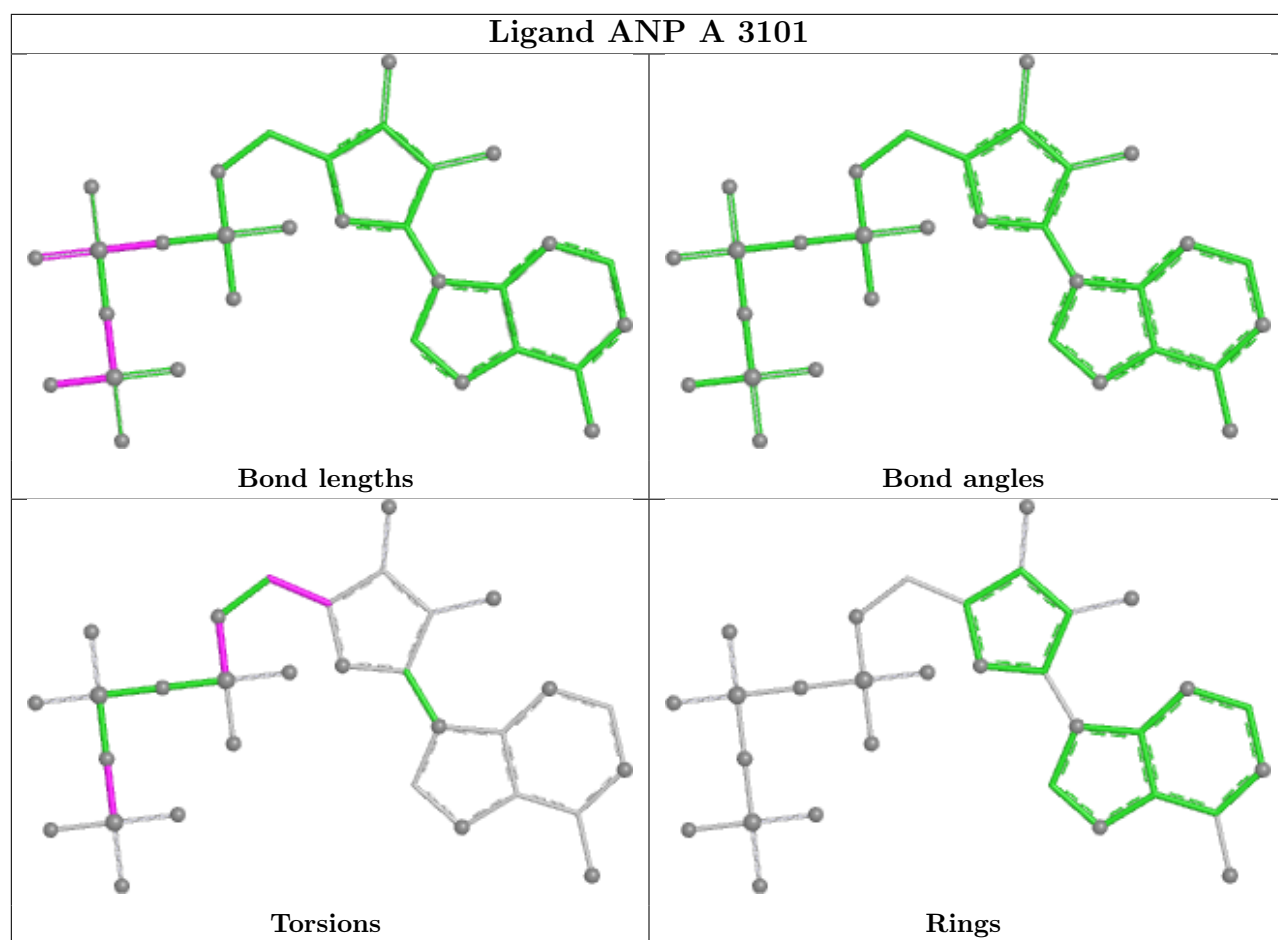
Mol	Chain	Res	Type	Atoms
3	A	3101	ANP	O4'-C4'-C5'-O5'
3	B	3101	ANP	PB-N3B-PG-O1G

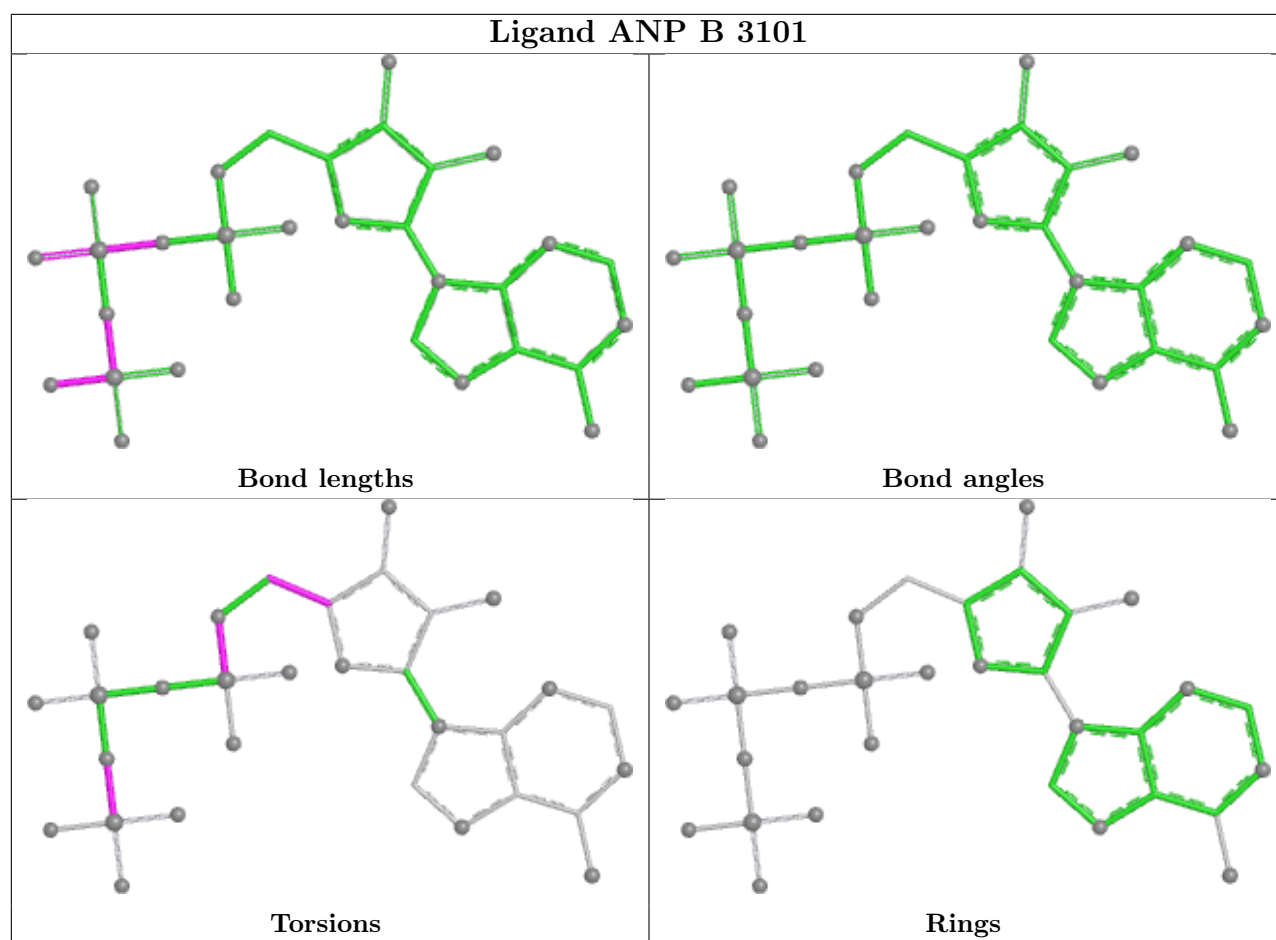
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3101	ANP	1	0
3	B	3101	ANP	3	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.

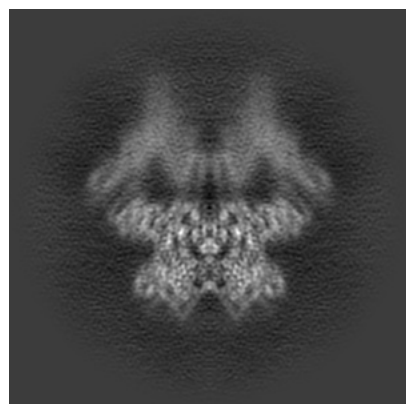
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17265. These allow visual inspection of the internal detail of the map and identification of artifacts.

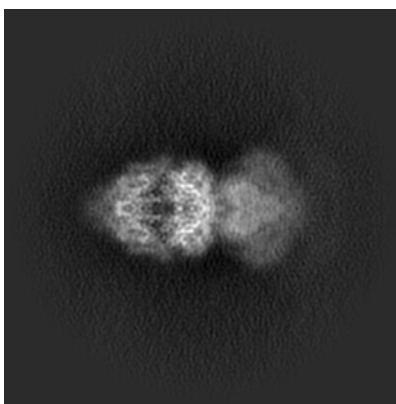
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

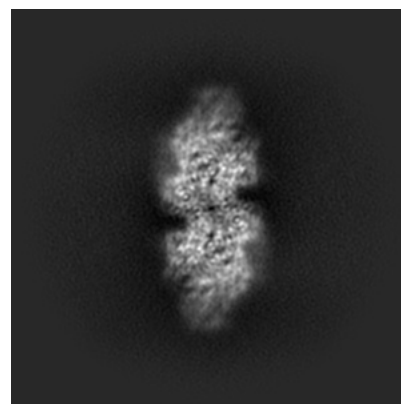
6.1.1 Primary map



X

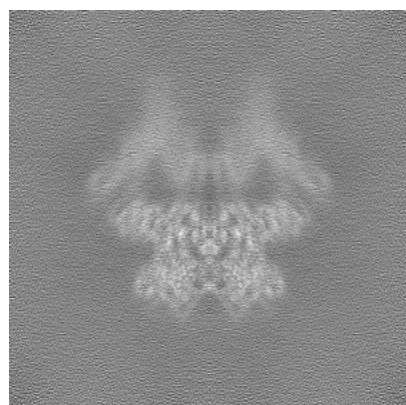


Y

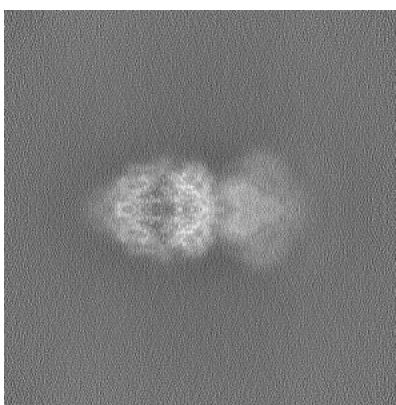


Z

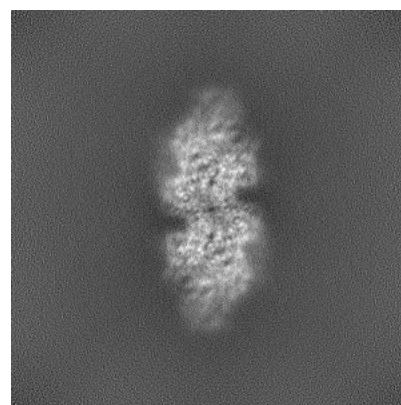
6.1.2 Raw map



X



Y

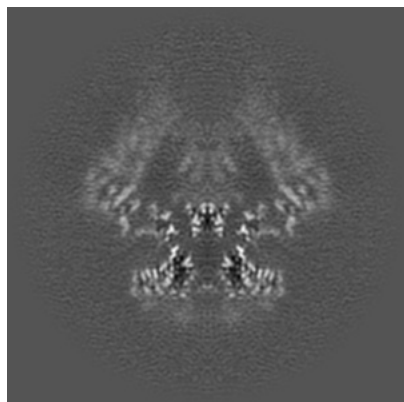


Z

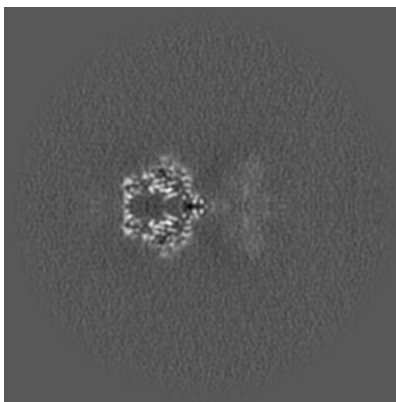
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

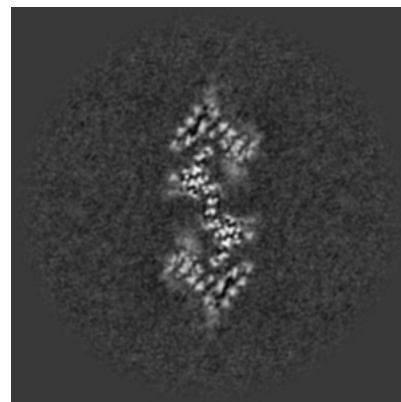
6.2.1 Primary map



X Index: 200

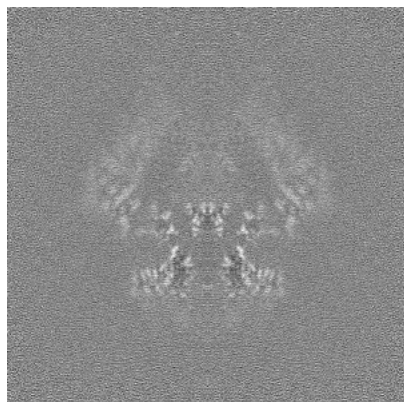


Y Index: 200

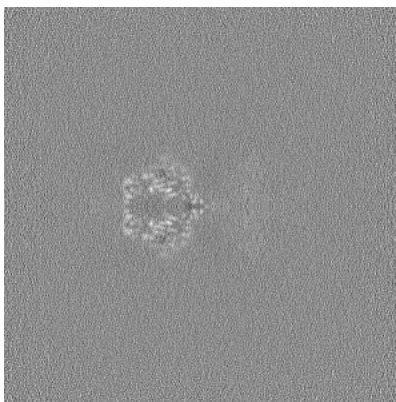


Z Index: 200

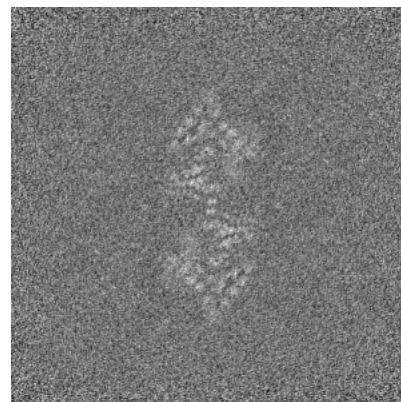
6.2.2 Raw map



X Index: 200



Y Index: 200

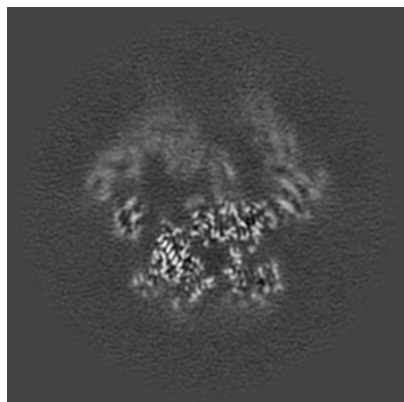


Z Index: 200

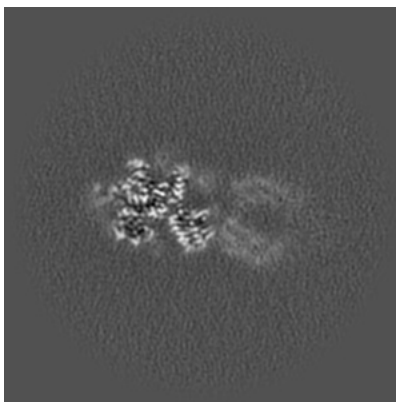
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

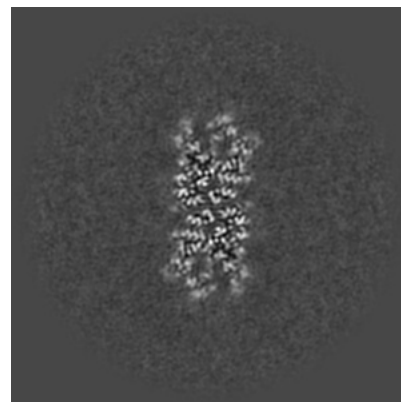
6.3.1 Primary map



X Index: 191

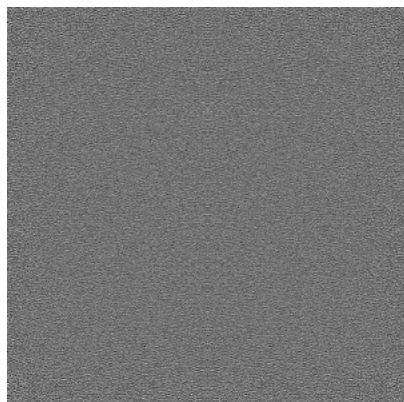


Y Index: 229

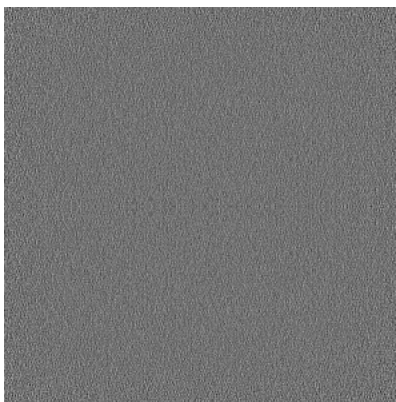


Z Index: 177

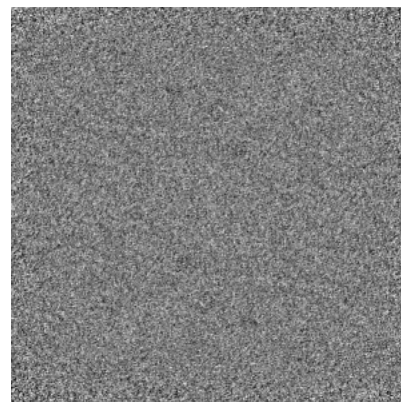
6.3.2 Raw map



X Index: 0



Y Index: 0

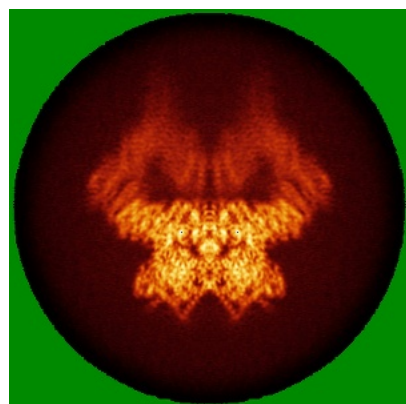


Z Index: 0

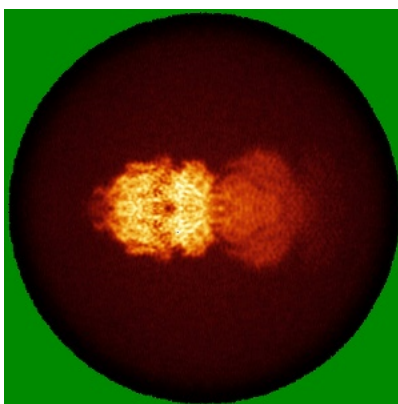
The images above show the largest variance slices of the map in three orthogonal directions.

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

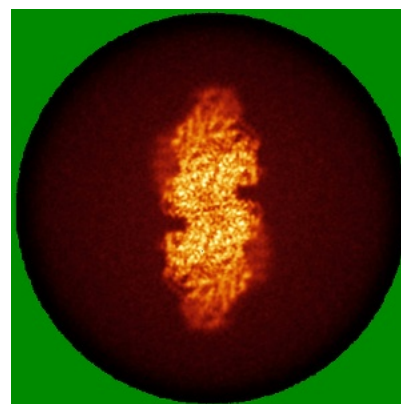
6.4.1 Primary map



X

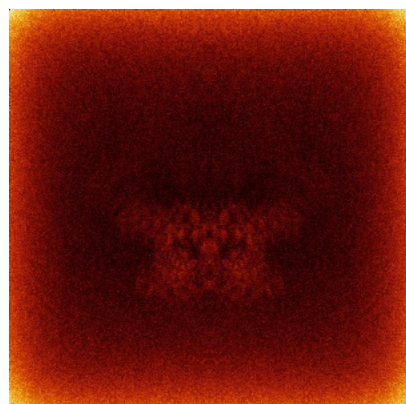


Y

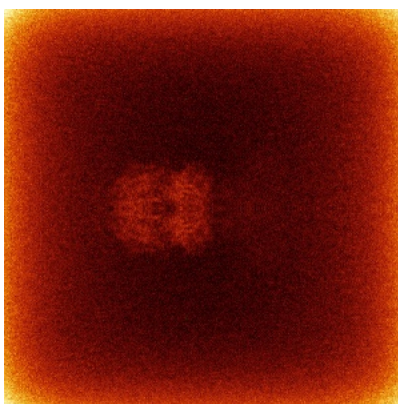


Z

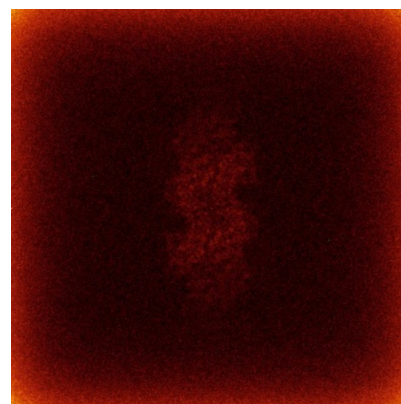
6.4.2 Raw map



X



Y

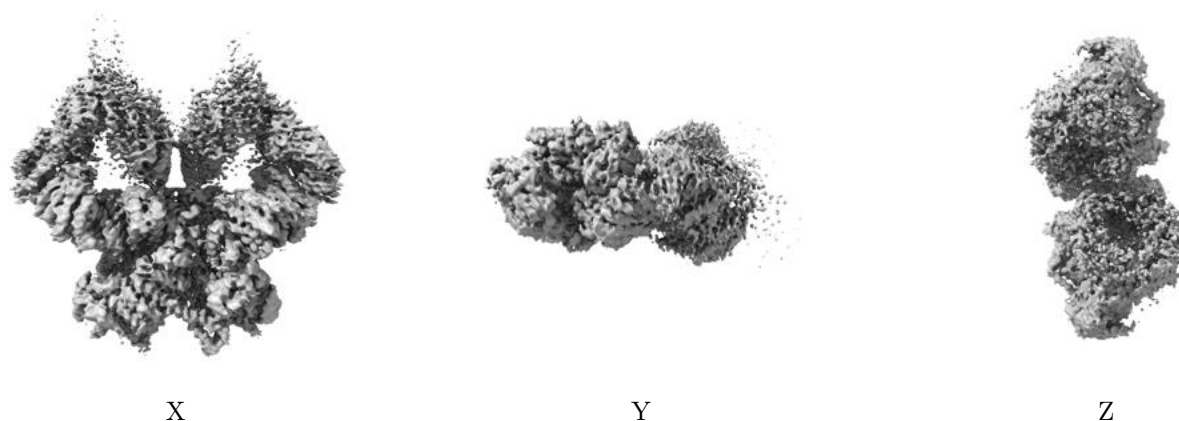


Z

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.

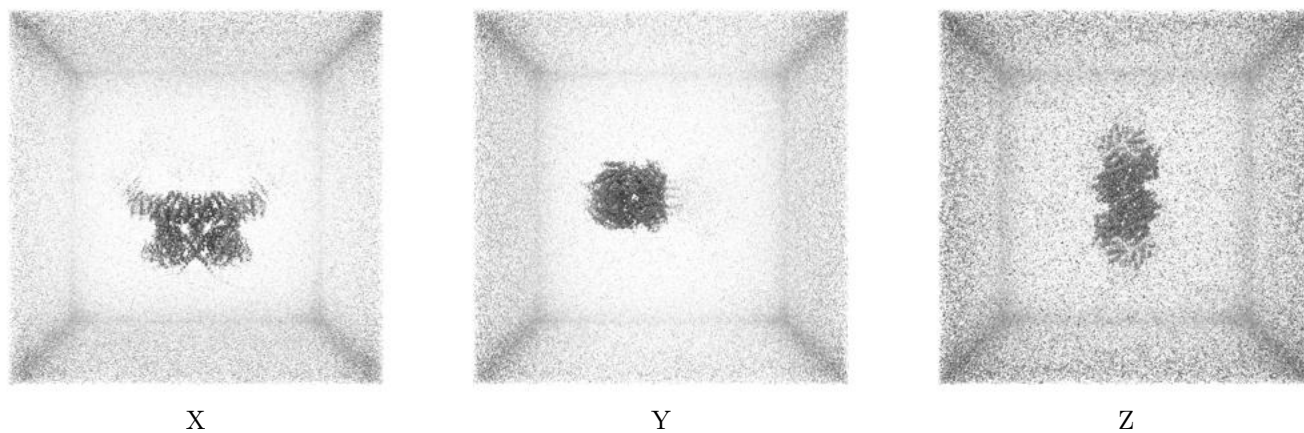
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

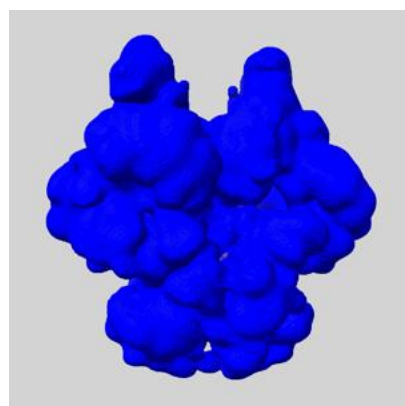
6.6 Mask visualisation [i](#)

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

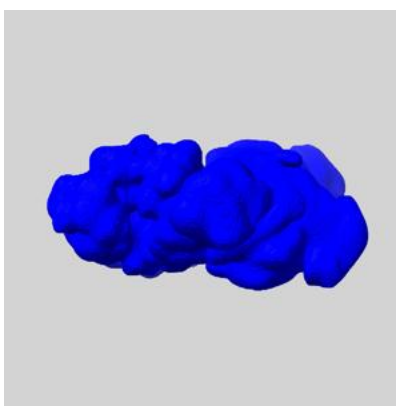
A mask typically either:

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

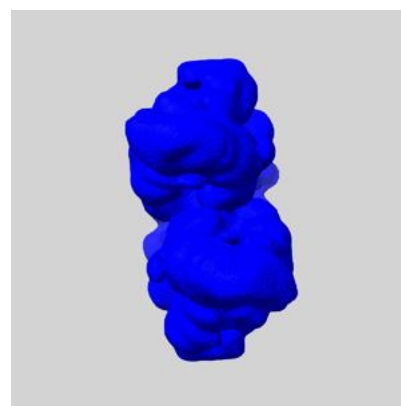
6.6.1 emd_17265_msk_1.map [i](#)



X



Y

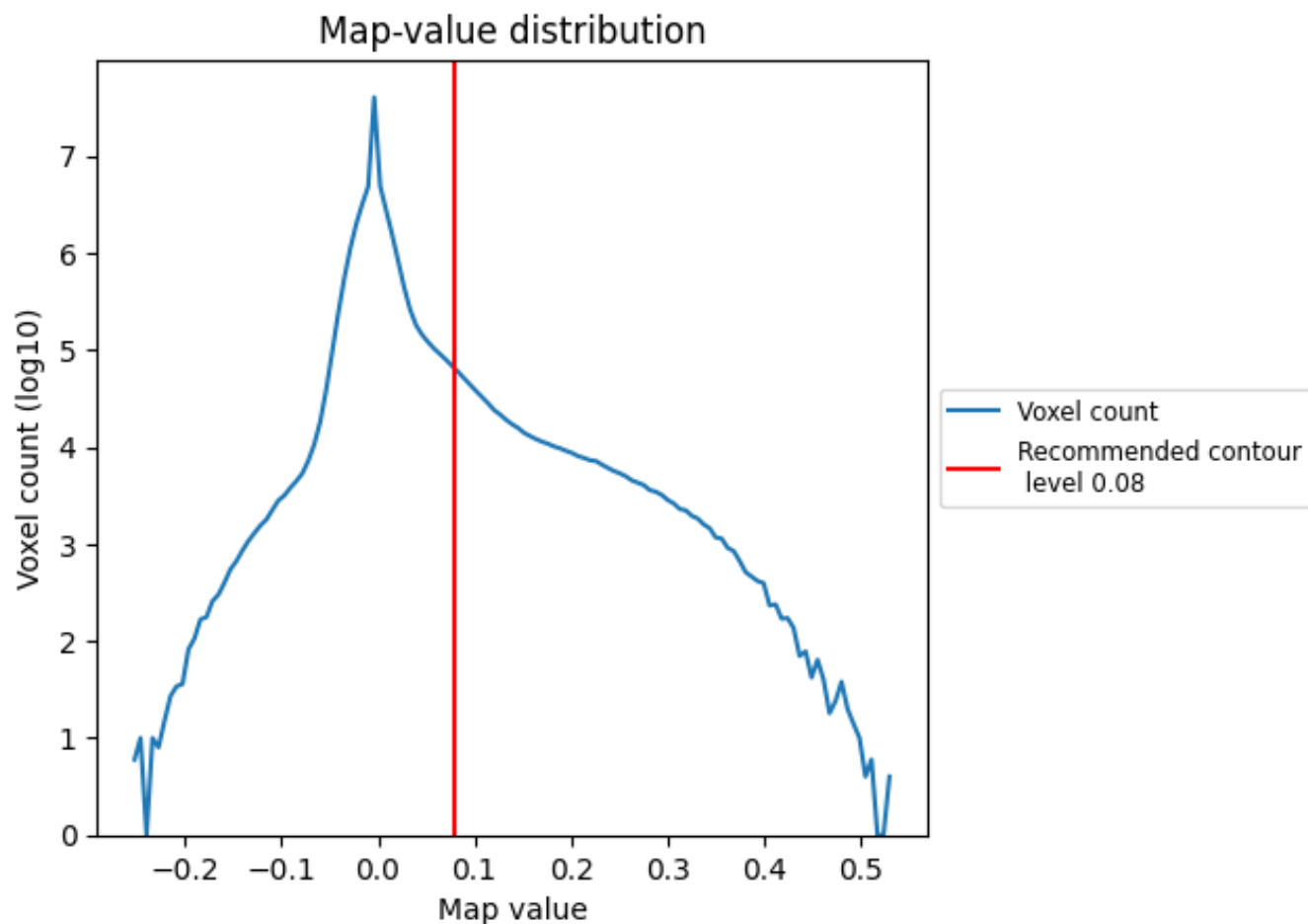


Z

7 Map analysis [i](#)

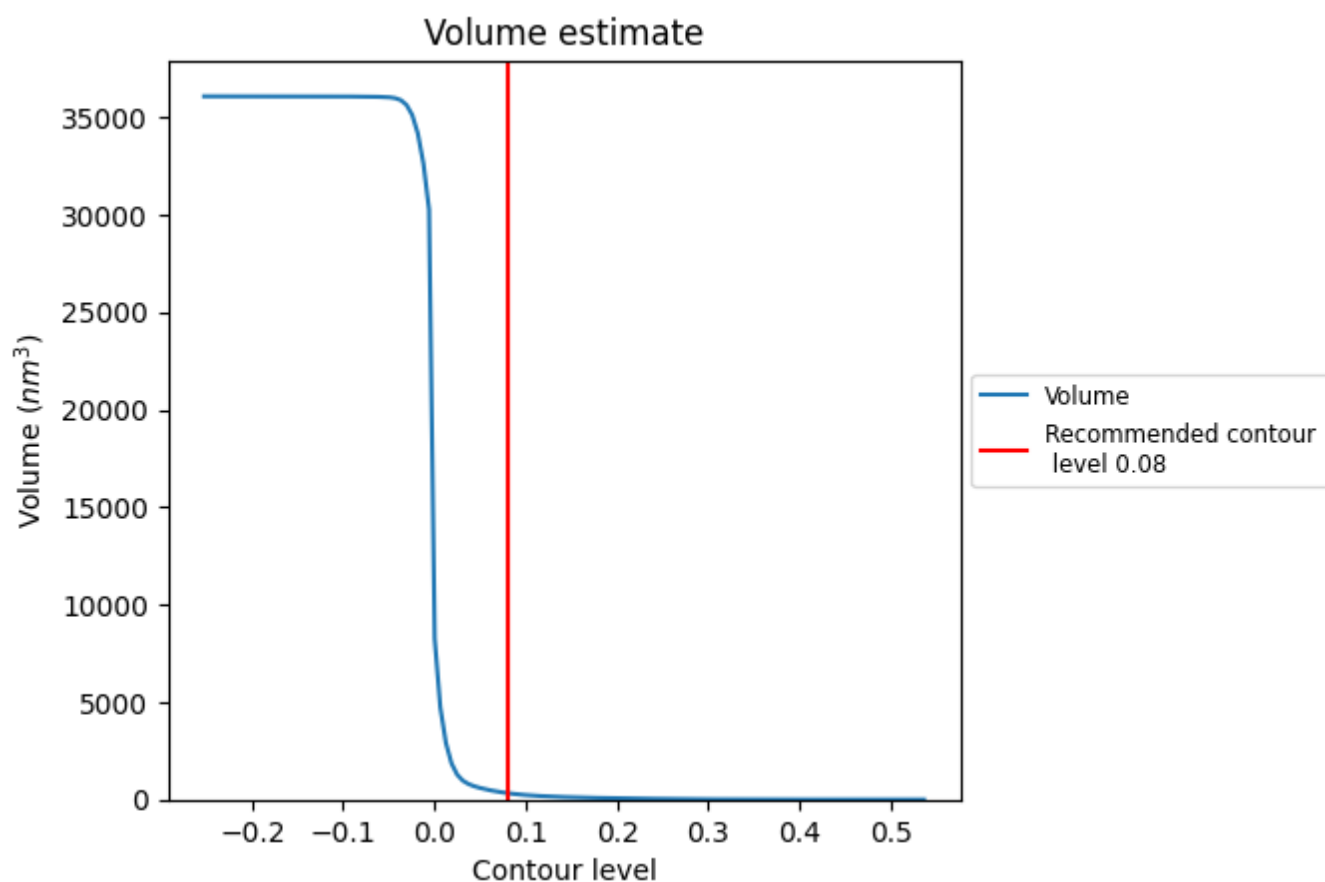
This section contains the results of statistical analysis of the map.

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.

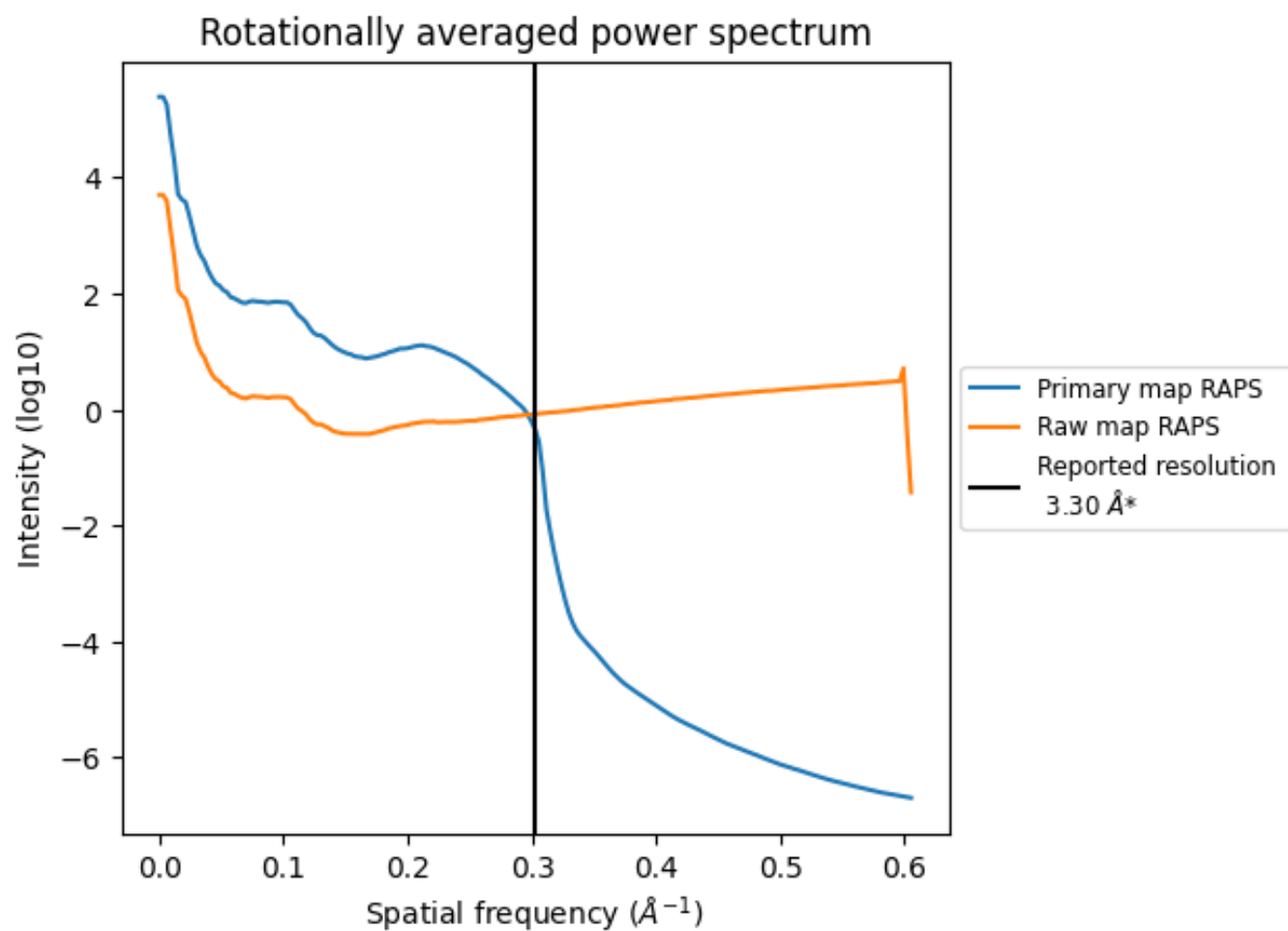
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm³; this corresponds to an approximate mass of 299 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 ⓘ

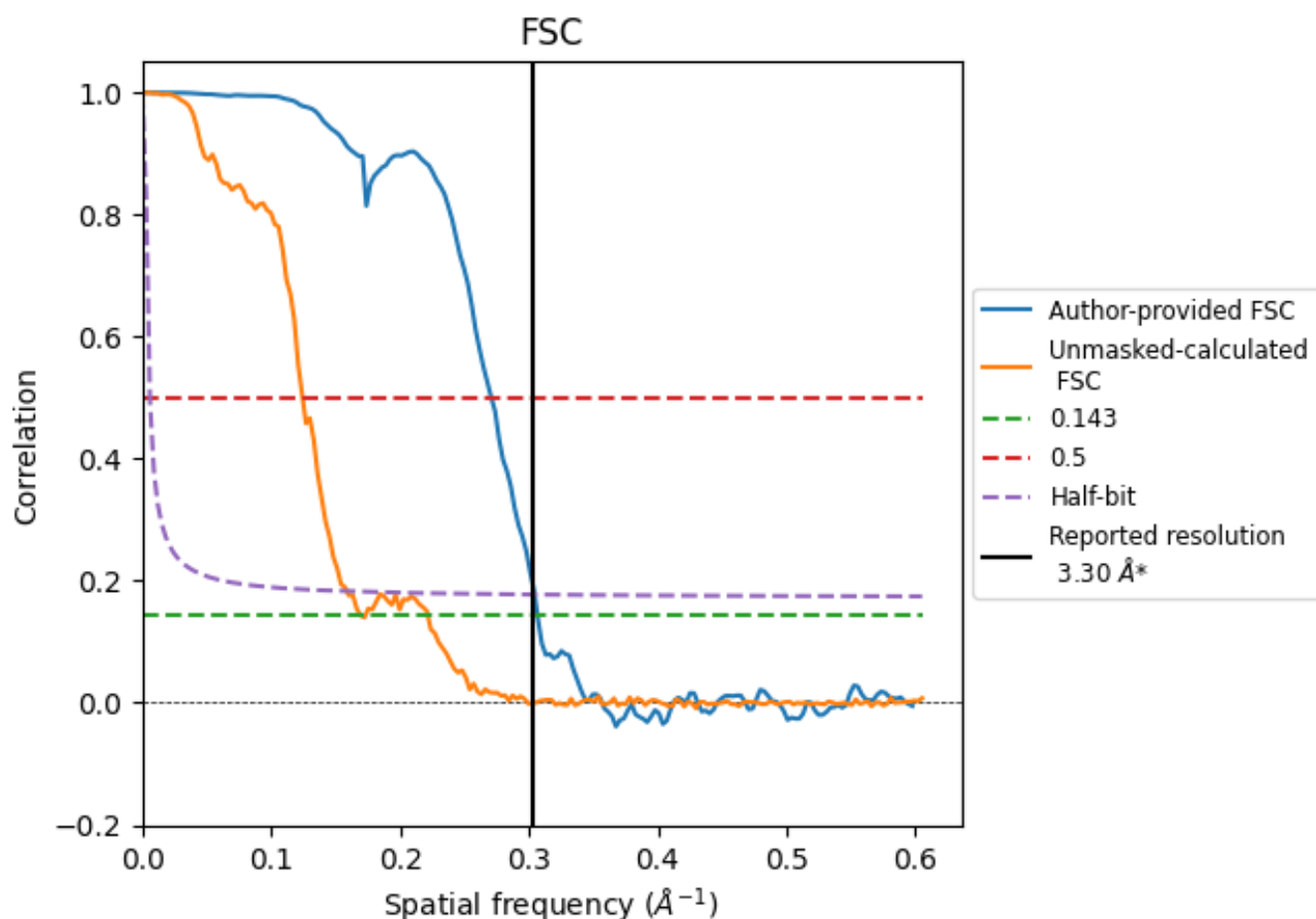


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

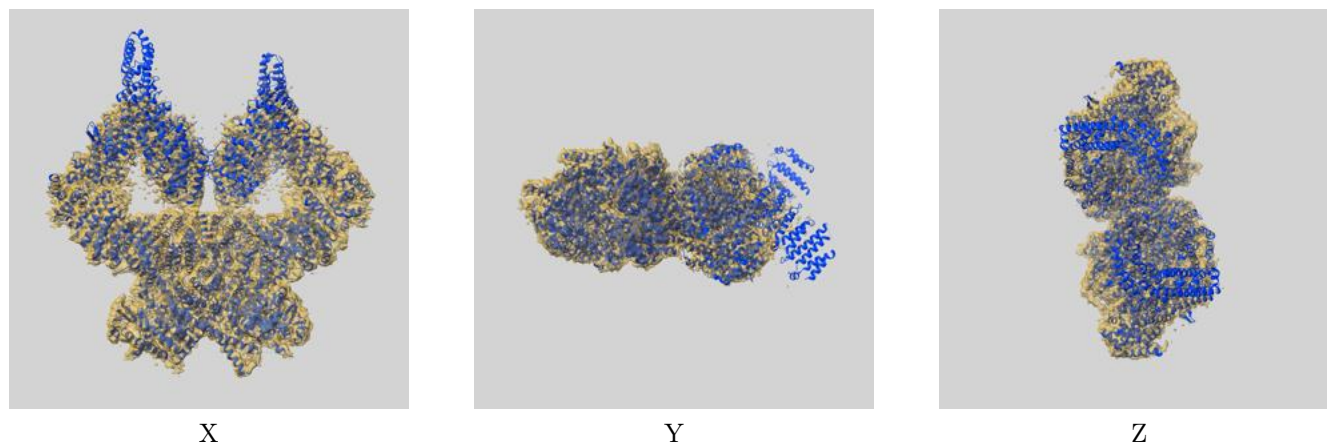
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.69	3.28
Unmasked-calculated*	5.90	8.04	6.29

*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 5.90 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

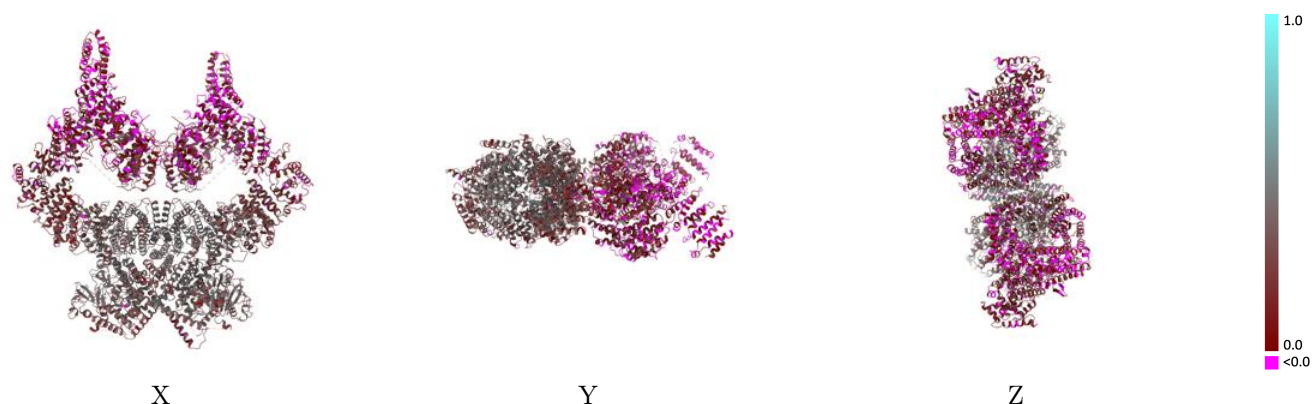
This section contains information regarding the fit between EMDB map EMD-17265 and PDB model 8OXM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



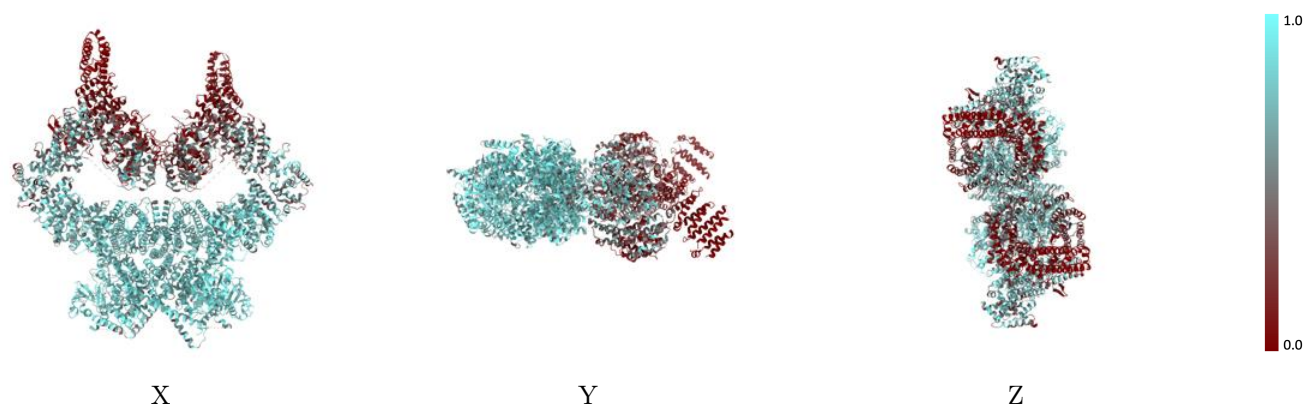
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



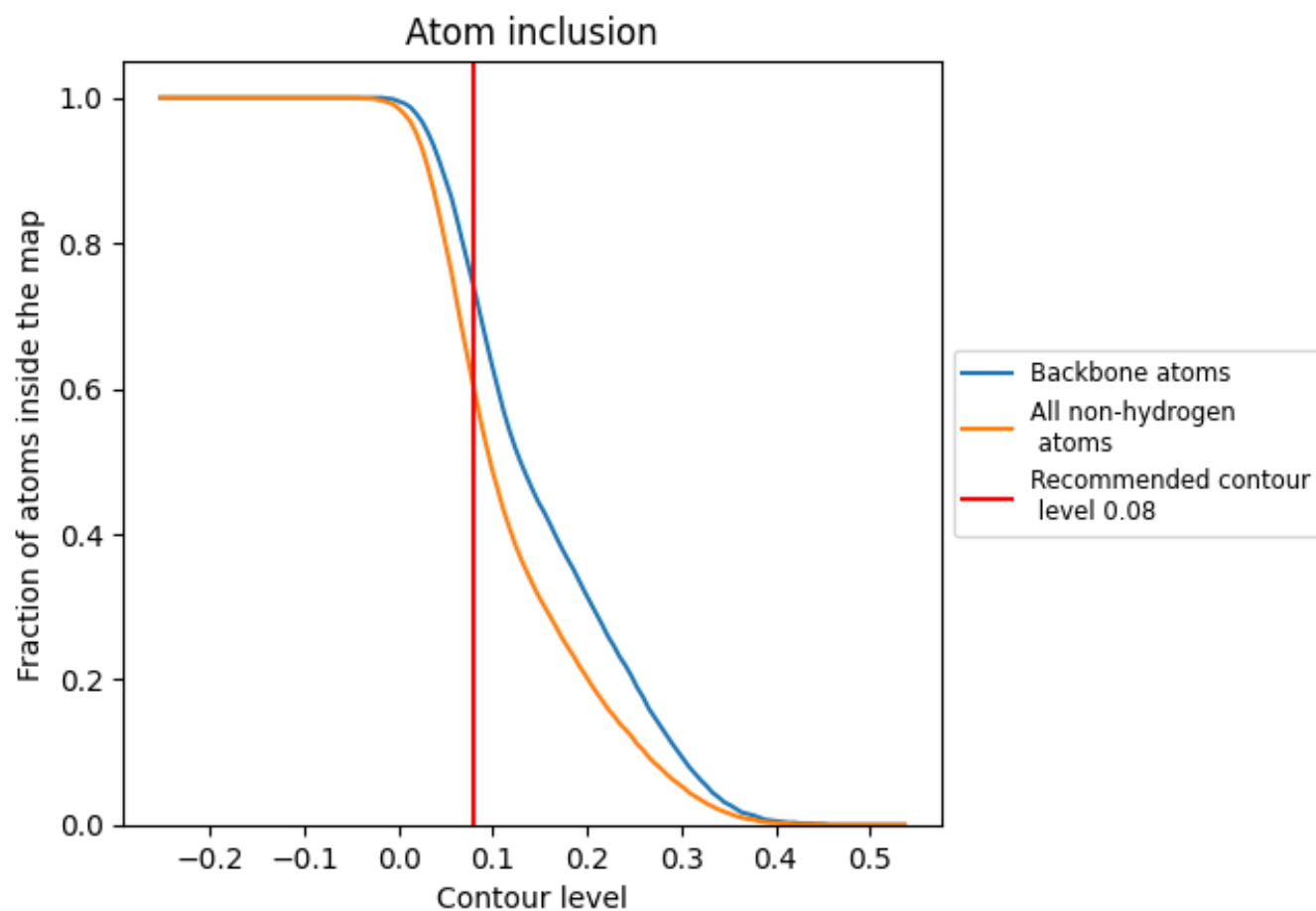
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 60% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.2450
A	0.5960	0.2410
B	0.6020	0.2480
E	0.2830	0.2750
F	0.2830	0.2820

