



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 02:02 AM UTC

PDB ID : 8OXQ / pdb_00008oxq
EMDB ID : EMD-17268
Title : ATM(Q2971A) dimeric C-terminal region in complex with Mg AMP-PNP
Authors : Howes, A.C.; Perisic, O.; Williams, R.L.
Deposited on : 2023-05-02
Resolution : 2.50 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

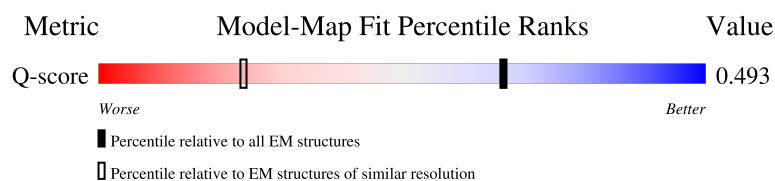
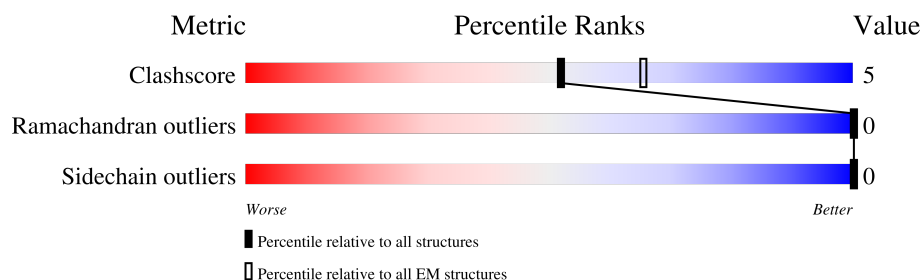
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	3184	 41% 7% 51%
1	B	3184	 41% 7% 51%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25078 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	1550	Total	C	N	O	S	0	0
			12506	7960	2138	2321	87		
1	B	1550	Total	C	N	O	S	0	0
			12506	7960	2138	2321	87		

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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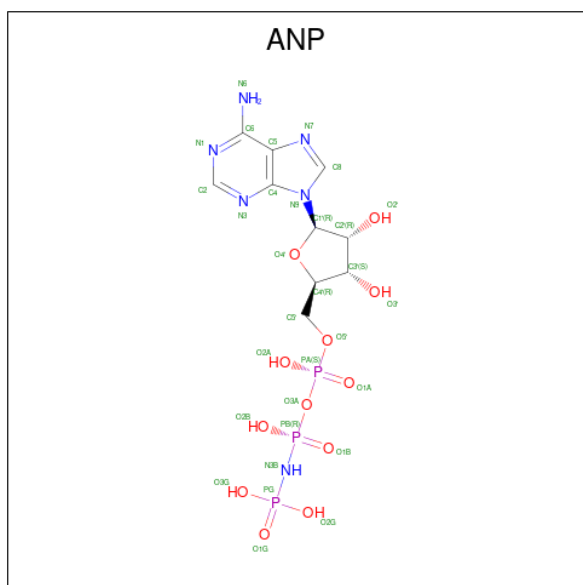
Chain	Residue	Modelled	Actual	Comment	Reference
B	-62	VAL	-	expression tag	UNP Q13315
B	-61	ILE	-	expression tag	UNP Q13315
B	-60	ARG	-	expression tag	UNP Q13315
B	-59	GLY	-	expression tag	UNP Q13315
B	-58	TRP	-	expression tag	UNP Q13315
B	-57	GLU	-	expression tag	UNP Q13315
B	-56	GLU	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 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	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

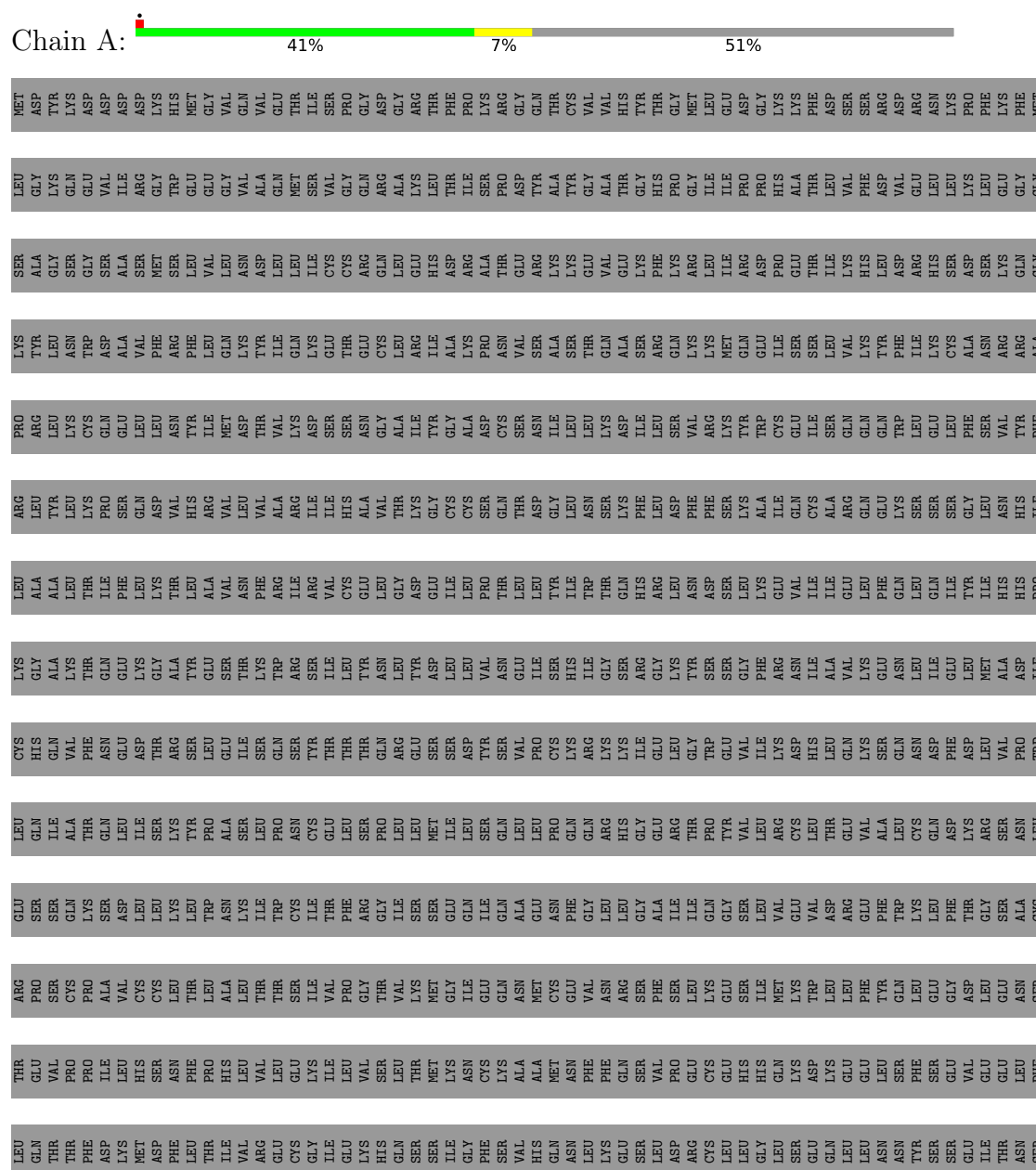
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

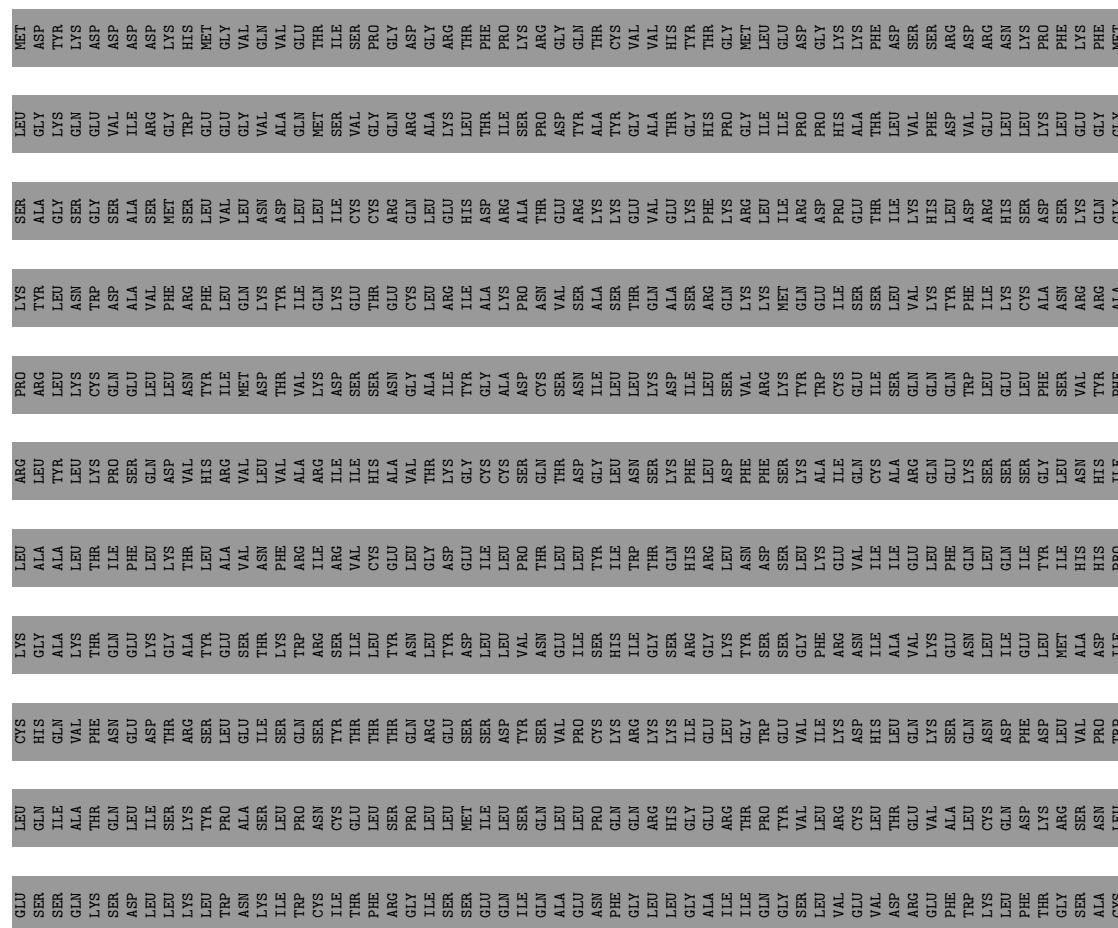
3 Residue-property plots

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

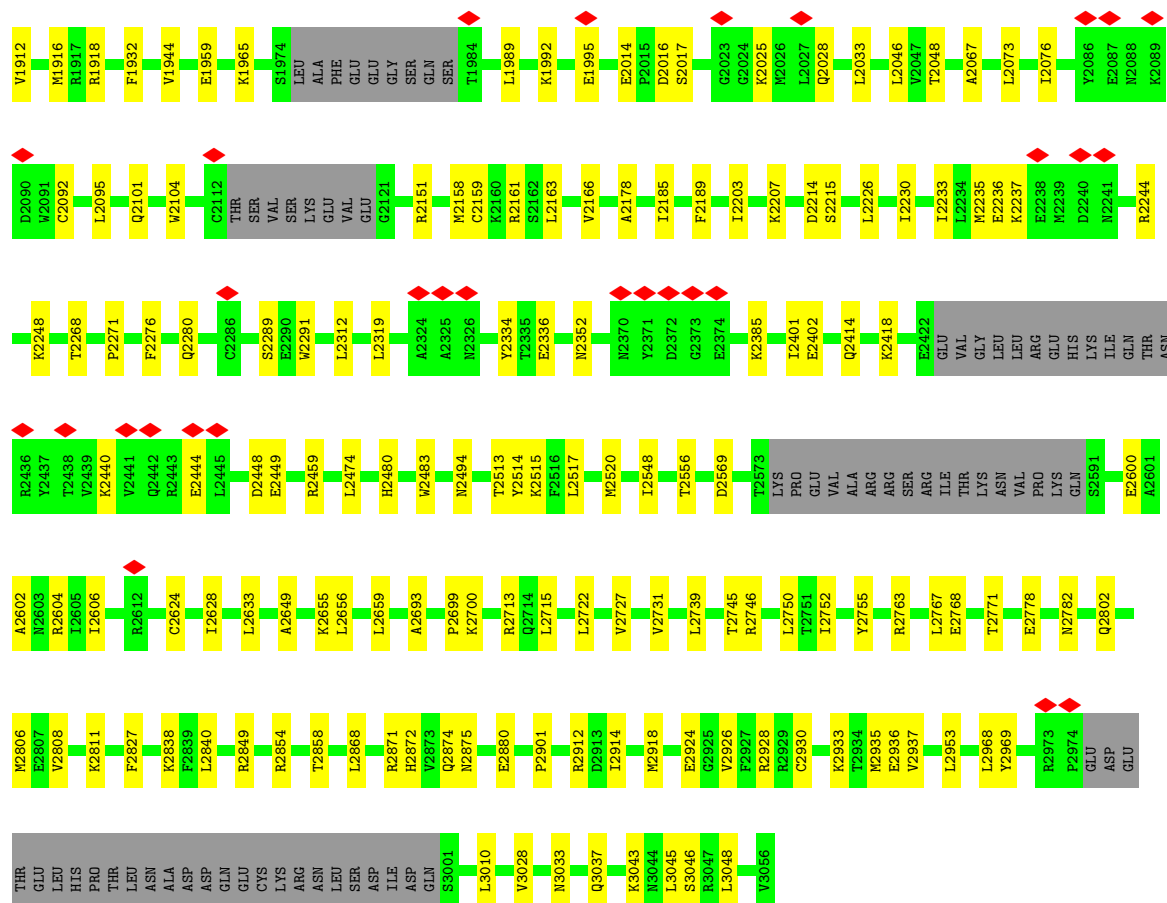
• Molecule 1: Serine-protein kinase ATM



I2076	T2086	E2087	N2088	K2089	D2090	W2091	C2092	L2095	Q2101	W2104	C2112	THR	SER	VAL	SER	LYS	GLU	VAL	GLU	GLY	GLU	ALA	GLN	SER	THR	R2151	M2158	C2159	K2160	R2161	S2162	L2163	V2166	A2178	I2185	L2188	F2189	L2198	I2203	K2207	D2214	L2226	I2230	I2233		
ARG	C1899	C1900	D1902	K1903	R1907	V1912	M1916	F1932	V1944	E1959	K1965	S1974	LEU	ALA	PHE	GLU	GLU	GLY	SER	GLN	SER	T1984	L1989	K1992	E1995	E2014	P2015	D2016	S2017	G2023	G2024	M2026	L2027	Q2028	L2033	L2046	V2047	T2048	A2067	L2073						
E1751	P1766	K1772	R1779	F1780	D1781	K1782	E1783	I1796	P1797	L1798	K1820	C1821	E1822	L1823	L1824	Q1825	L1826	P1843	Y1844	L1845	I1849	L1850	R1859	F1870	C1873	L1874	R1875	H1876	PHE	SER	GLN	THR	SER	ARG	THR	THR	PRO	ALA	ASN	ASP	SER	GLU	SER	HIS	PHE	
L1590	H1596	V1600	S1601	A1605	L1606	P1607	L1608	D1616	L1617	R1618	R1619	Q1620	L1621	D1626	Q1627	D1630	R1633	I1643	L1652	K1656	T1662	V1667	S1673	T1685	S1691	K1692	K1698	L1702	K1706	W1710	M1714	L1715	L1737	K1738	M1739	H1747										
K1454	A1460	L1465	I1469	I1476	R1479	P1480	S1481	C1482	D1485	F1491	L1497	K1510	V1521	L1524	P1526	L1527	E1533	Q1537	K1543	I1547	D1548	D1551	K1560	L1561	L1562	P1566	D1567	H1568	K1572	R1575	I1576	T1577	Q1578	K1582												
ASP	PRO	ALA	ASN	PRO	PRO	HIS	ASN	VAL	THR	PHE	GLU	ILE	LYS	THR	GLN	ASP	ASN	LYS	PRO	GLU	ILE	VAL	GLU	GLY	VAL	P1412	D1413	S1414	K1417	I1418	A1421	Q1425	A1426	E1427	E1428	Y1433	I1438	H1443	K1451							
GLU	THR	ALA	THR	LYS	VAL	THR	VAL	THR	GLY	GLU	GLN	ILE	ASP	ASN	GLN	ILE	PHE	GLU	ILE	SER	VAL	GLU	THR	GLY	THR	HIS	GLU	PRO	ALA	ASN	PRO	PHE	THR	GLN	THR	ASP	CYS	GLY	PHE	SER	GLY	LEU				
LYS	VAL	LEU	ILE	PRO	VAL	ARG	GLY	TYR	THR	LEU	ASP	ARG	VAL	THR	ASN	ASP	TRP	LYS	SER	THR	LEU	VAL	GLY	VAL	ALA	ASN	GLN	VAL	PRO	LEU	THR	ILE	GLY	THR	VAL	ASP	GLY	THR	VAL	GLY	THR	VAL	LYS	ARG		
VAL	LEU	GLU	VAL	SER	GLU	THR	GLY	ARG	ASP	VAL	GLU	ILE	GLY	THR	ASN	ASP	TRP	LYS	GLU	THR	ILE	VAL	TRP	VAL	ALA	GLN	GLY	THR	LEU	ALA	ASN	PRO	THR	ALA	VAL	THR	GLY	LEU	GLY	THR	VAL	GLY	VAL	TYR		
THR	GLY	SER	LEU	ARG	GLN	ASP	THR	GLY	THR	VAL	GLN	THR	LEU	GLY	GLN	PHE	GLN	ILE	GLU	THR	VAL	GLY	THR	ILE	LEU	THR	GLY	GLU	VAL	THR	GLY	THR	VAL	THR	GLY	LEU	GLY	THR	VAL	GLY	THR	VAL	GLY	THR		
GLU	THR	VAL	ARG	CYS	SER	LEU	CYS	VAL	THR	GLY	THR	ASN	THR	VAL	ASN	THR	VAL	ARG	LEU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1207435	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	0.543	Depositor
Minimum map value	-0.219	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	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

5.1 Standard geometry

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

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	0.08	0/12737	0.22	0/17196
1	B	0.08	0/12737	0.22	0/17196
All	All	0.08	0/25474	0.22	0/34392

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

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	12506	0	12633	137	0
1	B	12506	0	12633	140	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
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	25078	0	25292	271	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 5.

The worst 5 of 271 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:1875:ARG:O	1:A:1876:HIS:ND1	2.09	0.85
1:B:1875:ARG:O	1:B:1876:HIS:ND1	2.10	0.84
1:A:3045:LEU:HA	1:A:3048:LEU:HD12	1.76	0.68
1:A:2656:LEU:HD13	1:A:2659:LEU:HD11	1.76	0.67
1:B:3045:LEU:HA	1:B:3048:LEU:HD12	1.76	0.67

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	1536/3184 (48%)	1511 (98%)	25 (2%)	0	100	100
1	B	1536/3184 (48%)	1511 (98%)	25 (2%)	0	100	100
All	All	3072/6368 (48%)	3022 (98%)	50 (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	1396/2883 (48%)	1396 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1396/2883 (48%)	1396 (100%)	0	100	100
All	All	2792/5766 (48%)	2792 (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 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2069	GLN
1	B	2684	GLN
1	B	2874	GLN
1	B	2658	ASN
1	A	2684	GLN

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, 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
2	ANP	A	3101	3	33,33,33	1.16	4 (12%)	45,52,52	0.60	1 (2%)
2	ANP	B	3101	-	33,33,33	1.16	4 (12%)	45,52,52	0.60	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	-	0/18/38/38	0/3/3/3
2	ANP	B	3101	-	-	0/18/38/38	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	B	3101	ANP	PG-O2G	-3.17	1.48	1.56
2	A	3101	ANP	PG-O2G	-3.17	1.48	1.56
2	A	3101	ANP	PG-O3G	-3.15	1.48	1.56
2	B	3101	ANP	PG-O3G	-3.14	1.48	1.56
2	A	3101	ANP	PB-O2B	-3.14	1.48	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3101	ANP	O2B-PB-O1B	2.01	114.18	109.87

There are no chirality outliers.

There are no torsion outliers.

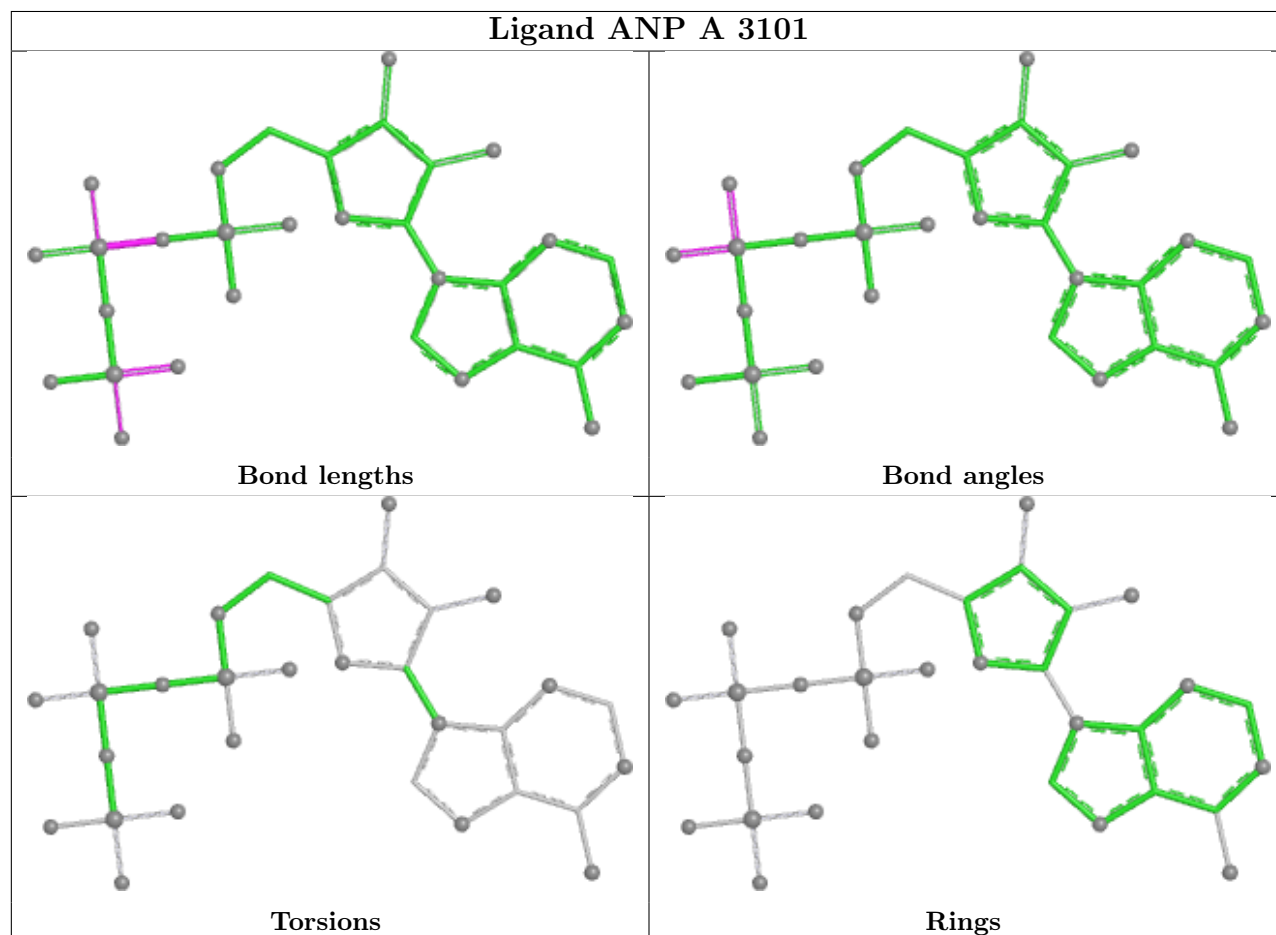
There are no ring outliers.

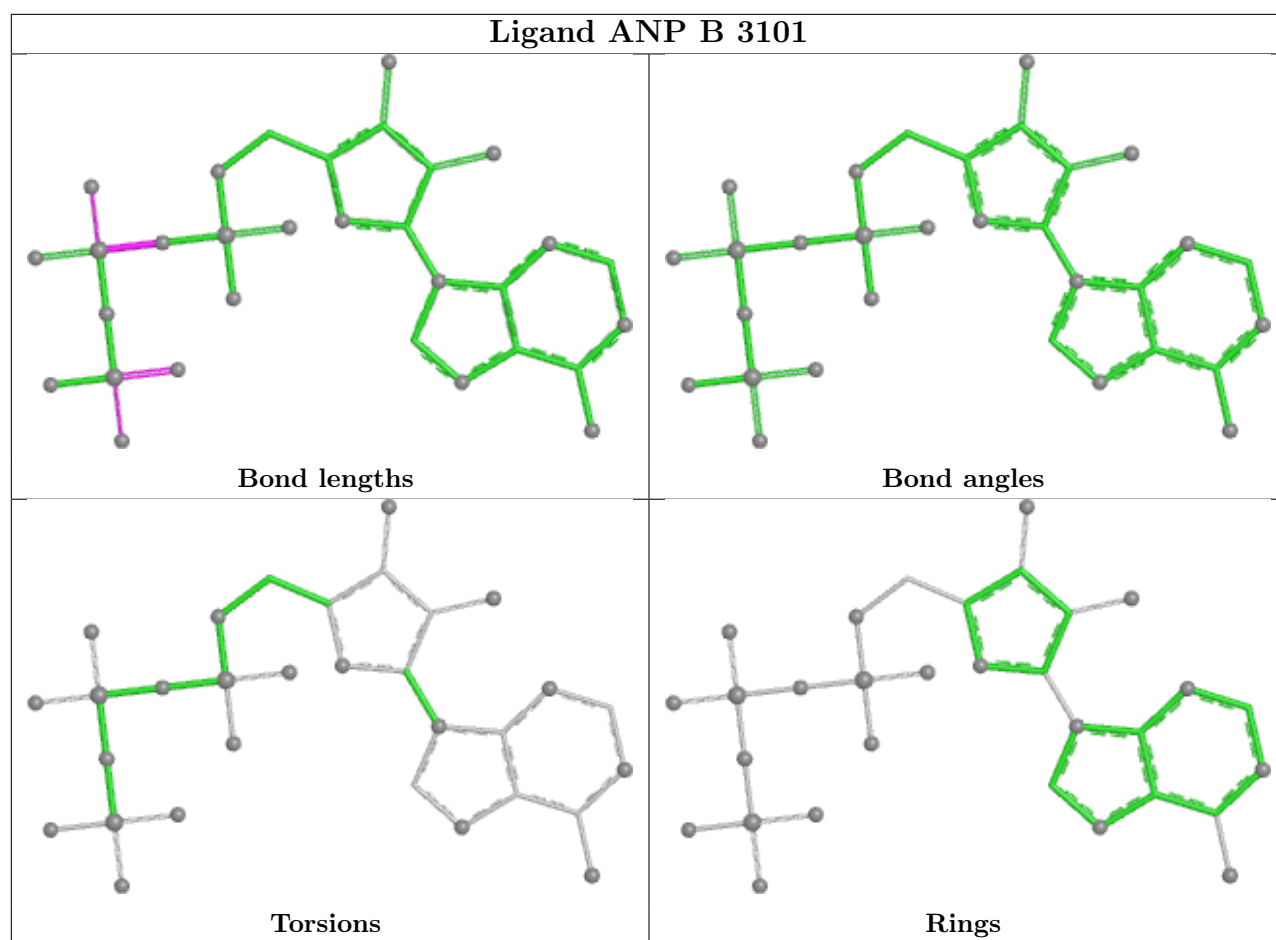
2 monomers are involved in 2 short contacts:

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.

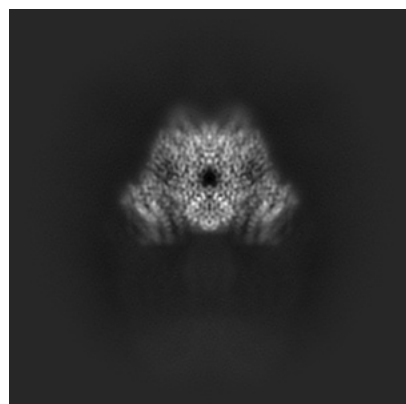
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17268. These allow visual inspection of the internal detail of the map and identification of artifacts.

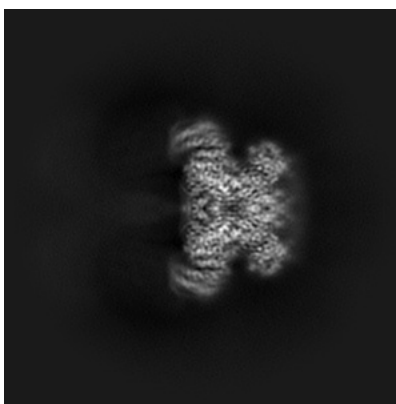
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

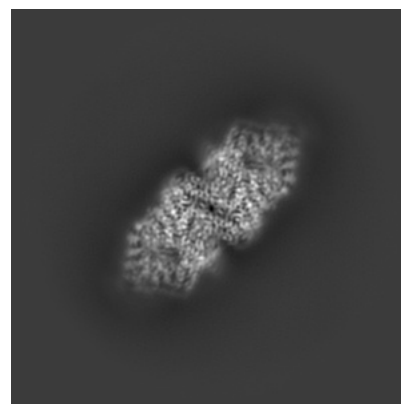
6.1.1 Primary map



X

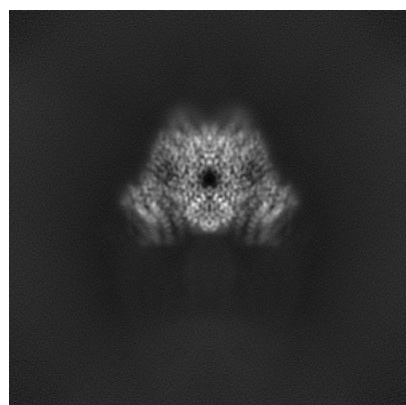


Y

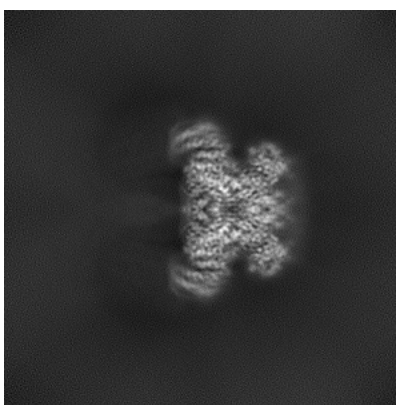


Z

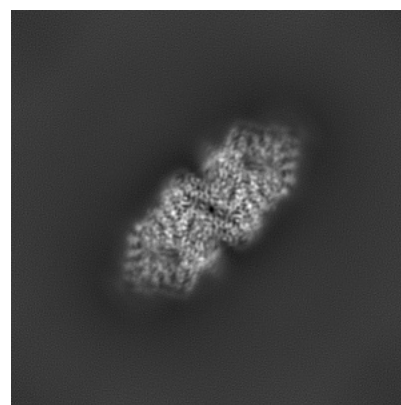
6.1.2 Raw map



X



Y

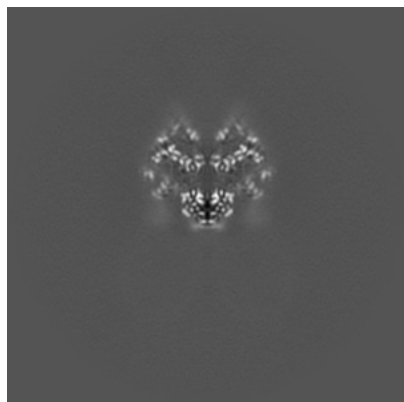


Z

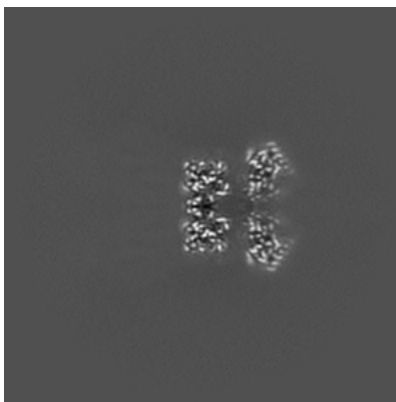
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

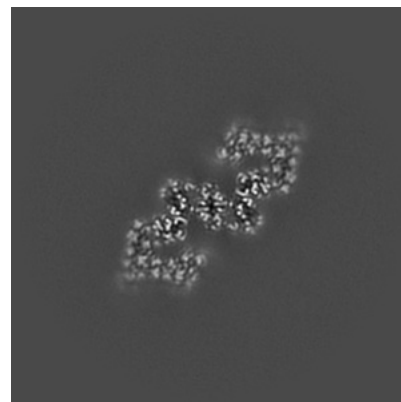
6.2.1 Primary map



X Index: 200

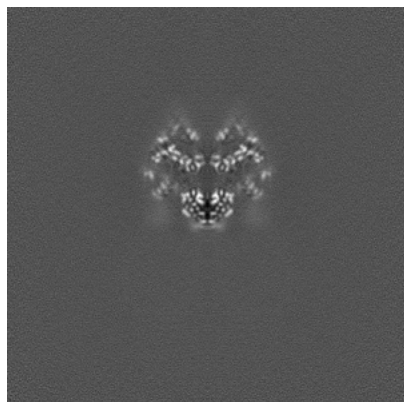


Y Index: 200

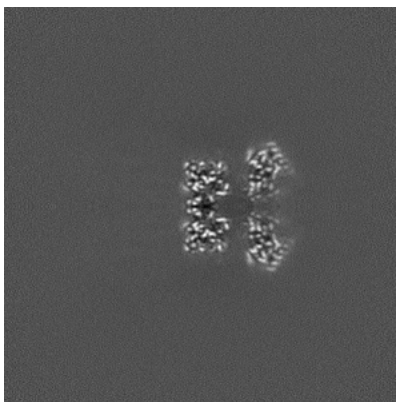


Z Index: 200

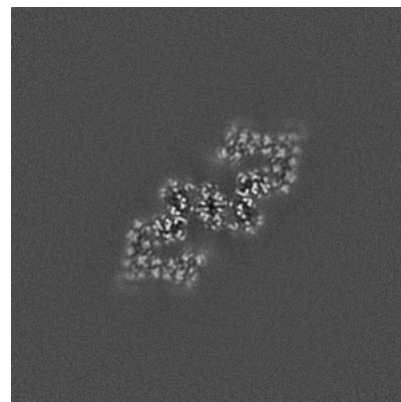
6.2.2 Raw map



X Index: 200



Y Index: 200

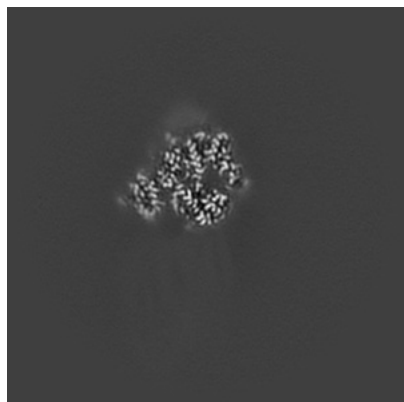


Z Index: 200

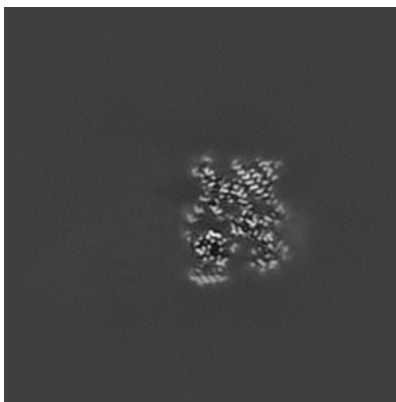
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

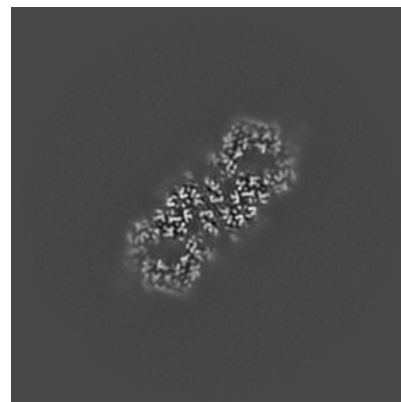
6.3.1 Primary map



X Index: 171

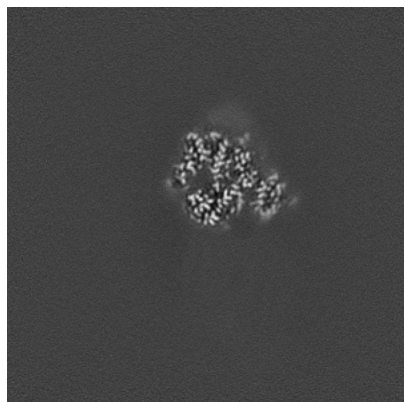


Y Index: 182

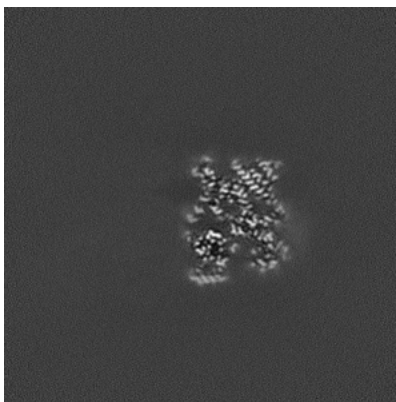


Z Index: 210

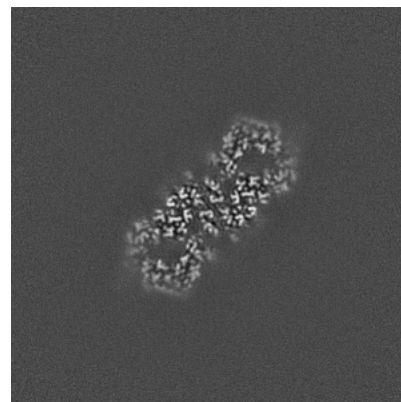
6.3.2 Raw map



X Index: 229



Y Index: 182

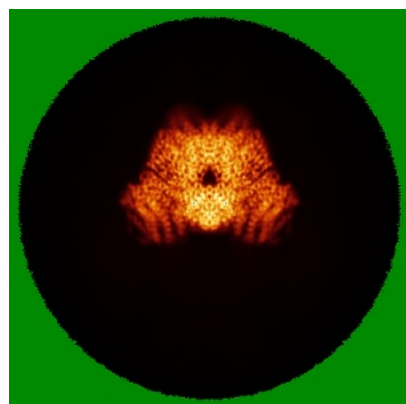


Z Index: 210

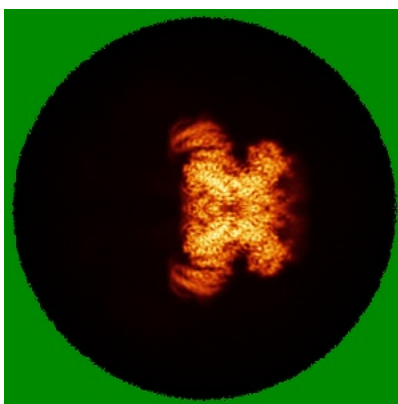
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

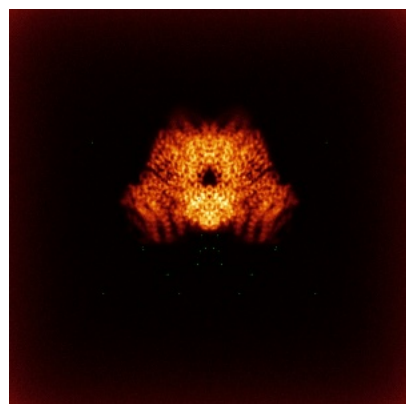


Y

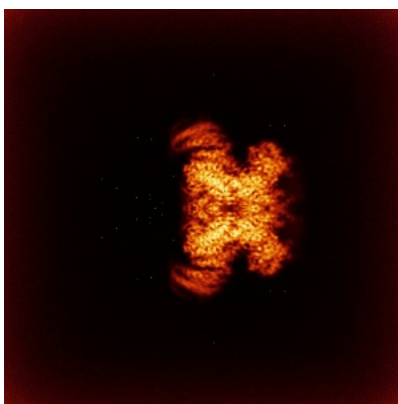


Z

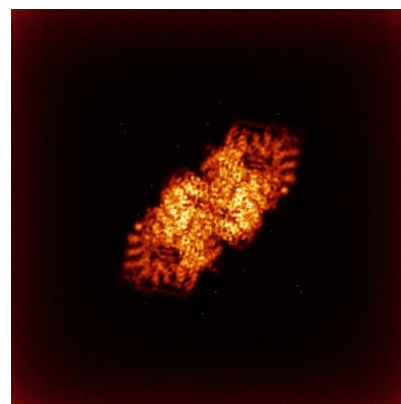
6.4.2 Raw map



X



Y

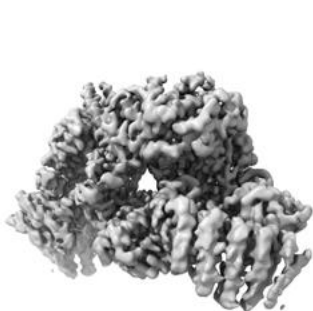


Z

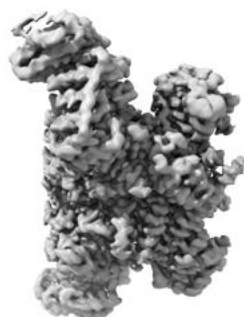
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

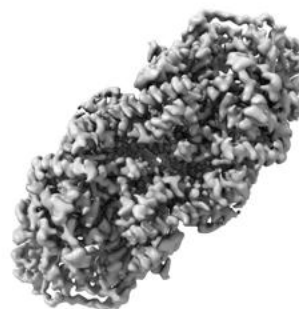
6.5.1 Primary map



X



Y



Z

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.

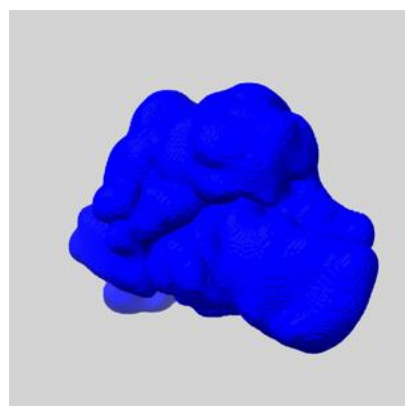
6.6 Mask visualisation [i](#)

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

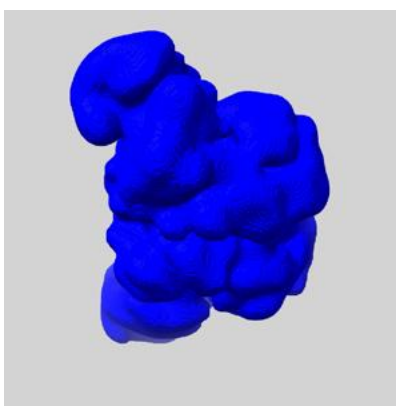
A mask typically either:

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

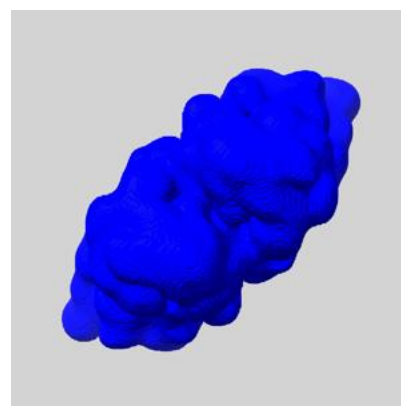
6.6.1 emd_17268_msk_1.map [i](#)



X



Y

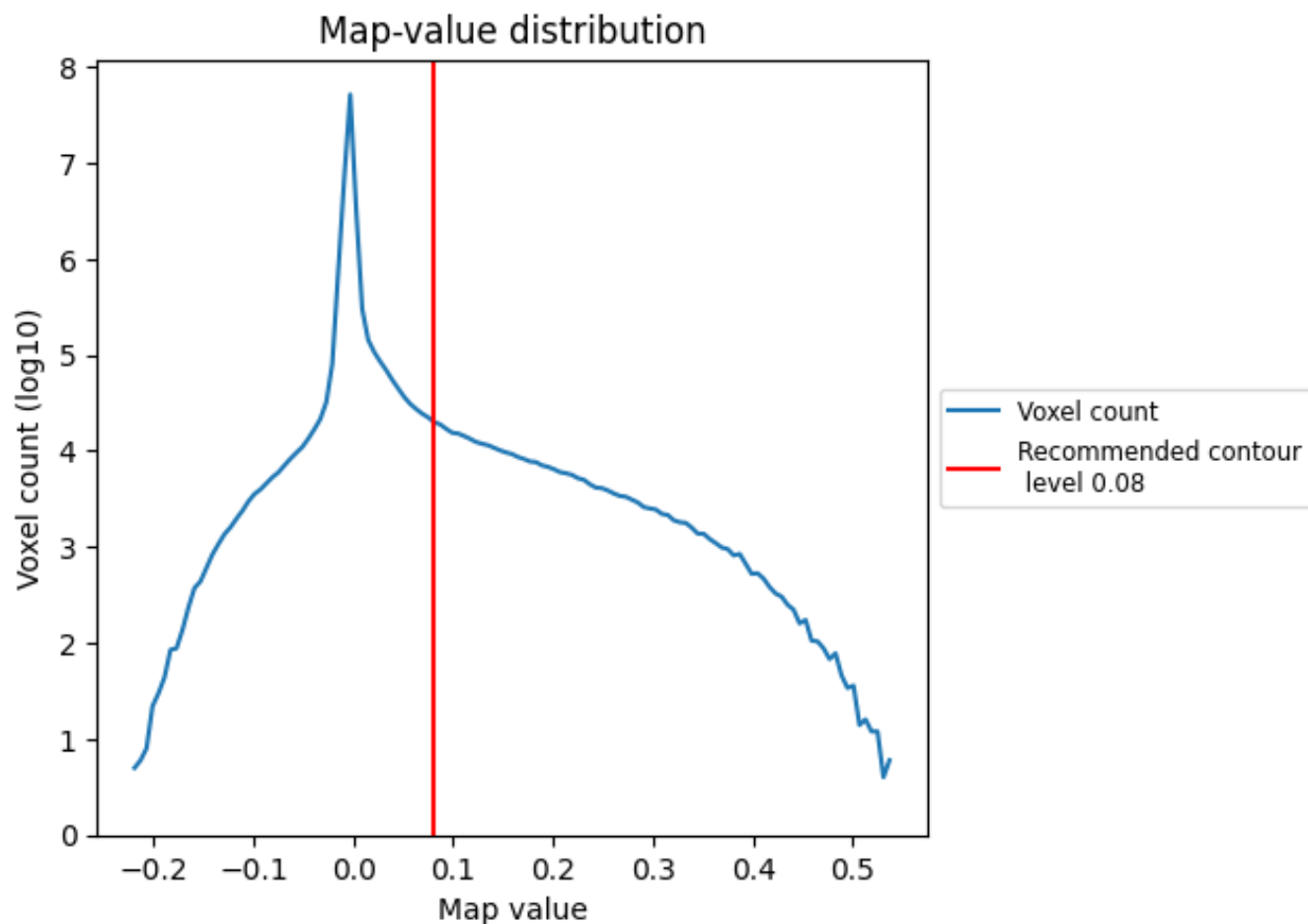


Z

7 Map analysis [i](#)

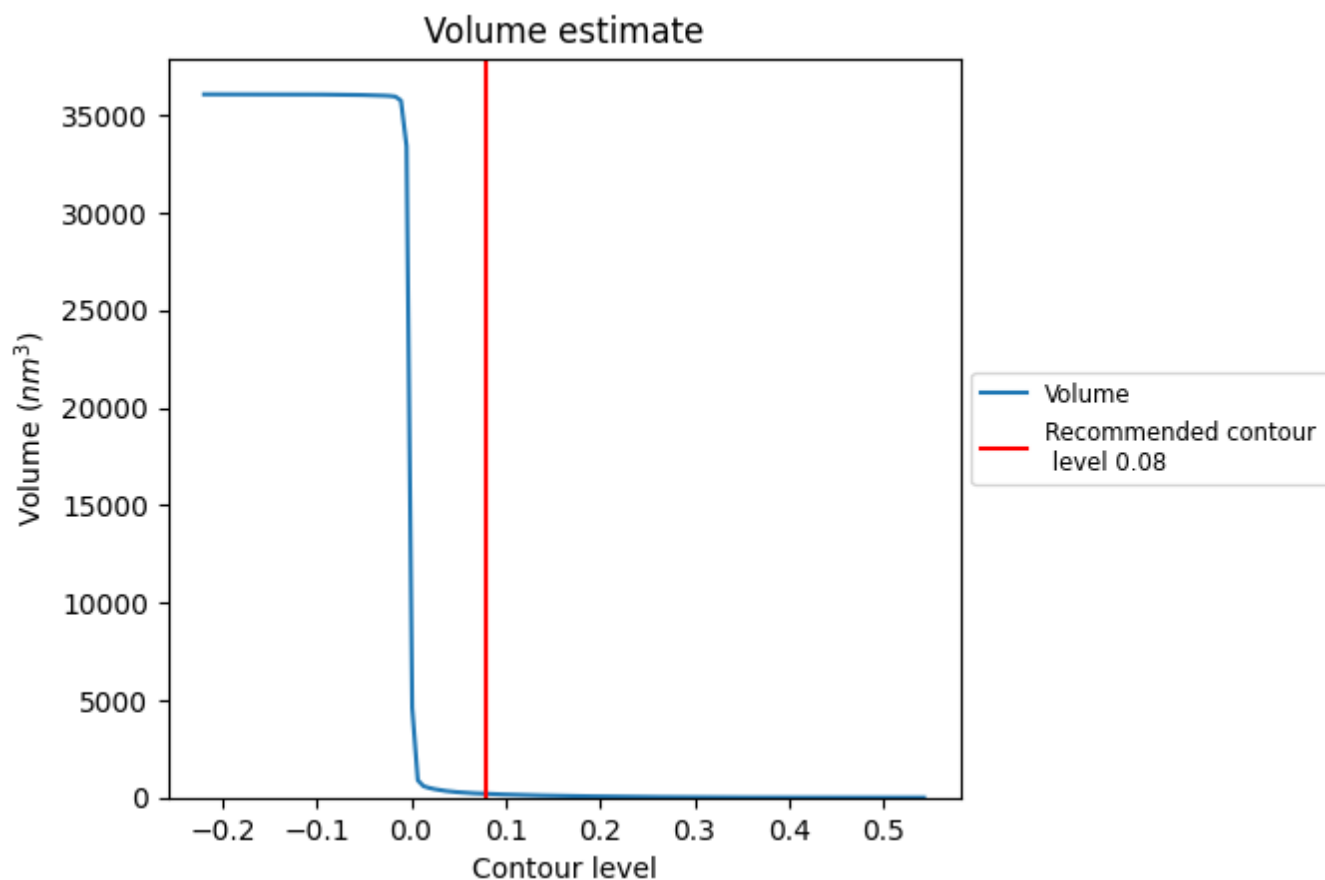
This section contains the results of statistical analysis of the map.

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.

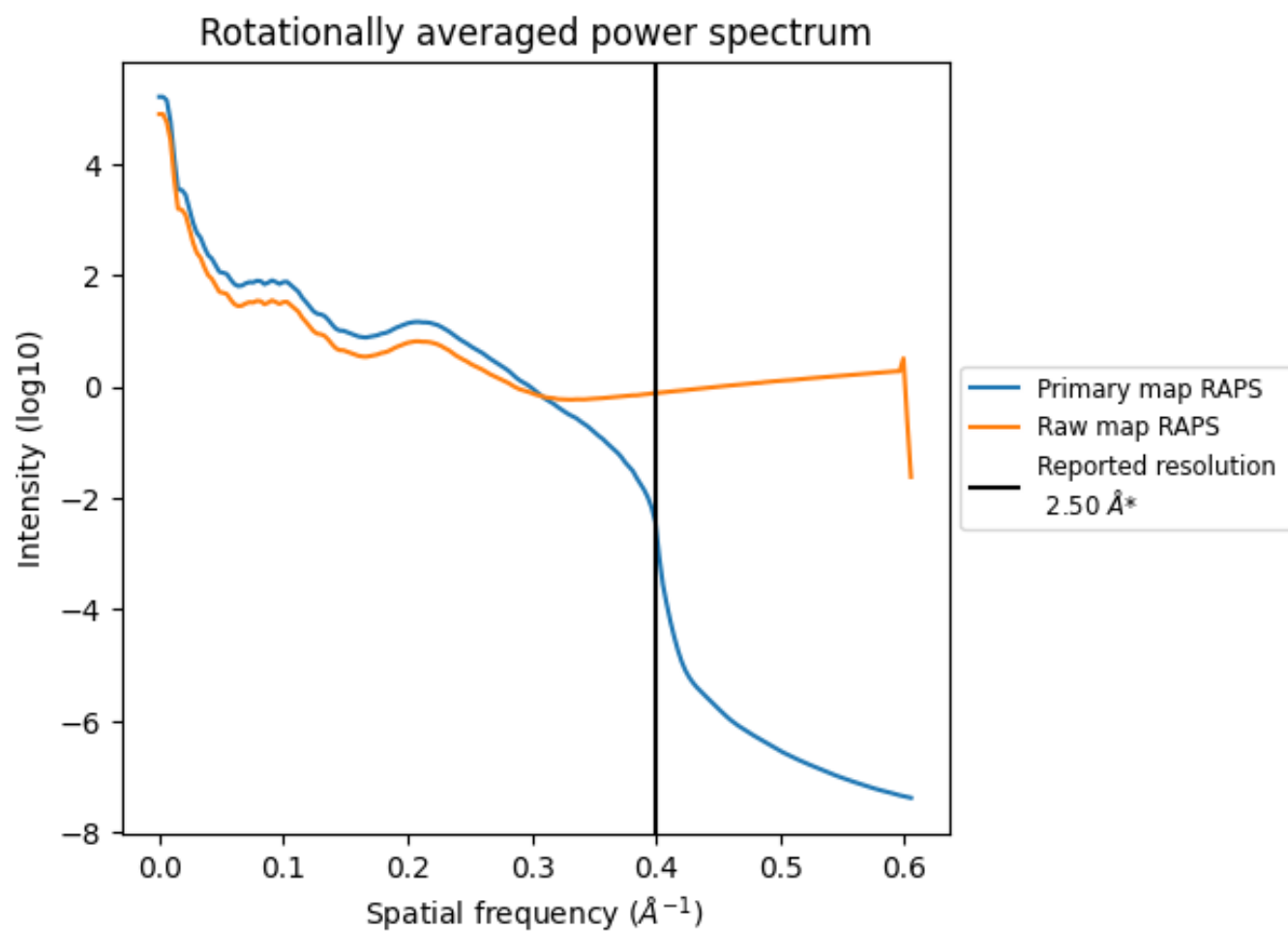
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 ⓘ

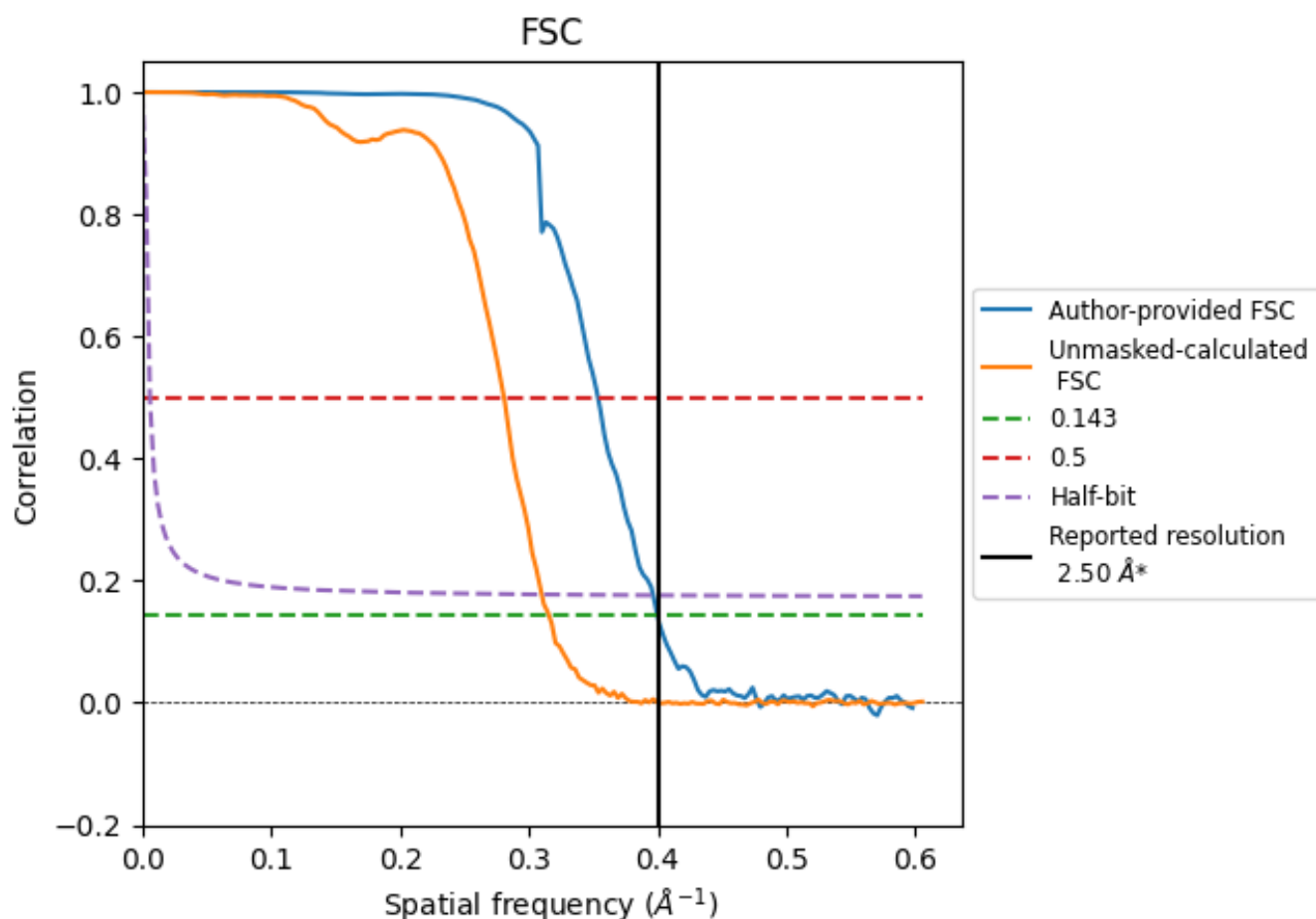


*Reported resolution corresponds to spatial frequency of $0.400 \text{ \AA}^{-1}$

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

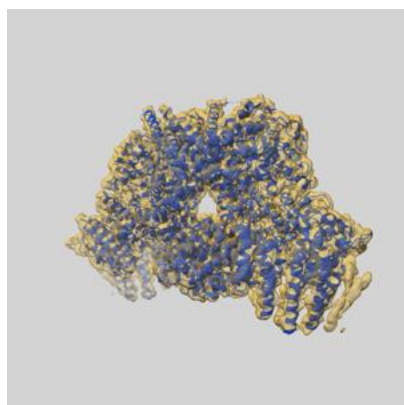
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.83	2.52
Unmasked-calculated*	3.17	3.56	3.22

*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 3.17 differs from the reported value 2.5 by more than 10 %

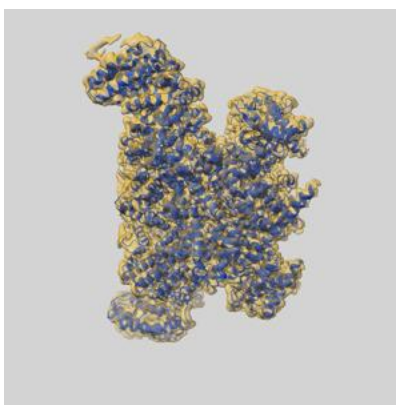
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17268 and PDB model 8OXQ. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

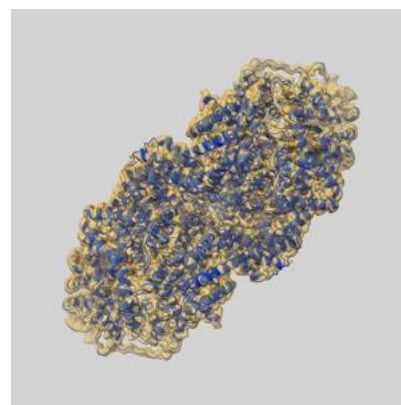
9.1 Map-model overlay [i](#)



X



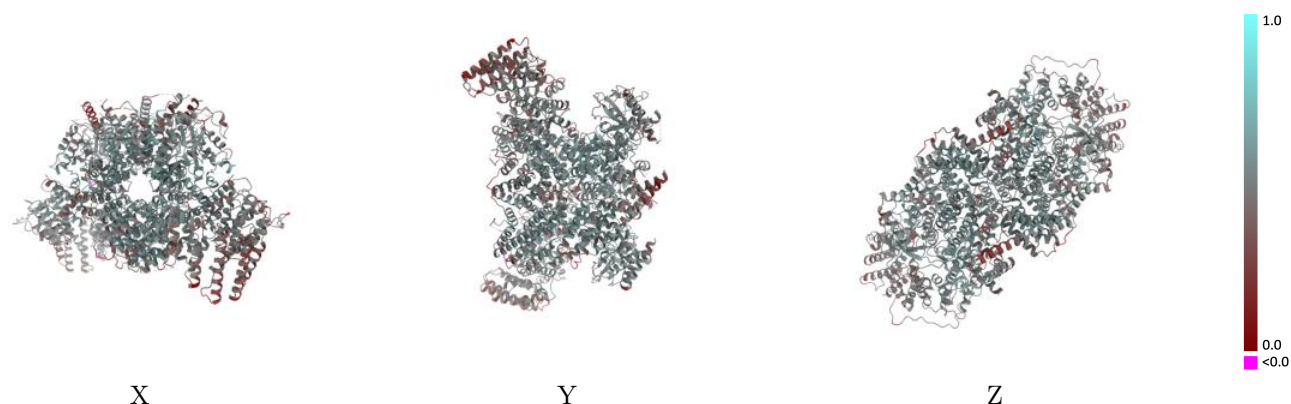
Y



Z

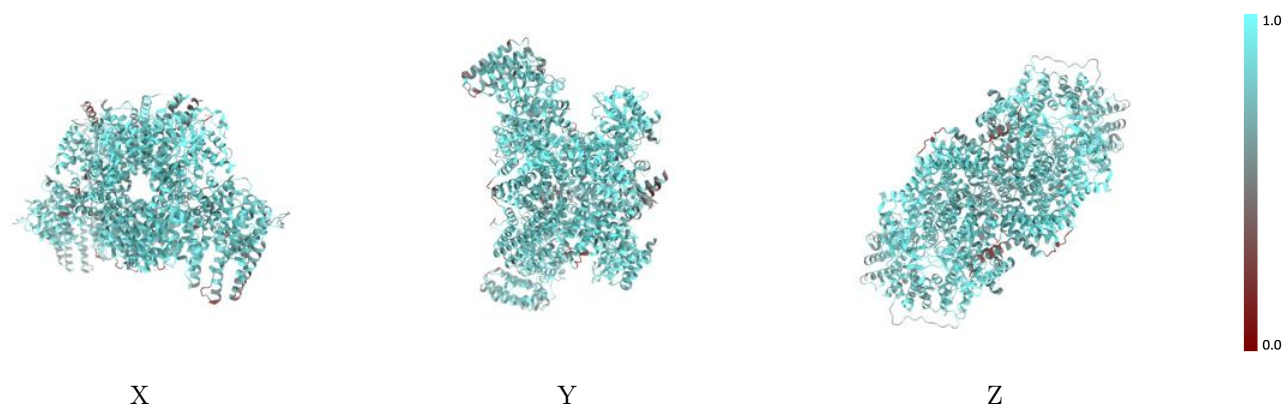
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



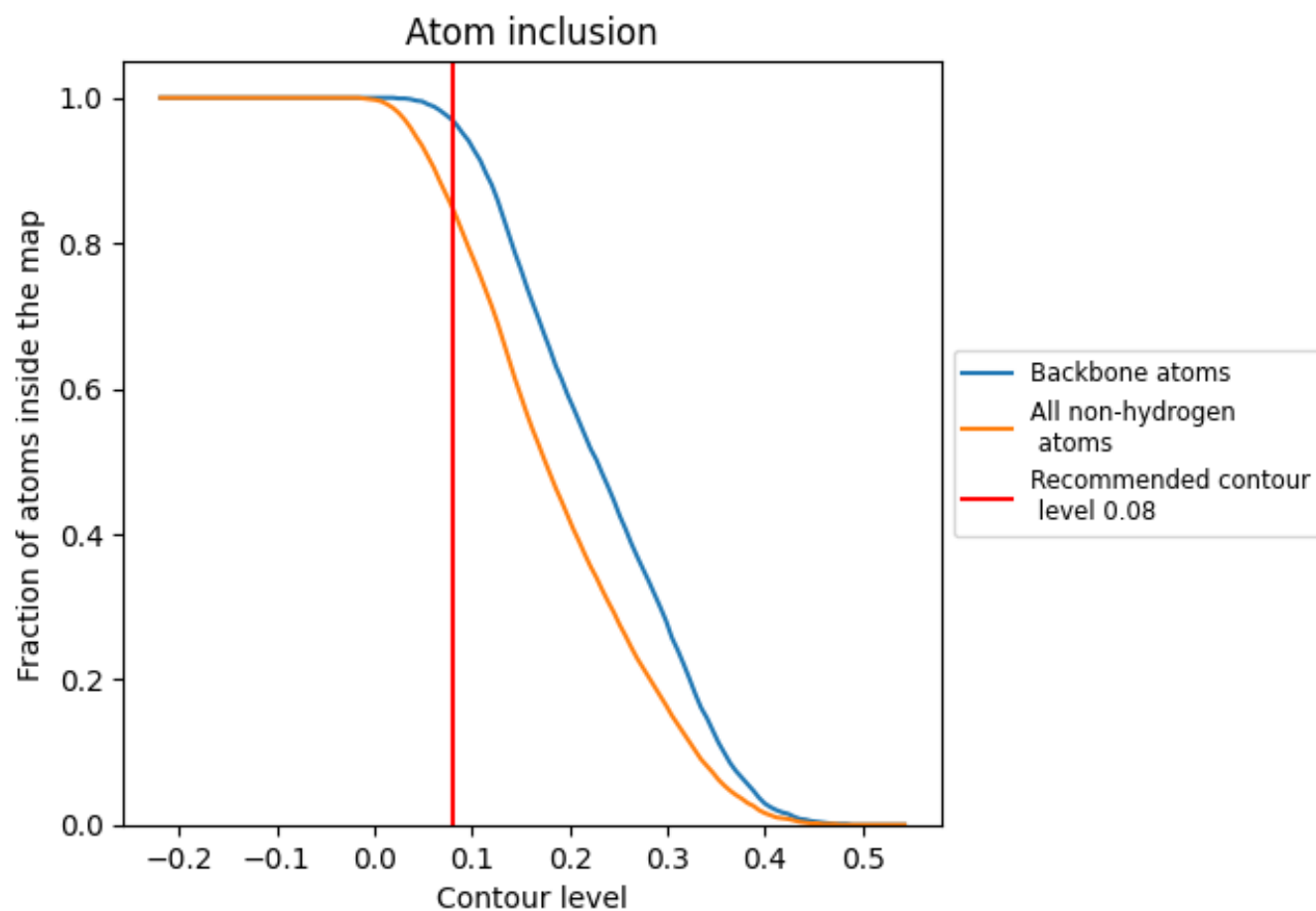
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 97% of all backbone atoms, 85% 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	0.8480	0.4930
A	0.8490	0.4960
B	0.8470	0.4890

