wwPDB EM Validation Summary Report

Dec 19, 2022 – 07:59 am GMT

PDB ID	:	7NJ0
EMDB ID	:	EMD-12368
Title	:	CryoEM structure of the human Separase-Cdk1-cyclin B1-Cks1 complex
Authors	:	Yu, J.; Raia, P.; Ghent, C.M.; Raisch, T.; Sadian, Y.; Barford, D.; Raunser, S.; Morgan, D.O.; Boland, A.
Deposited on	:	2021-02-14
Resolution	:	3.60 Å(reported)
Based on initial models	:	1QMZ, 4YC3

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 (i) 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 (i)) were used in the production of this report:

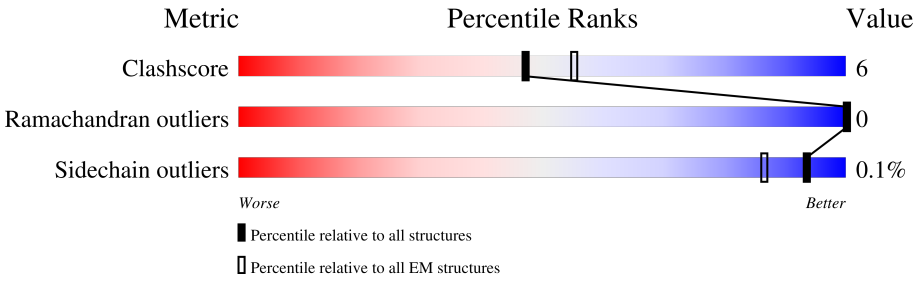
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2233	10% 45% 8% 47%
2	B	318	23% 76% 15% 9%
3	C	473	. 45% 12% 43%
4	D	79	33% 73% 15% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14330 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 Securin,Separin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	1188	9198	5863	1597	1696	1	41	0	0

There are 77 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-72	MET	-	initiating methionine	UNP O95997
A	-28	GLY	-	linker	UNP O95997
A	-27	GLY	-	linker	UNP O95997
A	-26	SER	-	linker	UNP O95997
A	-25	GLY	-	linker	UNP O95997
A	-24	GLY	-	linker	UNP O95997
A	-23	SER	-	linker	UNP O95997
A	-22	GLY	-	linker	UNP O95997
A	-21	GLY	-	linker	UNP O95997
A	-20	GLY	-	linker	UNP O95997
A	-19	SER	-	linker	UNP O95997
A	-18	GLY	-	linker	UNP O95997
A	-17	GLY	-	linker	UNP O95997
A	-16	GLY	-	linker	UNP O95997
A	-15	SER	-	linker	UNP O95997
A	-14	GLY	-	linker	UNP O95997
A	-13	GLU	-	linker	UNP O95997
A	-12	ASN	-	linker	UNP O95997
A	-11	LEU	-	linker	UNP O95997
A	-10	TYR	-	linker	UNP O95997
A	-9	PHE	-	linker	UNP O95997
A	-8	GLN	-	linker	UNP O95997
A	-7	GLY	-	linker	UNP O95997
A	-6	GLY	-	linker	UNP O95997
A	-5	GLY	-	linker	UNP O95997
A	-4	SER	-	linker	UNP O95997
A	-3	GLY	-	linker	UNP O95997
A	-2	GLY	-	linker	UNP O95997

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	linker	UNP O95997
A	0	GLY	-	linker	UNP O95997
A	25	ASP	ALA	conflict	UNP Q14674
A	116	VAL	ALA	conflict	UNP Q14674
A	693	ILE	MET	conflict	UNP Q14674
A	1329	SER	ARG	conflict	UNP Q14674
A	1561	GLN	ARG	conflict	UNP Q14674
A	2029	SER	CYS	conflict	UNP Q14674
A	2037	HIS	ARG	conflict	UNP Q14674
A	2121	SER	-	expression tag	UNP Q14674
A	2122	SER	-	expression tag	UNP Q14674
A	2123	LEU	-	expression tag	UNP Q14674
A	2124	ALA	-	expression tag	UNP Q14674
A	2125	GLU	-	expression tag	UNP Q14674
A	2126	GLU	-	expression tag	UNP Q14674
A	2127	ASN	-	expression tag	UNP Q14674
A	2128	LEU	-	expression tag	UNP Q14674
A	2129	TYR	-	expression tag	UNP Q14674
A	2130	PHE	-	expression tag	UNP Q14674
A	2131	GLN	-	expression tag	UNP Q14674
A	2132	SER	-	expression tag	UNP Q14674
A	2133	TRP	-	expression tag	UNP Q14674
A	2134	SER	-	expression tag	UNP Q14674
A	2135	HIS	-	expression tag	UNP Q14674
A	2136	PRO	-	expression tag	UNP Q14674
A	2137	GLN	-	expression tag	UNP Q14674
A	2138	PHE	-	expression tag	UNP Q14674
A	2139	GLU	-	expression tag	UNP Q14674
A	2140	LYS	-	expression tag	UNP Q14674
A	2141	GLY	-	expression tag	UNP Q14674
A	2142	GLY	-	expression tag	UNP Q14674
A	2143	GLY	-	expression tag	UNP Q14674
A	2144	SER	-	expression tag	UNP Q14674
A	2145	GLY	-	expression tag	UNP Q14674
A	2146	GLY	-	expression tag	UNP Q14674
A	2147	GLY	-	expression tag	UNP Q14674
A	2148	SER	-	expression tag	UNP Q14674
A	2149	GLY	-	expression tag	UNP Q14674
A	2150	GLY	-	expression tag	UNP Q14674
A	2151	GLY	-	expression tag	UNP Q14674
A	2152	SER	-	expression tag	UNP Q14674
A	2153	TRP	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2154	SER	-	expression tag	UNP Q14674
A	2155	HIS	-	expression tag	UNP Q14674
A	2156	PRO	-	expression tag	UNP Q14674
A	2157	GLN	-	expression tag	UNP Q14674
A	2158	PHE	-	expression tag	UNP Q14674
A	2159	GLU	-	expression tag	UNP Q14674
A	2160	LYS	-	expression tag	UNP Q14674

- Molecule 2 is a protein called Cyclin-dependent kinase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	290	Total	C	N	O	P	S	0	0
			2349	1514	395	431	1	8		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	ILE	-	expression tag	UNP P06493
B	299	ALA	-	expression tag	UNP P06493
B	300	ALA	-	expression tag	UNP P06493
B	301	GLU	-	expression tag	UNP P06493
B	302	ALA	-	expression tag	UNP P06493
B	303	LEU	-	expression tag	UNP P06493
B	304	GLU	-	expression tag	UNP P06493
B	305	VAL	-	expression tag	UNP P06493
B	306	LEU	-	expression tag	UNP P06493
B	307	PHE	-	expression tag	UNP P06493
B	308	GLN	-	expression tag	UNP P06493
B	309	GLY	-	expression tag	UNP P06493
B	310	PRO	-	expression tag	UNP P06493
B	311	HIS	-	expression tag	UNP P06493
B	312	HIS	-	expression tag	UNP P06493
B	313	HIS	-	expression tag	UNP P06493
B	314	HIS	-	expression tag	UNP P06493
B	315	HIS	-	expression tag	UNP P06493
B	316	HIS	-	expression tag	UNP P06493
B	317	HIS	-	expression tag	UNP P06493
B	318	HIS	-	expression tag	UNP P06493

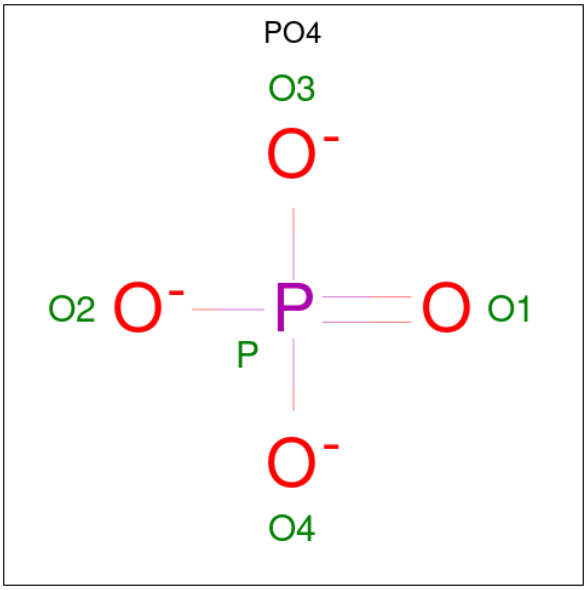
- Molecule 3 is a protein called G2/mitotic-specific cyclin-B1,G2/mitotic-specific cyclin-B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2173	1398	366	390	19		

- Molecule 4 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	70	Total	C	N	O	S	0	0
			605	392	103	107	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



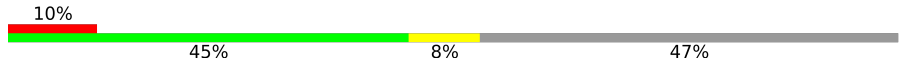
Mol	Chain	Residues	Atoms			AltConf
5	D	1	Total	O	P	0
			5	4	1	

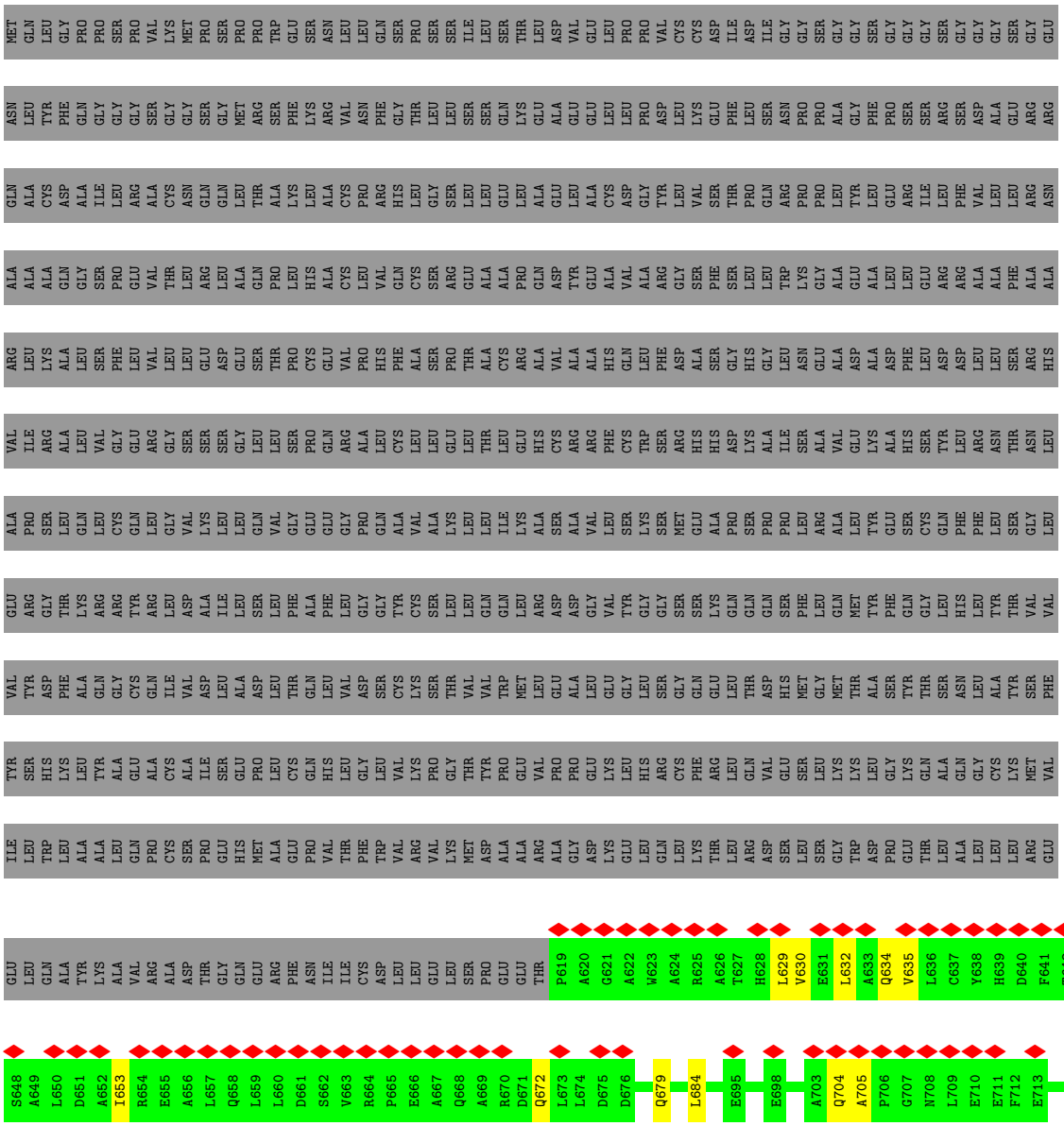
3 Residue-property plots (i)

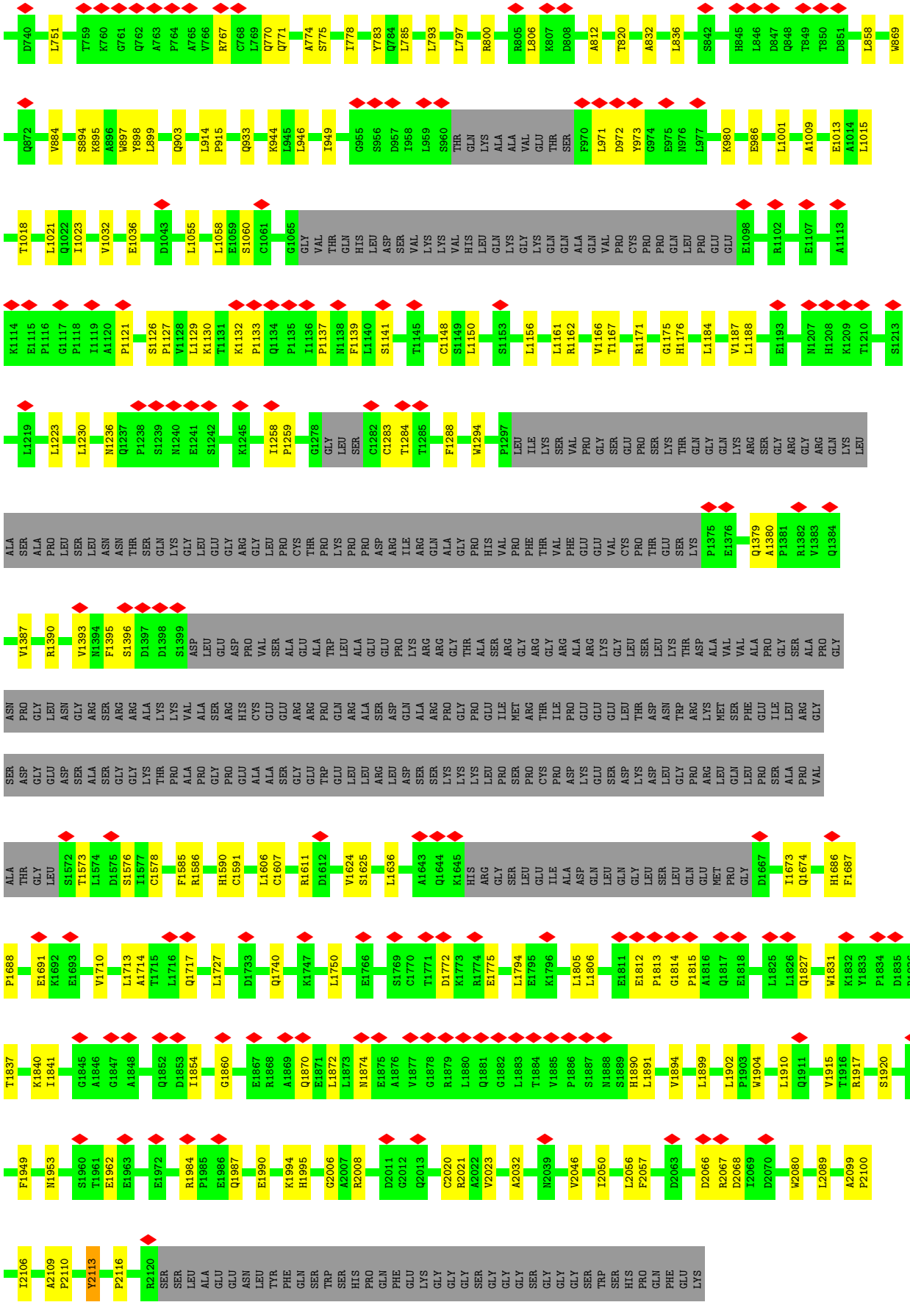
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Securin,Separin

Chain A:

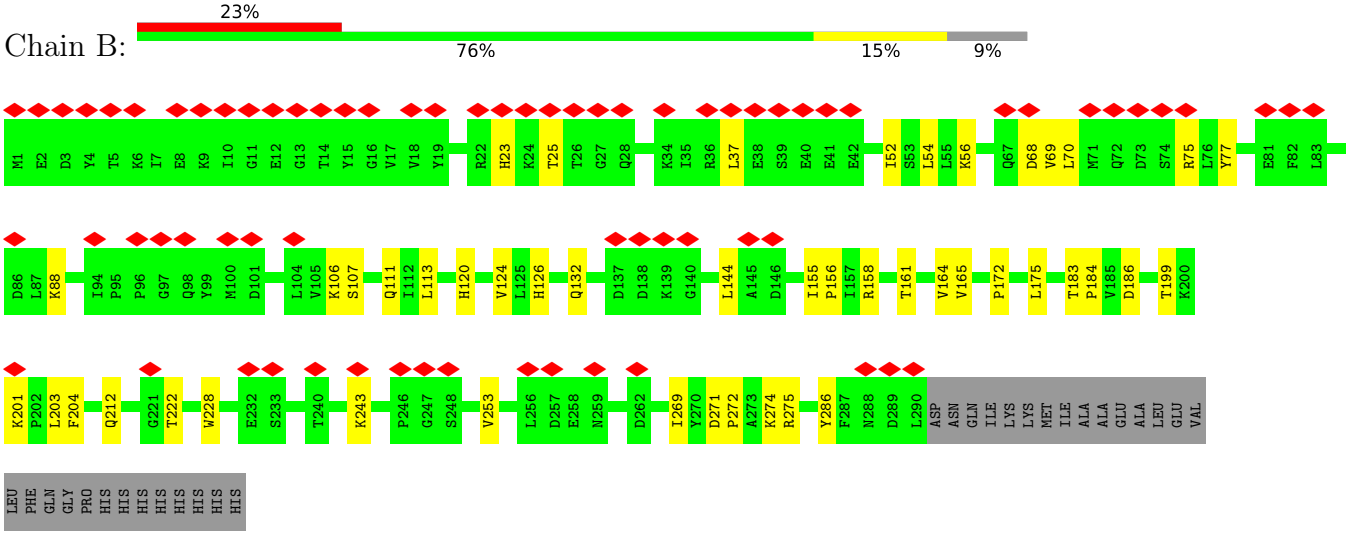





D740 L751 T759 K760 G761 Q762 A763 P764 A765 V766 R767 C768 L769 Q770 Q771 A774 S775 I778 Y783 Q784 L785 L793 L797 R800 R805 L806 K807 D808 A812 T820 A832 L836 S842 H845 L846 D847 Q848 T849 T850 D851 L858 W869
Q872 V884 S894 K895 A896 W897 Y898 L899 Q903 L914 P915 Q933 K944 L945 L946 I949 G955 S956 D957 I958 L959 S960 THR GLN LYS ALA ALA VAL GLU THR SER F970 L971 D972 Y973 G974 E975 N976 L977 K980 E986 L1001 A1009 E1013 A1014 L1015
T1018 L1021 Q1022 I1023 V1032 E1036 D1043 L1055 L1058 E1059 S1060 C1061 G1065 GLY VAL THR GLN HIS LEU ASP SER VAL LYS LYS VAL HIS LEU GLN LYS GLY LYS GLN GLN ALA GLN VAL PRO CYS PRO PRO GLN LEU PRO GLU GLU E1098 R1102 E1107 A1113
K1114 E1115 P1116 G1117 P1118 I1119 A1120 P1121 S1126 P1127 V1128 L1129 K1130 T1131 K1132 P1133 Q1134 P1135 I1136 P1137 N1138 F1139 L1140 S1141 T1145 C1148 S1149 L1150 S1153 L1156 L1161 R1162 V1166 T1167 R1171 G1175 H1176 L1184 V1187 L1188 E1193 N1207 H1208 K1209 T1210 S1213
L1219 L1223 L1230 N1236 Q1237 P1238 S1239 N1240 E1241 S1242 K1245 I1258 P1259 G1278 GLY LEU SER C1282 C1283 T1284 T1285 F1288 W1294 P1297 LEU ILE LYS SER VAL PRO GLY SER GLU PRO SER LYS THR GLN GLY GLN LYS ARG SER GLY ARG GLY ARG GLN LYS LEU
ALA SER ALA PRO LEU SER LEU ASN ASN THR SER GLN LYS GLY LEU GLU GLY ARG GLY LEU PRO CYS THR PRO LYS PRO PRO ASP ARG ILE ARG GLN ALA GLY PRO HIS VAL PRO PHE THR VAL PHE GLU GLU VAL CYS PRO THR GLU SER LYS P1375 E1376 Q1379 A1380 P1381 R1382 V1383 Q1384
V1387 R1390 V1393 N1394 F1395 S1396 D1397 D1398 S1399 ASP LEU GLU ASP PRO VAL SER ALA GLU ALA TRP LEU ALA ALA GLU GLU PRO LYS ARG ARG GLY THR ALA SER ARG GLY ARG GLY ARG ALA ARG LYS GLY LEU SER LEU LYS THR ASP ALA VAL VAL ALA PRO GLY SER ALA PRO GLY
ASN PRO GLY LEU ASN GLY ARG SER ARG ARG ALA LYS LYS VAL ALA SER ARG HIS CYS GLU GLU ARG PRO ALA PRO GLY PRO GLU ILE MET ARG THR ILE PRO GLU GLU GLU LEU THR ASP ASN TRP ARG LYS MET SER PHE GLU ILE LEU ARG GLY
SER ASP GLY GLU ASP SER ALA SER GLY TRP LYS THR PRO ALA PRO GLY PRO GLU ALA ALA SER GLY GLU TRP GLU LEU LEU ARG LEU ASP SER SER LYS LYS LEU PRO SER PRO CYS PRO ASP LYS GLU SER ASP LYS ASP LEU GLY PRO ARG LEU GLN LEU PRO SER ALA PRO VAL
ALA THR GLY LEU S1572 T1573 L1574 D1575 S1576 I1577 C1578 F1585 R1586 H1590 C1591 L1606 C1607 R1611 D1612 V1624 S1625 L1636 A1643 Q1644 K1645 HIS ARG GLY SER LEU GLU ILE ALA ASP GLN LEU GLN LEU GLY LEU SER LEU GLN GLU MET PRO GLY D1667 I1673 Q1674 H1686 F1687
P1688 E1691 K1692 E1693 V1710 L1713 A1714 T1715 L1716 Q1717 L1727 D1733 Q1740 K1747 L1750 E1766 S1769 C1770 T1771 D1772 K1773 R1774 E1775 L1794 E1795 K1796 L1805 L1806 E1811 E1812 P1813 G1814 P1815 A1816 Q1817 E1818 L1825 L1826 Q1827 W1831 K1832 Y1833 P1834 D1835 R1836
T1837 K1840 I1841 G1845 A1846 G1847 A1848 Q1852 D1853 I1854 G1860 E1867 R1868 A1869 Q1870 E1871 L1872 L1873 N1874 E1875 A1876 V1877 G1878 R1879 L1880 Q1881 G1882 L1883 T1884 V1885 P1886 S1887 N1888 S1889 H1890 L1891 V1894 L1899 L1902 P1903 W1904 L1910 Q1911 V1915 T1916 R1917 S1920 A1935
F1949 N1963 S1960 T1961 E1962 E1963 E1972 R1984 P1985 E1986 Q1987 E1990 K1994 H1995 G2006 A2007 R2008 D2011 G2012 Q2013 C2020 R2021 A2022 V2023 A2032 N2039 V2046 I2050 L2056 F2057 D2063 D2066 R2067 D2068 I2069 D2070 W2080 L2089 A2099 P2100
I2106 A2109 P2110 Y2113 P2116 R2120 SER SER LEU ALA GLU GLU ASN LEU TYR PHE GLN SER TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS

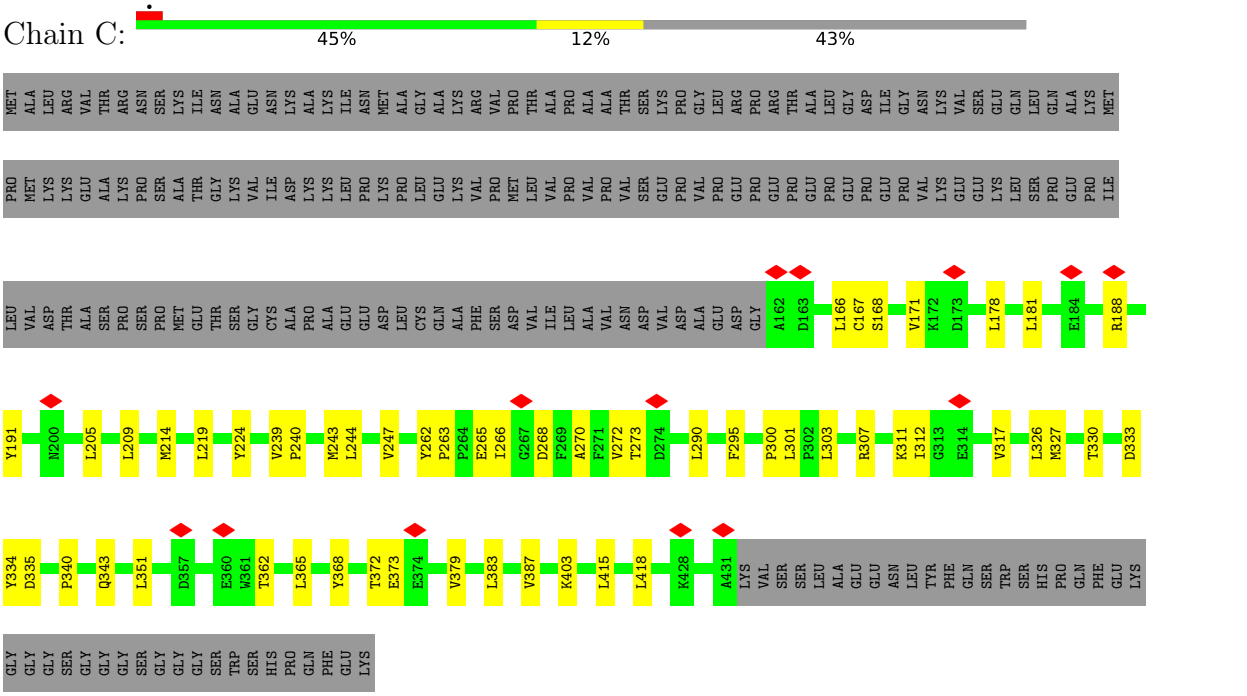
• Molecule 2: Cyclin-dependent kinase 1

Chain B:



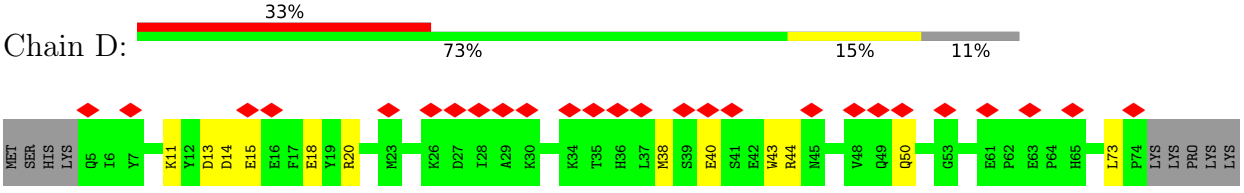
• Molecule 3: G2/mitotic-specific cyclin-B1,G2/mitotic-specific cyclin-B1

Chain C:



• Molecule 4: Cyclin-dependent kinases regulatory subunit 1

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	312836	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 ($e^-/Å^2$)	78	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, PO4, SEP

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	0.28	0/9373	0.44	0/12750
2	B	0.27	0/2392	0.43	0/3234
3	C	0.29	0/2218	0.44	0/3001
4	D	0.27	0/626	0.44	0/849
All	All	0.28	0/14609	0.44	0/19834

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	9198	0	9354	118	0
2	B	2349	0	2381	30	0
3	C	2173	0	2221	36	0
4	D	605	0	581	9	0
5	D	5	0	0	0	0
All	All	14330	0	14537	186	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 186 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)
4:D:11:LYS:HE2	4:D:20:ARG:HH21	1.53	0.74
1:A:1236:ASN:OD1	1:A:1717:GLN:NE2	2.21	0.73
1:A:1150:LEU:HA	1:A:1156:LEU:HD23	1.71	0.72
1:A:1727:LEU:HD23	1:A:1805:LEU:HD12	1.72	0.71
1:A:1127:PRO:HB3	3:C:311:LYS:HD3	1.72	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	1173/2233 (52%)	1064 (91%)	109 (9%)	0	100	100
2	B	287/318 (90%)	254 (88%)	33 (12%)	0	100	100
3	C	268/473 (57%)	255 (95%)	13 (5%)	0	100	100
4	D	68/79 (86%)	61 (90%)	7 (10%)	0	100	100
All	All	1796/3103 (58%)	1634 (91%)	162 (9%)	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	1004/1869 (54%)	1003 (100%)	1 (0%)	93 98
2	B	259/283 (92%)	259 (100%)	0	100 100
3	C	239/407 (59%)	239 (100%)	0	100 100
4	D	67/76 (88%)	67 (100%)	0	100 100
All	All	1569/2635 (60%)	1568 (100%)	1 (0%)	93 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2113	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	679	GLN
1	A	771	GLN
1	A	1740	GLN
1	A	1874	ASN
2	B	126	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	TPO	B	161	2	8,10,11	0.99	0	10,14,16	1.80	1 (10%)
1	SEP	A	1126	1	8,9,10	1.51	1 (12%)	8,12,14	1.52	2 (25%)

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	TPO	B	161	2	-	3/9/11/13	-
1	SEP	A	1126	1	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1126	SEP	P-O1P	3.29	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	161	TPO	P-OG1-CB	-5.15	107.64	123.21
1	A	1126	SEP	P-OG-CB	-3.03	109.94	118.30
1	A	1126	SEP	OG-CB-CA	2.49	110.56	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	161	TPO	O-C-CA-CB
2	B	161	TPO	CB-OG1-P-O2P
2	B	161	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
5	PO4	D	101	-	4,4,4	0.93	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

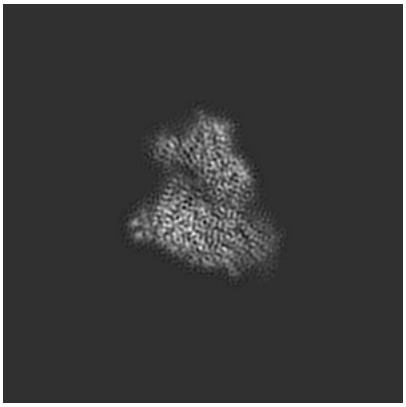
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12368. These allow visual inspection of the internal detail of the map and identification of artifacts.

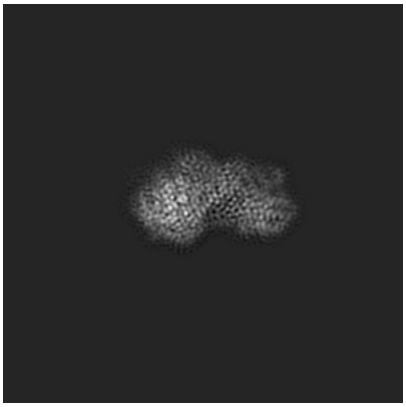
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

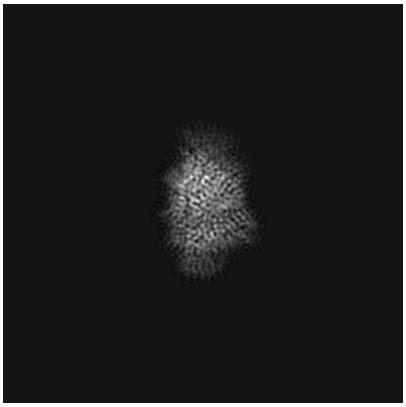
6.1.1 Primary map



X



Y

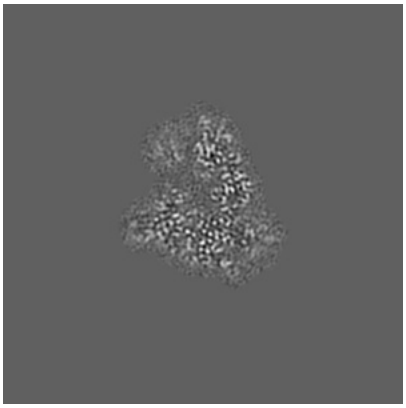


Z

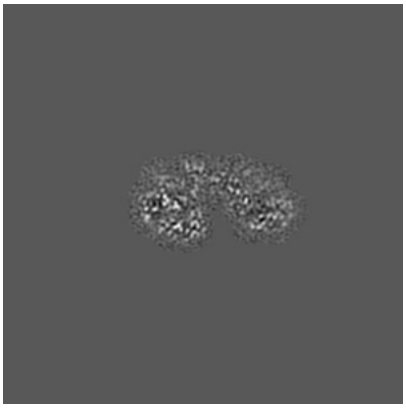
The images above show the map projected in three orthogonal directions.

6.2 Central slices

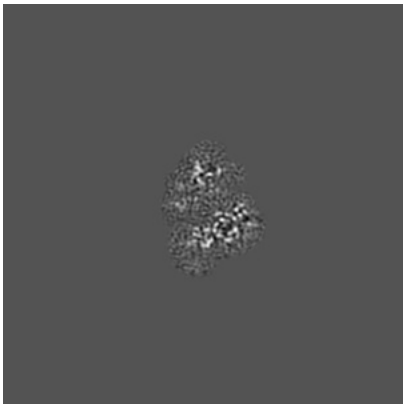
6.2.1 Primary map



X Index: 180



Y Index: 180

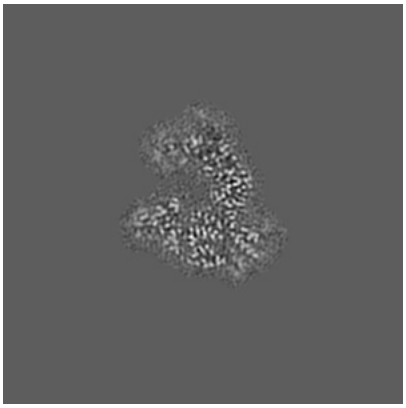


Z Index: 180

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: 176

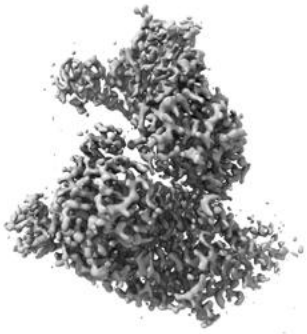
Y Index: 200

Z Index: 159

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

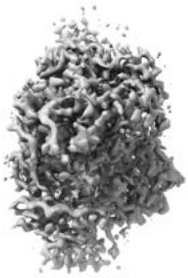
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

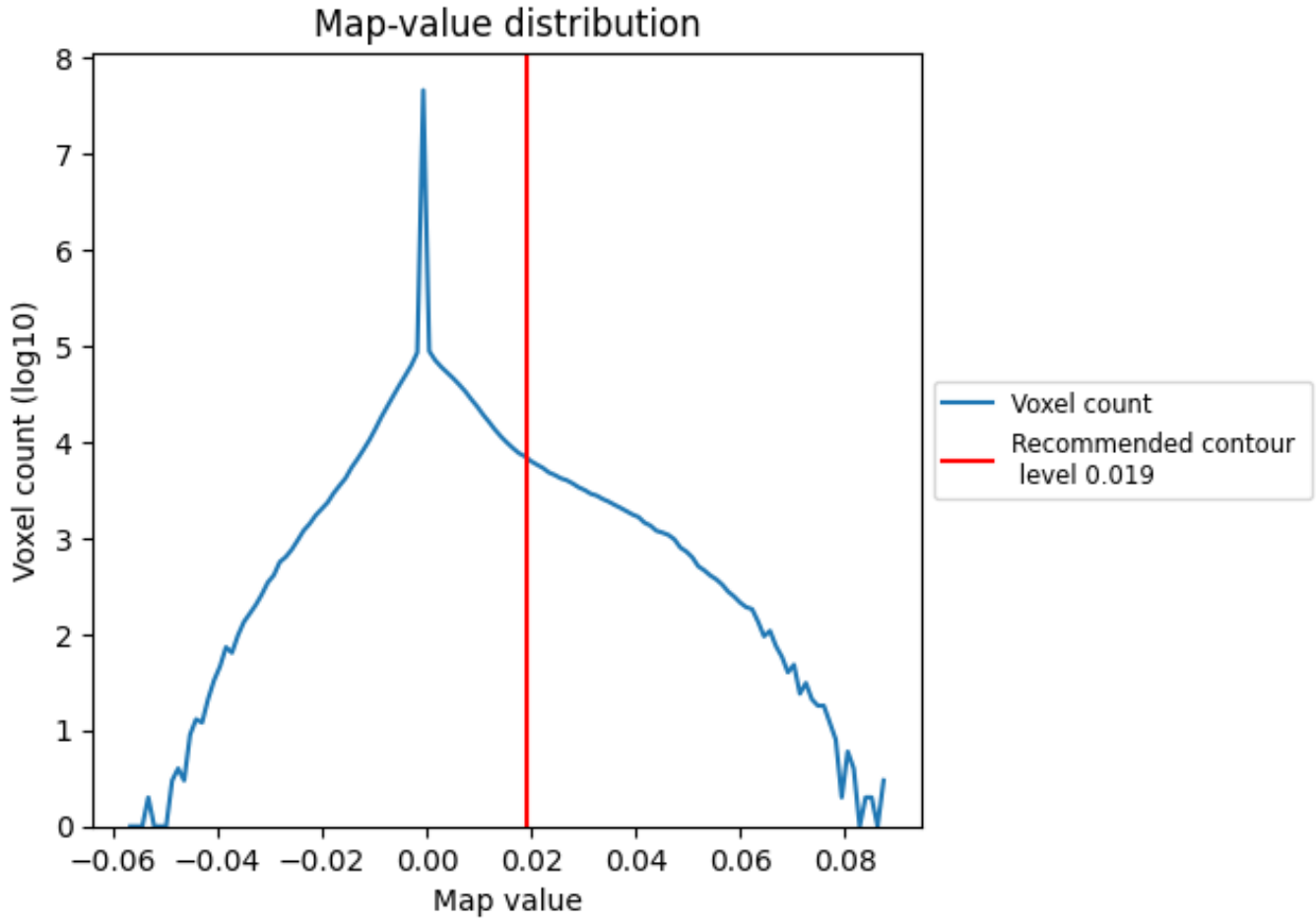
6.5 Mask visualisation (i)

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

7 Map analysis

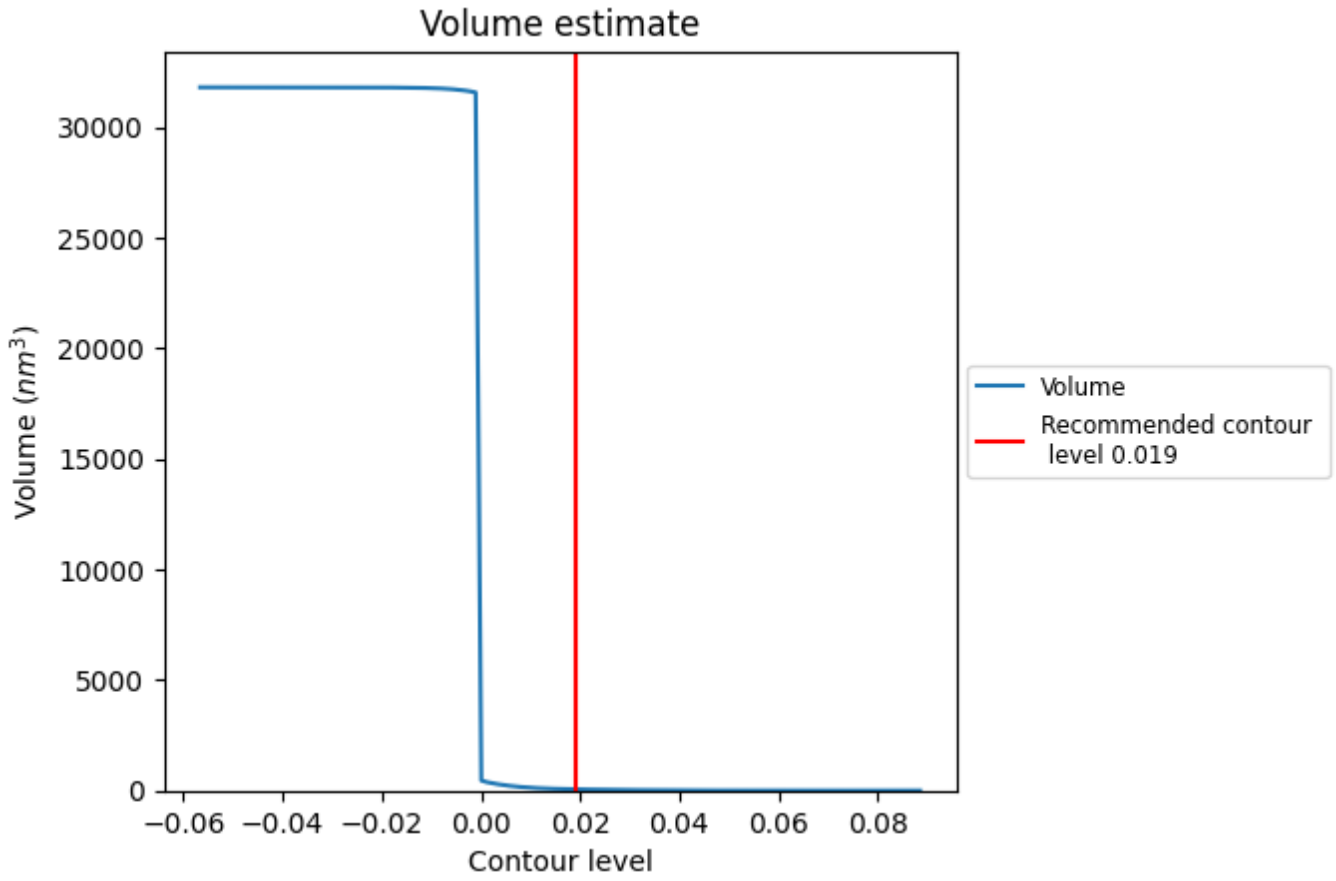
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

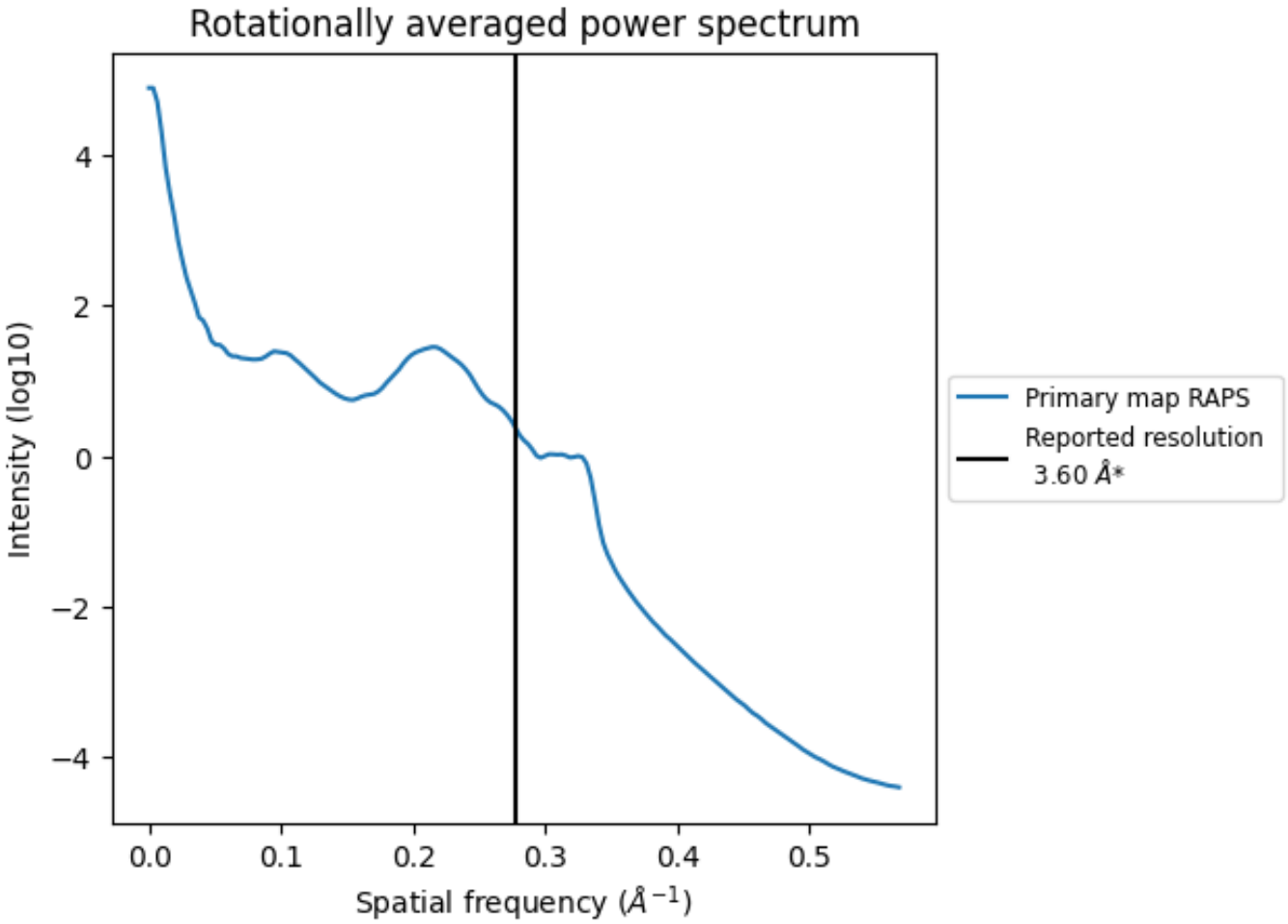
7.2 Volume estimate (i)



The volume at the recommended contour level is 58 nm^3; this corresponds to an approximate mass of 52 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 (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

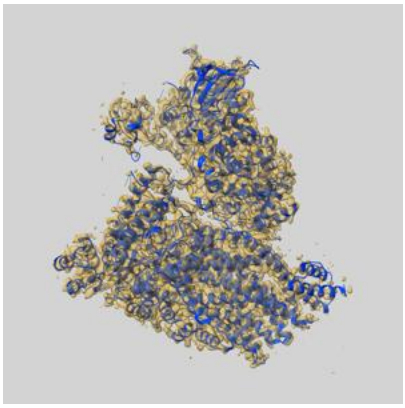
8 Fourier-Shell correlation (i)

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

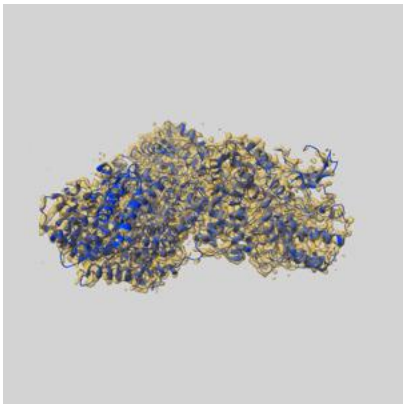
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12368 and PDB model 7NJ0. Per-residue inclusion information can be found in section 3 on page 7.

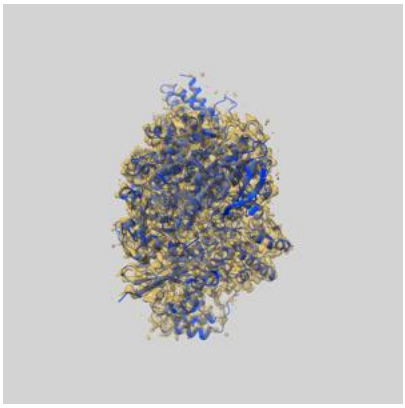
9.1 Map-model overlay



X



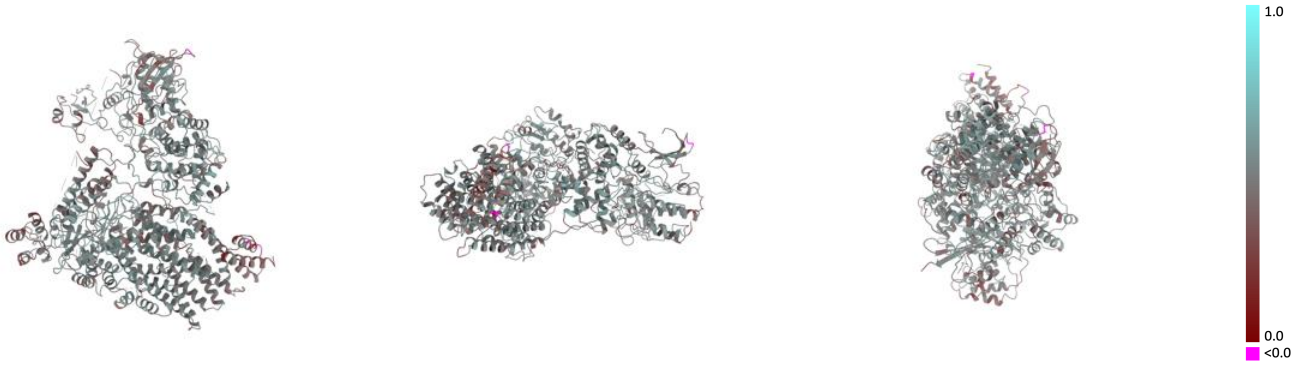
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 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.

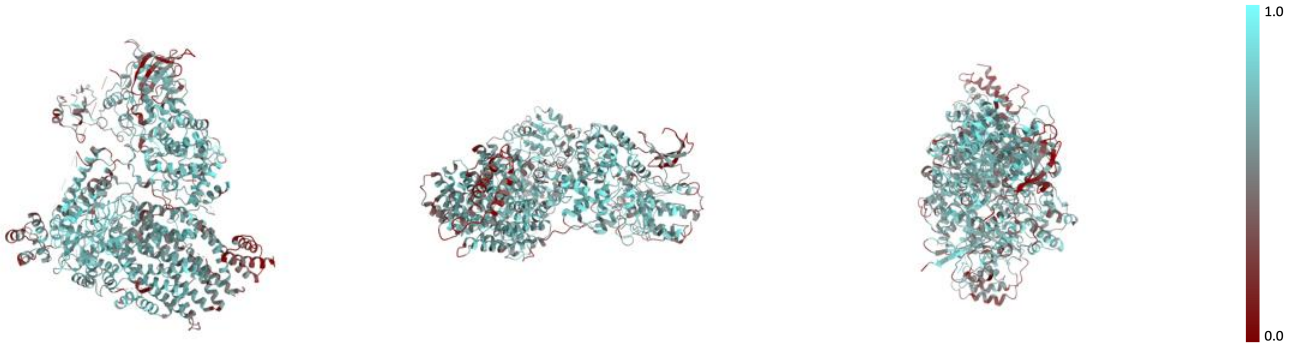
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

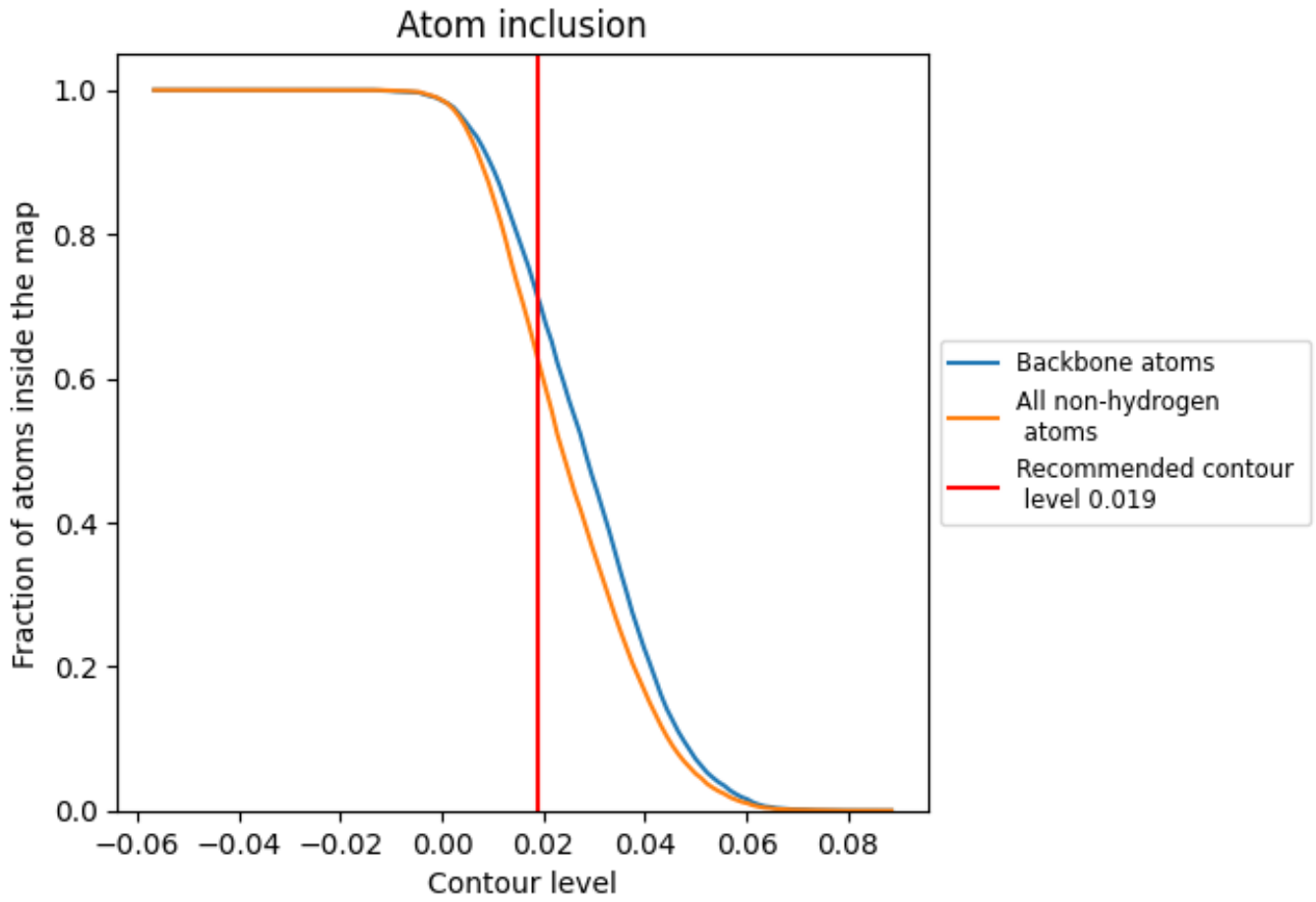
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 62% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6234	0.4870
A	0.6217	0.4850
B	0.5741	0.4790
C	0.7154	0.5170
D	0.5092	0.4580