wwPDB EM Validation Summary Report (i)

May 14, 2025 – 07:45 AM EDT

PDB ID	:	9BM6 / pdb_00009bm6
EMDB ID	:	EMD-44689
Title	:	State-7a of motor domain from full-length human dynein-1 in 5 mM ATP
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	3.22 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

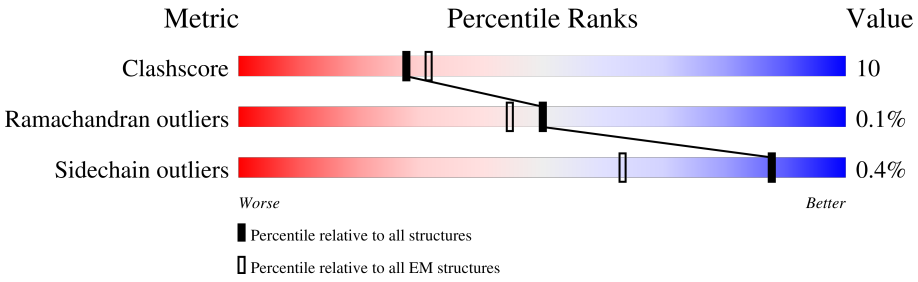
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.22 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4646	8% 47% 14% 38%

2 Entry composition

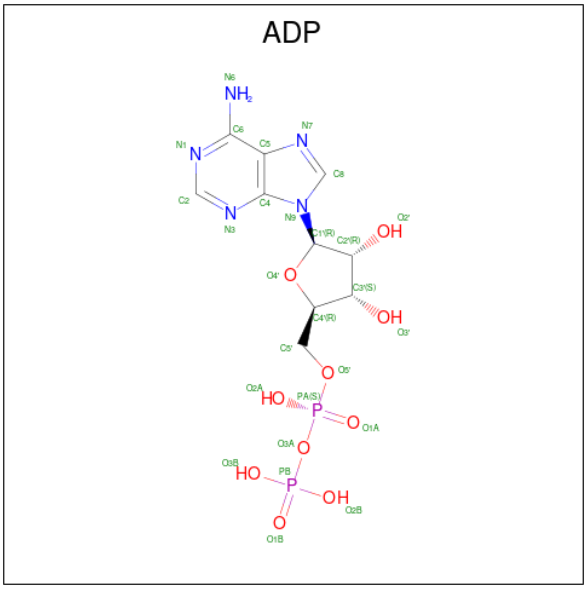
There are 4 unique types of molecules in this entry. The entry contains 23111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytoplasmic dynein 1 heavy chain 1.

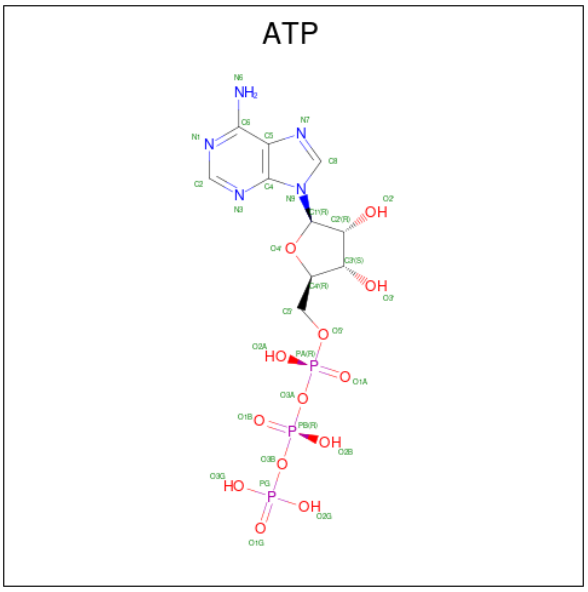
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2858	22994	14663	3967	4249	115	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

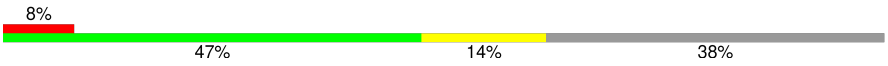
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

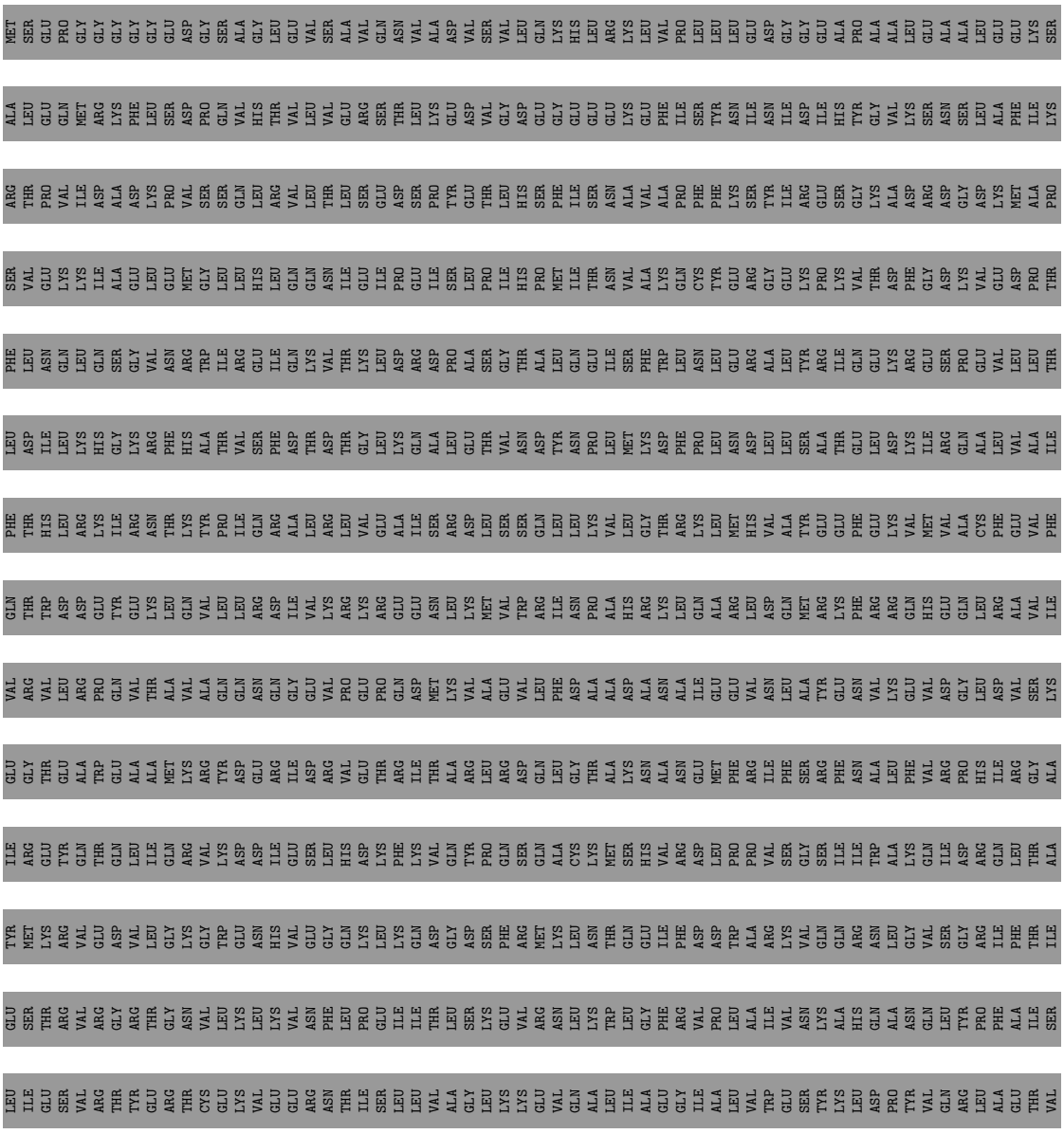
3 Residue-property plots (i)

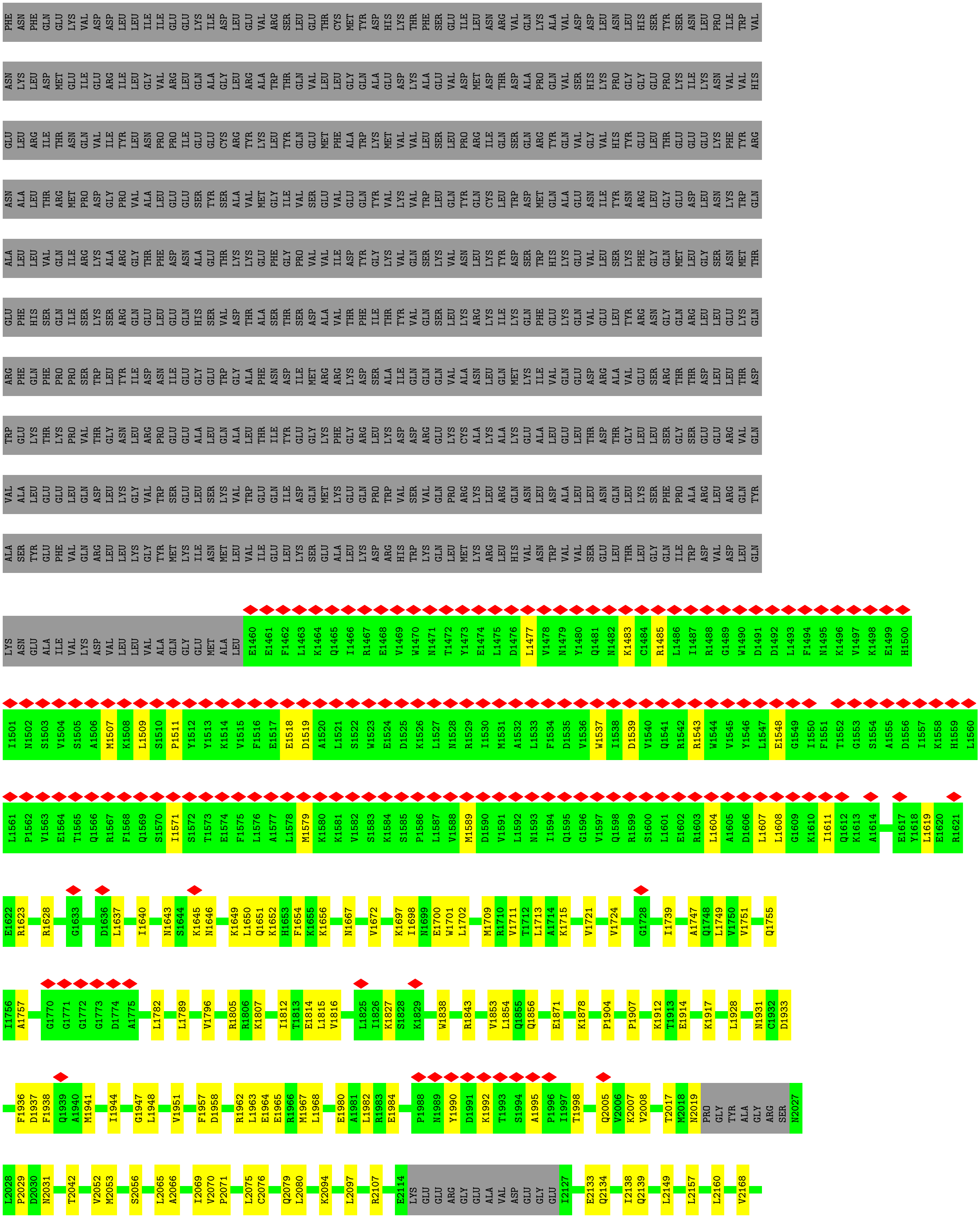
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

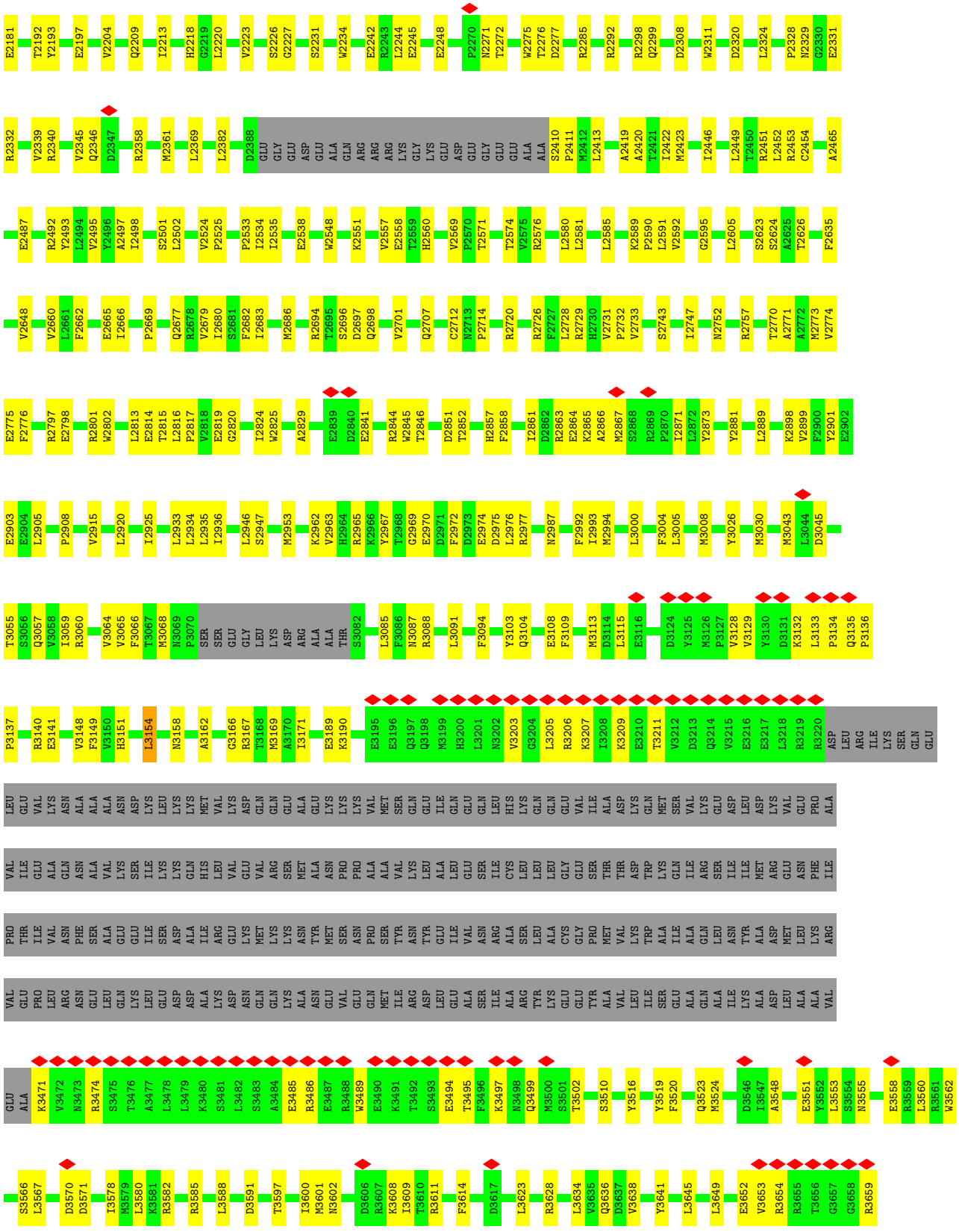
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

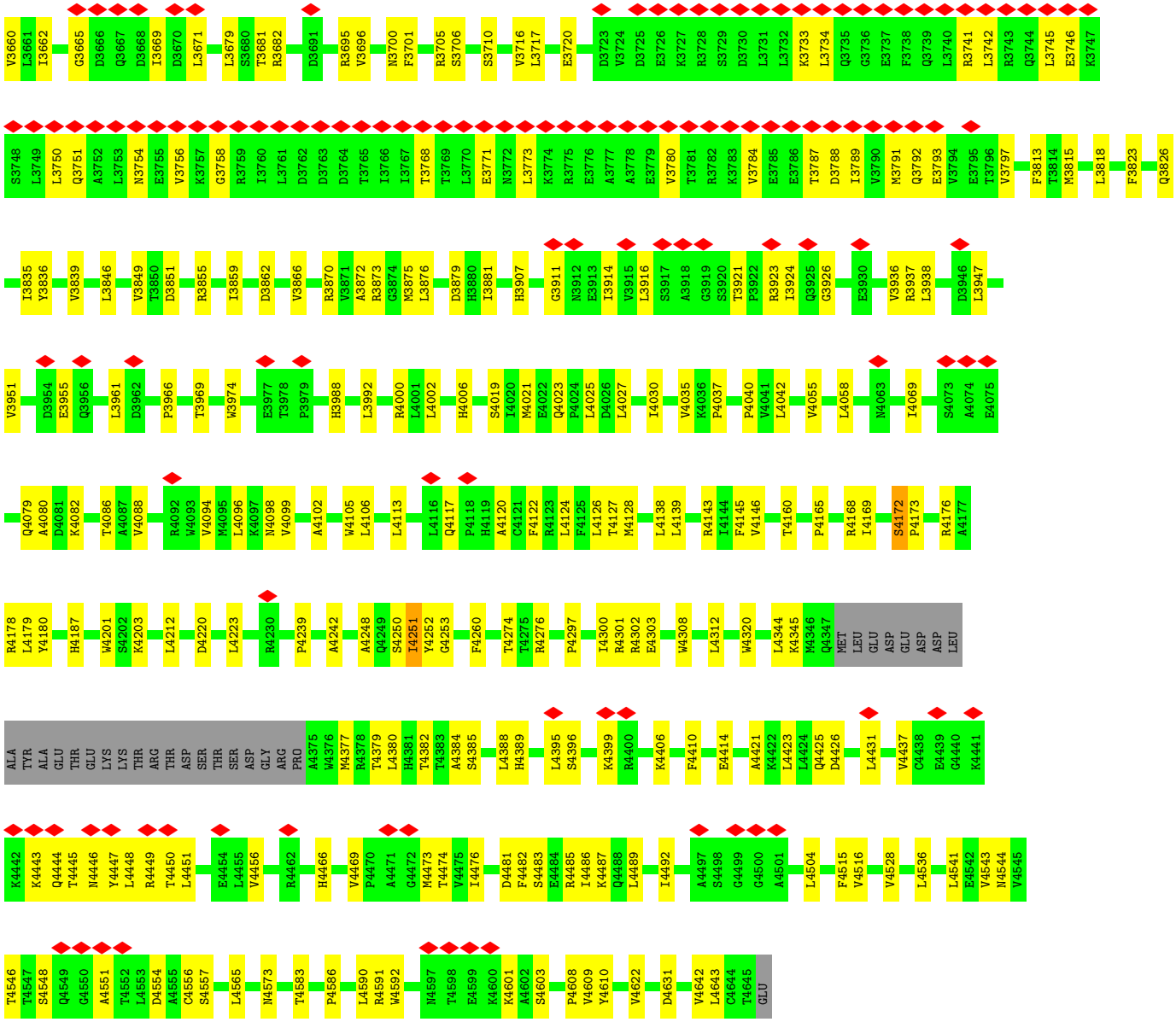
Chain A:






PHE ASN PHE GLN GLU LYS VAL ASP ASP LEU LEU ILE ILE GLU GLU LYS ILE ASP LEU GLU VAL ARG SER LEU GLU THR CYS MET TYR ASP HIS LYS THR PHE SER GLU ILE LEU ASN ARG VAL GLN LYS ALA VAL ASP ASP LEU ASN LEU HIS SER TYR SER ASN LEU PRO ILE TRP VAL
ASN LYS LEU ASP MET GLU ILE GLU ARG ILE LEU GLY VAL ARG LEU GLN ALA GLY LEU ARG ALA TRP THR GLN VAL LEU LEU GLY GLN ALA GLU ASP LYS ALA GLU VAL ASP MET ASP THR ASP ALA PRO GLN VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN VAL VAL HIS
GLU LEU ARG ILE THR ASN GLN VAL ILE TYR LEU ASN PRO PRO ILE GLU GLU CYS ARG TYR LYS LEU TYR GLN GLU MET PHE ALA TRP LYS MET VAL VAL LEU SER LEU PRO ARG ILE GLN SER GLN ARG TYR GLN VAL GLY VAL HIS TYR GLU LEU THR GLU GLU GLU LYS PHE TYR ARG
ASN ALA LEU THR ARG MET PRO ASP GLY PRO VAL ALA LEU GLU GLU SER TYR SER ALA VAL VAL MET GLY ILE VAL SER GLU VAL GLU GLN TYR VAL LYS VAL TRP LEU GLN TYR GLN CYS LEU TRP ASP MET GLN ALA GLU ASN ILE TYR ASN ARG LEU GLY GLU ASP LEU ASN LYS TRP GLN
ALA LEU LEU VAL GLN ILE ARG LYS ALA ARG GLY THR PHE ASP ASN ALA GLU THR LYS LYS GLU PHE GLY PRO VAL VAL ILE ASP TYR GLY LYS VAL GLN SER LYS VAL ASN LEU LYS TYR ASP SER TRP HIS LYS GLU VAL LEU SER LYS PHE GLY GLN MET LEU GLY SER ASN MET THR
GLU PHE HIS SER GLN ILE SER LYS SER ARG GLN GLU LEU GLU GLN HIS SER VAL ASP THR ALA SER THR SER ASP ALA ALA VAL THR PHE ILE THR TYR VAL GLN SER LEU LYS ARG LYS ILE LYS GLN PHE GLU LYS GLN VAL GLU LEU TYR ARG ASN GLY GLN ARG LEU LEU GLU LYS GLN
ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ASN ILE GLU GLY GLU TRP GLY ALA PHE ASN ASP ILE MET ARG ARG LYS ASP SER ALA ILE GLN GLN GLN VAL ALA ASN LEU GLN MET LYS ILE VAL GLN GLU ASP ARG ALA VAL GLU SER ARG THR THR ASP LEU LEU THR ASP
TRP GLU LYS THR LYS PRO VAL THR GLY ASN LEU ARG PRO GLU GLU ALA LEU GLN ALA LEU THR ILE TYR GLU GLY LYS PHE GLY ARG LEU LYS ASP ASP ARG GLU LYS CYS ALA LYS ALA LYS GLU ALA LEU GLU LEU THR ASP THR GLY LEU LEU SER GLY SER GLU GLU ARG VAL GLN
VAL ALA LEU GLU GLU LEU GLN ASP LEU LYS GLY VAL TRP SER GLU LEU SER LYS VAL TRP GLU GLN ILE ASP GLN MET LYS GLU GLN PRO TRP VAL SER VAL GLN PRO ARG LYS LEU ARG GLN ASN LEU ASP ALA LEU LEU ASN GLN LEU LYS SER PHE PRO ALA ARG LEU ARG GLN TYR
ALA SER TYR GLU PHE VAL GLN ARG LEU LEU LYS GLY TYR MET LYS ILE ASN MET LEU VAL ILE GLU LEU LYS SER GLU ALA LEU LYS ASP ARG HIS TRP LYS GLN LEU MET LYS ARG LEU HIS VAL ASN TRP VAL SER GLU LEU THR LEU GLY GLN ILE TRP ASP VAL ASP LEU GLN
LYS ASN GLU ALA ILE VAL LYS ASP VAL LEU LEU VAL ALA GLN GLY GLU MET ALA LEU E1460 E1461 F1462 L1463 K1464 Q1465 I1466 R1467 E1468 V1469 W1470 N1471 T1472 Y1473 E1474 L1475 D1476 L1477 V1478 N1479 Y1480 Q1481 N1482 K1483 C1484 R1485 L1486 I1487 R1488 G1489 W1490 D1491 D1492 L1493 F1494 N1495 K1496 V1497 K1498 E1499 H1500
I1501 N1502 S1503 V1504 S1505 A1506 M1507 K1508 L1509 S1510 P1511 Y1512 Y1513 K1514 V1515 F1516 E1517 E1518 D1519 A1520 L1521 S1522 W1523 E1524 D1525 K1526 L1527 N1528 R1529 I1530 M1531 A1532 L1533 F1534 D1535 V1536 W1537 I1538 D1539 V1540 Q1541 R1542 R1543 W1544 V1545 Y1546 L1547 E1548 G1549 I1550 F1551 T1552 G1553 S1554 A1555 D1556 I1557 K1558 H1559 L1560
L1561 P1562 V1563 E1564 T1565 Q1566 R1567 F1568 Q1569 S1570 I1571 S1572 T1573 E1574 F1575 L1576 A1577 L1578 M1579 K1580 K1581 V1582 S1583 K1584 S1585 P1586 L1587 V1588 M1589 D1590 V1591 L1592 N1593 I1594 Q1595 G1596 V1597 Q1598 R1599 S1600 L1601 E1602 R1603 L1604 A1605 D1606 L1607 L1608 G1609 K1610 I1611 Q1612 K1613 A1614 E1617 Y1618 L1619 E1620 R1621
E1622 R1623 R1628 G1633 D1636 L1637 I1640 N1643 S1644 K1645 N1646 K1649 L1650 Q1651 K1652 H1653 F1654 K1655 K1656 N1667 V1672 K1697 I1698 N1699 E1700 W1701 L1702 M1709 R1710 V1711 T1712 L1713 A1714 K1715 V1721 V1724 G1728 I1739 A1747 Q1748 L1749 V1750 V1751 Q1755
I1756 A1757 G1770 G1771 G1772 G1773 D1774 A1775 L1782 L1789 V1796 R1805 R1806 K1807 I1812 T1813 E1814 L1815 V1816 L1825 I1826 K1827 S1828 K1829 W1838 R1843 V1853 L1854 Q1855 Q1856 E1871 K1878 P1904 P1907 K1912 T1913 E1914 K1917 L1928 N1931 C1932 D1933
F1936 D1937 F1938 Q1939 A1940 M1941 I1944 G1947 L1948 V1951 F1957 D1958 R1962 L1963 E1964 E1965 R1966 M1967 L1968 E1980 A1981 L1982 R1983 E1984 P1988 N1989 Y1990 D1991 K1992 T1993 S1994 A1995 P1996 I1997 T1998 Q2005 V2006 K2007 V2008 T2017 M2018 N2019 PRO GLY TYR ALA GLY ARG SER N2027
L2028 P2029 D2030 N2031 T2042 V2052 M2053 S2056 L2065 A2066 I2069 V2070 P2071 L2075 C2076 Q2079 L2080 K2094 L2097 R2107 E2114 LYS GLU GLU ARG GLY GLU ALA VAL ASP GLU GLY GLU I2127 E2133 Q2134 I2138 Q2139 L2149 L2157 L2160 V2168




V3660 L3661 I3662 G3665 D3666 Q3667 D3668 I3669 D3670 L3671 L3679 S3680 T3681 R3682 D3691 R3695 V3696 M3700 F3701 R3705 S3706 S3710 V3716 L3717 E3720 D3723 V3724 D3725 E3726 K3727 R3728 S3729 D3730 L3731 L3732 K3733 L3734 Q3735 G3736 E3737 F3738 Q3739 L3740 R3741 L3742 R3743 Q3744 L3745 E3746 K3747
S3748 L3749 L3750 Q3751 A3752 L3753 N3754 E3755 V3756 K3757 G3758 R3759 I3760 L3761 D3762 D3763 D3764 T3765 I3766 I3767 T3768 T3769 L3770 E3771 N3772 L3773 K3774 R3775 E3776 A3777 A3778 E3779 V3780 T3781 R3782 K3783 V3784 E3785 E3786 T3787 D3788 I3789 V3790 M3791 Q3792 E3793 V3794 E3795 T3796 V3797 F3813 T3814 M3815 L3818 F3823 Q3826
I3835 Y3836 V3839 L3846 V3849 T3850 D3851 R3855 I3859 D3862 V3866 R3870 V3871 A3872 R3873 G3874 M3875 L3876 D3879 H3880 I3881 H3907 G3911 N3912 E3913 I3914 V3915 L3916 S3917 A3918 G3919 S3920 T3921 P3922 R3923 I3924 Q3925 G3926 E3930 V3936 R3937 L3938 D3946 L3947
V3951 D3954 E3955 Q3956 L3961 D3962 P3966 T3969 W3974 E3977 T3978 P3979 H3988 L3992 R4000 L4001 L4002 H4006 S4019 I4020 M4021 E4022 Q4023 P4024 L4025 D4026 L4027 I4030 V4035 K4036 P4037 P4040 V4041 L4042 V4055 L4058 N4063 I4069 S4073 A4074 E4075
Q4079 A4080 D4081 K4082 T4086 A4087 V4088 R4092 W4093 V4094 M4095 L4096 K4097 N4098 V4099 A4102 W4105 L4106 L4113 L4116 Q4117 P4118 H4119 A4120 C4121 F4122 R4123 L4124 F4125 L4126 T4127 M4128 L4138 L4139 R4143 I4144 F4145 V4146 T4160 P4165 R4168 I4169 S4172 P4173 R4176 A4177
R4178 L4179 Y4180 H4187 W4201 S4202 K4203 L4212 D4220 L4223 R4230 P4239 A4242 A4248 Q4249 S4250 I4251 Y4252 G4253 F4260 T4274 T4275 R4276 P4297 I4300 R4301 R4302 E4303 W4308 L4312 W4320 L4344 K4345 M4346 Q4347 MET LEU GLU ASP GLU ASP ASP ASP LEU
ALA TYR ALA GLU THR GLU LYS LYS THR ARG THR ASP SER THR SER ASP GLY ARG PRO A4375 W4376 M4377 R4378 T4379 L4380 H4381 T4382 T4383 A4384 S4385 L4388 H4389 L4395 S4396 K4399 R4400 K4406 F4410 E4414 A4421 K4422 L4423 L4424 Q4425 D4426 L4431 V4437 C4438 E4439 G4440 K4441
K4442 K4443 Q4444 T4445 N4446 Y4447 L4448 R4449 T4450 L4451 E4454 L4455 V4456 R4462 H4466 V4469 P4470 A4471 G4472 M4473 T4474 V4475 T4476 D4481 F4482 S4483 E4484 R4485 I4486 K4487 Q4488 L4489 I4492 A4497 S4498 G4499 G4500 A4501 L4504 F4515 V4516 V4528 L4536 L4541 E4542 V4543 N4544 V4545
T4546 T4547 S4548 Q4549 G4550 A4551 T4552 L4553 D4554 A4555 C4556 S4557 L4565 N4573 T4583 P4586 L4590 R4591 W4592 N4597 T4598 E4599 K4600 K4601 A4602 S4603 P4608 V4609 Y4610 V4622 D4631 V4642 L4643 C4644 T4645 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67951	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.933	Depositor
Minimum map value	-0.458	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, 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	A	0.13	0/23487	0.30	1/31835 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3045	ASP	CB-CA-C	-5.74	109.98	116.63

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	22994	0	23054	438	0
2	A	54	0	24	1	0
3	A	62	0	24	2	0
4	A	1	0	0	0	0
All	All	23111	0	23102	438	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 10.

The worst 5 of 438 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:3151:HIS:HD1	1:A:3516:TYR:HH	1.13	0.95
1:A:2498:ILE:HG23	1:A:2502:LEU:HD22	1.63	0.80
1:A:2863:ARG:HH21	1:A:2866:ALA:HB1	1.46	0.79
1:A:2816:LEU:HD11	1:A:2820:GLY:HA3	1.65	0.79
1:A:2053:MET:HE1	1:A:2094:LYS:HG2	1.64	0.79

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	2844/4646 (61%)	2766 (97%)	75 (3%)	3 (0%)	48 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	2871	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2544/4125 (62%)	2535 (100%)	9 (0%)	89 93

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3710	SER
1	A	3961	LEU
1	A	2276	THR
1	A	2454	CYS
1	A	2953	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3622	ASN
1	A	3772	ASN
1	A	4549	GLN
1	A	3709	GLN
1	A	3822	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)

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 (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	4703	4	28,33,33	0.66	0	34,52,52	0.60	1 (2%)
2	ADP	A	4701	-	24,29,29	0.87	0	29,45,45	1.23	2 (6%)
3	ATP	A	4702	-	28,33,33	0.67	0	34,52,52	0.59	1 (2%)
2	ADP	A	4704	-	24,29,29	0.88	0	29,45,45	1.26	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4703	4	-	5/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	7/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4704	ADP	N3-C2-N1	-3.67	123.69	128.67
2	A	4701	ADP	N3-C2-N1	-3.65	123.72	128.67
2	A	4704	ADP	C4-C5-N7	-2.65	106.53	109.34
2	A	4701	ADP	C4-C5-N7	-2.55	106.64	109.34
3	A	4703	ATP	C5-C6-N6	2.35	123.89	120.31

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	O4'-C4'-C5'-O5'

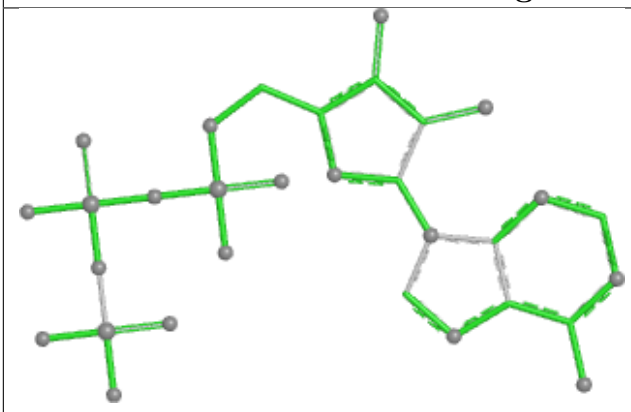
There are no ring outliers.

2 monomers are involved in 3 short contacts:

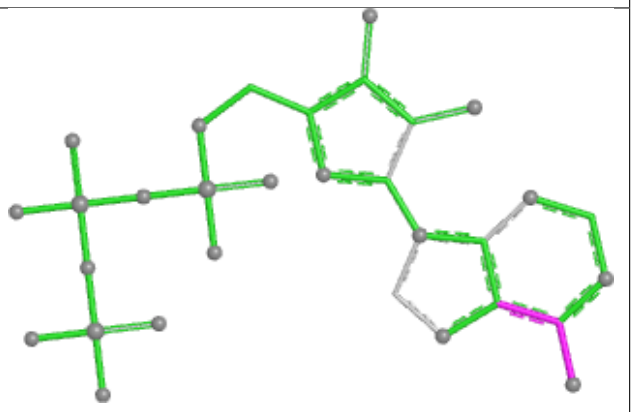
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	1	0
3	A	4702	ATP	2	0

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 then 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.

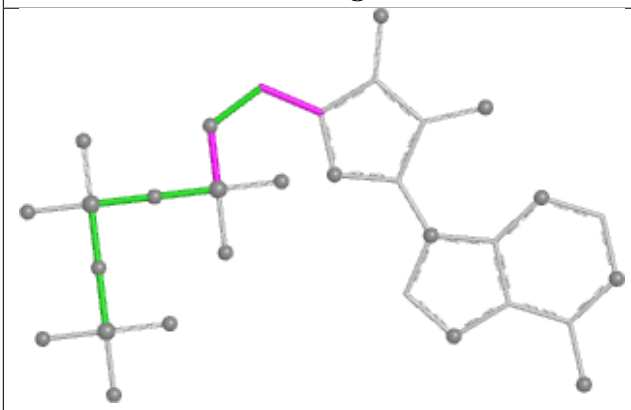
Ligand ATP A 4703



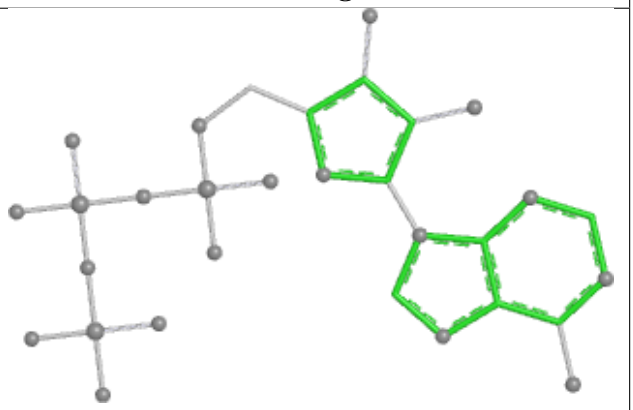
Bond lengths



Bond angles

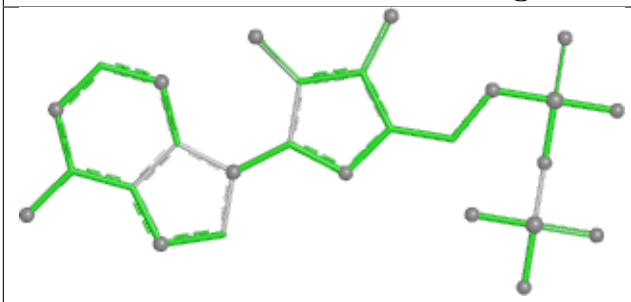


Torsions

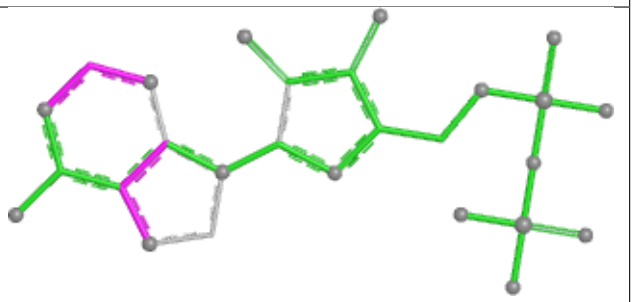


Rings

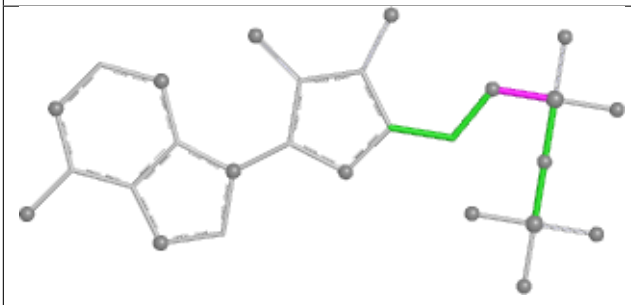
Ligand ADP A 4701



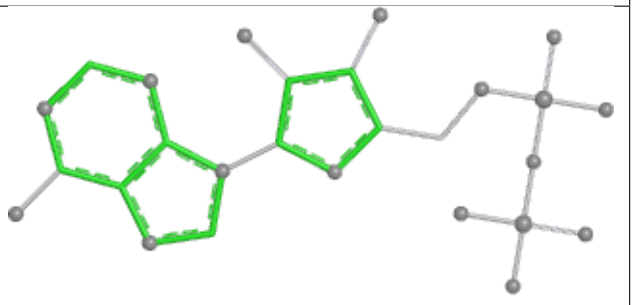
Bond lengths



Bond angles

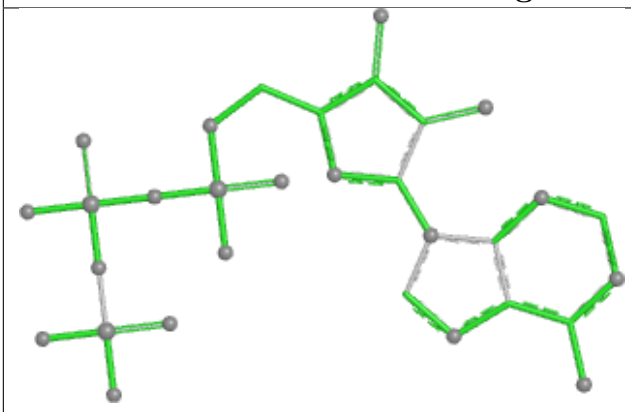


Torsions

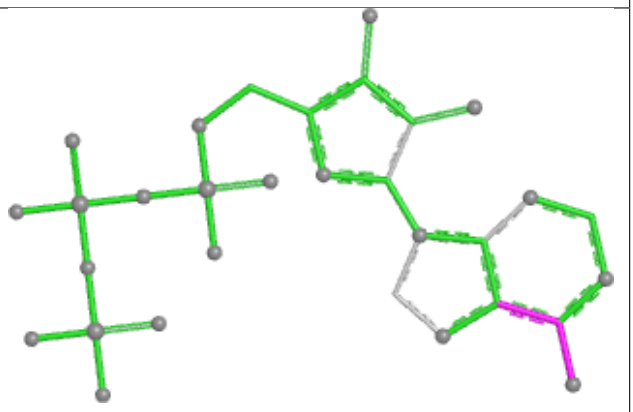


Rings

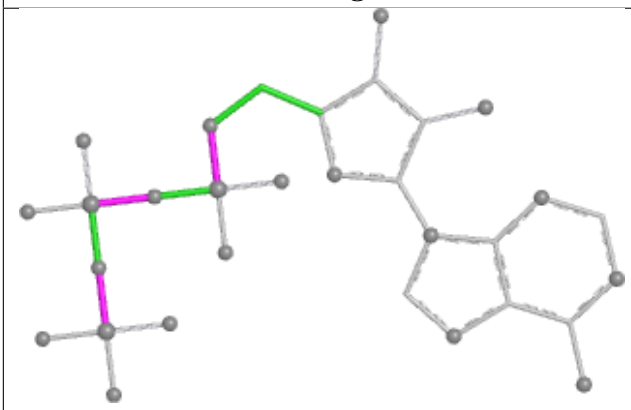
Ligand ATP A 4702



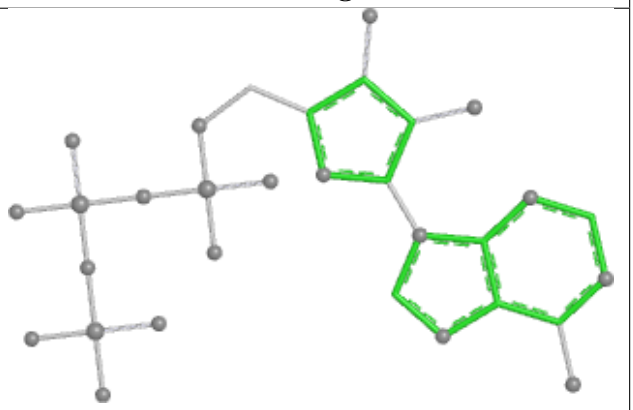
Bond lengths



Bond angles

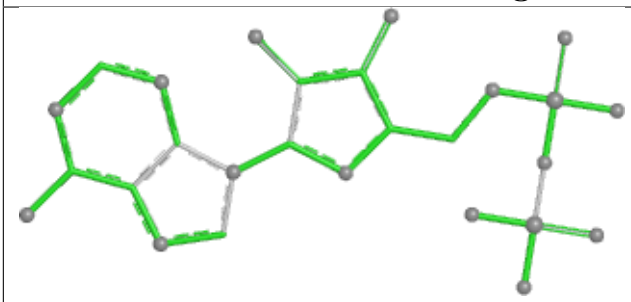


Torsions

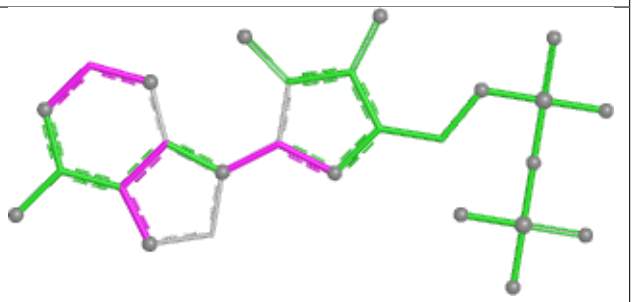


Rings

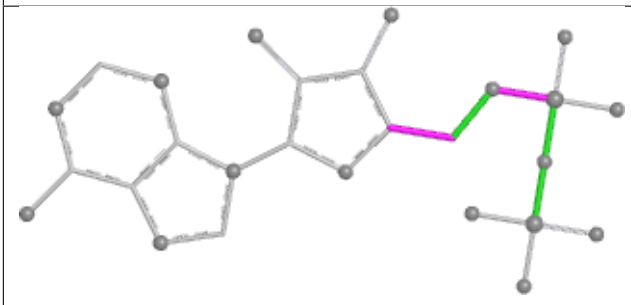
Ligand ADP A 4704



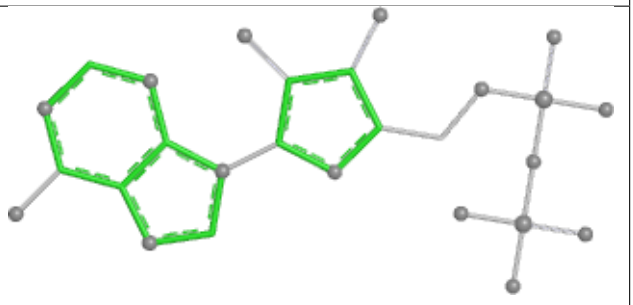
Bond lengths



Bond angles



Torsions



Rings

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.

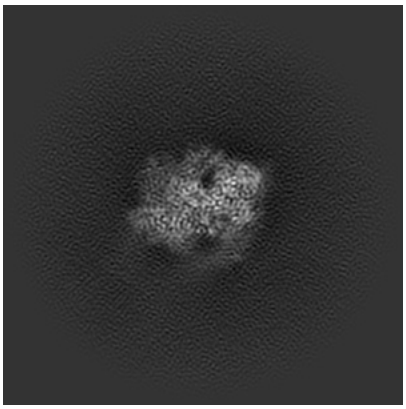
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44689. These allow visual inspection of the internal detail of the map and identification of artifacts.

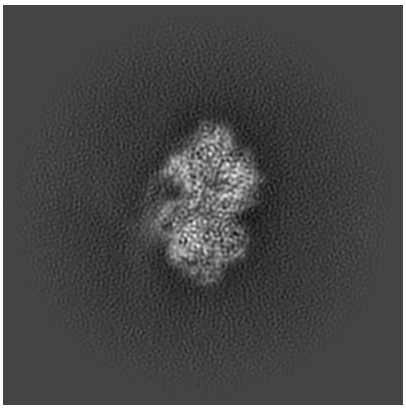
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

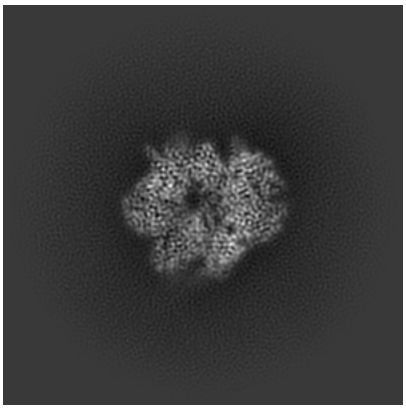
6.1.1 Primary map



X

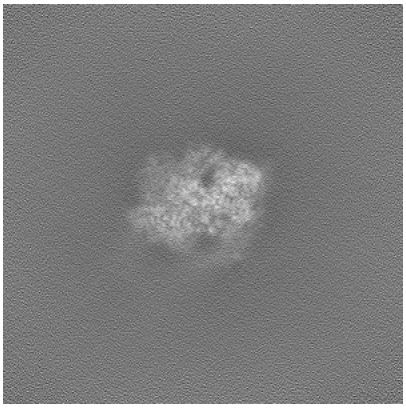


Y

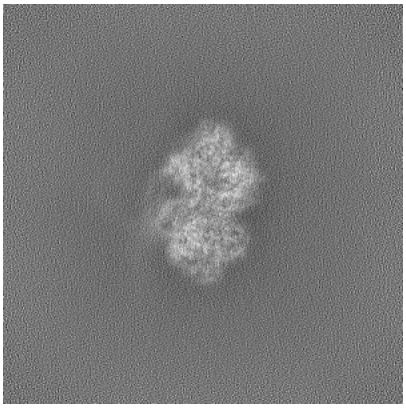


Z

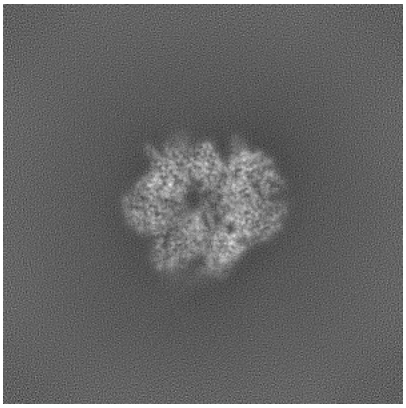
6.1.2 Raw map



X



Y

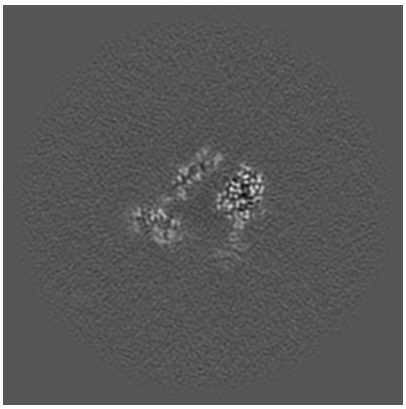


Z

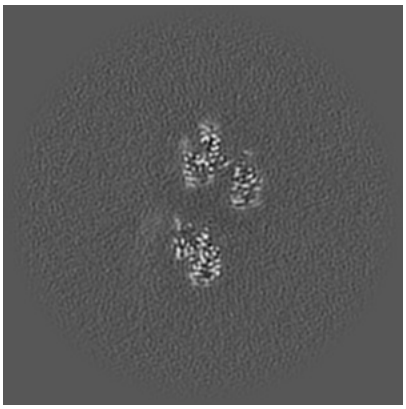
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

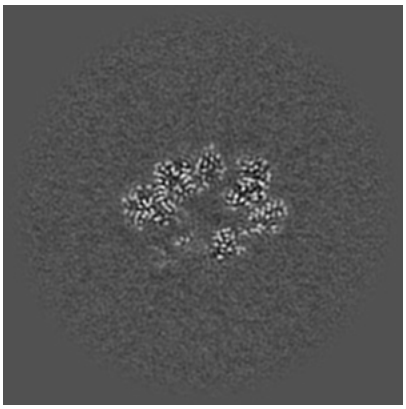
6.2.1 Primary map



X Index: 200

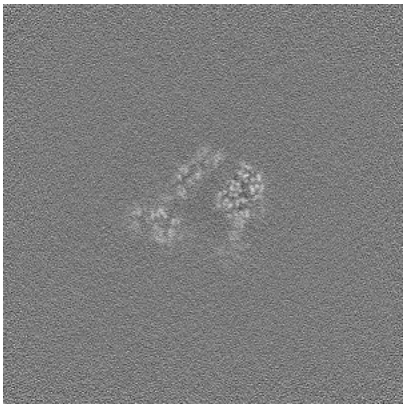


Y Index: 200

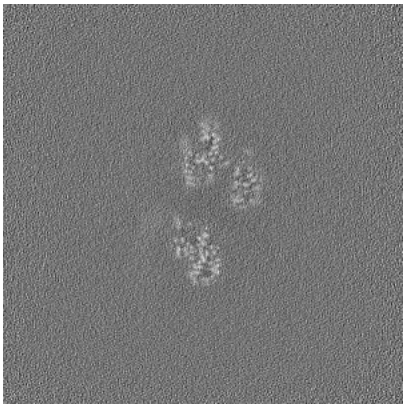


Z Index: 200

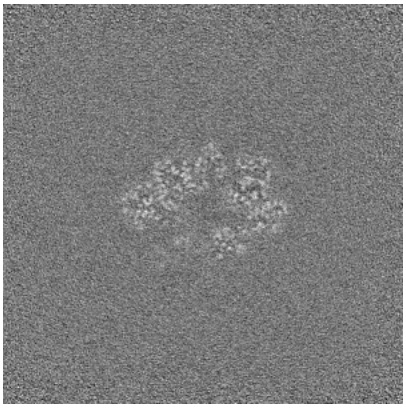
6.2.2 Raw map



X Index: 200



Y Index: 200

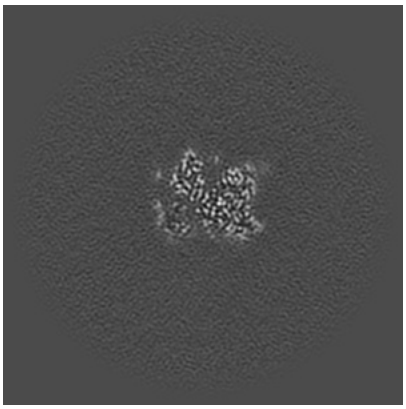


Z Index: 200

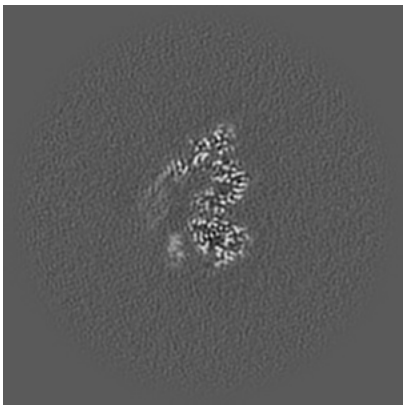
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

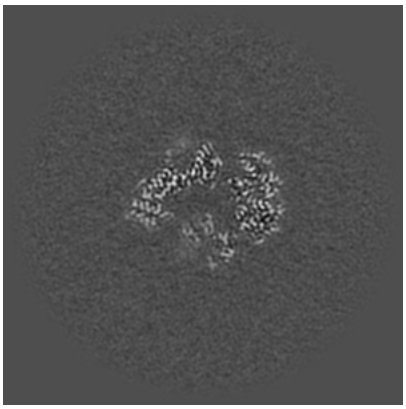
6.3.1 Primary map



X Index: 240

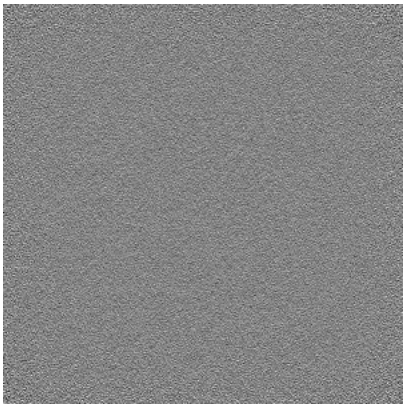


Y Index: 224

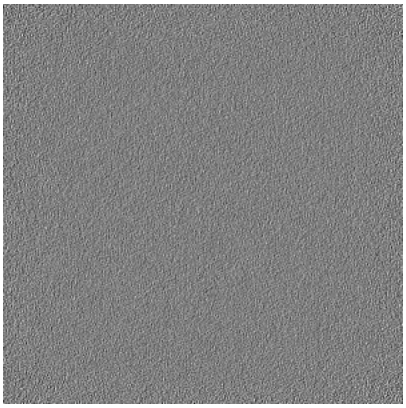


Z Index: 214

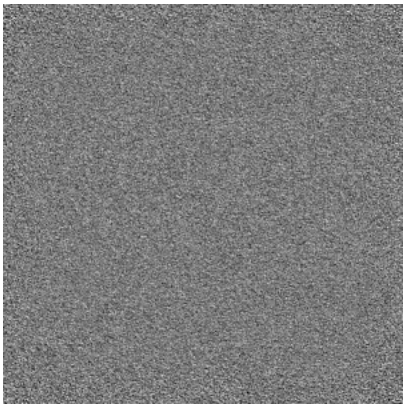
6.3.2 Raw map



X Index: 0



Y Index: 0

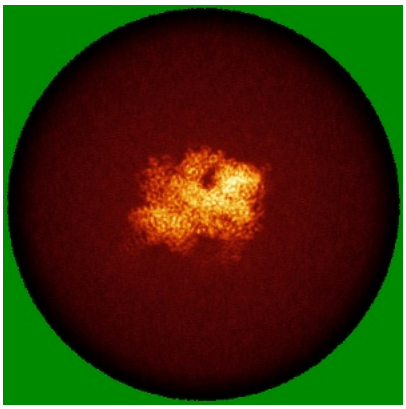


Z Index: 0

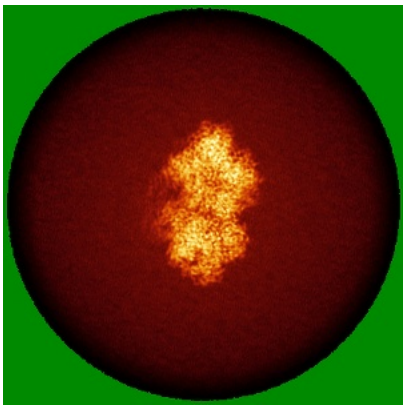
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

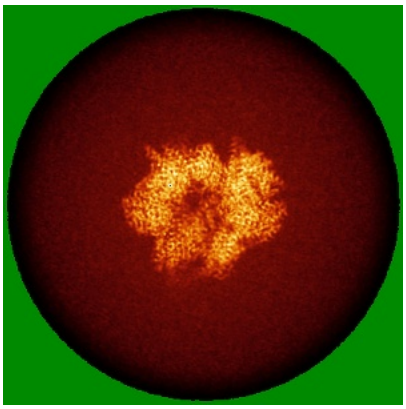
6.4.1 Primary map



X

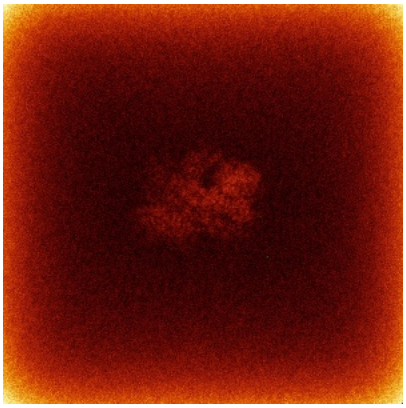


Y

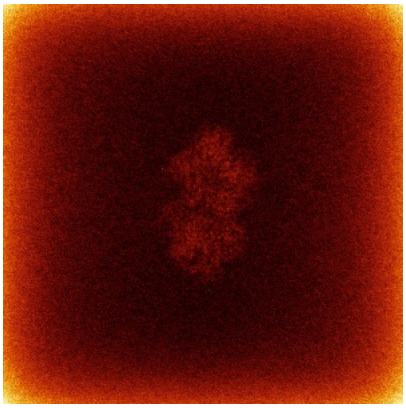


Z

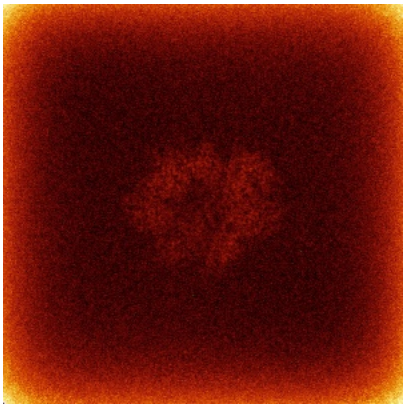
6.4.2 Raw map



X



Y

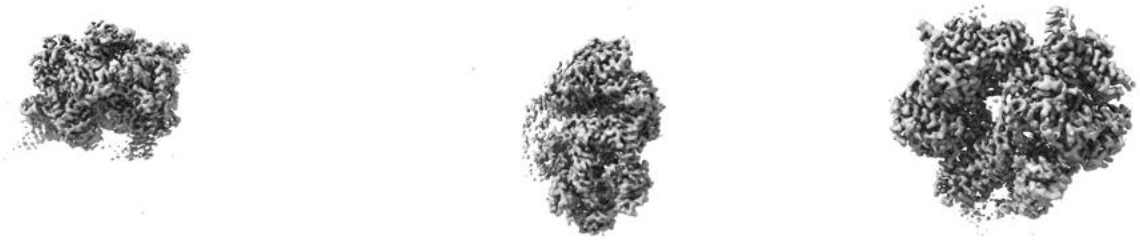


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. 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

X Y Z

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.

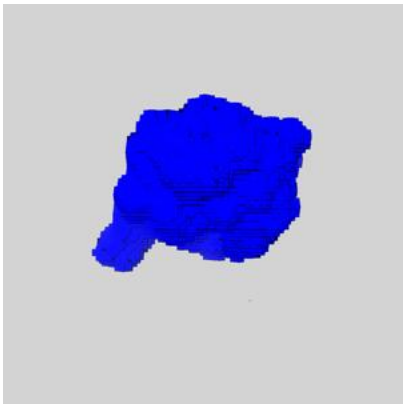
6.6 Mask visualisation

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

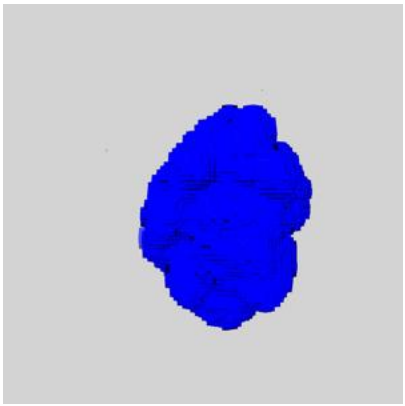
A mask typically either:

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

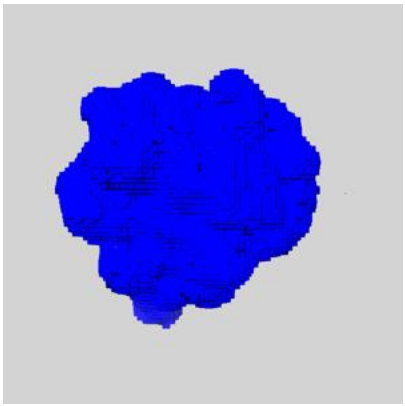
6.6.1 emd_44689_msk_1.map



X



Y

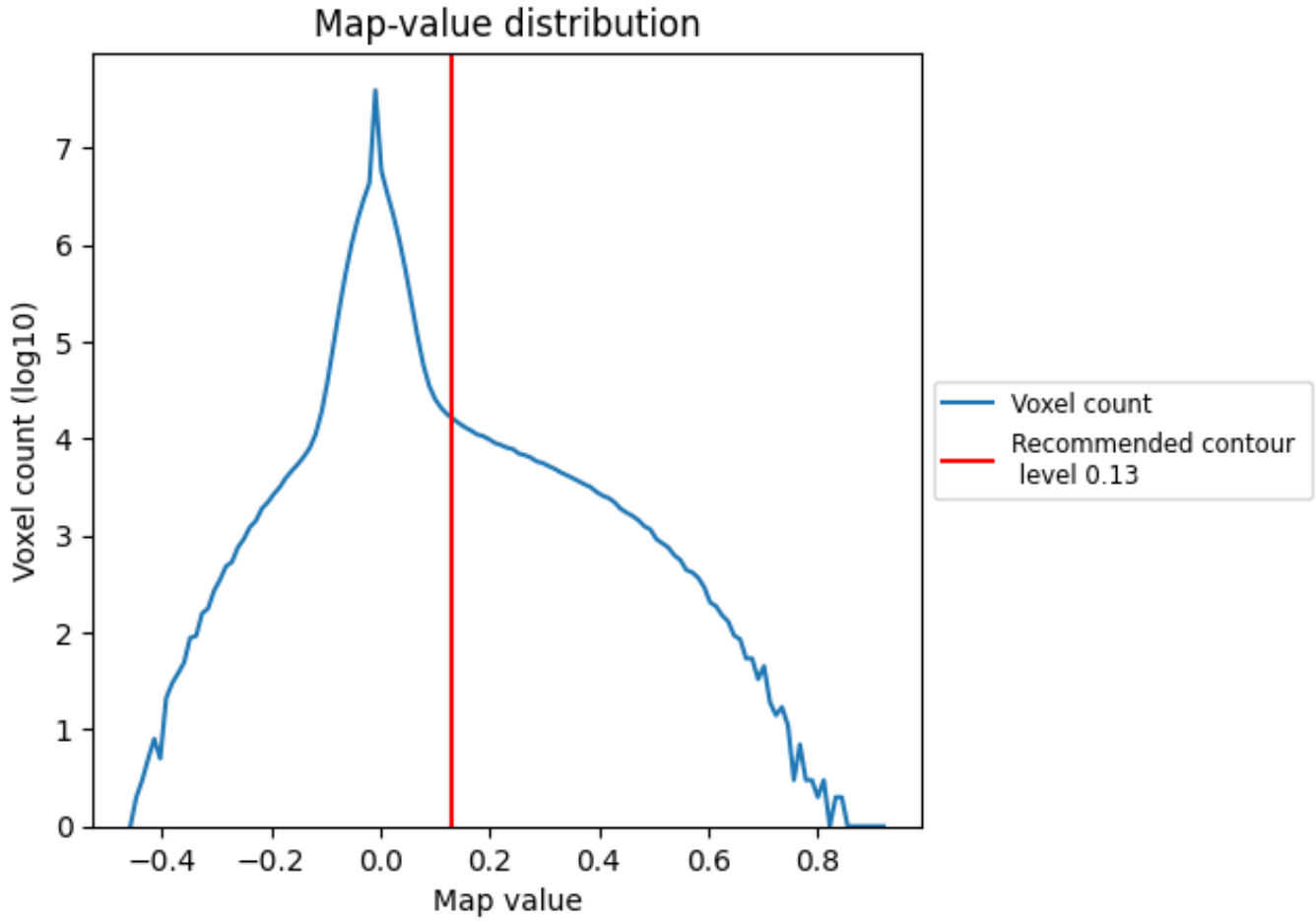


Z

7 Map analysis

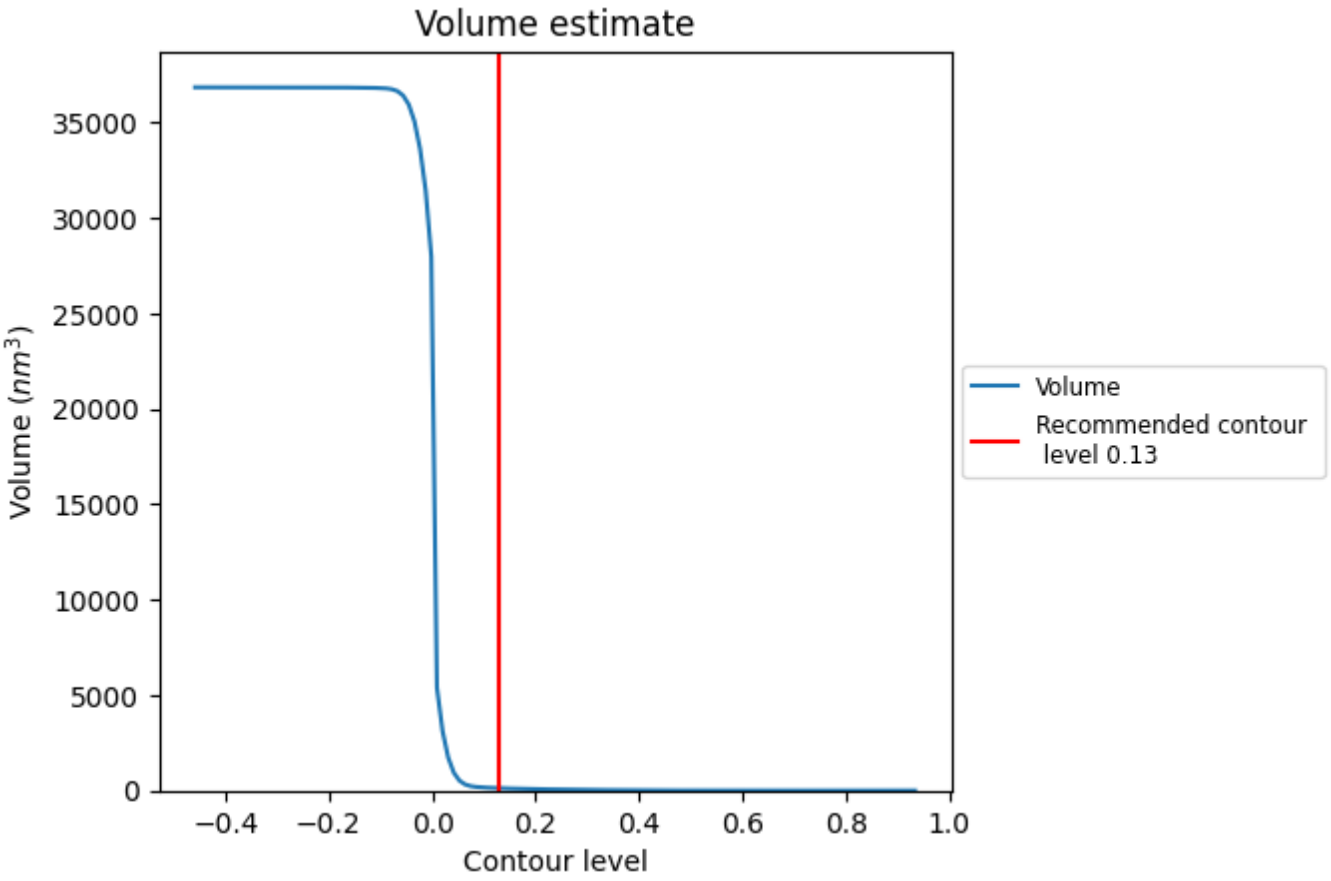
This section contains the results of statistical analysis of the map.

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.

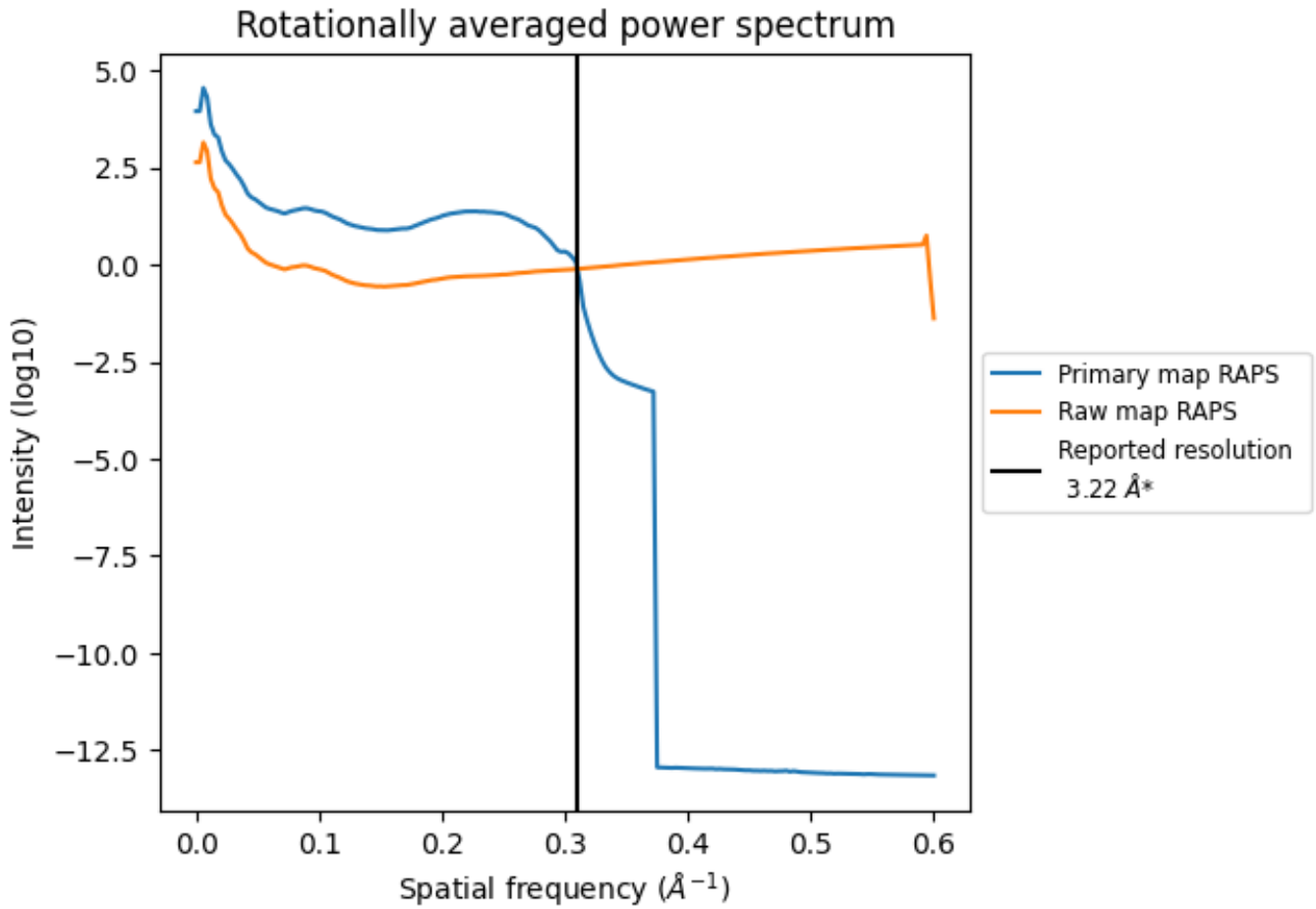
7.2 Volume estimate (i)



The volume at the recommended contour level is 124 nm^3; this corresponds to an approximate mass of 112 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)

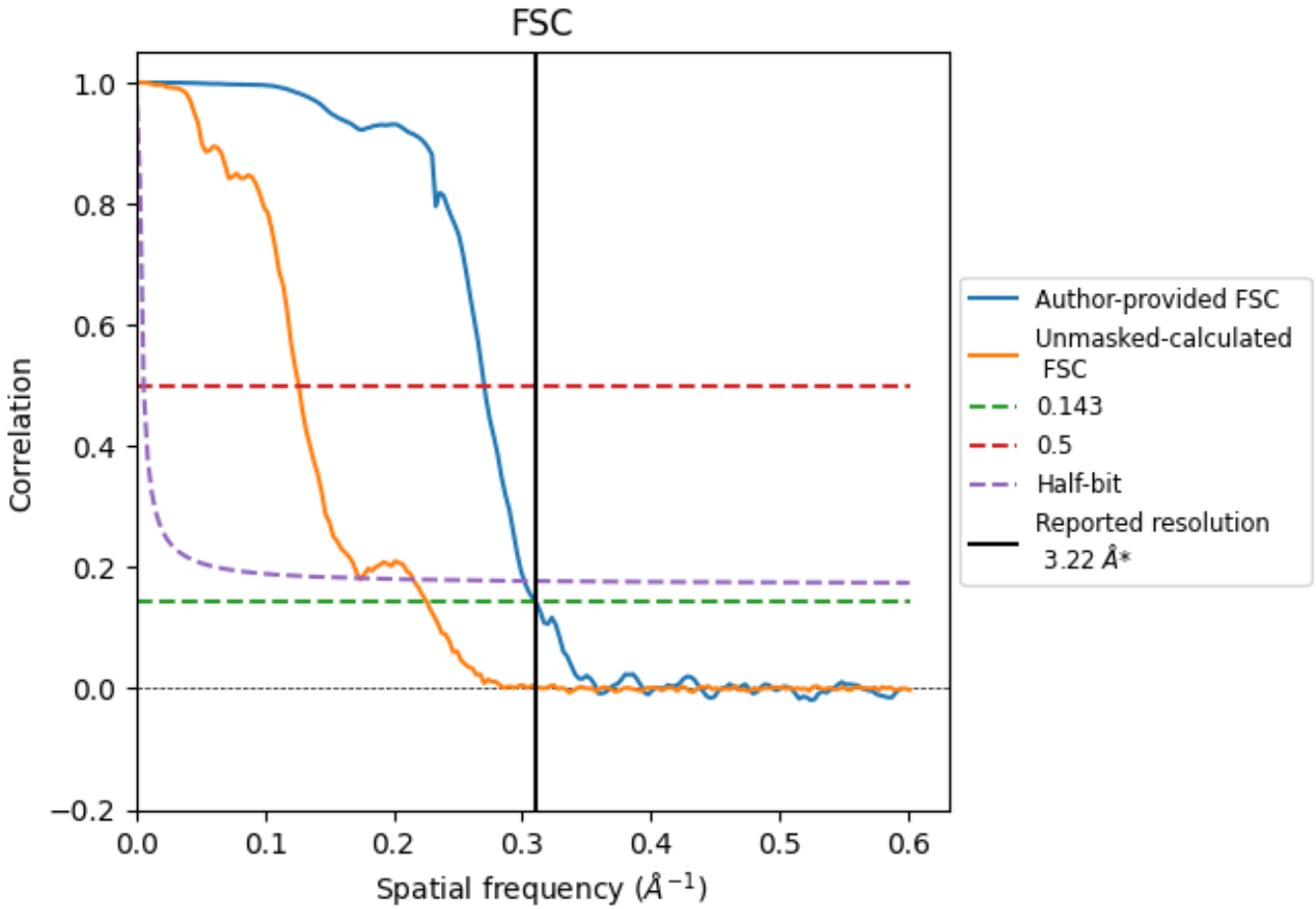


*Reported resolution corresponds to spatial frequency of 0.311 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.311 Å^{-1}

8.2 Resolution estimates (i)

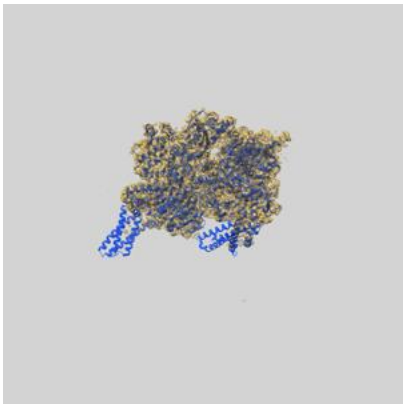
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.22	-	-
Author-provided FSC curve	3.22	3.70	3.32
Unmasked-calculated*	4.43	7.92	5.76

*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 4.43 differs from the reported value 3.22 by more than 10 %

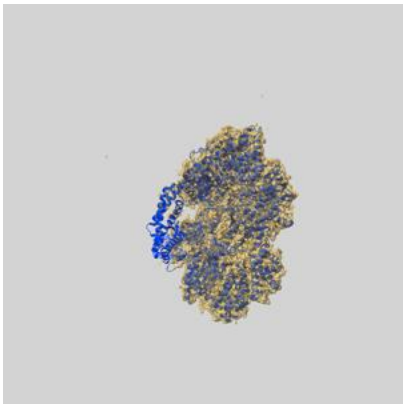
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44689 and PDB model 9BM6. Per-residue inclusion information can be found in section 3 on page 5.

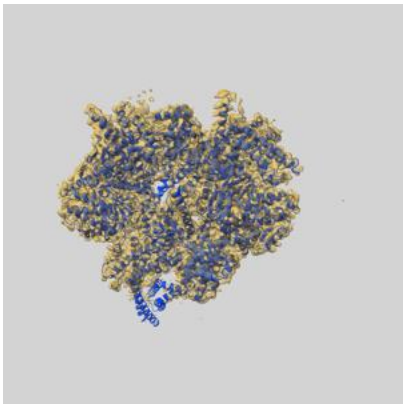
9.1 Map-model overlay



X



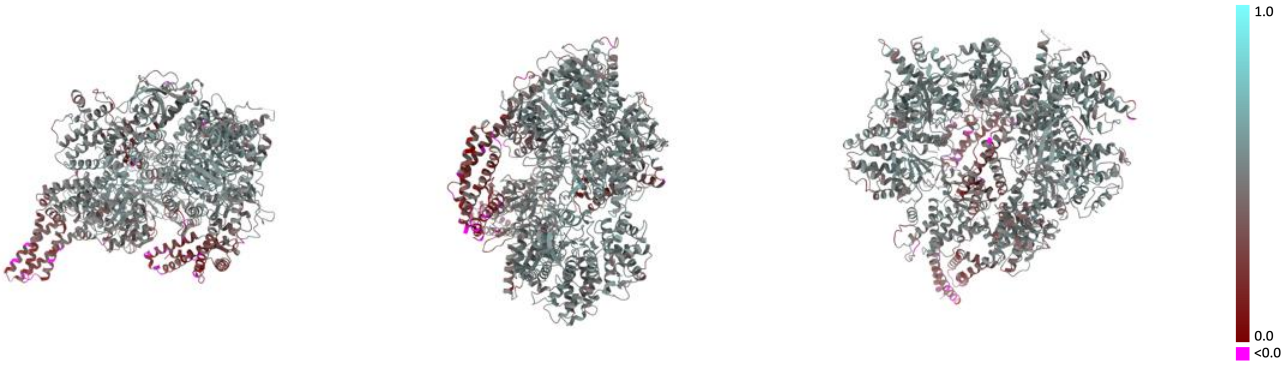
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

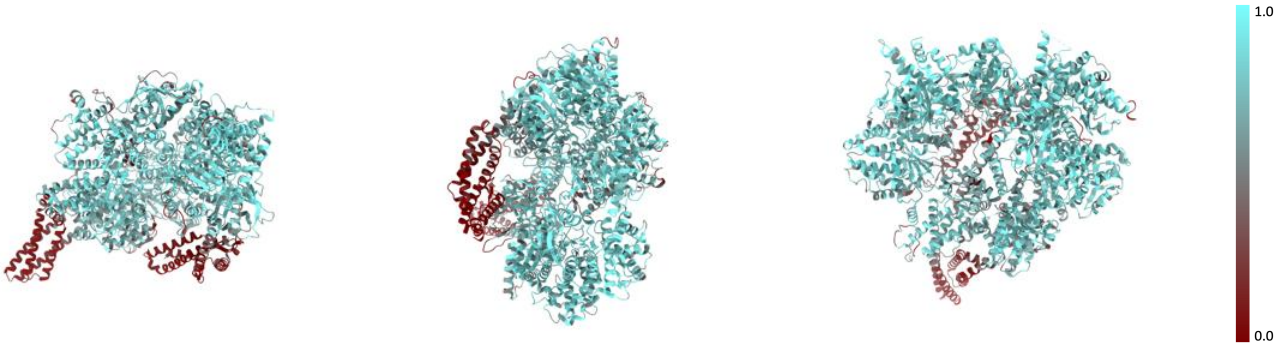
9.2 Q-score mapped to coordinate model



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.

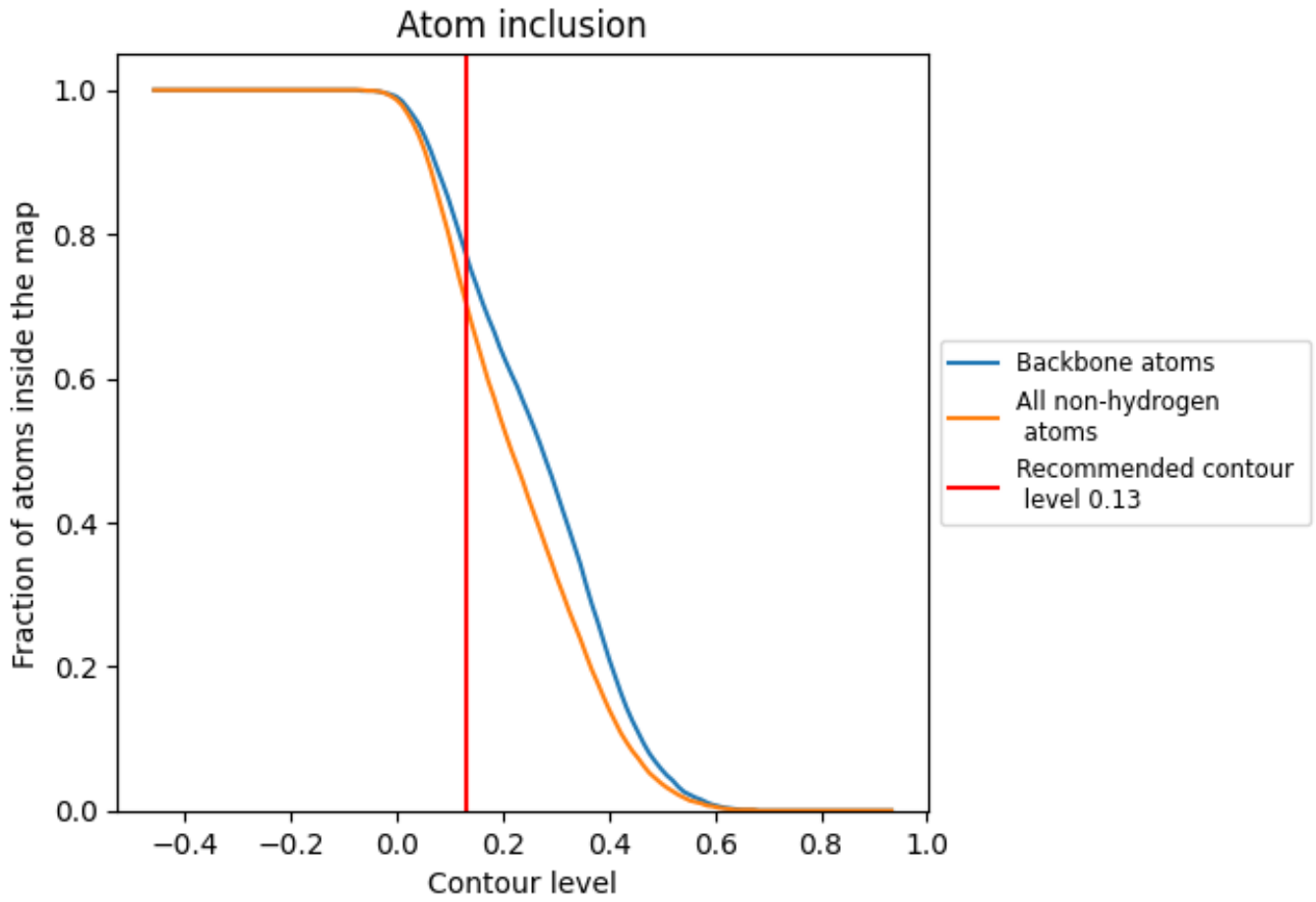
9.3 Atom inclusion mapped to coordinate model



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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.4690
A	0.7050	0.4690