wwPDB EM Validation Summary Report (i)

Aug 5, 2026 – 02:48 AM EDT

PDB ID	:	9BMG / pdb_00009bmg
EMDB ID	:	EMD-44698
Title	:	State-2 of full-length human dynein-1 in 5mM ATPVi
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	2.86 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:

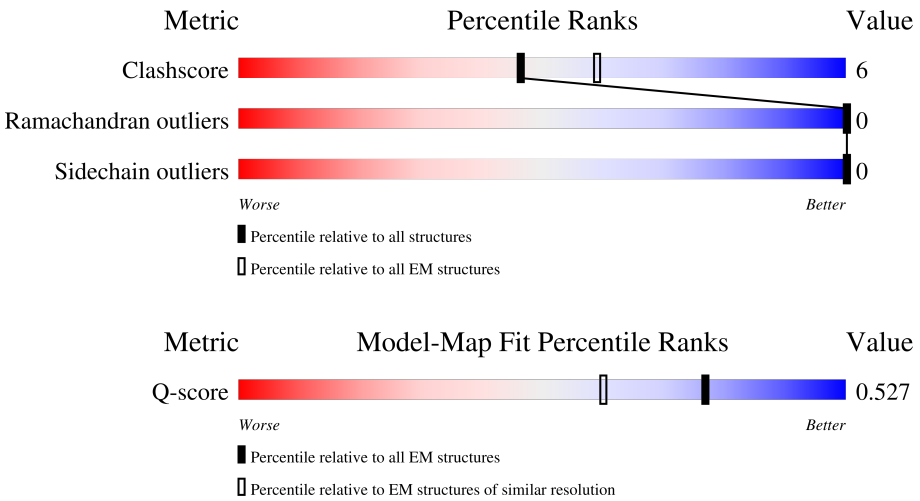
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

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 2.86 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	12017 (2.36 - 3.36)

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	10% 53% 10% 37%

2 Entry composition (i)

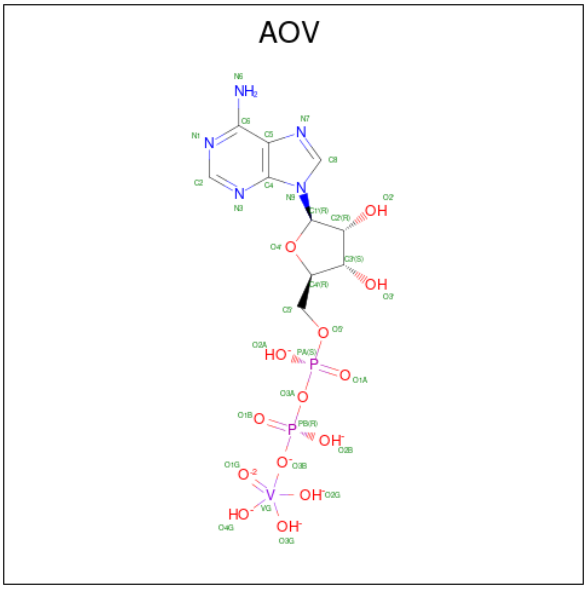
There are 5 unique types of molecules in this entry. The entry contains 23712 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

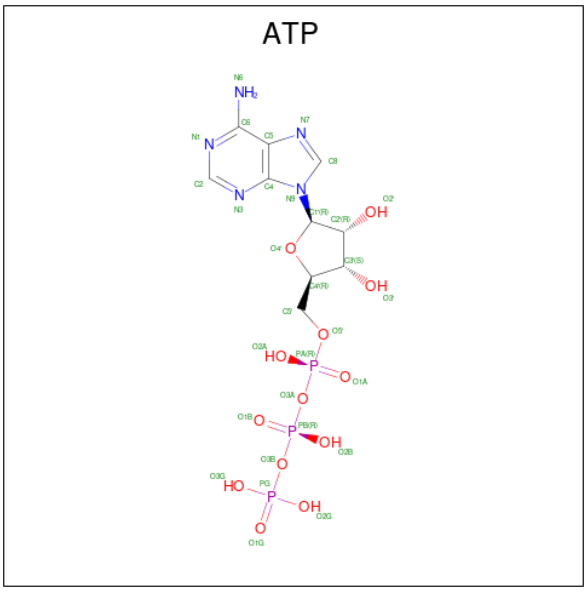
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2937	23593	15028	4070	4378	117	0	0

- Molecule 2 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$) (labeled as "Ligand of Interest" by depositor).



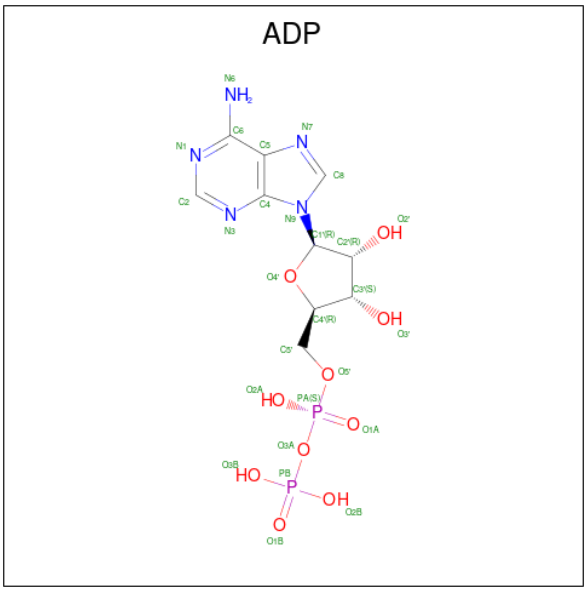
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	V	
2	A	1	32	10	5	14	2	1	0

- 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
			Total	C	N	O	P	
3	A	1	31	10	5	13	3	0

- Molecule 4 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	
4	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
4	A	1	27	10	5	10	2	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

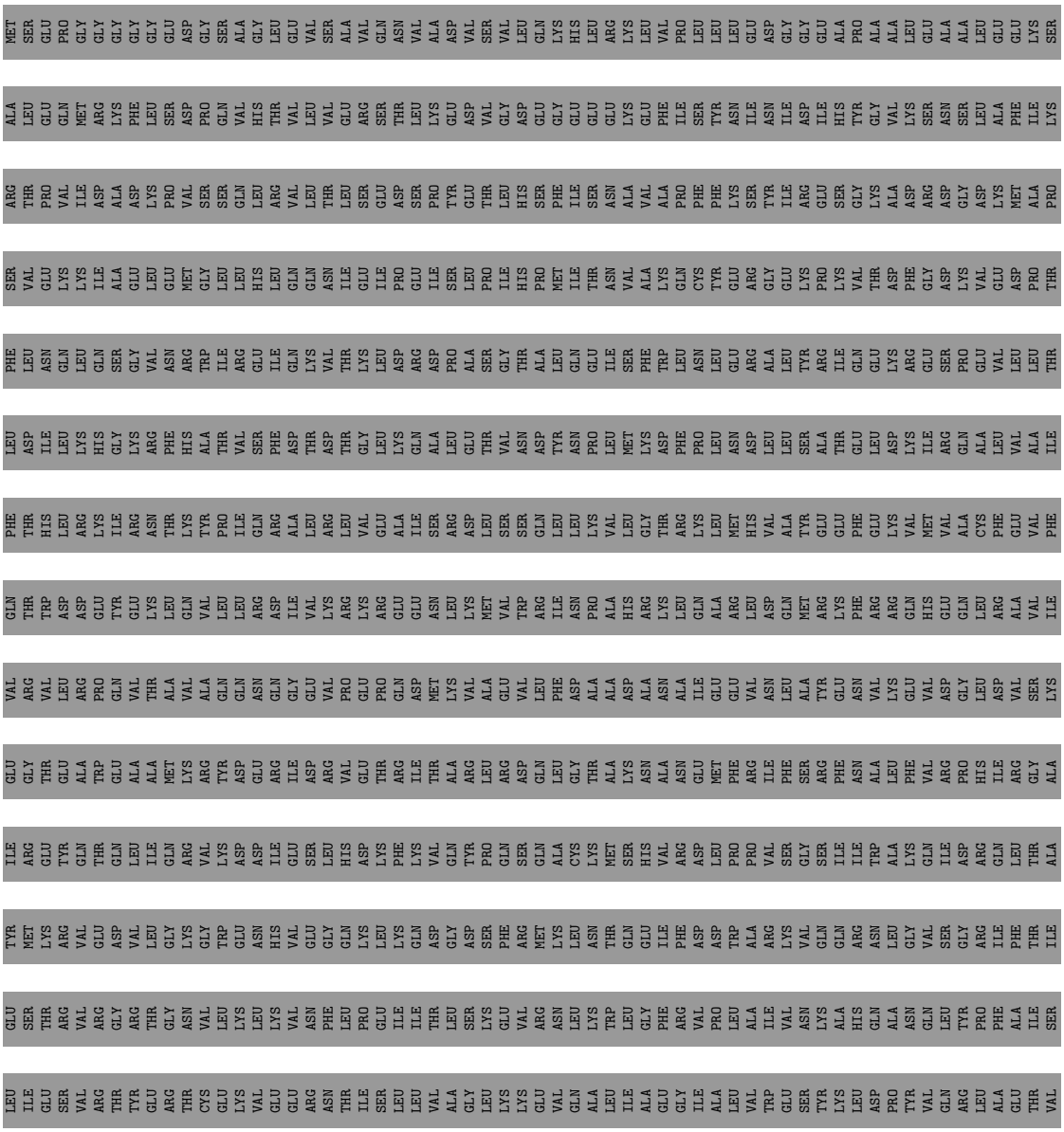
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	2	2	2	0

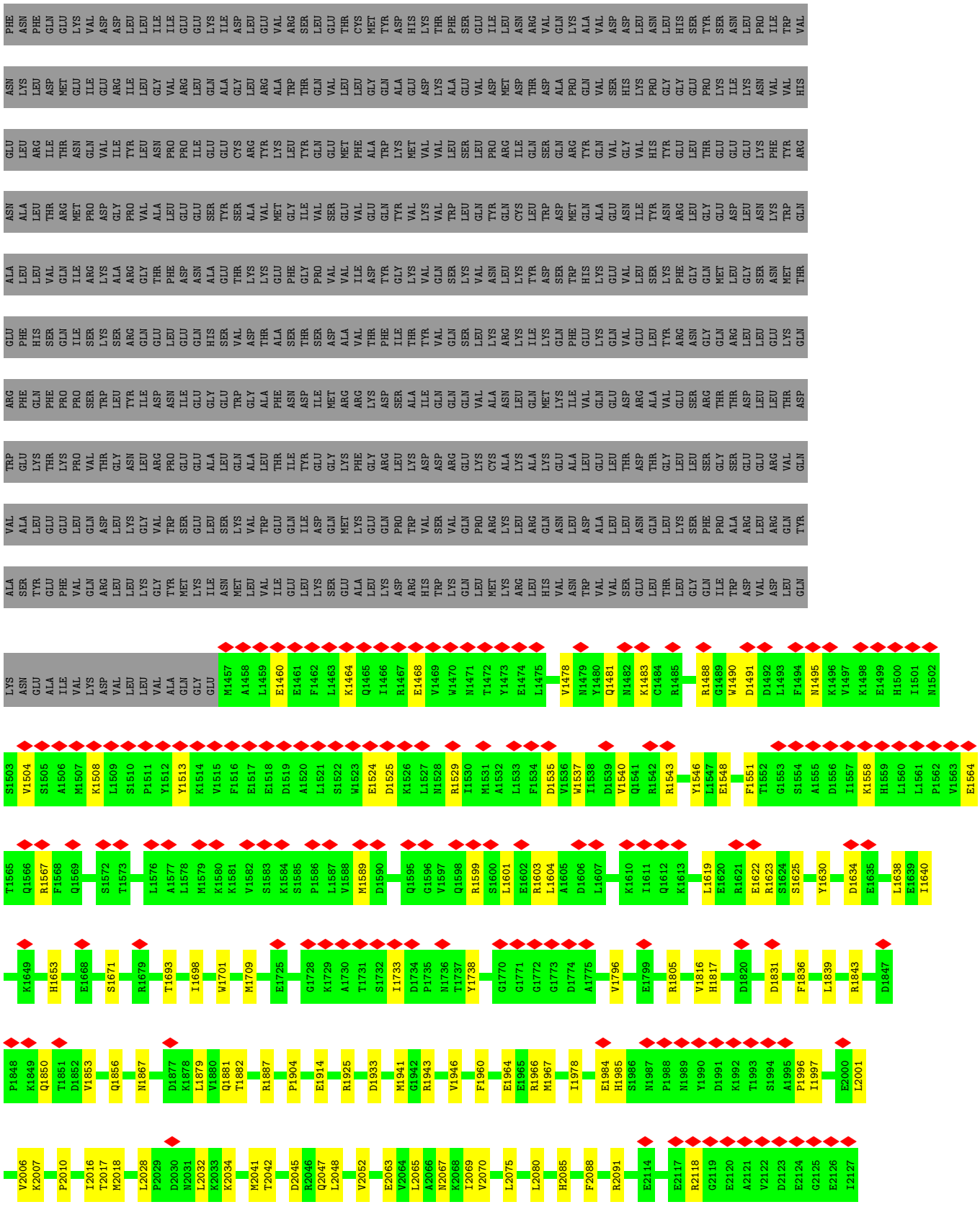
3 Residue-property plots (i)

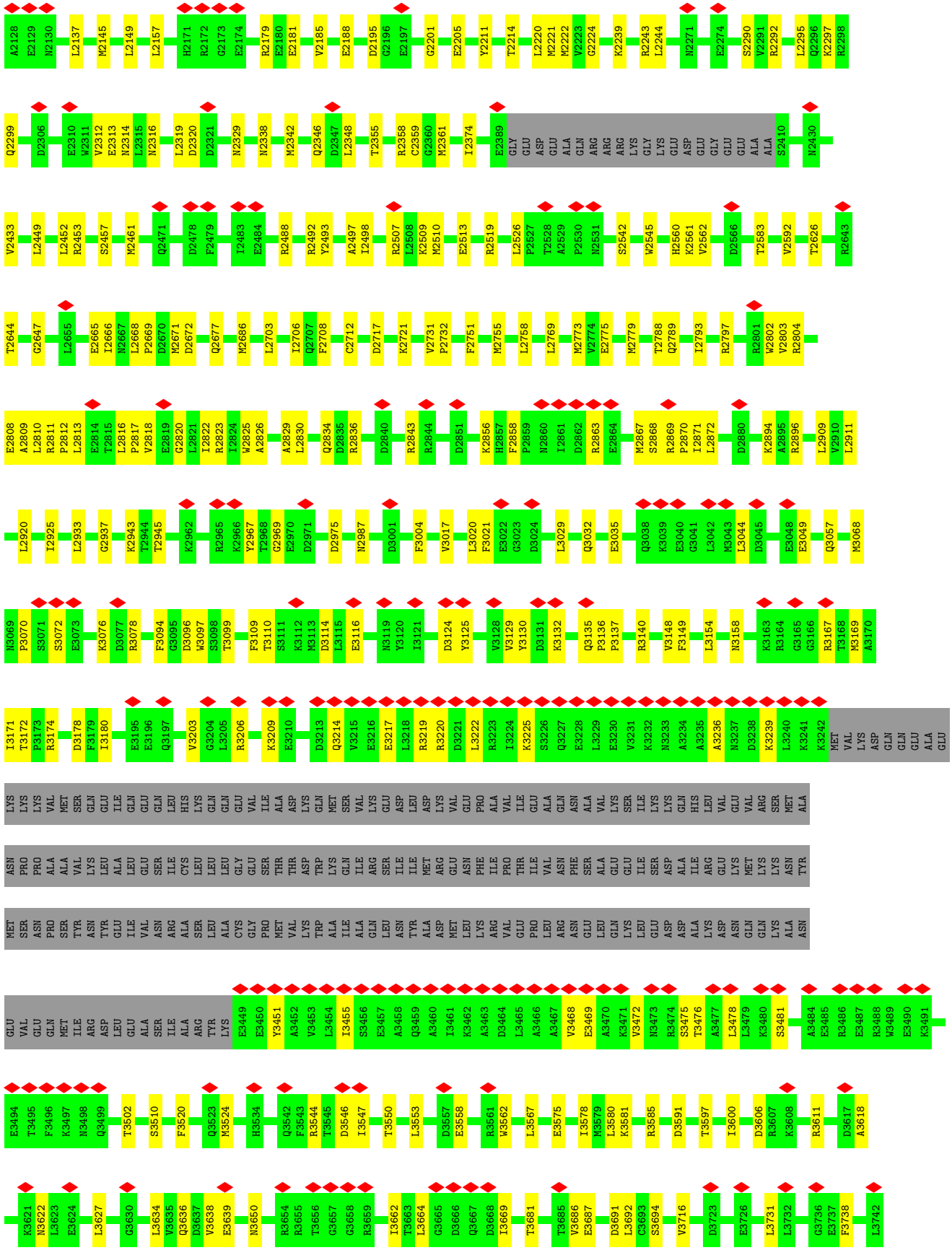
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 MET ASP THR ASP ALA PRO GLN VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN 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 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 THR 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 VAL THR PHE ILE THR TYR GLN SER LEU LYS ARG LYS GLN PHE GLU GLU ASN GLY GLN GLU LEU GLU GLN GLU GLU GLU GLU GLU LYS
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 GLN GLU GLN ARG ALA VAL GLU GLN GLN ARG THR THR ASP
TRP GLU LYS THR LYS PRO VAL THR GLY ASN LEU ARG PRO GLU GLU ALA LEU GLN LEU 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 GLY THR THR GLY LEU GLU GLU ARG VAL GLN
VAL ALA LEU GLU 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 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 ASP ARG HIS TRP LYS GLN GLN LEU MET LYS ARG LEU HIS VAL ASN TRP VAL 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 M1457 A1458 L1459 E1460 E1461 F1462 L1463 K1464 Q1465 I1466 R1467 E1468 V1469 W1470 N1471 T1472 Y1473 E1474 L1475 V1478 N1479 Y1480 Q1481 N1482 K1483 C1484 R1485 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 Y1546 L1547 E1548 F1551 T1552 G1553 S1554 A1555 D1556 I1557 K1558 H1559 L1560 L1561 P1562 V1563 E1564
T1565 Q1566 R1567 F1568 Q1569 S1572 T1573 L1576 A1577 L1578 M1579 K1580 K1581 V1582 S1583 K1584 S1585 P1586 L1587 V1588 M1589 D1590 Q1595 G1596 V1597 Q1598 R1599 S1600 L1601 E1602 R1603 L1604 A1605 D1606 L1607 K1610 I1611 Q1612 K1613 L1619 E1620 R1621 E1622 R1623 S1624 S1625 Y1630 D1634 E1635 L1638 E1639 I1640
K1649 H1653 E1668 S1671 R1679 T1693 I1698 W1701 M1709 E1725 G1728 K1729 A1730 T1731 S1732 I1733 D1734 P1735 N1736 T1737 Y1738 G1770 G1771 G1772 G1773 D1774 A1775 V1796 E1799 R1805 V1816 H1817 D1820 D1831 F1836 L1839 R1843 D1847
P1848 K1849 Q1850 T1851 D1852 V1853 Q1856 N1867 D1877 K1878 L1879 V1880 Q1881 T1882 R1887 P1904 E1914 R1925 D1933 M1941 G1942 R1943 V1946 F1960 E1964 E1965 R1966 M1967 I1978 E1984 H1985 S1986 N1987 P1988 N1989 Y1990 D1991 K1992 T1993 S1994 A1995 P1996 I1997 E2000 L2001
V2006 K2007 P2010 I2016 T2017 M2018 L2028 P2029 D2030 N2031 L2032 K2033 K2034 M2041 T2042 D2045 R2046 Q2047 L2048 V2052 E2063 V2064 L2065 A2066 N2067 K2068 I2069 V2070 L2075 L2080 H2085 F2088 R2091 E2114 E2117 R2118 G2119 E2120 A2121 V2122 D2123 E2124 G2125 E2126 I2127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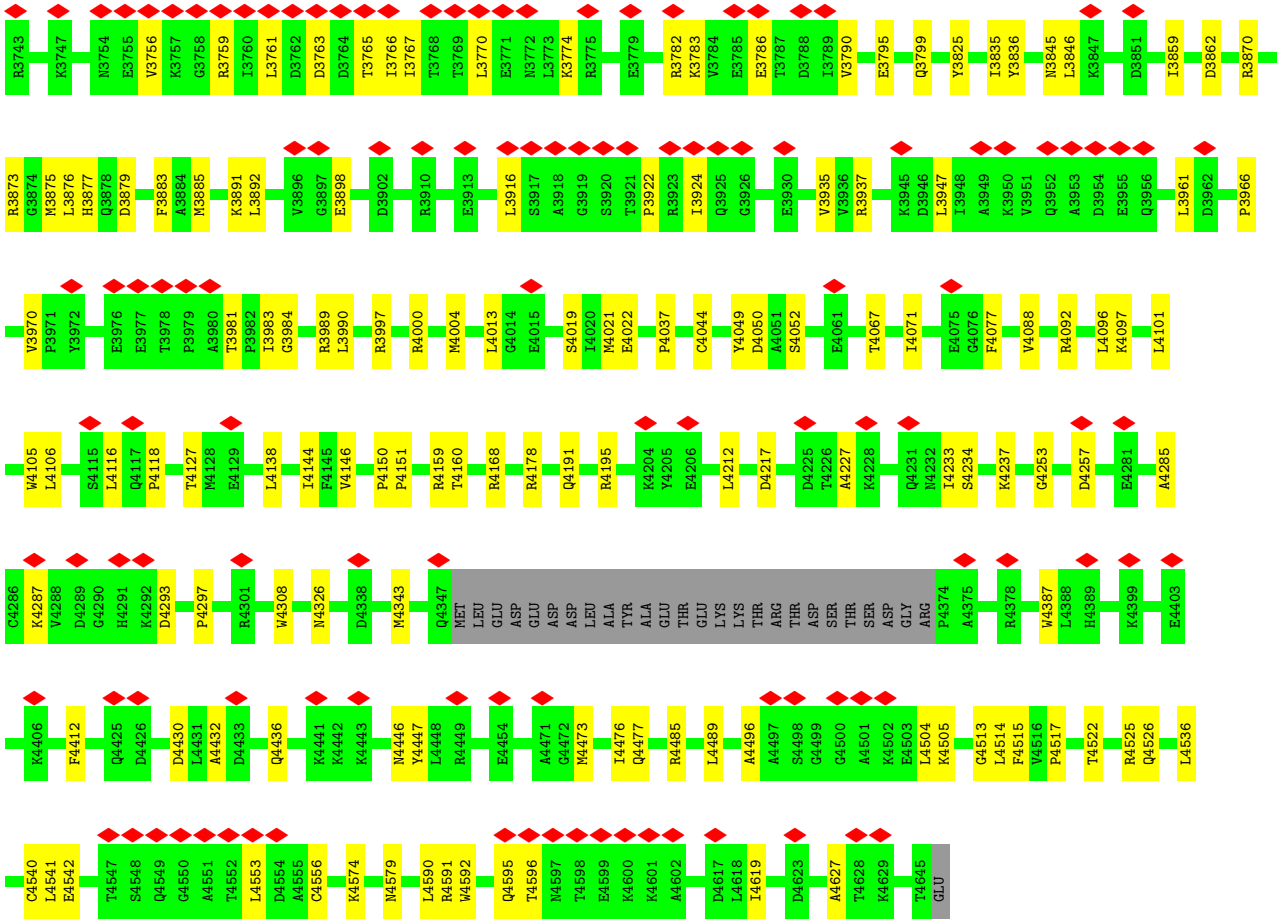
Q2299 D2306 E2310 W2311 V2312 E2313 N2314 L2315 N2316 L2319 D2320 D2321 N2329 N2338 M2342 Q2346 D2347 L2348 T2355 R2358 C2359 G2360 M2361 I2374 E2389 GLY GLU ASP GLU ALA GLN ARG ARG ARG LYS GLY LYS GLU ASP GLU GLY GLU GLU ALA ALA S2410 N2430
V2433 L2449 L2452 R2453 S2457 M2461 Q2471 D2478 F2479 I2483 E2484 R2488 R2492 Y2493 A2497 I2498 R2507 L2508 K2509 M2510 E2513 R2519 L2526 P2527 T2528 A2529 P2530 N2531 S2542 W2545 H2560 K2561 V2562 D2566 T2583 V2592 T2626 R2643
T2644 G2647 L2655 E2665 I2666 N2667 L2668 P2669 D2670 M2671 D2672 Q2677 M2686 L2703 I2706 Q2707 F2708 C2712 D2717 K2721 V2731 P2732 F2751 M2755 L2758 L2769 M2773 V2774 E2775 M2779 T2788 Q2789 I2793 R2797 R2801 W2802 V2803 R2804
E2808 A2809 L2810 R2811 P2812 L2813 E2814 T2815 L2816 P2817 V2818 E2819 G2820 L2821 I2822 R2823 I2824 W2825 A2826 A2829 L2830 Q2834 D2835 R2836 D2840 R2843 R2844 D2851 K2856 H2857 F2858 P2859 N2860 I2861 D2862 R2863 E2864 M2867 S2868 R2869 P2870 I2871 L2872 D2880 K2894 A2895 R2896 L2909 V2910 L2911
L2920 I2925 L2933 G2937 K2943 T2944 T2945 K2962 R2965 K2966 Y2967 T2968 G2969 E2970 D2971 D2975 N2987 D3001 F3004 V3017 L3020 F3021 E3022 G3023 D3024 L3029 Q3032 E3035 Q3038 K3039 E3040 G3041 L3042 M3043 L3044 D3045 E3048 E3049 Q3057 M3068
N3069 P3070 S3071 S3072 E3073 K3076 D3077 R3078 F3094 G3095 D3096 W3097 S3098 T3099 F3109 T3110 S3111 K3112 M3113 D3114 L3115 E3116 N3119 Y3120 I3121 D3124 Y3125 V3128 V3129 Y3130 D3131 K3132 Q3135 P3136 P3137 R3140 V3148 F3149 L3154 N3158 K3163 R3164 G3165 G3166 R3167 T3168 M3169 A3170
I3171 T3172 P3173 R3174 D3178 F3179 I3180 E3195 E3196 Q3197 V3203 G3204 L3205 R3206 K3209 E3210 D3213 Q3214 V3215 E3216 E3217 L3218 R3219 R3220 D3221 L3222 R3223 I3224 K3225 S3226 Q3227 E3228 L3229 E3230 V3231 K3232 N3233 A3234 A3235 A3236 N3237 D3238 K3239 L3240 K3241 K3242 MET VAL LYS ASP GLN GLN GLU ALA GLU
LYS LYS LYS VAL MET SER GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN GLN GLU VAL ILE ALA ASP LYS GLN MET SER VAL LYS GLU ASP LEU ASP LYS VAL GLU PRO ALA VAL ILE GLU ALA GLN ASN ALA VAL LYS SER ILE LYS LYS GLN HIS LEU VAL GLU VAL ARG SER MET ALA
ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU LEU SER ILE CYS LEU LEU LEU GLY GLU SER THR THR ASP TRP LYS GLN ILE ARG GLU ILE ILE MET ARG GLU ASN PHE ILE PRO THR ILE VAL ASN PHE SER ALA GLU GLU ILE SER ASP ALA ILE ARG GLU LYS MET LYS LYS ASN TYR
MET SER ASN PRO SER TYR ASN TYR GLU ILE VAL ASN ARG ALA SER LEU ALA CYS GLY PRO MET VAL LYS TRP ALA ILE ALA GLN GLN LEU ASN TYR ALA ASP MET LEU LYS ARG VAL GLU PRO LEU ARG ASN GLU LEU ASP ASP ALA LYS ASP ASN GLN GLN LYS ALA ASN
GLU VAL GLU GLN MET ILE ARG ASP LEU GLU ALA SER ILE ALA ARG TYR LYS E3449 E3450 Y3451 A3452 V3453 L3454 I3455 S3456 E3457 A3458 Q3459 A3460 I3461 K3462 A3463 D3464 L3465 A3466 A3467 V3468 E3469 A3470 K3471 V3472 N3473 R3474 S3475 T3476 A3477 L3478 L3479 K3480 S3481 A3484 E3485 R3486 E3487 R3488 W3489 E3490 K3491
E3494 T3495 F3496 K3497 N3498 Q3499 T3502 S3510 F3520 Q3523 M3524 H3534 Q3542 F3543 R3544 T3545 D3546 I3547 T3550 L3553 D3557 E3558 R3561 W3562 L3567 E3575 I3578 M3579 L3580 K3581 R3585 D3591 T3597 I3600 D3606 R3607 K3608 R3611 D3617 A3618
K3621 N3622 L3623 E3624 L3627 G3630 L3634 V3635 Q3636 D3637 V3638 E3639 N3650 R3654 R3655 T3656 G3657 G3658 R3659 I3662 T3663 L3664 G3665 D3666 Q3667 D3668 I3669 T3681 T3685 V3686 E3687 D3691 L3692 C3693 S3694 V3716 D3723 E3726 L3731 L3732 G3736 E3737 F3738 L3742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R3873 G3874 M3875 L3876 H3877 Q3878 D3879 F3883 A3884 M3885 K3891 L3892 V3896 G3897 E3898 D3902 R3910 E3913 L3916 S3917 A3918 G3919 S3920 T3921 P3922 R3923 I3924 Q3925 G3926 E3930 V3935 V3936 R3937 K3945 D3946 L3947 I3948 A3949 K3950 V3951 Q3952 A3953 D3954 E3955 Q3956 L3961 D3962 P3966
V3970 P3971 Y3972 E3976 E3977 T3978 P3979 A3980 T3981 P3982 I3983 G3984 R3989 L3990 R3997 R4000 M4004 L4013 G4014 E4015 S4019 I4020 M4021 E4022 P4037 C4044 Y4049 D4050 A4051 S4052 E4061 T4067 I4071 E4075 G4076 F4077 V4088 R4092 L4096 K4097 L4101
W4105 L4106 S4115 L4116 Q4117 P4118 T4127 M4128 E4129 L4138 I4144 F4145 V4146 P4150 P4151 R4159 T4160 R4168 R4178 Q4191 R4195 K4204 Y4205 E4206 L4212 D4217 D4225 T4226 A4227 K4228 Q4231 M4232 I4233 S4234 K4237 G4253 D4257 E4281 A4285
C4286 K4287 V4288 D4289 G4290 H4291 K4292 D4293 P4297 R4301 W4308 N4326 D4338 M4343 Q4347 MET LEU GLU ASP GLU ASP ASP LEU ALA TYR ALA GLU THR GLU LYS LYS THR ARG THR ASP SER THR SER ASP GLY ARG P4374 A4375 R4378 W4387 L4388 H4389 K4399 E4403
K4406 F4412 Q4425 D4426 D4430 L4431 A4432 D4433 Q4436 K4441 K4442 K4443 N4446 Y4447 L4448 R4449 E4454 A4471 G4472 M4473 I4476 Q4477 R4485 L4489 A4496 A4497 S4498 G4499 G4500 A4501 K4502 E4503 L4504 K4505 G4513 L4514 F4515 V4516 P4517 T4522 R4525 Q4526 L4536
C4540 L4541 E4542 T4547 S4548 Q4549 G4550 A4551 T4552 L4553 D4554 A4555 C4556 K4574 N4579 L4590 R4591 W4592 Q4595 T4596 M4597 T4598 E4599 K4600 K4601 A4602 D4617 L4618 I4619 D4623 A4627 T4628 K4629 T4645 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136324	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)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.050	Depositor
Minimum map value	-1.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AOV, ADP, ATP

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	0.10	0/24093	0.24	0/32651

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23593	0	23657	287	0
2	A	32	0	12	3	0
3	A	31	0	12	0	0
4	A	54	0	24	2	0
5	A	2	0	0	0	0
All	All	23712	0	23705	287	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 287 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:1490:TRP:HH2	1:A:1537:TRP:HD1	1.34	0.74
1:A:4574:LYS:HB3	1:A:4627:ALA:HB2	1.70	0.72
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.71	0.72
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.71	0.72
1:A:4049:TYR:OH	1:A:4191:GLN:NE2	2.24	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	2929/4646 (63%)	2886 (98%)	43 (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	2605/4125 (63%)	2605 (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 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2781	GLN
1	A	4335	GLN
1	A	3063	HIS
1	A	4429	GLN
1	A	4038	ASN

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 6 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
4	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
3	ATP	A	4702	5	32,33,33	0.32	0	48,52,52	0.28	0
2	AOV	A	4701	5	32,34,34	5.09	7 (21%)	42,56,56	2.25	12 (28%)
4	ADP	A	4704	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)

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
4	ADP	A	4703	-	-	5/16/32/32	0/3/3/3
3	ATP	A	4702	5	-	3/22/38/38	0/3/3/3
2	AOV	A	4701	5	-	2/16/39/39	0/3/3/3
4	ADP	A	4704	-	-	1/16/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	AOV	O1G-VG	27.64	2.10	1.61
4	A	4703	ADP	C5-C4	4.71	1.47	1.39
4	A	4704	ADP	C5-C4	4.71	1.47	1.39
2	A	4701	AOV	C5-C4	4.63	1.47	1.39
4	A	4704	ADP	C5-C6	2.72	1.48	1.41

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4701	AOV	C5-C4-N3	-7.22	116.78	126.72
4	A	4703	ADP	C5-C4-N3	-6.10	118.32	126.72
4	A	4704	ADP	C5-C4-N3	-5.82	118.70	126.72
2	A	4701	AOV	N3-C4-N9	5.75	136.94	127.17
4	A	4703	ADP	N3-C4-N9	4.92	135.53	127.17

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4703	ADP	C5'-O5'-PA-O1A
4	A	4703	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	O4'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'
4	A	4703	ADP	O4'-C4'-C5'-O5'

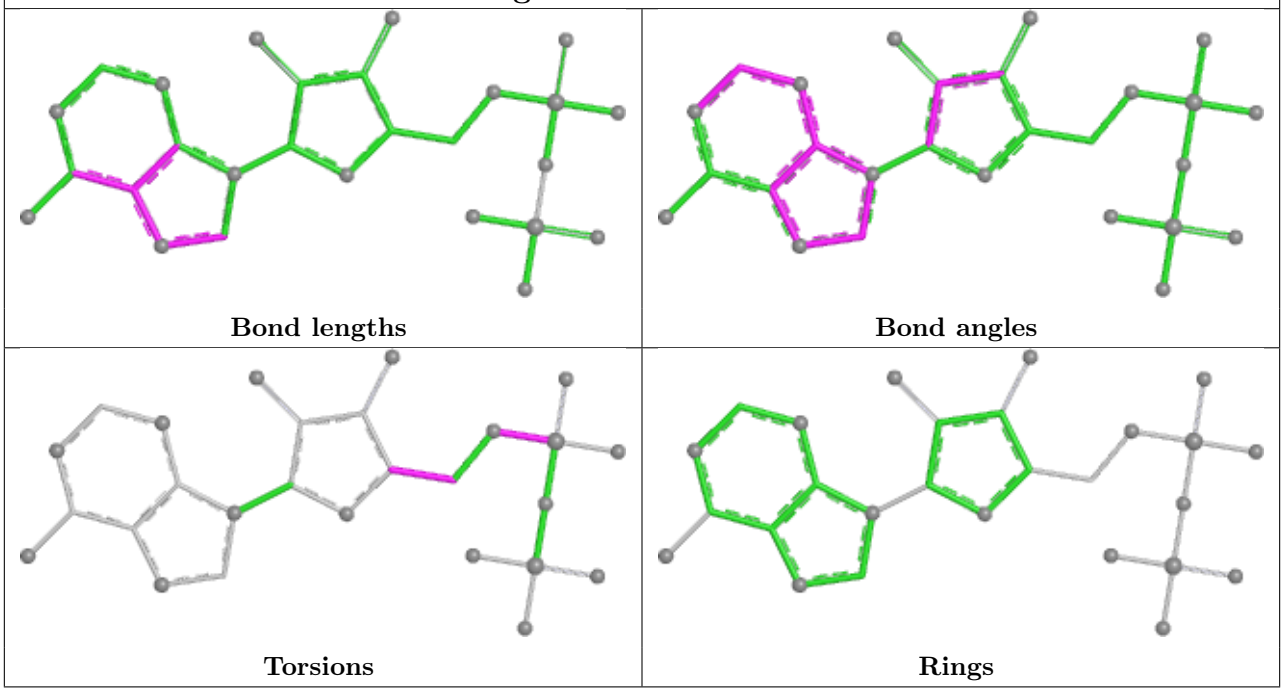
There are no ring outliers.

3 monomers are involved in 5 short contacts:

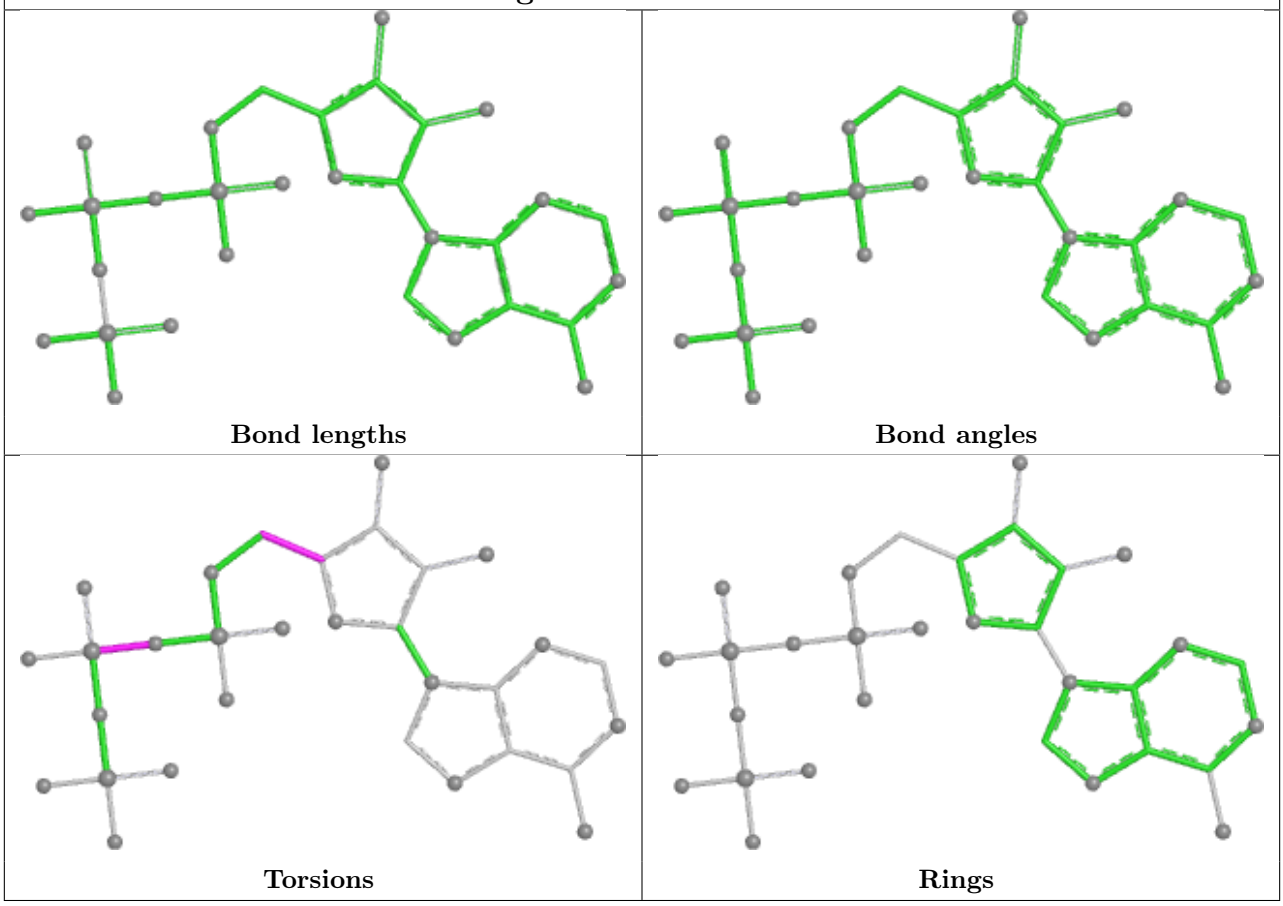
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4703	ADP	1	0
2	A	4701	AOV	3	0
4	A	4704	ADP	1	0

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 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.

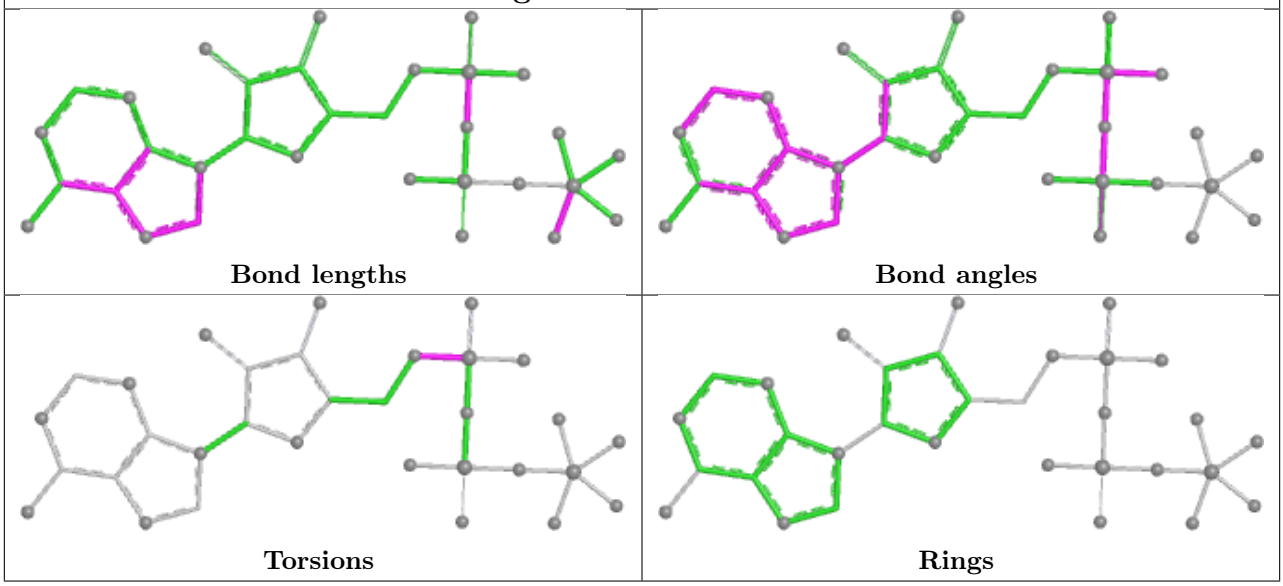
Ligand ADP A 4703

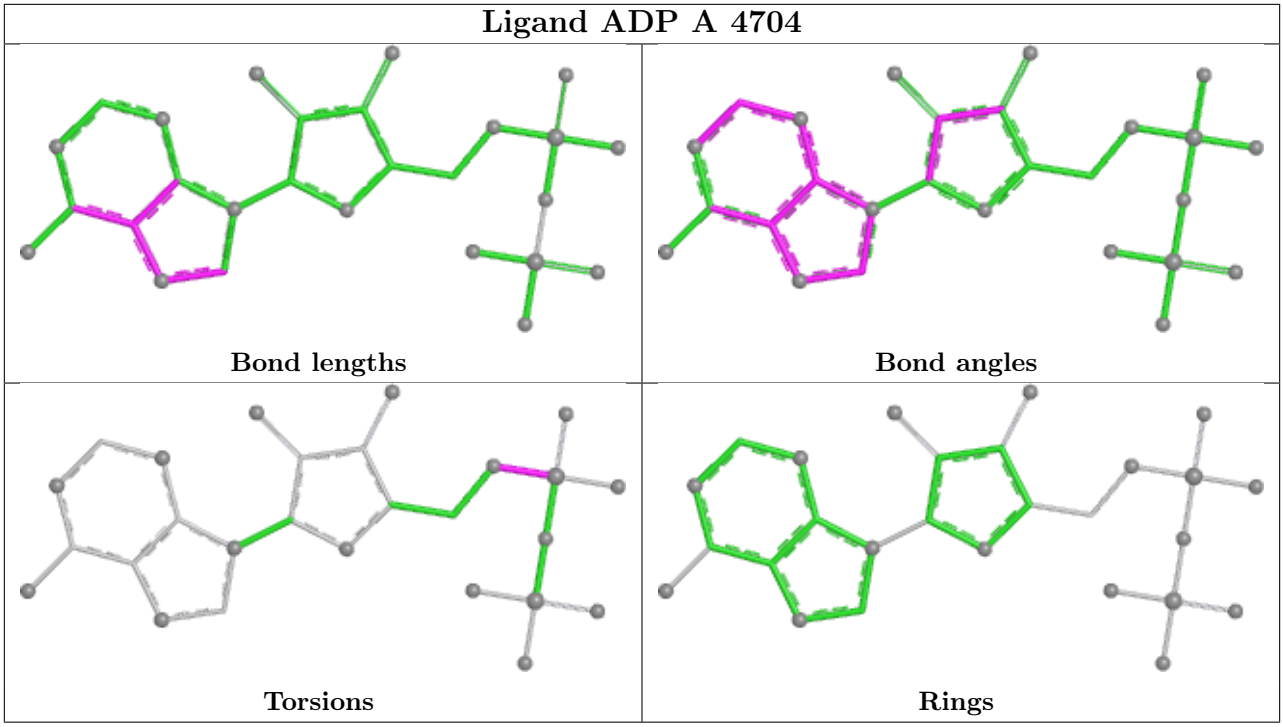


Ligand ATP A 4702



Ligand AOV A 4701





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.

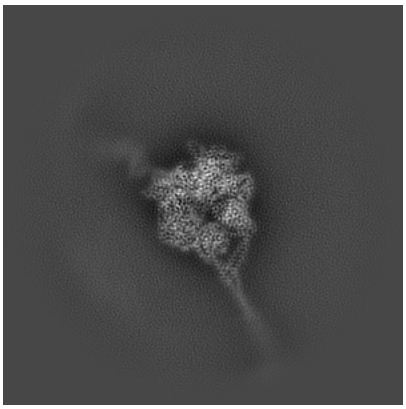
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-44698. These allow visual inspection of the internal detail of the map and identification of artifacts.

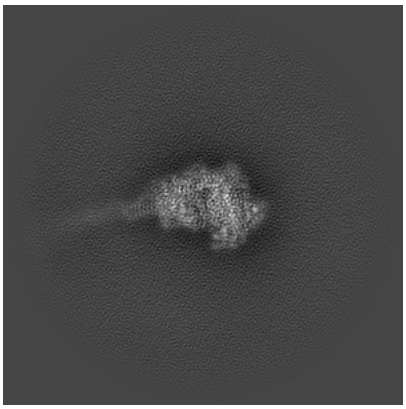
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

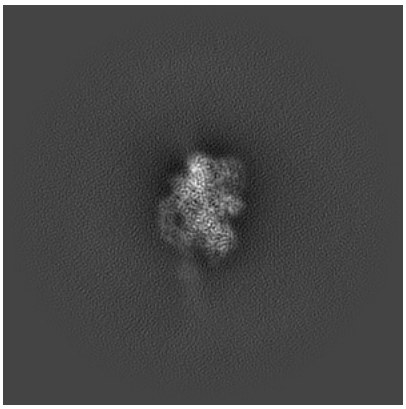
6.1.1 Primary map



X

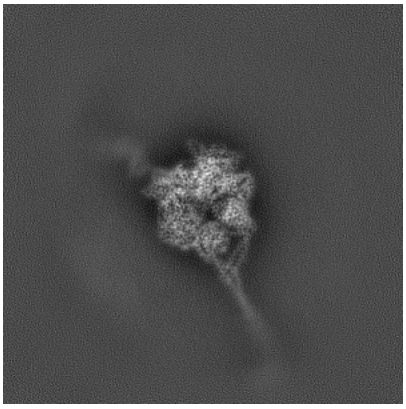


Y

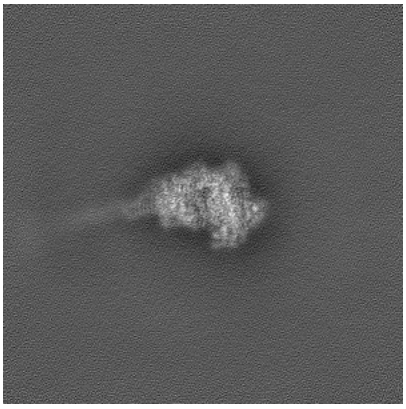


Z

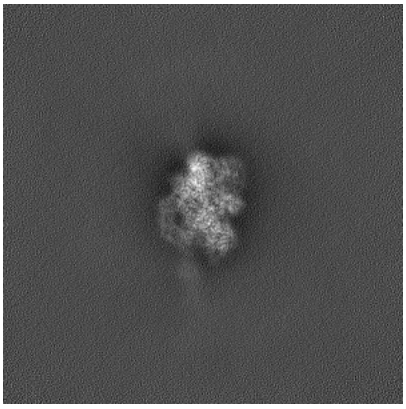
6.1.2 Raw map



X



Y

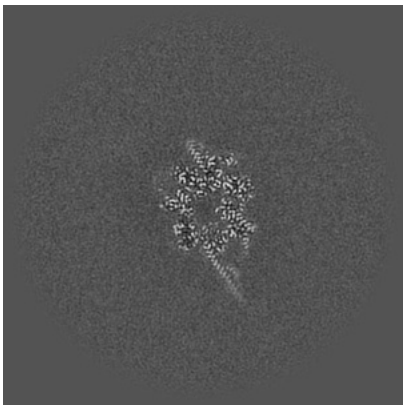


Z

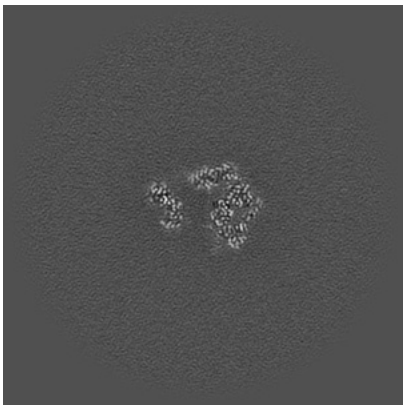
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



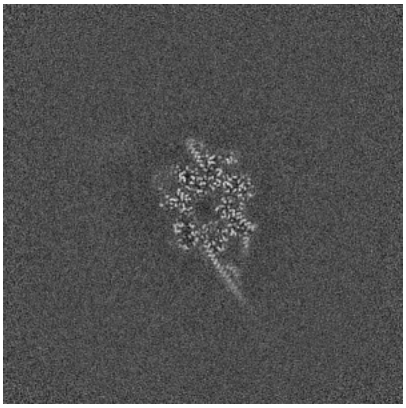
X Index: 192



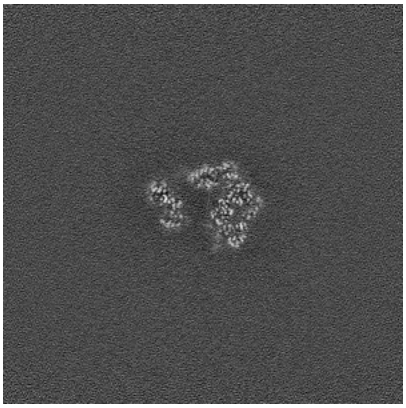
Y Index: 192

Z Index: 192

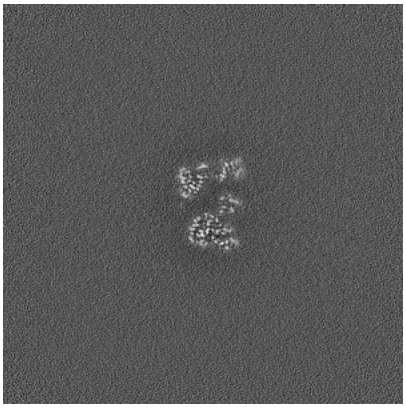
6.2.2 Raw map



X Index: 192



Y Index: 192

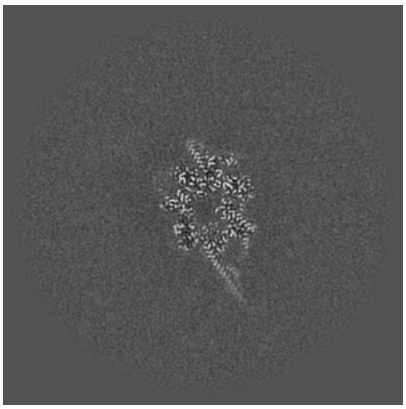


Z Index: 192

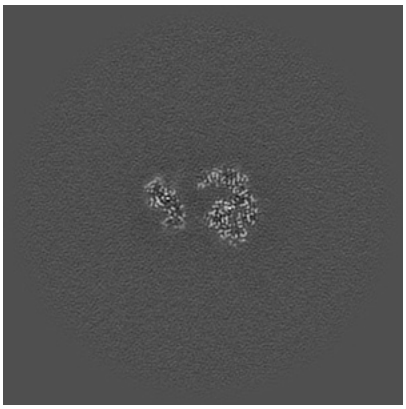
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

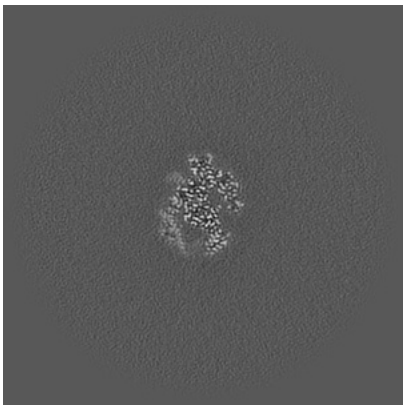
6.3.1 Primary map



X Index: 192

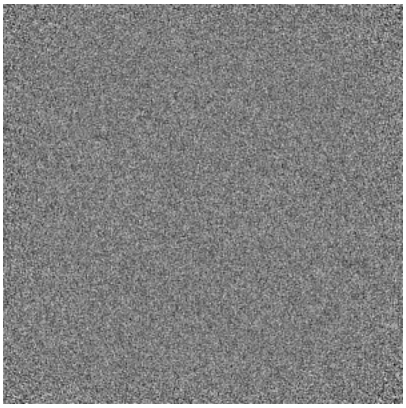


Y Index: 197

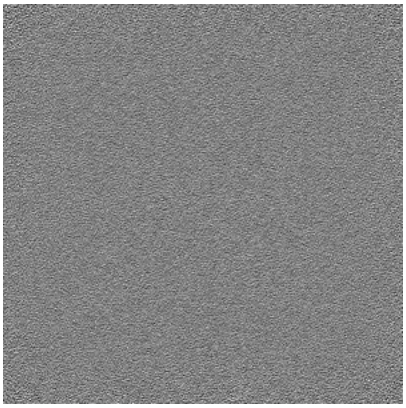


Z Index: 213

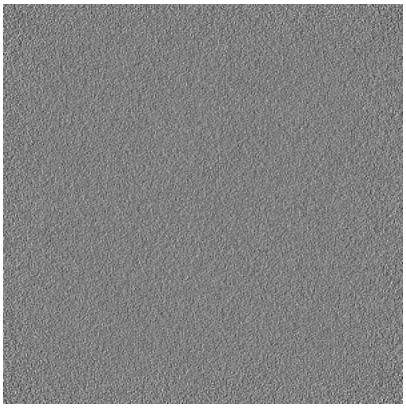
6.3.2 Raw map



X Index: 0



Y Index: 0

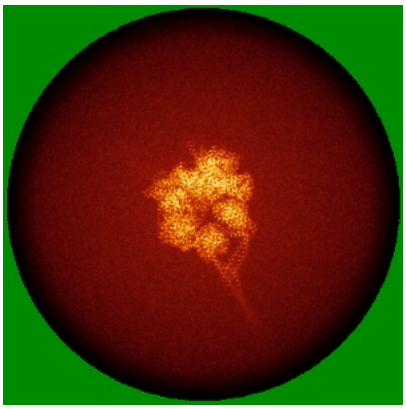


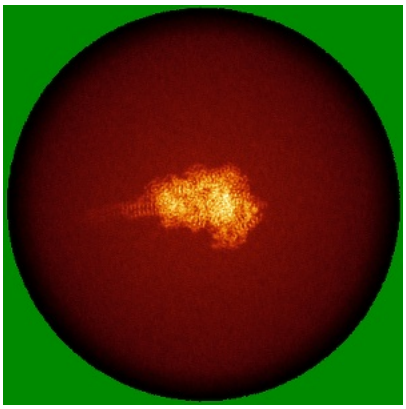
Z Index: 0

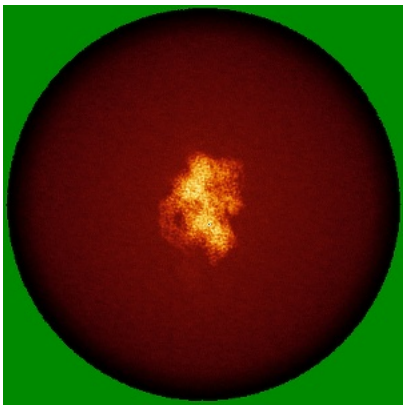
The images above show the largest variance slices of the map in three orthogonal directions.

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

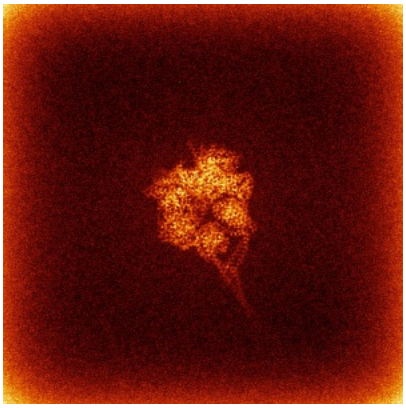
6.4.1 Primary map

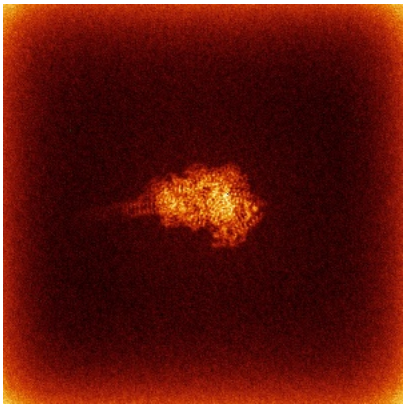

X

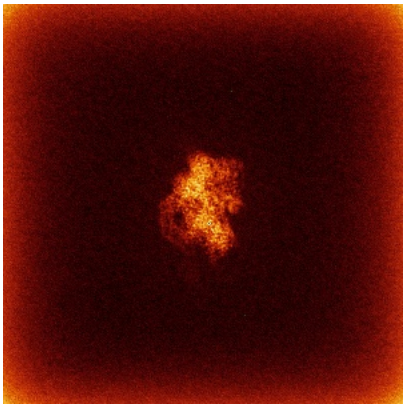

Y


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 0.4. 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.

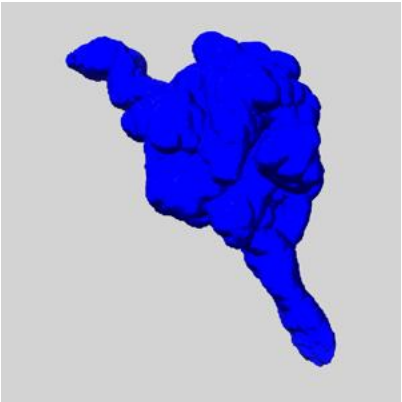
6.6 Mask visualisation (i)

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

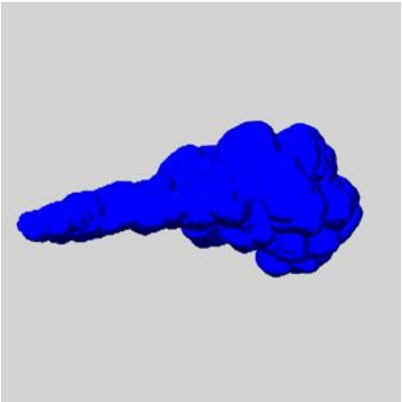
A mask typically either:

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

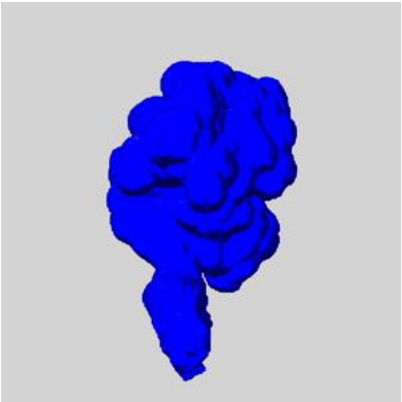
6.6.1 emd_44698_msk_1.map (i)



X



Y

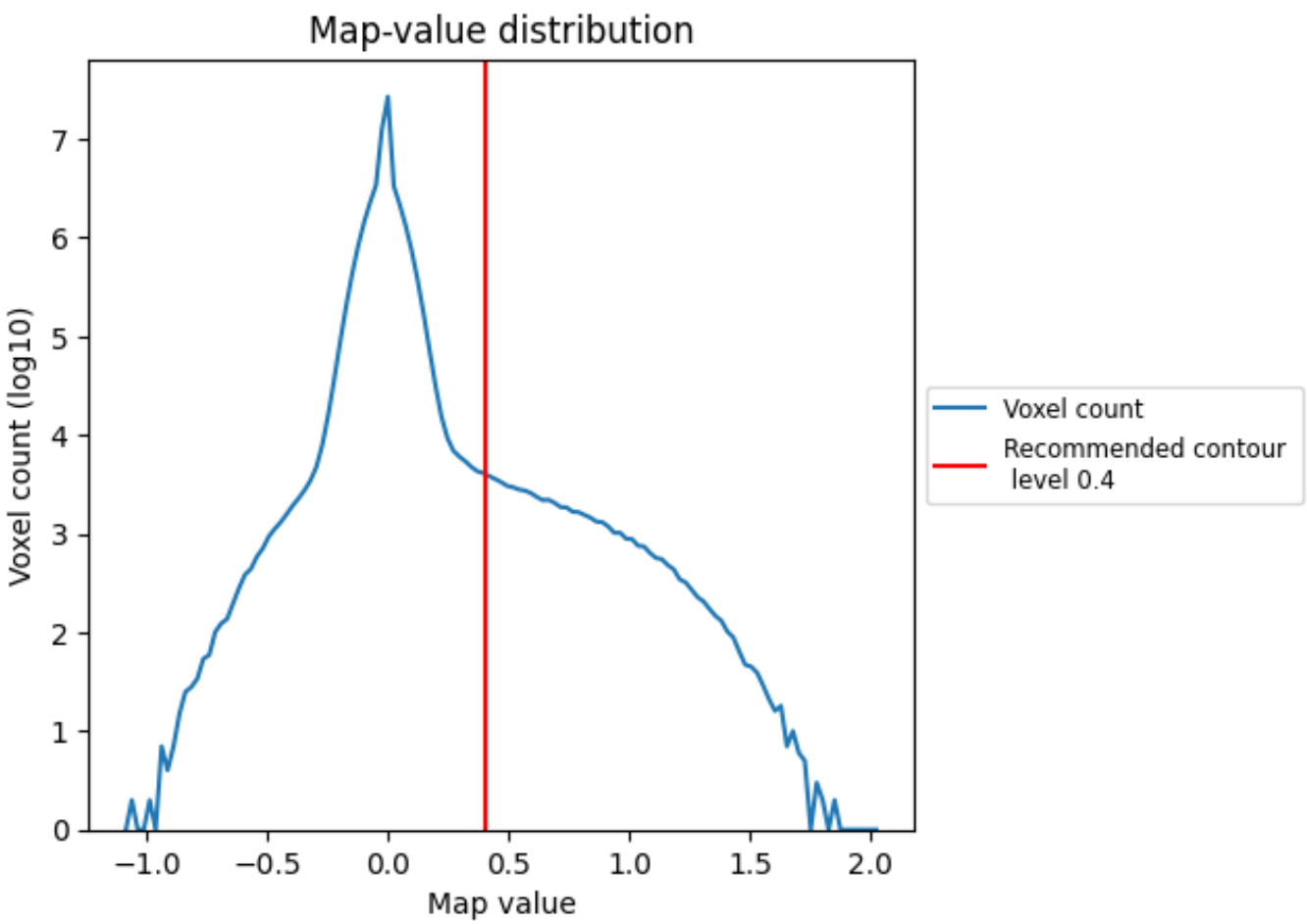


Z

7 Map analysis (i)

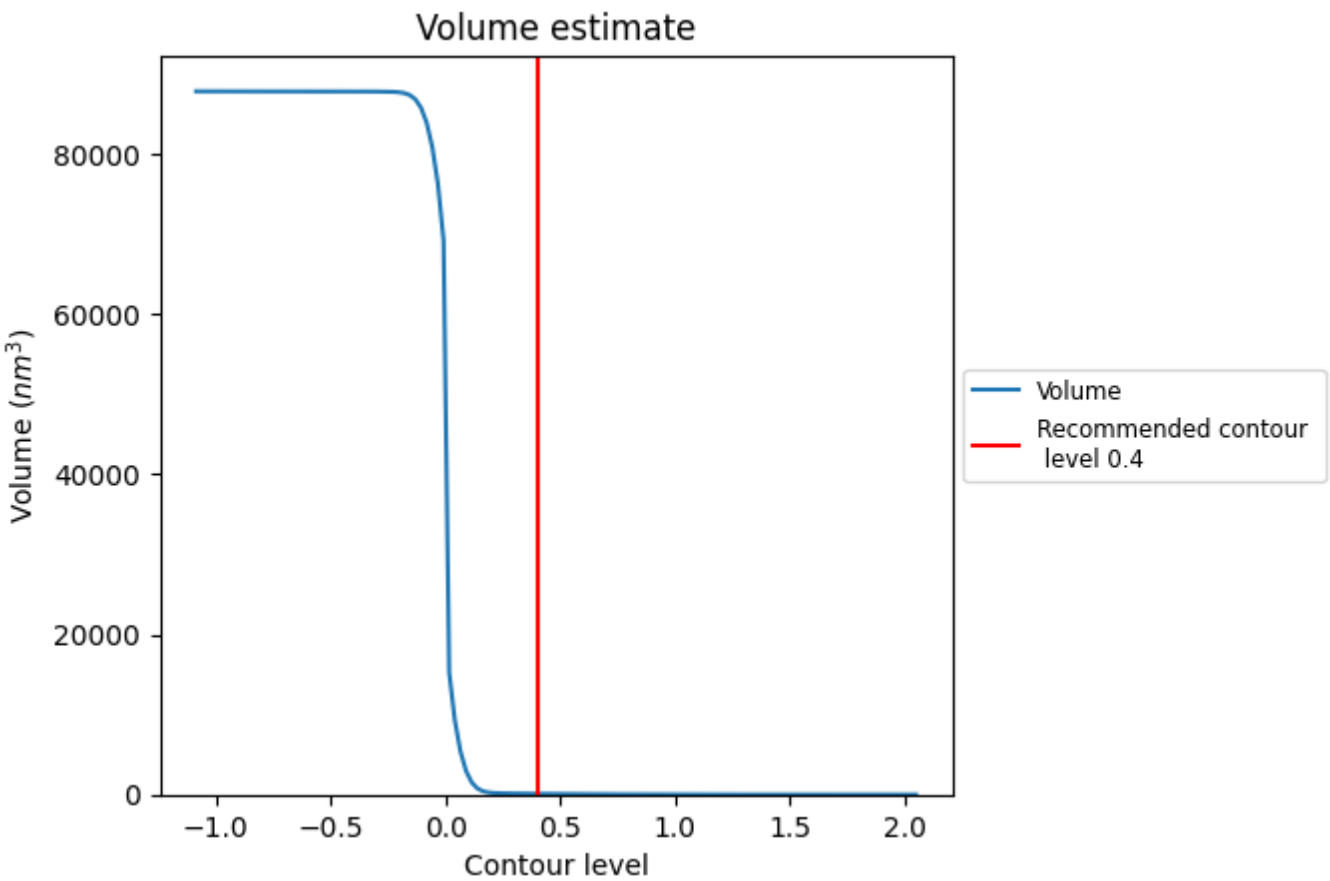
This section contains the results of statistical analysis of the map.

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.

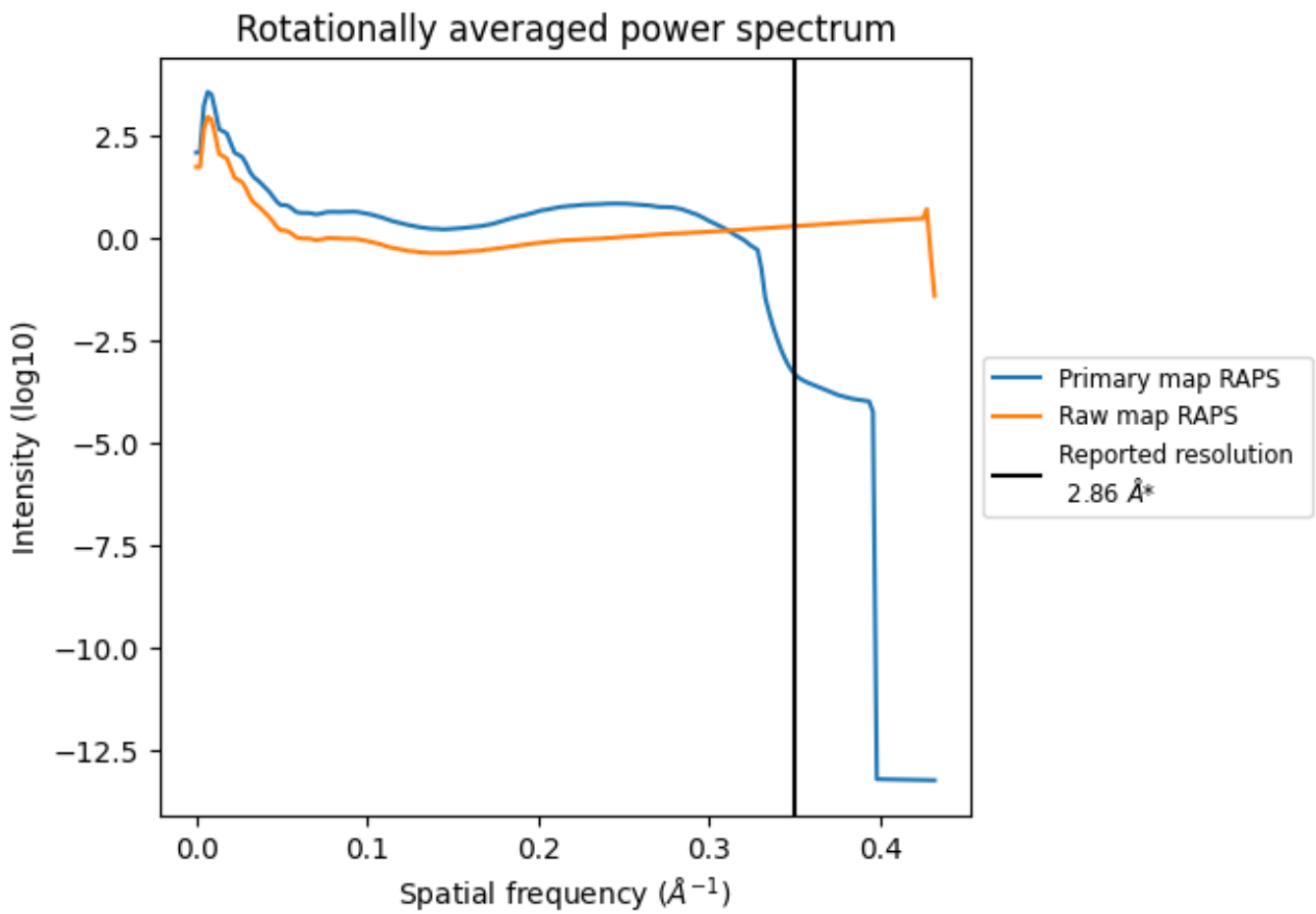
7.2 Volume estimate (i)



The volume at the recommended contour level is 95 nm^3; this corresponds to an approximate mass of 86 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)

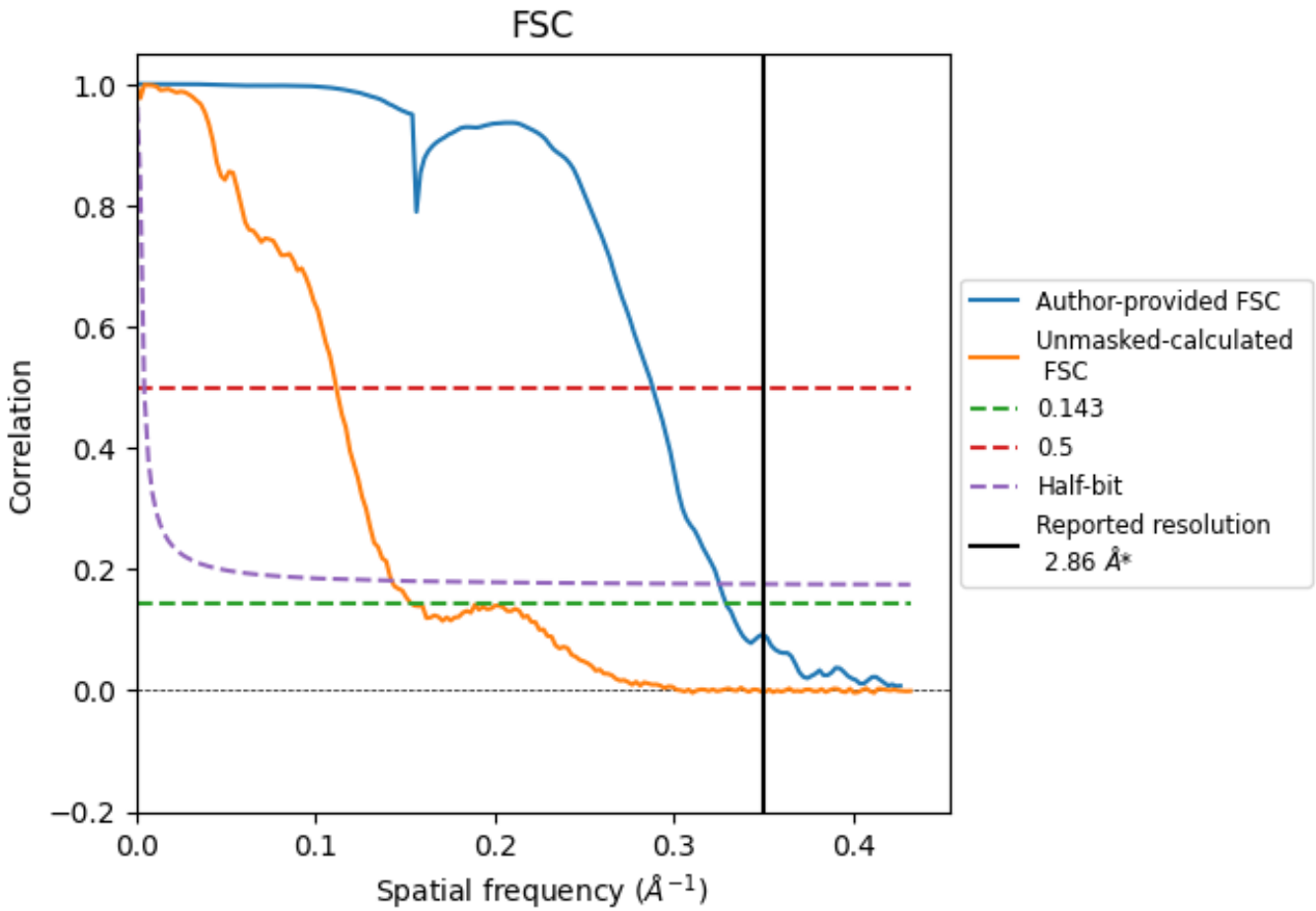


*Reported resolution corresponds to spatial frequency of 0.350 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.350 Å^{-1}

8.2 Resolution estimates (i)

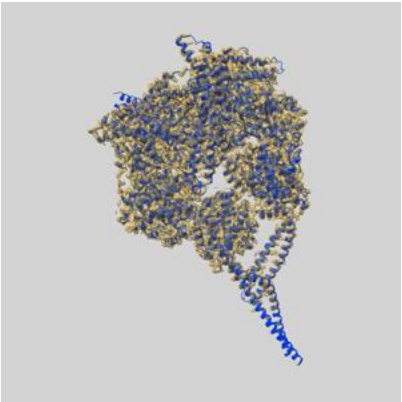
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	3.04	3.47	3.07
Unmasked-calculated*	6.50	8.96	7.01

*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 6.50 differs from the reported value 2.86 by more than 10 %

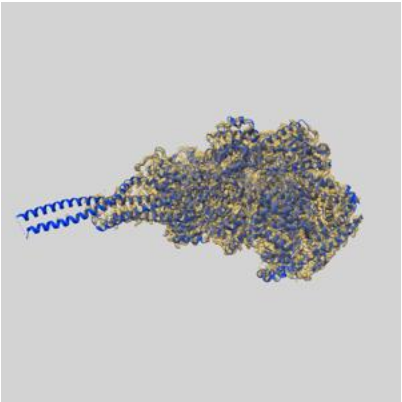
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-44698 and PDB model 9BMG. Per-residue inclusion information can be found in section 3 on page 6.

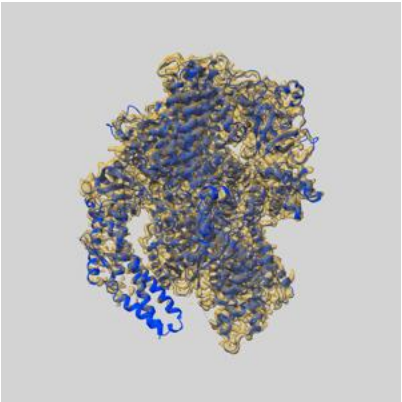
9.1 Map-model overlay (i)



X



Y



Z

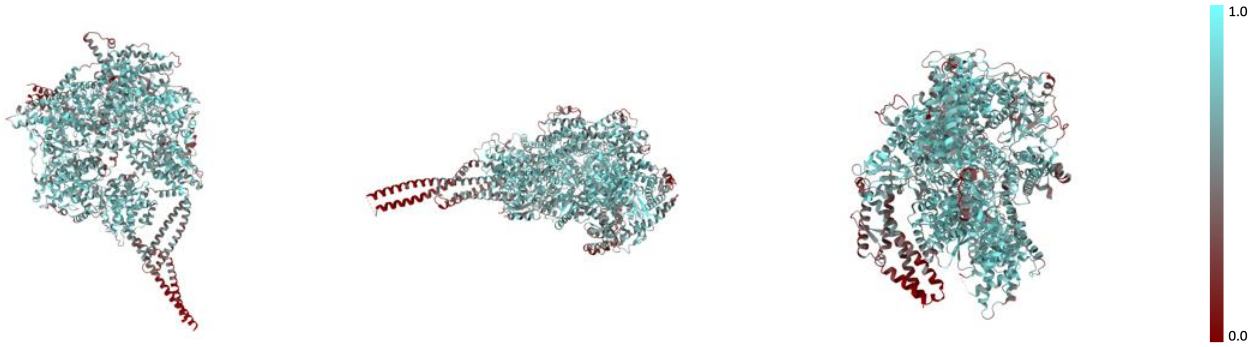
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

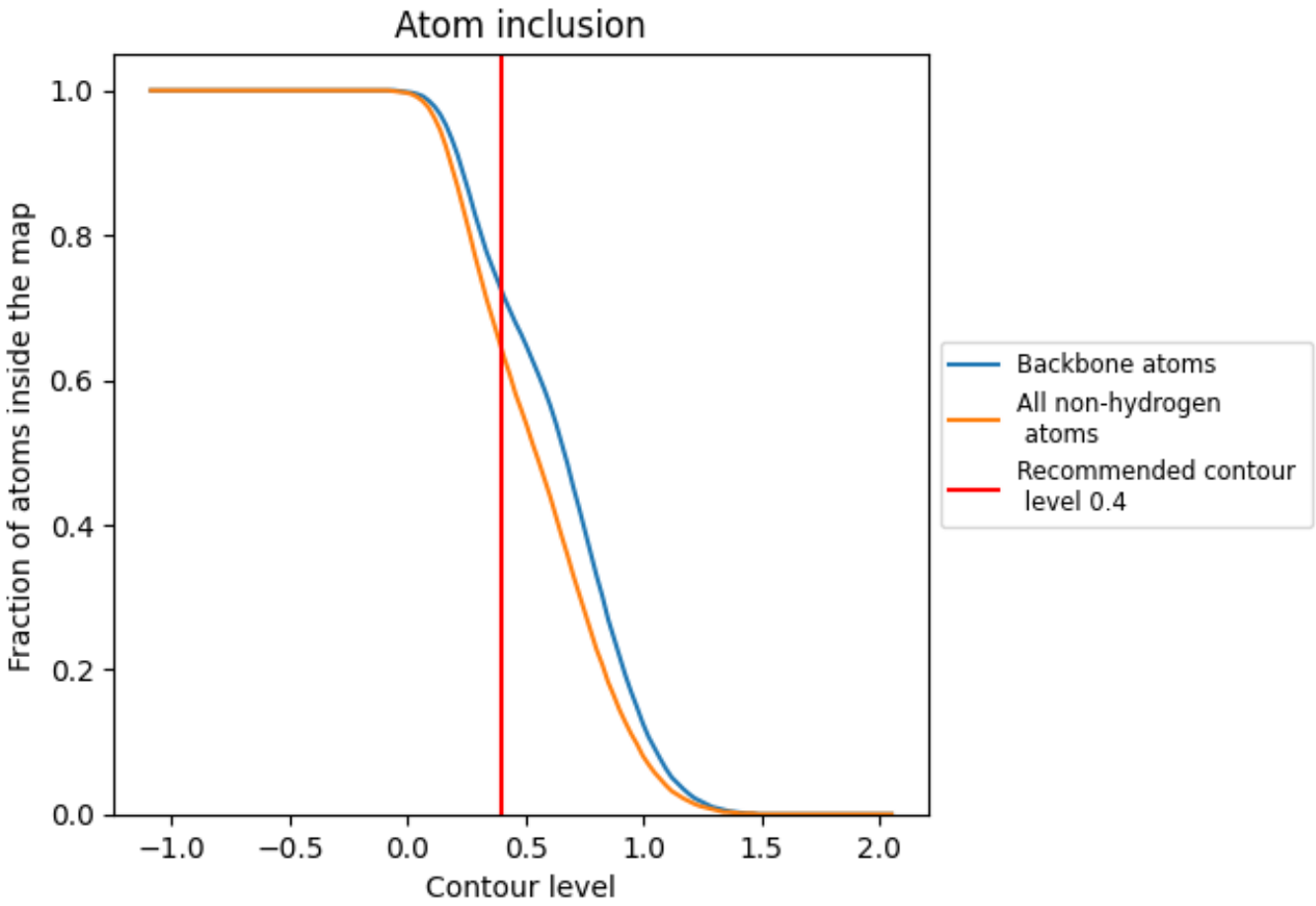
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.5270
A	0.6410	0.5270