wwPDB EM Validation Summary Report

May 18, 2025 – 02:21 AM EDT

PDB ID	:	9BMU / pdb_00009bmu
EMDB ID	:	EMD-44711
Title	:	State-6 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors	:	Chai, P.; Zhang, K.
Deposited on	:	2024-05-02
Resolution	:	3.70 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

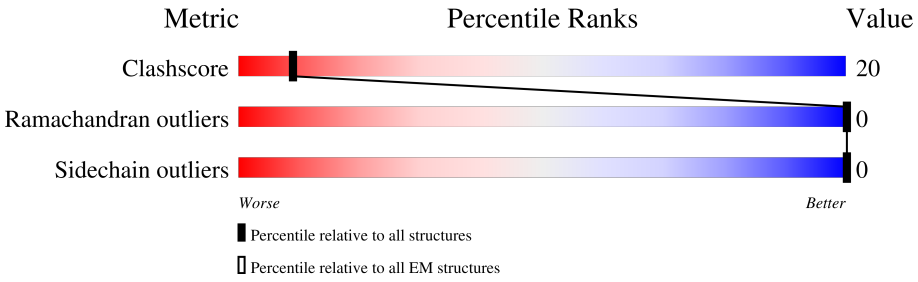
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 3.70 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	5% 35% 24% 42%

2 Entry composition (i)

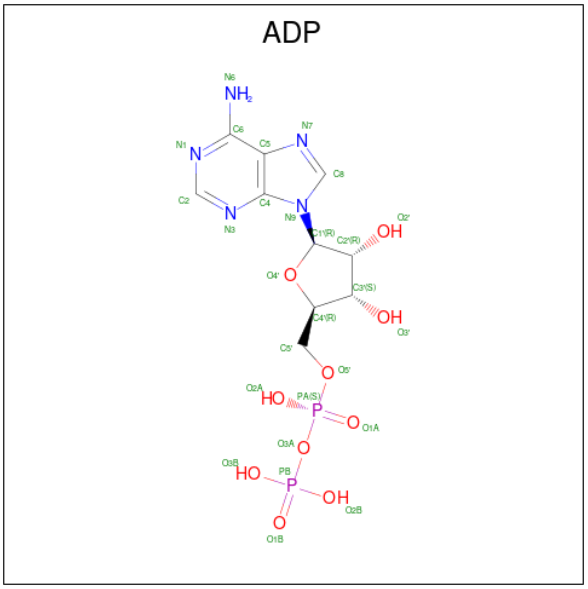
There are 3 unique types of molecules in this entry. The entry contains 21776 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

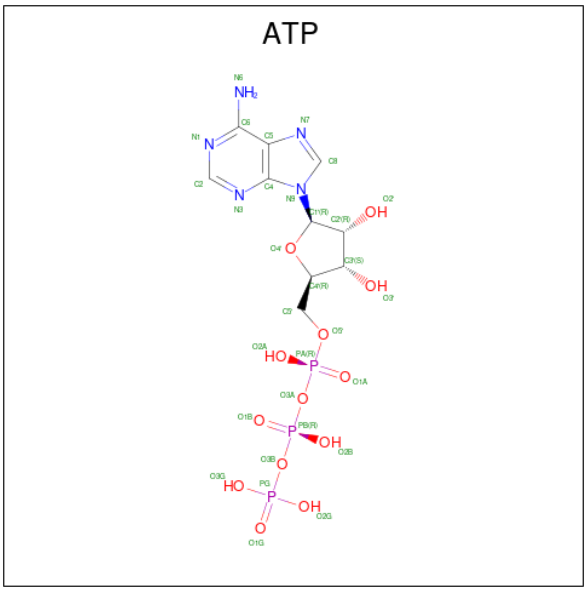
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2698	21664	13799	3740	4014	111	0	0

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

- 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).



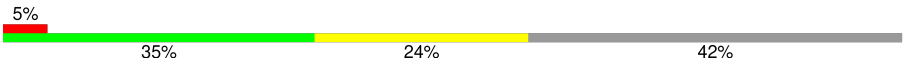
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

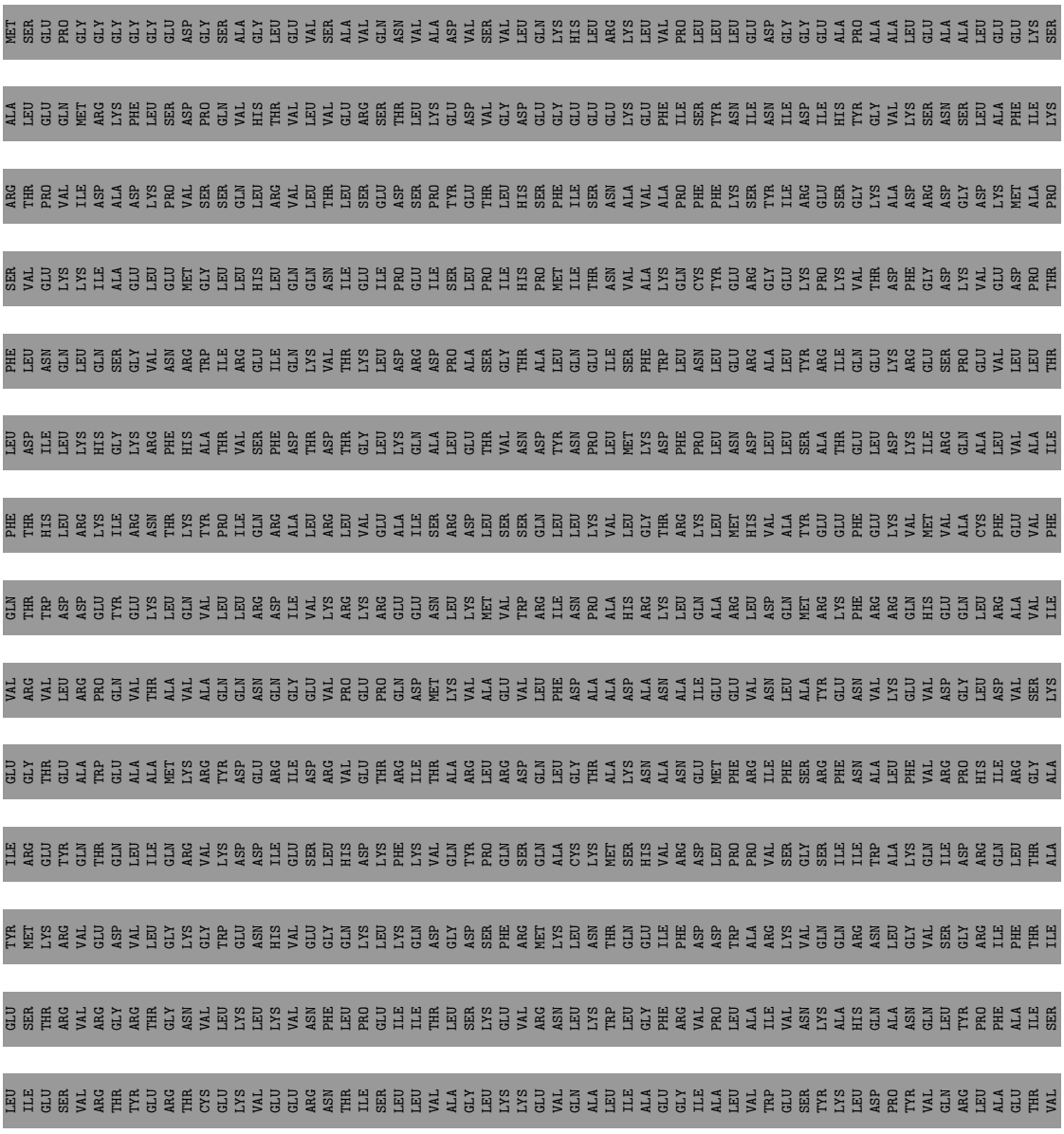
3 Residue-property plots (i)

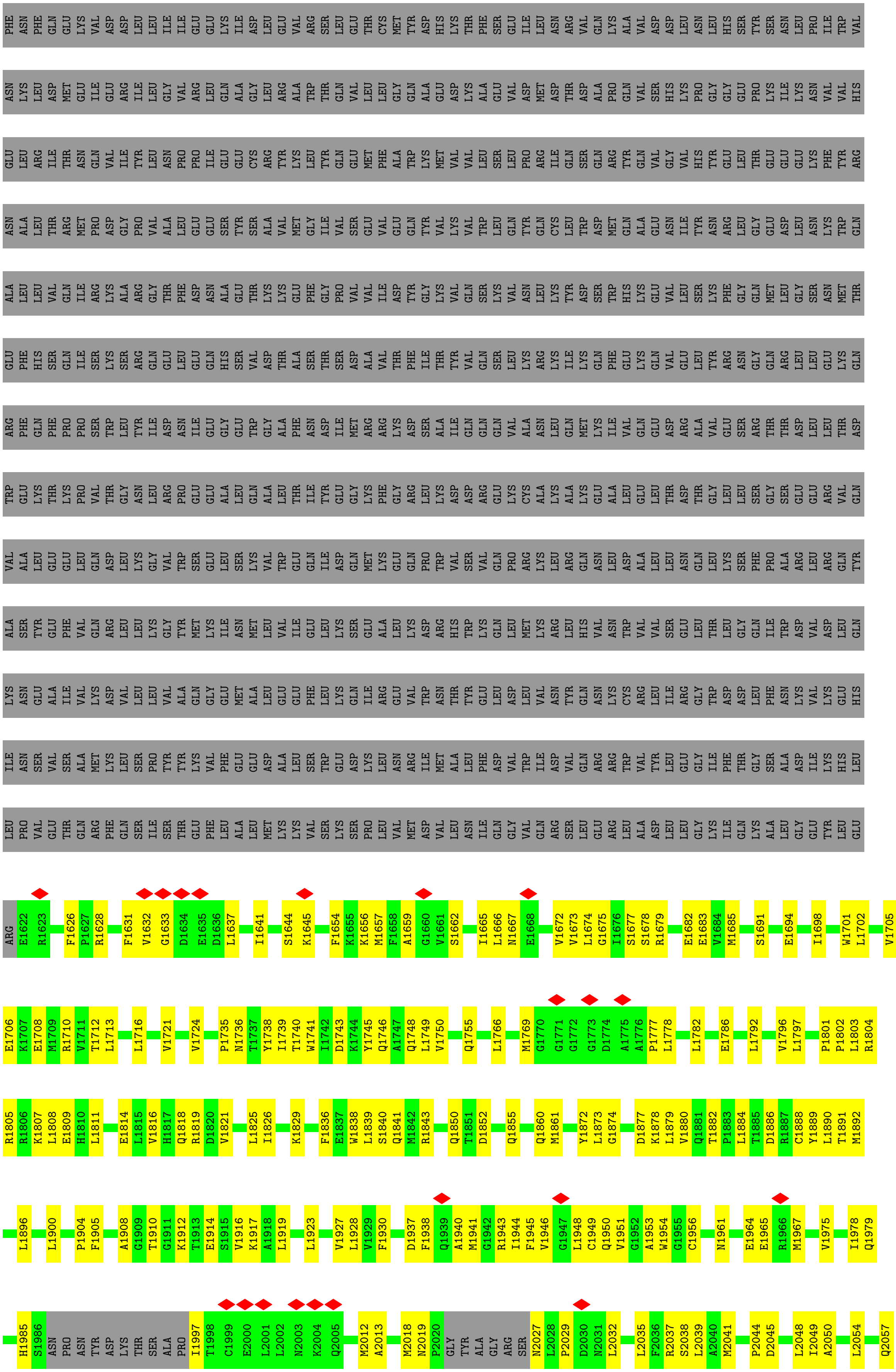
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

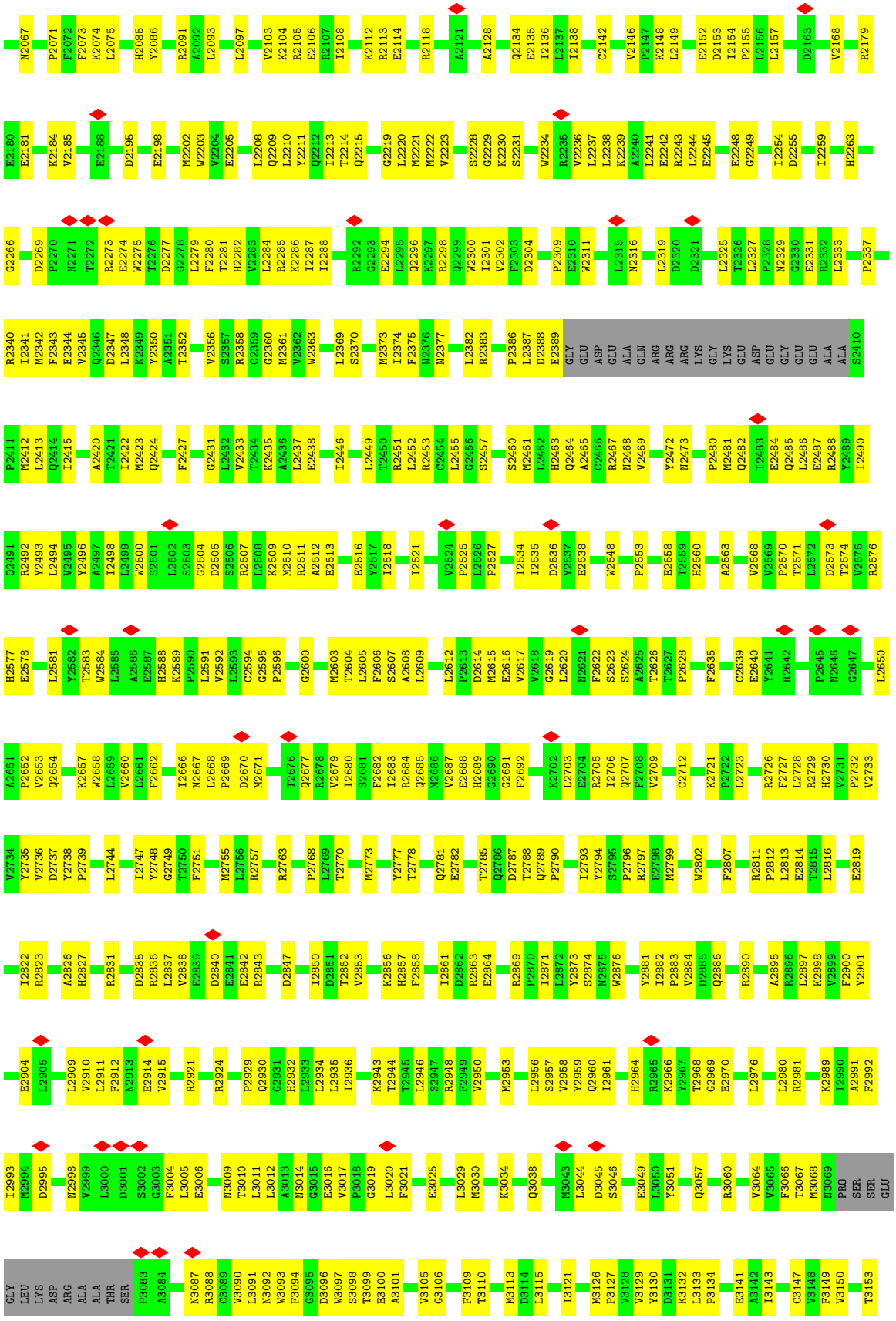
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

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 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 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 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 GLU GLU PHE LEU LYS GLN ILE ARG GLU VAL TRP ASN THR TYR GLU LEU ASP LEU VAL ASN TYR GLN ASN LYS CYS ARG LEU ILE ARG GLY TRP ASP ASP LEU PHE ASN LYS VAL LYS GLU HIS
ILE ASN SER VAL SER ALA MET LYS LEU SER PRO TYR TYR LYS VAL PHE GLU GLU ASP ALA LEU SER TRP GLU ASP LYS LEU ASN ARG ILE MET ALA LEU PHE ASP VAL TRP ILE ASP VAL GLN ARG ARG TRP VAL TYR LEU GLU GLY ILE PHE THR GLY SER ALA ASP ILE LYS HIS LEU
LEU PRO VAL GLU THR GLN ARG PHE GLN SER ILE SER THR GLU PHE LEU ALA LEU MET LYS LYS VAL SER LYS SER PRO LEU VAL MET ASP VAL LEU ASN ILE GLN GLY VAL GLN ARG SER LEU GLU ARG LEU ALA ASP LEU LEU GLY LYS ILE GLN LYS ALA LEU GLY GLU TYR LEU GLU
ARG E1622 R1623 F1626 P1627 R1628 F1631 V1632 G1633 D1634 E1635 D1636 L1637 I1641 S1644 K1645 F1654 K1655 K1656 M1657 F1658 A1659 G1660 V1661 S1662 I1665 L1666 N1667 E1668 V1672 V1673 L1674 G1675 I1676 S1677 S1678 R1679 E1682 E1683 V1684 M1685 S1691 E1694 I1698 W1701 L1702 V1705
E1706 K1707 E1708 M1709 R1710 V1711 T1712 L1713 L1716 V1721 V1724 P1735 N1736 T1737 Y1738 I1739 T1740 W1741 I1742 D1743 K1744 Y1745 Q1746 A1747 Q1748 L1749 V1750 Q1755 L1766 M1769 G1770 G1771 G1772 G1773 D1774 A1775 A1776 P1777 L1778 L1782 E1786 L1792 V1796 L1797 P1801 P1802 L1803 R1804
R1805 R1806 K1807 L1808 E1809 H1810 L1811 E1814 L1815 V1816 H1817 Q1818 R1819 D1820 V1821 L1825 I1826 K1829 F1836 E1837 W1838 L1839 S1840 Q1841 M1842 R1843 Q1850 T1851 D1852 Q1855 Q1860 M1861 Y1872 L1873 G1874 D1877 K1878 L1879 V1880 Q1881 T1882 P1883 L1884 T1885 D1886 R1887 C1888 Y1889 L1890 T1891 M1892
L1896 L1900 P1904 F1905 A1908 G1909 T1910 G1911 K1912 T1913 E1914 S1915 V1916 K1917 A1918 L1919 L1923 V1927 L1928 V1929 F1930 D1937 F1938 Q1939 A1940 M1941 G1942 R1943 I1944 F1945 V1946 G1947 L1948 C1949 Q1950 V1951 G1952 A1953 W1954 G1955 C1956 N1961 E1964 E1965 R1966 M1967 V1975 I1978 Q1979
H1985 S1986 ASN PRO ASN TYR ASP LYS THR SER ALA PRO I1997 T1998 C1999 E2000 L2001 L2002 N2003 K2004 Q2005 M2012 A2013 M2018 N2019 P2020 GLY TYR ALA GLY ARG SER N2027 L2028 P2029 D2030 N2031 L2032 L2035 F2036 R2037 S2038 L2039 A2040 M2041 P2044 D2045 L2048 I2049 A2050 L2054 Q2057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E2180 E2181 K2184 V2185 E2188 D2195 E2198 M2202 W2203 V2204 E2205 L2208 Q2209 L2210 Y2211 Q2212 I2213 T2214 Q2215 G2219 L2220 M2221 M2222 V2223 S2228 G2229 K2230 S2231 W2234 R2235 V2236 L2237 L2238 K2239 A2240 L2241 E2242 R2243 L2244 E2245 E2248 G2249 I2254 D2255 I2259 H2263
G2266 D2269 P2270 N2271 T2272 R2273 E2274 W2275 T2276 D2277 G2278 L2279 F2280 T2281 H2282 W2283 L2284 R2285 K2286 I2287 I2288 R2292 G2293 E2294 L2295 Q2296 K2297 R2298 Q2299 W2300 I2301 V2302 F2303 D2304 P2309 E2310 W2311 L2315 W2316 L2319 D2320 D2321 L2325 T2326 L2327 P2328 N2329 G2330 E2331 R2332 L2333 P2337
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P2411 M2412 L2413 Q2414 I2415 A2420 T2421 I2422 M2423 Q2424 F2427 G2431 L2432 V2433 T2434 K2435 A2436 L2437 E2438 I2446 L2449 T2450 R2451 L2452 R2453 C2454 L2455 G2456 S2457 S2460 M2461 L2462 H2463 Q2464 A2465 C2466 R2467 N2468 V2469 Y2472 N2473 P2480 M2481 Q2482 I2483 E2484 Q2485 L2486 E2487 R2488 Y2489 I2490
Q2491 R2492 Y2493 L2494 V2495 Y2496 A2497 I2498 L2499 W2500 S2501 L2502 S2503 G2504 D2505 S2506 R2507 L2508 K2509 M2510 R2511 A2512 E2513 E2516 Y2517 I2518 I2521 V2524 P2525 L2526 P2527 I2534 I2535 D2536 Y2537 E2538 W2548 P2553 E2558 T2559 H2560 A2563 V2568 V2569 P2570 T2571 L2572 D2573 T2574 V2575 R2576
H2577 E2578 L2581 Y2582 T2583 W2584 L2585 A2586 E2587 H2588 K2589 P2590 L2591 V2592 L2593 C2594 G2595 P2596 G2600 M2603 T2604 L2605 F2606 S2607 A2608 L2609 L2612 P2613 D2614 M2615 E2616 V2617 W2618 G2619 L2620 N2621 F2622 S2623 S2624 A2625 T2626 T2627 P2628 F2635 C2639 E2640 Y2641 R2642 P2645 N2646 G2647 L2650
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I2822 R2823 A2826 H2827 R2831 D2835 R2836 L2837 V2838 E2839 D2840 E2841 E2842 R2843 D2847 I2850 D2851 T2852 V2853 K2856 H2857 F2858 I2861 D2862 R2863 E2864 R2869 P2870 I2871 L2872 Y2873 S2874 N2875 W2876 Y2881 I2882 P2883 V2884 D2885 Q2886 R2890 A2895 R2896 L2897 K2898 V2899 F2900 Y2901
E2904 L2905 L2909 V2910 L2911 F2912 N2913 E2914 V2915 R2921 R2924 P2929 Q2930 G2931 H2932 L2933 L2934 L2935 I2936 K2943 T2944 T2945 L2946 S2947 R2948 F2949 V2950 M2953 L2956 S2957 V2958 Y2959 Q2960 I2961 H2964 R2965 K2966 Y2967 T2968 G2969 E2970 L2976 L2980 R2981 K2989 I2990 A2991 F2992
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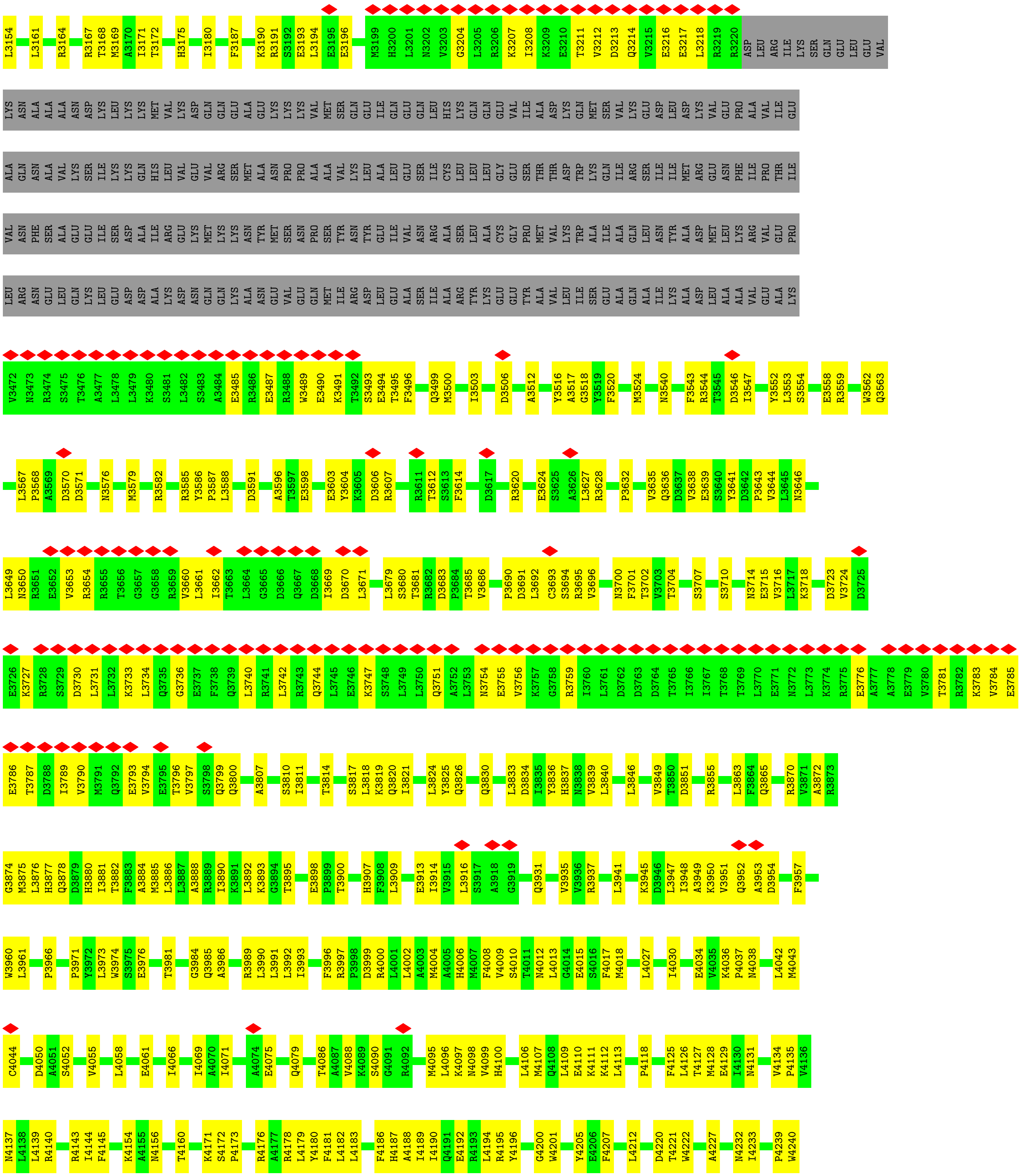
GLY LEU LYS ASP ARG ALA ALA THR SER P3083 A3084 N3087 R3088 C3089 V3090 L3091 N3092 W3093 F3094 G3095 D3096 W3097 S3098 T3099 E3100 A3101 V3105 G3106 F3109 T3110 M3113 D3114 L3115 I3121 M3126 P3127 V3128 V3129 Y3130 D3131 K3132 L3133 P3134 E3141 A3142 I3143 C3147 V3148 F3149 V3150 T3153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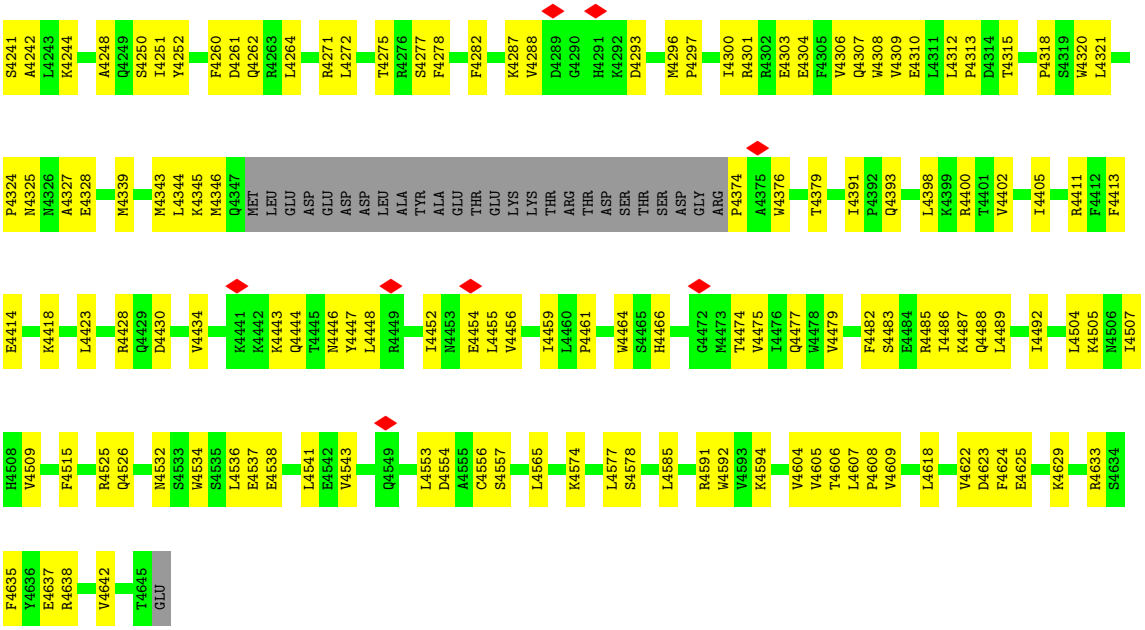
LYS ASN ALA ALA ALA ASN ASP LYS LEU LYS LYS MET VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS VAL MET SER GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN GLN GLU VAL ILE ALA ASP LYS GLN MET SER VAL LYS GLU ASP LEU ASP LYS VAL GLU PRO ALA VAL ILE GLU
ALA GLN ASN ALA VAL LYS SER ILE LYS LYS GLN HIS LEU VAL GLU VAL ARG SER MET ALA ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU SER ILE CYS LEU LEU LEU GLY GLU SER THR THR ASP TRP LYS GLN ILE ARG SER 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 LEU ASN TYR ALA ASP MET LEU LYS ARG VAL GLU PRO
LEU ARG ASN GLU LEU GLN LYS LEU GLU 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 GLU GLU TYR ALA VAL LEU ILE SER GLU ALA GLN ALA ILE LYS ALA ASP LEU ALA ALA VAL GLU ALA LYS
V3472 N3473 R3474 S3475 T3476 A3477 L3478 L3479 K3480 S3481 L3482 S3483 A3484 E3485 R3486 E3487 R3488 W3489 E3490 K3491 T3492 S3493 E3494 T3495 F3496 Q3499 M3500 I3503 D3506 A3512 Y3516 A3517 G3518 Y3519 F3520 M3524 N3540 F3543 R3544 T3545 D3546 I3547 Y3552 L3553 S3554 E3558 R3559 W3562 Q3563
L3567 P3568 A3569 D3570 D3571 N3576 M3579 R3582 R3585 Y3586 P3587 L3588 D3591 A3596 T3597 E3598 E3603 Y3604 K3605 D3606 R3607 R3611 T3612 S3613 F3614 D3617 R3620 E3624 S3625 A3626 L3627 R3628 P3632 V3635 Q3636 D3637 V3638 E3639 S3640 Y3641 D3642 P3643 V3644 L3645 N3646
L3649 N3650 R3651 E3652 V3653 R3654 R3655 T3656 G3657 G3658 R3659 V3660 L3661 I3662 T3663 L3664 G3665 D3666 Q3667 D3668 I3669 D3670 L3671 L3679 S3680 T3681 R3682 D3683 P3684 T3685 V3686 P3690 D3691 L3692 C3693 S3694 R3695 V3696 N3700 F3701 T3702 V3703 T3704 S3707 S3710 N3714 E3715 V3716 L3717 K3718 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 S3798 Q3799 Q3800 A3807 S3810 I3811 T3814 S3817 L3818 K3819 Q3820 I3821 L3824 Y3825 Q3826 Q3830 L3833 D3834 I3835 Y3836 H3837 N3838 V3839 L3840 L3846 V3849 T3850 D3851 R3855 L3863 F3864 Q3865 R3870 V3871 A3872 R3873
G3874 M3875 L3876 H3877 Q3878 D3879 H3880 I3881 T3882 F3883 A3884 M3885 L3886 L3887 A3888 R3889 I3890 K3891 L3892 K3893 G3894 T3895 E3898 P3899 T3900 H3907 F3908 L3909 E3913 I3914 V3915 L3916 S3917 A3918 G3919 Q3931 V3935 V3936 R3937 L3941 K3945 D3946 L3947 I3948 A3949 K3950 V3951 Q3952 A3953 D3954 F3957
W3960 L3961 P3966 P3971 Y3972 L3973 W3974 S3975 E3976 T3981 G3984 Q3985 A3986 R3989 L3990 L3991 L3992 I3993 F3996 R3997 P3998 D3999 R4000 L4001 L4002 A4003 M4004 A4005 H4006 M4007 F4008 V4009 S4010 T4011 N4012 L4013 G4014 E4015 S4016 F4017 M4018 L4027 I4030 E4034 V4035 K4036 P4037 N4038 L4042 M4043
C4044 D4050 A4051 S4052 V4055 L4058 E4061 I4066 I4069 A4070 I4071 A4074 E4075 Q4079 T4086 A4087 V4088 K4089 S4090 G4091 R4092 M4095 L4096 K4097 N4098 V4099 H4100 L4106 M4107 Q4108 L4109 E4110 K4111 K4112 L4113 P4118 F4125 L4126 T4127 M4128 E4129 I4130 N4131 V4134 P4135 V4136
N4137 L4138 L4139 R4140 R4143 I4144 F4145 K4154 A4155 N4156 T4160 K4171 S4172 P4173 R4176 A4177 R4178 L4179 Y4180 F4181 L4182 L4183 F4186 H4187 A4188 I4189 I4190 Q4191 E4192 R4193 L4194 R4195 Y4196 G4200 W4201 Y4205 E4206 F4207 L4212 D4220 T4221 W4222 A4227 N4232 I4233 P4239 W4240


S4241 A4242 L4243 K4244 A4248 Q4249 S4250 I4251 Y4252 F4260 D4261 Q4262 R4263 L4264 R4271 L4272 T4275 R4276 S4277 F4278 F4282 K4287 V4288 D4289 G4290 H4291 K4292 D4293 M4296 P4297 I4300 R4301 R4302 E4303 E4304 F4305 V4306 Q4307 W4308 V4309 E4310 L4311 L4312 P4313 D4314 T4315 P4318 S4319 W4320 L4321
P4324 N4325 N4326 A4327 E4328 M4339 M4343 L4344 K4345 M4346 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 W4376 T4379 I4391 P4392 Q4393 L4398 K4399 R4400 T4401 V4402 I4405 R4411 F4412 F4413
E4414 K4418 L4423 R4428 Q4429 D4430 V4434 K4441 K4442 K4443 Q4444 T4445 N4446 Y4447 L4448 R4449 I4452 N4453 E4454 L4455 V4456 I4459 L4460 P4461 W4464 S4465 H4466 G4472 M4473 T4474 V4475 I4476 Q4477 W4478 V4479 F4482 S4483 E4484 R4485 I4486 K4487 Q4488 L4489 I4492 L4504 K4505 N4506 I4507
H4508 V4509 F4515 R4525 Q4526 N4532 S4533 W4534 S4535 L4536 E4537 E4538 L4541 E4542 V4543 Q4549 L4553 D4554 A4555 C4556 S4557 L4565 K4574 L4577 S4578 L4585 R4591 W4592 V4593 K4594 V4604 V4605 T4606 L4607 P4608 V4609 L4618 V4622 D4623 F4624 E4625 K4629 R4633 S4634
F4635 V4636 E4637 R4638 V4642 T4645 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93339	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	0.603	Depositor
Minimum map value	-0.336	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	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

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	0.20	0/22127	0.40	0/29993

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2229	GLY	Peptide

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	21664	0	21700	885	0
2	A	81	0	36	14	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	5	0
All	All	21776	0	21748	886	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 20.

The worst 5 of 886 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:3126:MET:HE3	1:A:3127:PRO:HD2	1.50	0.93
1:A:2603:MET:HE1	2:A:4703:ADP:C4	2.04	0.93
1:A:2688:GLU:HB2	1:A:2730:HIS:HE1	1.33	0.90
1:A:2619:GLY:HA2	1:A:2662:PHE:HB3	1.58	0.84
1:A:2473:ASN:HB2	1:A:2481:MET:HE1	1.60	0.83

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	2684/4646 (58%)	2592 (97%)	92 (3%)	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	2397/4125 (58%)	2397 (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 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3667	GLN
1	A	3772	ASN
1	A	4466	HIS
1	A	3714	ASN
1	A	3792	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\|>2$
3	ATP	A	4702	-	28,33,33	0.99	2 (7%)	34,52,52	0.65	1 (2%)
2	ADP	A	4701	-	24,29,29	0.86	0	29,45,45	1.32	5 (17%)
2	ADP	A	4704	-	24,29,29	0.81	0	29,45,45	1.28	2 (6%)
2	ADP	A	4703	-	24,29,29	0.83	0	29,45,45	1.33	4 (13%)

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	4702	-	-	5/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4702	ATP	PA-O3A	-2.72	1.56	1.59
3	A	4702	ATP	PB-O3B	-2.64	1.56	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4704	ADP	N3-C2-N1	-3.69	123.66	128.67
2	A	4701	ADP	N3-C2-N1	-3.35	124.12	128.67
2	A	4703	ADP	N3-C2-N1	-3.21	124.32	128.67
2	A	4703	ADP	C4'-O4'-C1'	2.90	112.58	109.92
2	A	4704	ADP	C4-C5-N7	-2.67	106.52	109.34

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A

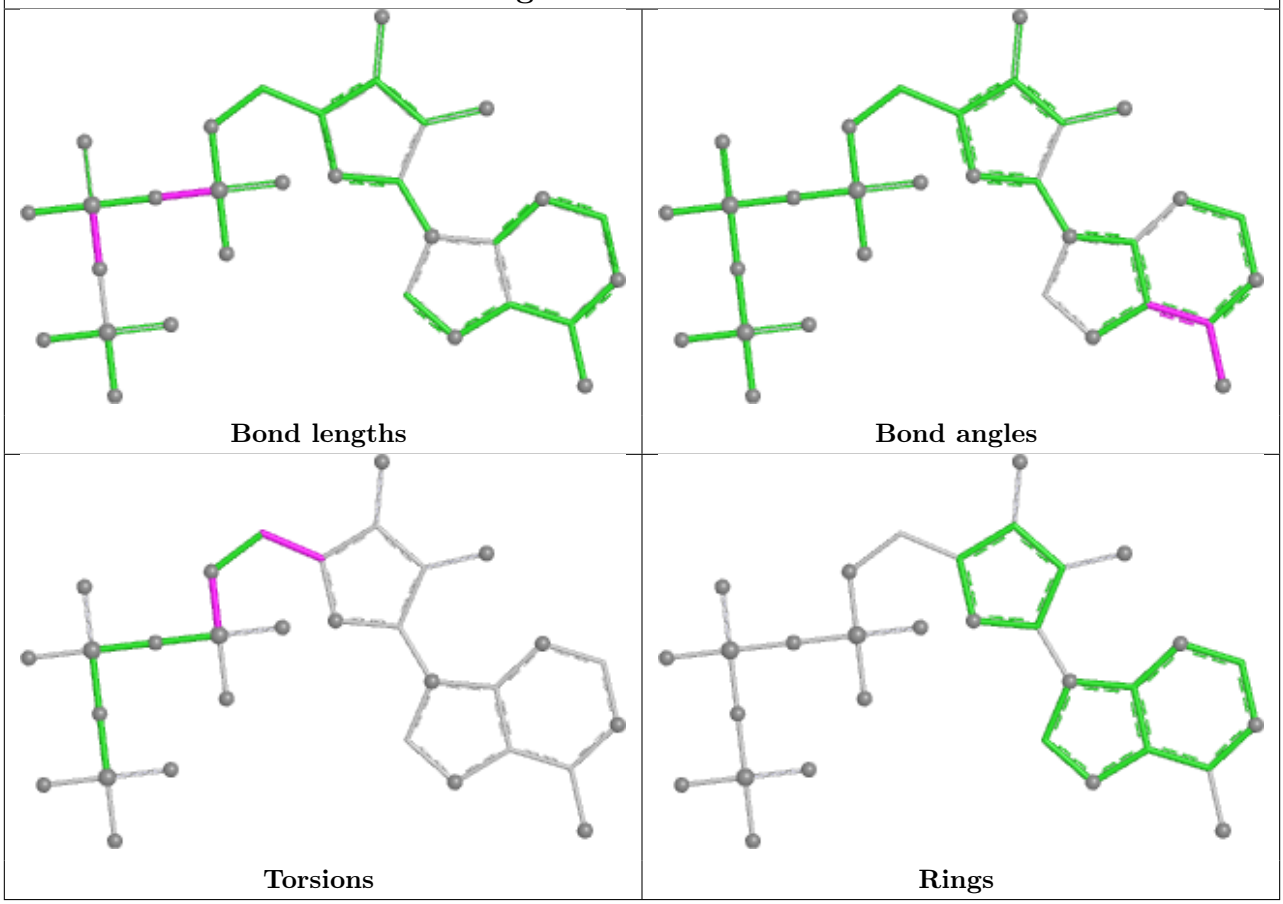
There are no ring outliers.

4 monomers are involved in 19 short contacts:

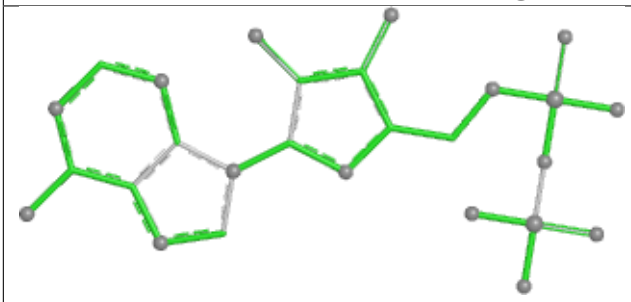
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	5	0
2	A	4701	ADP	6	0
2	A	4704	ADP	2	0
2	A	4703	ADP	6	0

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.

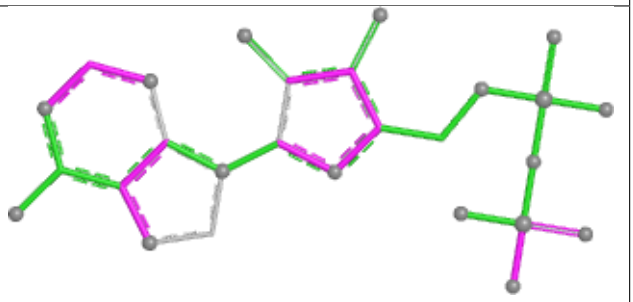
Ligand ATP A 4702



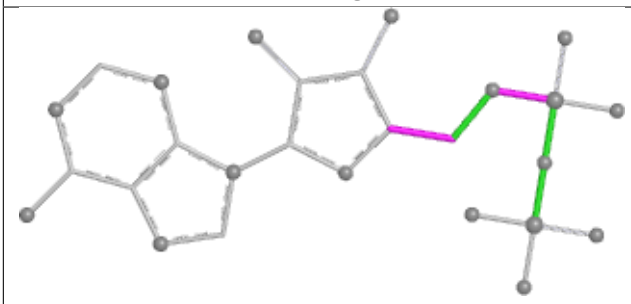
Ligand ADP A 4701



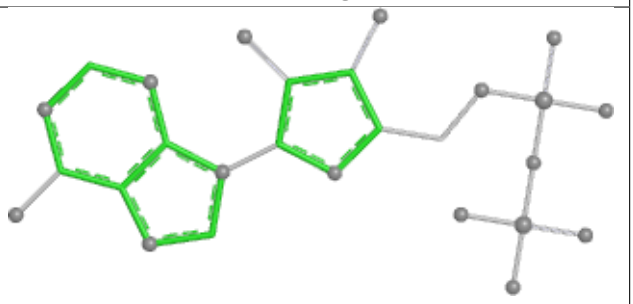
Bond lengths



Bond angles

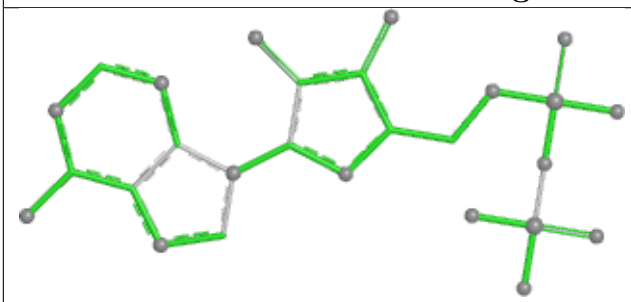


Torsions

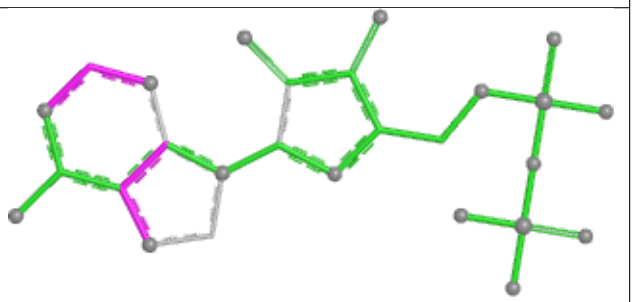


Rings

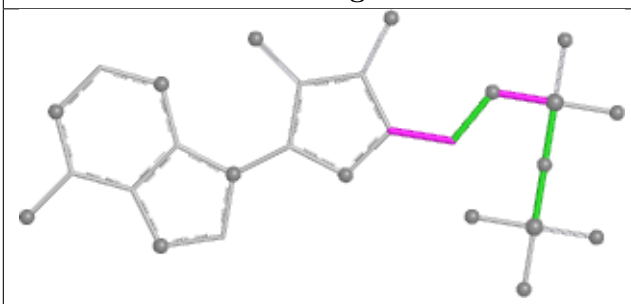
Ligand ADP A 4704



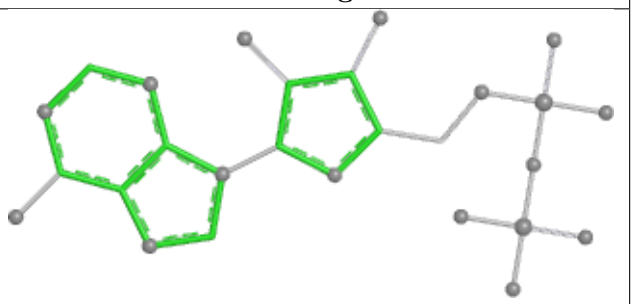
Bond lengths



Bond angles

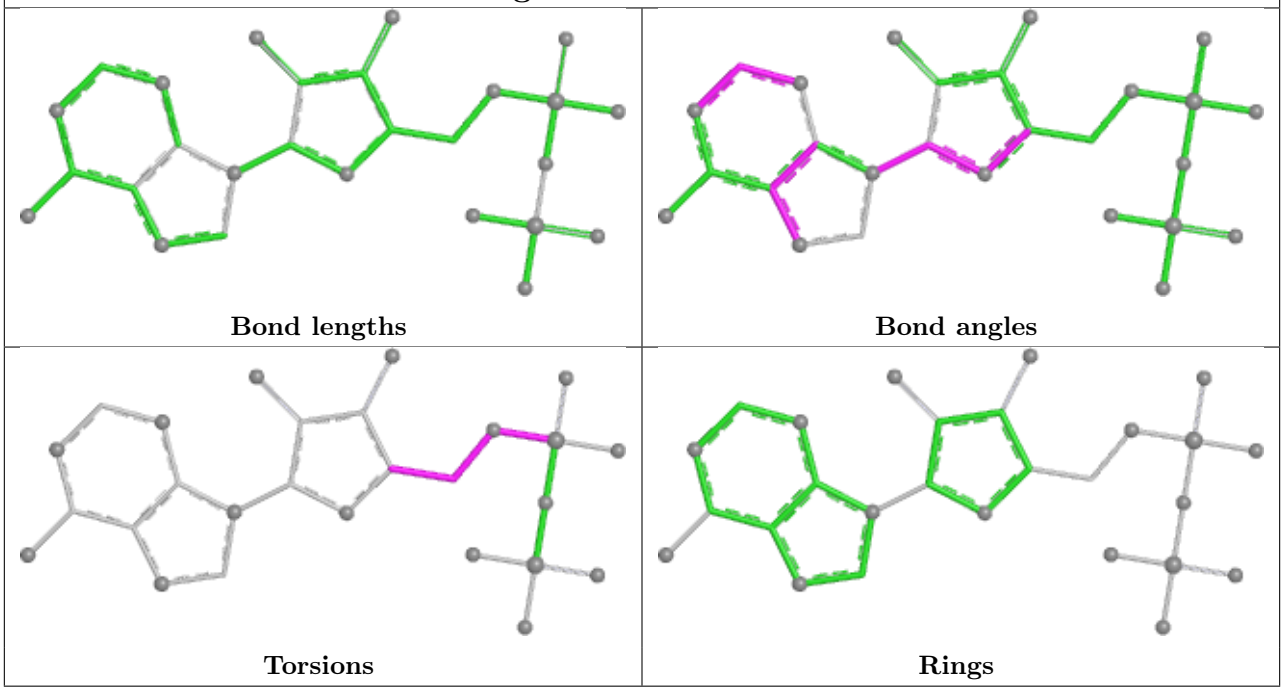


Torsions



Rings

Ligand ADP A 4703



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.

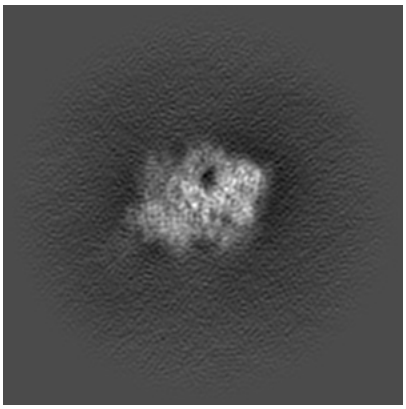
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44711. These allow visual inspection of the internal detail of the map and identification of artifacts.

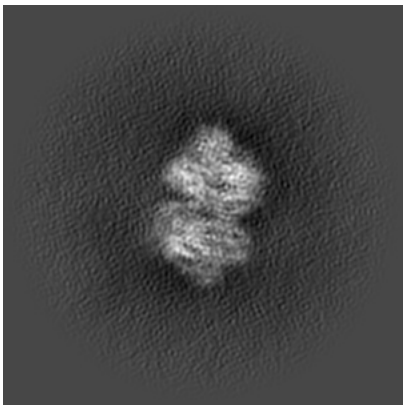
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

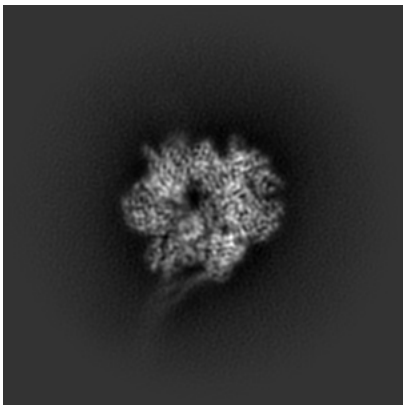
6.1.1 Primary map



X

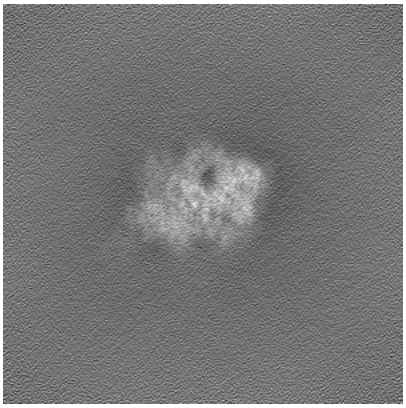


Y

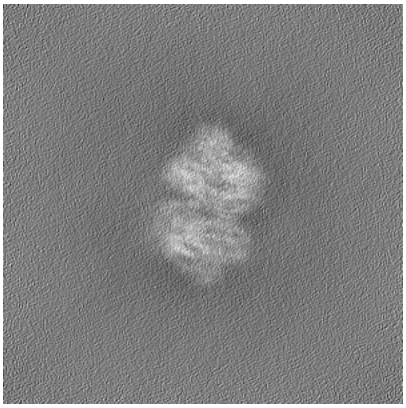


Z

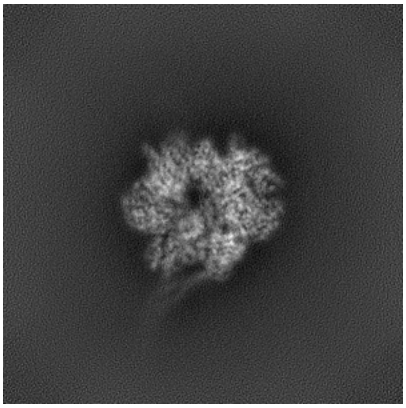
6.1.2 Raw map



X



Y

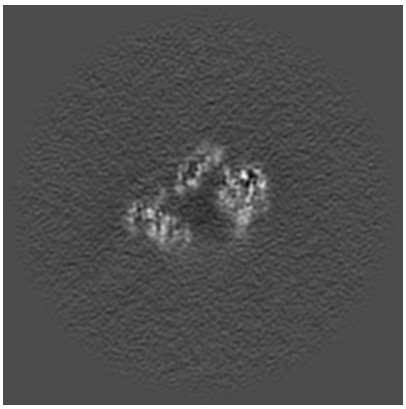


Z

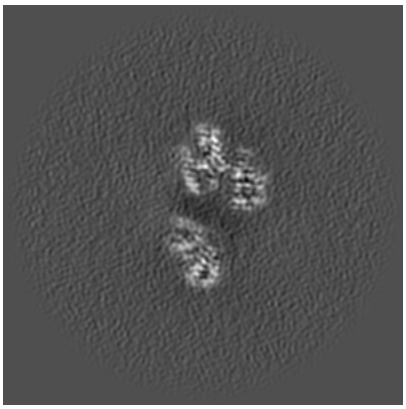
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

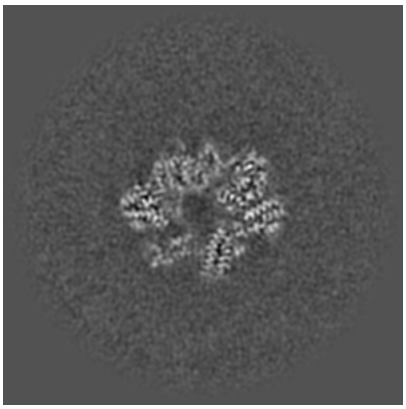
6.2.1 Primary map



X Index: 160



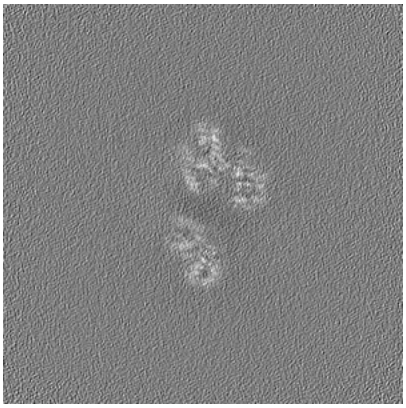
Y Index: 160



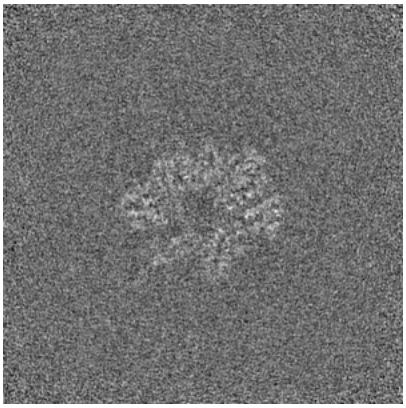
Z Index: 160

6.2.2 Raw map

X Index: 160



Y Index: 160

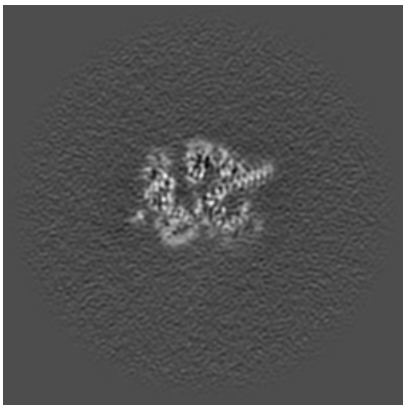


Z Index: 160

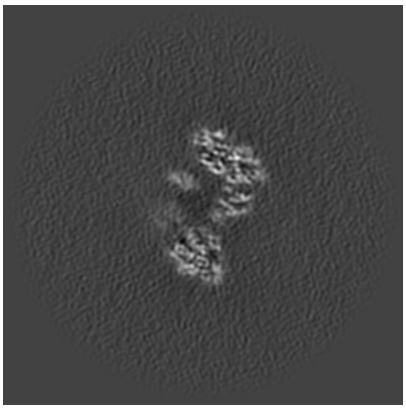
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

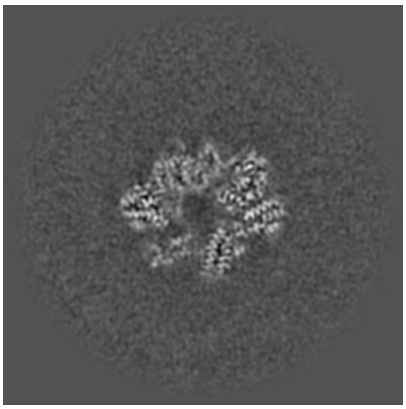
6.3.1 Primary map



X Index: 182

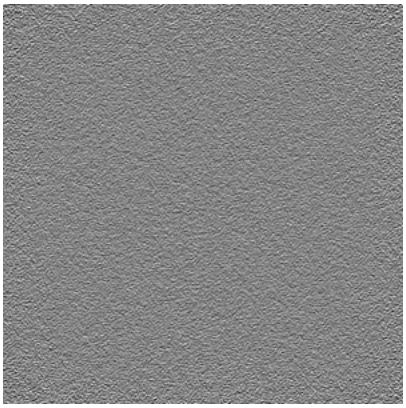


Y Index: 150

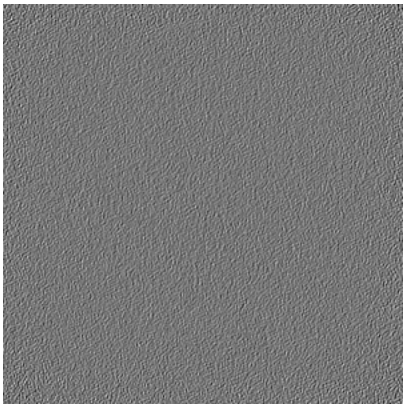


Z Index: 160

6.3.2 Raw map



X Index: 0



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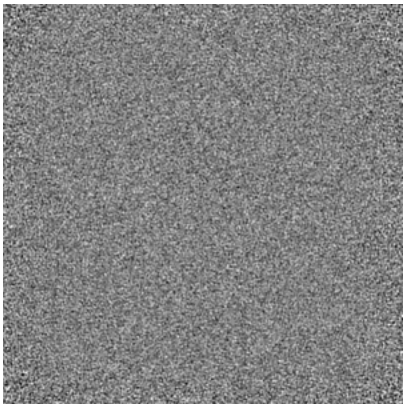
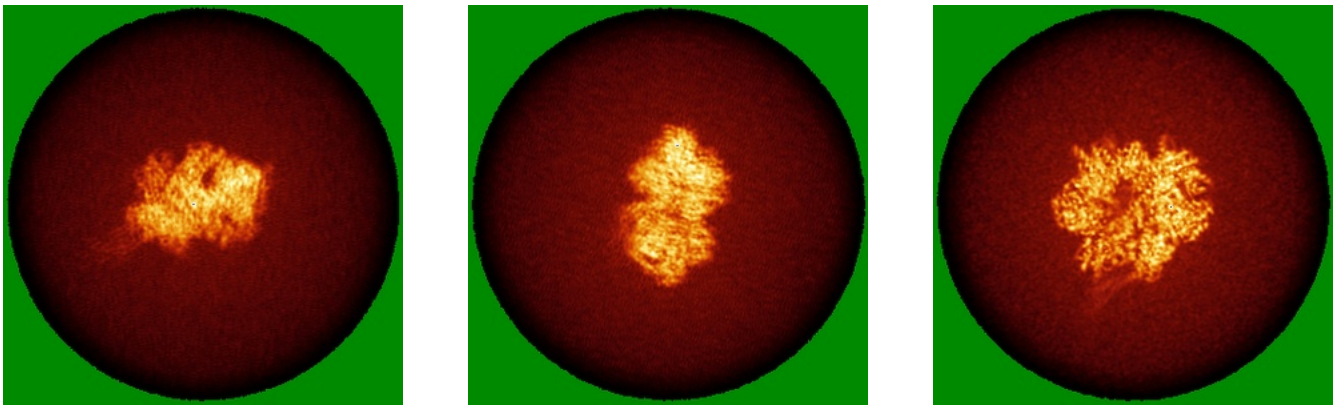


Z Index: 0

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

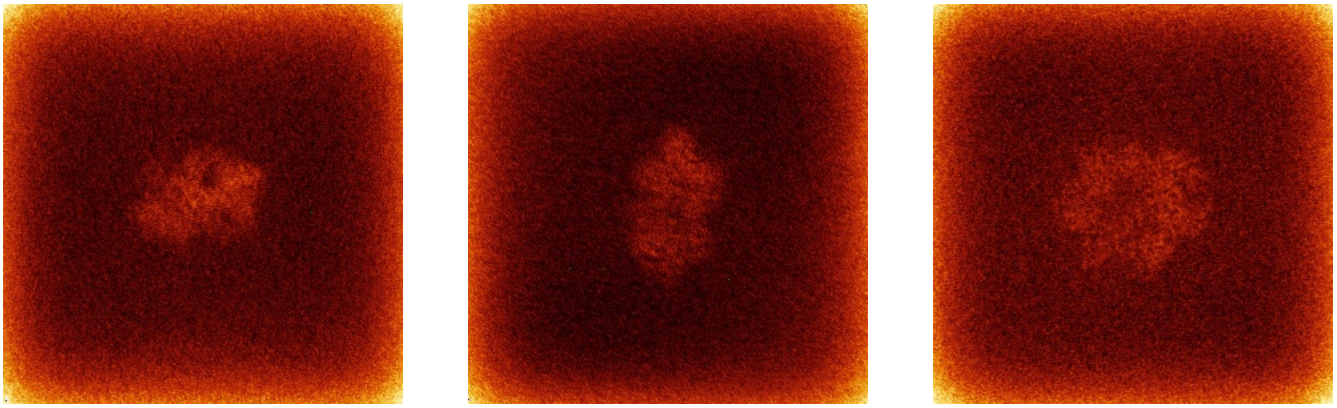
6.4 Orthogonal standard-deviation projections (False-color) (i)

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 0.1. 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.

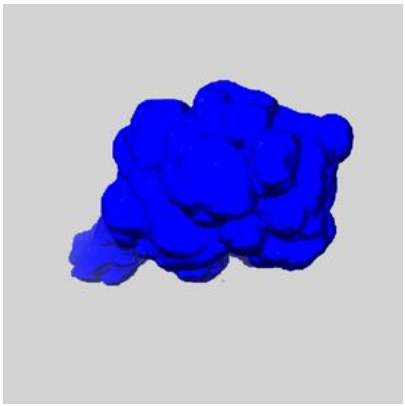
6.6 Mask visualisation (i)

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

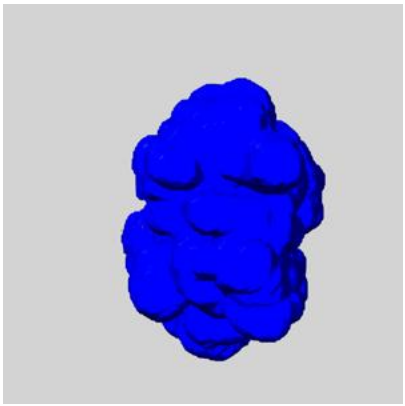
A mask typically either:

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

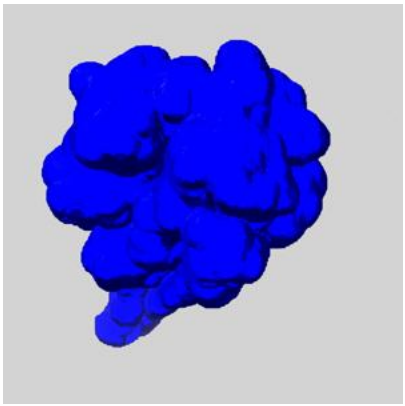
6.6.1 emd_44711_msk_1.map (i)



X



Y

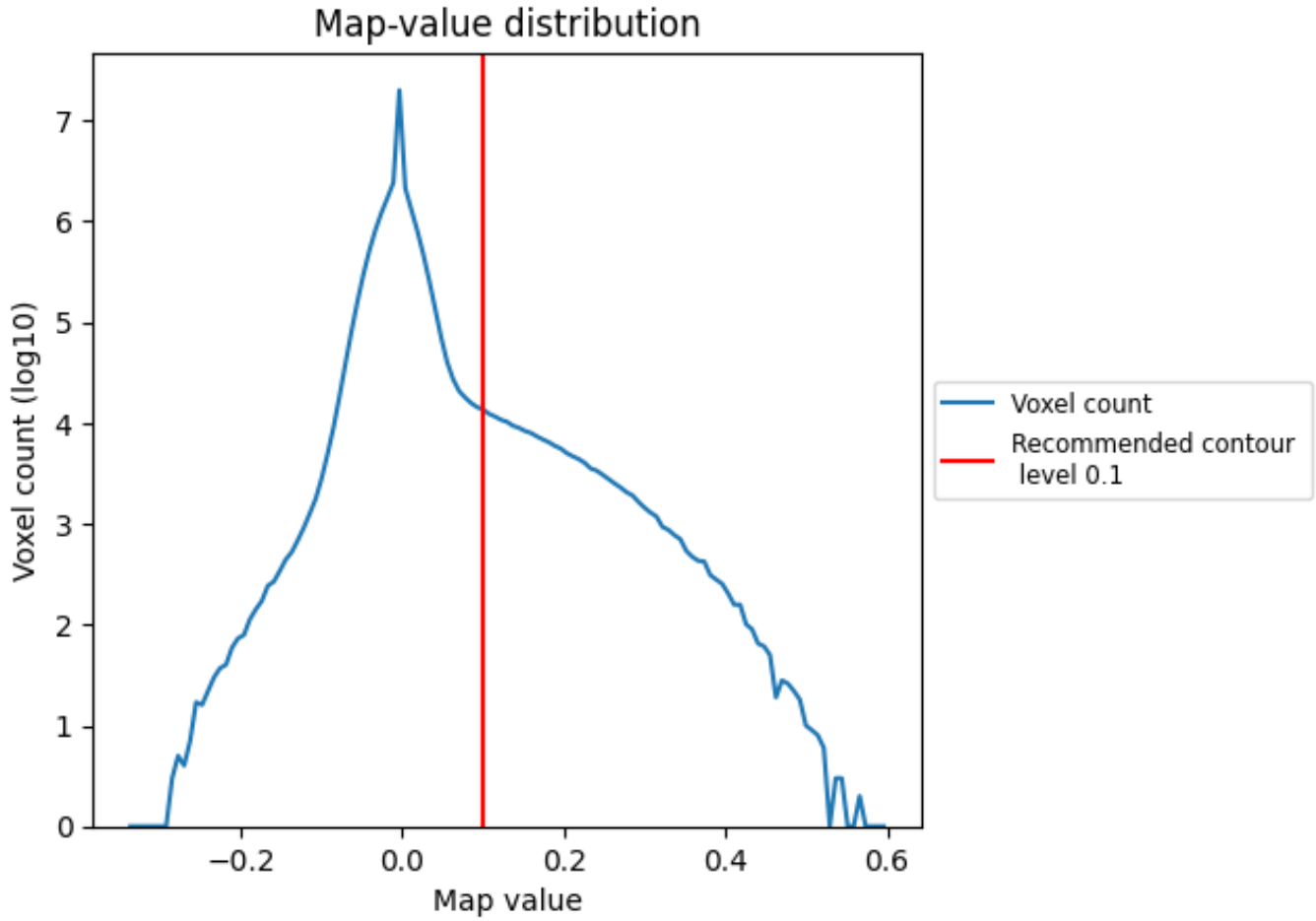


Z

7 Map analysis

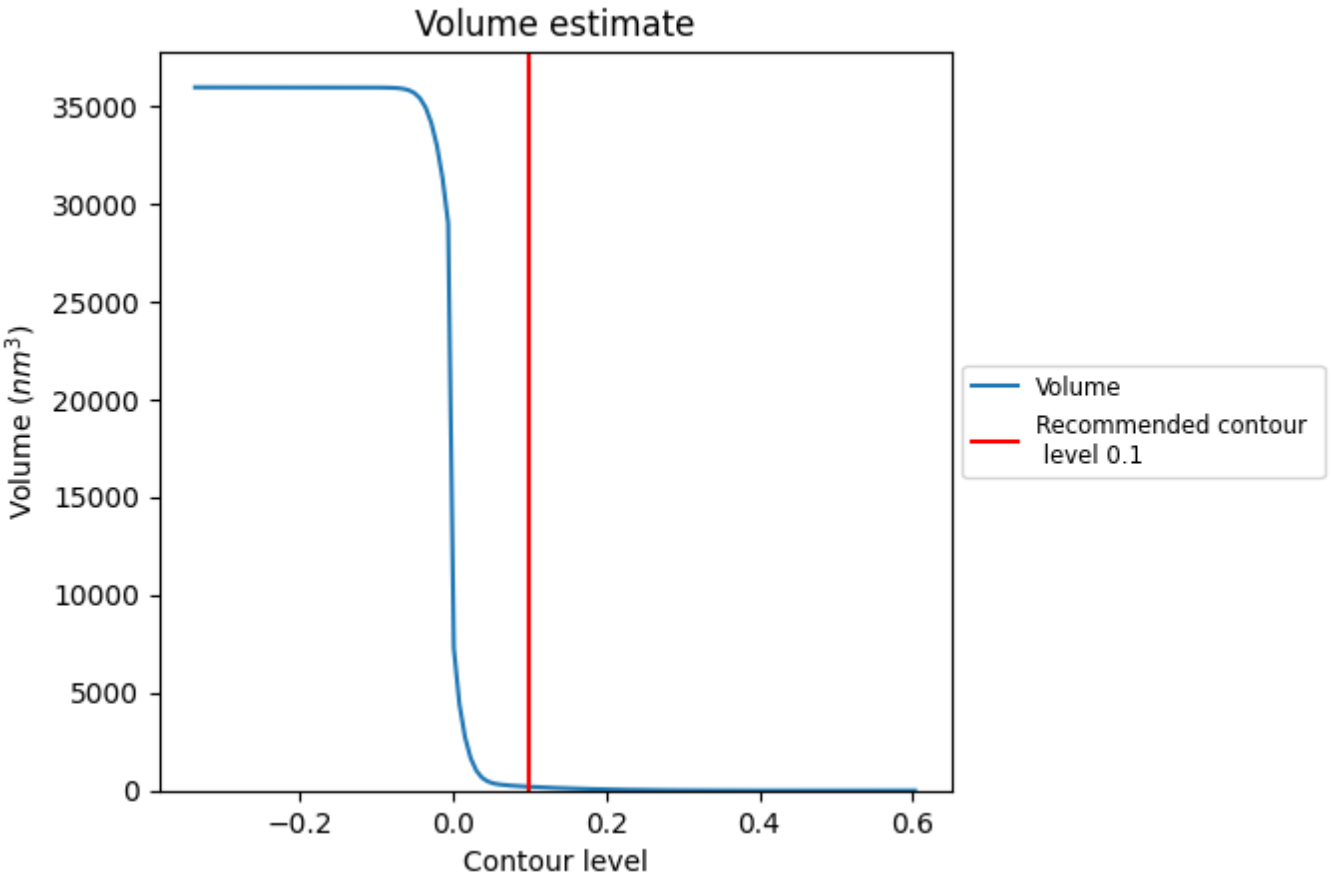
This section contains the results of statistical analysis of the map.

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.

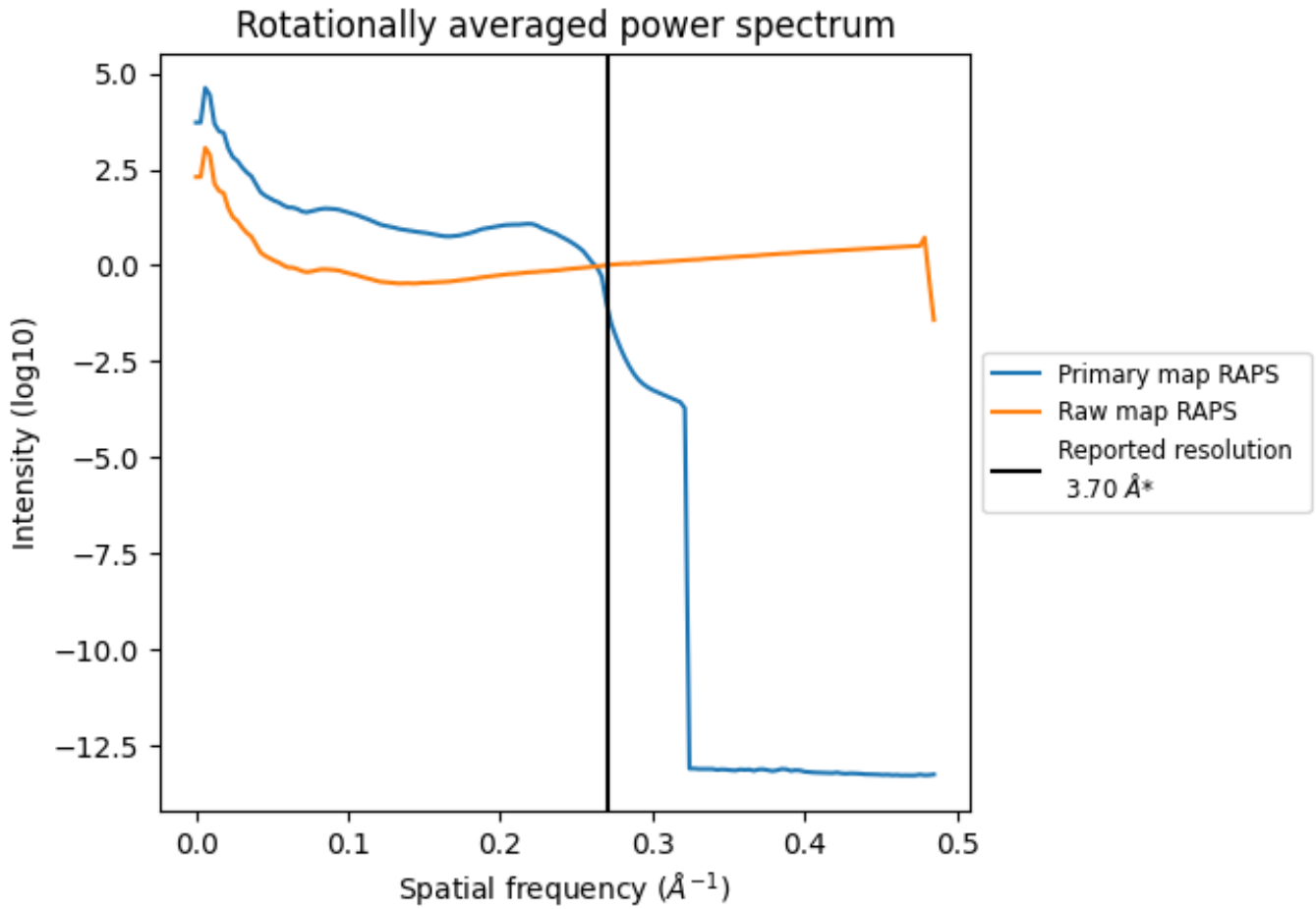
7.2 Volume estimate (i)



The volume at the recommended contour level is 195 nm^3; this corresponds to an approximate mass of 176 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)

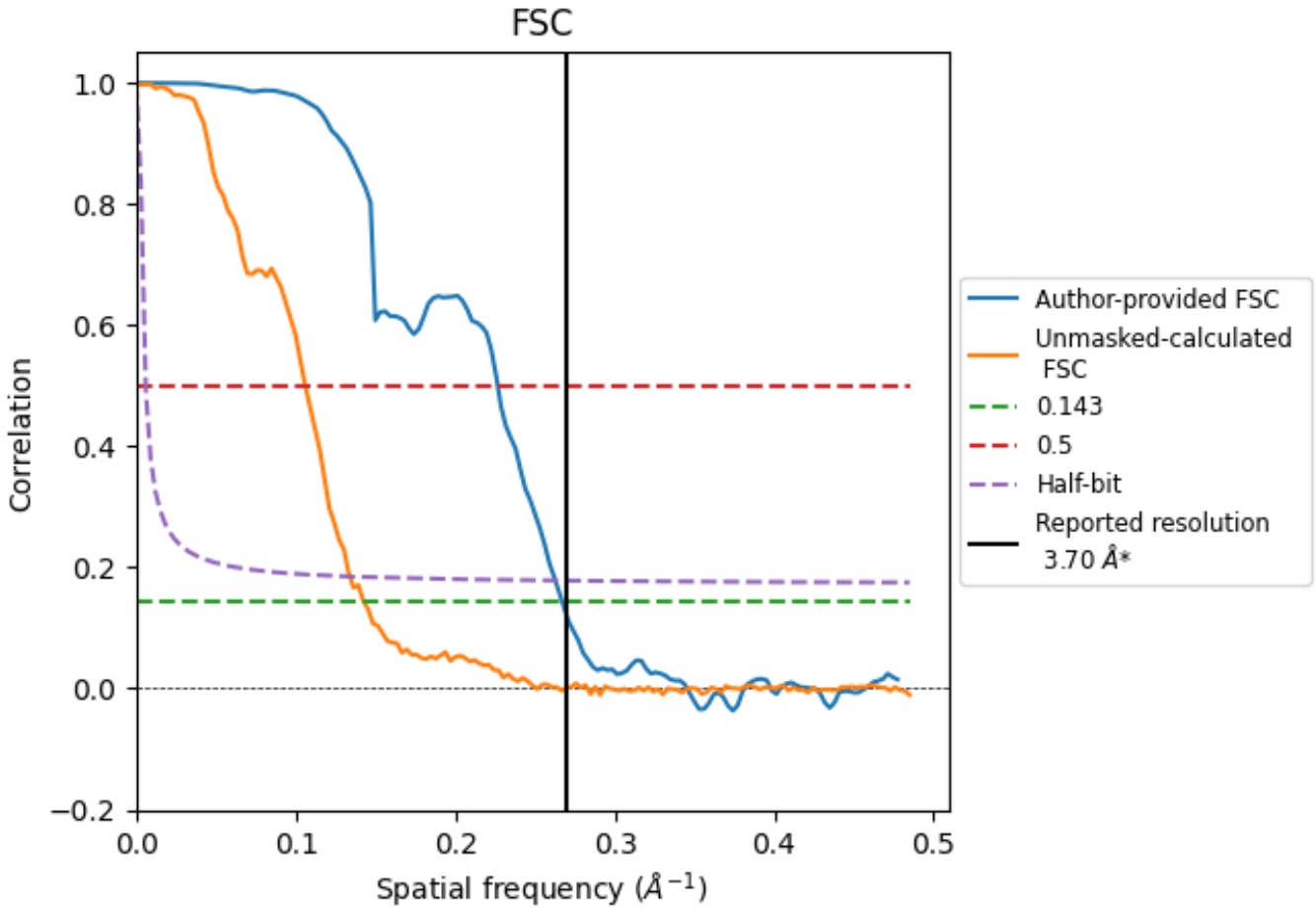


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

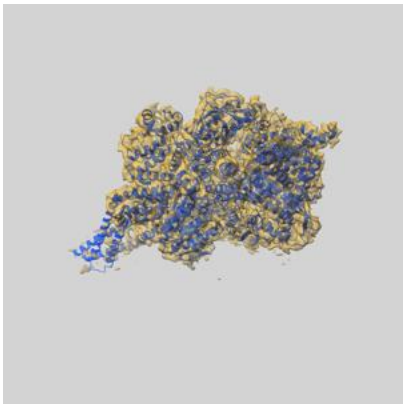
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.41	3.81
Unmasked-calculated*	7.00	9.43	7.46

*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 7.00 differs from the reported value 3.7 by more than 10 %

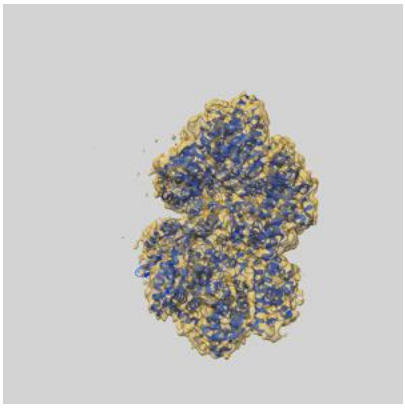
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44711 and PDB model 9BMU. Per-residue inclusion information can be found in section 3 on page 5.

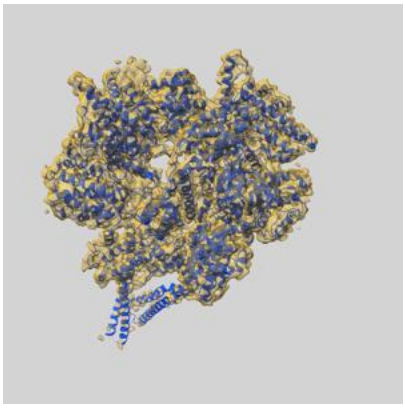
9.1 Map-model overlay



X



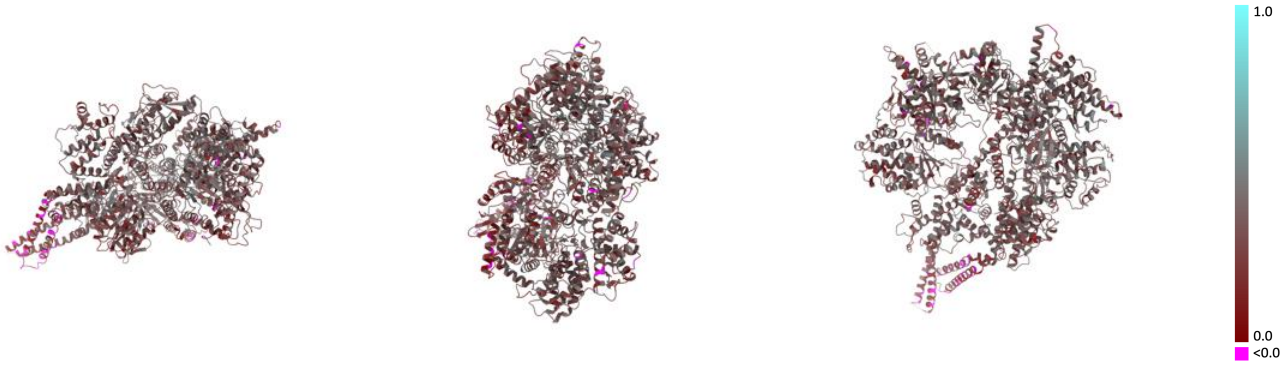
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

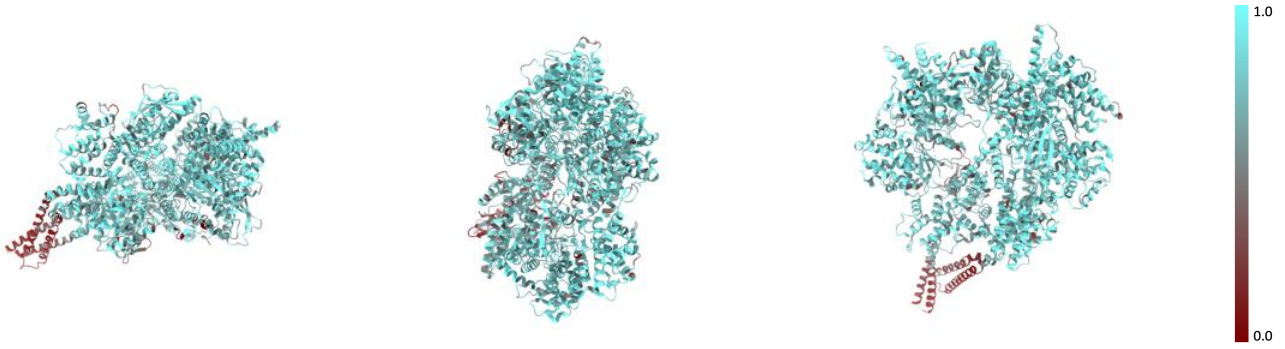
9.2 Q-score mapped to coordinate model



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.

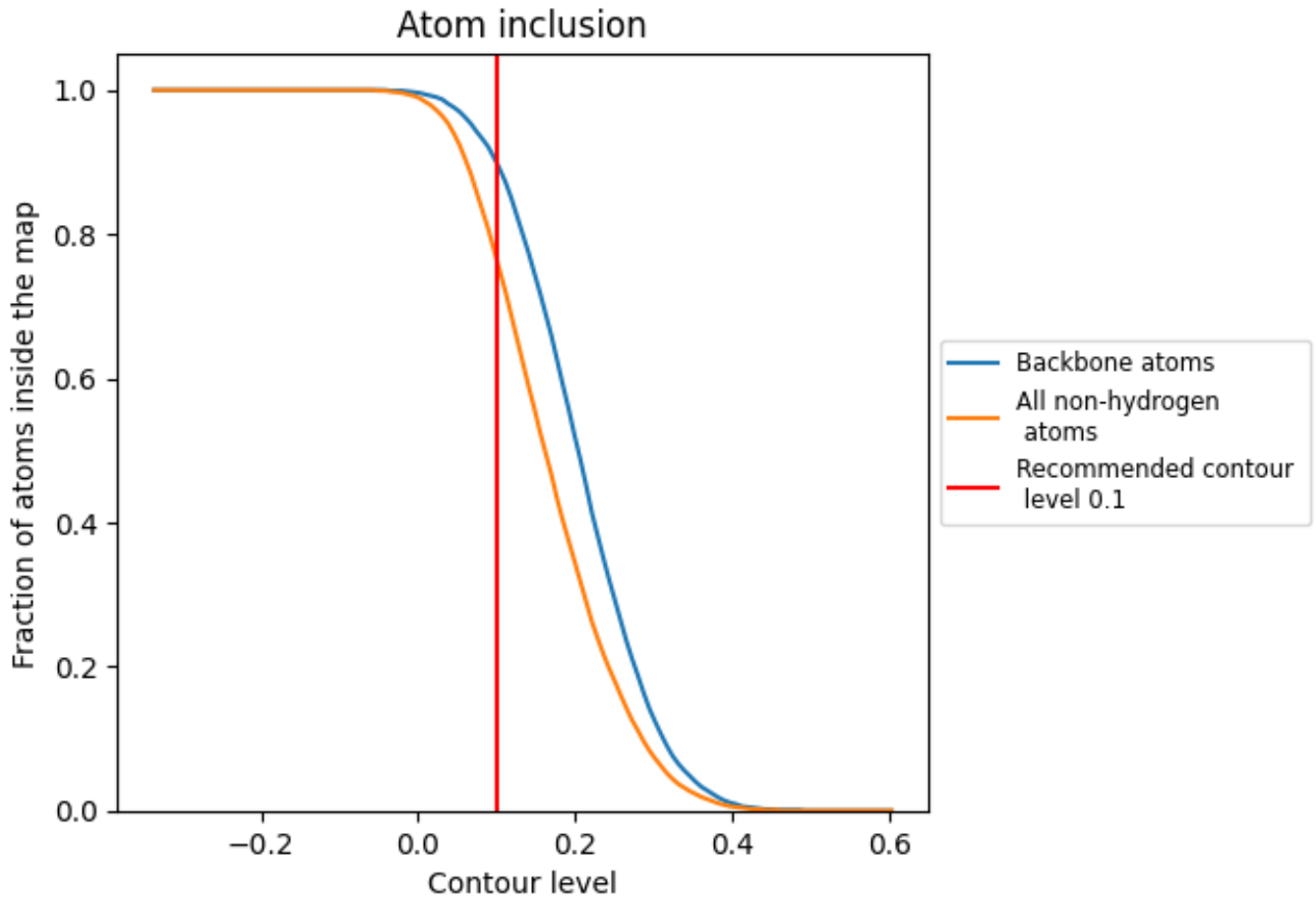
9.3 Atom inclusion mapped to coordinate model



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.3330
A	0.7650	0.3330