Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 04:12 am GMT

PDB ID	:	6ZYW
EMDB ID	:	EMD-11576
Title	:	Outer Dynein Arm-Shulin complex - overall structure (Tetrahymena thermophila)
Authors	:	Mali, G.R.; Abid Ali, F.; Lau, C.K.; Carter, A.P.
Deposited on	:	2020-08-03
Resolution	:	8.78 Å(reported)

This is a Full wwPDB EM Validation 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:

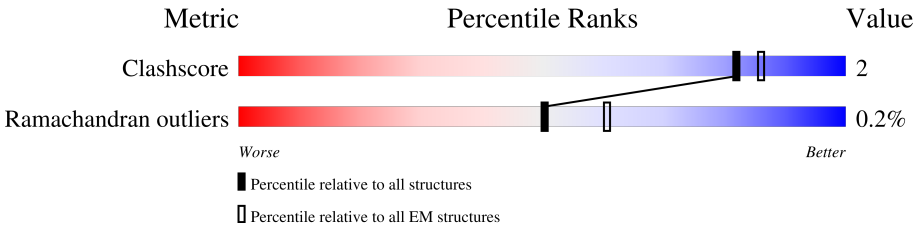
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.78 Å.

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



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

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	4168	35% 85% 6% 9%
2	B	4595	16% 91% 5%
3	C	4620	13% 94%
4	D	667	47% 52%
4	d	667	19% 81%
5	E	670	51% 49%
5	e	670	15% 85%
6	F	133	74% 26%
7	G	103	90% 8%

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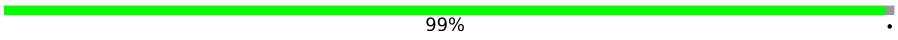
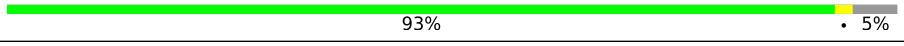
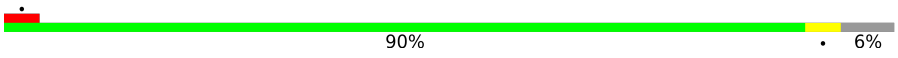
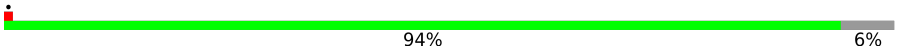
Mol	Chain	Length	Quality of chain
8	H	92	
9	I	110	
10	J	93	
11	K	111	
12	L	111	
13	M	87	
14	N	132	
15	O	117	
16	P	110	
17	Y	1200	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 73897 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 Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	3795	Total 18787	C 11198	N 3795	O 3794	0	0

- Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	4370	Total 20008	C 12102	N 3953	O 3953	0	417

- Molecule 3 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	4433	Total 19737	C 11997	N 3870	O 3870	0	563

- Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	321	Total 1588	C 946	N 321	O 321	0	0
4	d	128	Total 637	C 381	N 128	O 128	0	0

- Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	341	Total 1678	C 996	N 341	O 341	0	0
5	e	102	Total 501	C 297	N 102	O 102	0	0

- Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	98	Total 486	C 290	N 98	O 98	0	0

- Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	95	Total 470	C 280	N 95	O 95	0	0

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	85	Total 420	C 250	N 85	O 85	0	0

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	89	Total 439	C 261	N 89	O 89	0	0

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	84	Total 416	C 248	N 84	O 84	0	0

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	95	Total 470	C 280	N 95	O 95	0	0

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	97	Total 479	C 285	N 97	O 97	0	0

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	86	Total 426	C 254	N 86	O 86	0	0

- Molecule 14 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	109	Total 537	C 319	N 109	O 109	0	0

- Molecule 15 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	111	Total 550	C 328	N 111	O 111	0	0

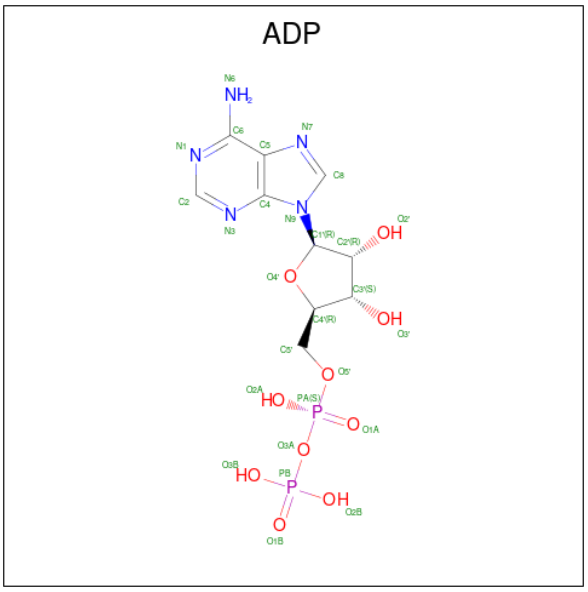
- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	103	Total 513	C 307	N 103	O 103	0	0

- Molecule 17 is a protein called Shulin.

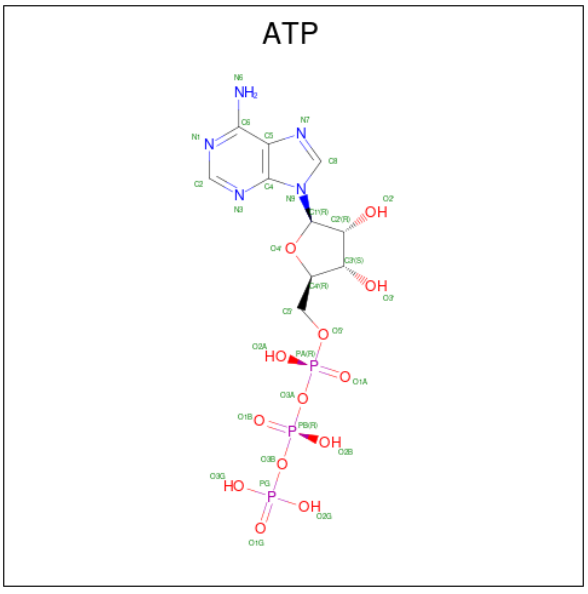
Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	1133	Total 5611	C 3345	N 1133	O 1133	0	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



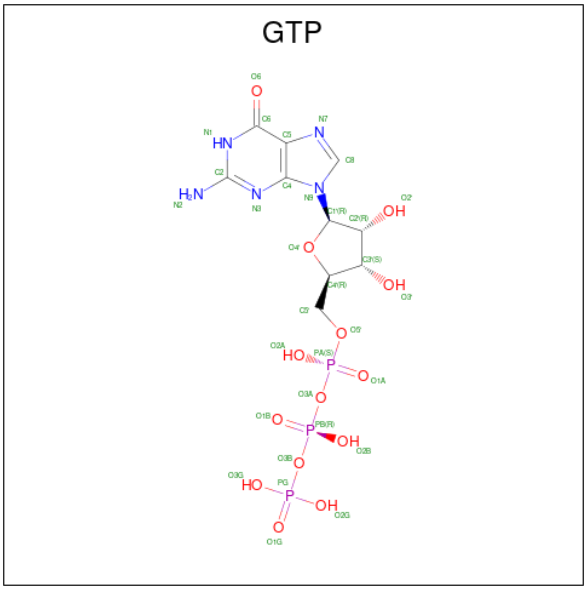
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			81	30	15	30	6	
18	C	1	Total	C	N	O	P	0
			81	30	15	30	6	
18	C	1	Total	C	N	O	P	0
			81	30	15	30	6	

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 20 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



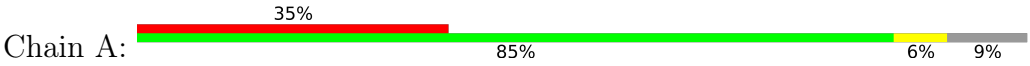
Mol	Chain	Residues	Atoms					AltConf
20	Y	1	Total	C	N	O	P	0
			32	10	5	14	3	

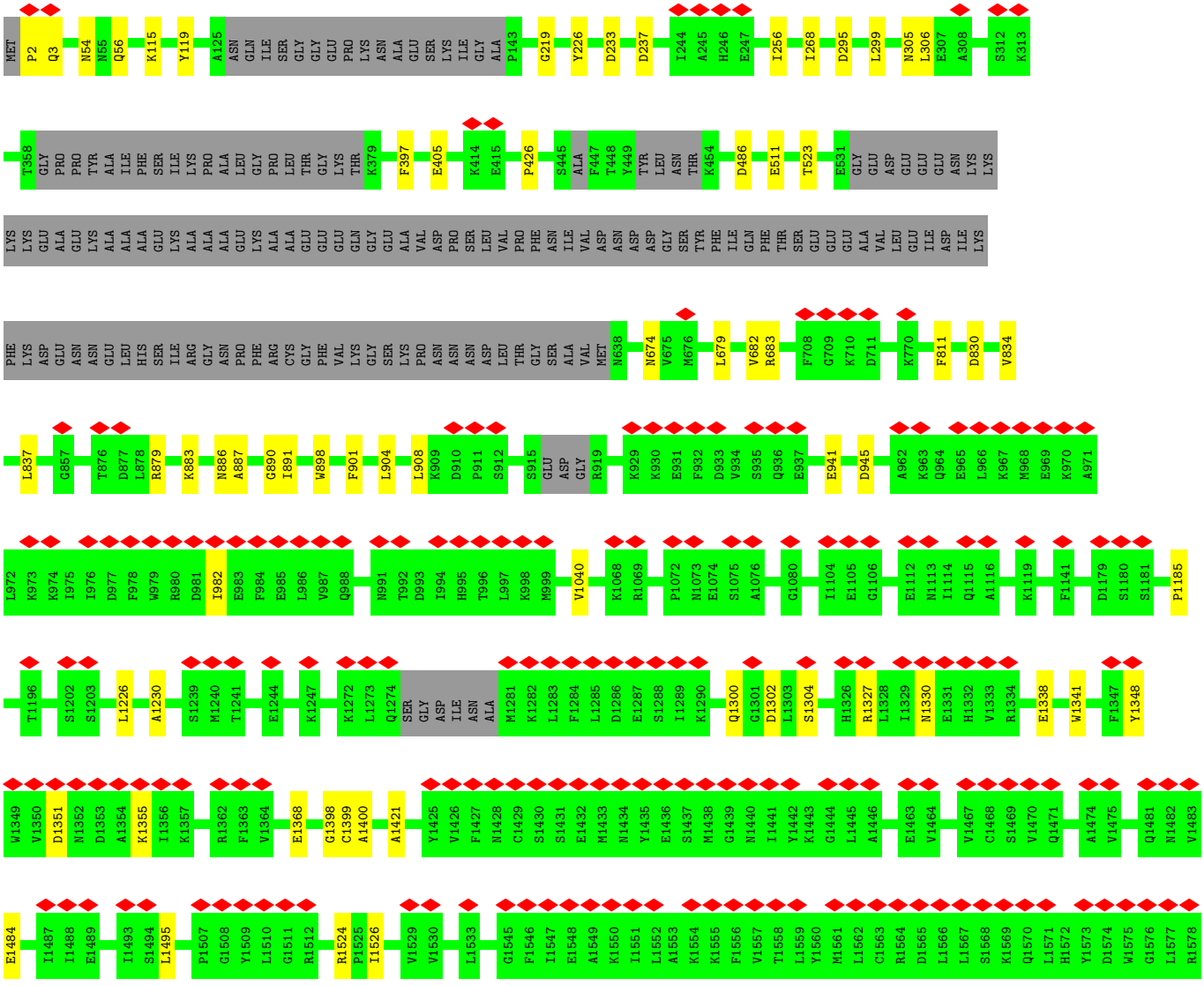
3 Residue-property plots (i)

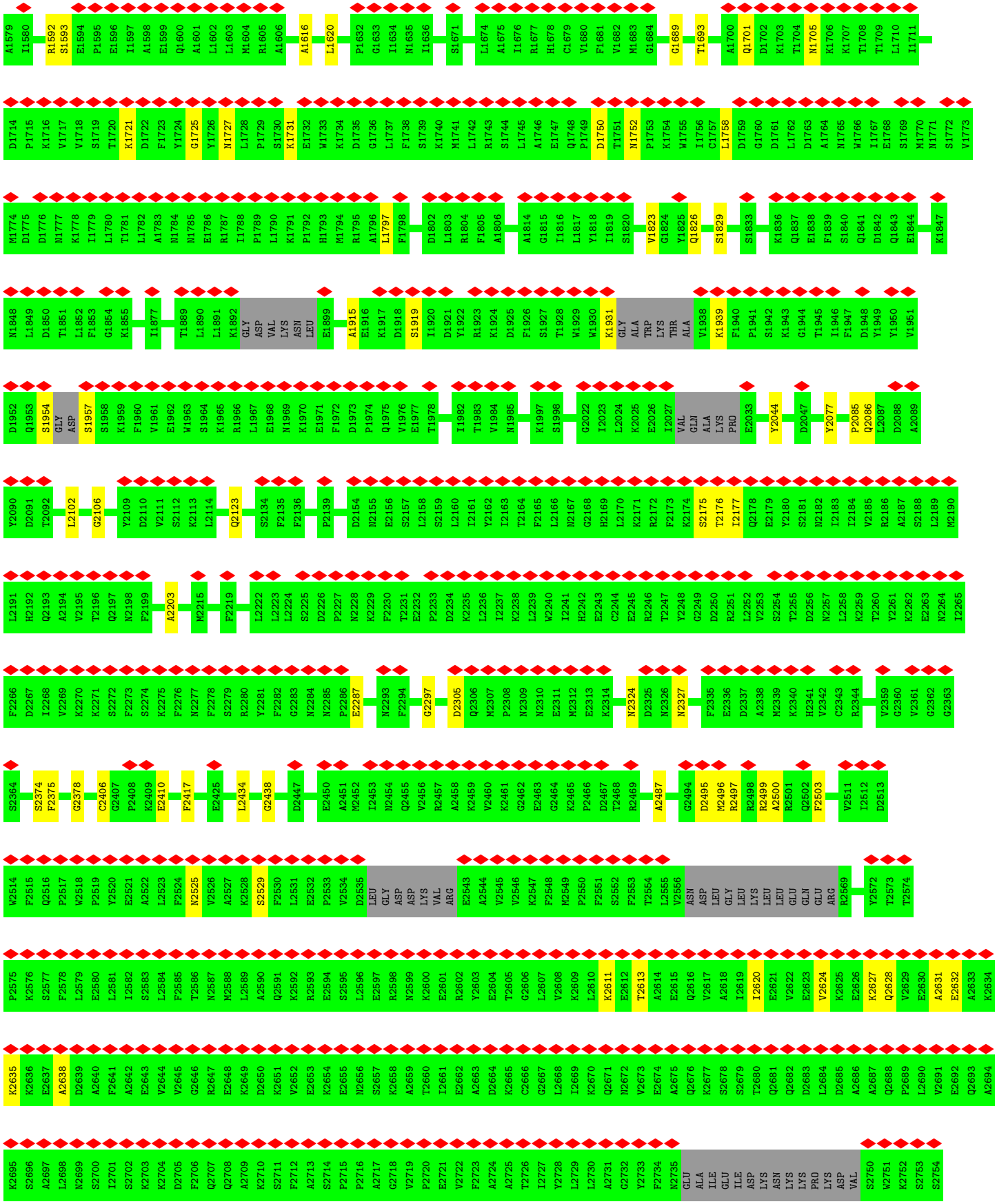
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative

Chain A:



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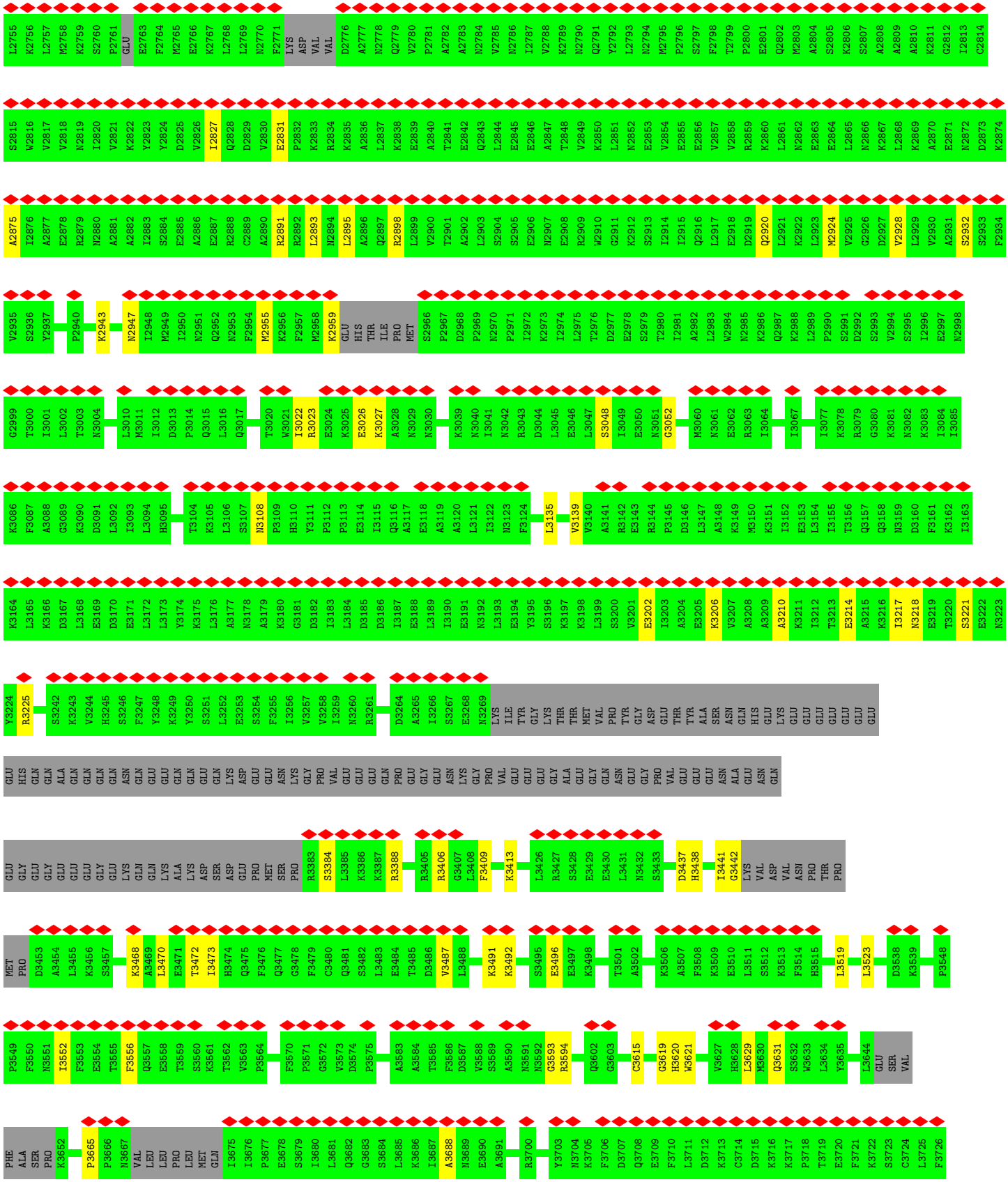
D1714 P1715 K1716 V1717 V1718 S1719 T1720 K1721 D1722 F1723 Y1724 G1725 Y1726 N1727 L1728 P1729 S1730 K1731 E1732 W1733 K1734 D1735 G1736 L1737 F1738 S1739 K1740 M1741 L1742 R1743 S1744 L1745 A1746 E1747 Q1748 P1749 D1750 T1751 N1752 P1753 K1754 W1755 I1756 C1757 L1758 D1759 G1760 D1761 L1762 D1763 A1764 N1765 W1766 I1767 E1768 S1769 M1770 N1771 S1772 V1773
M1774 D1775 D1776 N1777 K1778 I1779 L1780 T1781 L1782 A1783 N1784 N1785 E1786 R1787 I1788 P1789 L1790 K1791 P1792 H1793 M1794 R1795 A1796 L1797 F1798 D1802 L1803 R1804 F1805 A1806 A1814 G1815 I1816 L1817 Y1818 I1819 S1820 V1823 G1824 Y1825 Q1826 S1829 S1833 K1836 Q1837 E1838 F1839 S1840 Q1841 D1842 Q1843 E1844 K1847
N1848 L1849 D1850 T1851 L1852 F1853 G1854 K1855 I1877 T1889 L1890 L1891 K1892 GLY ASP VAL LYS ASN LEU E1899 A1915 E1916 K1917 D1918 S1919 I1920 D1921 Y1922 R1923 K1924 D1925 F1926 S1927 T1928 W1929 W1930 K1931 GLY ALA TRP LYS THR ALA V1938 K1939 F1940 P1941 S1942 K1943 G1944 T1945 I1946 F1947 D1948 Y1949 Y1950 V1951
D1952 Q1953 S1954 GLY ASP S1957 S1958 K1959 F1960 V1961 E1962 W1963 S1964 K1965 R1966 L1967 E1968 N1969 K1970 E1971 F1972 D1973 P1974 Q1975 V1976 E1977 T1978 I1982 T1983 V1984 N1985 K1997 S1998 G2022 I2023 L2024 K2025 E2026 I2027 VAL GLN ALA LYS PRO E2033 Y2044 D2047 Y2077 P2085 Q2086 L2087 D2088 A2089
Y2090 D2091 T2092 L2102 G2106 Y2109 D2110 V2111 S2112 K2113 L2114 Q2123 S2134 P2135 F2136 P2139 D2154 N2155 E2156 S2157 L2158 S2159 L2160 I2161 Y2162 I2163 T2164 F2165 L2166 N2167 G2168 H2169 L2170 K2171 R2172 F2173 K2174 S2175 T2176 I2177 Q2178 E2179 Y2180 S2181 N2182 I2183 I2184 V2185 R2186 A2187 S2188 L2189 M2190
L2191 H2192 Q2193 A2194 V2195 T2196 Q2197 N2198 F2199 A2203 M2215 F2219 L2222 L2223 L2224 S2225 D2226 P2227 N2228 K2229 F2230 T2231 E2232 P2233 D2234 K2235 L2236 I2237 K2238 L2239 W2240 I2241 H2242 E2243 C2244 E2245 R2246 T2247 Y2248 G2249 D2250 R2251 L2252 V2253 S2254 T2255 D2256 N2257 L2258 K2259 T2260 Y2261 K2262 E2263 N2264 I2265
F2266 D2267 I2268 V2269 K2270 K2271 S2272 F2273 S2274 K2275 F2276 N2277 F2278 S2279 R2280 Y2281 F2282 G2283 N2284 N2285 P2286 E2287 N2293 F2294 G2297 D2305 Q2306 M2307 P2308 N2309 N2310 E2311 M2312 E2313 K2314 M2324 D2325 N2326 N2327 F2335 E2336 D2337 A2338 M2339 K2340 H2341 V2342 C2343 R2344 V2359 G2360 V2361 G2362 G2363
S2364 S2374 F2375 G2378 C2406 G2407 P2408 K2409 E2410 F2417 E2425 L2434 G2438 D2447 E2450 A2451 M2452 I2453 N2454 Q2455 V2456 R2457 A2458 K2459 V2460 K2461 G2462 E2463 G2464 K2465 P2466 D2467 T2468 R2469 A2487 G2494 D2495 M2496 R2497 R2498 R2499 A2500 R2501 Q2502 F2503 V2511 I2512 D2513
W2514 F2515 Q2516 P2517 W2518 P2519 Y2520 E2521 A2522 L2523 F2524 N2525 V2526 A2527 K2528 S2529 F2530 L2531 E2532 P2533 V2534 D2535 LEU GLY ASP ASP LYS VAL ARG E2543 A2544 V2545 V2546 K2547 F2548 M2549 P2550 F2551 S2552 F2553 T2554 L2555 V2556 ASN ASP LEU GLY LEU LYS LEU LEU GLU GLN GLU ARG R2569 Y2572 T2573 T2574
P2575 K2576 S2577 F2578 L2579 E2580 L2581 I2582 S2583 L2584 F2585 T2586 N2587 M2588 L2589 A2590 Q2591 K2592 R2593 E2594 S2595 L2596 E2597 R2598 N2599 K2600 E2601 R2602 Y2603 E2604 T2605 G2606 L2607 V2608 K2609 L2610 K2611 E2612 T2613 A2614 E2615 Q2616 V2617 A2618 I2619 I2620 E2621 V2622 E2623 V2624 K2625 E2626 K2627 Q2628 V2629 E2630 A2631 E2632 A2633 K2634
K2635 K2636 E2637 A2638 D2639 A2640 F2641 A2642 E2643 V2644 V2645 G2646 R2647 E2648 K2649 D2650 K2651 V2652 E2653 K2654 E2655 N2656 S2657 K2658 A2659 T2660 I2661 E2662 A2663 D2664 K2665 C2666 G2667 L2668 I2669 K2670 Q2671 N2672 V2673 E2674 A2675 Q2676 K2677 S2678 S2679 T2680 Q2681 Q2682 D2683 L2684 D2685 A2686 A2687 Q2688 P2689 L2690 V2691 E2692 Q2693 A2694
K2695 S2696 A2697 L2698 N2699 S2700 I2701 S2702 K2703 K2704 D2705 F2706 Q2707 Q2708 A2709 K2710 S2711 F2712 A2713 S2714 P2715 P2716 A2717 G2718 V2719 P2720 E2721 V2722 F2723 A2724 A2725 T2726 I2727 Y2728 L2729 L2730 A2731 G2732 Y2733 F2734 N2735 GLU ALA ILE GLU ILE ASP LYS ASN LYS LYS PRO LYS ASP VAL S2750 W2751 K2752 S2753 S2754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S2815 W2816 V2817 V2818 N2819 I2820 V2821 K2822 Y2823 Y2824 D2825 V2826 I2827 Q2828 D2829 V2830 E2831 P2832 K2833 R2834 K2835 A2836 L2837 K2838 E2839 A2840 T2841 E2842 Q2843 L2844 E2845 E2846 A2847 T2848 V2849 K2850 L2851 N2852 E2853 V2854 E2855 E2856 V2857 V2858 R2859 K2860 L2861 N2862 E2863 E2864 L2865 N2866 K2867 L2868 K2869 A2870 E2871 N2872 D2873 K2874
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V2935 S2936 Y2937 P2940 K2943 N2947 I2948 M2949 I2950 N2951 Q2952 N2953 F2954 M2955 K2956 F2957 M2958 K2959 GLU HIS THR ILE PRO MET S2966 P2967 D2968 P2969 N2970 P2971 I2972 K2973 I2974 L2975 T2976 D2977 E2978 S2979 T2980 I2981 A2982 L2983 W2984 N2985 K2986 Q2987 K2988 L2989 P2990 S2991 D2992 S2993 V2994 S2995 I2996 E2997 N2998
G2999 T3000 I3001 L3002 T3003 N3004 L3010 M3011 I3012 D3013 P3014 Q3015 L3016 Q3017 T3020 W3021 I3022 R3023 E3024 K3025 E3026 K3027 A3028 N3029 N3030 K3039 N3040 I3041 N3042 R3043 D3044 L3045 E3046 L3047 S3048 I3049 E3050 N3051 G3052 M3060 N3061 E3062 R3063 I3064 I3067 I3077 K3078 R3079 G3080 K3081 N3082 K3083 I3084 I3085
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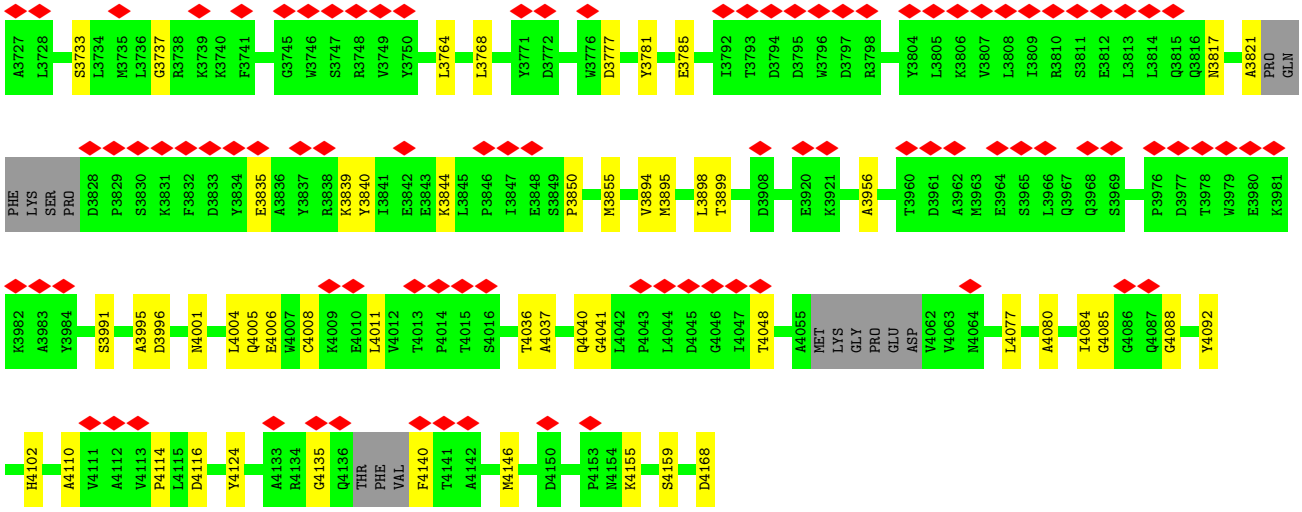
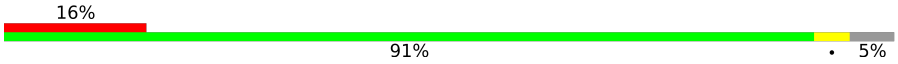
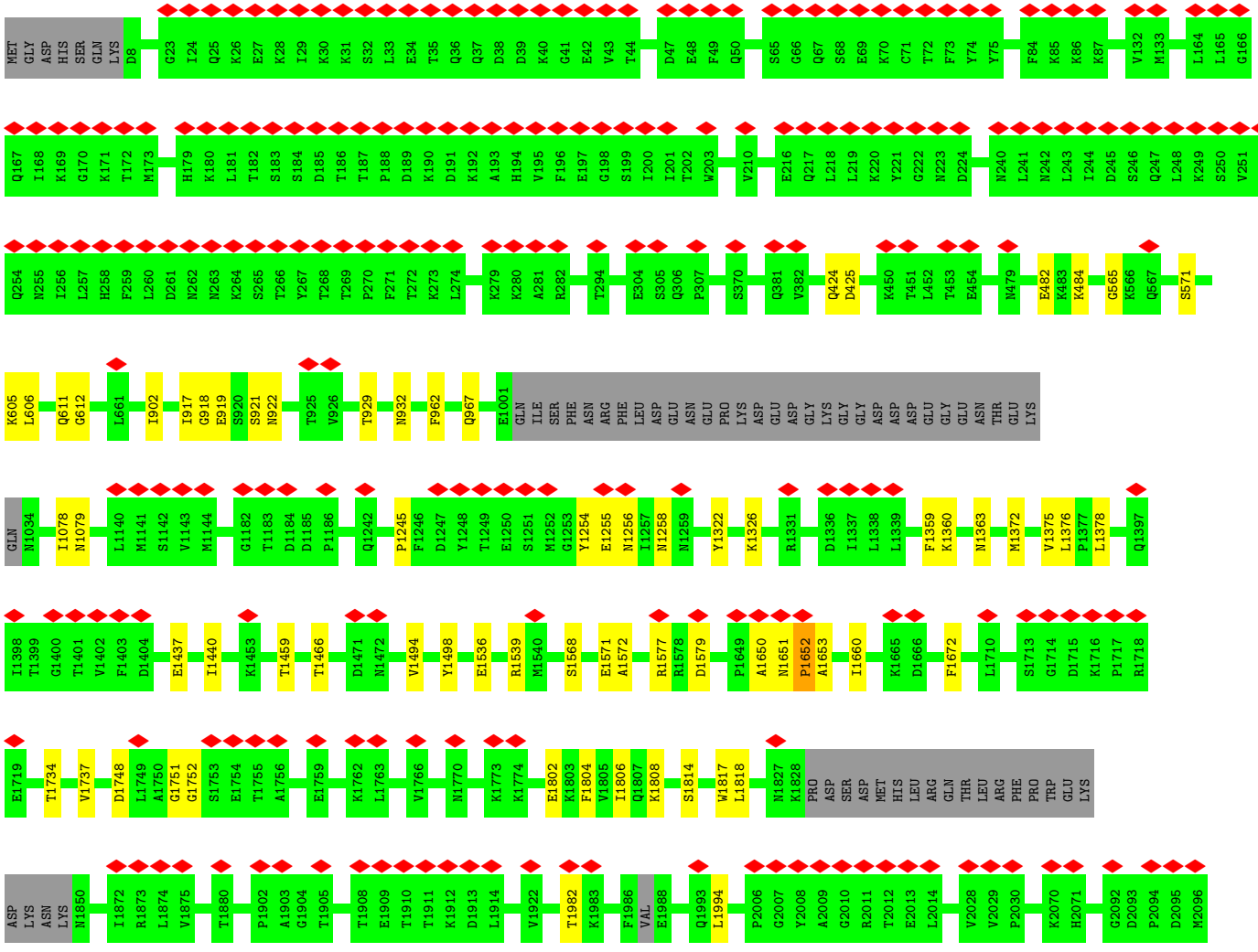
K3164 L3165 K3166 D3167 L3168 E3169 D3170 E3171 L3172 L3173 Y3174 K3175 L3176 A3177 N3178 A3179 K3180 G3181 D3182 I3183 L3184 D3185 D3186 I3187 E3188 L3189 I3190 E3191 N3192 L3193 E3194 Y3195 S3196 K3197 K3198 L3199 S3200 V3201 E3202 I3203 A3204 E3205 K3206 V3207 A3208 A3209 A3210 K3211 I3212 T3213 E3214 A3215 K3216 I3217 N3218 E3219 T3220 S3221 E3222 N3223
Y3224 R3225 S3242 K3243 V3244 H3245 S3246 F3247 Y3248 K3249 Y3250 S3251 L3252 E3253 S3254 F3255 I3256 V3257 V3258 I3259 N3260 R3261 D3264 A3265 I3266 S3267 E3268 N3269 LYS ILE TYR GLY LYS THR THR MET VAL PRO TYR GLY ASP GLU THR TYR ALA SER ASN GLN HIS GLU LYS GLU GLU GLU GLU GLU GLU
GLU HIS GLN GLN ALA GLN GLN GLN GLN ASN GLN GLU GLU GLN GLN LYS ASP GLU GLU ASN LYS GLY PRO VAL GLU GLU GLU GLN PRO GLU GLY GLU ASN LYS GLY PRO VAL GLU GLU GLU GLY ALA GLU GLY GLN ASN GLU GLY PRO VAL GLU GLU GLU ASN ALA GLU GLN
GLU GLY GLU GLY GLU GLU GLU GLY GLU LYS GLN GLN LYS ALA LYS ASP SER ASP GLU PRO MET SER PRO R3383 S3384 L3385 K3386 K3387 R3388 R3405 R3406 G3407 L3408 F3409 K3413 L3426 R3427 S3428 E3429 E3430 L3431 N3432 S3433 D3437 H3438 I3441 G3442 LYS VAL ASP VAL ASN PRO THR PRO
MET PRO D3453 A3454 L3455 K3456 S3457 K3468 A3469 L3470 E3471 T3472 T3473 H3474 Q3475 F3476 Q3477 G3478 F3479 C3480 Q3481 S3482 L3483 E3484 T3485 D3486 V3487 L3488 K3491 K3492 S3495 E3496 E3497 K3498 T3501 A3502 K3506 A3507 F3508 K3509 E3510 L3511 S3512 K3513 F3514 H3515 L3519 L3523 D3538 K3539 P3548
P3549 F3550 N3551 I3552 E3553 E3554 T3555 F3556 Q3557 E3558 T3559 S3560 K3561 T3562 V3563 P3564 F3570 P3571 G3572 V3573 D3574 P3575 A3583 A3584 T3585 F3586 D3587 V3588 S3589 A3590 N3591 N3592 G3593 R3594 Q3602 G3603 C3615 G3619 H3620 W3621 V3627 H3628 L3629 M3630 Q3631 S3632 W3633 L3634 Y3635 L3644 GLU SER VAL
PHE ALA SER PRO K3652 P3665 P3666 N3667 VAL LEU LEU PRO LEU MET GLN I3675 I3676 P3677 E3678 S3679 I3680 L3681 Q3682 G3683 S3684 L3685 K3686 I3687 A3688 N3689 E3690 A3691 R3700 Y3703 N3704 K3705 F3706 D3707 Q3708 E3709 F3710 L3711 D3712 K3713 C3714 D3715 K3716 K3717 P3718 T3719 E3720 F3721 K3722 S3723 C3724 L3725 F3726

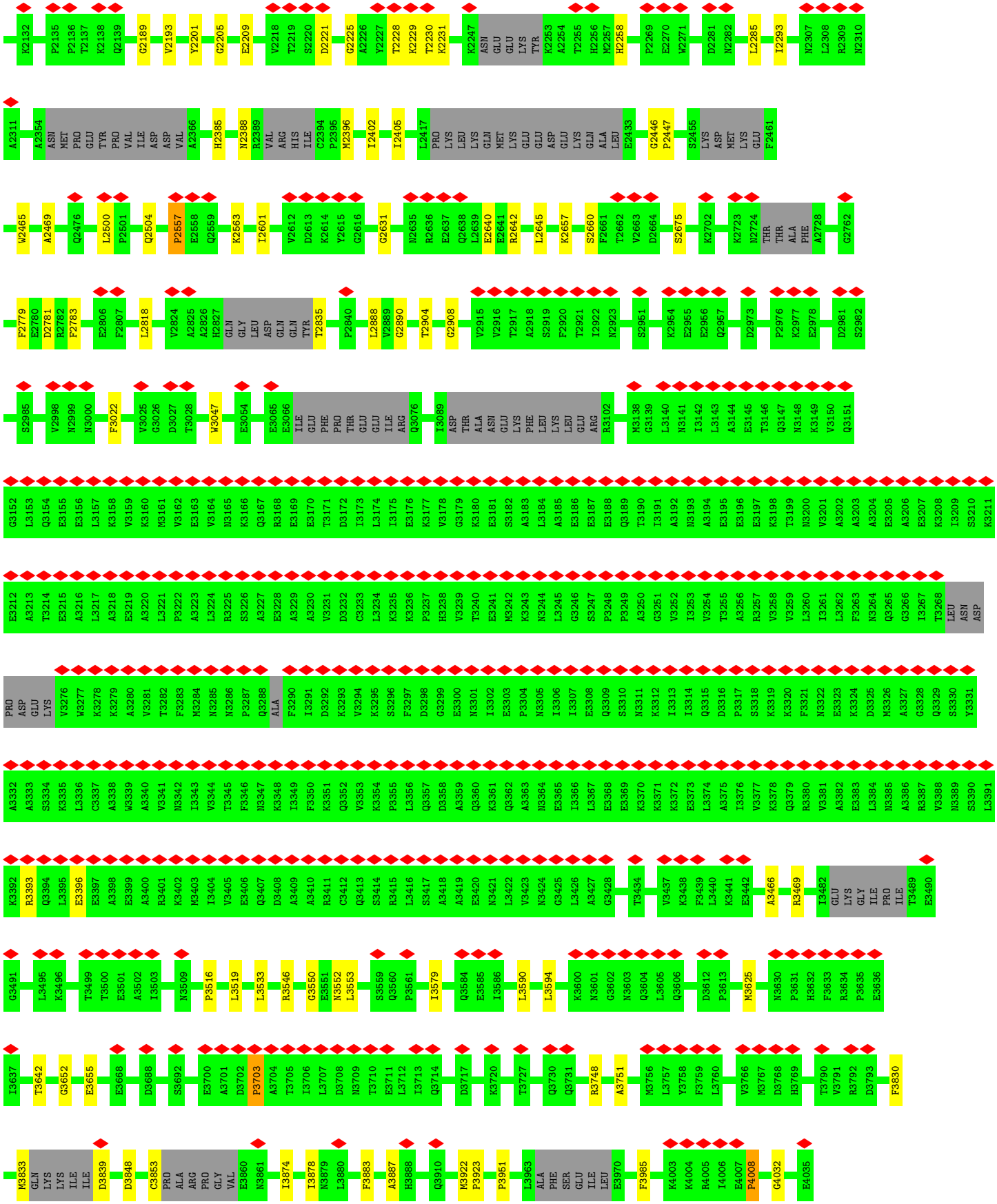


• Molecule 2: Outer arm dynein beta heavy chain

Chain B:



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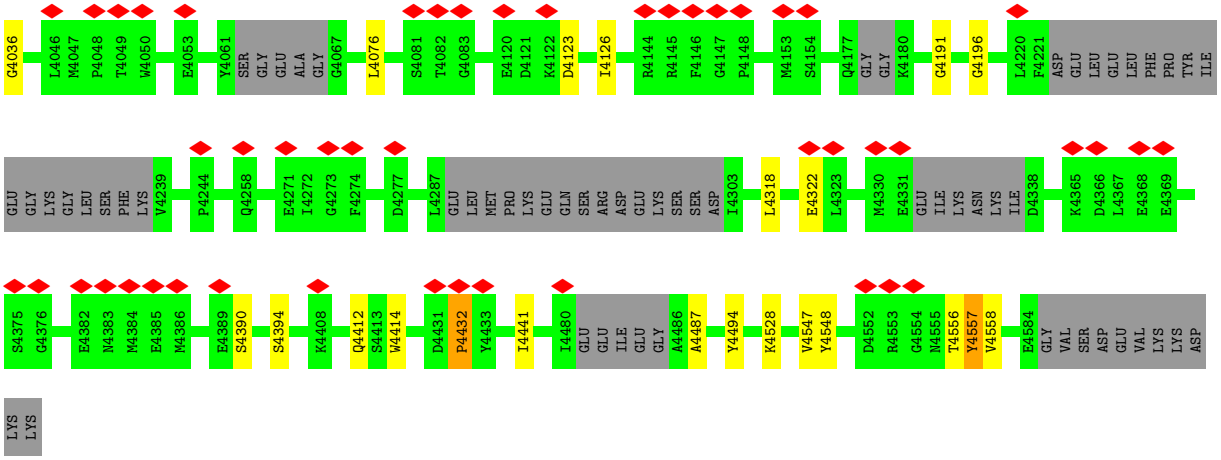
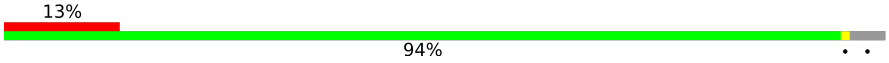
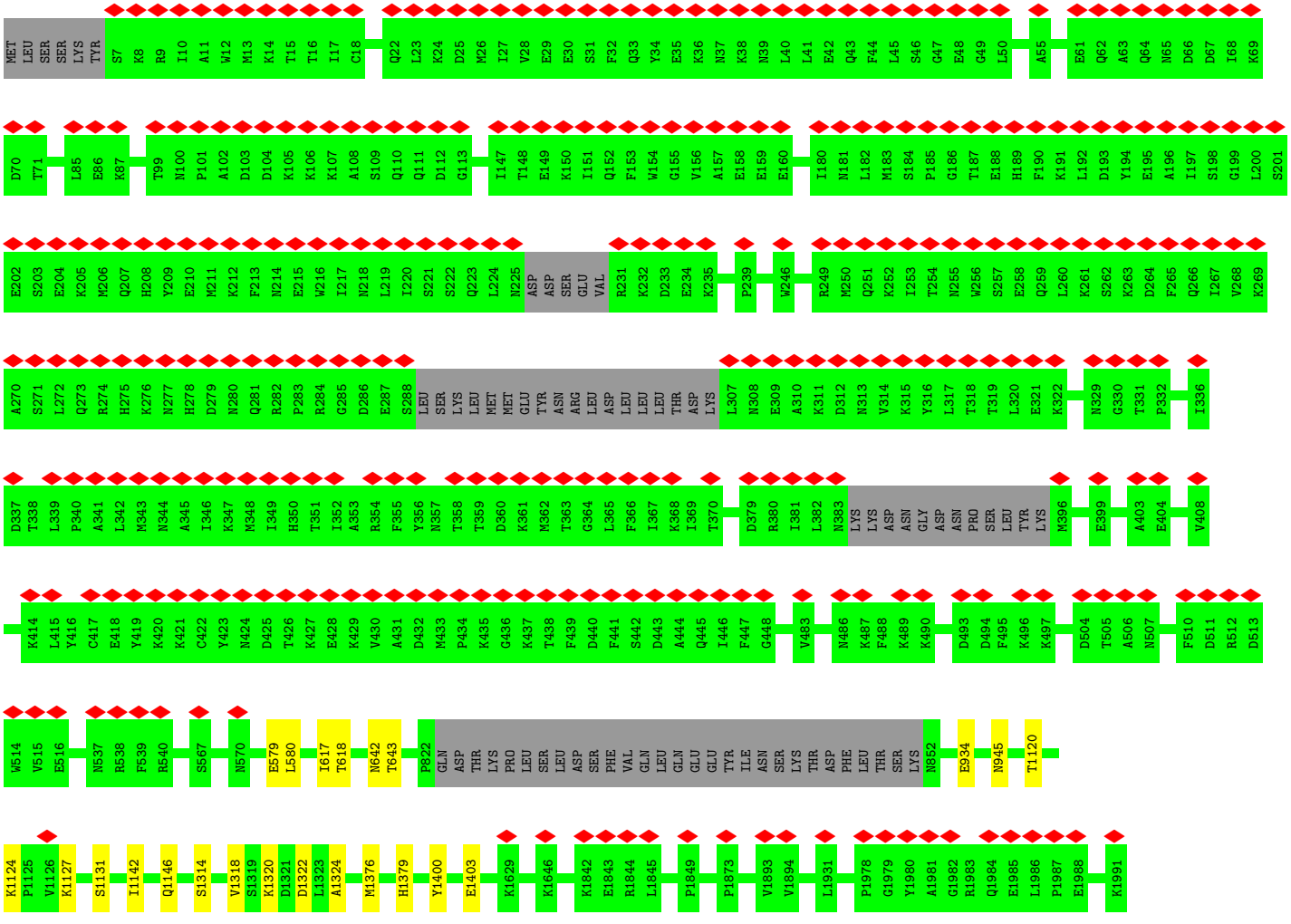
A2311 A2354 ASN MET PRO GLU TYR PRO VAL ILE ASP ASP VAL A2366 H2385 N2388 R2389 VAL ARG HIS ILE C2394 P2395 N2396 I2402 I2405 L2417 PRO LYS LEU LYS GLN MET LYS GLU GLU ASP GLU LYS GLN ALA LEU E2433 G2446 P2447 S2455 LYS ASP MET LYS GLU F2461
W2465 A2469 Q2476 L2500 P2501 Q2504 P2557 E2558 Q2559 K2563 I2601 V2612 D2613 K2614 Y2615 G2616 G2631 N2635 R2636 E2637 Q2638 L2639 E2640 E2641 R2642 L2645 K2657 S2660 F2661 T2662 V2663 D2664 S2675 K2702 K2723 N2724 THR THR ALA PHE A2728 G2762
F2779 E2780 D2781 R2782 F2783 E2806 F2807 L2818 V2824 A2825 A2826 H2827 GLN GLY LEU ASP GLN GLN TYR T2835 P2840 L2888 V2889 G2890 T2904 G2908 V2915 V2916 T2917 A2918 S2919 F2920 T2921 I2922 N2923 S2951 K2954 E2955 E2956 Q2957 D2973 P2976 K2977 E2978 D2981 S2982
S2985 V2998 N2999 N3000 F3022 V3025 G3026 D3027 T3028 W3047 E3054 E3065 E3066 ILE GLU PHE PRO THR GLU GLU ILE ARG Q3076 I3089 ASP THR ALA ASN GLU LYS PHE LEU LYS LEU GLU ARG R3102 M3138 G3139 L3140 N3141 I3142 L3143 A3144 E3145 T3146 Q3147 N3148 K3149 V3150 Q3151
G3152 L3153 Q3154 E3155 E3156 L3157 K3158 V3159 K3160 M3161 V3162 E3163 V3164 N3165 K3166 Q3167 R3168 E3169 E3170 T3171 D3172 I3173 L3174 I3175 E3176 K3177 V3178 G3179 K3180 E3181 S3182 A3183 L3184 A3185 E3186 E3187 E3188 Q3189 T3190 I3191 A3192 N3193 A3194 E3195 E3196 E3197 K3198 T3199 N3200 V3201 A3202 A3203 A3204 E3205 A3206 E3207 K3208 I3209 S3210 K3211
E3212 A3213 T3214 E3215 A3216 L3217 A3218 E3219 A3220 L3221 P3222 A3223 L3224 R3225 S3226 A3227 E3228 A3229 A3230 V3231 D3232 C3233 L3234 K3235 K3236 P3237 H3238 V3239 T3240 E3241 M3242 K3243 N3244 L3245 G3246 S3247 P3248 P3249 A3250 G3251 V3252 I3253 V3254 T3255 A3256 R3257 V3258 K3259 L3260 I3261 L3262 F3263 N3264 Q3265 G3266 I3267 T3268 LEU ASN ASP
PRO ASP GLU LYS V3276 W3277 K3278 K3279 A3280 V3281 T3282 F3283 M3284 N3285 N3286 P3287 Q3288 ALA F3290 I3291 D3292 K3293 V3294 K3295 S3296 F3297 D3298 G3299 E3300 N3301 I3302 E3303 P3304 N3305 I3306 I3307 E3308 Q3309 S3310 N3311 K3312 I3313 I3314 Q3315 D3316 P3317 S3318 K3319 K3320 F3321 N3322 E3323 K3324 D3325 M3326 A3327 G3328 Q3329 S3330 Y3331
A3332 A3333 S3334 K3335 L3336 C3337 A3338 W3339 A3340 V3341 N3342 I3343 V3344 T3345 F3346 N3347 K3348 I3349 F3350 K3351 Q3352 V3353 K3354 P3355 L3356 Q3357 D3358 A3359 Q3360 K3361 Q3362 A3363 N3364 E3365 I3366 L3367 E3368 E3369 K3370 K3371 K3372 E3373 L3374 A3375 I3376 V3377 K3378 Q3379 R3380 Y3381 A3382 E3383 L3384 N3385 A3386 R3387 Y3388 N3389 S3390 L3391
K3392 R3393 Q3394 L3395 E3396 E3397 A3398 E3399 A3400 R3401 K3402 M3403 I3404 V3405 E3406 Q3407 D3408 A3409 A3410 R3411 C3412 Q3413 S3414 R3415 L3416 S3417 A3418 A3419 E3420 N3421 L4422 V3423 N3424 G3425 L3426 A3427 G3428 T3434 V3437 K3438 F3439 L3440 K3441 E3442 A3466 R3469 I3482 GLU LYS GLY ILE PRO ILE T3489 E3490
G3491 L3495 K3496 T3499 T3500 E3501 A3502 I3503 N3509 P3516 L3519 L3533 R3546 G3550 E3551 N3552 L3553 S3559 Q3560 P3561 I3579 Q3584 E3585 I3586 L3590 L3594 K3600 N3601 G3602 N3603 Q3604 L3605 Q3606 D3612 P3613 M3625 N3630 P3631 H3632 F3633 R3634 P3635 E3636
I3637 T3642 G3652 E3655 E3668 D3688 S3692 E3700 A3701 D3702 P3703 A3704 T3705 I3706 L3707 D3708 N3709 T3710 E3711 L3712 I3713 Q3714 D3717 K3720 T3727 Q3730 Q3731 R3748 A3751 M3756 L3757 Y3758 F3759 L3760 V3766 M3767 D3768 H3769 T3790 V3791 R3792 D3793 F3830
M3833 GLN LYS LYS ILE ILE D3839 D3848 C3853 PRO ALA ARG PRO GLY VAL E3860 N3861 I3874 I3878 N3879 L3880 F3883 A3887 H3888 Q3910 M3922 P3923 P3951 L3963 ALA PHE SER GLU ILE LEU E3970 F3985 K4003 K4004 R4005 I4006 E4007 P4008 G4032 E4035

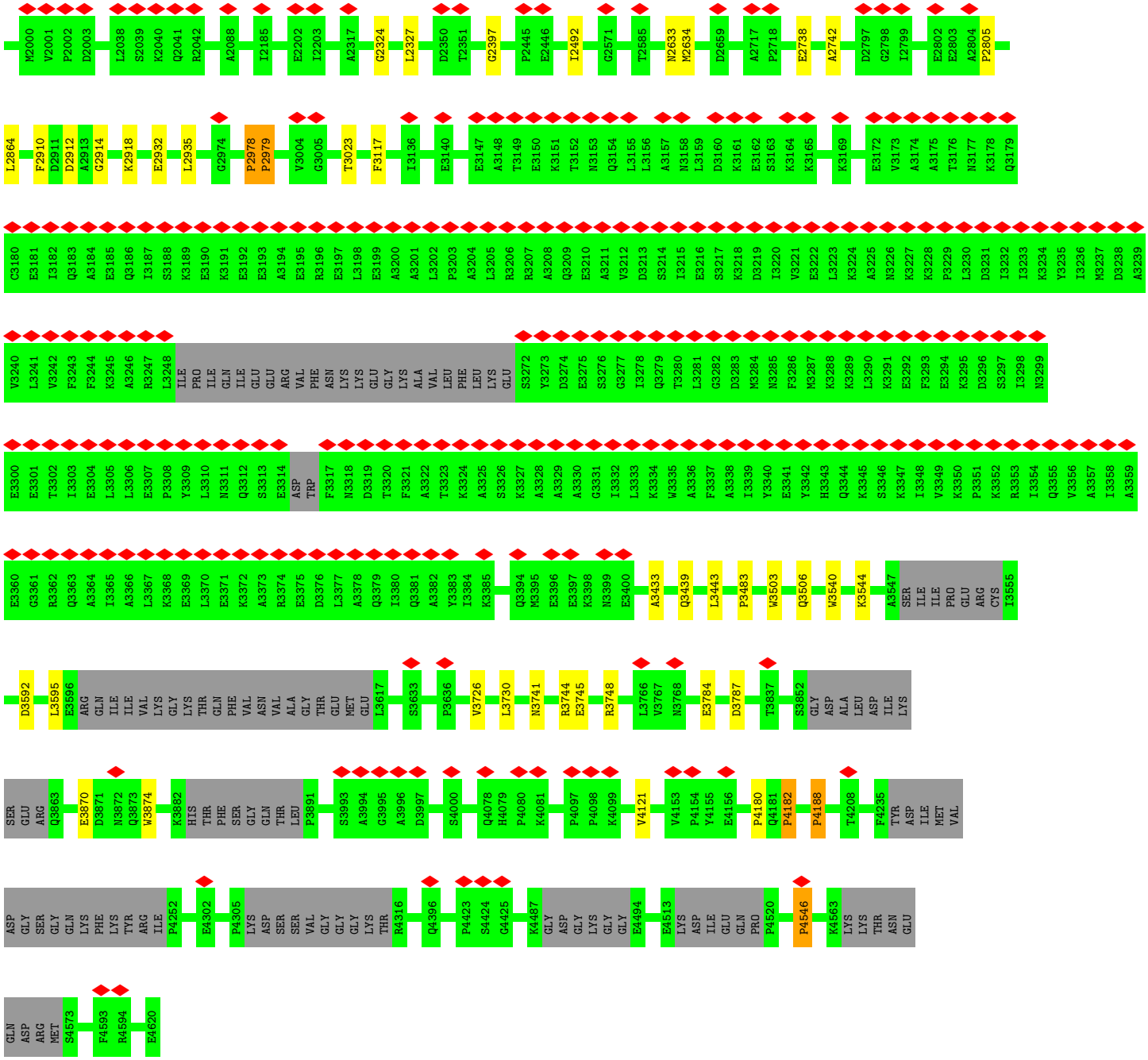


• Molecule 3: Dynein heavy chain, outer arm protein

Chain C:

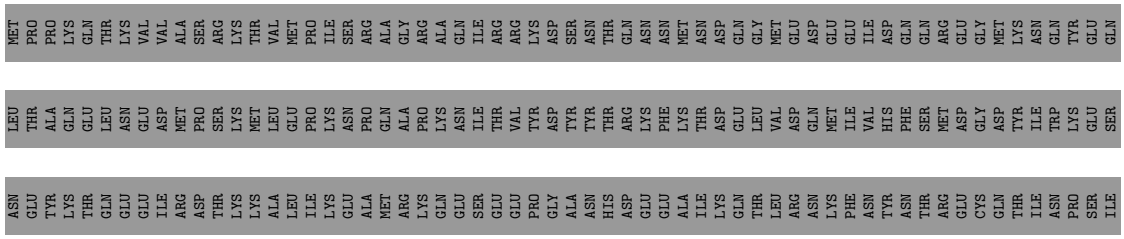


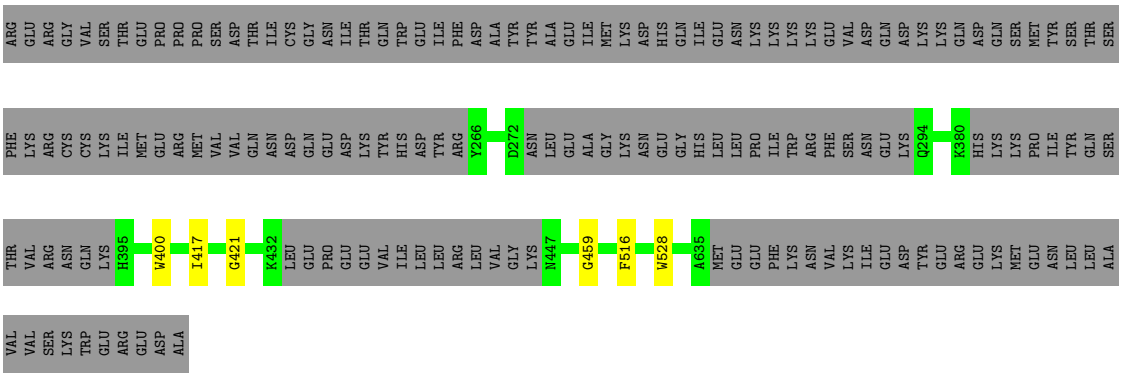




• Molecule 4: Dynein intermediate chain 2

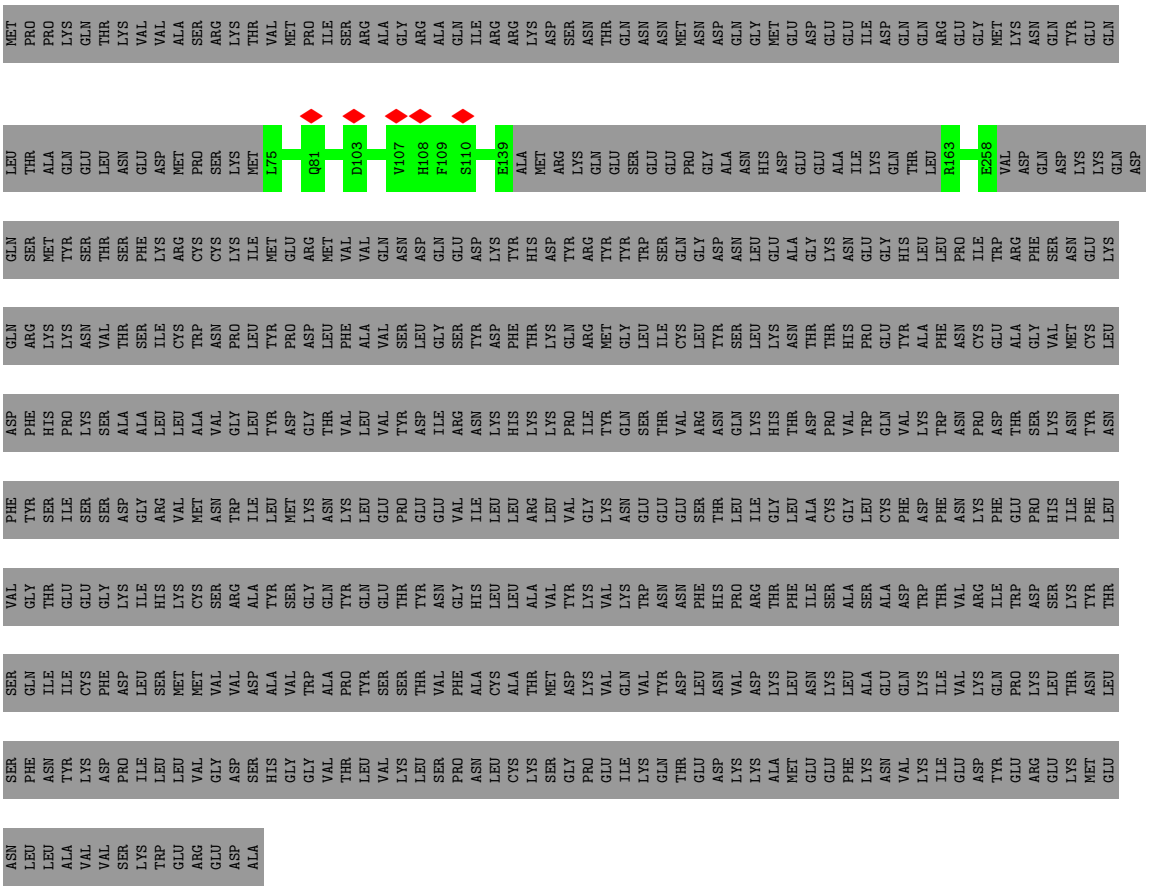
Chain D: 47% • 52%





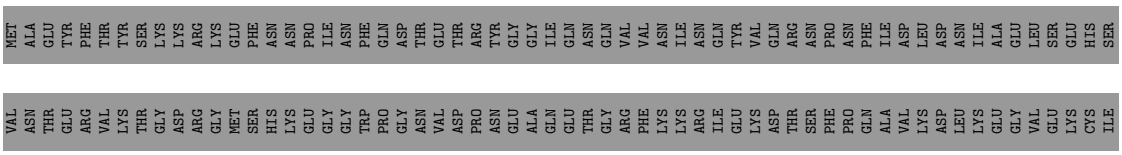
• Molecule 4: Dynein intermediate chain 2

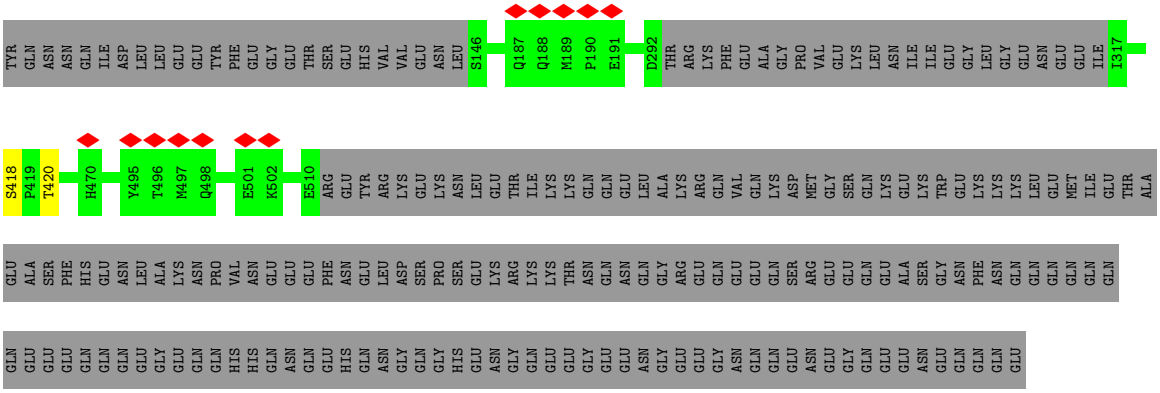
Chain d:



• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

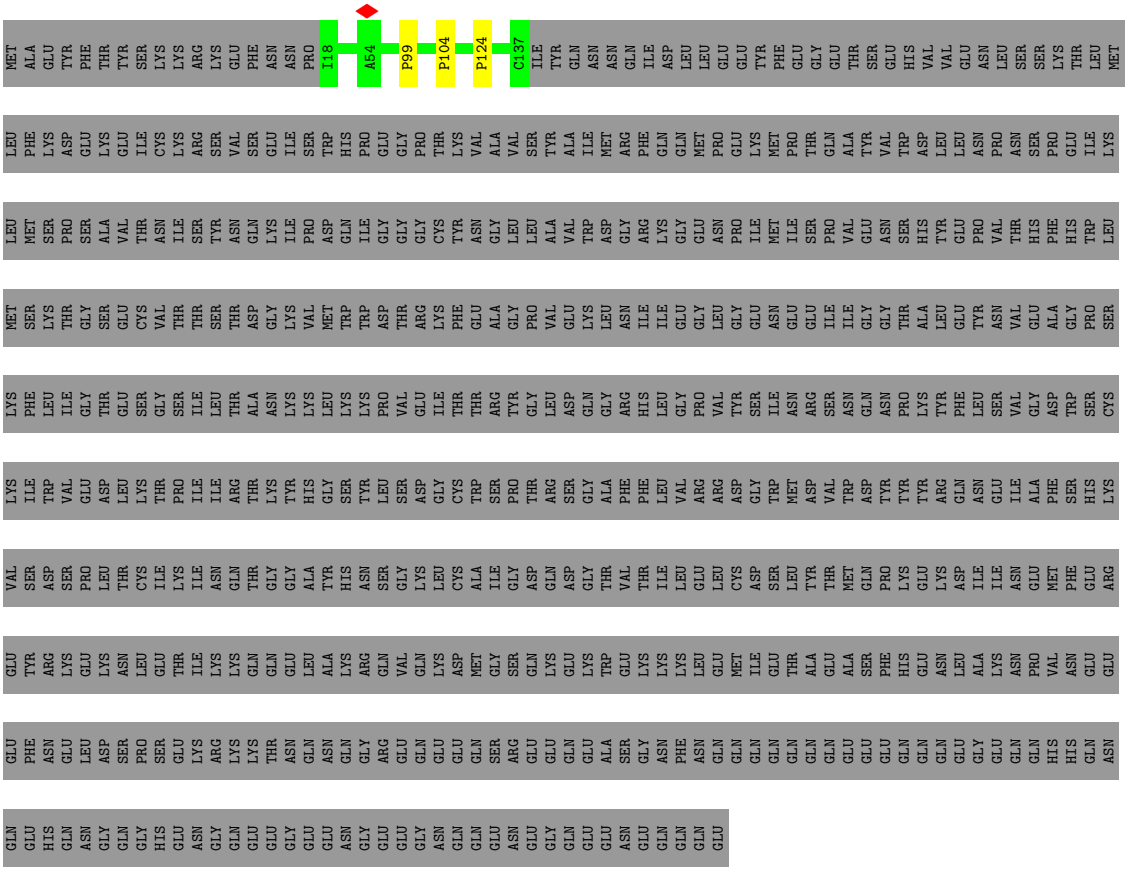
Chain E:





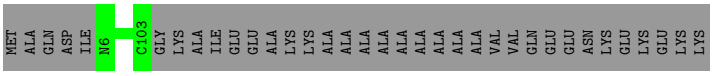
• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

Chain e:



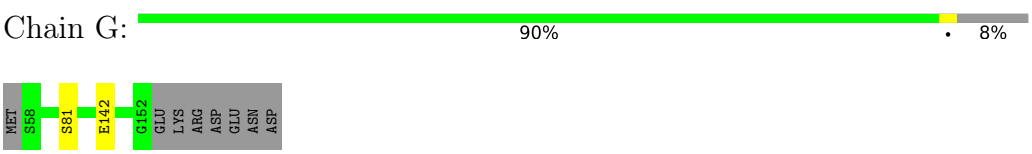
• Molecule 6: Dynein light chain roadblock-type 2 protein

Chain F:



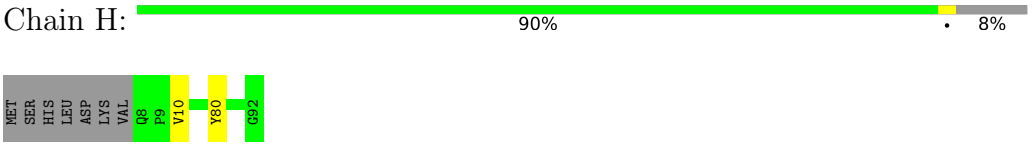
• Molecule 7: Dynein light chain roadblock-type 2 protein

Chain G:



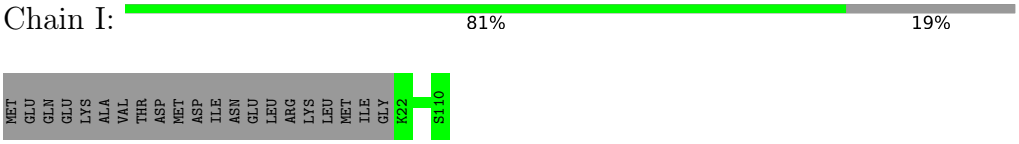
• Molecule 8: Dynein light chain

Chain H:



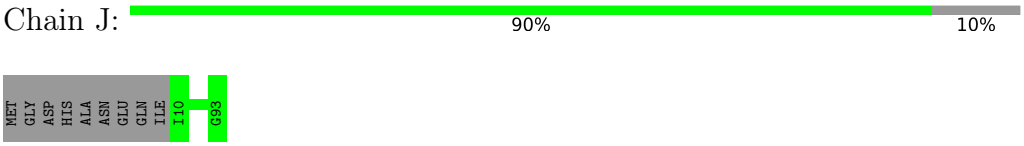
• Molecule 9: Dynein light chain

Chain I:



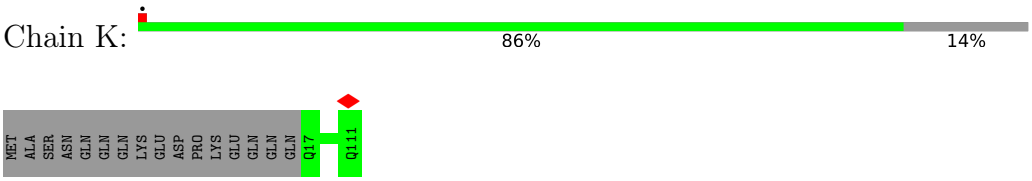
• Molecule 10: Dynein light chain

Chain J:



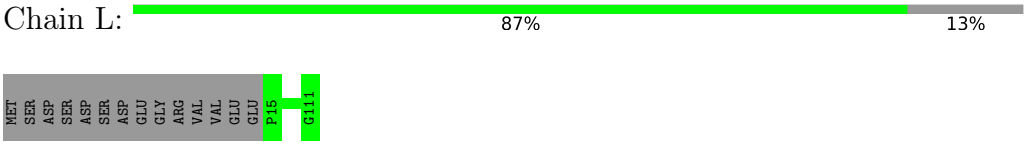
• Molecule 11: Dynein light chain

Chain K:



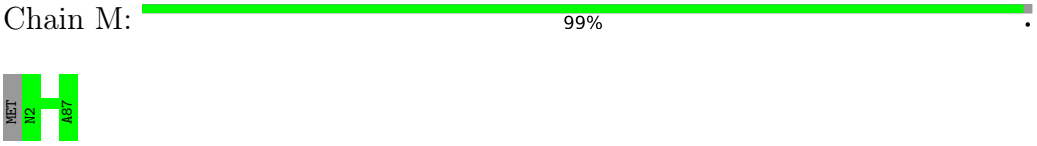
• Molecule 12: Dynein light chain

Chain L:



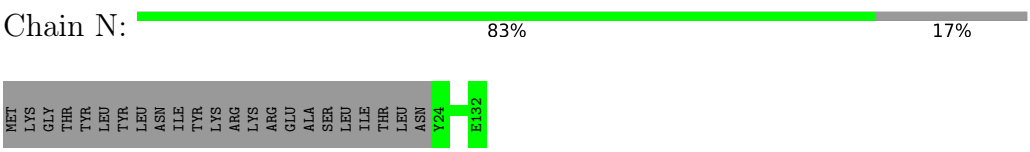
• Molecule 13: Dynein light chain

Chain M:



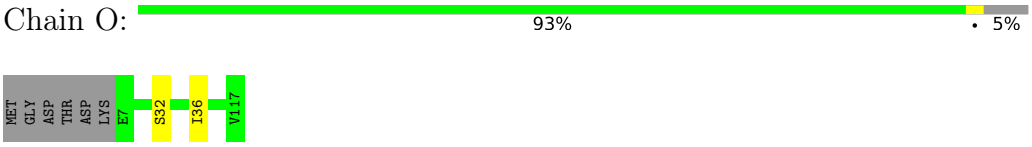
• Molecule 14: Dynein light chain 2A

Chain N:



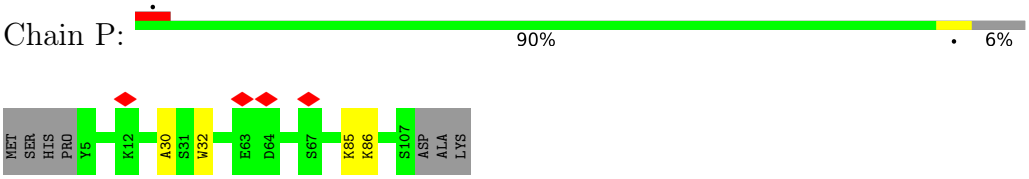
• Molecule 15: Dynein light chain tctex-type 1 protein

Chain O:



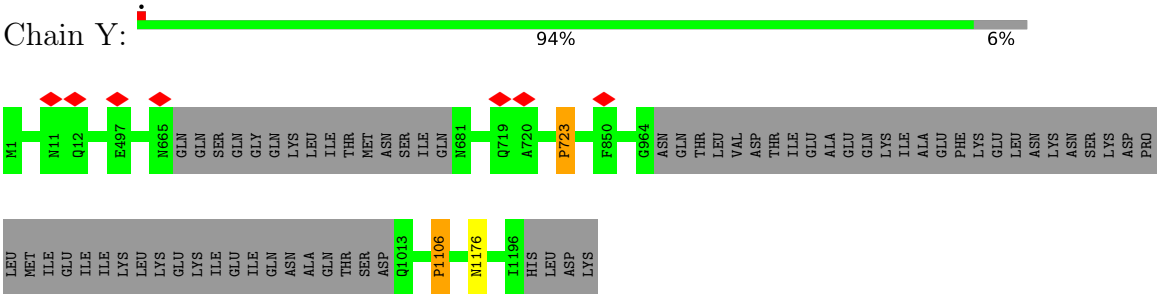
• Molecule 16: Thioredoxin

Chain P:



• Molecule 17: Shulin

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0008	Depositor
Map size (Å)	499.5, 499.5, 499.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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, GTP, 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	0.34	0/18743	0.69	1/26057 (0.0%)
2	B	0.39	0/19561	0.65	6/27233 (0.0%)
3	C	0.31	0/19162	0.56	8/26702 (0.0%)
4	D	0.36	0/1584	0.84	0/2201
4	d	0.31	0/634	0.61	0/881
5	E	0.36	0/1676	0.78	0/2327
5	e	0.44	0/498	0.76	3/687 (0.4%)
6	F	0.46	0/485	0.86	0/675
7	G	0.37	0/469	0.73	0/652
8	H	0.42	0/419	0.84	0/582
9	I	0.40	0/438	0.86	0/608
10	J	0.31	0/415	0.57	0/577
11	K	0.28	0/469	0.56	0/652
12	L	0.28	0/478	0.57	0/664
13	M	0.29	0/425	0.55	0/591
14	N	0.28	0/536	0.57	0/744
15	O	0.24	0/549	0.50	0/764
16	P	0.78	0/512	0.92	0/714
17	Y	0.29	1/5608 (0.0%)	0.55	2/7814 (0.0%)
All	All	0.35	1/72661 (0.0%)	0.64	20/101125 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	1176	ASN	C-N	6.01	1.47	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4432	PRO	N-CA-CB	8.75	113.80	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4182	PRO	N-CA-CB	6.65	111.28	103.30
3	C	4188	PRO	N-CA-CB	6.65	111.28	103.30
17	Y	1106	PRO	N-CA-CB	6.55	111.16	103.30
3	C	2978	PRO	N-CA-CB	6.33	110.89	103.30
3	C	4180	PRO	N-CA-CB	6.29	110.85	103.30
17	Y	723	PRO	N-CA-CB	6.25	110.81	103.30
2	B	4008	PRO	N-CA-CB	6.21	110.76	103.30
5	e	99	PRO	N-CA-CB	6.21	110.76	103.30
3	C	4546	PRO	N-CA-CB	6.21	110.75	103.30
2	B	3703	PRO	N-CA-CB	6.20	110.74	103.30
3	C	2979	PRO	N-CA-CB	6.20	110.73	103.30
2	B	1652	PRO	N-CA-CB	5.83	110.29	103.30
5	e	124	PRO	N-CA-CB	5.76	110.21	103.30
1	A	1185	PRO	N-CA-CB	5.71	110.16	103.30
3	C	2805	PRO	N-CA-CB	5.63	110.06	103.30
3	C	3483	PRO	N-CA-CB	5.61	110.03	103.30
5	e	104	PRO	N-CA-CB	5.38	109.75	103.30
2	B	3951	PRO	N-CA-CB	5.29	109.65	103.30
2	B	2557	PRO	N-CA-CB	5.08	109.40	103.30

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	18787	0	8282	131	0
2	B	20008	0	8566	89	0
3	C	19737	0	8300	29	0
4	D	1588	0	693	3	0
4	d	637	0	261	0	0
5	E	1678	0	724	1	0
5	e	501	0	215	0	0
6	F	486	0	218	0	0
7	G	470	0	203	1	0
8	H	420	0	185	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	439	0	202	0	0
10	J	416	0	184	0	0
11	K	470	0	215	0	0
12	L	479	0	209	0	0
13	M	426	0	189	0	0
14	N	537	0	231	0	0
15	O	550	0	247	1	0
16	P	513	0	213	2	0
17	Y	5611	0	2410	0	0
18	C	81	0	36	0	0
19	C	31	0	12	0	0
20	Y	32	0	12	0	0
All	All	73897	0	31807	258	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 2.

All (258) 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)
2:B:917:ILE:O	2:B:921:SER:CB	2.17	0.92
3:C:617:ILE:C	3:C:618:THR:CA	2.46	0.84
2:B:4318:LEU:O	2:B:4322:GLU:N	2.12	0.83
3:C:642:ASN:CA	3:C:643:THR:N	2.43	0.81
2:B:2229:LYS:O	2:B:2230:THR:N	2.13	0.81
2:B:4032:GLY:O	2:B:4036:GLY:N	2.15	0.80
2:B:424:GLN:CA	2:B:425:ASP:N	2.45	0.80
1:A:4124:TYR:N	1:A:4146:MET:O	2.15	0.79
3:C:1314:SER:O	3:C:1318:VAL:N	2.14	0.79
1:A:2611:LYS:O	1:A:2613:THR:N	2.15	0.78
2:B:3830:PHE:O	2:B:3839:ASP:N	2.16	0.78
1:A:4048:THR:O	1:A:4110:ALA:N	2.16	0.78
1:A:2631:ALA:O	1:A:2635:LYS:N	2.16	0.77
2:B:3552:ASN:O	2:B:3553:LEU:N	2.18	0.76
2:B:3546:ARG:O	2:B:3550:GLY:N	2.19	0.76
3:C:579:GLU:CA	3:C:580:LEU:N	2.49	0.75
2:B:2201:TYR:O	2:B:2205:GLY:N	2.19	0.75
2:B:2228:THR:O	2:B:2231:LYS:N	2.21	0.74
1:A:2496:MET:O	1:A:2500:ALA:N	2.20	0.74
1:A:2297:GLY:N	1:A:2375:PHE:O	2.21	0.73
1:A:4004:LEU:O	1:A:4008:CYS:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1954:SER:O	1:A:1957:SER:N	2.21	0.73
2:B:1568:SER:O	2:B:1572:ALA:N	2.21	0.73
2:B:2396:MET:N	2:B:2447:PRO:O	2.22	0.72
1:A:3:GLN:N	1:A:305:ASN:O	2.23	0.72
2:B:1650:ALA:N	2:B:1653:ALA:O	2.22	0.72
1:A:2627:LYS:O	1:A:2631:ALA:N	2.23	0.71
1:A:3895:MET:O	1:A:3899:THR:N	2.24	0.71
1:A:1400:ALA:N	1:A:1524:ARG:O	2.23	0.71
1:A:426:PRO:O	1:A:486:ASP:N	2.24	0.70
2:B:2209:GLU:N	2:B:2258:HIS:O	2.25	0.70
2:B:2221:ASP:O	2:B:2225:GLY:N	2.23	0.69
1:A:3221:SER:O	1:A:3225:ARG:N	2.25	0.69
2:B:3848:ASP:O	2:B:3853:CYS:N	2.24	0.69
1:A:2044:TYR:O	1:A:2086:GLN:N	2.26	0.68
1:A:2893:LEU:O	1:A:2898:ARG:N	2.26	0.68
2:B:3833:MET:O	2:B:3839:ASP:N	2.25	0.68
1:A:886:ASN:O	1:A:890:GLY:N	2.27	0.68
1:A:1484:GLU:O	1:A:1495:LEU:N	2.27	0.68
1:A:3519:LEU:O	1:A:3523:LEU:N	2.26	0.68
1:A:3384:SER:O	1:A:3388:ARG:N	2.26	0.68
1:A:898:TRP:O	1:A:901:PHE:N	2.27	0.67
1:A:3781:TYR:O	1:A:3785:GLU:N	2.26	0.67
2:B:4441:ILE:N	2:B:4494:TYR:O	2.27	0.67
1:A:1931:LYS:O	1:A:1939:LYS:N	2.28	0.67
1:A:3470:LEU:O	1:A:3473:ILE:N	2.28	0.67
2:B:606:LEU:HA	2:B:612:GLY:HA2	1.77	0.67
2:B:4123:ASP:O	2:B:4126:ILE:N	2.26	0.67
1:A:3835:GLU:O	1:A:3839:LYS:N	2.27	0.67
3:C:3741:ASN:O	3:C:3745:GLU:N	2.27	0.67
1:A:3594:ARG:O	1:A:3621:TRP:N	2.26	0.67
2:B:918:GLY:O	2:B:921:SER:C	2.34	0.67
1:A:679:LEU:O	1:A:683:ARG:N	2.26	0.66
1:A:2495:ASP:O	1:A:2496:MET:N	2.29	0.65
3:C:1127:LYS:O	3:C:1131:SER:N	2.29	0.65
1:A:2374:SER:O	1:A:2378:GLY:N	2.29	0.65
2:B:2285:LEU:N	2:B:2293:ILE:O	2.30	0.65
2:B:1804:PHE:O	2:B:1808:LYS:N	2.28	0.65
2:B:2465:TRP:O	2:B:2469:ALA:N	2.30	0.65
1:A:1592:ARG:O	1:A:1593:SER:N	2.29	0.65
3:C:2492:ILE:O	3:C:2634:MET:N	2.29	0.65
2:B:2890:GLY:N	2:B:3022:PHE:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1398:GLY:O	1:A:1524:ARG:N	2.32	0.63
2:B:2189:GLY:O	2:B:2193:VAL:N	2.31	0.63
1:A:2928:VAL:O	1:A:2932:SER:N	2.29	0.63
1:A:1616:ALA:O	1:A:1620:LEU:N	2.32	0.62
3:C:3870:GLU:O	3:C:3874:TRP:N	2.31	0.62
3:C:2910:PHE:O	3:C:2914:GLY:N	2.31	0.62
2:B:1748:ASP:O	2:B:1752:GLY:N	2.31	0.62
1:A:3406:ARG:O	1:A:3688:ALA:N	2.33	0.62
1:A:2175:SER:O	1:A:2177:ILE:N	2.32	0.62
2:B:605:LYS:CB	2:B:611:GLN:CB	2.79	0.61
2:B:3393:ARG:O	2:B:3396:GLU:N	2.34	0.61
2:B:3516:PRO:O	2:B:3519:LEU:N	2.32	0.61
1:A:834:VAL:O	1:A:837:LEU:N	2.34	0.61
1:A:3487:VAL:O	1:A:3491:LYS:N	2.33	0.61
1:A:1915:ALA:O	1:A:1919:SER:N	2.33	0.61
2:B:918:GLY:O	2:B:922:ASN:N	2.34	0.60
7:G:81:SER:N	7:G:142:GLU:O	2.34	0.60
2:B:2904:THR:O	2:B:2908:GLY:N	2.34	0.60
2:B:3590:LEU:O	2:B:3594:LEU:N	2.31	0.60
1:A:1348:TYR:O	1:A:1355:LYS:N	2.34	0.60
1:A:3206:LYS:O	1:A:3210:ALA:N	2.32	0.60
2:B:1802:GLU:O	2:B:1806:ILE:N	2.30	0.60
1:A:3135:LEU:O	1:A:3139:VAL:N	2.35	0.59
2:B:1660:ILE:O	2:B:1672:PHE:N	2.35	0.59
1:A:1701:GLN:O	1:A:1705:ASN:N	2.35	0.59
2:B:902:ILE:O	2:B:1079:ASN:N	2.36	0.59
1:A:3214:GLU:O	1:A:3218:ASN:N	2.35	0.59
1:A:2628:GLN:O	1:A:2632:GLU:N	2.34	0.58
2:B:2657:LYS:O	2:B:2660:SER:N	2.36	0.58
1:A:3023:ARG:O	1:A:3027:LYS:N	2.37	0.58
2:B:1734:THR:O	2:B:1737:VAL:N	2.37	0.58
3:C:2912:ASP:O	3:C:2918:LYS:N	2.37	0.58
5:E:418:SER:O	5:E:420:THR:N	2.37	0.58
2:B:2781:ASP:O	2:B:3047:TRP:N	2.37	0.57
1:A:3615:CYS:O	1:A:3619:GLY:N	2.37	0.57
2:B:606:LEU:HA	2:B:612:GLY:CA	2.34	0.57
2:B:4547:VAL:O	2:B:4558:VAL:N	2.36	0.57
1:A:1400:ALA:O	1:A:1526:ILE:N	2.38	0.57
2:B:4191:GLY:O	2:B:4196:GLY:N	2.38	0.57
1:A:4135:GLY:O	1:A:4140:PHE:N	2.38	0.57
4:D:400:TRP:N	4:D:417:ILE:O	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:ASP:O	1:A:834:VAL:N	2.38	0.56
2:B:2818:LEU:N	2:B:2835:THR:O	2.38	0.56
1:A:674:ASN:HA	1:A:811:PHE:HA	1.87	0.56
1:A:1689:GLY:O	1:A:1693:THR:N	2.38	0.56
3:C:3117:PHE:CB	3:C:3433:ALA:HB2	2.36	0.56
1:A:2417:PHE:N	1:A:2487:ALA:O	2.38	0.56
2:B:1255:GLU:O	2:B:1256:ASN:C	2.43	0.55
3:C:1120:THR:O	3:C:1124:LYS:N	2.40	0.55
2:B:3579:ILE:O	2:B:3625:MET:N	2.39	0.55
1:A:3492:LYS:O	1:A:3496:GLU:N	2.39	0.55
1:A:1727:ASN:O	1:A:1731:LYS:N	2.39	0.55
1:A:4080:ALA:HB1	1:A:4092:TYR:O	2.07	0.55
3:C:1376:MET:O	3:C:1379:HIS:N	2.40	0.54
1:A:2102:LEU:O	1:A:2106:GLY:N	2.40	0.54
1:A:2499:ARG:O	1:A:2503:PHE:N	2.40	0.54
2:B:1437:GLU:O	2:B:1440:ILE:N	2.41	0.54
2:B:1254:TYR:O	2:B:1258:ASN:CB	2.55	0.54
1:A:3733:SER:O	1:A:3737:GLY:N	2.41	0.54
1:A:3438:HIS:O	1:A:3442:GLY:N	2.41	0.53
1:A:2176:THR:O	1:A:2177:ILE:N	2.40	0.53
1:A:3048:SER:O	1:A:3052:GLY:N	2.41	0.53
1:A:4006:GLU:O	1:A:4011:LEU:N	2.41	0.53
1:A:3894:VAL:O	1:A:3898:LEU:N	2.39	0.53
1:A:219:GLY:O	1:A:226:TYR:N	2.41	0.53
2:B:3874:ILE:O	2:B:3878:ILE:N	2.40	0.53
3:C:2324:GLY:O	3:C:2327:LEU:N	2.41	0.53
1:A:3817:ASN:O	1:A:3821:ALA:N	2.41	0.52
2:B:1982:THR:O	2:B:1994:LEU:N	2.42	0.52
1:A:1327:ARG:O	1:A:1330:ASN:N	2.42	0.52
2:B:4390:SER:O	2:B:4394:SER:N	2.43	0.51
1:A:2287:GLU:N	1:A:2305:ASP:O	2.43	0.51
15:O:32:SER:O	15:O:36:ILE:N	2.43	0.51
1:A:3850:PRO:O	1:A:3855:MET:N	2.43	0.51
1:A:3991:SER:O	1:A:3995:ALA:HB3	2.10	0.51
1:A:2920:GLN:O	1:A:2924:MET:N	2.41	0.51
2:B:3533:LEU:N	2:B:3642:THR:O	2.43	0.51
1:A:3409:PHE:O	1:A:3413:LYS:N	2.43	0.51
2:B:902:ILE:O	2:B:1078:ILE:HA	2.11	0.51
1:A:1302:ASP:O	1:A:1304:SER:N	2.44	0.51
1:A:3552:ILE:O	1:A:3556:PHE:N	2.43	0.51
1:A:679:LEU:O	1:A:682:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:565:GLY:HA2	2:B:571:SER:H	1.75	0.50
3:C:2397:GLY:O	3:C:2633:ASN:N	2.43	0.50
1:A:2077:TYR:N	1:A:2123:GLN:O	2.42	0.50
2:B:3985:PHE:N	2:B:4076:LEU:O	2.42	0.50
1:A:3615:CYS:O	1:A:3620:HIS:N	2.43	0.50
4:D:516:PHE:O	4:D:528:TRP:N	2.45	0.50
1:A:4036:THR:O	1:A:4040:GLN:N	2.45	0.49
2:B:605:LYS:O	2:B:612:GLY:HA3	2.12	0.49
1:A:4155:LYS:O	1:A:4159:SER:N	2.45	0.49
1:A:4037:ALA:O	1:A:4041:GLY:N	2.41	0.49
1:A:115:LYS:O	1:A:119:TYR:N	2.46	0.49
1:A:2324:ASN:HA	1:A:2327:ASN:O	2.13	0.49
1:A:4085:GLY:O	1:A:4088:GLY:N	2.46	0.49
2:B:1577:ARG:O	2:B:1579:ASP:N	2.45	0.49
1:A:3764:LEU:O	1:A:3768:LEU:N	2.38	0.49
3:C:2932:GLU:O	3:C:2935:LEU:N	2.42	0.49
1:A:3217:ILE:O	1:A:3221:SER:N	2.40	0.48
2:B:2446:GLY:O	2:B:2675:SER:N	2.43	0.48
1:A:3840:TYR:O	1:A:3844:LYS:N	2.44	0.48
1:A:2891:ARG:O	1:A:2895:LEU:N	2.44	0.48
1:A:3468:LYS:O	1:A:3472:THR:N	2.44	0.48
1:A:4077:LEU:O	1:A:4102:HIS:N	2.47	0.48
1:A:3996:ASP:HA	1:A:4168:ASP:HA	1.96	0.48
3:C:2864:LEU:N	3:C:3023:THR:O	2.45	0.48
1:A:1721:LYS:O	1:A:1725:GLY:N	2.45	0.48
2:B:2888:LEU:O	2:B:3022:PHE:N	2.46	0.48
3:C:3592:ASP:O	3:C:3595:LEU:N	2.47	0.48
1:A:4124:TYR:O	1:A:4146:MET:N	2.46	0.47
1:A:2827:ILE:O	1:A:2831:GLU:N	2.44	0.47
2:B:1814:SER:O	2:B:1818:LEU:N	2.39	0.47
3:C:1142:ILE:O	3:C:1146:GLN:N	2.47	0.47
2:B:919:GLU:O	2:B:921:SER:O	2.33	0.47
1:A:4001:ASN:O	1:A:4005:GLN:N	2.39	0.47
2:B:1322:TYR:O	2:B:1326:LYS:N	2.47	0.47
2:B:1459:THR:N	2:B:1466:THR:O	2.43	0.47
2:B:4548:TYR:HA	2:B:4557:TYR:HA	1.97	0.47
1:A:2955:MET:O	1:A:2959:LYS:N	2.47	0.47
1:A:2406:CYS:O	1:A:2410:GLU:N	2.38	0.47
2:B:1372:MET:O	2:B:1376:LEU:N	2.48	0.46
2:B:4412:GLN:O	2:B:4414:TRP:N	2.48	0.46
3:C:3744:ARG:O	3:C:3748:ARG:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1372:MET:O	2:B:1375:VAL:N	2.48	0.46
2:B:962:PHE:O	2:B:967:GLN:N	2.37	0.46
1:A:1300:GLN:O	1:A:1302:ASP:N	2.44	0.46
1:A:2638:ALA:HB2	1:A:2875:ALA:HB1	1.97	0.46
2:B:1568:SER:O	2:B:1571:GLU:N	2.44	0.46
2:B:2631:GLY:O	2:B:2645:LEU:N	2.42	0.46
1:A:233:ASP:O	1:A:237:ASP:N	2.48	0.45
1:A:1826:GLN:O	1:A:1829:SER:N	2.50	0.45
3:C:2738:GLU:O	3:C:2742:ALA:N	2.49	0.45
1:A:1338:GLU:O	1:A:1341:TRP:N	2.50	0.45
2:B:2500:LEU:O	2:B:2504:GLN:N	2.50	0.45
3:C:1320:LYS:HA	3:C:1324:ALA:HB1	1.99	0.45
1:A:887:ALA:O	1:A:891:ILE:N	2.32	0.44
2:B:1359:PHE:O	2:B:1363:ASN:N	2.41	0.44
2:B:1814:SER:O	2:B:1817:TRP:N	2.50	0.44
2:B:2779:PHE:O	2:B:2783:PHE:N	2.50	0.44
1:A:3777:ASP:O	1:A:3781:TYR:N	2.46	0.44
1:A:2525:ASN:O	1:A:2529:SER:CB	2.66	0.44
2:B:929:THR:O	2:B:932:ASN:N	2.50	0.44
16:P:85:LYS:O	16:P:86:LYS:CB	2.65	0.44
1:A:54:ASN:C	1:A:56:GLN:H	2.21	0.44
1:A:879:ARG:O	1:A:883:LYS:N	2.45	0.44
1:A:1399:CYS:HA	1:A:1524:ARG:C	2.38	0.44
1:A:3996:ASP:HA	1:A:4168:ASP:O	2.17	0.44
3:C:3439:GLN:O	3:C:3443:LEU:N	2.42	0.44
1:A:2:PRO:HA	1:A:306:LEU:HA	2.00	0.43
1:A:256:ILE:O	1:A:268:ILE:HA	2.18	0.43
1:A:4114:PRO:O	1:A:4116:ASP:N	2.51	0.43
2:B:1375:VAL:O	2:B:1378:LEU:N	2.51	0.43
16:P:30:ALA:C	16:P:32:TRP:H	2.21	0.43
1:A:1399:CYS:HA	1:A:1524:ARG:O	2.18	0.43
2:B:3748:ARG:O	2:B:3751:ALA:HB3	2.18	0.43
1:A:397:PHE:O	1:A:405:GLU:HA	2.19	0.43
1:A:2044:TYR:HA	1:A:2085:PRO:HA	2.00	0.43
2:B:482:GLU:O	2:B:484:LYS:N	2.52	0.43
3:C:1400:TYR:O	3:C:1403:GLU:N	2.47	0.43
3:C:3503:TRP:O	3:C:3506:GLN:N	2.52	0.43
1:A:1758:LEU:N	1:A:1797:LEU:O	2.47	0.43
1:A:3437:ASP:O	1:A:3441:ILE:N	2.44	0.42
1:A:2943:LYS:O	1:A:2947:ASN:N	2.44	0.42
2:B:3466:ALA:O	2:B:3469:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3726:VAL:O	3:C:3730:LEU:N	2.44	0.42
8:H:10:VAL:N	8:H:80:TYR:O	2.50	0.42
3:C:3540:TRP:O	3:C:3544:LYS:N	2.50	0.42
1:A:904:LEU:O	1:A:908:LEU:N	2.51	0.42
1:A:4077:LEU:N	1:A:4102:HIS:O	2.51	0.42
2:B:1494:VAL:O	2:B:1498:TYR:N	2.52	0.42
1:A:295:ASP:O	1:A:299:LEU:N	2.53	0.42
1:A:2203:ALA:HB2	1:A:3956:ALA:HA	2.02	0.42
2:B:3883:PHE:O	2:B:3887:ALA:N	2.44	0.42
3:C:3784:GLU:O	3:C:3787:ASP:N	2.53	0.42
1:A:2620:ILE:O	1:A:2624:VAL:N	2.48	0.41
2:B:2402:ILE:O	2:B:2405:ILE:N	2.52	0.41
2:B:3652:GLY:O	2:B:3655:GLU:N	2.53	0.41
2:B:2563:LYS:N	2:B:2601:ILE:O	2.52	0.41
2:B:1748:ASP:O	2:B:1751:GLY:N	2.46	0.41
2:B:1360:LYS:HA	2:B:1363:ASN:CB	2.50	0.41
4:D:421:GLY:HA2	4:D:459:GLY:O	2.20	0.41
1:A:3202:GLU:O	1:A:3206:LYS:N	2.52	0.41
1:A:2434:LEU:O	1:A:2438:GLY:N	2.48	0.41
2:B:1536:GLU:O	2:B:1539:ARG:N	2.53	0.41
1:A:3629:LEU:O	1:A:3631:GLN:N	2.54	0.41
3:C:934:GLU:O	3:C:945:ASN:N	2.41	0.41
1:A:1226:LEU:O	1:A:1230:ALA:HB2	2.20	0.41
1:A:1368:GLU:O	1:A:1421:ALA:HB1	2.21	0.41
1:A:3022:ILE:O	1:A:3026:GLU:N	2.51	0.41
2:B:2640:GLU:O	2:B:2642:ARG:N	2.54	0.41
2:B:4487:ALA:HB2	2:B:4528:LYS:H	1.86	0.41
1:A:2495:ASP:O	1:A:2497:ARG:N	2.54	0.40
2:B:2385:HIS:O	2:B:2388:ASN:N	2.54	0.40
1:A:941:GLU:O	1:A:945:ASP:CB	2.69	0.40
1:A:511:GLU:HA	1:A:523:THR:HA	2.02	0.40
1:A:1750:ASP:O	1:A:1752:ASN:N	2.55	0.40

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	3707/4168 (89%)	3206 (86%)	493 (13%)	8 (0%)	47	81
2	B	3893/4595 (85%)	3484 (90%)	398 (10%)	11 (0%)	41	77
3	C	3846/4620 (83%)	3509 (91%)	330 (9%)	7 (0%)	47	81
4	D	313/667 (47%)	268 (86%)	45 (14%)	0	100	100
4	d	122/667 (18%)	112 (92%)	10 (8%)	0	100	100
5	E	337/670 (50%)	287 (85%)	50 (15%)	0	100	100
5	e	96/670 (14%)	86 (90%)	10 (10%)	0	100	100
6	F	96/133 (72%)	79 (82%)	17 (18%)	0	100	100
7	G	93/103 (90%)	81 (87%)	12 (13%)	0	100	100
8	H	83/92 (90%)	76 (92%)	7 (8%)	0	100	100
9	I	87/110 (79%)	79 (91%)	8 (9%)	0	100	100
10	J	82/93 (88%)	77 (94%)	5 (6%)	0	100	100
11	K	93/111 (84%)	83 (89%)	10 (11%)	0	100	100
12	L	95/111 (86%)	90 (95%)	5 (5%)	0	100	100
13	M	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
14	N	107/132 (81%)	100 (94%)	7 (6%)	0	100	100
15	O	109/117 (93%)	99 (91%)	10 (9%)	0	100	100
16	P	101/110 (92%)	97 (96%)	4 (4%)	0	100	100
17	Y	1127/1200 (94%)	1071 (95%)	54 (5%)	2 (0%)	47	81
All	All	14471/18456 (78%)	12961 (90%)	1482 (10%)	28 (0%)	50	81

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1823	VAL
2	B	1651	ASN
2	B	1652	PRO
2	B	2557	PRO
2	B	3703	PRO
2	B	4008	PRO
2	B	4432	PRO
3	C	2978	PRO

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Mol	Chain	Res	Type
3	C	2979	PRO
3	C	4182	PRO
3	C	4188	PRO
3	C	4546	PRO
17	Y	723	PRO
17	Y	1106	PRO
1	A	1351	ASP
1	A	4084	ILE
2	B	4556	THR
3	C	1322	ASP
2	B	1245	PRO
2	B	3923	PRO
1	A	982	ILE
1	A	3108	ASN
2	B	4557	TYR
1	A	1040	VAL
1	A	3665	PRO
2	B	3922	MET
3	C	4121	VAL
1	A	3593	GLY

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

5 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	$\#\|Z\| > 2$
18	ADP	C	4704	-	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)
19	ATP	C	4702	-	26,33,33	0.87	1 (3%)	31,52,52	1.68	5 (16%)
20	GTP	Y	1301	-	26,34,34	1.21	2 (7%)	32,54,54	1.65	6 (18%)
18	ADP	C	4701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	3 (10%)
18	ADP	C	4703	-	24,29,29	0.93	1 (4%)	29,45,45	1.54	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
18	ADP	C	4704	-	-	3/12/32/32	0/3/3/3
19	ATP	C	4702	-	-	4/18/38/38	0/3/3/3
20	GTP	Y	1301	-	-	6/18/38/38	0/3/3/3
18	ADP	C	4701	-	-	1/12/32/32	0/3/3/3
18	ADP	C	4703	-	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	1301	GTP	C5-C6	-4.38	1.38	1.47
18	C	4704	ADP	C5-C4	2.25	1.46	1.40
18	C	4701	ADP	C5-C4	2.18	1.46	1.40
20	Y	1301	GTP	C2-N3	2.17	1.38	1.33
18	C	4703	ADP	C5-C4	2.13	1.46	1.40
19	C	4702	ATP	C5-C4	2.03	1.46	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	4702	ATP	PA-O3A-PB	-5.12	115.25	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	4701	ADP	PA-O3A-PB	-4.56	117.17	132.83
18	C	4704	ADP	PA-O3A-PB	-4.21	118.36	132.83
19	C	4702	ATP	PB-O3B-PG	-4.13	118.64	132.83
18	C	4703	ADP	PA-O3A-PB	-4.13	118.66	132.83
20	Y	1301	GTP	PA-O3A-PB	-4.09	118.78	132.83
20	Y	1301	GTP	PB-O3B-PG	-3.93	119.33	132.83
18	C	4703	ADP	N3-C2-N1	-3.65	122.97	128.68
19	C	4702	ATP	N3-C2-N1	-3.65	122.97	128.68
18	C	4704	ADP	N3-C2-N1	-3.52	123.17	128.68
20	Y	1301	GTP	C5-C6-N1	3.39	119.94	113.95
18	C	4703	ADP	C3'-C2'-C1'	3.17	105.76	100.98
20	Y	1301	GTP	C2-N1-C6	-3.14	119.31	125.10
18	C	4701	ADP	N3-C2-N1	-3.13	123.78	128.68
18	C	4701	ADP	C4-C5-N7	-2.94	106.34	109.40
20	Y	1301	GTP	C8-N7-C5	2.85	108.42	102.99
18	C	4704	ADP	C3'-C2'-C1'	2.79	105.18	100.98
18	C	4704	ADP	C4-C5-N7	-2.54	106.75	109.40
20	Y	1301	GTP	O6-C6-C5	-2.24	120.00	124.37
19	C	4702	ATP	C4-C5-N7	-2.15	107.16	109.40
19	C	4702	ATP	N6-C6-N1	2.15	123.03	118.57
18	C	4703	ADP	C4-C5-N7	-2.09	107.22	109.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	4703	ADP	C5'-O5'-PA-O1A
18	C	4703	ADP	C5'-O5'-PA-O2A
18	C	4704	ADP	C5'-O5'-PA-O2A
19	C	4702	ATP	C5'-O5'-PA-O1A
19	C	4702	ATP	C5'-O5'-PA-O3A
19	C	4702	ATP	C3'-C4'-C5'-O5'
20	Y	1301	GTP	C5'-O5'-PA-O3A
20	Y	1301	GTP	O4'-C4'-C5'-O5'
20	Y	1301	GTP	C3'-C4'-C5'-O5'
19	C	4702	ATP	O4'-C4'-C5'-O5'
18	C	4704	ADP	C5'-O5'-PA-O3A
18	C	4704	ADP	C5'-O5'-PA-O1A
20	Y	1301	GTP	C5'-O5'-PA-O1A
20	Y	1301	GTP	PB-O3A-PA-O5'
18	C	4703	ADP	C5'-O5'-PA-O3A
20	Y	1301	GTP	PG-O3B-PB-O2B

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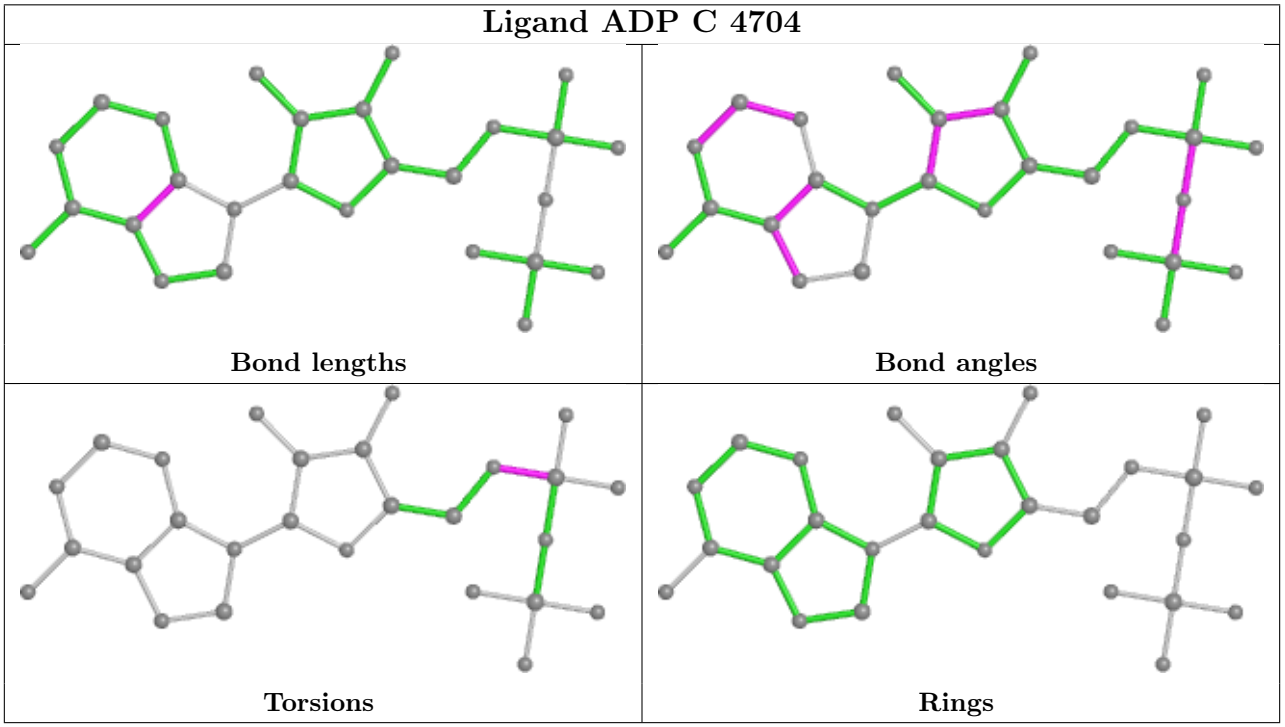
Mol	Chain	Res	Type	Atoms
18	C	4701	ADP	C5'-O5'-PA-O1A
18	C	4703	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

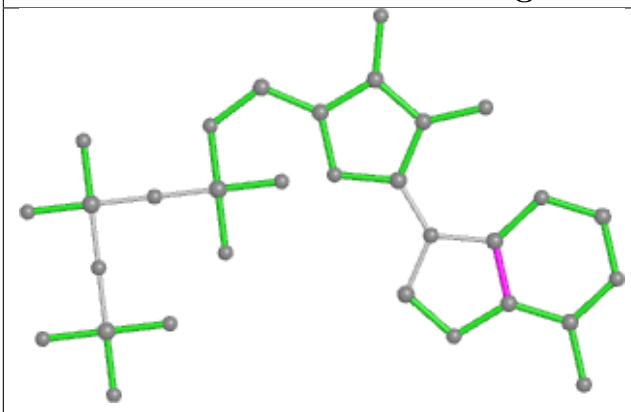
No monomer is involved in short contacts.

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.

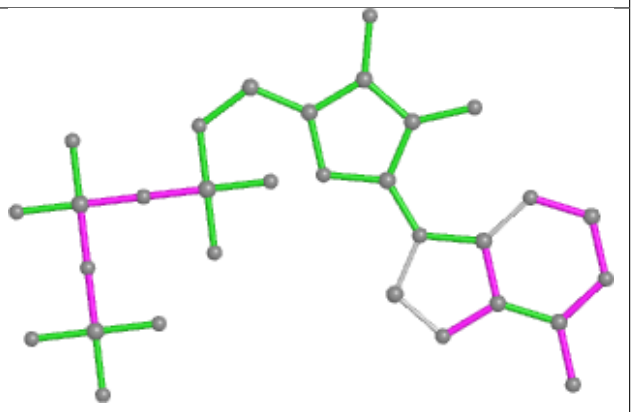
Ligand ADP C 4704



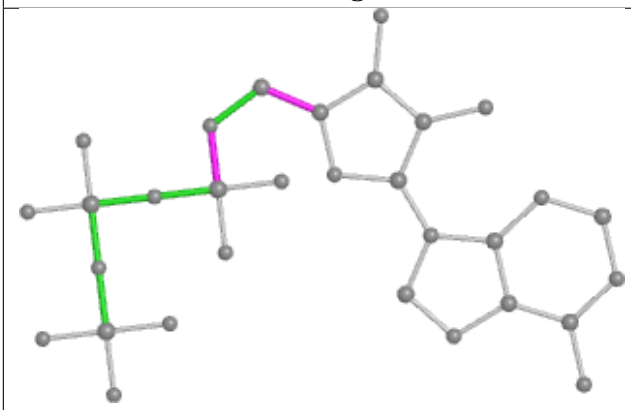
Ligand ATP C 4702



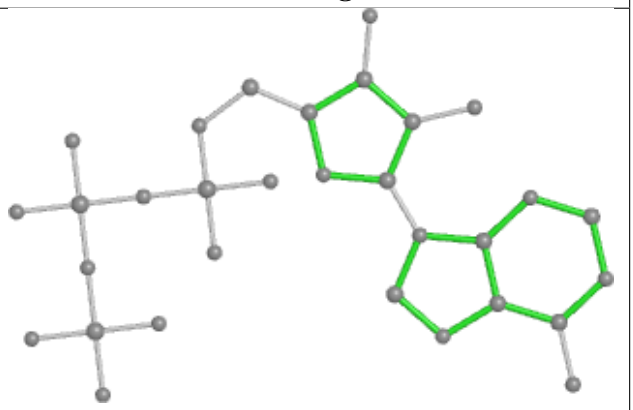
Bond lengths



Bond angles

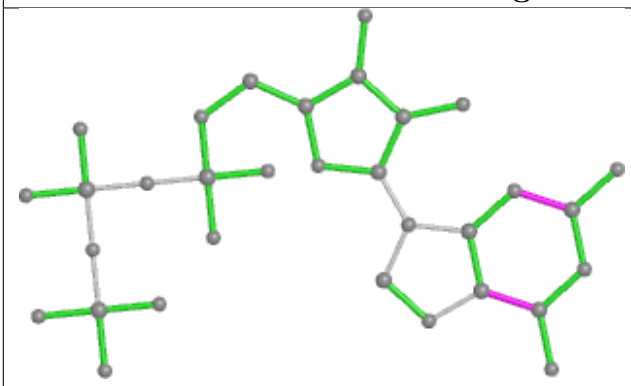


Torsions

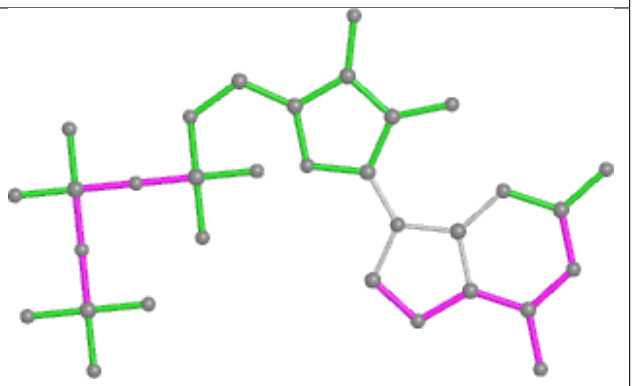


Rings

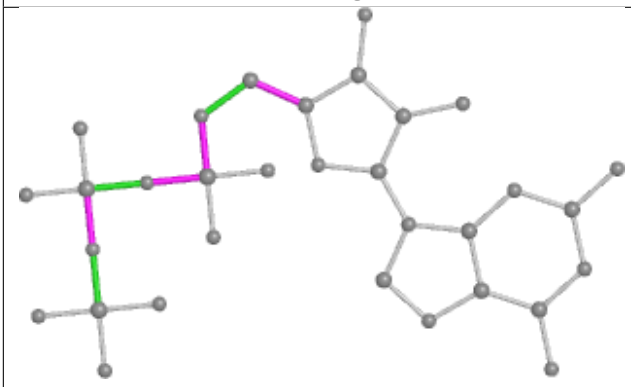
Ligand GTP Y 1301



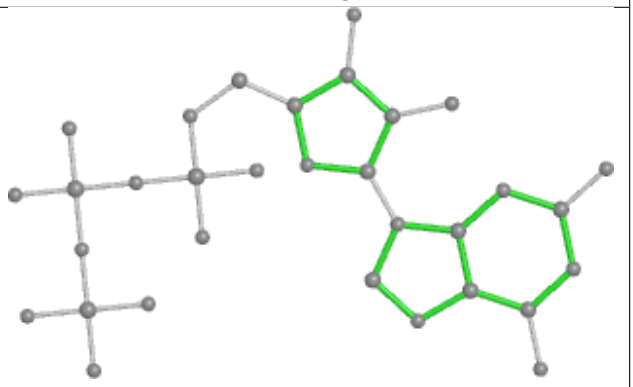
Bond lengths



Bond angles

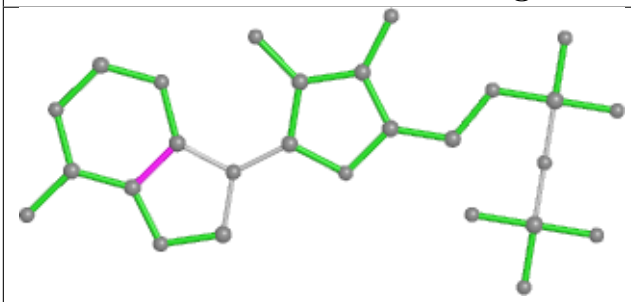


Torsions

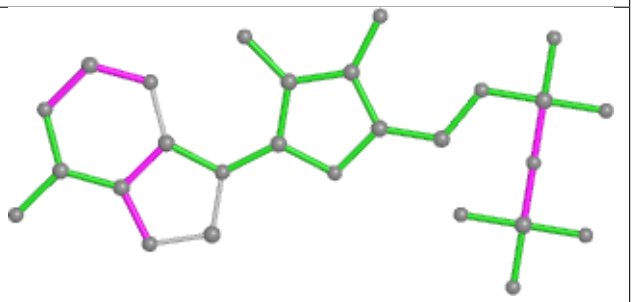


Rings

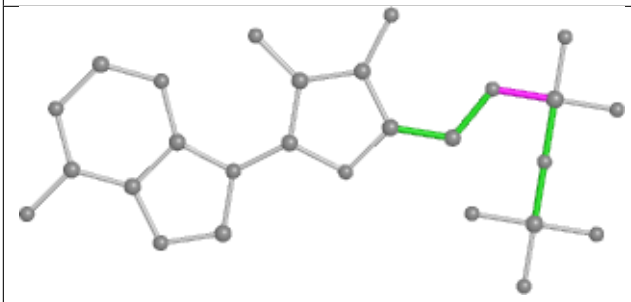
Ligand ADP C 4701



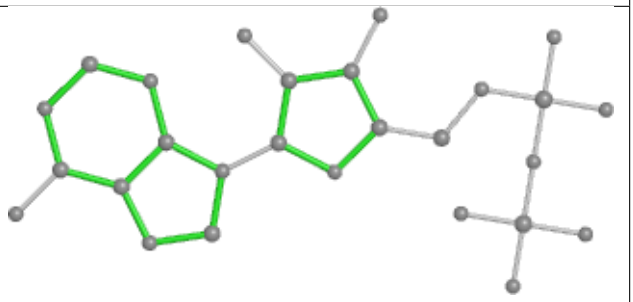
Bond lengths



Bond angles

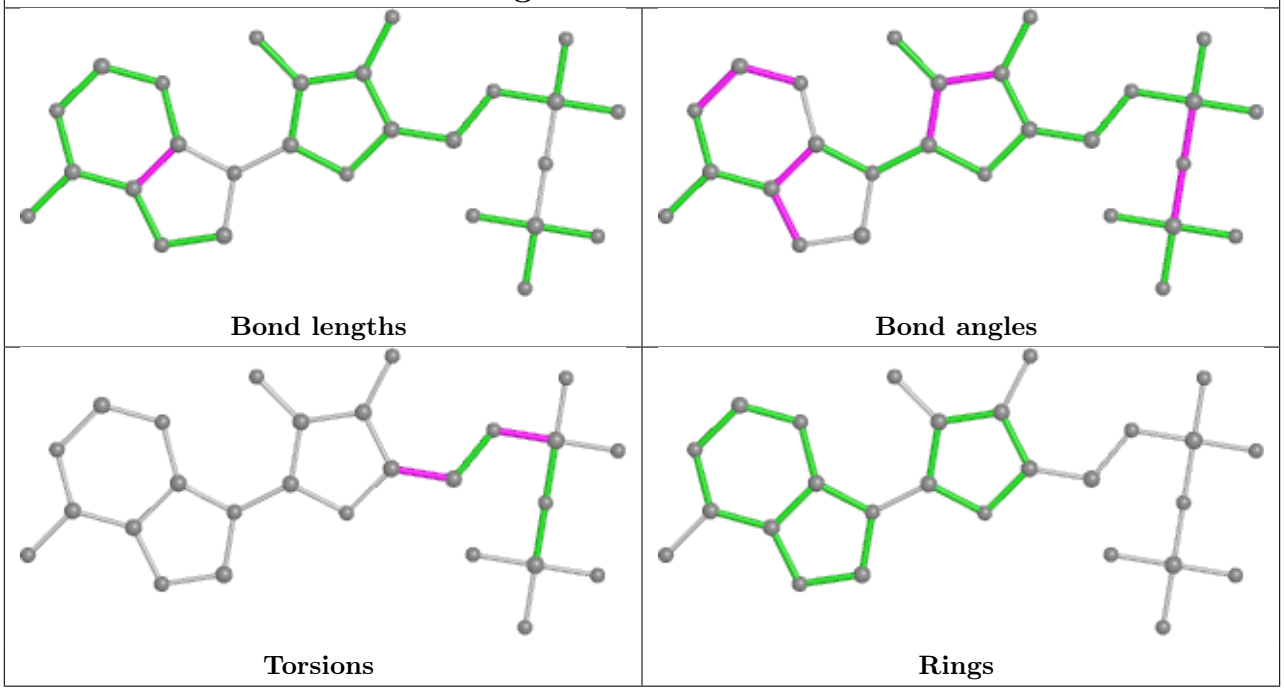


Torsions



Rings

Ligand ADP C 4703



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	23
2	B	12
5	e	2
4	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	201:GLN	C	235:TRP	N	31.73
1	A	389:ASP	C	390:THR	N	29.62
1	A	486:ASP	C	487:GLN	N	21.39
1	A	1299:VAL	C	1300:GLN	N	17.01
1	A	2300:SER	C	2301:ASP	N	13.90
1	A	2232:GLU	C	2233:PRO	N	13.48
1	B	4440:MET	C	4441:ILE	N	12.83

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1507:PRO	C	1508:GLY	N	12.62
1	B	2495:LYS	C	2496:VAL	N	12.29
1	A	2533:PRO	C	2534:VAL	N	10.43
1	A	4018:CYS	C	4019:ILE	N	10.38
1	B	2583:MET	C	2584:VAL	N	9.43
1	A	2296:ALA	C	2297:GLY	N	9.01
1	A	4109:ASN	C	4110:ALA	N	8.24
1	A	2058:THR	C	2059:LEU	N	8.10
1	A	2897:GLN	C	2898:ARG	N	6.96
1	A	1972:PHE	C	1973:ASP	N	6.76
1	B	1775:VAL	C	1776:ARG	N	6.38
1	e	66:VAL	C	72:LYS	N	6.29
1	e	81:LYS	C	95:GLU	N	6.23
1	A	2132:ALA	C	2133:GLY	N	5.82
1	A	3472:THR	C	3473:ILE	N	5.79
1	A	3921:LYS	C	3922:THR	N	5.38
1	B	2658:SER	C	2659:GLY	N	5.09
1	A	2630:GLU	C	2631:ALA	N	4.86
1	B	2091:ARG	C	2092:GLY	N	4.86
1	B	3793:ASP	C	3794:GLU	N	4.35
1	A	1725:GLY	C	1726:TYR	N	4.16
1	A	2000:LEU	C	2001:MET	N	3.91
1	A	2612:GLU	C	2613:THR	N	3.44
1	B	4123:ASP	C	4124:PRO	N	3.30
1	B	2229:LYS	C	2230:THR	N	3.20
1	B	3552:ASN	C	3553:LEU	N	3.19
1	A	2495:ASP	C	2496:MET	N	3.16
1	B	2702:LYS	C	2703:ALA	N	3.15
1	B	2006:PRO	C	2007:GLY	N	3.09
1	A	1592:ARG	C	1593:SER	N	3.08
1	A	2176:THR	C	2177:ILE	N	3.05

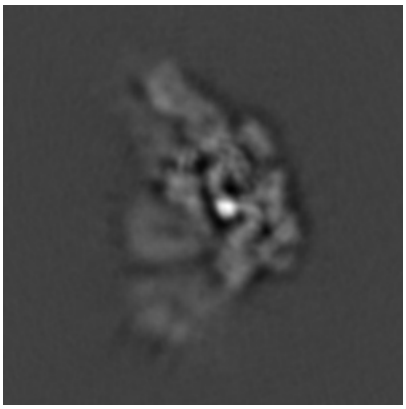
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11576. These allow visual inspection of the internal detail of the map and identification of artifacts.

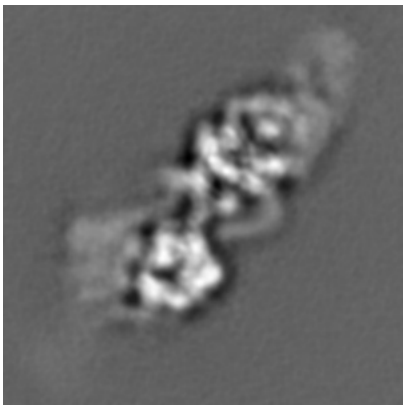
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

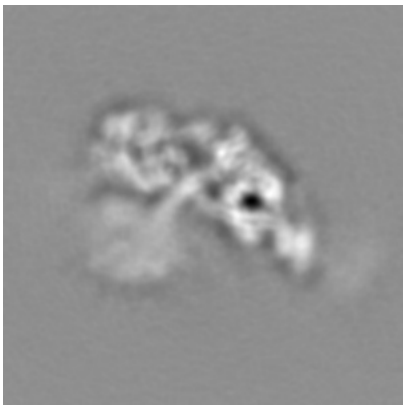
6.1.1 Primary map



X

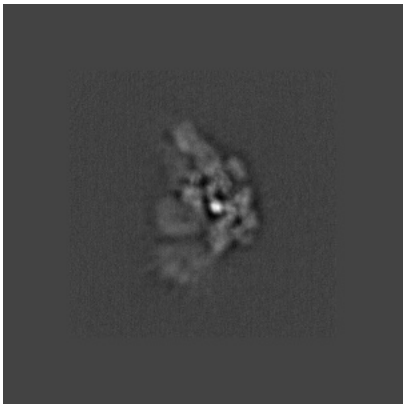


Y

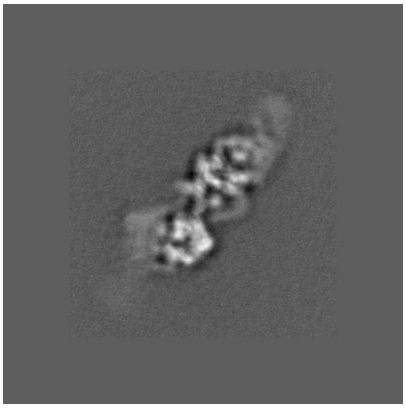


Z

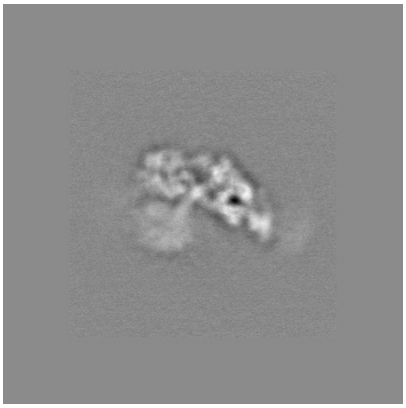
6.1.2 Raw map



X



Y

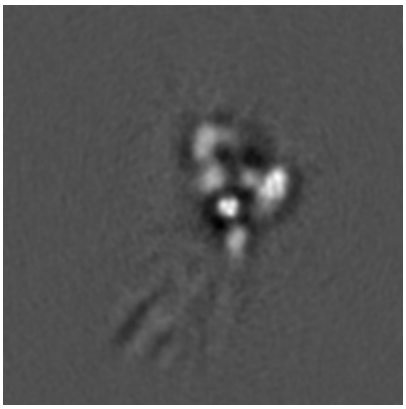


Z

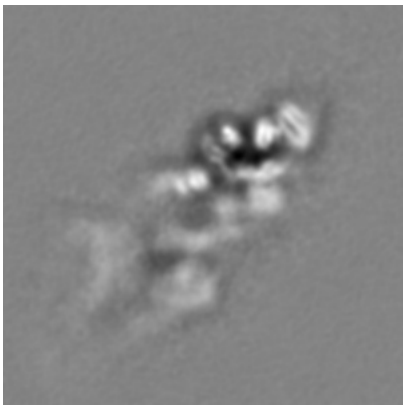
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

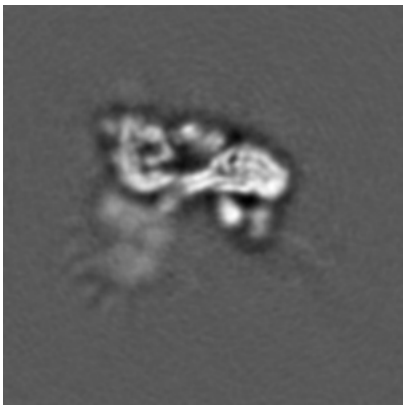
6.2.1 Primary map



X Index: 225

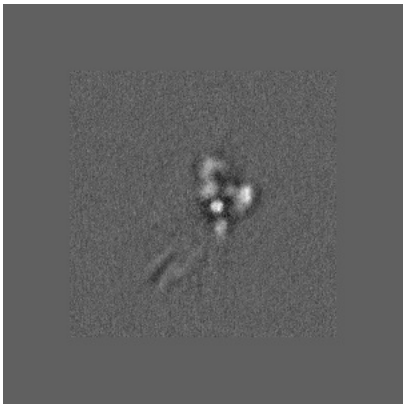


Y Index: 225

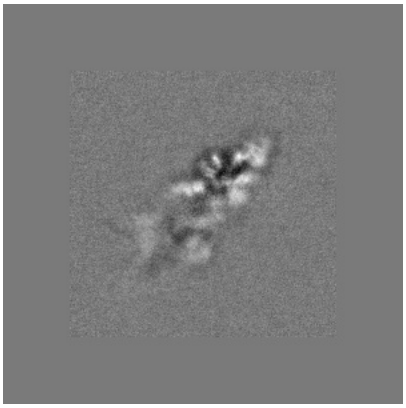


Z Index: 225

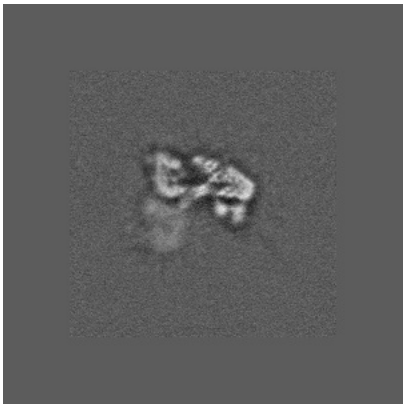
6.2.2 Raw map



X Index: 384



Y Index: 384

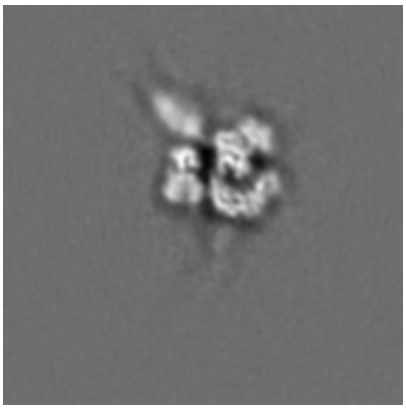


Z Index: 384

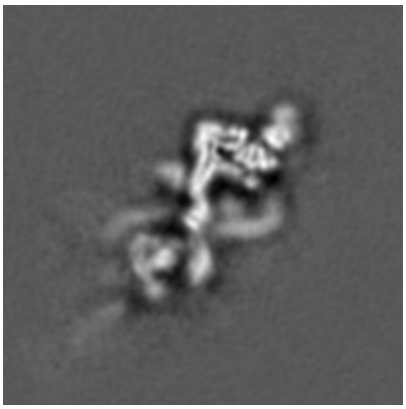
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

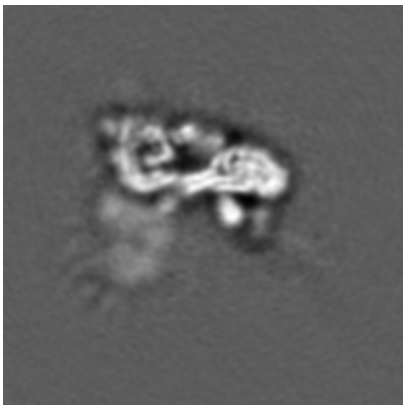
6.3.1 Primary map



X Index: 274

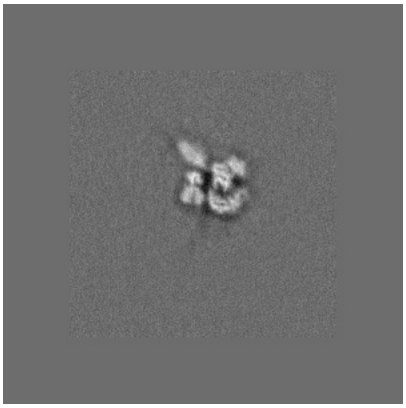


Y Index: 246

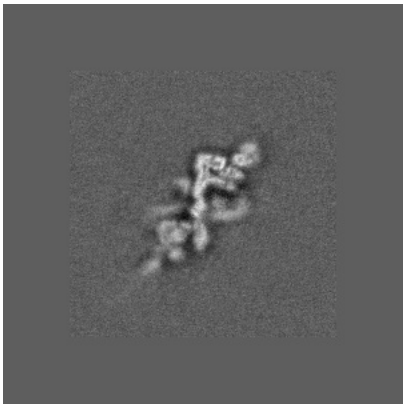


Z Index: 223

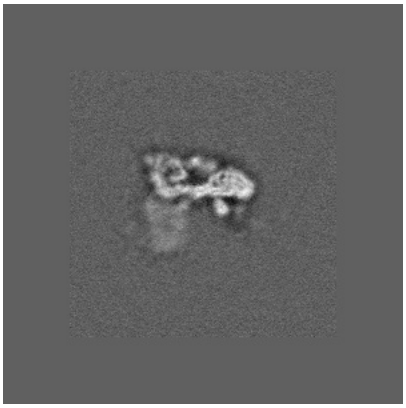
6.3.2 Raw map



X Index: 438



Y Index: 405



Z Index: 378

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

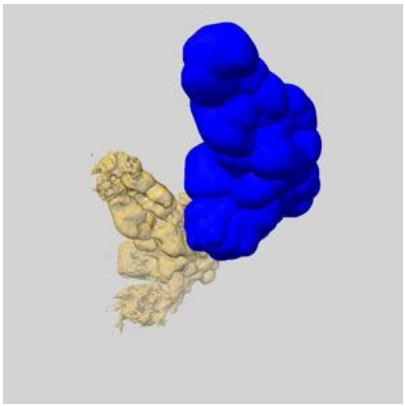
6.5 Mask visualisation (i)

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

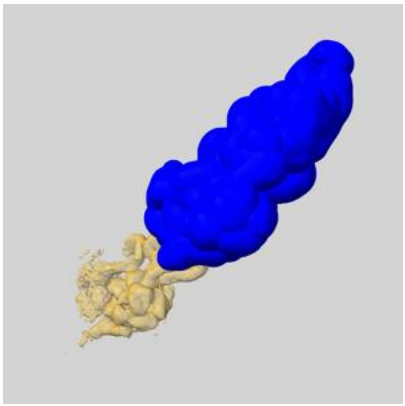
A mask typically either:

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

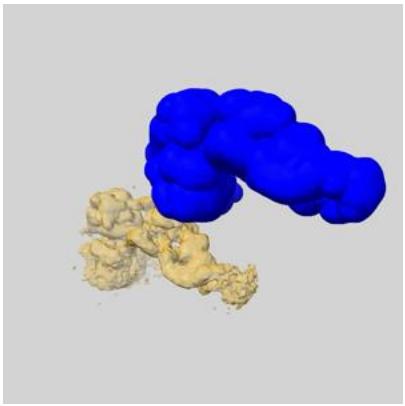
6.5.1 emd_11576_msk_1.map (i)



X



Y

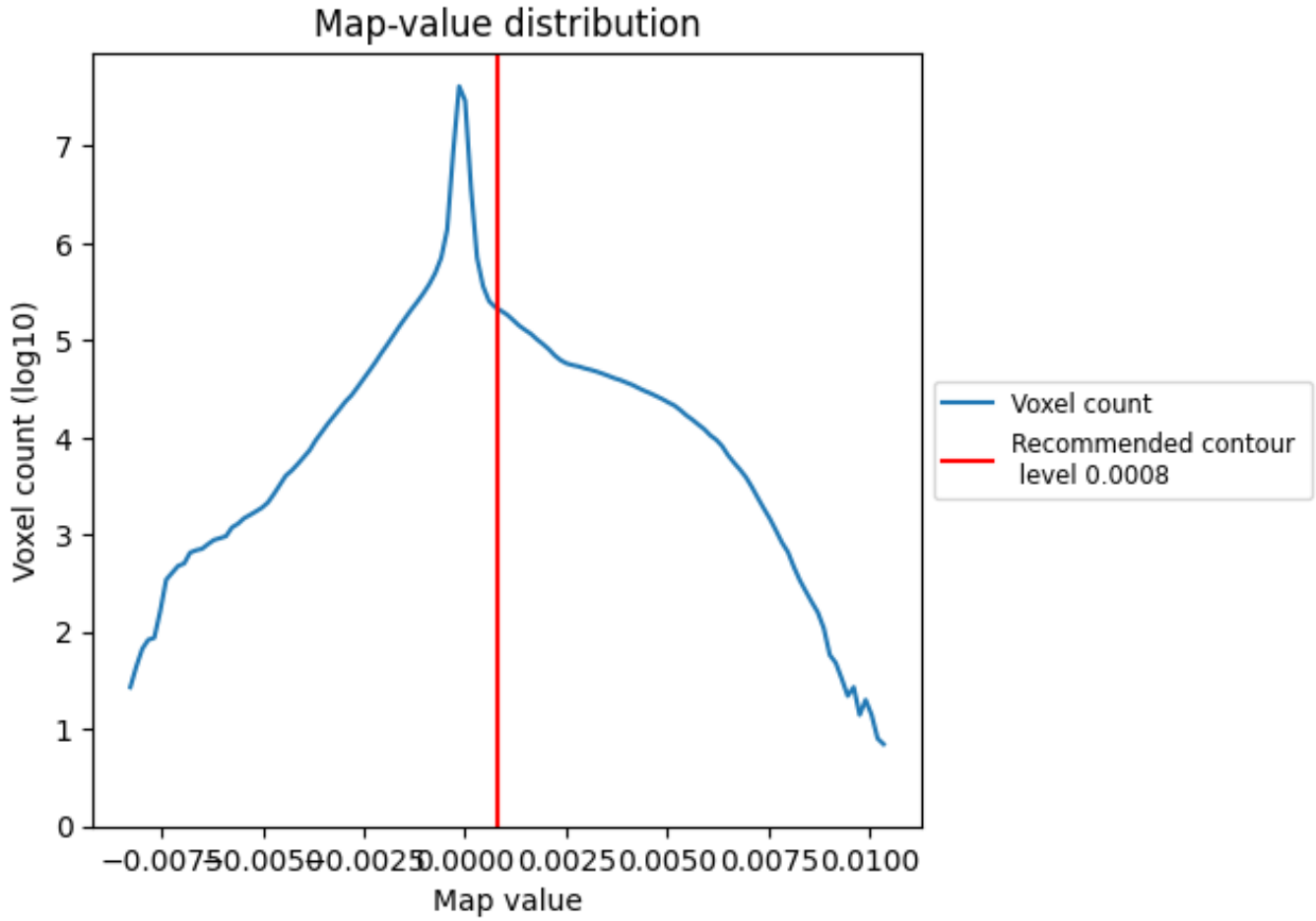


Z

7 Map analysis

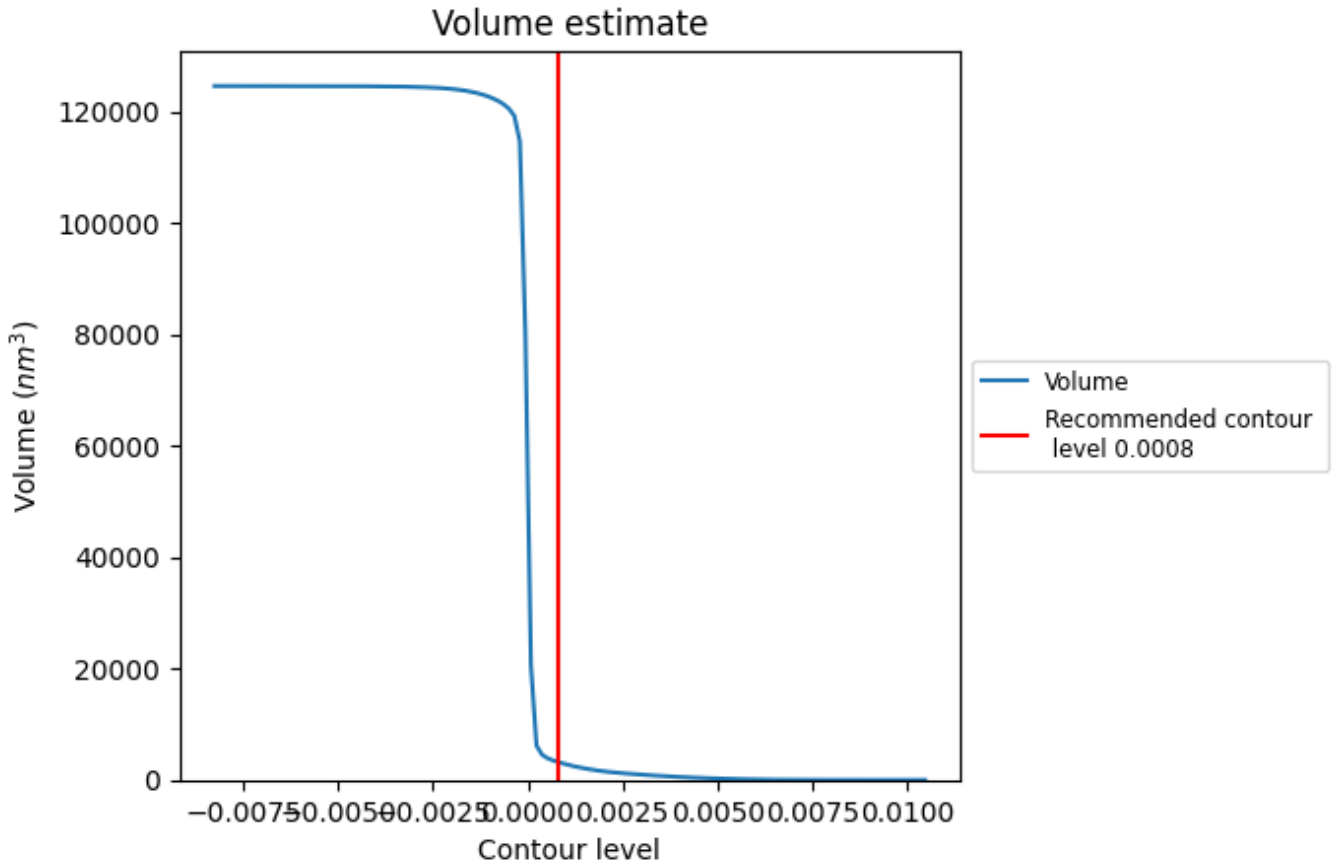
This section contains the results of statistical analysis of the map.

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.

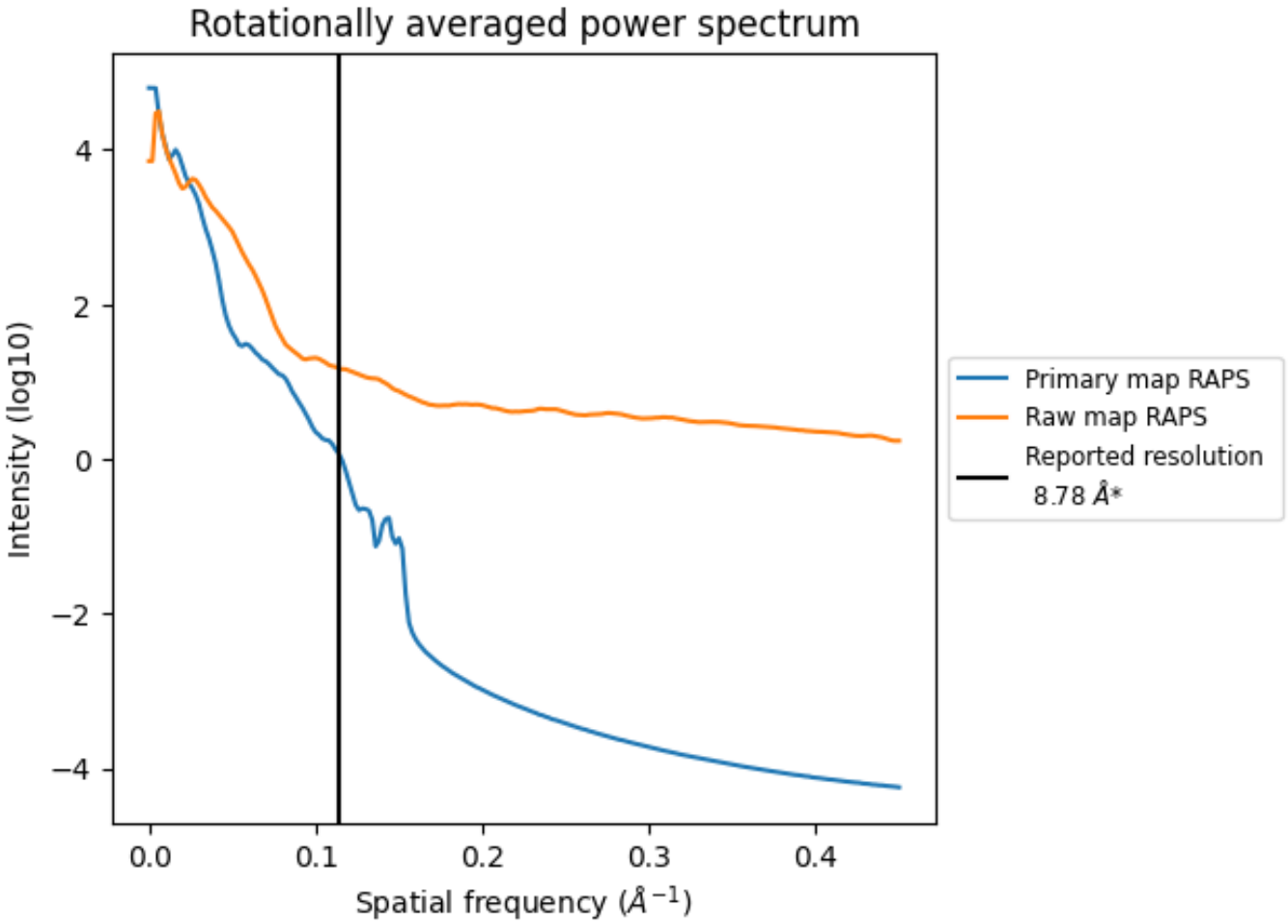
7.2 Volume estimate



The volume at the recommended contour level is 3222 nm^3; this corresponds to an approximate mass of 2910 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)

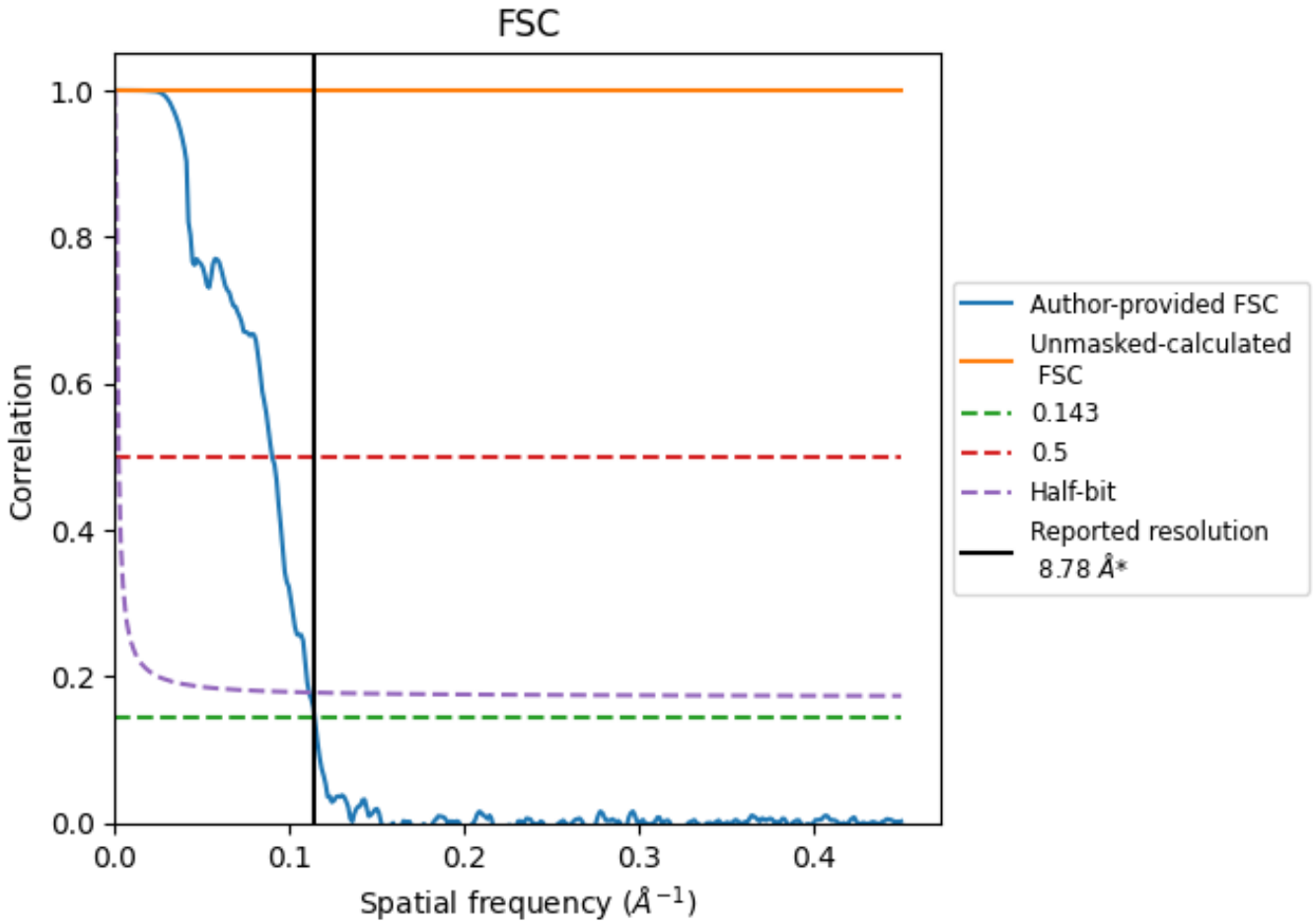


*Reported resolution corresponds to spatial frequency of 0.114 $Å^{-1}$

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 0.114 Å^{-1}

8.2 Resolution estimates (i)

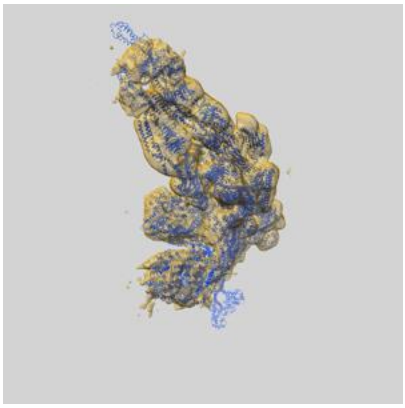
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.78	-	-
Author-provided FSC curve	8.73	11.09	8.98
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

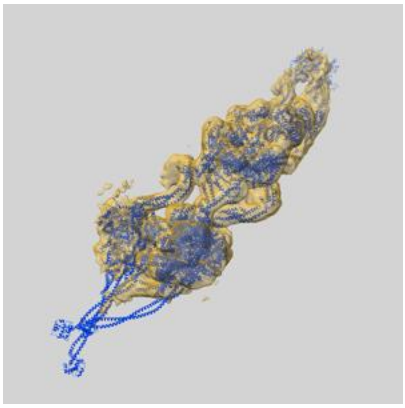
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11576 and PDB model 6ZYW. Per-residue inclusion information can be found in section 3 on page 9.

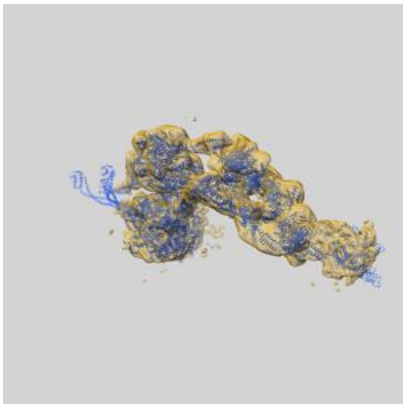
9.1 Map-model overlay



X



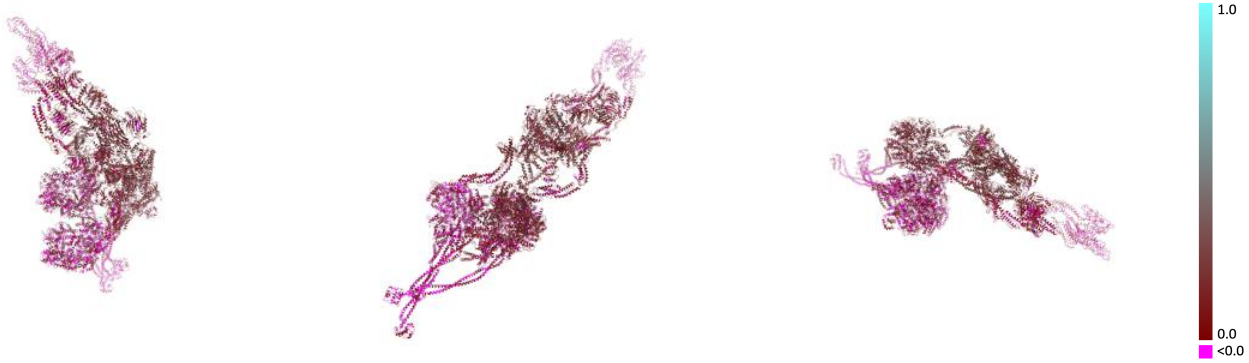
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0008 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.

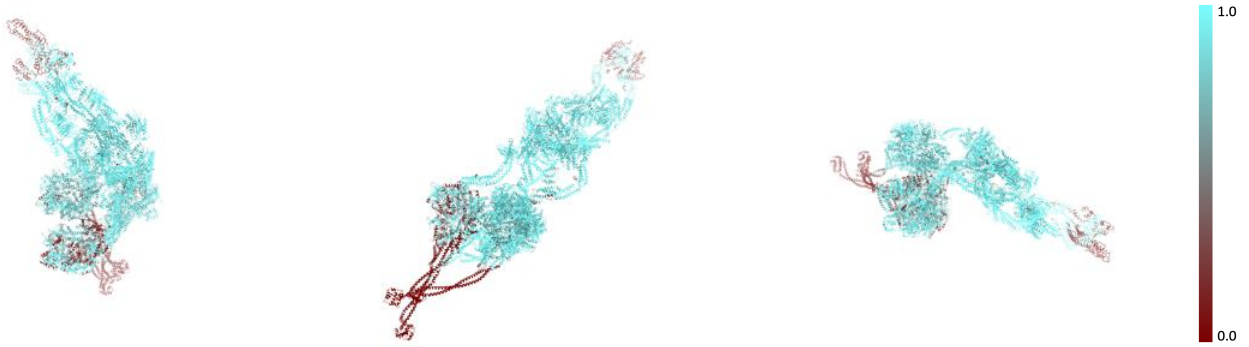
9.2 Q-score mapped to coordinate model



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.

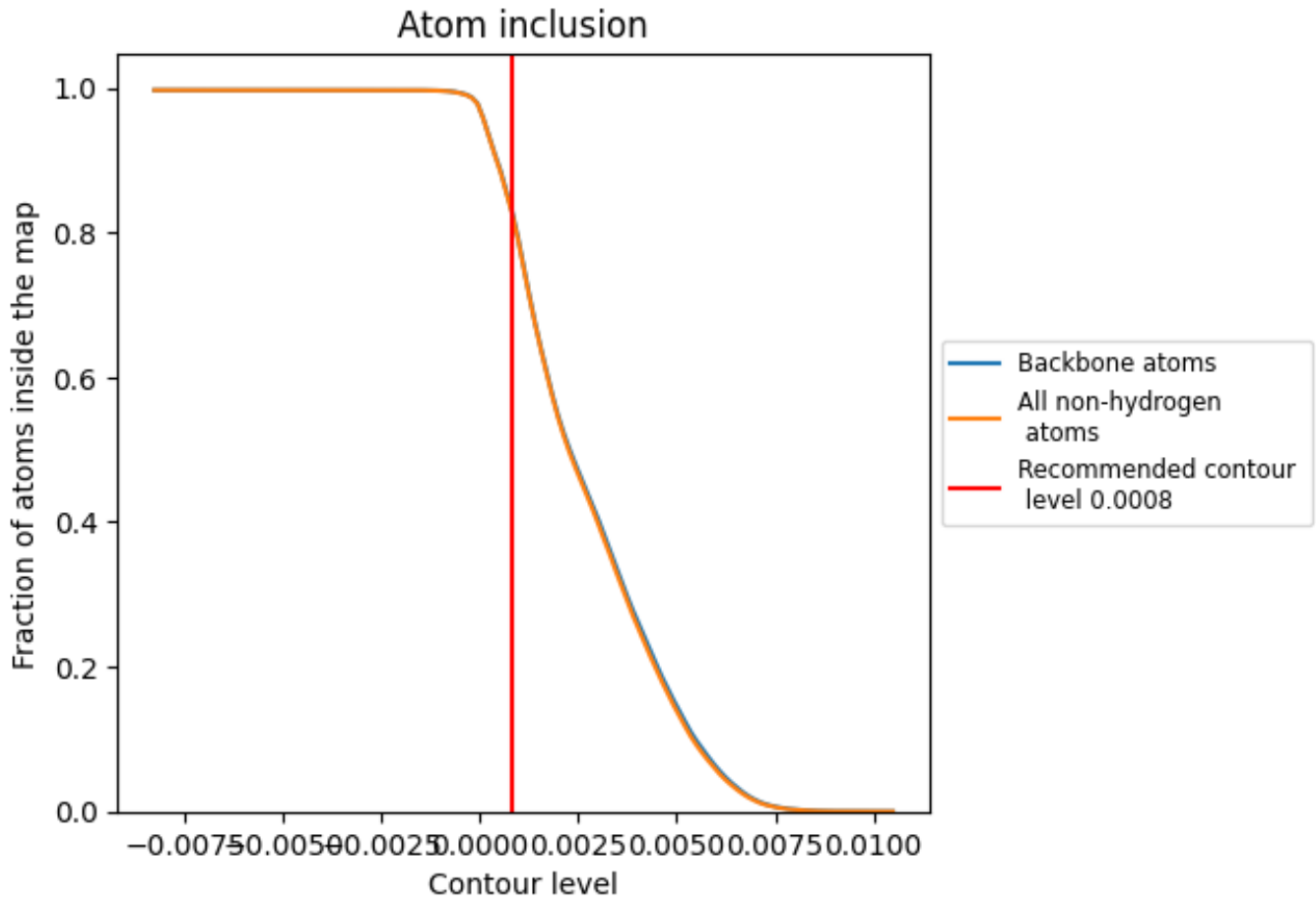
9.3 Atom inclusion mapped to coordinate model



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 (0.0008).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.0008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8305	0.1030
A	0.6147	0.0490
B	0.8391	0.0730
C	0.9056	0.1350
D	0.9994	0.1040
E	0.9636	0.0940
F	0.9979	0.1610
G	0.9957	0.1840
H	1.0000	0.1760
I	0.9932	0.2000
J	0.9952	0.2100
K	0.9915	0.2000
L	0.9937	0.2030
M	0.9977	0.2150
N	1.0000	0.1660
O	0.9982	0.1580
P	0.9552	0.0670
Y	0.9910	0.2020
d	0.9498	0.1750
e	0.9860	0.1510