wwPDB EM Validation Summary Report (i)

Oct 6, 2024 – 03:22 AM EDT

PDB ID	:	7KEK
EMDB ID	:	EMD-22840
Title	:	Structure of the free outer-arm dynein in pre-parallel state
Authors	:	Rao, Q.; Zhang, K.
Deposited on	:	2020-10-11
Resolution	:	8.00 Å(reported)

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

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

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

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

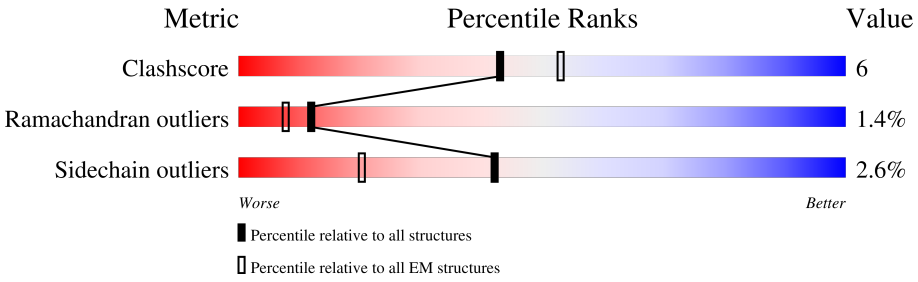
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 8.00 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	4620	12% 86% 10%
2	C	4168	8% 84% 10% 5%
3	Q	202	95% 90% 5% 5%
4	B	4595	13% 84% 13%
5	I	110	76% 17%
6	H	92	88% 10%
7	G	159	52% 8% 40%
8	F	133	68% 14% 17%

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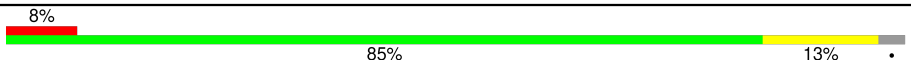
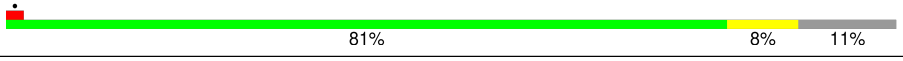
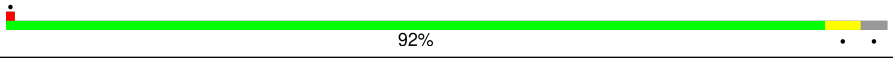
Mol	Chain	Length	Quality of chain
9	N	117	
10	O	132	
11	E	670	
12	D	667	
13	P	122	
14	L	111	
15	K	93	
16	J	111	
17	M	87	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 117936 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 alpha heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4443	33894	21519	5788	6429	158	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4488	LYS	GLY	conflict	UNP Q22A67

- Molecule 2 is a protein called Dynein gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	3943	30436	19390	5162	5735	149	0	0

- Molecule 3 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Q	192	1002	607	202	193	2	0

- Molecule 4 is a protein called Dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	4516	34604	21978	5928	6547	151	0	0

- Molecule 5 is a protein called Dynein light chain LC8_1a (LC10).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	106	827	526	134	161	6	0	0

- Molecule 6 is a protein called Dynein light chain LC8_1b (DLC82).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 7 is a protein called Dynein light chain roadblock LC7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	96	Total	C	N	O	S	0	0
			749	471	129	148	1		

- Molecule 8 is a protein called Dynein light chain roadblock LC7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	110	Total	C	N	O	S	0	0
			863	544	152	165	2		

- Molecule 9 is a protein called Dynein light chain Tctex_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	114	Total	C	N	O	S	0	0
			855	543	143	166	3		

- Molecule 10 is a protein called Dynein light chain Tctex_a (LC2A).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	120	Total	C	N	O	S	0	0
			986	634	172	177	3		

- Molecule 11 is a protein called Dynein intermediate chain DIC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	555	Total	C	N	O	S	0	0
			4423	2786	759	856	22		

- Molecule 12 is a protein called Dynein intermediate chain DIC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	579	Total	C	N	O	S	0	0
			4664	2964	787	883	30		

- Molecule 13 is a protein called Thioredoxin LC3BL.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	109	Total 541	C 323	N 109	O 109	0	0

- Molecule 14 is a protein called Dynein light chain LC8_3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	98	Total 783	C 511	N 132	O 137	S 3	0	0

- Molecule 15 is a protein called Dynein light chain LC8_2a (LC8E).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	90	Total 754	C 489	N 124	O 137	S 4	0	0

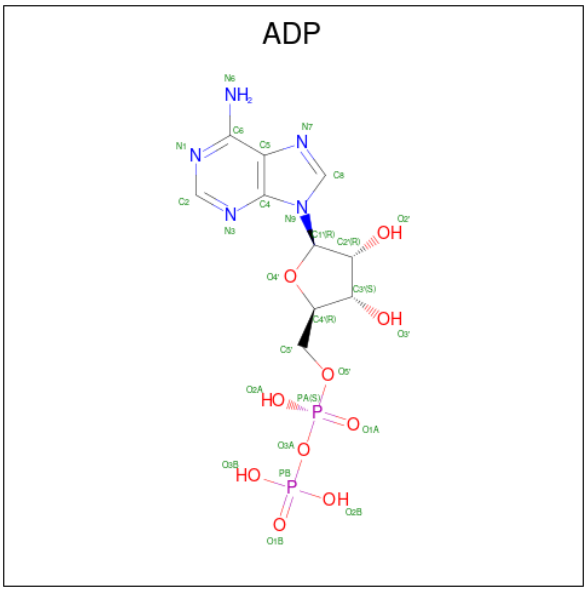
- Molecule 16 is a protein called Dynein light chain LC8_2b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	95	Total 806	C 527	N 135	O 140	S 4	0	0

- Molecule 17 is a protein called Dynein light chain LC8_3a.

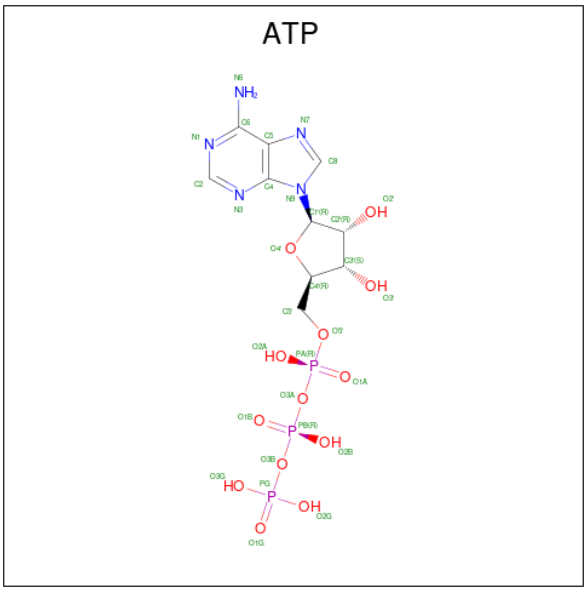
Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	87	Total 735	C 477	N 123	O 130	S 5	0	0

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

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

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

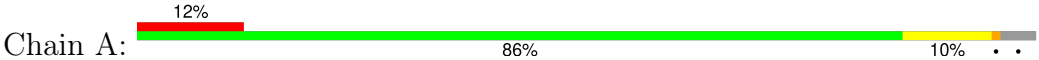
Mol	Chain	Residues	Atoms		AltConf
20	A	3	Total	Mg	0
			3	3	
20	C	3	Total	Mg	0
			3	3	
20	B	3	Total	Mg	0
			3	3	

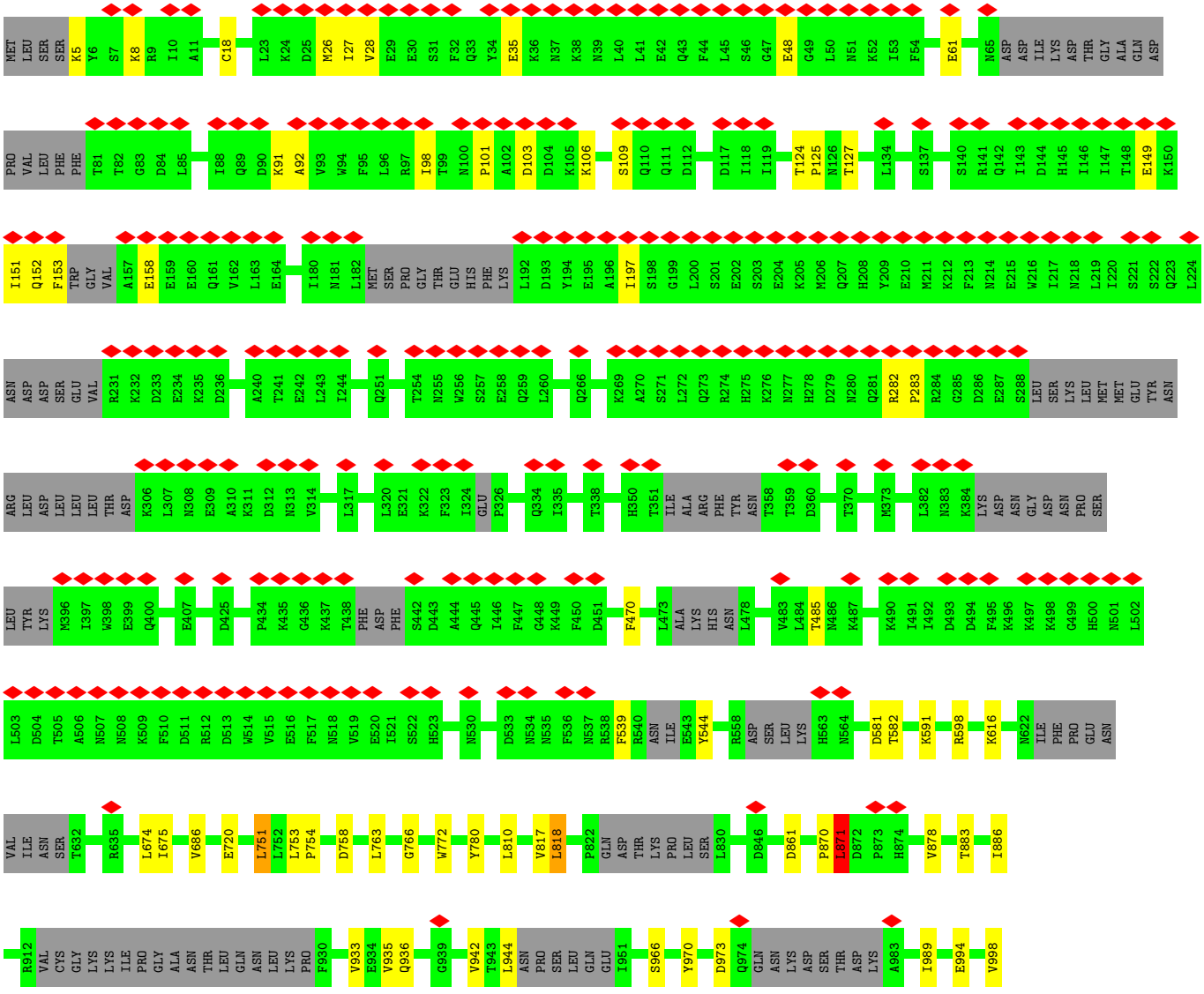
3 Residue-property plots (i)

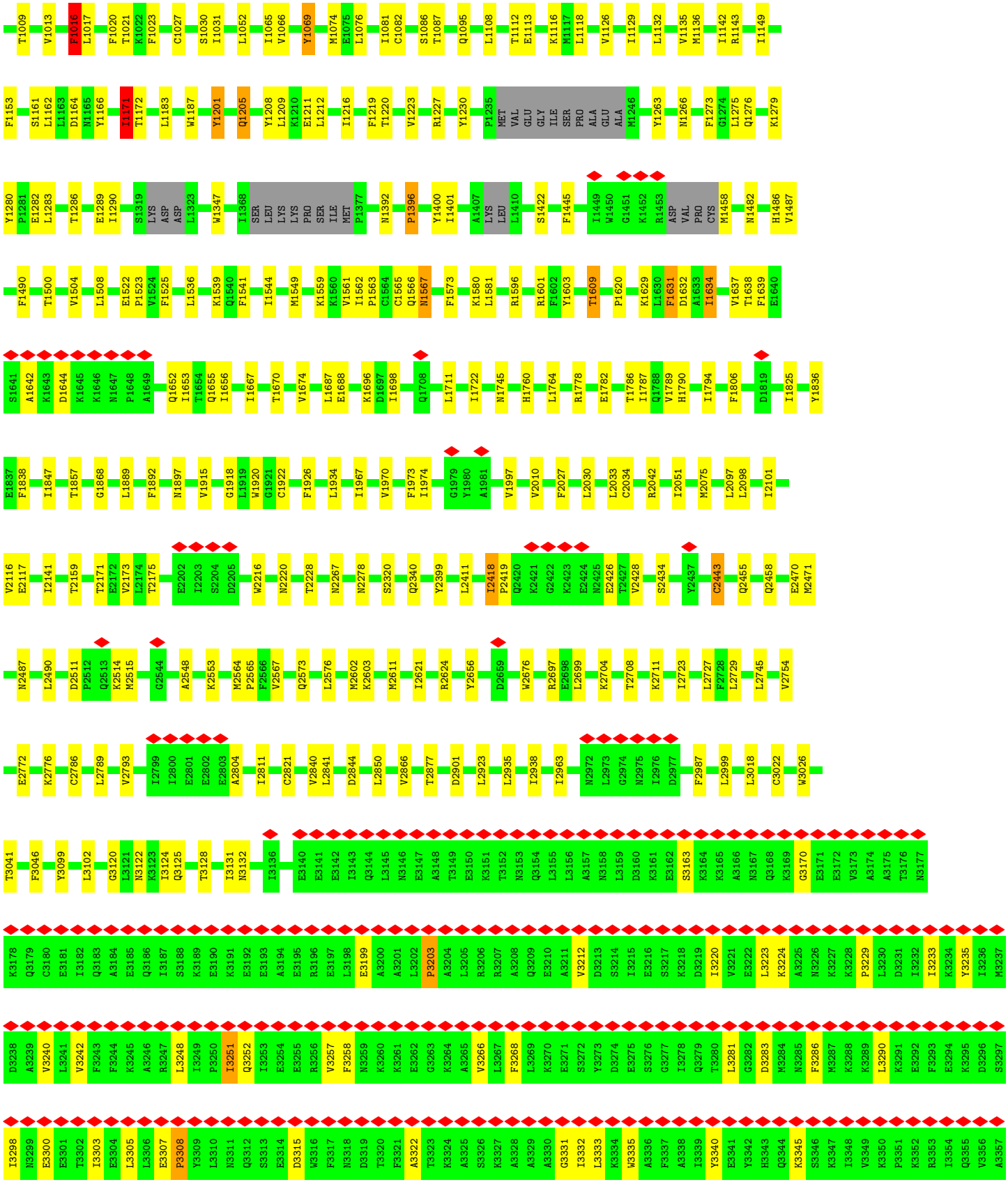
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:



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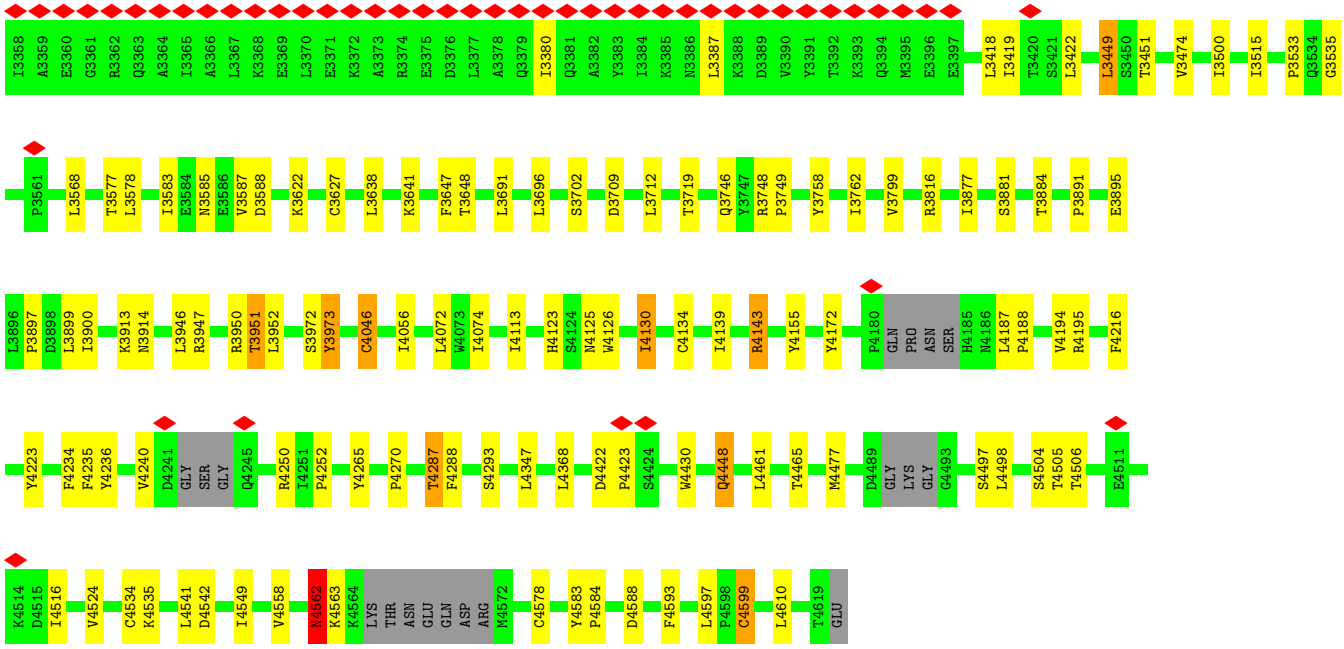
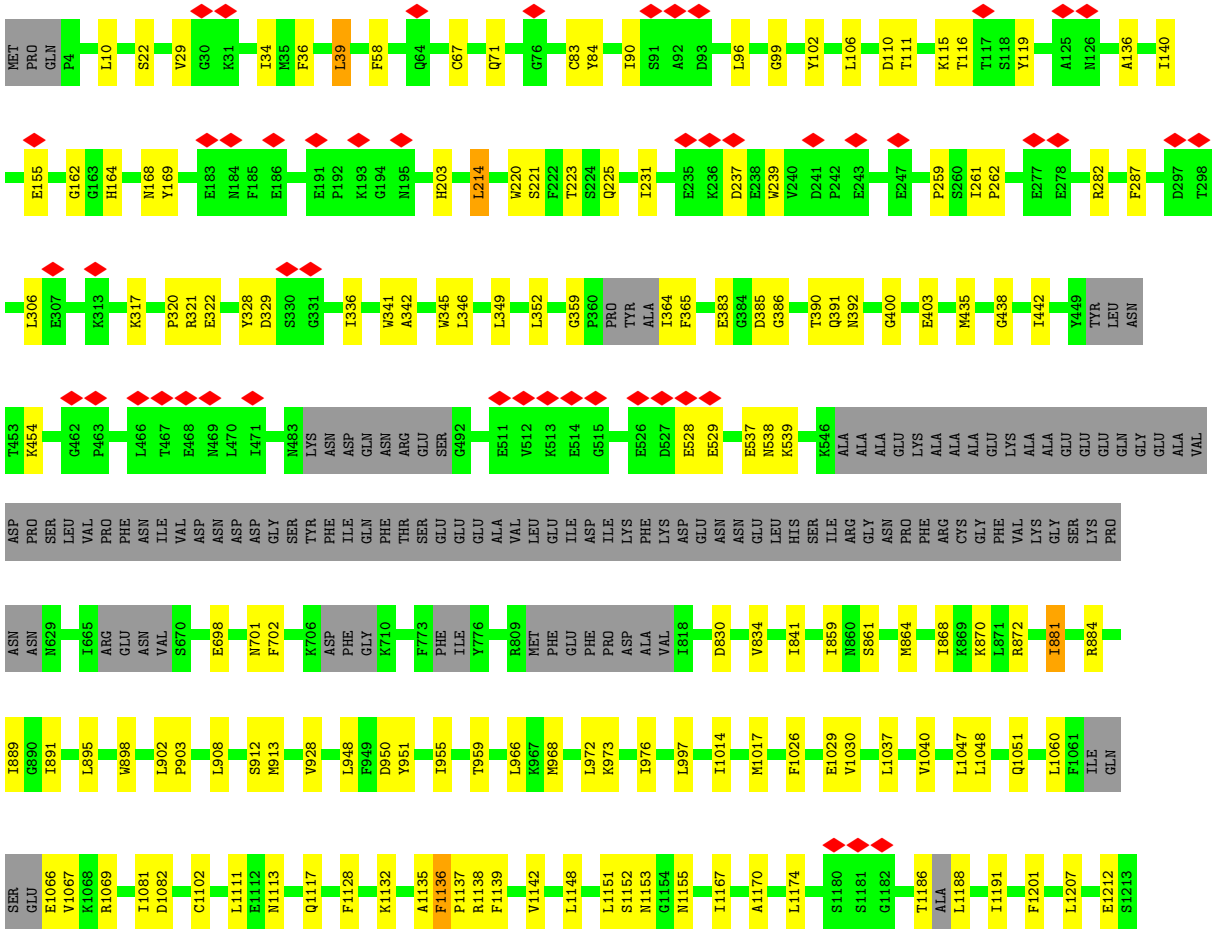
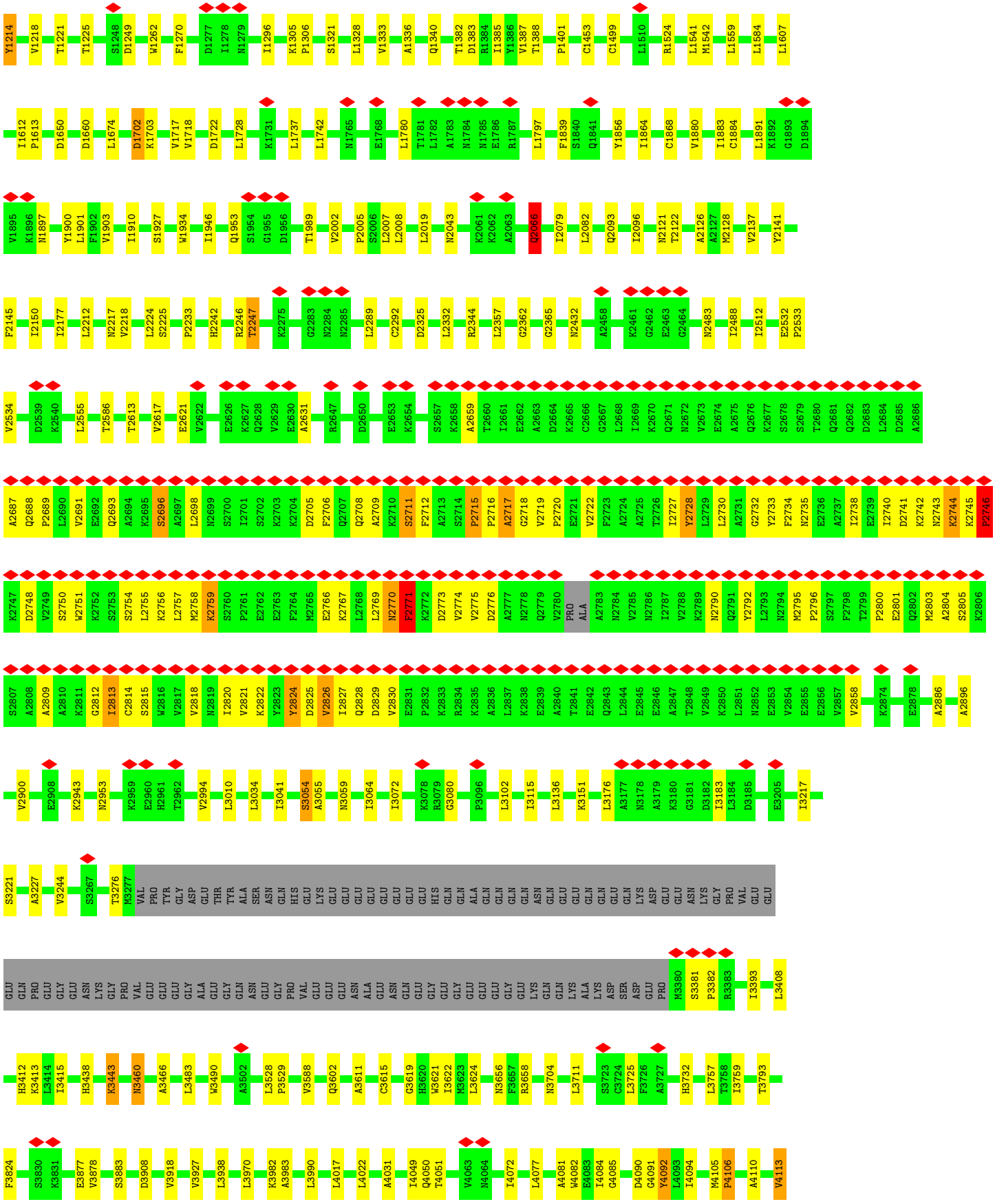
F1153 S1161 L1162 L1163 D1164 N1165 Y1166 I1171 T1172 L1183 W1187 Y1201 Q1205 Y1208 L1209 K1210 E1211 L1212 I1216 F1219 T1220 V1223 R1227 Y1230 P1235 MET VAL GLU GLY ILE SER PRO ALA GLU ALA M1246 Y1263 N1266 F1273 G1274 L1275 Q1276 K1279
Y1280 P1281 E1282 L1283 T1286 E1289 I1290 S1319 LYS ASP ASP L1323 W1347 T1368 SER LEU LYS LYS PRO SER ILE MET P1377 N1392 P1396 Y1400 I1401 A1407 LYS LEU L1410 S1422 F1445 I1449 W1450 G1451 K1452 R1453 ASP VAL PRO CYS M1458 N1482 H1486 V1487
F1490 T1500 V1504 L1508 E1522 P1523 V1524 F1525 L1536 K1539 Q1540 F1541 I1544 M1549 K1559 K1560 V1561 I1562 P1563 C1564 C1565 Q1566 N1567 F1573 K1580 L1581 R1596 R1601 F1602 Y1603 T1609 P1620 K1629 L1630 F1631 D1632 A1633 T1634 V1637 T1638 F1639 E1640
S1641 A1642 K1643 D1644 K1645 K1646 N1647 P1648 A1649 Q1652 I1653 T1654 Q1655 I1656 I1667 T1670 V1674 L1687 E1688 K1696 D1697 I1698 Q1708 L1711 I1722 N1745 H1760 L1764 R1778 E1782 T1786 I1787 Q1788 V1789 H1790 I1794 F1806 D1819 I1825 Y1836
E1837 F1838 I1847 T1857 G1868 L1889 F1892 N1897 V1915 G1918 L1919 W1920 G1921 C1922 F1926 L1934 I1967 V1970 F1973 I1974 G1979 Y1980 A1981 V1997 V2010 F2027 L2030 L2033 C2034 R2042 I2051 M2075 L2097 L2098 I2101
V2116 E2117 I2141 T2159 T2171 E2172 V2173 L2174 T2175 E2202 I2203 S2204 D2205 W2216 N2220 T2228 N2267 N2278 S2320 Q2340 Y2399 L2411 I2418 P2419 Q2420 K2421 G2422 K2423 E2424 N2425 E2426 T2427 V2428 S2434 Y2437 C2443 Q2455 Q2458 E2470 M2471
N2487 L2490 D2511 P2512 Q2513 K2514 M2515 G2544 A2548 K2553 M2564 P2565 F2566 V2567 Q2573 L2576 M2602 K2603 M2611 I2621 R2624 Y2656 D2659 W2676 R2697 E2698 L2699 K2704 T2708 K2711 I2723 L2727 F2728 L2729 L2745 V2754
E2772 K2776 C2786 L2789 V2793 I2799 I2800 E2801 E2802 E2803 A2804 I2811 C2821 V2840 L2841 D2844 L2850 V2866 T2877 D2901 L2923 L2935 I2938 I2963 N2972 L2973 G2974 N2975 I2976 D2977 F2987 L2999 L3018 C3022 W3026
T3041 F3046 Y3099 L3102 G3120 L3121 N3122 K3123 I3124 Q3125 T3128 I3131 N3132 I3136 E3140 E3141 E3142 I3143 Q3144 L3145 N3146 E3147 A3148 T3149 E3150 K3151 T3152 N3153 Q3154 L3155 L3156 A3157 N3158 L3159 D3160 K3161 E3162 S3163 K3164 K3165 A3166 N3167 Q3168 K3169 G3170 E3171 E3172 V3173 A3174 A3175 T3176 N3177
K3178 Q3179 C3180 E3181 I3182 Q3183 A3184 E3185 Q3186 I3187 S3188 K3189 E3190 K3191 E3192 E3193 A3194 E3195 R3196 E3197 L3198 E3199 A3200 A3201 L3202 P3203 A3204 L3205 R3206 R3207 A3208 Q3209 E3210 A3211 V3212 D3213 S3214 I3215 E3216 S3217 K3218 D3219 I3220 V3221 E3222 L3223 K3224 A3225 N3226 K3227 K3228 P3229 L3230 D3231 I3232 I3233 K3234 Y3235 I3236 M3237
D3238 A3239 V3240 L3241 V3242 F3243 F3244 K3245 A3246 R3247 L3248 I3249 P3250 I3251 Q3252 I3253 E3254 E3255 R3256 V3257 F3258 N3259 K3260 K3261 E3262 G3263 K3264 A3265 V3266 L3267 F3268 L3269 K3270 E3271 S3272 Y3273 D3274 E3275 S3276 G3277 I3278 Q3279 T3280 L3281 G3282 D3283 M3284 N3285 F3286 M3287 K3288 K3289 L3290 K3291 E3292 F3293 E3294 K3295 D3296 S3297
I3298 N3299 E3300 E3301 T3302 I3303 E3304 L3305 L3306 E3307 P3308 Y3309 L3310 N3311 Q3312 S3313 E3314 D3315 W3316 F3317 N3318 D3319 T3320 F3321 A3322 T3323 K3324 A3325 S3326 K3327 A3328 A3329 A3330 G3331 I3332 L3333 K3334 W3335 A3336 F3337 A3338 I3339 Y3340 E3341 Y3342 H3343 Q3344 K3345 S3346 K3347 I3348 V3349 K3350 P3351 K3352 R3353 I3354 Q3355 V3356 A3357



• Molecule 2: Dynein gamma heavy chain

Chain C:

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A2687 Q2688 P2689 L2690 V2691 E2692 Q2693 A2694 K2695 S2696 A2697 L2698 N2699 S2700 I2701 S2702 K2703 K2704 D2705 P2706 Q2707 Q2708 A2709 K2710 S2711 P2712 A2713 S2714 P2715 P2716 A2717 G2718 V2719 P2720 E2721 V2722 P2723 A2724 A2725 T2726 I2727 Y2728 L2729 L2730 A2731 G2732 Y2733 F2734 N2735 E2736 A2737 I2738 E2739 I2740 D2741 K2742 N2743 K2744 K2745 P2746
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S3221 A3227 V3244 S3267 T3276 M3277 VAL PRO TYR GLY ASP GLU THR TYR ALA SER ASN GLN HIS GLU LYS GLU GLU GLU GLU GLU GLU GLU GLU HIS GLN GLN ALA GLN GLN GLN GLN ASN GLN GLU GLU GLN GLN GLN GLU 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 ASN GLN GLU GLY GLU GLY GLU GLU GLU GLY GLU GLU GLU GLY GLU GLU LYS GLN GLN LYS ALA LYS ASP SER ASP GLU PRO M3380 S3381 P3382 R3383 I3393 L3408
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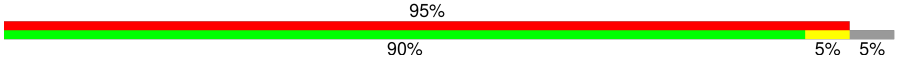
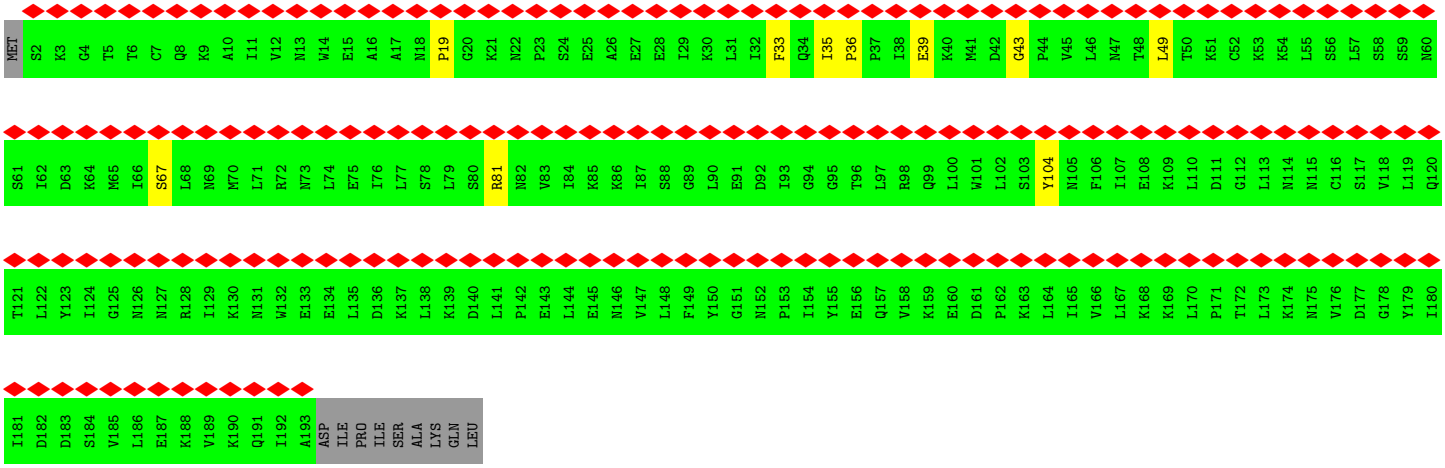
F3824 S3830 K3831 E3877 V3878 S3883 D3908 V3918 V3927 L3938 L3970 K3982 A3983 L3990 L4017 L4022 A4031 I4049 Q4050 T4051 V4063 N4064 I4072 L4077 A4081 W4082 E4083 I4084 G4085 D4090 G4091 Y4092 L4093 I4094 M4105 P4106 A4110 V4113

• Molecule 3: Dynein light chain 1

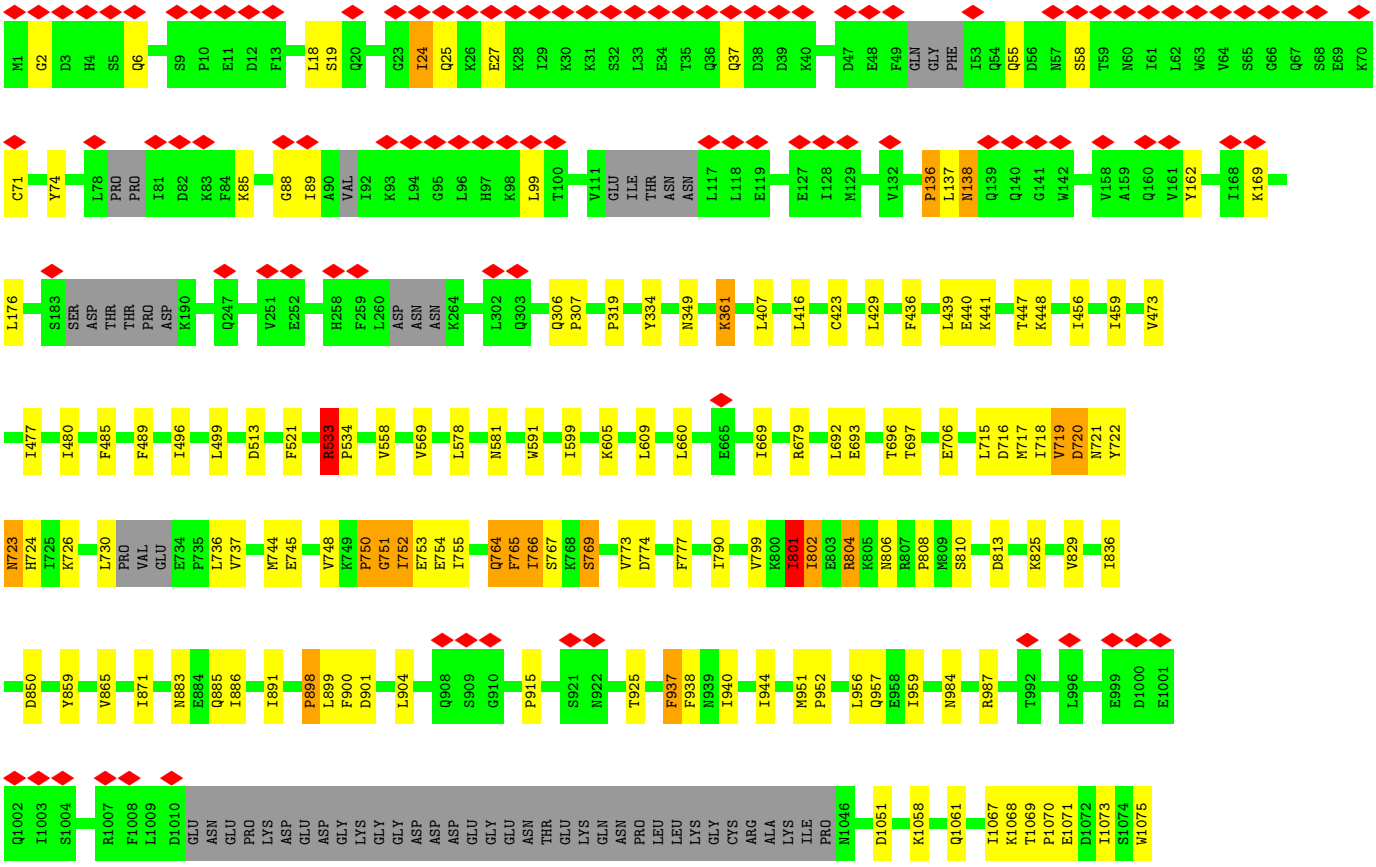
Chain Q:

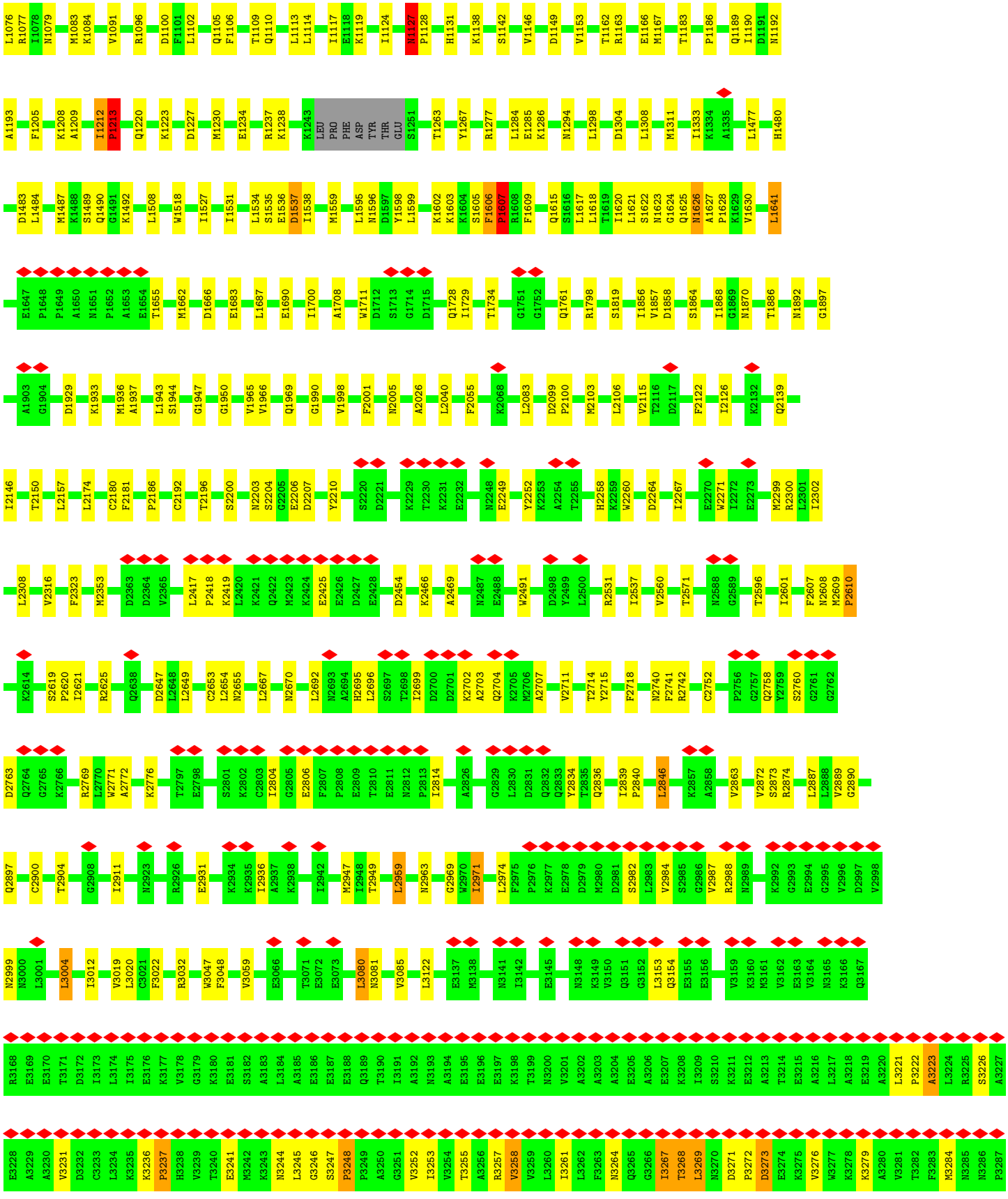


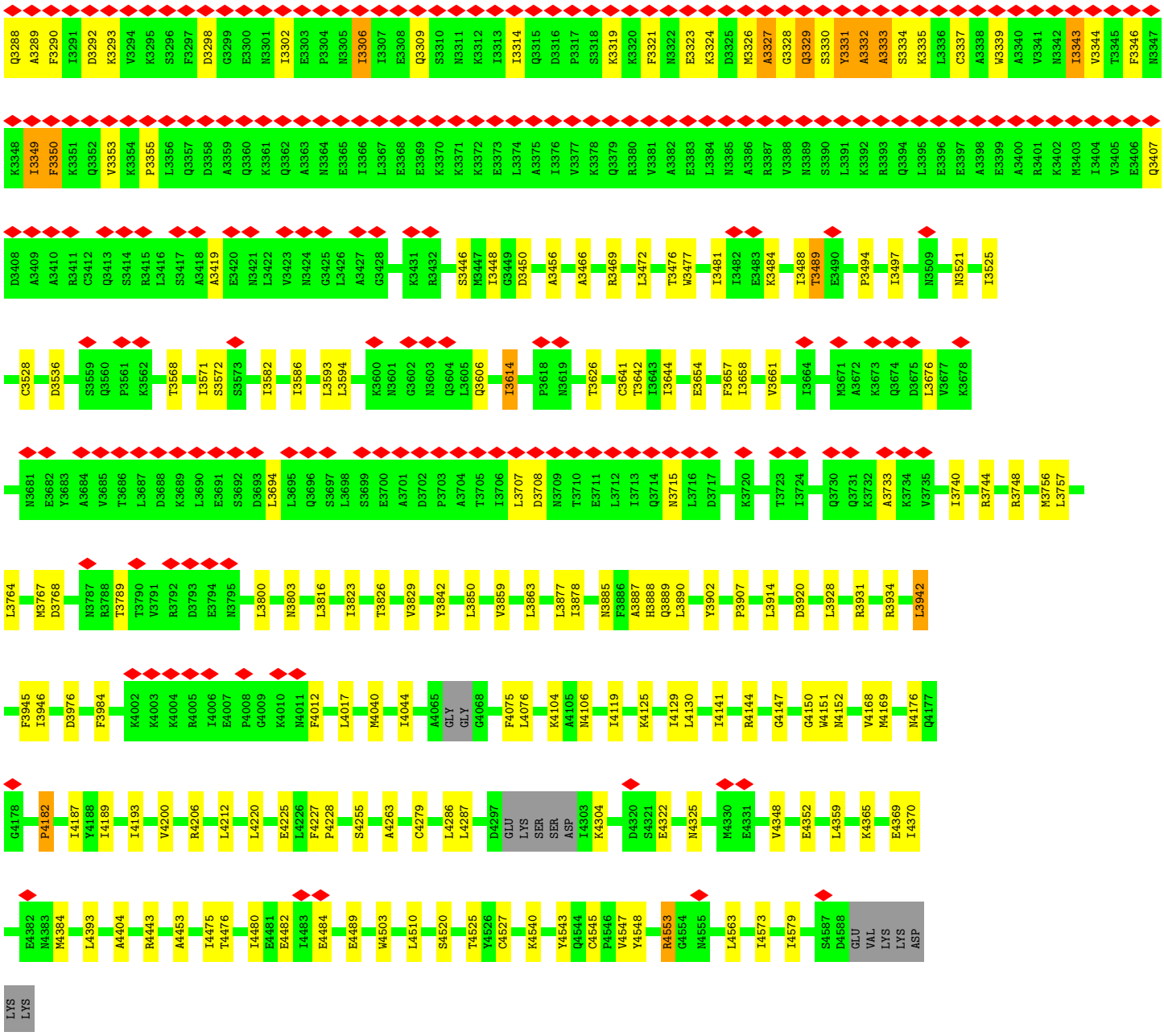


• Molecule 4: Dynein beta heavy chain

Chain B:

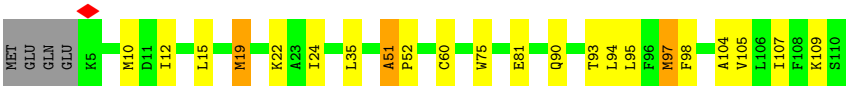



L1076 R1077 T1078 N1079 M1083 K1084 V1091 R1096 D1100 F1101 L1102 Q1105 F1106 T1109 Q1110 L1113 L1114 I1117 E1118 K1119 I1124 N1127 P1128 H1131 K1138 S1142 V1146 D1149 V1153 T1162 R1163 E1166 M1167 T1183 P1186 Q1189 T1190 D1191 N1192
A1193 F1205 K1208 A1209 I1212 P1213 Q1220 K1223 D1227 M1230 E1234 R1237 K1238 K1243 LEU PRO PHE ASP TYR THR GLU S1251 T1263 Y1267 R1277 L1284 E1285 K1286 N1294 L1298 D1304 L1308 M1311 I1333 K1334 A1335 L1477 H1480
D1483 L1484 M1487 K1488 S1489 Q1490 G1491 K1492 L1508 W1518 I1527 I1531 L1534 S1535 E1536 D1537 I1538 M1559 L1595 N1596 D1597 Y1598 L1599 K1602 K1603 K1604 S1605 F1606 R1607 R1608 F1609 Q1615 S1616 L1617 L1618 T1619 I1620 L1621 S1622 N1623 G1624 Q1625 N1626 A1627 P1628 K1629 V1630 L1641
E1647 P1648 P1649 A1650 N1651 P1652 A1653 E1654 T1655 M1662 D1666 E1683 L1687 E1690 I1700 A1708 W1711 D1712 S1713 G1714 D1715 Q1728 I1729 T1734 G1751 G1752 Q1761 R1798 S1819 I1856 V1857 D1858 S1864 I1868 G1869 N1870 T1886 N1892 G1897
A1903 G1904 D1929 K1933 M1936 A1937 L1943 S1944 G1947 G1950 V1965 V1966 Q1969 G1990 V1998 F2001 N2005 A2026 L2040 F2055 K2068 L2083 D2099 P2100 M2103 L2106 V2115 T2116 D2117 F2122 I2126 K2132 Q2139
I2146 T2150 L2157 L2174 C2180 F2181 P2186 C2192 T2196 S2200 N2203 S2204 G2205 E2206 D2207 Y2210 S2220 D2221 K2229 T2230 K2231 E2232 N2248 E2249 Y2252 K2253 A2254 T2255 H2258 K2259 W2260 D2264 I2267 E2270 W2271 I2272 E2273 M2299 R2300 L2301 I2302
L2308 V2316 F2323 M2353 D2363 D2364 V2365 L2417 P2418 K2419 L2420 K2421 Q2422 M2423 K2424 E2425 E2426 D2427 E2428 D2454 K2466 A2469 N2487 E2488 W2491 D2498 Y2499 L2500 R2531 I2537 V2560 T2571 N2588 G2589 T2596 I2601 F2607 N2608 M2609 P2610
K2614 S2619 P2620 I2621 R2625 Q2638 D2647 L2648 L2649 C2653 L2654 N2655 L2667 N2670 L2692 N2693 A2694 H2695 L2696 S2697 T2698 I2699 D2700 D2701 K2702 A2703 Q2704 K2705 M2706 A2707 V2711 T2714 Y2715 F2718 M2740 F2741 R2742 C2752 P2756 G2757 Q2758 Y2759 S2760 G2761 G2762
D2763 Q2764 G2765 K2766 R2769 L2770 W2771 A2772 K2776 T2797 E2798 S2801 K2802 C2803 I2804 G2805 E2806 F2807 P2808 E2809 T2810 E2811 N2812 P2813 I2814 A2826 G2829 L2830 D2831 Q2832 Q2833 Y2834 T2835 Q2836 I2839 P2840 L2846 K2857 A2858 V2863 V2872 S2873 R2874 L2887 L2888 V2889 G2890
Q2897 C2900 T2904 G2908 I2911 N2923 R2926 E2931 K2934 K2935 I2936 A2937 K2938 I2942 M2947 I2948 T2949 L2959 N2963 G2969 W2970 I2971 L2974 F2975 P2976 K2977 E2978 D2979 M2980 D2981 S2982 L2983 V2984 S2985 G2986 V2987 R2988 N2989 K2992 G2993 E2994 G2995 V2996 D2997 V2998
N2999 N3000 L3001 L3004 I3012 V3019 L3020 C3021 F3022 R3032 W3047 F3048 V3059 E3066 T3071 E3072 E3073 L3080 N3081 V3085 L3122 E3137 M3138 N3141 I3142 E3145 N3148 K3149 V3150 Q3151 G3152 L3153 Q3154 E3155 E3156 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 V3259 L3260 I3261 L3262 F3263 N3264 Q3265 G3266 I3267 T3268 L3269 N3270 D3271 P3272 D3273 E3274 K3275 V3276 W3277 K3278 K3279 A3280 V3281 T3282 F3283 M3284 N3285 N3286 P3287



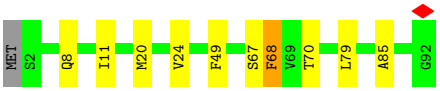
• Molecule 5: Dynein light chain LC8_1a (LC10)

Chain I:

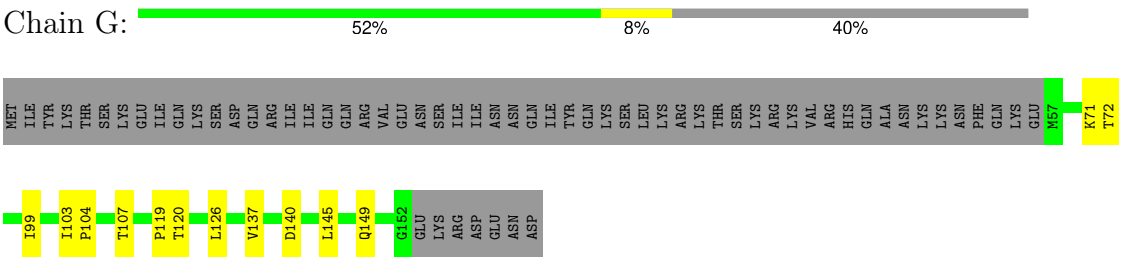


• Molecule 6: Dynein light chain LC8_1b (DLC82)

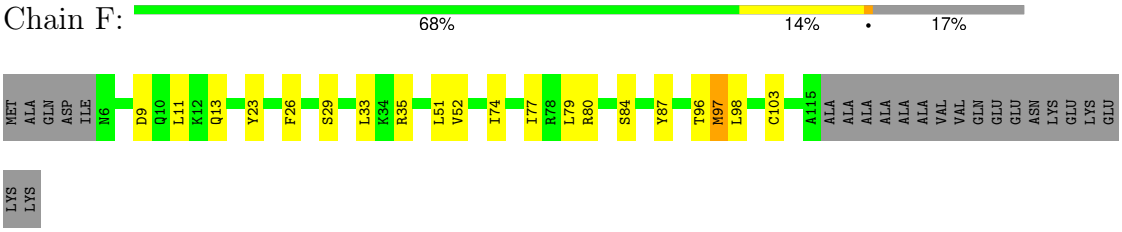
Chain H:



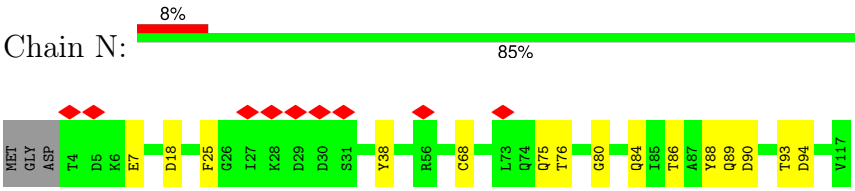
• Molecule 7: Dynein light chain roadblock LC7B



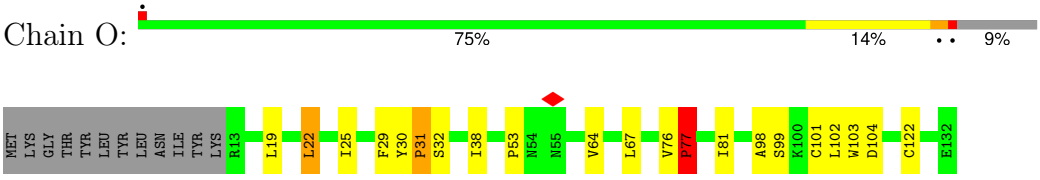
• Molecule 8: Dynein light chain roadblock LC7A



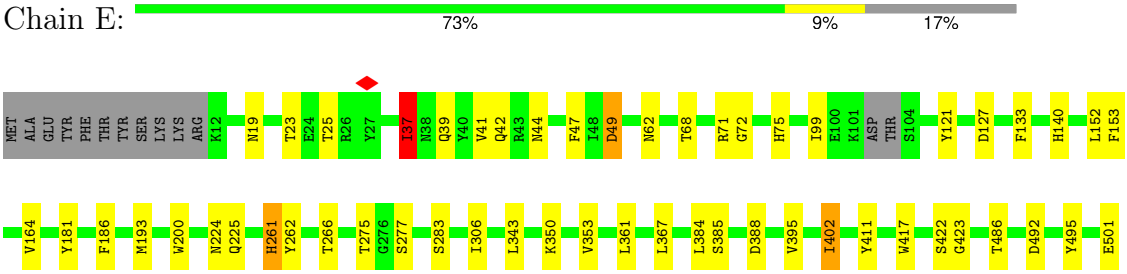
• Molecule 9: Dynein light chain Tctex_b

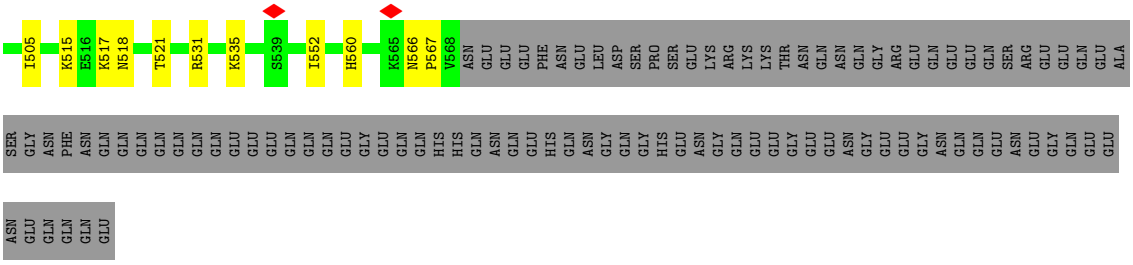


• Molecule 10: Dynein light chain Tctex_a (LC2A)



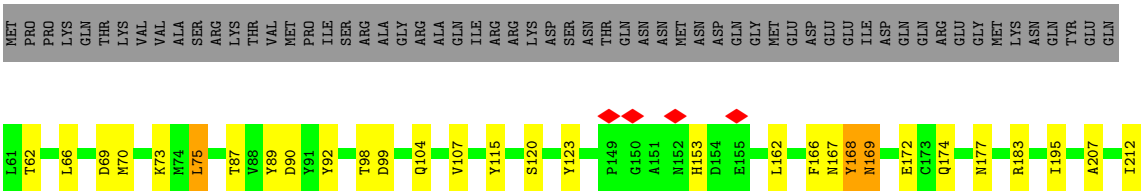
• Molecule 11: Dynein intermediate chain DIC3





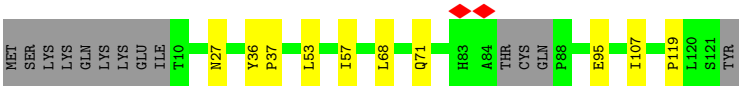
• Molecule 12: Dynein intermediate chain DIC2

Chain D:



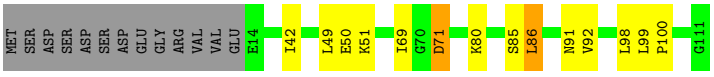
• Molecule 13: Thioredoxin LC3BL

Chain P:



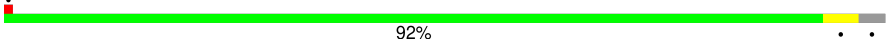
• Molecule 14: Dynein light chain LC8_3b

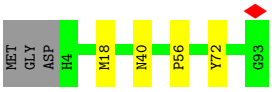
Chain L:



• Molecule 15: Dynein light chain LC8_2a (LC8E)

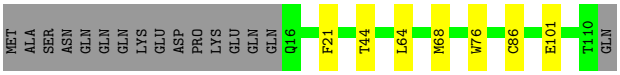
Chain K:





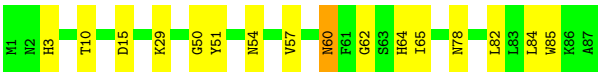
• Molecule 16: Dynein light chain LC8_2b

Chain J:



• Molecule 17: Dynein light chain LC8_3a

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	9.863	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	1015.746, 1061.068, 970.42395	wwPDB
Map dimensions	381, 398, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.666, 2.666, 2.666	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.69	0/34464	0.78	1/46623 (0.0%)
2	C	0.69	1/31037 (0.0%)	0.80	5/42000 (0.0%)
3	Q	0.86	0/1005	0.84	0/1388
4	B	0.70	2/35205 (0.0%)	0.81	7/47647 (0.0%)
5	I	0.68	0/838	0.77	0/1131
6	H	0.67	0/767	0.77	0/1031
7	G	0.69	0/755	0.77	0/1018
8	F	0.68	0/875	0.77	0/1178
9	N	0.69	0/867	0.78	0/1179
10	O	0.67	0/1004	0.80	0/1349
11	E	0.67	0/4522	0.78	0/6114
12	D	0.66	0/4772	0.78	1/6458 (0.0%)
13	P	0.87	0/538	0.86	0/746
14	L	0.66	0/800	0.76	0/1076
15	K	0.66	0/776	0.73	0/1038
16	J	0.63	0/831	0.74	0/1118
17	M	0.65	0/752	0.76	0/1006
All	All	0.69	3/119808 (0.0%)	0.79	14/162100 (0.0%)

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	2
2	C	0	3
4	B	0	4
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1606	PHE	C-N	20.47	1.73	1.34
2	C	1136	PHE	C-N	16.22	1.65	1.34
4	B	730	LEU	C-O	5.28	1.33	1.23

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1136	PHE	O-C-N	26.30	171.08	121.10
2	C	1136	PHE	C-N-CD	23.12	176.95	128.40
4	B	1606	PHE	O-C-N	-20.88	81.42	121.10
4	B	1606	PHE	C-N-CD	-20.37	75.80	120.60
2	C	1136	PHE	CA-C-N	-18.02	66.65	117.10

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	GLU	Peptide
1	A	4250	ARG	Peptide
2	C	2717	ALA	Peptide
2	C	2746	PRO	Peptide
2	C	528	GLU	Peptide

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	33894	0	32284	319	0
2	C	30436	0	29388	319	0
3	Q	1002	0	498	6	0
4	B	34604	0	33084	703	0
5	I	827	0	829	17	0
6	H	750	0	735	7	0
7	G	749	0	772	10	0
8	F	863	0	881	9	0
9	N	855	0	800	13	0
10	O	986	0	1002	11	0
11	E	4423	0	4291	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	4664	0	4484	65	0
13	P	541	0	220	2	0
14	L	783	0	811	9	0
15	K	754	0	716	3	0
16	J	806	0	769	2	0
17	M	735	0	738	9	0
18	A	54	0	24	2	0
18	B	54	0	24	0	0
18	C	54	0	24	3	0
19	A	31	0	12	0	0
19	B	31	0	12	1	0
19	C	31	0	12	0	0
20	A	3	0	0	0	0
20	B	3	0	0	0	0
20	C	3	0	0	0	0
All	All	117936	0	112410	1466	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1466 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1223:LYS:HE2	4:B:1277:ARG:CB	1.23	1.63
4:B:1599:LEU:HB3	4:B:1617:LEU:CG	1.18	1.61
1:A:1219:PHE:HZ	1:A:1263:TYR:CD2	1.17	1.60
1:A:1219:PHE:CE1	1:A:1263:TYR:HA	1.26	1.60
1:A:1219:PHE:CZ	1:A:1263:TYR:CD2	1.89	1.60

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	4381/4620 (95%)	4081 (93%)	258 (6%)	42 (1%)	13 49
2	C	3914/4168 (94%)	3582 (92%)	283 (7%)	49 (1%)	10 43
3	Q	190/202 (94%)	163 (86%)	24 (13%)	3 (2%)	8 38
4	B	4488/4595 (98%)	4017 (90%)	383 (8%)	88 (2%)	6 32
5	I	104/110 (94%)	95 (91%)	8 (8%)	1 (1%)	13 49
6	H	89/92 (97%)	83 (93%)	6 (7%)	0	100 100
7	G	92/159 (58%)	87 (95%)	5 (5%)	0	100 100
8	F	108/133 (81%)	96 (89%)	11 (10%)	1 (1%)	14 52
9	N	112/117 (96%)	92 (82%)	17 (15%)	3 (3%)	4 25
10	O	118/132 (89%)	103 (87%)	10 (8%)	5 (4%)	2 17
11	E	551/670 (82%)	496 (90%)	51 (9%)	4 (1%)	19 57
12	D	569/667 (85%)	510 (90%)	51 (9%)	8 (1%)	9 41
13	P	103/122 (84%)	86 (84%)	11 (11%)	6 (6%)	1 14
14	L	96/111 (86%)	91 (95%)	4 (4%)	1 (1%)	13 49
15	K	88/93 (95%)	79 (90%)	9 (10%)	0	100 100
16	J	93/111 (84%)	84 (90%)	8 (9%)	1 (1%)	12 47
17	M	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	5 27
All	All	15181/16189 (94%)	13817 (91%)	1150 (8%)	214 (1%)	12 41

5 of 214 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO
1	A	197	ILE
1	A	871	LEU
1	A	973	ASP
1	A	3251	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3420/4197 (82%)	3338 (98%)	82 (2%)	44	62
2	C	3149/3691 (85%)	3095 (98%)	54 (2%)	56	72
3	Q	10/186 (5%)	10 (100%)	0	100	100
4	B	3497/4145 (84%)	3399 (97%)	98 (3%)	38	57
5	I	91/95 (96%)	87 (96%)	4 (4%)	24	45
6	H	82/83 (99%)	80 (98%)	2 (2%)	44	62
7	G	86/149 (58%)	85 (99%)	1 (1%)	67	78
8	F	93/109 (85%)	86 (92%)	7 (8%)	11	31
9	N	85/104 (82%)	84 (99%)	1 (1%)	67	78
10	O	106/119 (89%)	99 (93%)	7 (7%)	14	34
11	E	484/597 (81%)	467 (96%)	17 (4%)	31	51
12	D	507/609 (83%)	482 (95%)	25 (5%)	21	42
14	L	87/99 (88%)	83 (95%)	4 (5%)	23	44
15	K	80/82 (98%)	79 (99%)	1 (1%)	65	77
16	J	81/97 (84%)	79 (98%)	2 (2%)	42	61
17	M	78/78 (100%)	74 (95%)	4 (5%)	20	41
All	All	11936/14440 (83%)	11627 (97%)	309 (3%)	42	59

5 of 309 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	4540	LYS
12	D	371	THR
6	H	8	GLN
11	E	127	ASP
14	L	71	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	4177	GLN
17	M	3	HIS
7	G	149	GLN
11	E	481	GLN
2	C	1888	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	ATP	A	4702	20	28,33,33	0.71	0	34,52,52	0.79	1 (2%)
18	ADP	B	4705	20	24,29,29	0.79	0	29,45,45	0.75	1 (3%)
18	ADP	B	4706	20	24,29,29	0.75	0	29,45,45	0.70	1 (3%)
18	ADP	A	4701	20	24,29,29	0.75	0	29,45,45	0.79	1 (3%)
18	ADP	C	4206	20	24,29,29	0.73	0	29,45,45	1.03	2 (6%)
18	ADP	C	4203	20	24,29,29	0.76	1 (4%)	29,45,45	1.25	2 (6%)
19	ATP	B	4701	20	28,33,33	0.71	0	34,52,52	0.84	1 (2%)
19	ATP	C	4201	20	28,33,33	0.69	0	34,52,52	0.78	1 (2%)
18	ADP	A	4703	-	24,29,29	0.75	0	29,45,45	1.05	2 (6%)

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
19	ATP	A	4702	20	-	5/18/38/38	0/3/3/3
18	ADP	B	4705	20	-	5/12/32/32	0/3/3/3
18	ADP	B	4706	20	-	2/12/32/32	0/3/3/3
18	ADP	A	4701	20	-	5/12/32/32	0/3/3/3
18	ADP	C	4206	20	-	4/12/32/32	0/3/3/3
18	ADP	C	4203	20	-	5/12/32/32	0/3/3/3
19	ATP	B	4701	20	-	0/18/38/38	0/3/3/3
19	ATP	C	4201	20	-	4/18/38/38	0/3/3/3
18	ADP	A	4703	-	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	4203	ADP	C8-N7	-2.02	1.31	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	4203	ADP	C4'-O4'-C1'	-4.29	106.00	109.92
18	A	4703	ADP	C4'-O4'-C1'	-3.95	106.31	109.92
18	C	4206	ADP	C4'-O4'-C1'	-3.56	106.67	109.92
18	C	4203	ADP	C1'-N9-C4	2.70	131.39	126.64
19	B	4701	ATP	C5-C6-N6	2.40	123.97	120.31

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	4701	ADP	PA-O3A-PB-O3B
18	C	4203	ADP	C5'-O5'-PA-O1A
18	C	4203	ADP	C5'-O5'-PA-O2A
18	C	4203	ADP	C5'-O5'-PA-O3A
18	C	4206	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	4701	ADP	1	0
18	C	4206	ADP	2	0

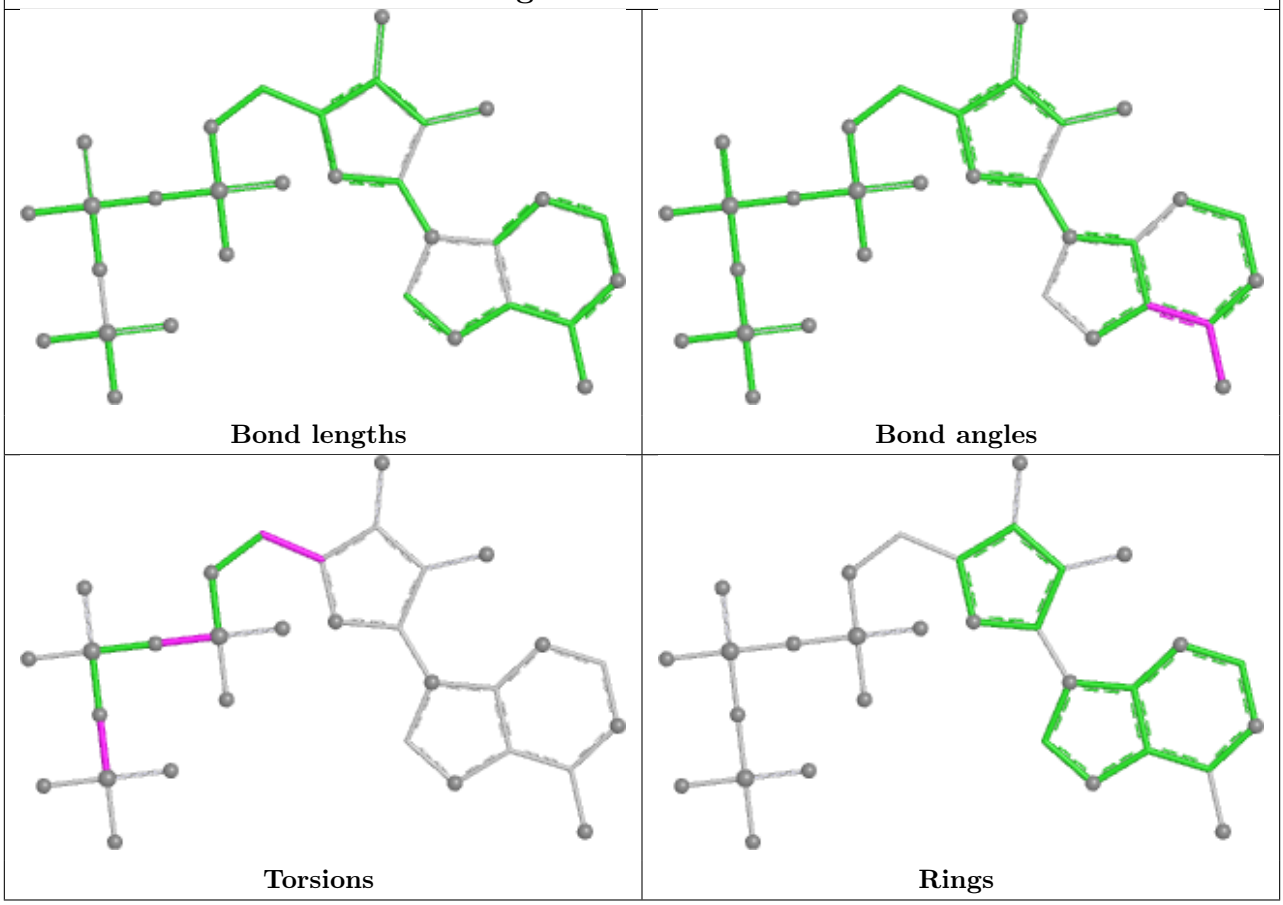
Continued on next page...

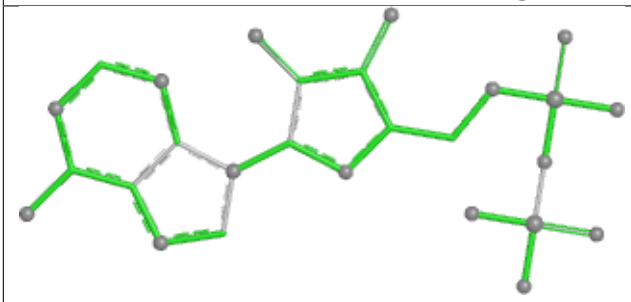
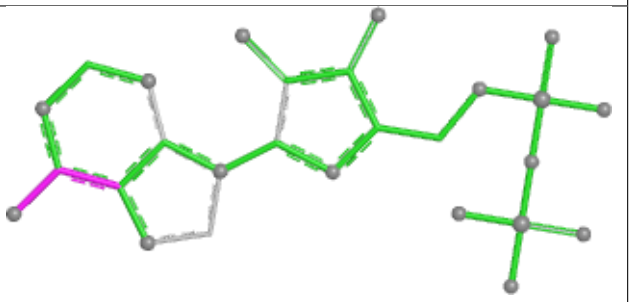
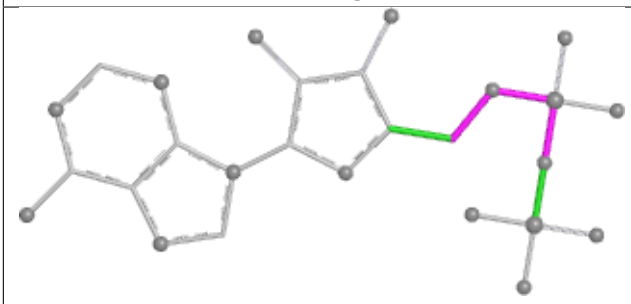
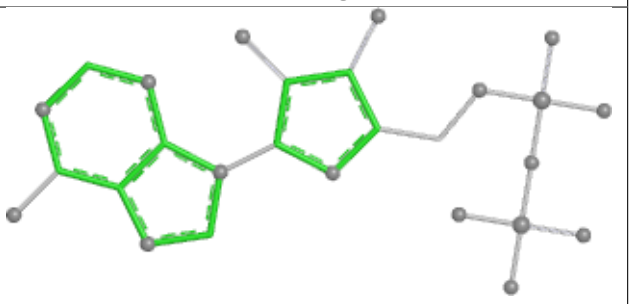
Continued from previous page...

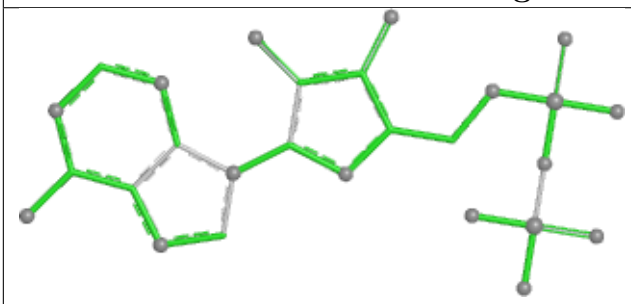
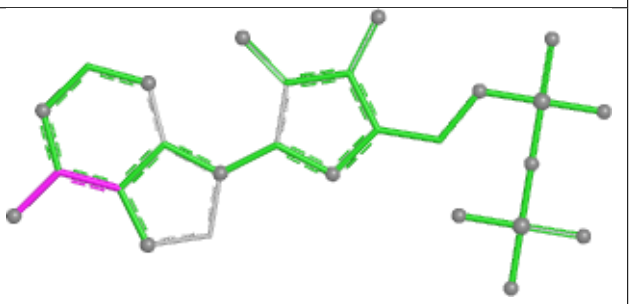
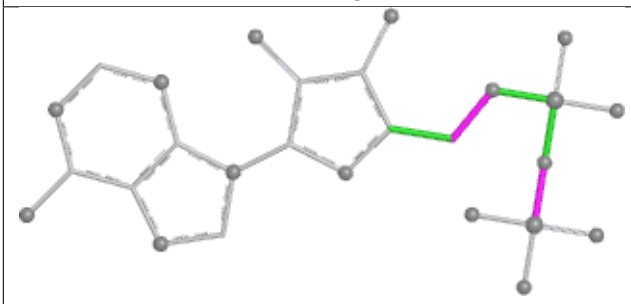
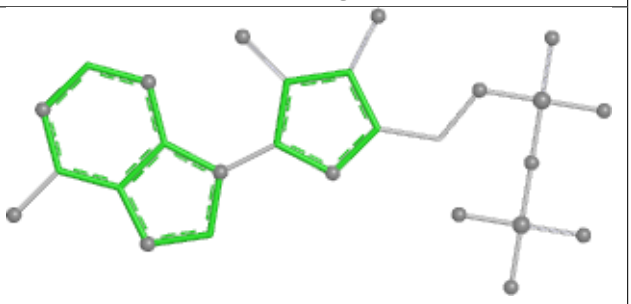
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	4203	ADP	1	0
19	B	4701	ATP	1	0
18	A	4703	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

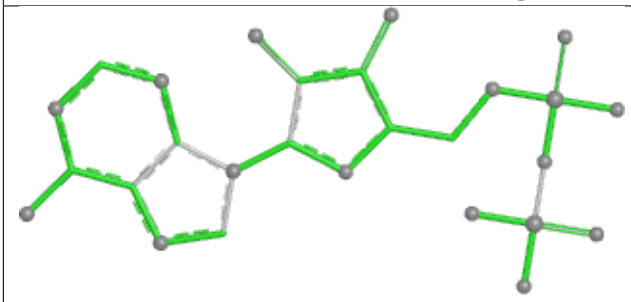
Ligand ATP A 4702



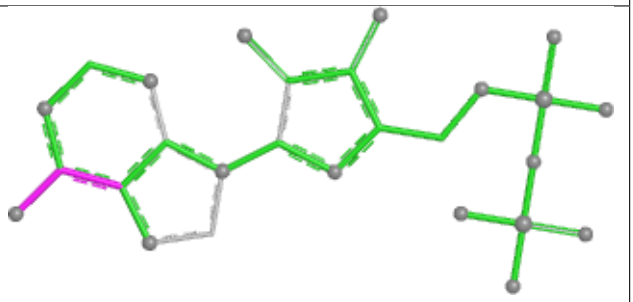
Ligand ADP B 4705	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 4706	
 Bond lengths	 Bond angles
 Torsions	 Rings

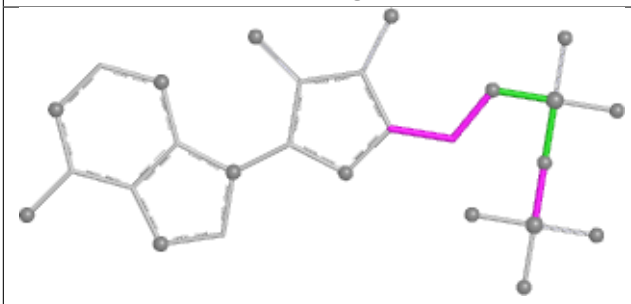
Ligand ADP A 4701



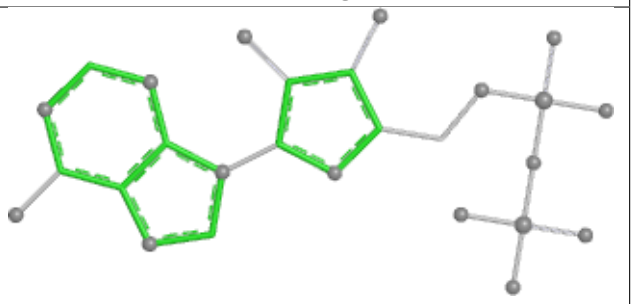
Bond lengths



Bond angles

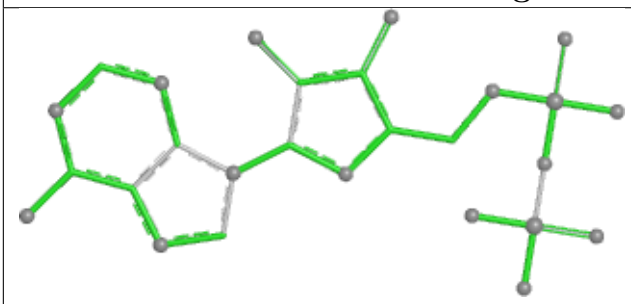


Torsions

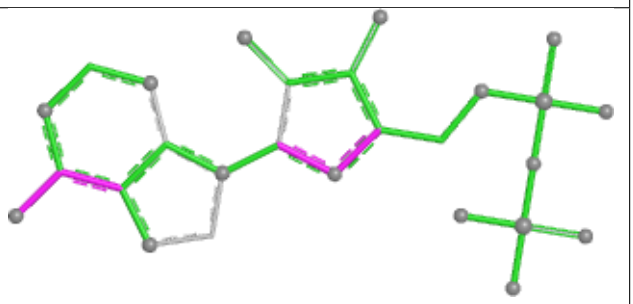


Rings

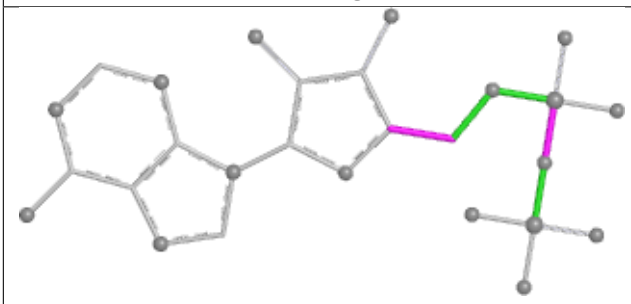
Ligand ADP C 4206



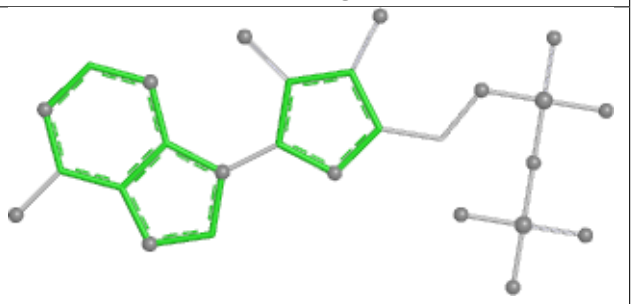
Bond lengths



Bond angles

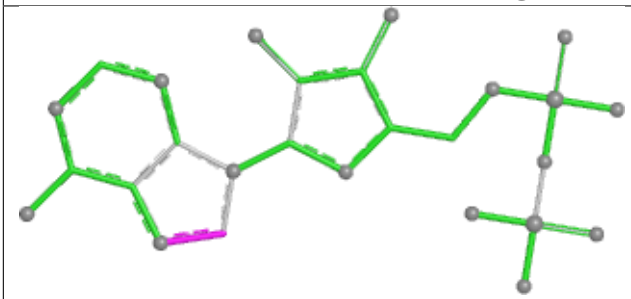


Torsions

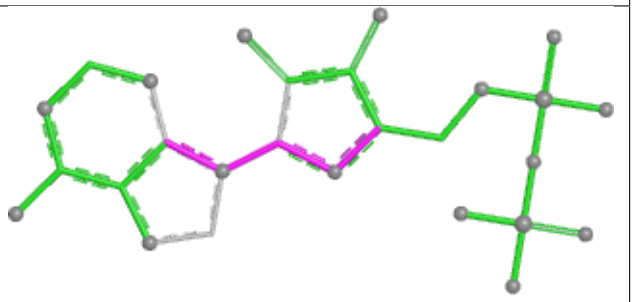


Rings

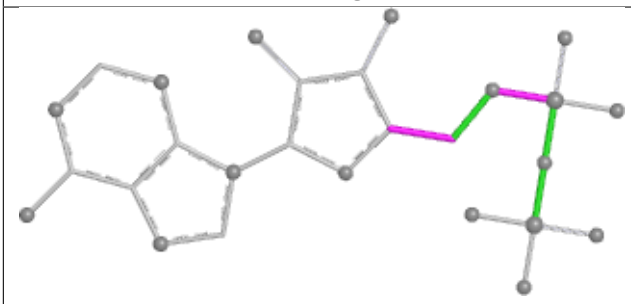
Ligand ADP C 4203



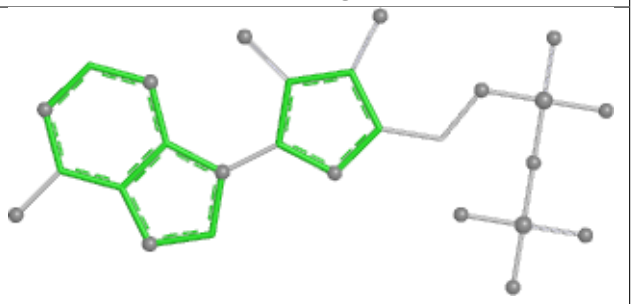
Bond lengths



Bond angles

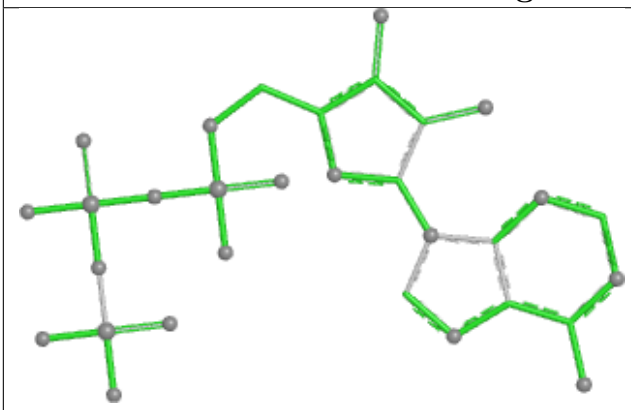


Torsions

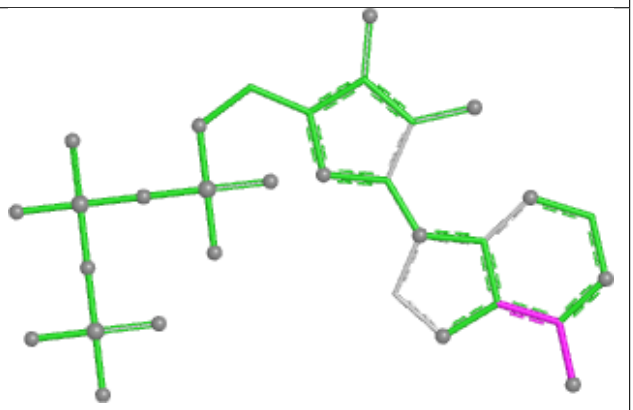


Rings

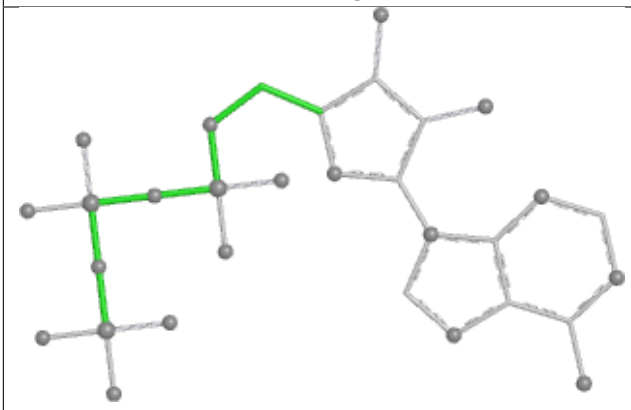
Ligand ATP B 4701



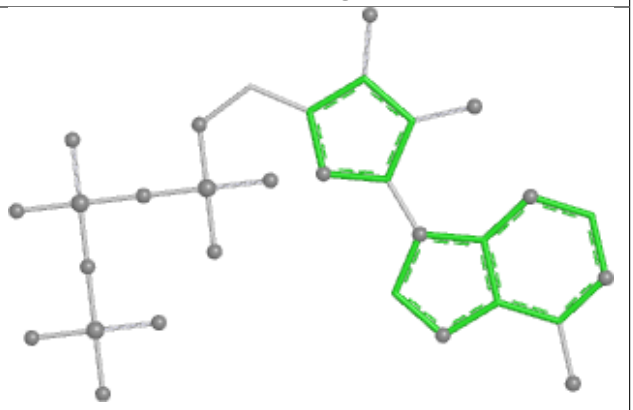
Bond lengths



Bond angles

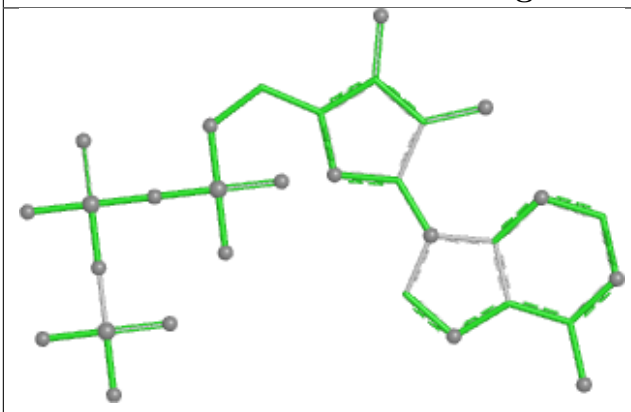


Torsions

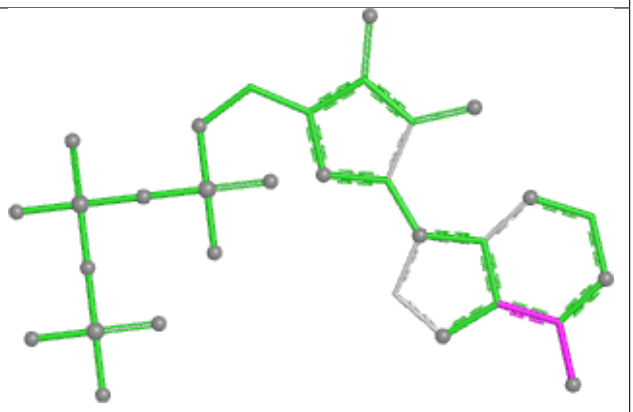


Rings

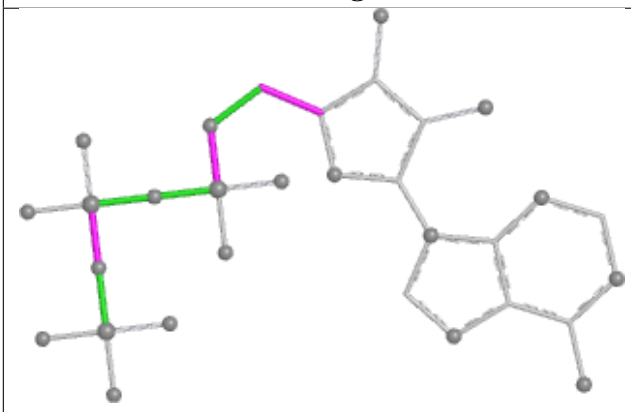
Ligand ATP C 4201



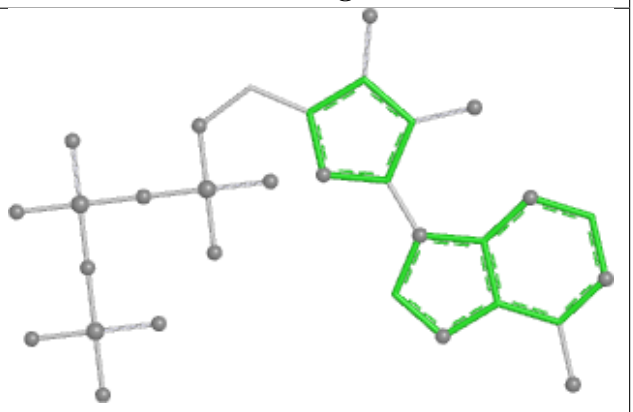
Bond lengths



Bond angles

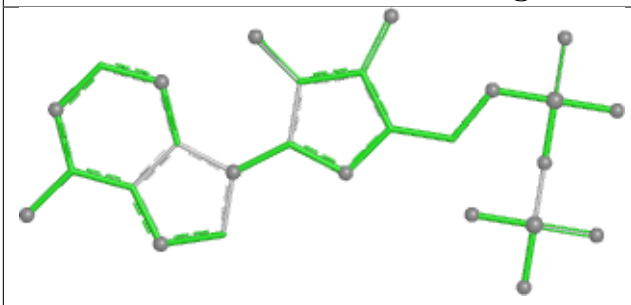


Torsions

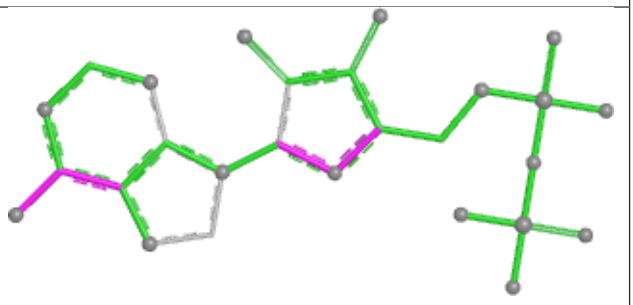


Rings

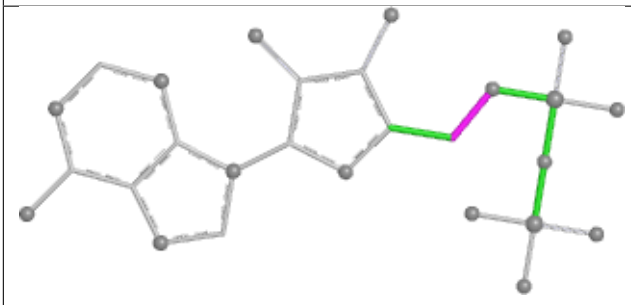
Ligand ADP A 4703



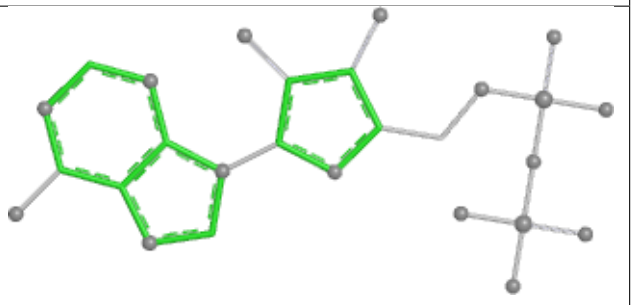
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
2	C	3
4	B	3
12	D	2
13	P	1
7	G	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	364:ILE	C	365:PHE	N	4.18
1	B	25:GLN	C	26:LYS	N	3.78
1	D	216:HIS	C	217:GLN	N	3.67
1	A	53:ILE	C	54:PHE	N	3.57
1	A	115:ASP	C	116:ASN	N	3.46

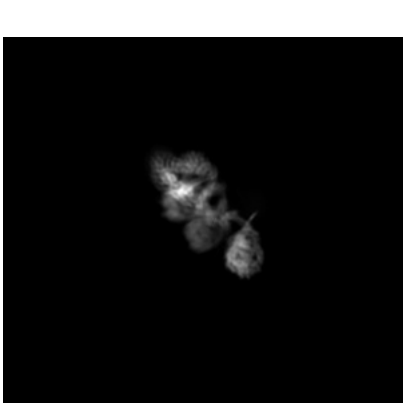
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22840. These allow visual inspection of the internal detail of the map and identification of artifacts.

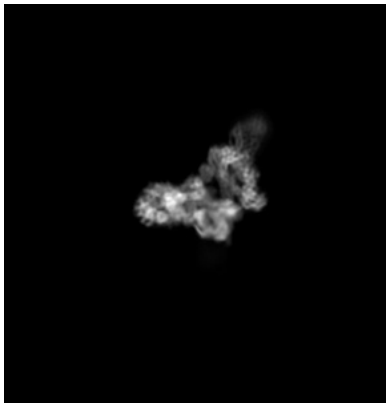
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

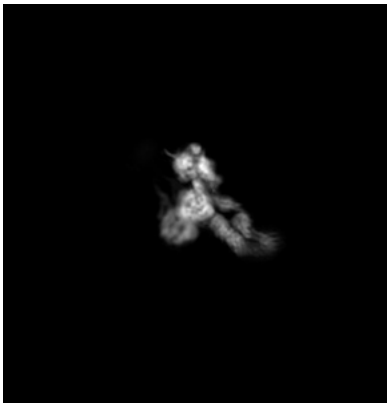
6.1.1 Primary map



X



Y



Z

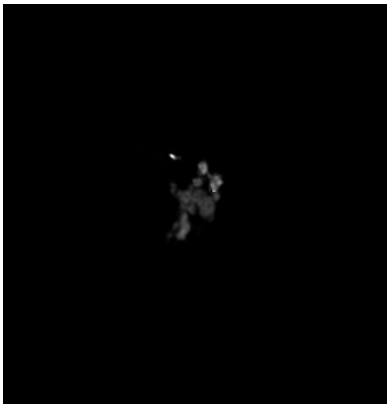
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 190

Y Index: 199

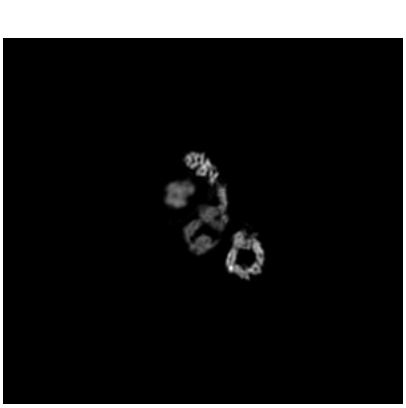


Z Index: 182

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: 189

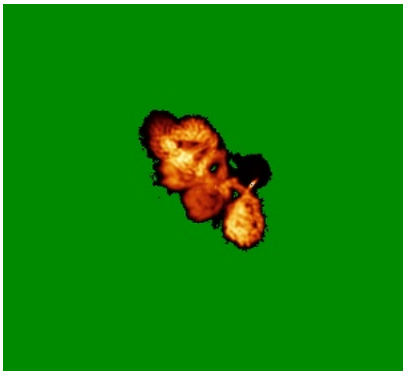
Y Index: 186

Z Index: 209

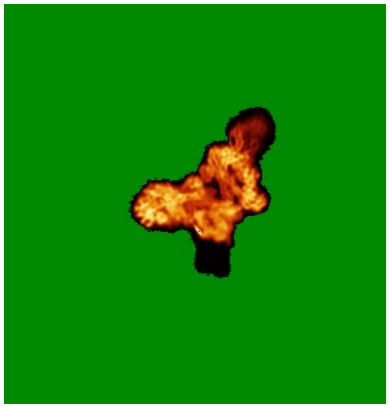
The images above show the largest variance slices of the map in three orthogonal directions.

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

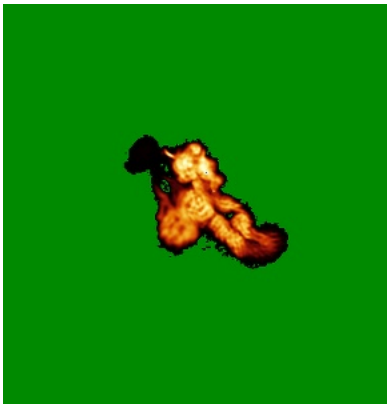
6.4.1 Primary map



X



Y

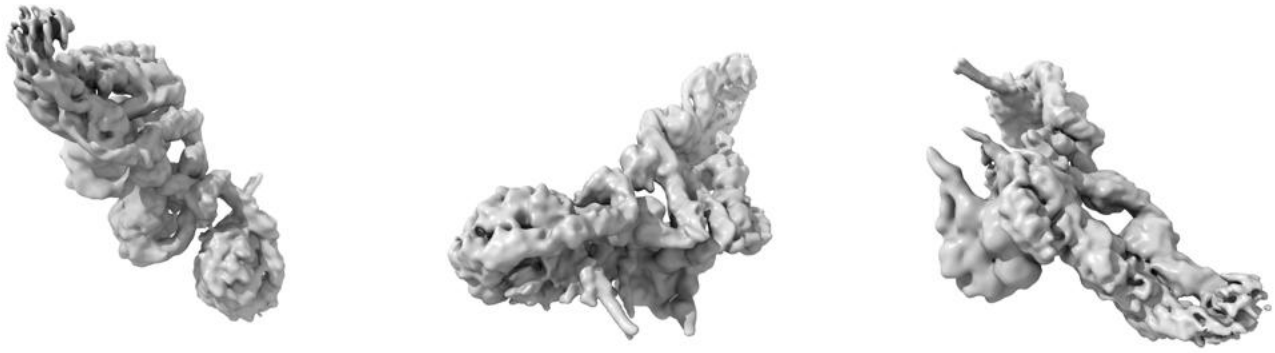


Z

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 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

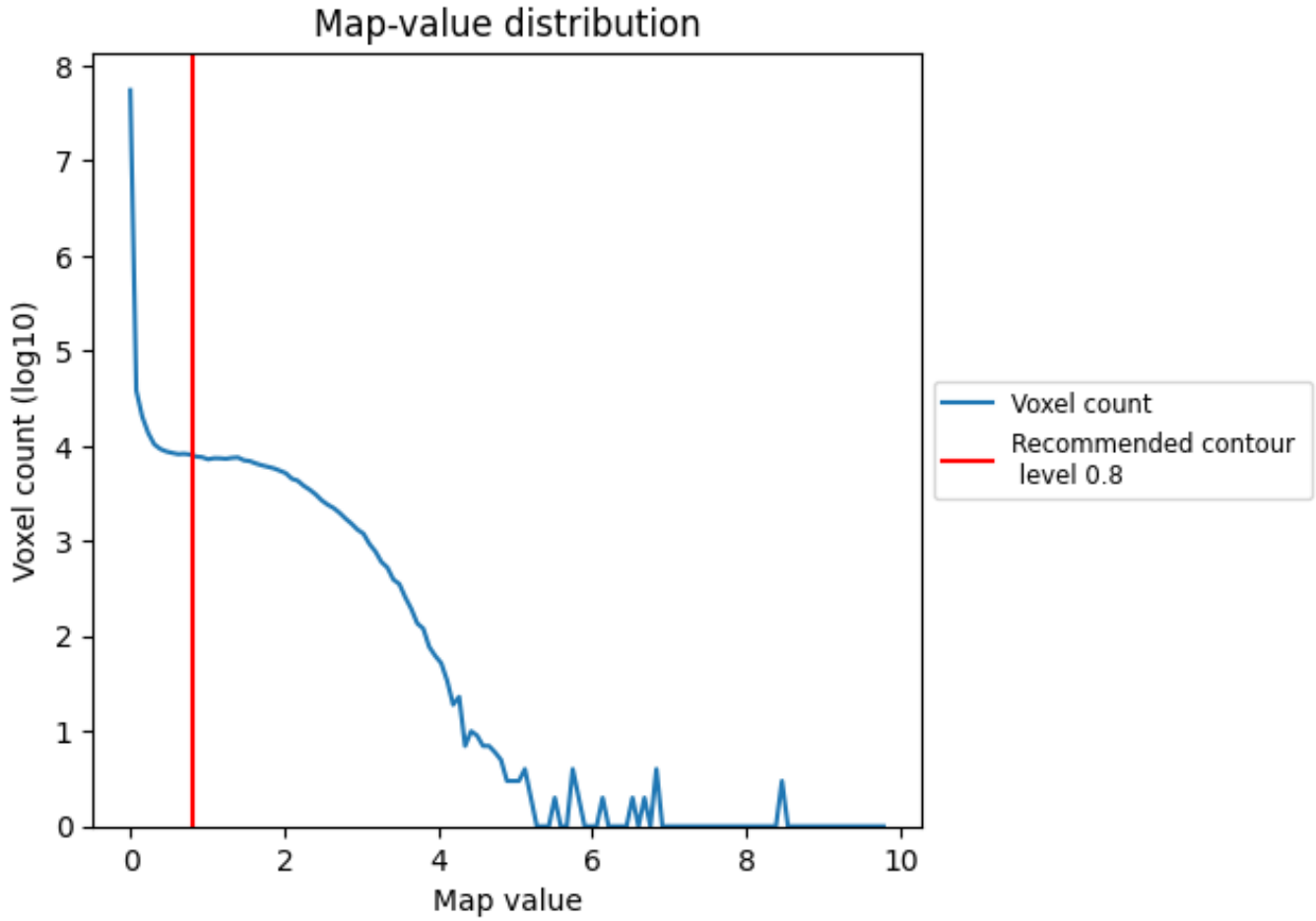
6.6 Mask visualisation (i)

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

7 Map analysis

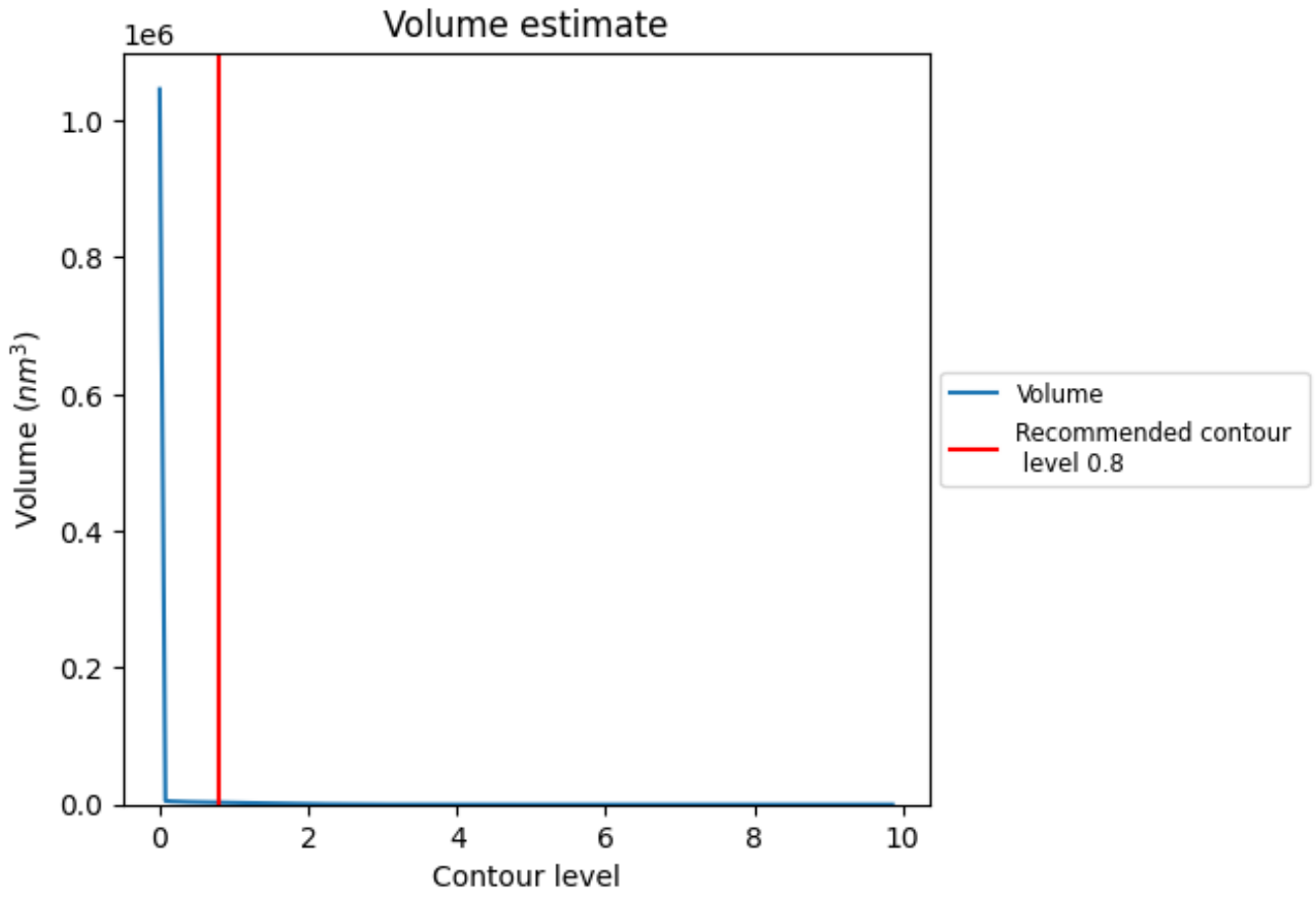
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 2909 nm^3; this corresponds to an approximate mass of 2628 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

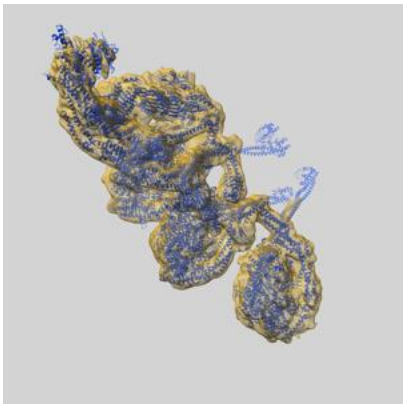
8 Fourier-Shell correlation (i)

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

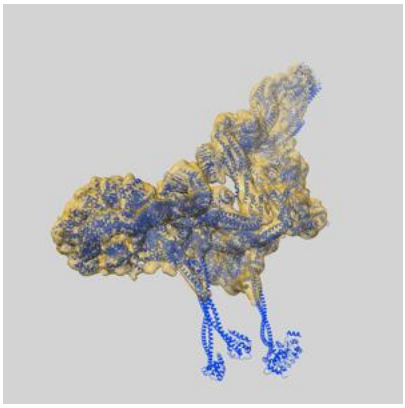
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22840 and PDB model 7KEK. Per-residue inclusion information can be found in section 3 on page 9.

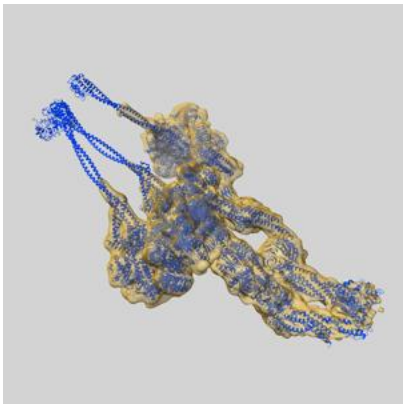
9.1 Map-model overlay



X



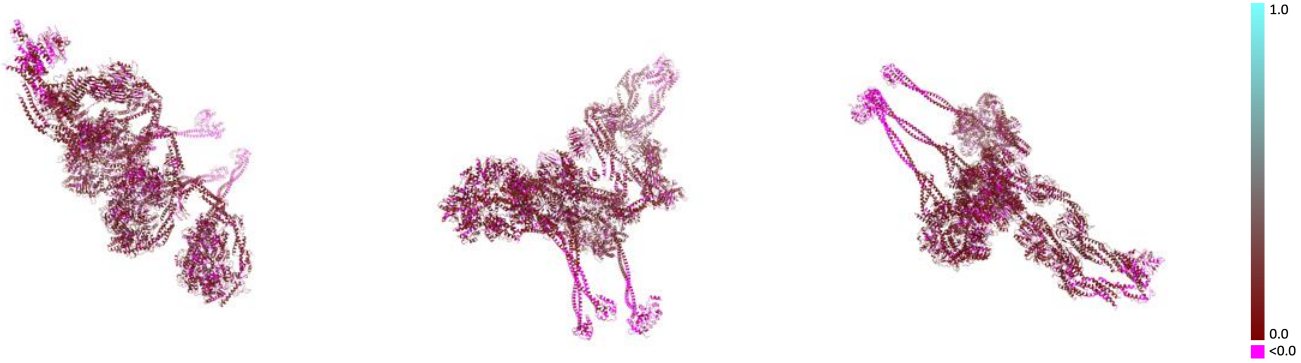
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

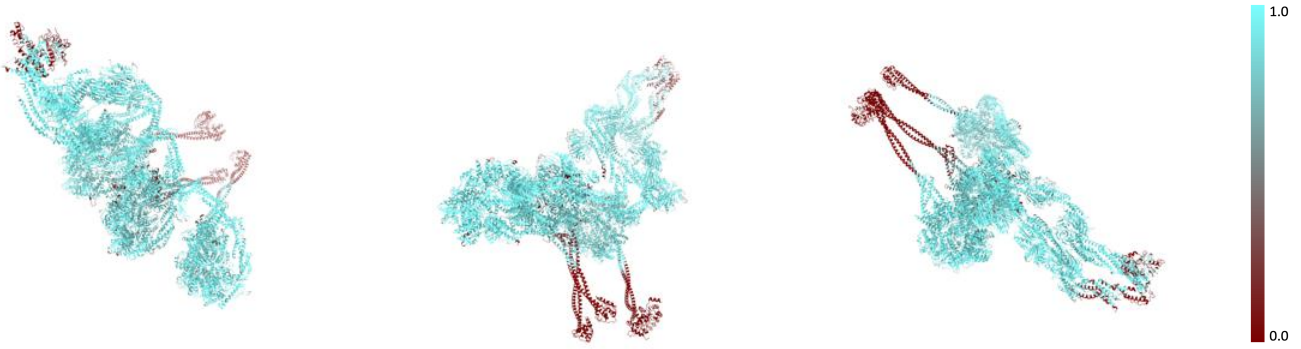
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

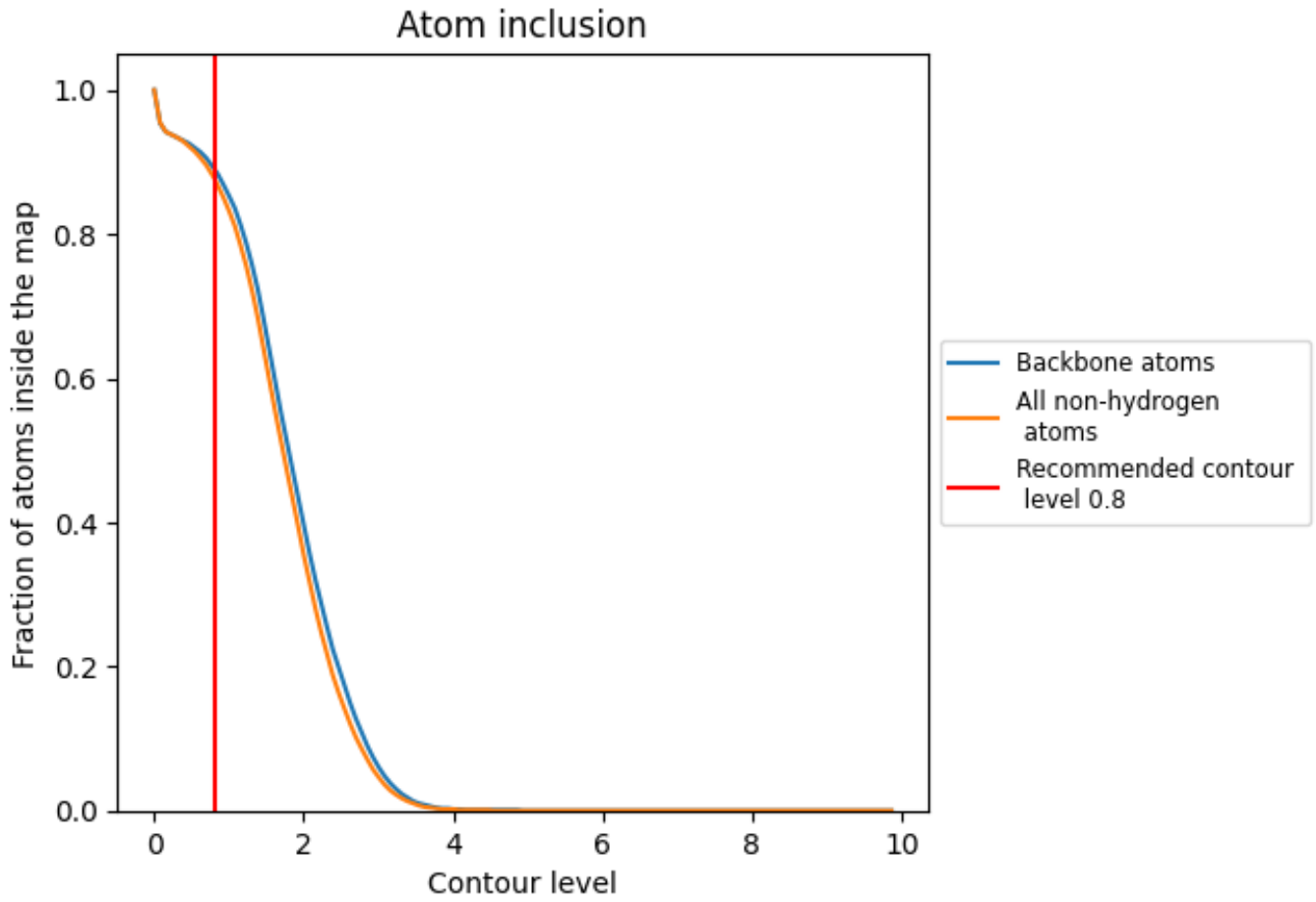
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.0820
A	0.8690	0.0750
B	0.8440	0.0940
C	0.9000	0.0720
D	0.9770	0.0930
E	0.9660	0.0980
F	0.9940	0.1140
G	0.9730	0.1140
H	0.9880	0.1000
I	0.9670	0.1140
J	0.9860	0.0810
K	0.9850	0.0970
L	0.9870	0.1020
M	0.9720	0.0830
N	0.9110	0.0660
O	0.9670	0.0780
P	0.9760	0.1150
Q	0.0000	-0.0550