wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 12:56 PM EST

PDB ID	:	7K5B
EMDB ID	:	EMD-22679
Title	:	Structure of outer-arm dynein bound to microtubule doublet in microtubule binding state 2 (MTBS-2)
Authors	:	Rao, Q.; Zhang, K.
Deposited on	:	2020-09-16
Resolution	:	4.50 Å(reported)

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

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

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

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

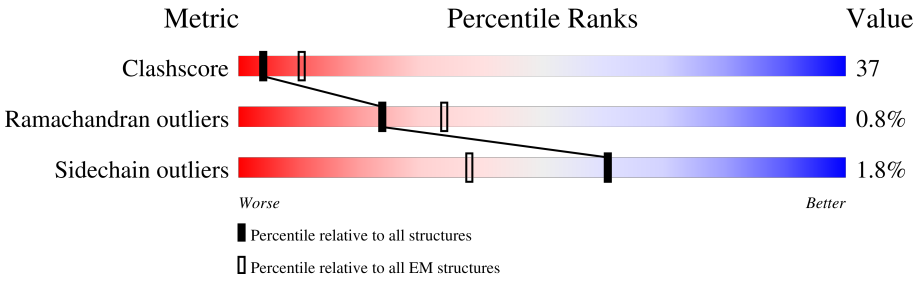
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.50 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
Sidechain outliers	154315	3826

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	4615	6% 73% 23%
2	B	4588	72% 25%
3	C	3947	82% 17%
4	D	595	6% 43% 52%
5	E	557	45% 54%
6	F	128	13% 50% 49%
7	G	151	32% 52% 38% 7%
8	H	91	5% 37% 63%

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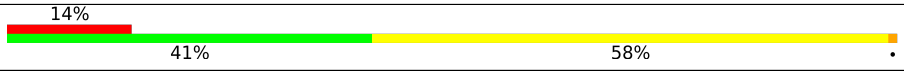
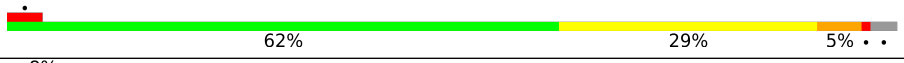
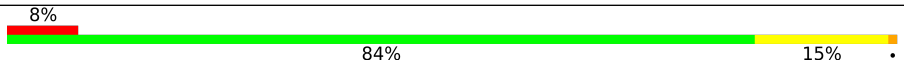
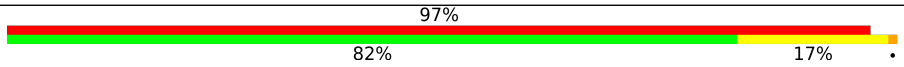
Mol	Chain	Length	Quality of chain
9	I	106	
10	J	95	
11	K	90	
12	L	111	
13	M	87	
14	N	114	
15	O	120	
16	P	112	
17	Q	192	
18	R	150	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	ADP	A	4701	-	-	X	-
19	ADP	A	4901	-	-	X	-
19	ADP	B	5501	-	-	X	-
19	ADP	C	4702	-	-	X	-
20	ATP	A	4801	-	-	X	-
20	ATP	B	5601	-	-	X	-
21	MG	A	5002	-	-	X	-

2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 119573 atoms, of which 156 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 heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4453	33975	21575	5802	6440	158	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3238	ASN	ASP	conflict	UNP Q22A67

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4524	34751	22080	5950	6571	150	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	ALA	GLN	conflict	UNP I7M9J2
B	1287	ALA	LEU	conflict	UNP I7M9J2
B	3977	ALA	SER	conflict	UNP I7M9J2

- Molecule 3 is a protein called gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	3947	30427	19395	5159	5724	149	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	579	4680	2975	791	883	31	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	555	Total	C	N	O	S	0	0
			4440	2798	762	858	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	128	Total	C	N	O	S	0	0
			996	625	176	193	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1024	636	184	203	1		

- Molecule 8 is a protein called Dynein light chain.

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

- Molecule 9 is a protein called Dynein light chain.

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

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	95	Total	C	N	O	S	0	0
			807	527	135	140	5		

- Molecule 11 is a protein called Dynein light chain.

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

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	111	Total	C	N	O	S	0	0
			855	555	145	152	3		

- Molecule 13 is a protein called Dynein light chain.

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

- Molecule 14 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	N	O	S	0	0
			852	542	142	165	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	92	ALA	ASN	conflict	UNP A4VEB3

- Molecule 15 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	120	Total	C	N	O	S	0	0
			994	639	173	179	3		

- Molecule 16 is a protein called Thioredoxin.

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

- Molecule 17 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	192	Total	C	N	O	0	0
			1006	610	203	193		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	2	ALA	SER	conflict	UNP Q1HGH9

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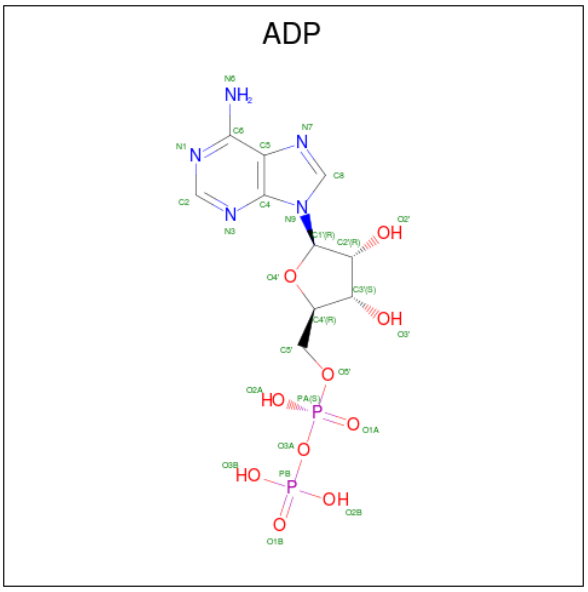
Chain	Residue	Modelled	Actual	Comment	Reference
Q	179	MET	TYR	conflict	UNP Q1HGH9

- Molecule 18 is a protein called Dynein light chain 4A.

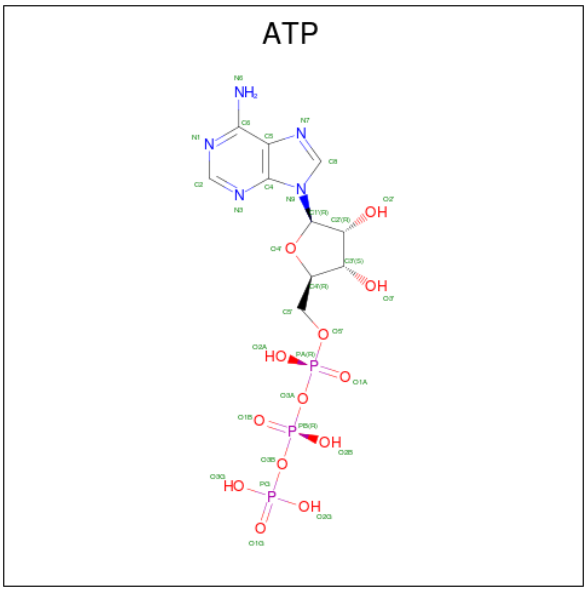
Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	150	Total	C	H	N	O	0	0
			895	439	156	150	150		

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
19	A	1	Total	C	N	O	P	0
			54	20	10	20	4	
19	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
19	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
19	C	1	Total	C	N	O	P	0
			54	20	10	20	4	
19	C	1	Total	C	N	O	P	0
			54	20	10	20	4	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

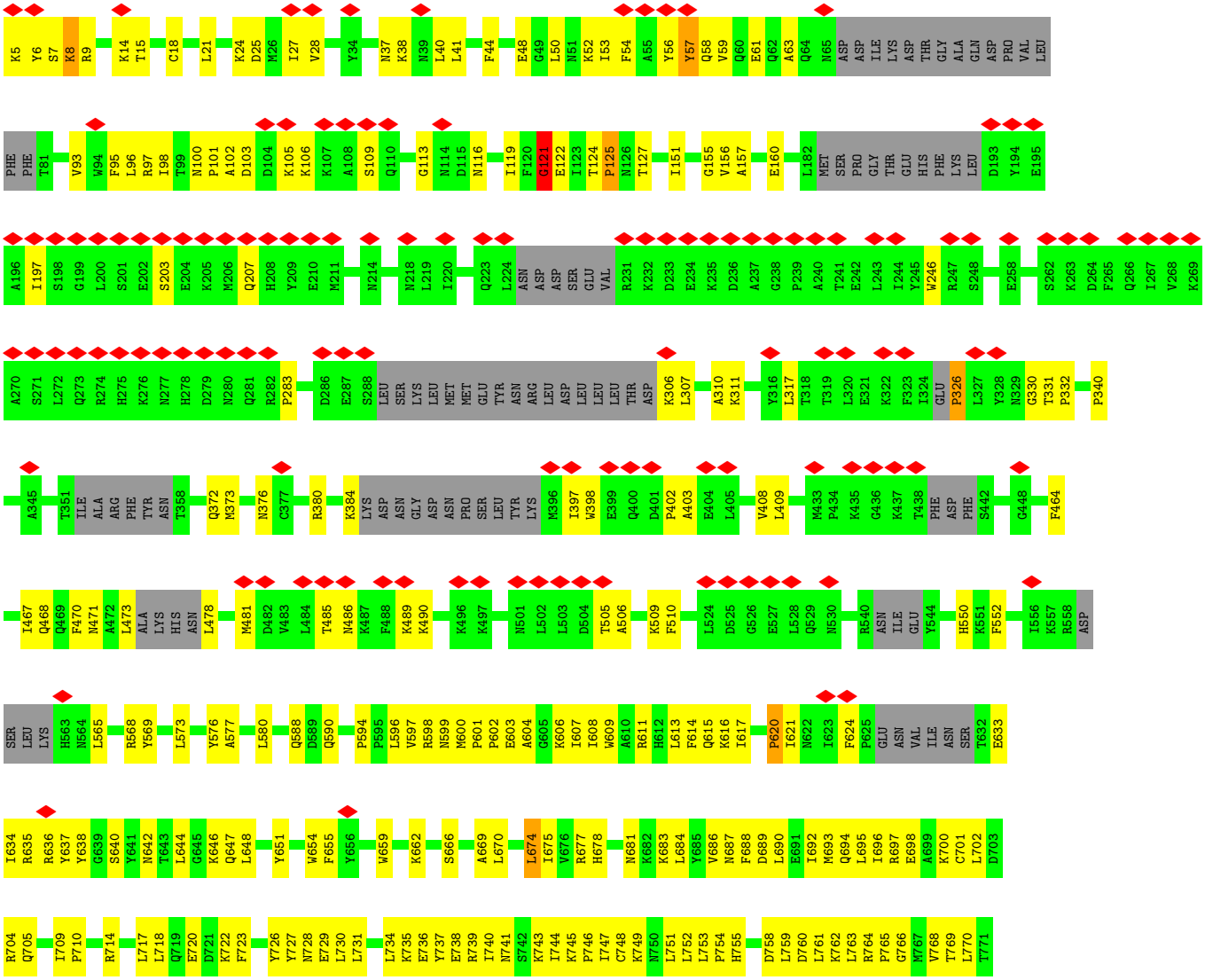
Mol	Chain	Residues	Atoms		AltConf
21	A	3	Total	Mg	0
			3	3	
21	B	3	Total	Mg	0
			3	3	
21	C	3	Total	Mg	0
			3	3	

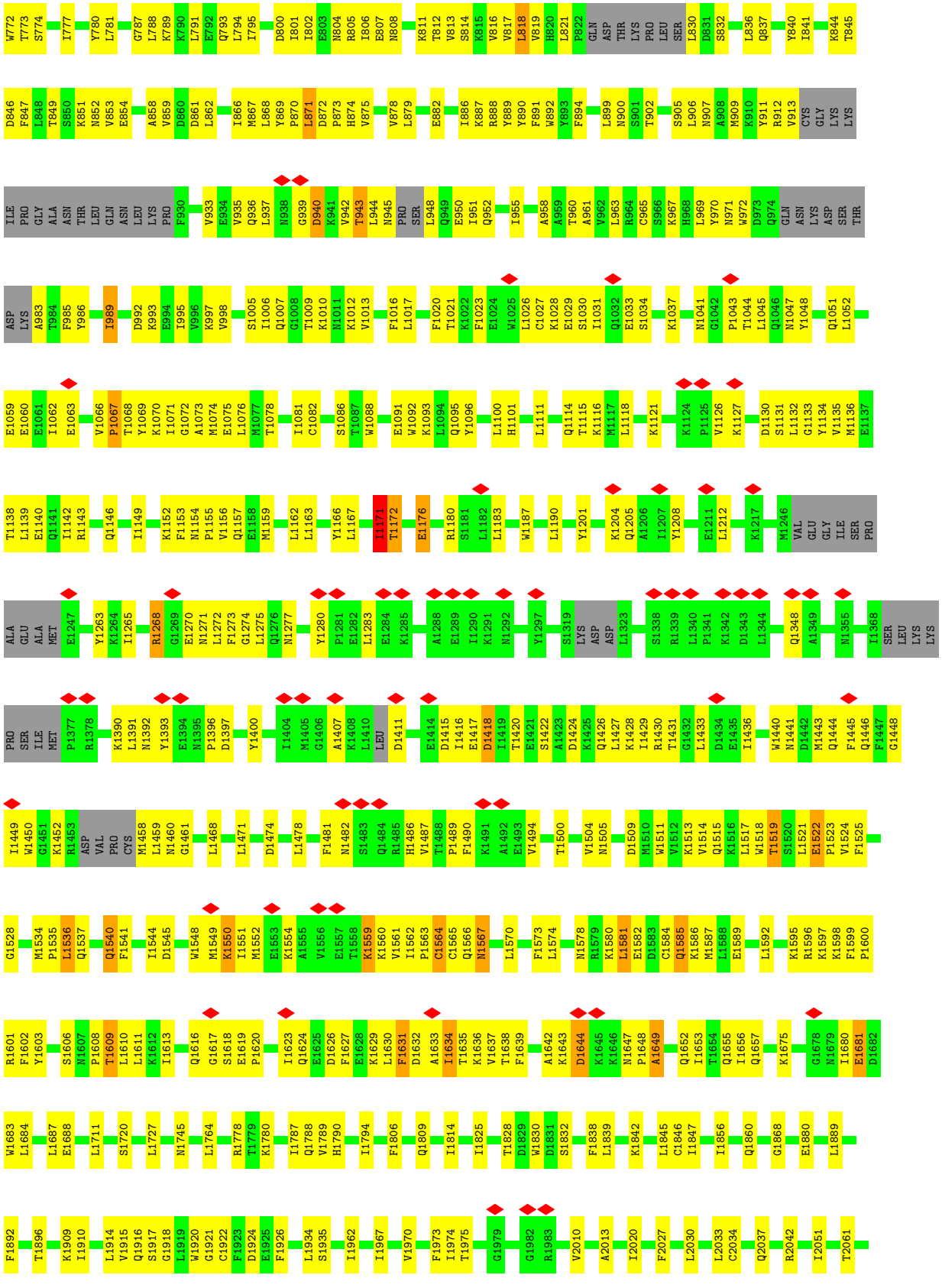
3 Residue-property plots (i)

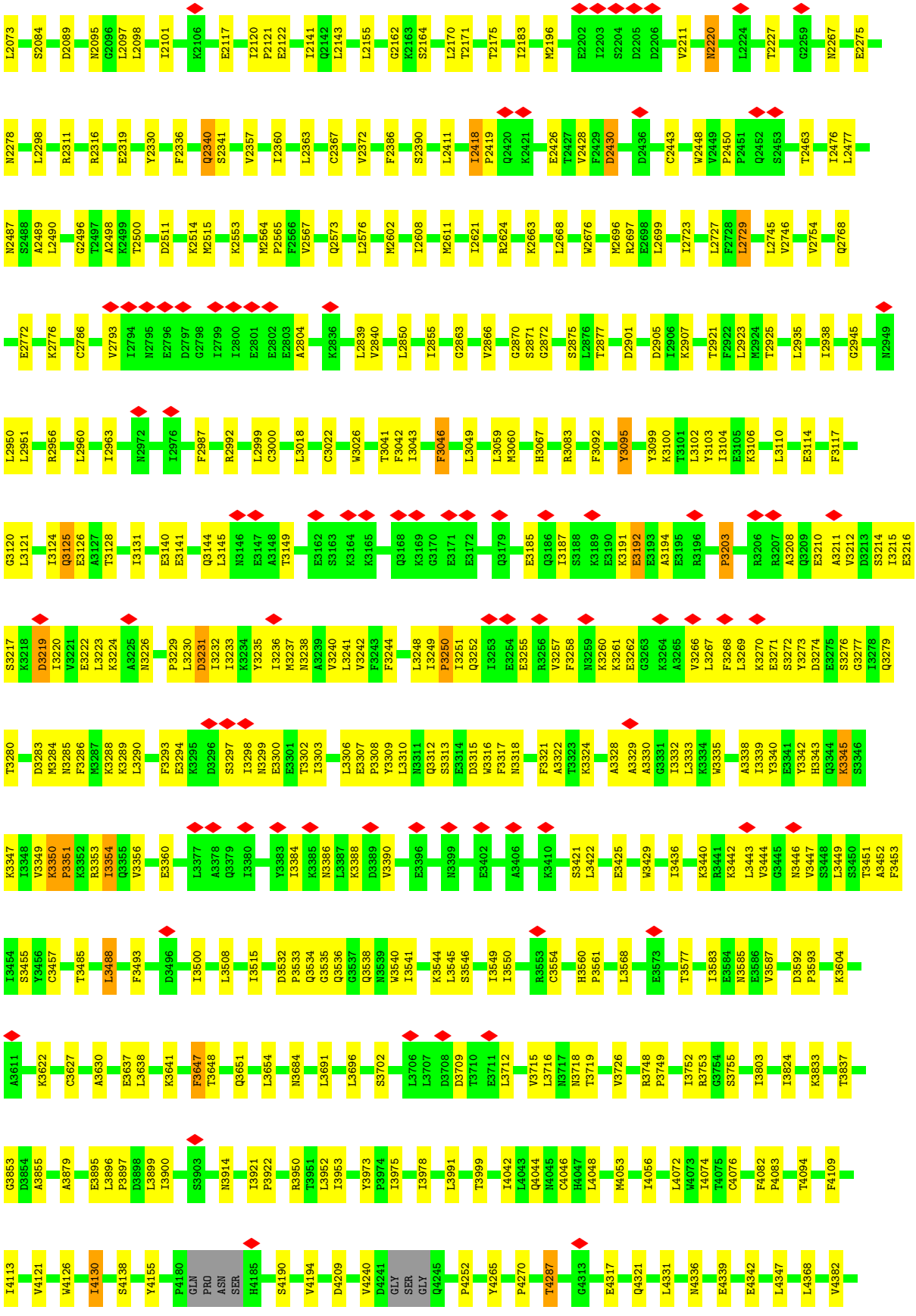
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

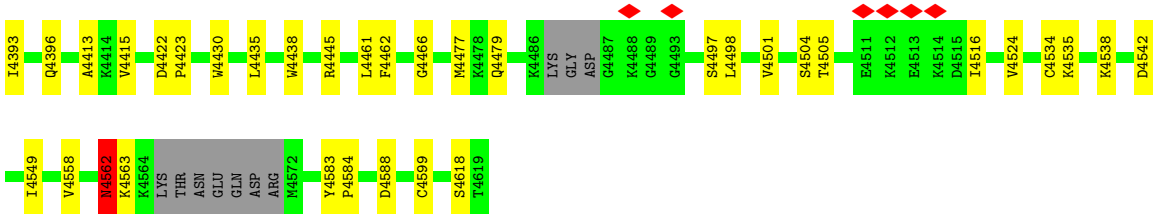
• Molecule 1: Dynein heavy chain, outer arm protein

Chain A:



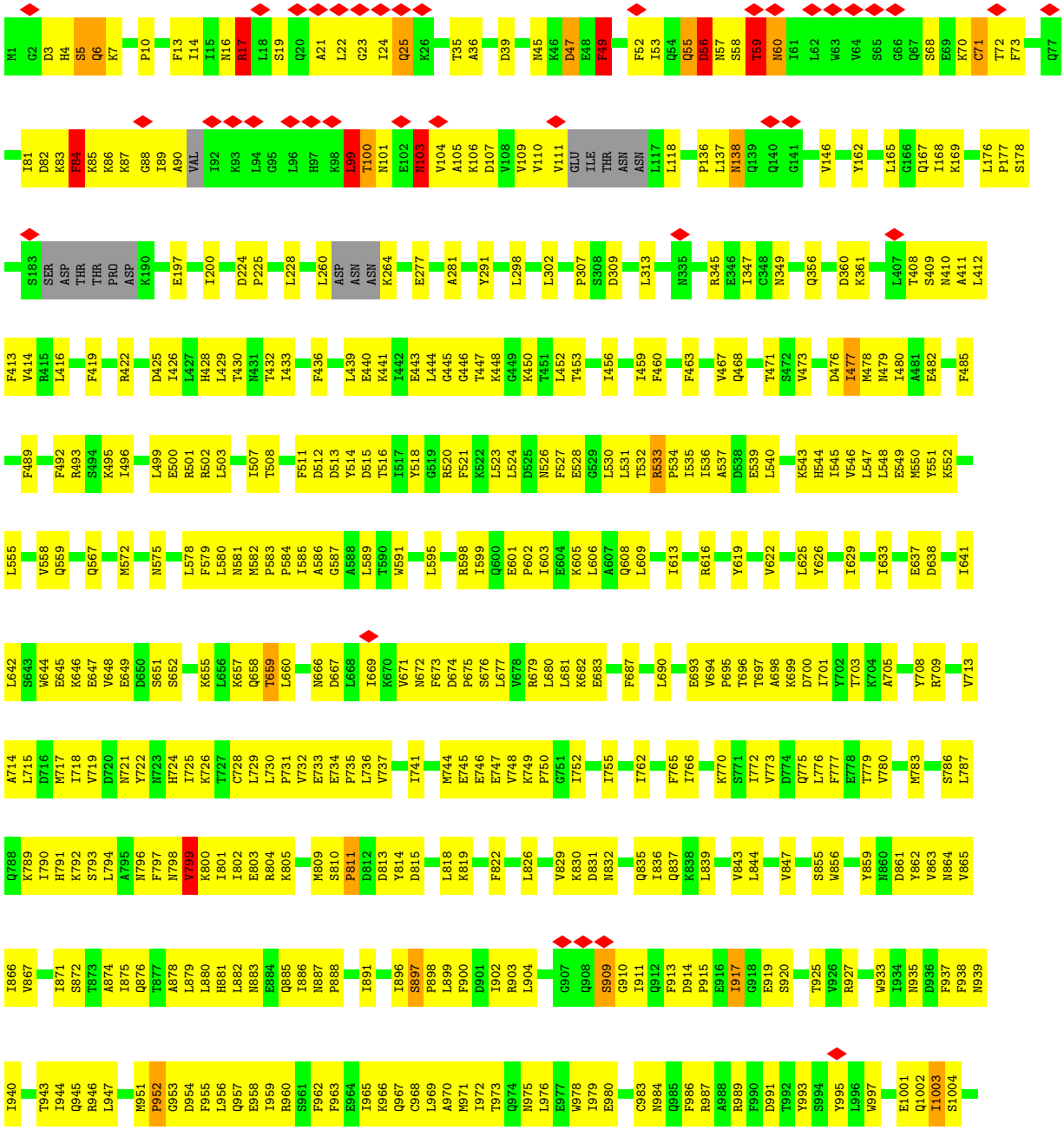


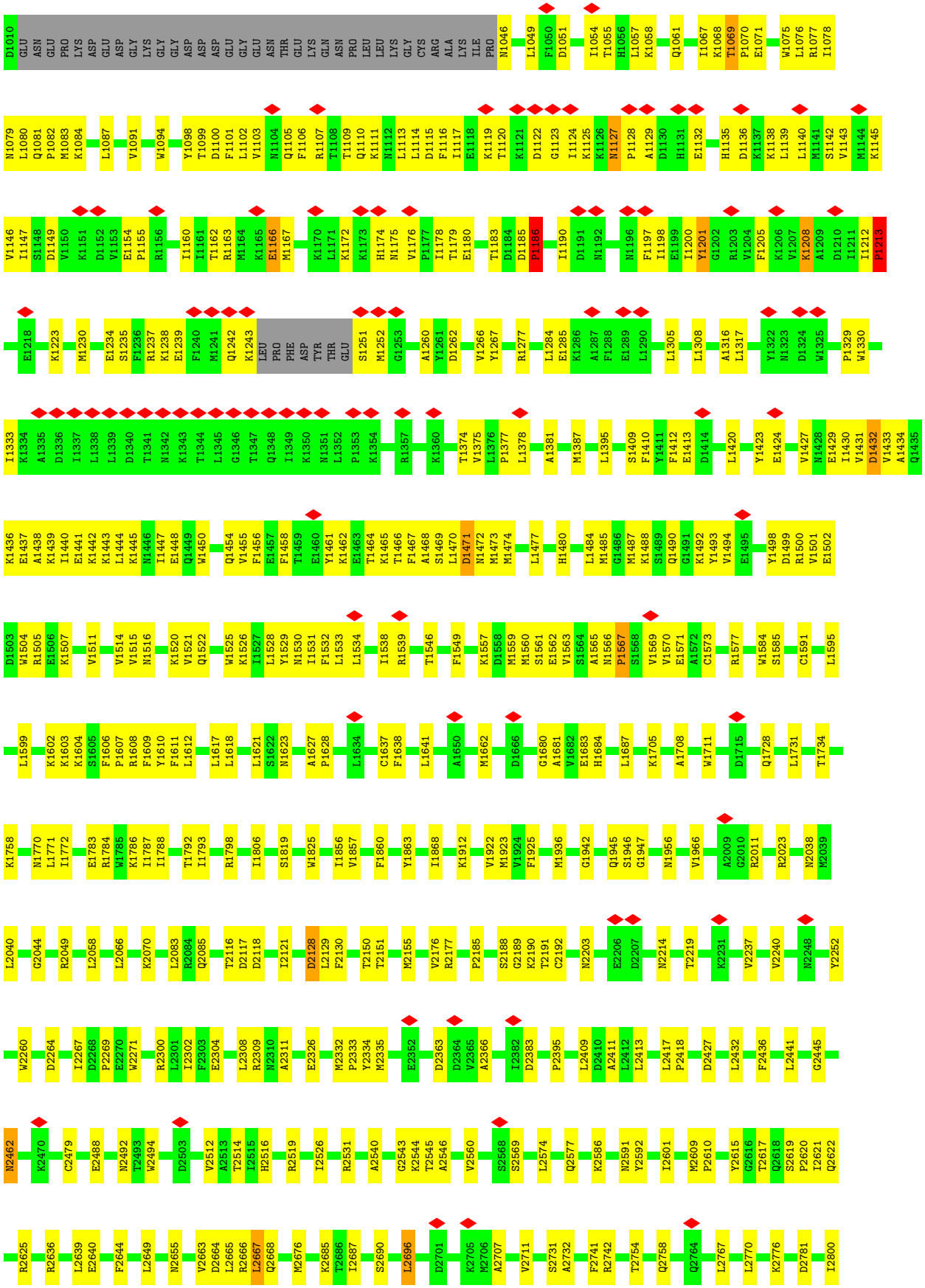


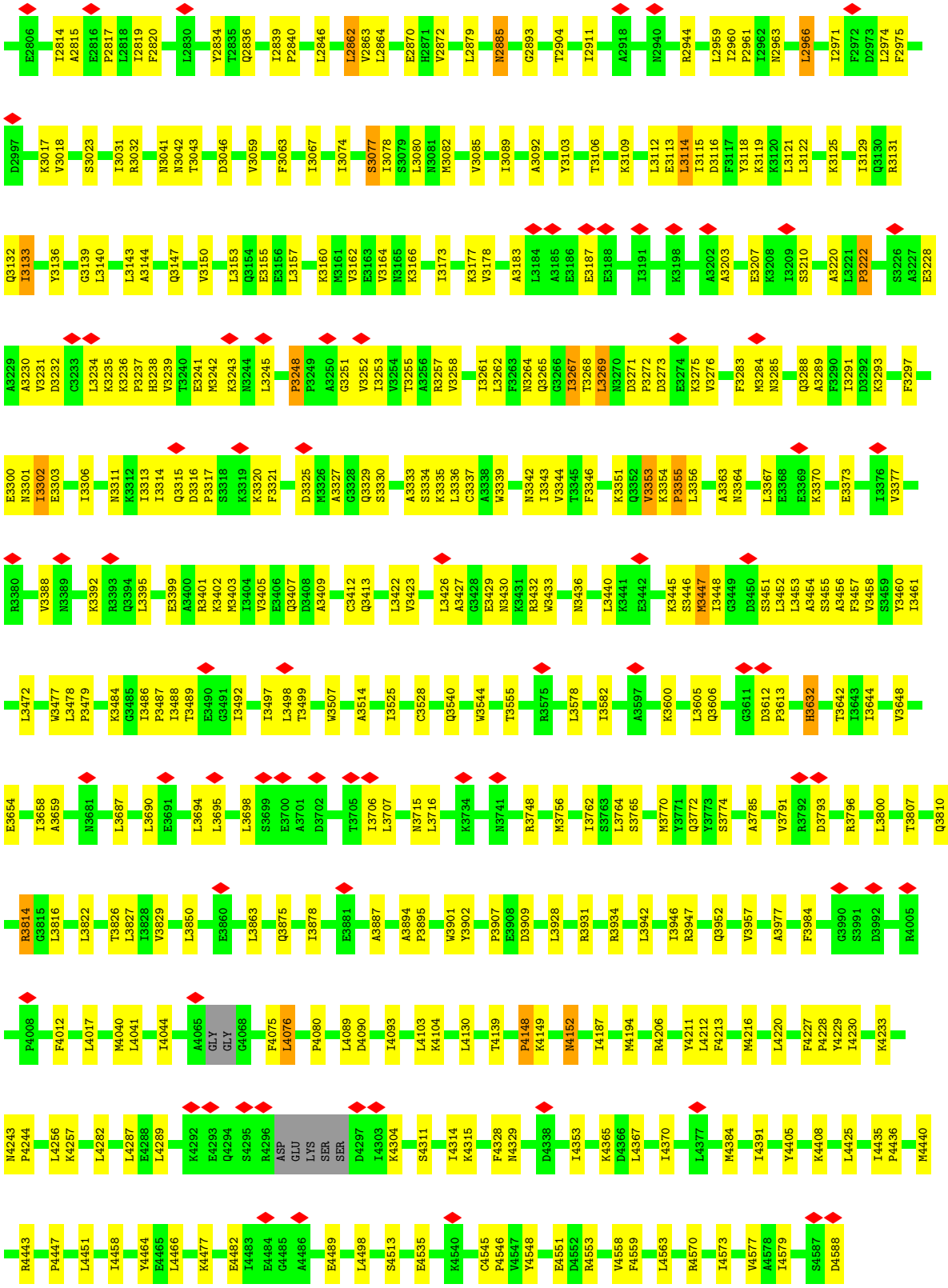


• Molecule 2: Outer arm dynein beta heavy chain

Chain B:

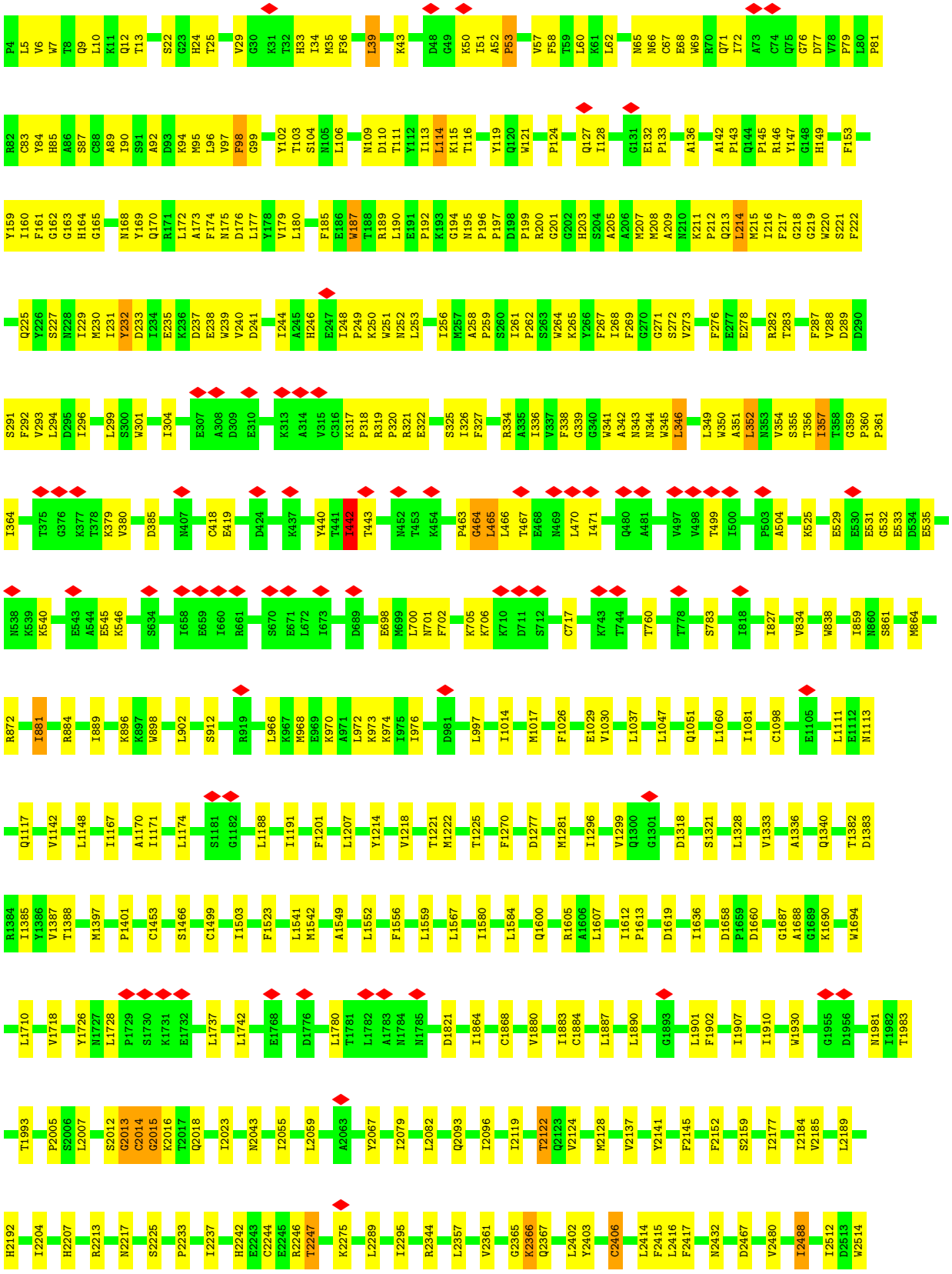



D1010 GLU ASN GLU PRO LYS ASP GLU ASP GLY LYS GLY GLY ASP ASP GLU GLY GLU ASN THR GLU LYS GLN ASN PRO LEU LEU LYS GLY CYS ARG ALA LYS ILE PRO N1046 L1049 F1050 D1051 I1054 T1055 H1056 L1057 K1058 Q1061 I1067 K1068 T1069 P1070 E1071 W1075 L1076 R1077 I1078
N1079 L1080 Q1081 P1082 M1083 K1084 L1087 V1091 W1094 Y1098 T1099 D1100 F1101 L1102 V1103 N1104 Q1105 F1106 R1107 T1108 T1109 Q1110 K1111 N1112 L1113 L1114 D1115 F1116 I1117 E1118 K1119 T1120 K1121 D1122 G1123 I1124 K1125 K1126 N1127 P1128 A1129 D1130 H1131 E1132 H1135 D1136 K1137 K1138 L1139 L1140 M1141 S1142 V1143 M1144 K1145
V1146 I1147 S1148 D1149 V1150 K1151 D1152 V1153 E1154 P1155 R1156 I1160 I1161 T1162 R1163 M1164 K1165 E1166 M1167 K1170 L1171 K1172 K1173 H1174 N1175 V1176 P1177 I1178 T1179 E1180 T1183 D1184 D1185 P1186 I1190 D1191 N1192 N1196 F1197 I1198 E1199 I1200 Y1201 G1202 R1203 V1204 F1205 K1206 V1207 K1208 A1209 D1210 I1211 I1212 P1213
E1218 K1223 M1230 E1234 S1235 F1236 R1237 K1238 E1239 F1240 M1241 Q1242 K1243 LEU PRO PHE ASP TYR THR GLU S1251 M1252 G1253 A1260 Y1261 D1262 V1266 Y1267 R1277 L1284 E1285 K1286 A1287 F1288 E1289 L1290 L1305 L1308 A1316 L1317 Y1322 N1323 D1324 W1325 P1329 W1330
I1333 K1334 A1335 D1336 I1337 L1338 L1339 D1340 T1341 N1342 K1343 T1344 L1345 G1346 T1347 Q1348 I1349 K1350 N1351 L1352 P1353 K1354 R1357 K1360 T1374 V1375 L1376 P1377 L1378 A1381 M1387 L1395 S1409 F1410 Y1411 F1412 E1413 D1414 L1420 Y1423 E1424 V1427 N1428 E1429 I1430 V1431 D1432 V1433 A1434 Q1435
K1436 E1437 A1438 K1439 I1440 E1441 K1442 K1443 L1444 K1445 N1446 I1447 E1448 Q1449 W1450 Q1454 V1455 F1456 E1457 F1458 T1459 E1460 Y1461 K1462 E1463 T1464 K1465 T1466 F1467 A1468 S1469 L1470 D1471 N1472 M1473 M1474 L1477 H1480 L1484 M1485 G1486 M1487 K1488 S1489 Q1490 G1491 K1492 Y1493 V1494 E1495 Y1498 D1499 R1500 V1501 E1502
D1503 W1504 R1505 E1506 K1507 V1511 V1514 V1515 N1516 K1520 V1521 Q1522 W1525 K1526 I1527 L1528 Y1529 N1530 I1531 F1532 L1533 L1534 I1538 R1539 T1546 F1549 K1557 D1558 M1559 M1560 S1561 E1562 V1563 S1564 A1565 N1566 P1567 S1568 V1569 V1570 E1571 A1572 C1573 R1577 W1584 S1585 C1591 L1595
L1599 K1602 K1603 K1604 S1605 F1606 P1607 R1608 F1609 Y1610 F1611 L1612 L1617 L1618 L1621 S1622 N1623 A1627 P1628 L1634 C1637 F1638 L1641 A1650 M1662 D1666 G1680 A1681 V1682 E1683 H1684 L1687 K1705 A1708 W1711 D1715 Q1728 L1731 T1734
K1758 N1770 L1771 I1772 E1783 R1784 W1785 K1786 I1787 I1788 T1792 I1793 R1798 I1806 S1819 W1825 I1856 V1857 F1860 Y1863 I1868 K1912 V1922 M1923 V1924 F1925 M1936 G1942 Q1945 S1946 G1947 N1956 V1966 A2009 G2010 R2011 R2023 N2038 M2039
L2040 G2044 R2049 L2058 L2066 K2070 L2083 R2084 Q2085 T2116 D2117 D2118 I2121 D2128 L2129 F2130 T2150 T2151 M2155 V2176 R2177 P2185 S2188 G2189 K2190 T2191 C2192 N2203 E2206 D2207 N2214 T2219 K2231 V2237 V2240 N2248 Y2252
W2260 D2264 I2267 D2268 P2269 E2270 W2271 R2300 L2301 I2302 F2303 E2304 L2308 R2309 N2310 A2311 E2326 M2332 P2333 Y2334 M2335 E2352 D2363 D2364 V2365 A2366 I2382 D2383 P2395 L2409 D2410 A2411 L2412 L2413 L2417 P2418 D2427 L2432 F2436 L2441 G2445
N2462 K2470 C2479 E2488 N2492 T2493 W2494 D2503 V2512 A2513 T2514 I2515 H2516 R2519 I2526 R2531 A2540 G2543 K2544 T2545 A2546 V2560 S2568 S2569 L2574 Q2577 K2586 N2591 Y2592 I2601 M2609 P2610 Y2615 G2616 T2617 Q2618 S2619 P2620 I2621 Q2622
R2625 R2636 L2639 E2640 F2644 L2649 N2655 V2663 D2664 L2665 R2666 L2667 Q2668 M2676 K2685 T2686 I2687 S2690 L2696 D2701 K2705 M2706 A2707 V2711 S2731 A2732 F2741 R2742 T2754 Q2758 Q2764 L2767 L2770 K2776 D2781 I2800



• Molecule 3: gamma heavy chain

Chain C: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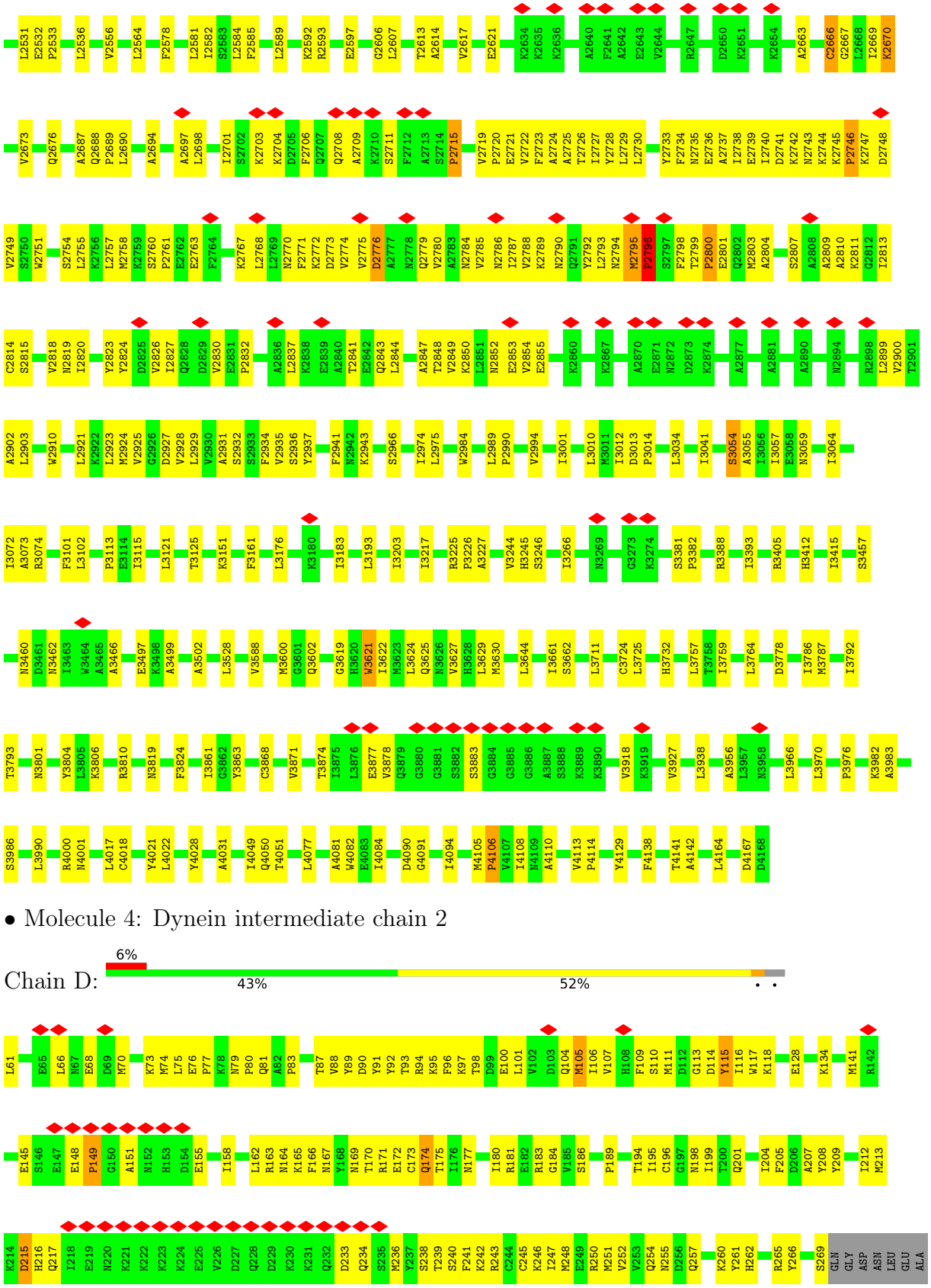
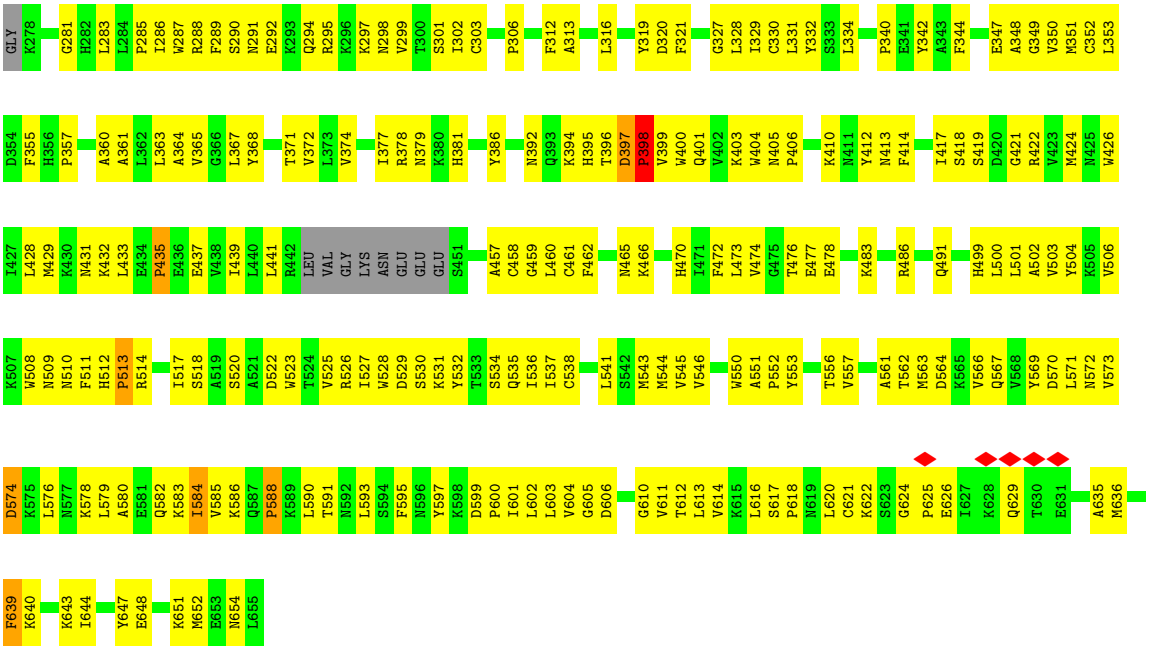
R82 C83 Y84 H85 A86 S87 C88 A89 I90 S91 A92 D93 K94 M95 L96 V97 F98 G99 Y102 T103 S104 N105 L106 N109 D110 T111 Y112 I113 L114 K115 T116 Y119 Q120 W121 P124 Q127 I128 G131 E132 P133 A136 A142 P143 Q144 P145 R146 Y147 G148 H149 F153
Y159 I160 F161 G162 G163 H164 G165 N168 Y169 Q170 R171 L172 A173 F174 N175 D176 L177 Y178 V179 L180 F185 E186 W187 T188 R189 L190 E191 P192 K193 G194 N195 P196 P197 D198 P199 R200 G201 G202 H203 S204 A205 A206 M207 M208 A209 N210 K211 P212 Q213 L214 M215 I216 F217 G218 G219 W220 S221 F222
Q225 Y226 S227 N228 I229 M230 I231 Y232 D233 I234 E235 K236 D237 E238 W239 V240 D241 I244 A245 H246 E247 I248 P249 K250 W251 N252 L253 I256 M257 A258 P259 S260 I261 P262 S263 W264 K265 Y266 F267 I268 F269 G270 G271 S272 V273 F276 E277 E278 R282 T283 F287 V288 D289 D290
S291 F292 V293 L294 D295 I296 L299 S300 W301 I304 E307 A308 D309 E310 K313 A314 V315 C316 K317 P318 R319 P320 R321 E322 S325 I326 F327 R334 A335 I336 V337 F338 G339 G340 W341 A342 N343 N344 W345 L346 L349 W350 A351 L352 N353 V354 S355 T356 I357 T358 G359 P360 P361
I364 T375 G376 K377 T378 K379 V380 D385 N407 C418 E419 D424 K437 Y440 T441 I442 T443 N452 T453 K454 P463 G464 L465 L466 T467 E468 N469 L470 I471 Q480 A481 V497 V498 T499 I500 P503 A504 K525 E529 E530 E531 G532 E533 D534 E535
N538 K539 K540 E543 A544 E545 K546 S634 I658 E659 I660 R661 S670 E671 L672 I673 D689 E698 M699 L700 N701 F702 K705 K706 K710 D711 S712 C717 K743 T744 T760 T778 S783 I818 I827 V834 W838 I859 N860 S861 M864
R872 I881 R884 I889 K896 K897 W898 L902 S912 R919 L966 K967 M968 E969 K970 A971 L972 K973 K974 I975 I976 D981 L997 I1014 M1017 F1026 E1029 V1030 L1037 L1047 Q1051 L1060 I1081 C1098 E1105 L1111 E1112 N1113
Q1117 V1142 L1148 I1167 A1170 I1171 L1174 S1181 G1182 L1188 I1191 F1201 L1207 Y1214 V1218 T1221 M1222 T1225 F1270 D1277 M1281 I1296 V1299 Q1300 G1301 D1318 S1321 L1328 V1333 A1336 Q1340 T1382 D1383
R1384 I1385 Y1386 V1387 T1388 M1397 P1401 C1453 S1466 C1499 I1503 F1523 L1541 M1542 A1549 L1552 F1556 L1559 L1567 I1580 L1584 Q1600 R1605 A1606 L1607 I1612 P1613 D1619 I1636 D1658 P1659 D1660 G1687 A1688 G1689 K1690 W1694
L1710 V1718 Y1726 N1727 L1728 P1729 S1730 K1731 E1732 L1737 L1742 E1768 D1776 L1780 T1781 L1782 A1783 N1784 N1785 D1821 I1864 C1868 V1880 I1883 C1884 L1887 L1890 G1893 L1901 F1902 I1907 I1910 W1930 G1955 D1956 N1981 I1982 T1983
T1993 P2005 S2006 L2007 S2012 G2013 C2014 G2015 K2016 T2017 Q2018 I2023 N2043 I2055 L2059 A2063 Y2067 I2079 L2082 Q2093 I2096 I2119 T2122 Q2123 V2124 M2128 V2137 Y2141 F2145 F2152 S2159 I2177 I2184 V2185 L2189
H2192 I2204 H2207 R2213 N2217 S2225 P2233 I2237 H2242 E2243 C2244 E2245 R2246 T2247 K2275 L2289 I2295 R2344 L2357 V2361 G2365 K2366 Q2367 L2402 Y2403 C2406 L2414 F2415 L2416 F2417 N2432 D2467 V2480 I2488 I2512 D2513 W2514



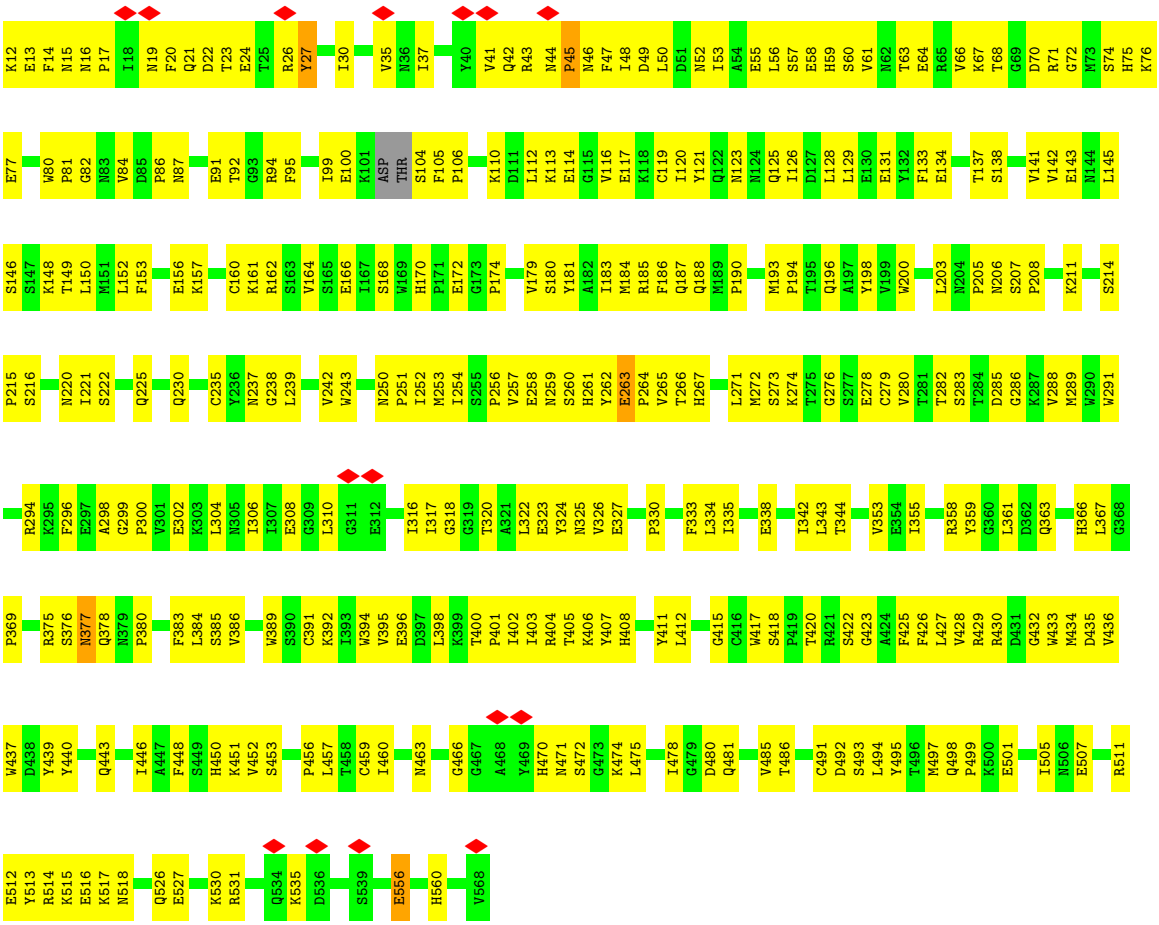
• Molecule 4: Dynein intermediate chain 2

Chain D:



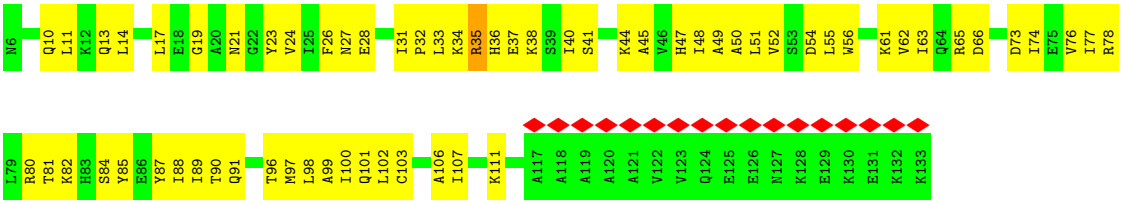
• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

Chain E:



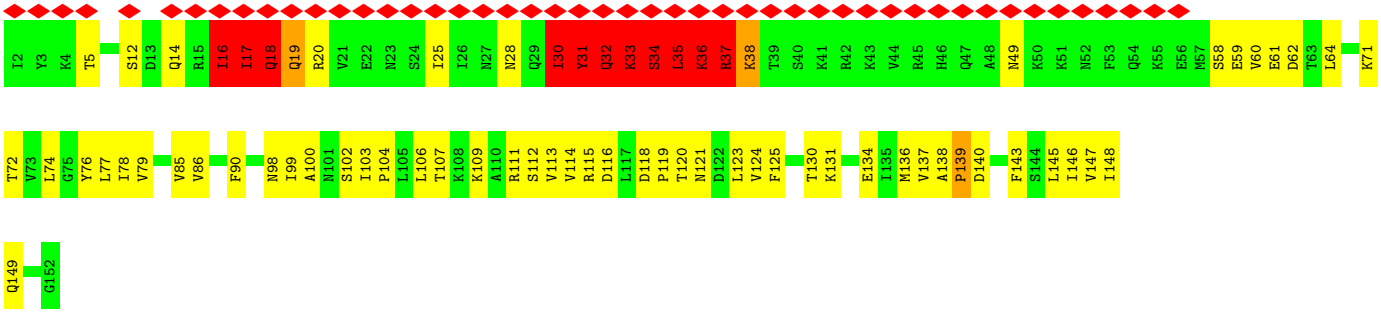
• Molecule 6: Dynein light chain roadblock-type 2 protein

Chain F:



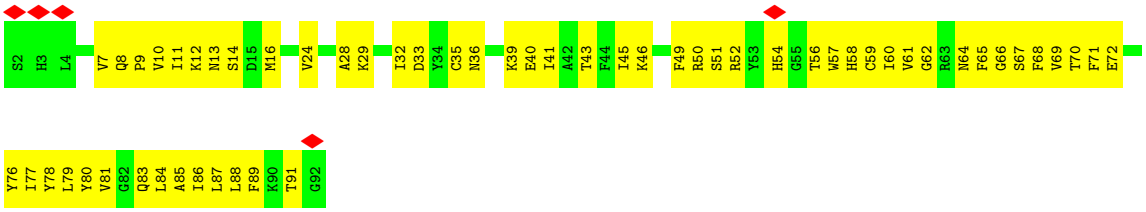
• Molecule 7: Dynein light chain roadblock-type 2 protein

Chain G:



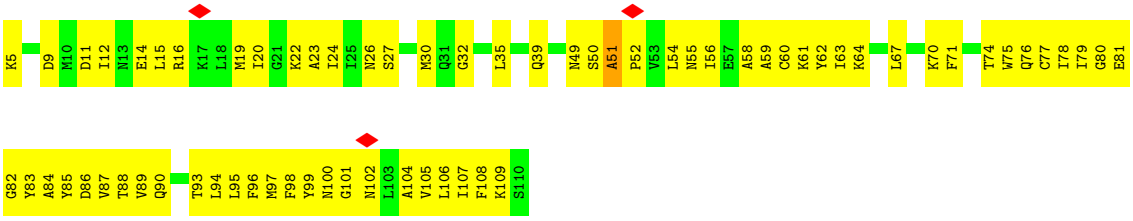
• Molecule 8: Dynein light chain

Chain H:



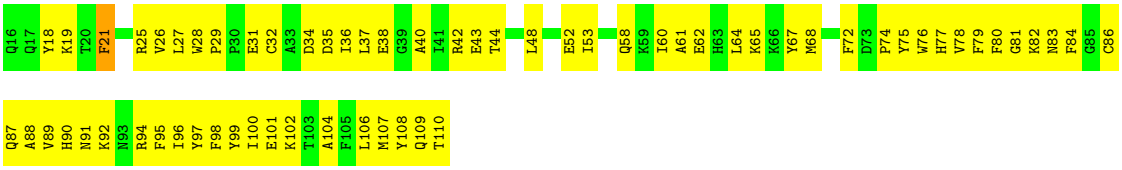
• Molecule 9: Dynein light chain

Chain I:



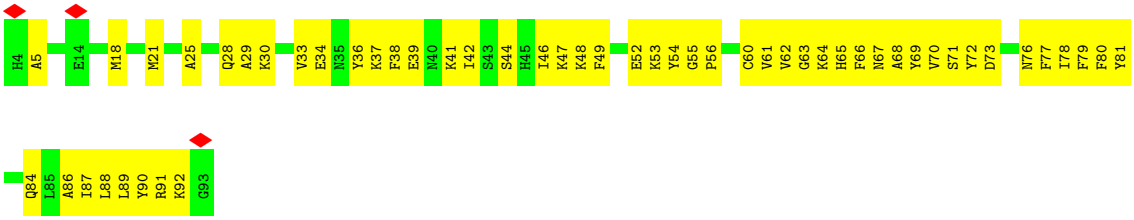
• Molecule 10: Dynein light chain

Chain J:



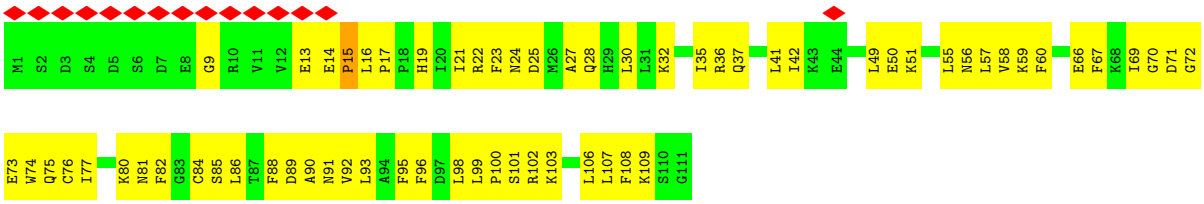
• Molecule 11: Dynein light chain

Chain K:



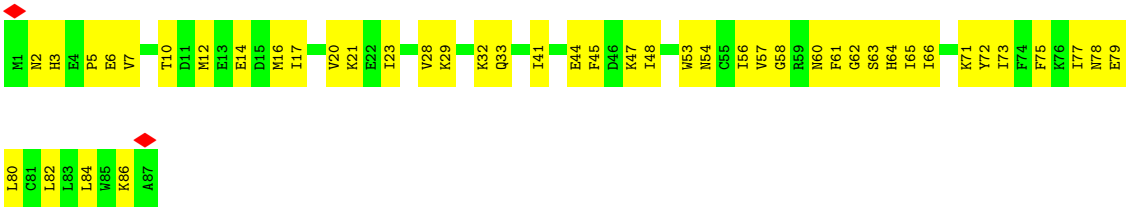
• Molecule 12: Dynein light chain

Chain L:



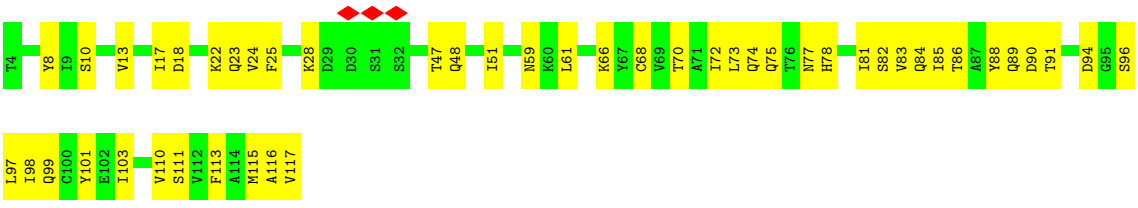
• Molecule 13: Dynein light chain

Chain M:



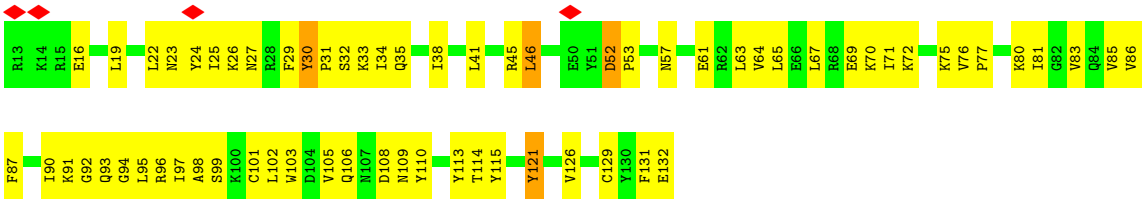
• Molecule 14: Dynein light chain tctex-type 1 protein

Chain N:



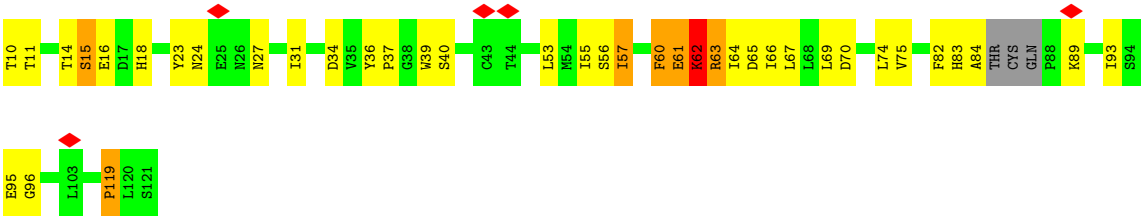
• Molecule 15: Dynein light chain 2A

Chain O:



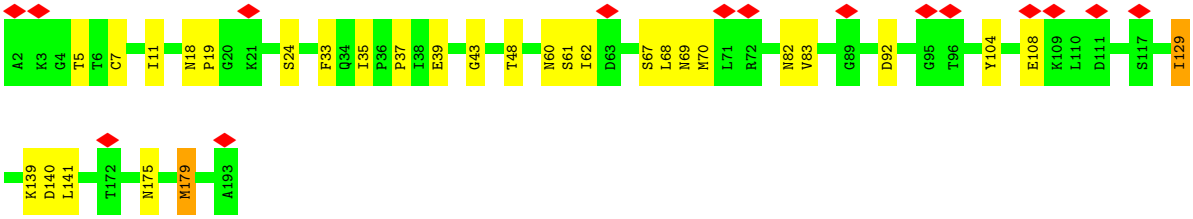
• Molecule 16: Thioredoxin

Chain P:



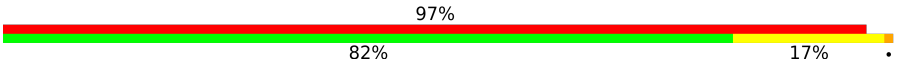
• Molecule 17: Dynein light chain 1

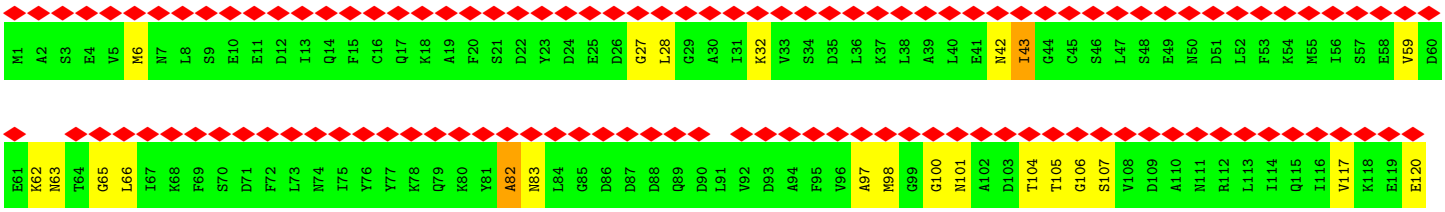
Chain Q:



• Molecule 18: Dynein light chain 4A

Chain R:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76936	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	8.594	Depositor
Minimum map value	0.000	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.189	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	527.86786, 493.20984, 462.55084	wwPDB
Map dimensions	396, 370, 347	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3329996, 1.3329996, 1.3329996	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, MG, 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	0.71	7/34544 (0.0%)	0.81	27/46728 (0.1%)
2	B	0.72	7/35358 (0.0%)	0.82	36/47850 (0.1%)
3	C	0.67	2/31033 (0.0%)	0.77	24/42007 (0.1%)
4	D	0.63	1/4789 (0.0%)	0.74	6/6477 (0.1%)
5	E	0.61	0/4540	0.64	0/6136
6	F	0.57	0/1008	0.58	0/1355
7	G	0.63	0/1030	0.98	11/1403 (0.8%)
8	H	0.63	0/767	0.61	0/1031
9	I	0.65	0/838	0.59	0/1131
10	J	0.61	0/832	0.65	0/1119
11	K	0.62	0/776	0.60	0/1038
12	L	0.60	0/872	0.61	0/1176
13	M	0.61	0/752	0.61	0/1006
14	N	0.66	0/864	0.67	0/1175
15	O	0.64	0/1012	0.64	0/1358
16	P	1.92	3/538 (0.6%)	1.60	15/746 (2.0%)
17	Q	0.33	0/1009	0.59	3/1392 (0.2%)
18	R	0.83	1/738 (0.1%)	0.95	2/1025 (0.2%)
All	All	0.70	21/121300 (0.0%)	0.79	124/164153 (0.1%)

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	4
2	B	0	11
3	C	0	1
4	D	0	1
7	G	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	2
All	All	0	31

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1067	PRO	N-CD	51.30	2.19	1.47
2	B	59	THR	C-N	-39.10	0.44	1.34
16	P	62	LYS	C-N	-30.53	0.63	1.34
16	P	15	SER	C-N	20.51	1.81	1.34
1	A	1649	ALA	C-N	-17.37	0.94	1.34

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1171	ILE	CA-C-N	-49.31	8.71	117.20
1	A	1171	ILE	C-N-CA	-46.87	4.53	121.70
2	B	59	THR	O-C-N	-39.33	59.78	122.70
2	B	49	PHE	O-C-N	-27.89	78.07	122.70
3	C	467	THR	N-CA-CB	23.73	155.38	110.30

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1171	ILE	Mainchain,Peptide
1	A	121	GLY	Mainchain
1	A	1649	ALA	Mainchain
2	B	25	GLN	Peptide
2	B	49	PHE	Mainchain

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	33975	0	32379	2211	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	34751	0	33289	2334	0
3	C	30427	0	29352	1238	0
4	D	4680	0	4511	1070	0
5	E	4440	0	4311	909	0
6	F	996	0	1019	263	0
7	G	1024	0	883	189	0
8	H	750	0	734	219	0
9	I	827	0	826	293	0
10	J	807	0	772	268	0
11	K	754	0	716	122	0
12	L	855	0	854	211	0
13	M	735	0	738	192	0
14	N	852	0	799	201	0
15	O	994	0	1017	311	0
16	P	541	0	217	56	0
17	Q	1006	0	512	51	0
18	R	739	156	339	45	0
19	A	54	0	23	31	0
19	B	54	0	24	18	0
19	C	54	0	22	32	0
20	A	31	0	12	10	0
20	B	31	0	12	43	0
20	C	31	0	12	2	0
21	A	3	0	0	2	0
21	B	3	0	0	0	0
21	C	3	0	0	0	0
All	All	119417	156	113373	8535	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 37.

The worst 5 of 8535 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)
10:J:86:CYS:SG	11:K:61:VAL:HG22	1.24	1.72
1:A:3235:TYR:CE2	1:A:3269:LEU:HD13	1.25	1.71
3:C:196:PRO:HA	3:C:239:TRP:CZ2	1.23	1.67
2:B:3118:TYR:CE2	2:B:3452:LEU:HA	1.25	1.64
4:D:170:THR:CG2	13:M:66:ILE:CG1	1.74	1.64

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	4391/4615 (95%)	4176 (95%)	190 (4%)	25 (1%)	25 65
2	B	4498/4588 (98%)	4258 (95%)	203 (4%)	37 (1%)	19 60
3	C	3923/3947 (99%)	3698 (94%)	202 (5%)	23 (1%)	25 65
4	D	569/595 (96%)	546 (96%)	16 (3%)	7 (1%)	13 50
5	E	551/557 (99%)	531 (96%)	18 (3%)	2 (0%)	34 72
6	F	126/128 (98%)	120 (95%)	6 (5%)	0	100 100
7	G	147/151 (97%)	134 (91%)	7 (5%)	6 (4%)	3 25
8	H	89/91 (98%)	88 (99%)	1 (1%)	0	100 100
9	I	104/106 (98%)	100 (96%)	3 (3%)	1 (1%)	15 54
10	J	93/95 (98%)	90 (97%)	3 (3%)	0	100 100
11	K	88/90 (98%)	85 (97%)	3 (3%)	0	100 100
12	L	109/111 (98%)	104 (95%)	4 (4%)	1 (1%)	17 56
13	M	85/87 (98%)	83 (98%)	2 (2%)	0	100 100
14	N	112/114 (98%)	105 (94%)	7 (6%)	0	100 100
15	O	118/120 (98%)	112 (95%)	4 (3%)	2 (2%)	9 43
16	P	103/112 (92%)	90 (87%)	7 (7%)	6 (6%)	1 20
17	Q	190/192 (99%)	174 (92%)	13 (7%)	3 (2%)	9 45
18	R	148/150 (99%)	121 (82%)	19 (13%)	8 (5%)	2 22
All	All	15444/15849 (97%)	14615 (95%)	708 (5%)	121 (1%)	24 60

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	PRO
1	A	125	PRO
1	A	127	THR
1	A	151	ILE

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Mol	Chain	Res	Type
1	A	1171	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	3430/4191 (82%)	3358 (98%)	72 (2%)	53 72
2	B	3525/4135 (85%)	3447 (98%)	78 (2%)	52 71
3	C	3139/3505 (90%)	3091 (98%)	48 (2%)	65 80
4	D	511/545 (94%)	507 (99%)	4 (1%)	81 89
5	E	488/496 (98%)	484 (99%)	4 (1%)	81 89
6	F	105/105 (100%)	104 (99%)	1 (1%)	76 86
7	G	86/141 (61%)	86 (100%)	0	100 100
8	H	82/82 (100%)	82 (100%)	0	100 100
9	I	91/91 (100%)	91 (100%)	0	100 100
10	J	82/82 (100%)	81 (99%)	1 (1%)	71 84
11	K	80/80 (100%)	80 (100%)	0	100 100
12	L	90/99 (91%)	90 (100%)	0	100 100
13	M	78/78 (100%)	78 (100%)	0	100 100
14	N	84/101 (83%)	84 (100%)	0	100 100
15	O	108/108 (100%)	106 (98%)	2 (2%)	57 75
17	Q	11/176 (6%)	11 (100%)	0	100 100
All	All	11990/14015 (86%)	11780 (98%)	210 (2%)	61 77

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3077	SER
2	B	4464	TYR
4	D	174	GLN
2	B	3269	LEU

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Mol	Chain	Res	Type
2	B	3800	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 204 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	105	ASN
3	C	2951	ASN
14	N	89	GLN
3	C	213	GLN
3	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 monosaccharides 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	ADP	B	5501	21	24,29,29	0.66	0	29,45,45	0.93	2 (6%)
19	ADP	C	4702	21	24,29,29	0.69	1 (4%)	29,45,45	1.04	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	ATP	B	5601	21	26,33,33	0.67	0	31,52,52	0.83	1 (3%)
19	ADP	A	4701	21	24,29,29	0.96	1 (4%)	29,45,45	1.43	4 (13%)
20	ATP	C	4201	21	26,33,33	0.70	0	31,52,52	0.89	2 (6%)
19	ADP	B	5602	21	24,29,29	0.67	0	29,45,45	0.73	1 (3%)
19	ADP	C	4703	21	24,29,29	0.65	0	29,45,45	0.87	2 (6%)
19	ADP	A	4901	21	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
20	ATP	A	4801	21	26,33,33	0.93	1 (3%)	31,52,52	1.39	4 (12%)

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	ADP	B	5501	21	-	1/12/32/32	0/3/3/3
19	ADP	C	4702	21	-	5/12/32/32	0/3/3/3
20	ATP	B	5601	21	-	1/18/38/38	0/3/3/3
19	ADP	A	4701	21	-	8/12/32/32	0/3/3/3
20	ATP	C	4201	21	-	1/18/38/38	0/3/3/3
19	ADP	B	5602	21	-	2/12/32/32	0/3/3/3
19	ADP	C	4703	21	-	3/12/32/32	0/3/3/3
19	ADP	A	4901	21	-	6/12/32/32	0/3/3/3
20	ATP	A	4801	21	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	4901	ADP	C5-C4	2.35	1.47	1.40
19	A	4701	ADP	C5-C4	2.26	1.46	1.40
19	C	4702	ADP	C8-N7	-2.07	1.31	1.34
20	A	4801	ATP	C5-C4	2.07	1.46	1.40

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	4801	ATP	PB-O3B-PG	-3.69	120.15	132.83
19	A	4901	ADP	PA-O3A-PB	-3.56	120.61	132.83
19	A	4701	ADP	C3'-C2'-C1'	3.48	106.22	100.98
19	A	4901	ADP	C3'-C2'-C1'	3.42	106.12	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	4801	ATP	N3-C2-N1	-3.28	123.56	128.68

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	4701	ADP	PB-O3A-PA-O5'
19	A	4701	ADP	C5'-O5'-PA-O1A
19	A	4701	ADP	C5'-O5'-PA-O2A
19	A	4901	ADP	PB-O3A-PA-O5'
19	A	4901	ADP	C5'-O5'-PA-O2A

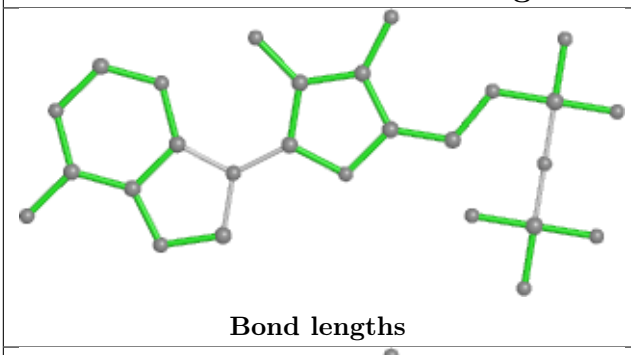
There are no ring outliers.

9 monomers are involved in 136 short contacts:

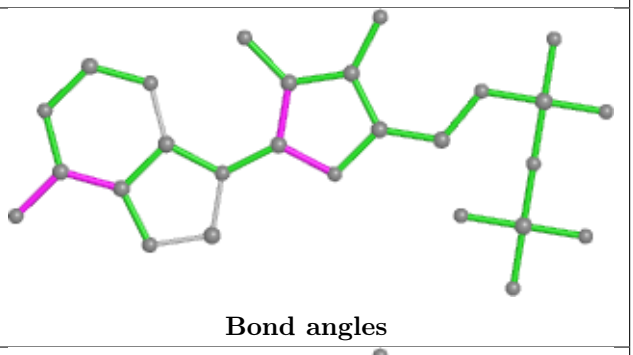
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	5501	ADP	16	0
19	C	4702	ADP	25	0
20	B	5601	ATP	43	0
19	A	4701	ADP	12	0
20	C	4201	ATP	2	0
19	B	5602	ADP	2	0
19	C	4703	ADP	7	0
19	A	4901	ADP	19	0
20	A	4801	ATP	10	0

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

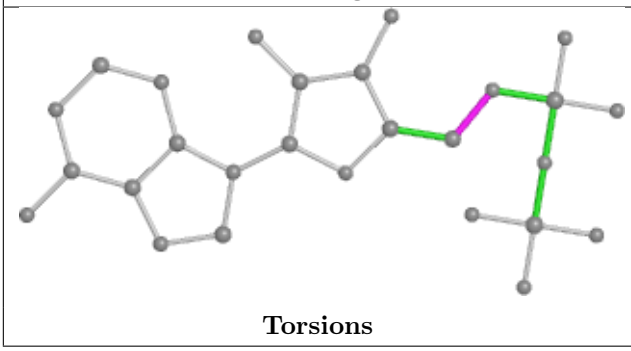
Ligand ADP B 5501



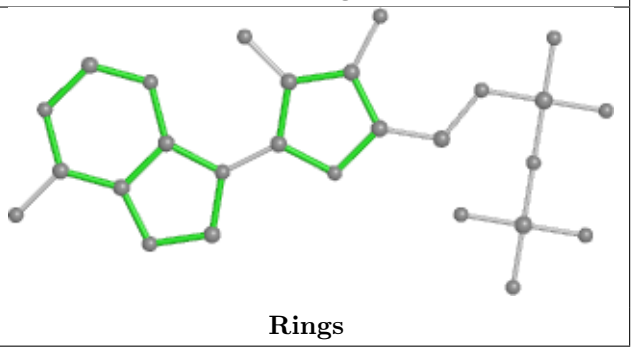
Bond lengths



Bond angles

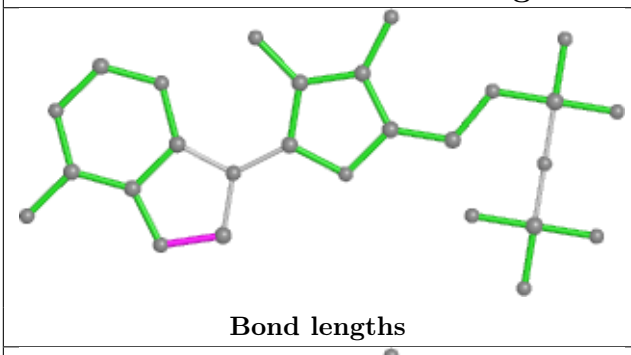


Torsions

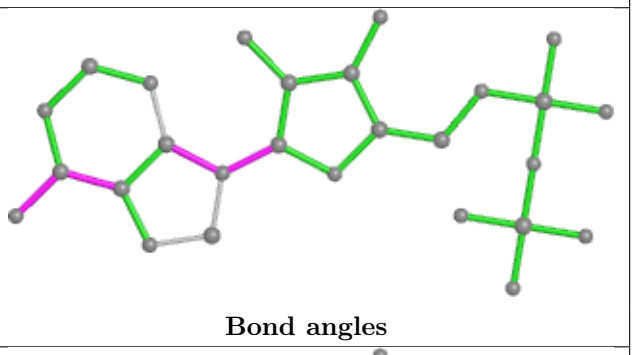


Rings

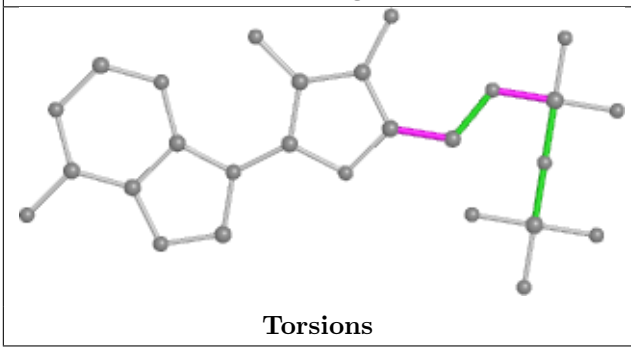
Ligand ADP C 4702



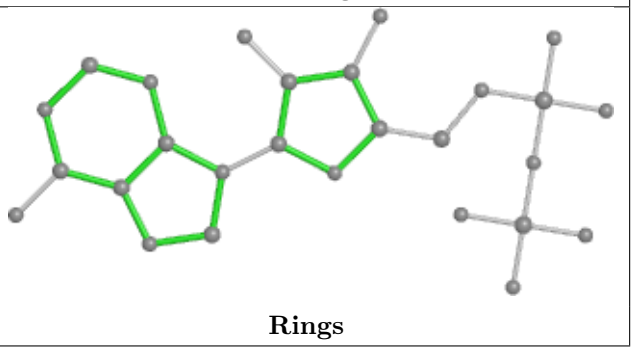
Bond lengths



Bond angles

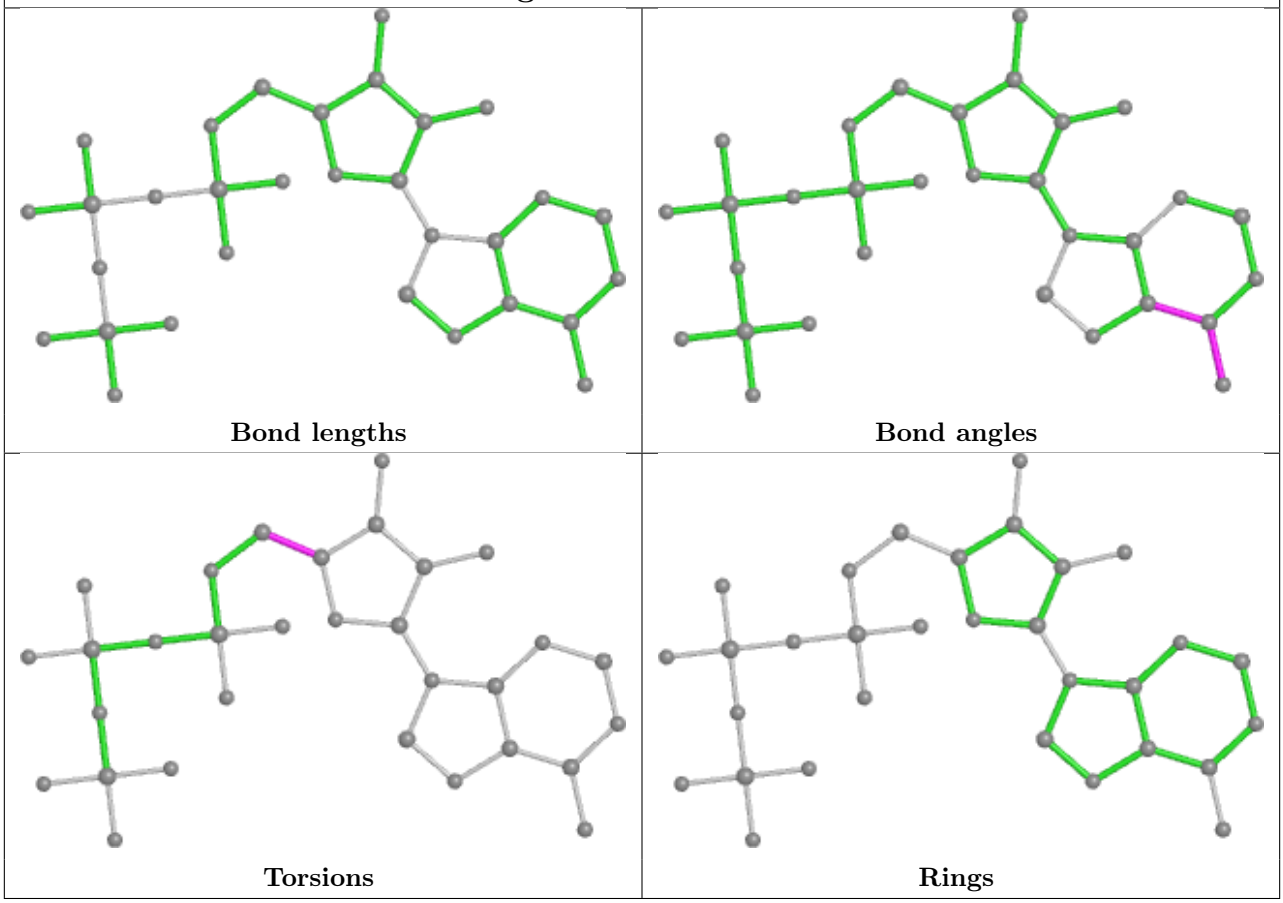


Torsions

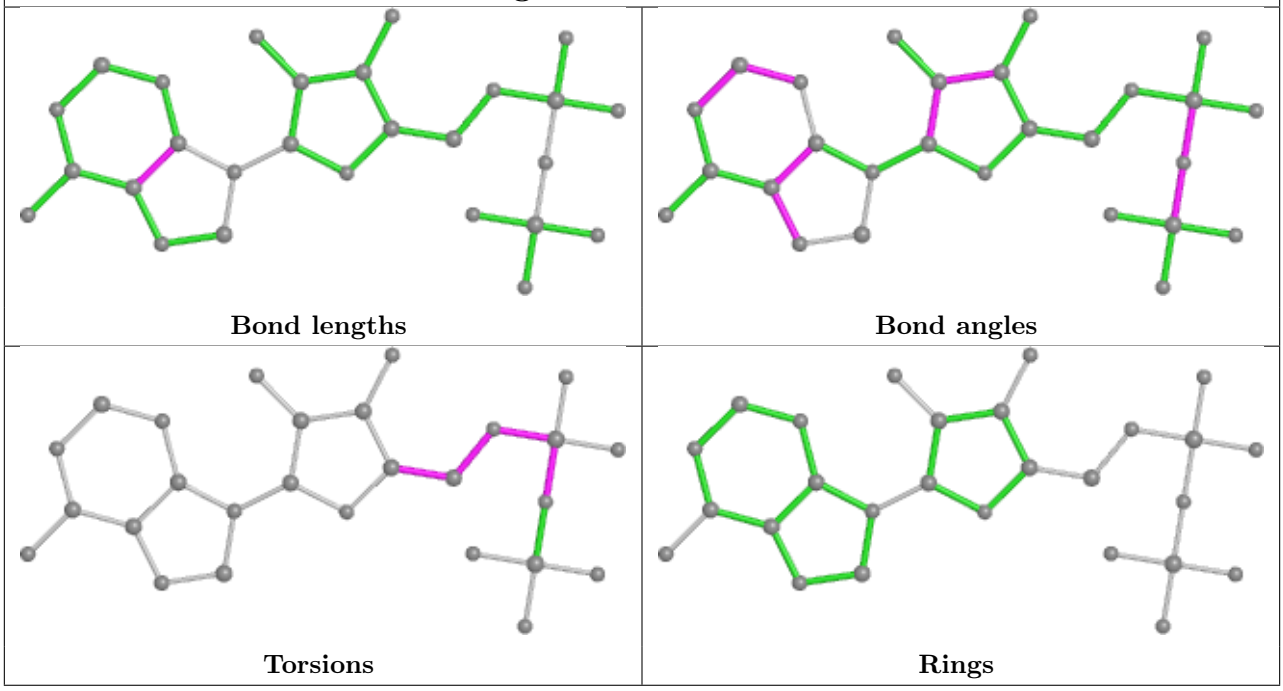


Rings

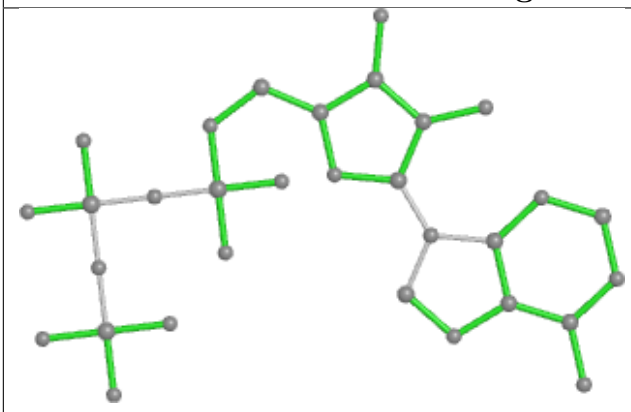
Ligand ATP B 5601



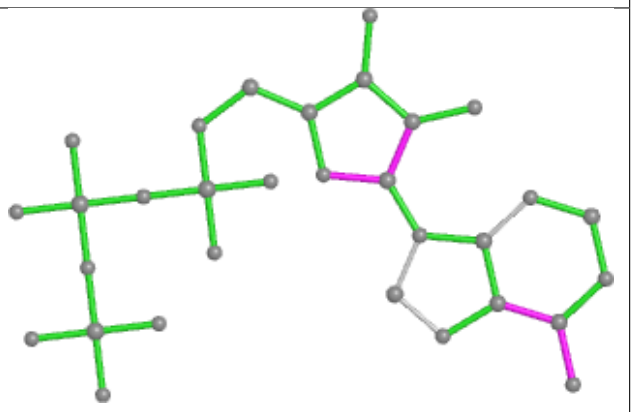
Ligand ADP A 4701



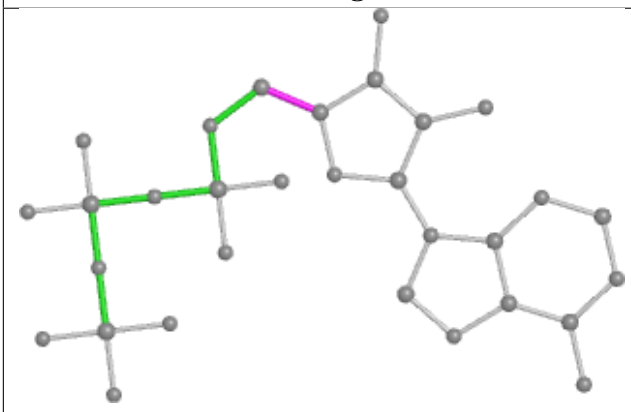
Ligand ATP C 4201



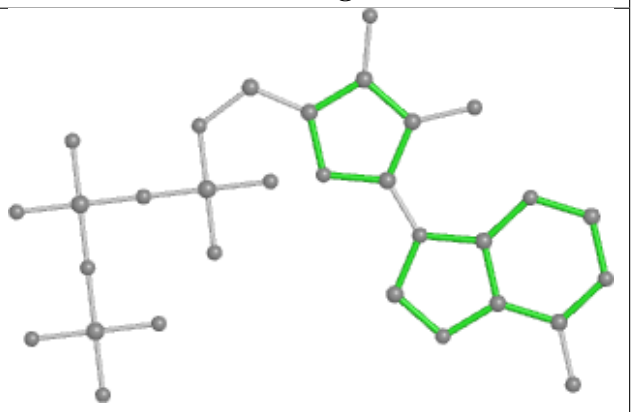
Bond lengths



Bond angles

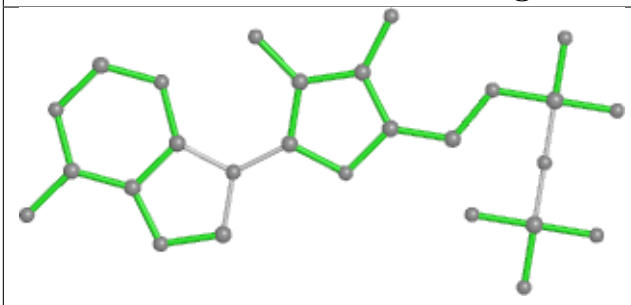


Torsions

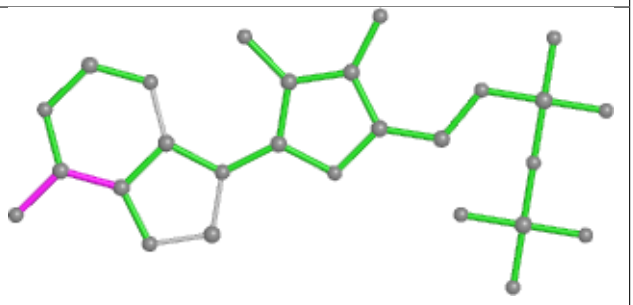


Rings

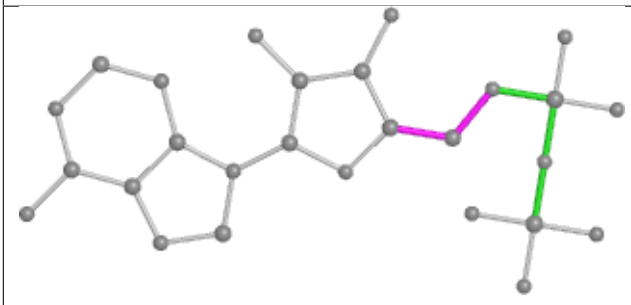
Ligand ADP B 5602



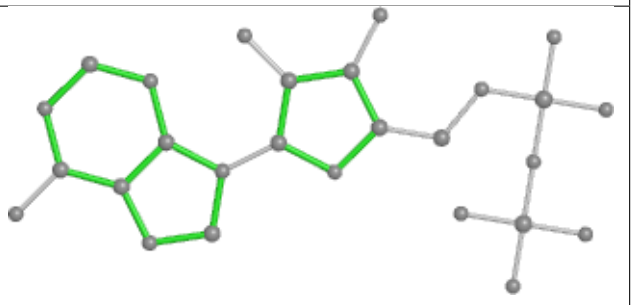
Bond lengths



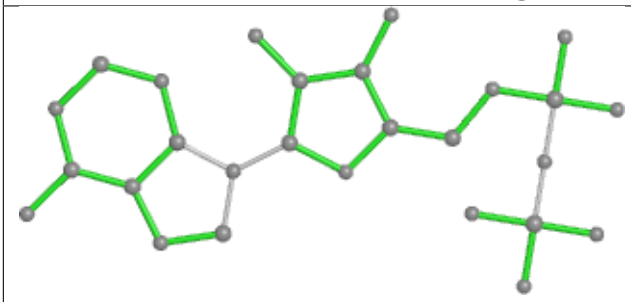
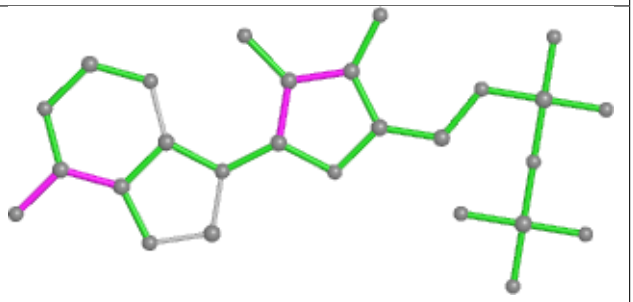
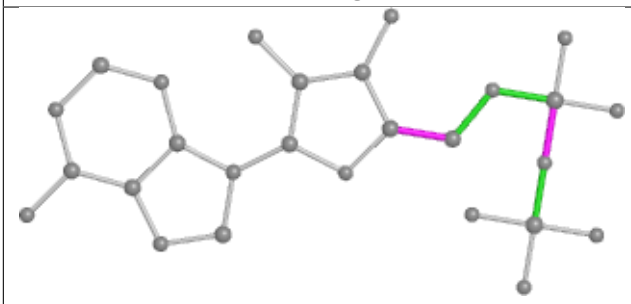
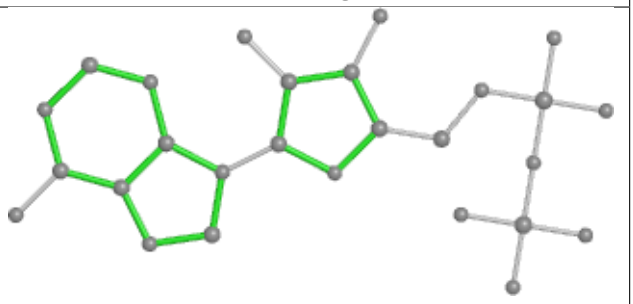
Bond angles

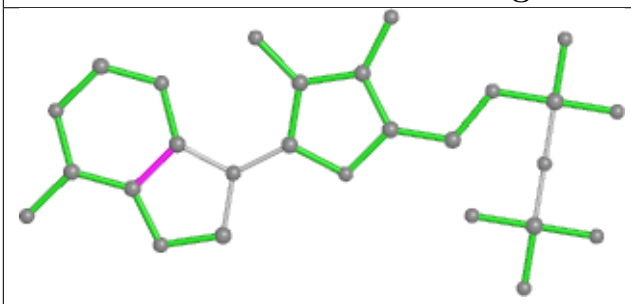
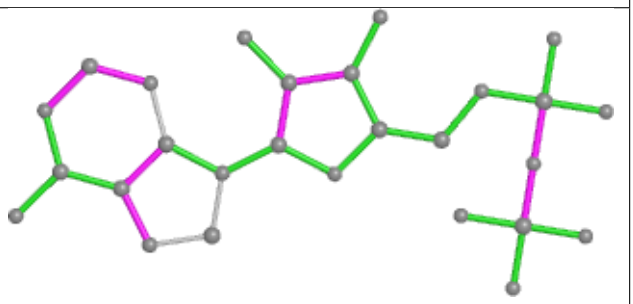
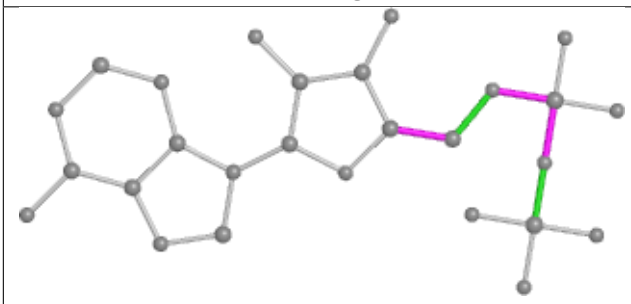
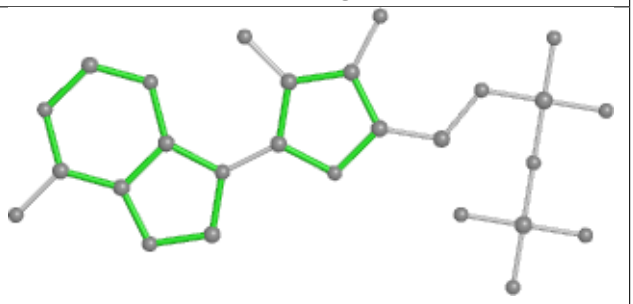


Torsions

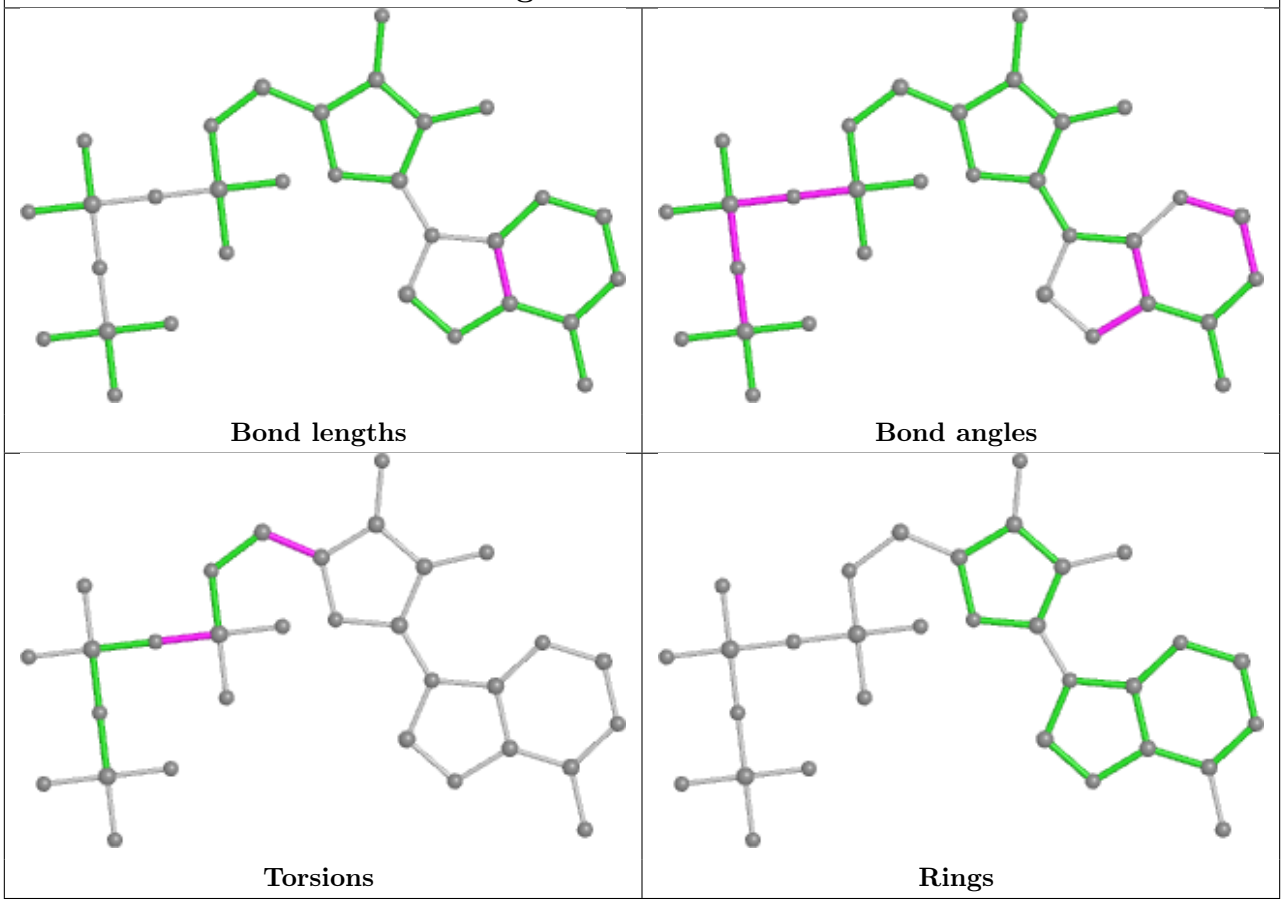


Rings

Ligand ADP C 4703	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 4901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP A 4801



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	12
3	C	11
2	B	11
16	P	4
4	D	2
7	G	1
18	R	1

The worst 5 of 42 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3277:MET	C	3380:MET	N	42.67
1	A	1235:PRO	C	1246:MET	N	14.08
1	C	809:ARG	C	818:ILE	N	13.93
1	C	449:TYR	C	452:ASN	N	13.33
1	C	665:ILE	C	670:SER	N	11.69

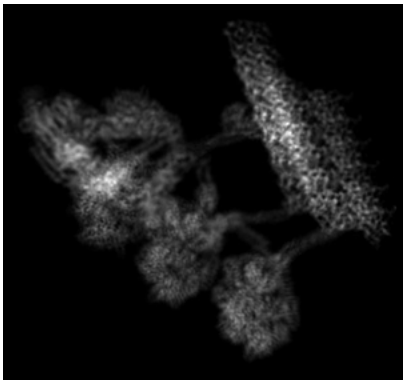
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22679. These allow visual inspection of the internal detail of the map and identification of artifacts.

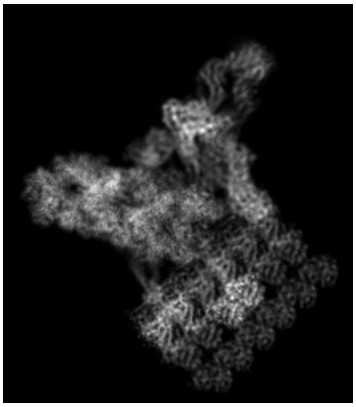
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

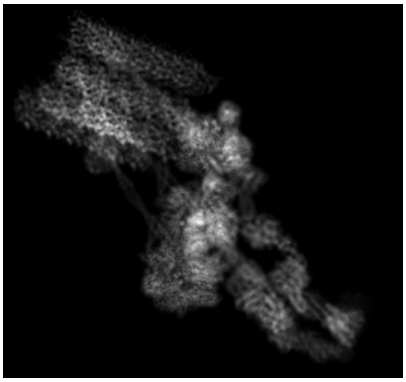
6.1.1 Primary map



X



Y

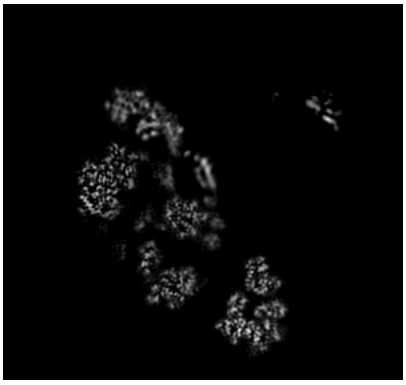


Z

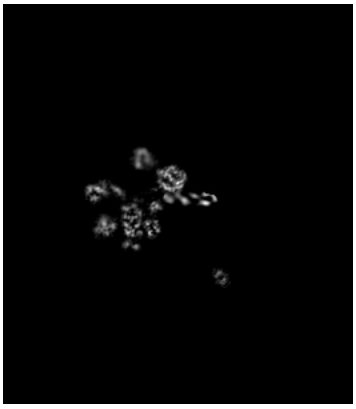
The images above show the map projected in three orthogonal directions.

6.2 Central slices

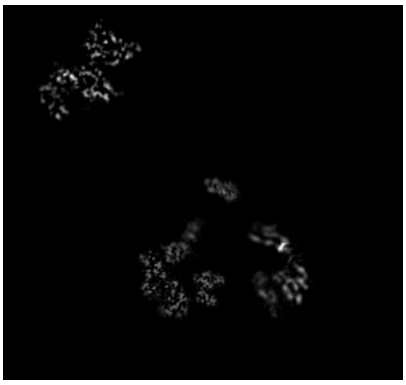
6.2.1 Primary map



X Index: 198



Y Index: 185

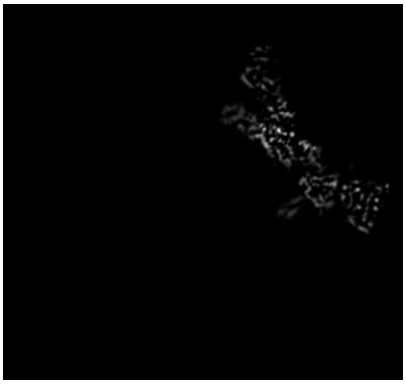


Z Index: 173

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

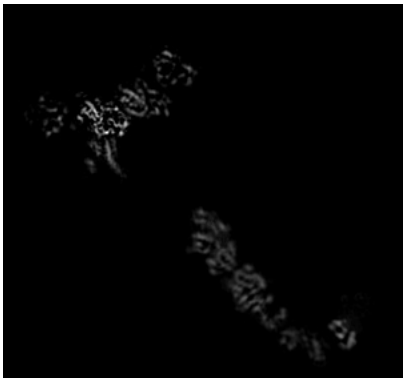
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 97

Y Index: 249



Z Index: 228

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

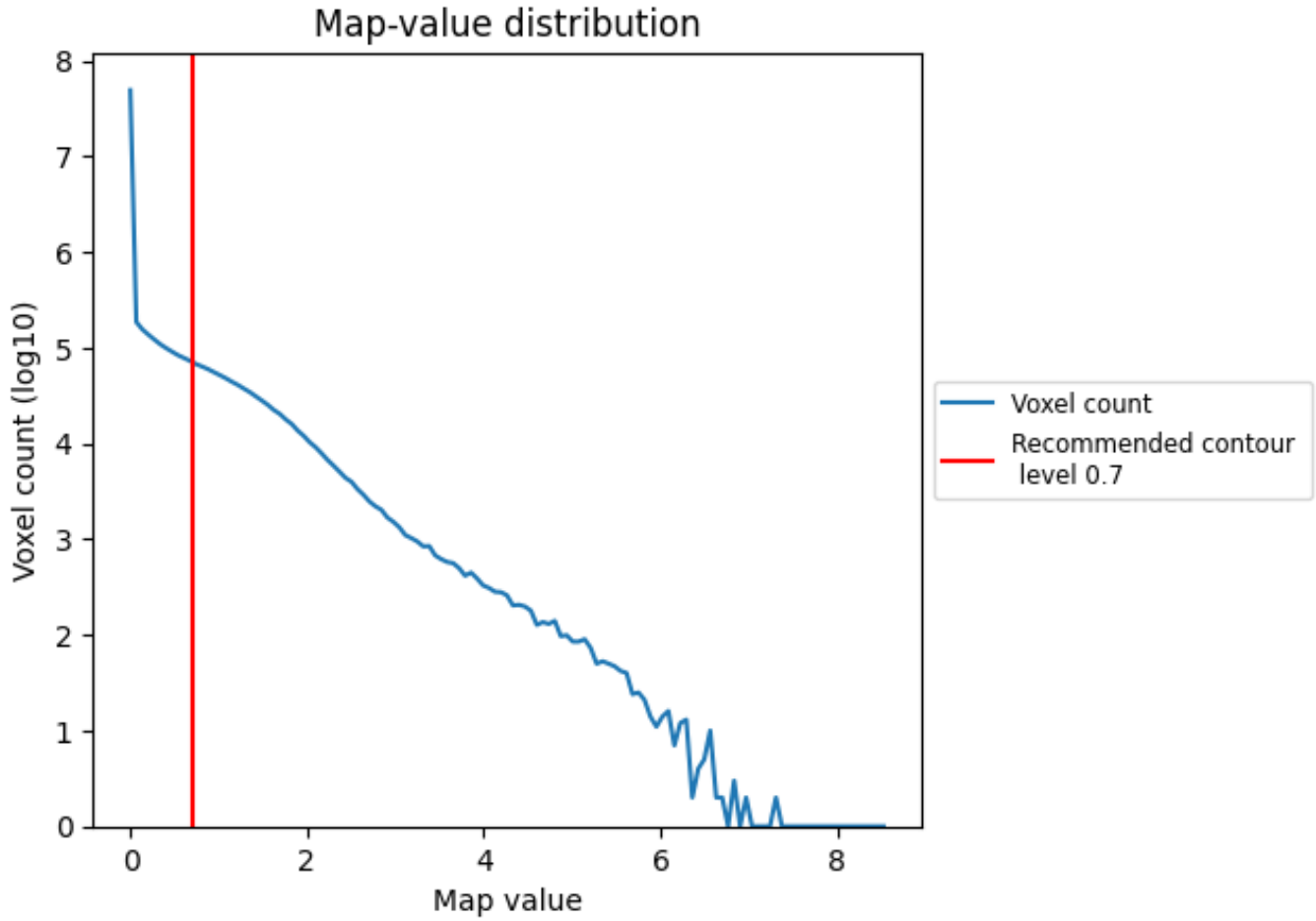
6.5 Mask visualisation (i)

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

7 Map analysis

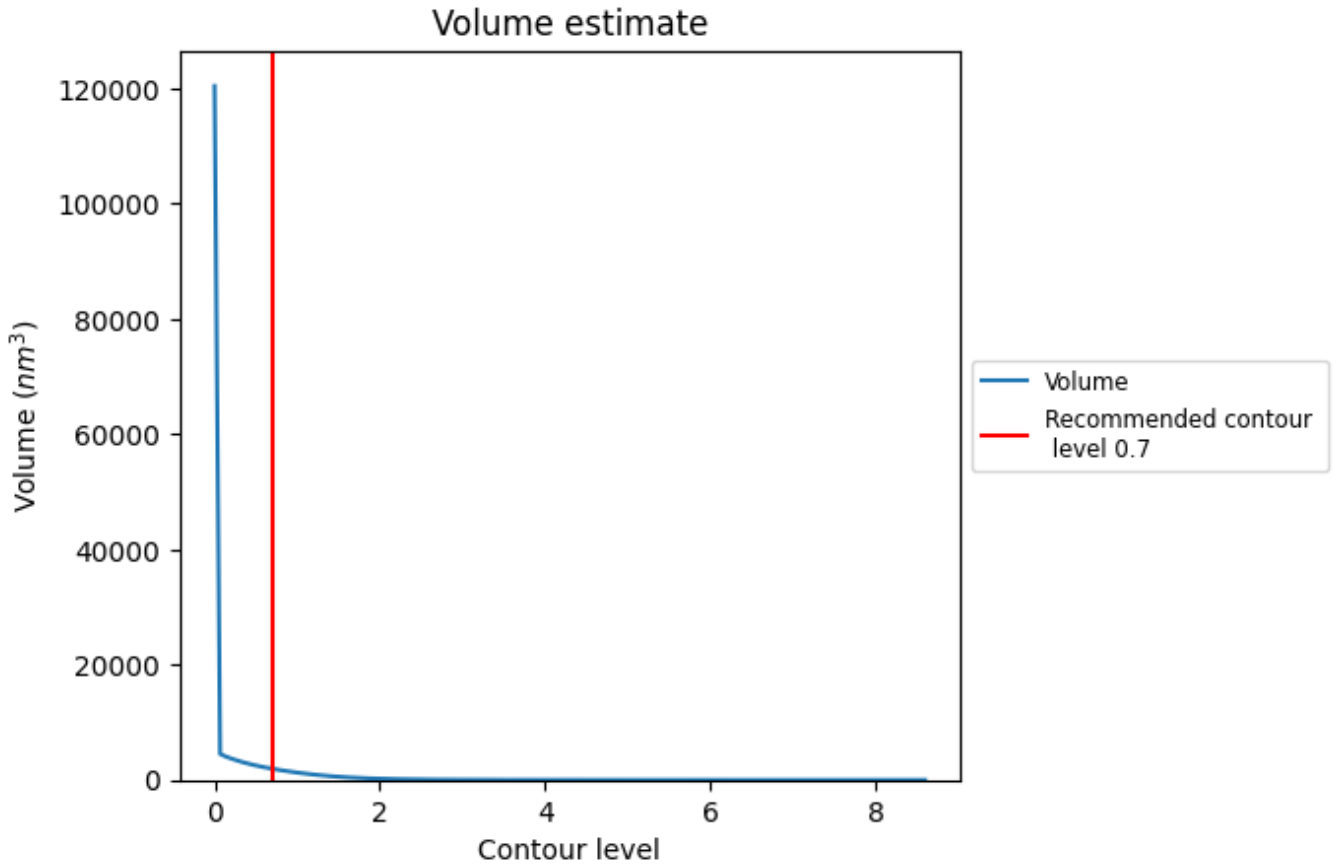
This section contains the results of statistical analysis of the map.

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 1940 nm^3; this corresponds to an approximate mass of 1753 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.

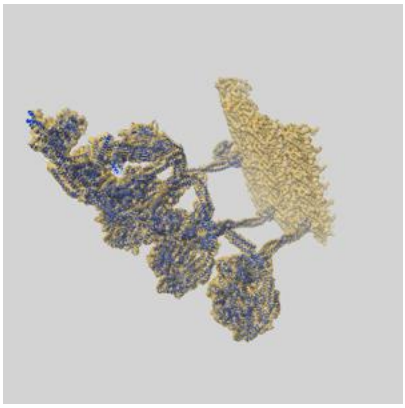
8 Fourier-Shell correlation

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

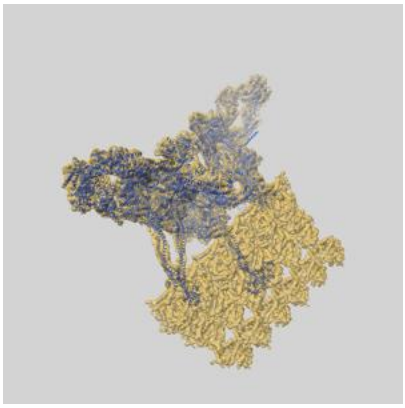
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22679 and PDB model 7K5B. Per-residue inclusion information can be found in section 3 on page 9.

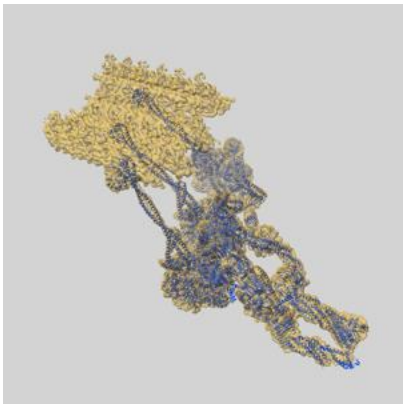
9.1 Map-model overlay



X



Y



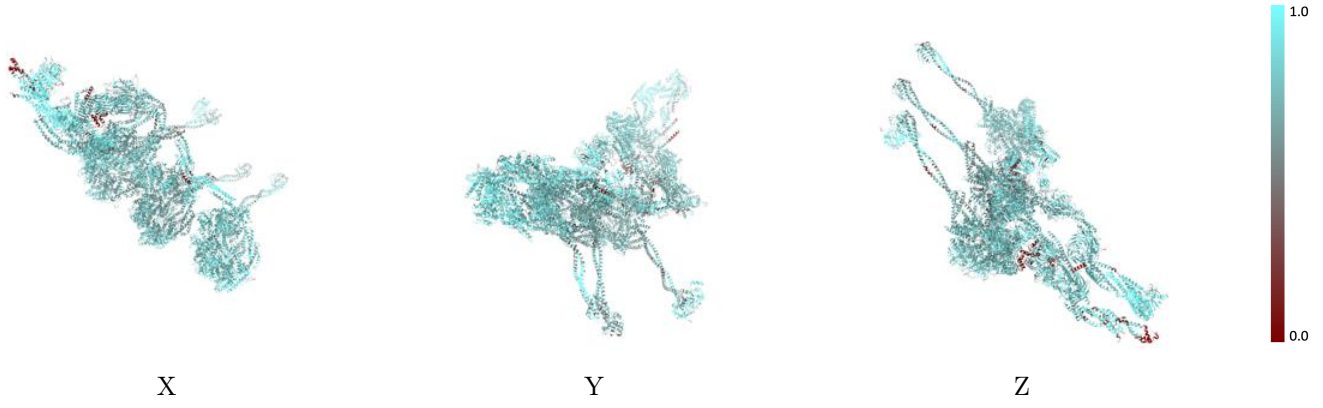
Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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)

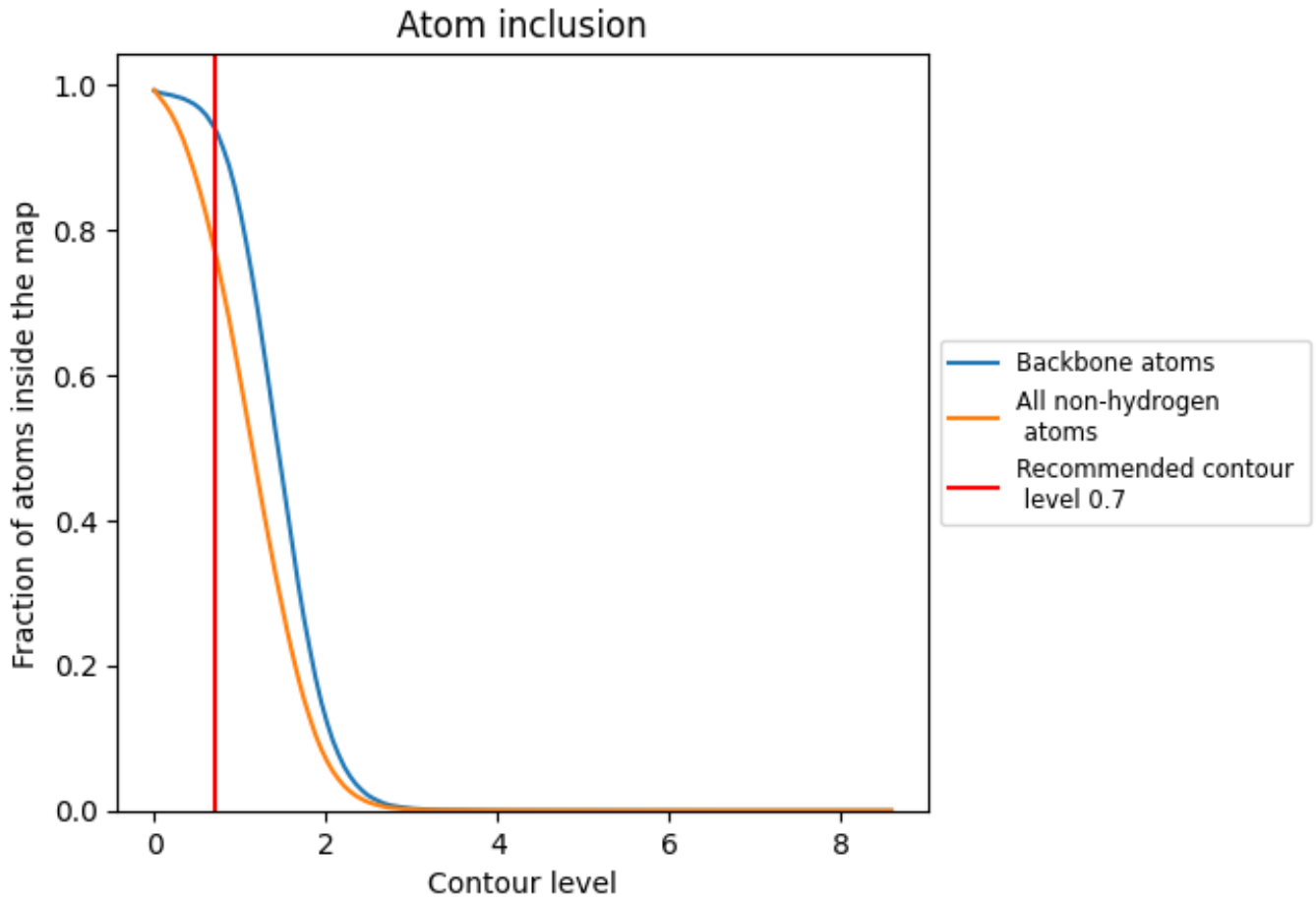
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 77% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7738	0.2640
A	0.7587	0.2830
B	0.7566	0.2730
C	0.8177	0.2860
D	0.8027	0.2060
E	0.8275	0.2060
F	0.7012	0.1850
G	0.6180	0.1440
H	0.7741	0.1860
I	0.8049	0.1730
J	0.7952	0.1850
K	0.8067	0.1780
L	0.6568	0.1780
M	0.7680	0.1590
N	0.7675	0.1640
O	0.7505	0.1440
P	0.8909	0.1510
Q	0.8493	0.2450
R	0.0271	-0.0320