wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 08:13 pm GMT

PDB ID	:	8RRS
EMDB ID	:	EMD-19463
Title	:	Structure of mouse RyR2 solubilised in detergent in open state in complex with Ca2+, ATP, caffeine and Nb9657.
Authors	:	Li, C.; Efremov, R.G.
Deposited on	:	2024-01-23
Resolution	:	3.40 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:

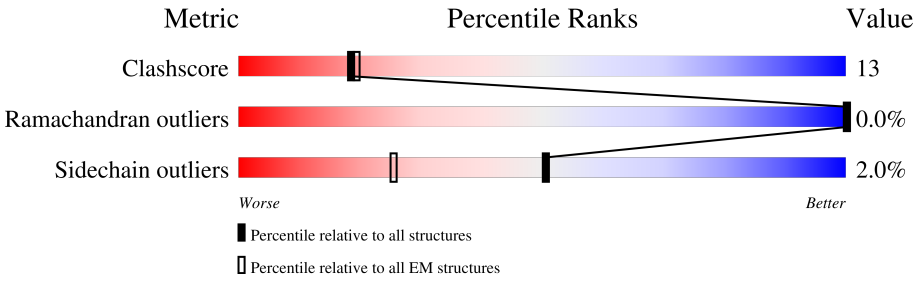
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	4966	58% 24% · 17%
1	C	4966	59% 24% · 17%
1	E	4966	58% 24% · 17%
1	F	4966	58% 24% · 17%
2	B	4966	37% 64% 28% 8%
2	D	4966	36% 66% 26% 8%
2	G	4966	36% 64% 28% 8%
2	I	4966	36% 64% 28% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 136400 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.

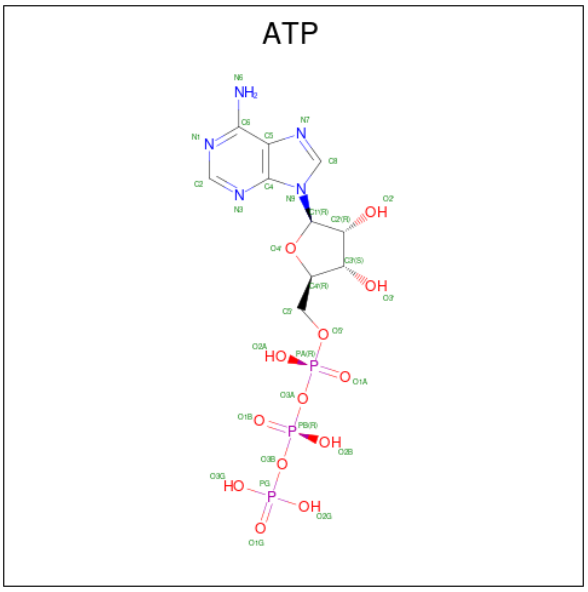
- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4142	Total 33088	C 21113	N 5650	O 6106	S 219	0	0
1	C	4142	Total 33088	C 21113	N 5650	O 6106	S 219	0	0
1	E	4142	Total 33088	C 21113	N 5650	O 6106	S 219	0	0
1	F	4142	Total 33088	C 21113	N 5650	O 6106	S 219	0	0

- Molecule 2 is a protein called Nanobody 9657.

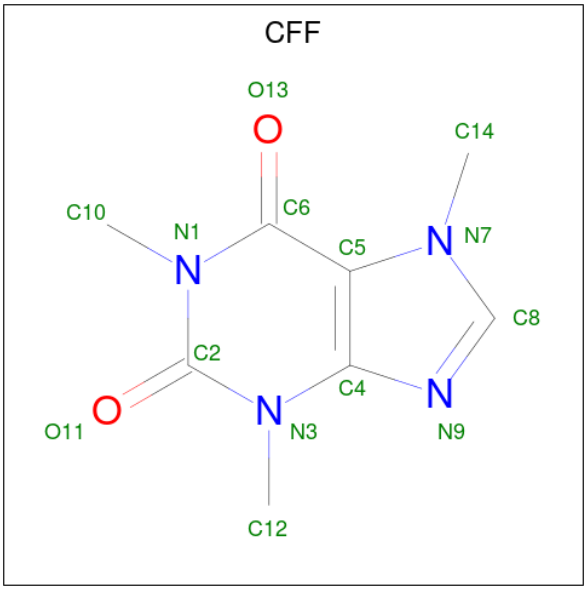
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total 965	C 595	N 170	O 195	S 5	0	0
2	D	126	Total 965	C 595	N 170	O 195	S 5	0	0
2	G	126	Total 965	C 595	N 170	O 195	S 5	0	0
2	I	126	Total 965	C 595	N 170	O 195	S 5	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	C	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	F	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	F	1	Total	Zn	0
			1	1	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

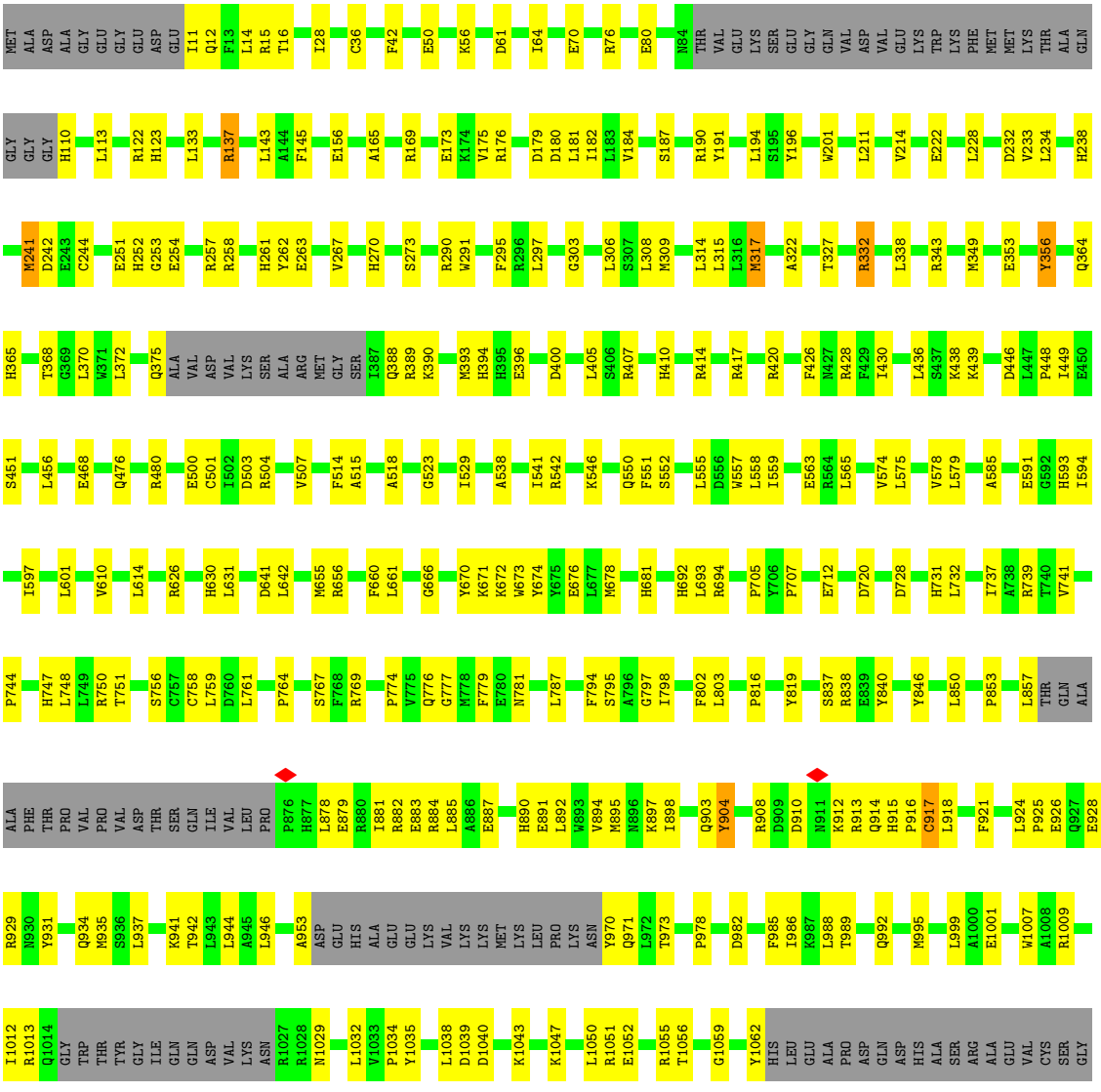
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	
6	F	1	Total	Ca	0
			1	1	

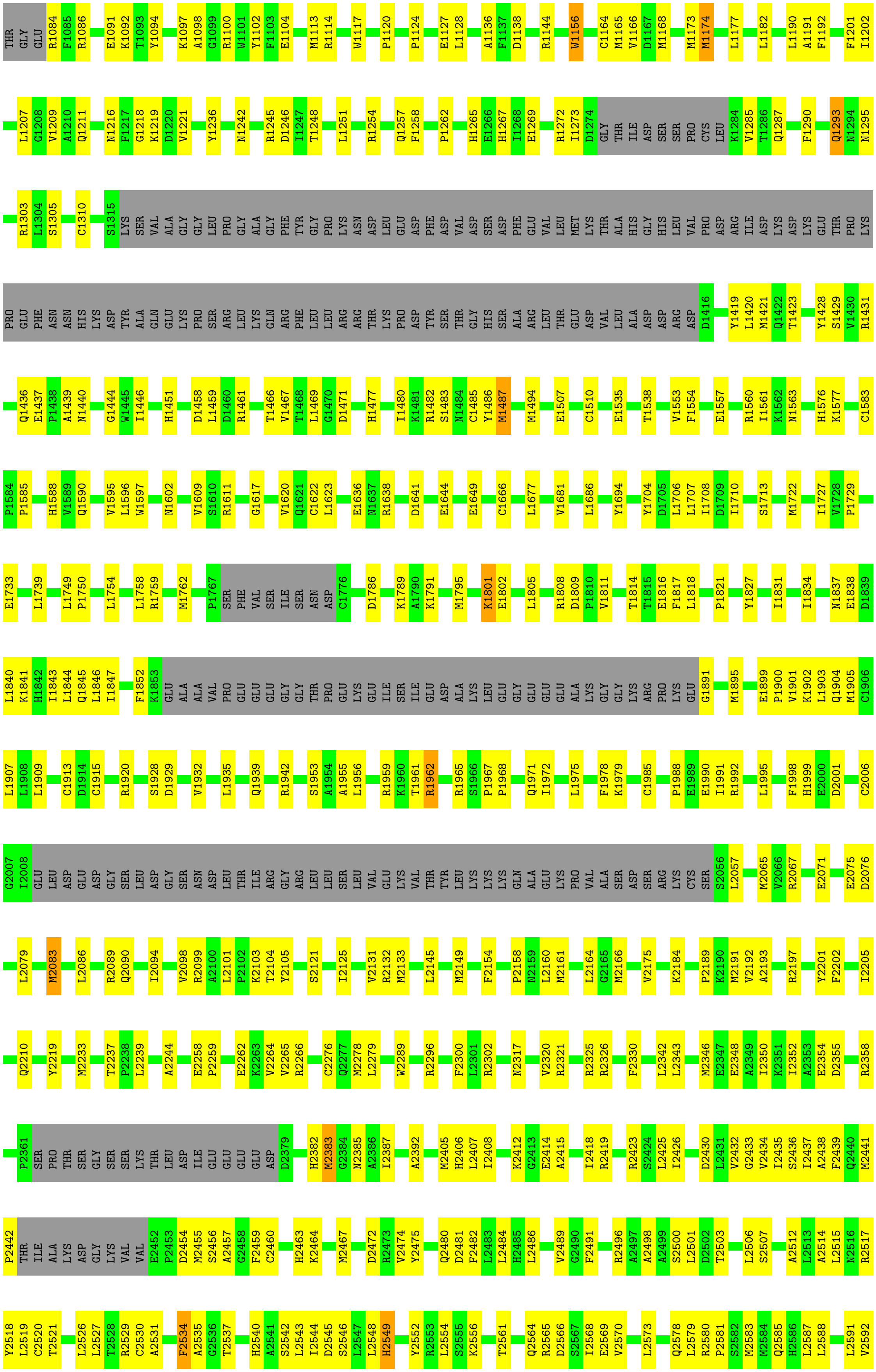
3 Residue-property plots (i)

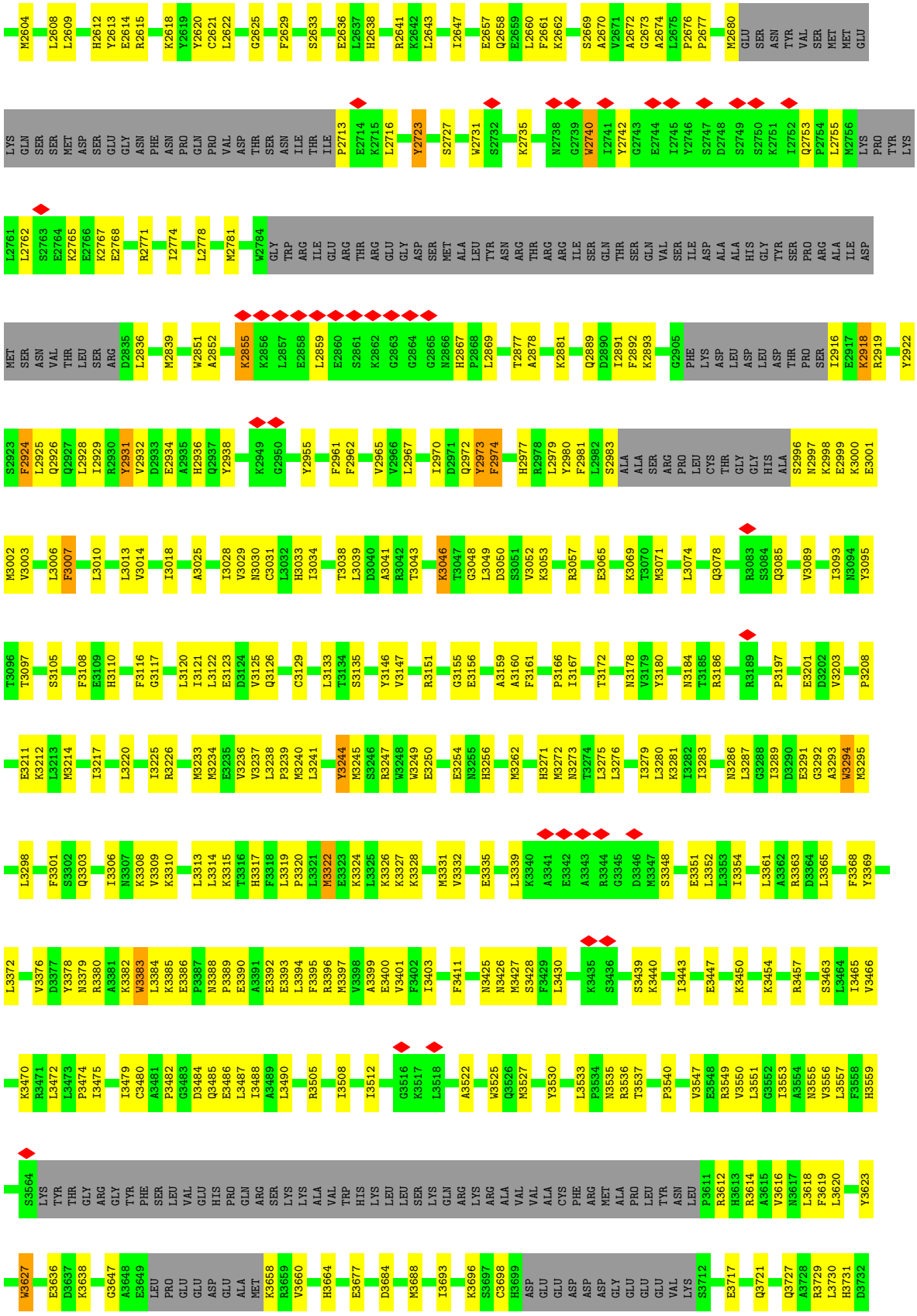
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

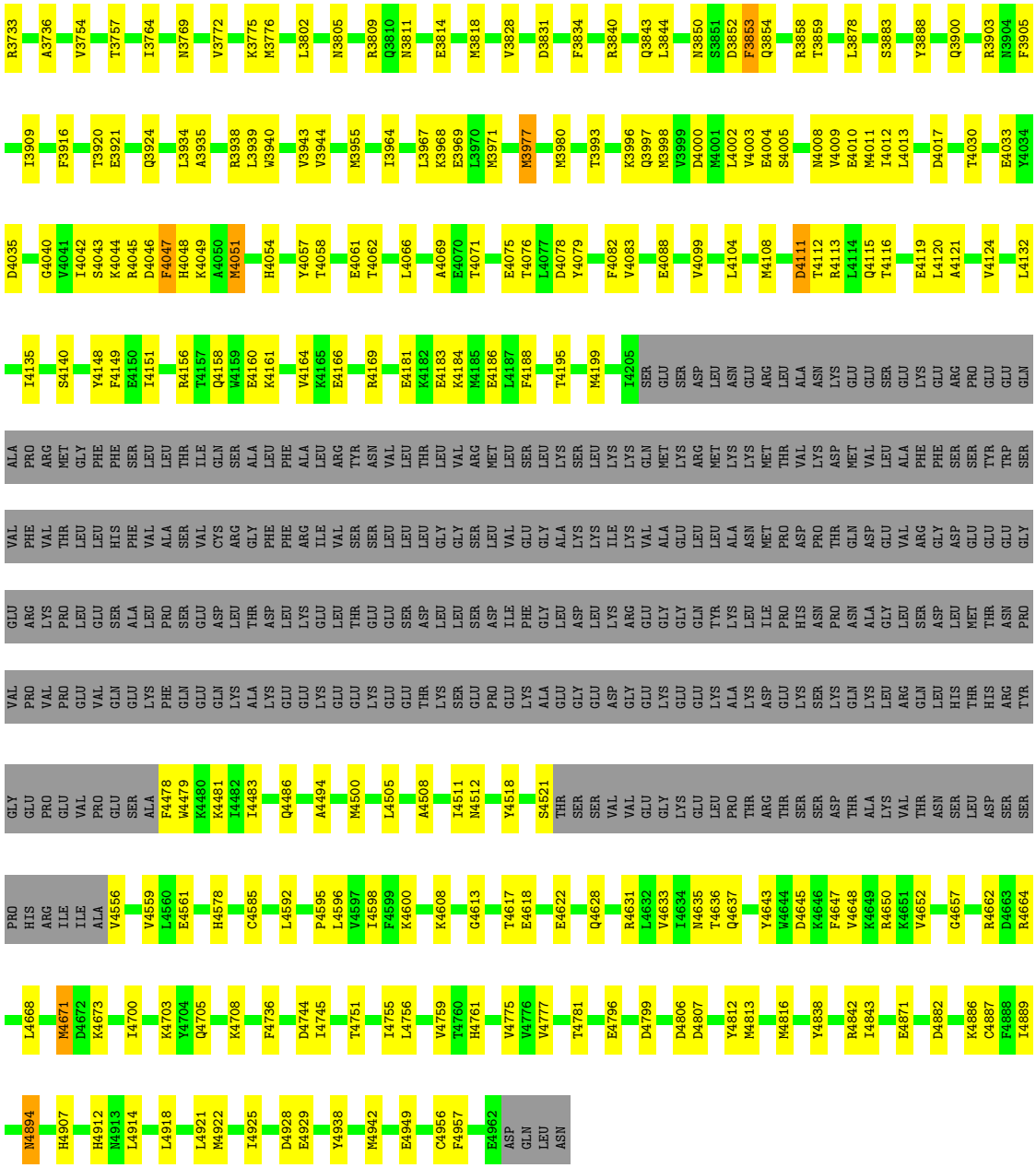
- Molecule 1: Ryanodine receptor 2

Chain A:



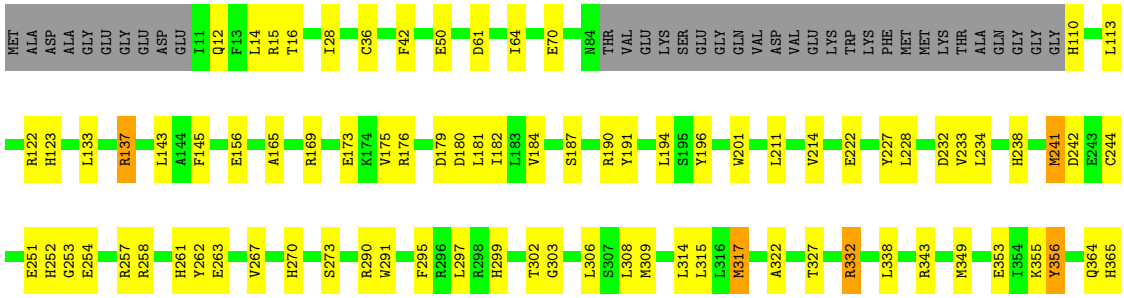

THR GLY GLU R1084 F1085 R1086 E1091 K1092 T1093 Y1094 K1097 A1098 G1099 R1100 W1101 Y1102 F1103 E1104 M1113 R1114 W1117 P1120 P1124 E1127 L1128 A1136 F1137 D1138 R1144 W1156 C1164 M1165 V1166 D1167 M1168 M1173 M1174 L1177 L1182 L1190 A1191 F1192 F1201 I1202
L1207 G1208 V1209 A1210 Q1211 N1216 F1217 G1218 K1219 D1220 V1221 Y1236 N1242 R1245 D1246 I1247 T1248 L1251 R1254 Q1257 F1258 P1262 H1265 E1266 H1267 I1268 E1269 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU K1284 V1285 T1286 Q1287 F1290 Q1293 N1294 N1295
R1303 L1304 S1305 C1310 S1315 LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS
PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1419 L1420 M1421 Q1422 T1423 Y1428 S1429 V1430 R1431
Q1436 E1437 P1438 A1439 N1440 G1444 W1445 I1446 H1451 D1458 L1459 D1460 R1461 T1466 V1467 T1468 L1469 G1470 D1471 H1477 I1480 K1481 R1482 S1483 N1484 C1485 Y1486 M1487 M1494 E1507 C1510 E1535 T1538 V1553 F1554 E1557 R1560 I1561 K1562 N1563 H1576 K1577 C1583
P1584 P1585 H1588 V1589 Q1590 V1595 L1596 W1597 N1602 V1609 S1610 R1611 G1617 V1620 Q1621 C1622 L1623 E1636 N1637 R1638 D1641 E1644 E1649 C1666 L1677 V1681 L1686 Y1694 Y1704 D1705 L1706 L1707 I1708 D1709 I1710 S1713 M1722 I1727 V1728 P1729
E1733 L1739 L1749 P1750 L1754 L1758 R1759 M1762 P1767 SER PHE VAL SER ILE SER ASN ASP C1776 D1786 K1789 A1790 K1791 M1795 K1801 E1802 L1805 R1808 D1809 P1810 V1811 T1814 T1815 E1816 F1817 L1818 P1821 Y1827 I1831 I1834 N1837 E1838 D1839
L1840 K1841 H1842 I1843 L1844 Q1845 L1846 I1847 F1852 K1853 GLU ALA ALA VAL PRO GLU GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU G1891 M1895 E1899 P1900 V1901 K1902 L1903 Q1904 M1905 C1906
L1907 L1908 L1909 C1913 D1914 C1915 R1920 S1928 D1929 V1932 L1935 Q1939 R1942 S1953 A1954 A1955 L1956 R1959 K1960 T1961 R1962 R1965 S1966 P1967 P1968 Q1971 I1972 L1975 F1978 K1979 C1985 P1988 E1989 E1990 I1991 R1992 L1995 F1998 H1999 E2000 D2001 C2006
G2007 I2008 GLU LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 L2057 M2065 V2066 R2067 E2071 E2075 D2076
L2079 M2083 L2086 R2089 Q2090 I2094 V2098 R2099 A2100 L2101 P2102 K2103 T2104 Y2105 S2121 I2125 V2131 R2132 M2133 L2145 M2149 F2154 P2158 N2159 L2160 M2161 L2164 G2165 M2166 V2175 K2184 P2189 K2190 M2191 V2192 A2193 R2197 Y2201 F2202 I2205
Q2210 Y2219 M2233 T2237 P2238 L2239 A2244 E2258 P2259 E2262 K2263 V2264 V2265 R2266 C2276 Q2277 M2278 L2279 W2289 R2296 F2300 L2301 R2302 N2317 V2320 R2321 R2325 R2326 F2330 L2342 L2343 M2346 E2347 E2348 A2349 I2350 K2351 I2352 A2353 E2354 D2355 R2358
P2361 SER PRO THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU ASP D2379 H2382 M2383 G2384 N2385 A2386 I2387 A2392 M2405 H2406 L2407 I2408 K2412 G2413 E2414 A2415 I2418 R2419 R2423 S2424 L2425 I2426 D2430 L2431 V2432 G2433 V2434 I2435 S2436 I2437 A2438 F2439 Q2440 M2441
P2442 THR ILE ALA LYS ASP GLY LYS VAL VAL E2452 P2453 D2454 M2455 S2456 A2457 G2458 F2459 C2460 H2463 K2464 M2467 D2472 R2473 V2474 Y2475 Q2480 D2481 F2482 L2483 L2484 H2485 L2486 V2489 G2490 F2491 R2496 A2497 A2498 A2499 S2500 L2501 D2502 T2503 L2506 S2507 A2512 L2513 A2514 L2515 N2516 R2517
Y2518 L2519 C2520 T2521 L2526 L2527 T2528 R2529 C2530 A2531 F2534 A2535 G2536 T2537 H2540 A2541 S2542 L2543 I2544 D2545 S2546 L2547 L2548 H2549 Y2552 R2553 L2554 S2555 K2556 T2561 Q2564 R2565 D2566 S2567 I2568 E2569 V2570 L2573 Q2578 L2579 R2580 P2581 S2582 M2583 M2584 Q2585 H2586 L2587 L2588 L2591 V2592

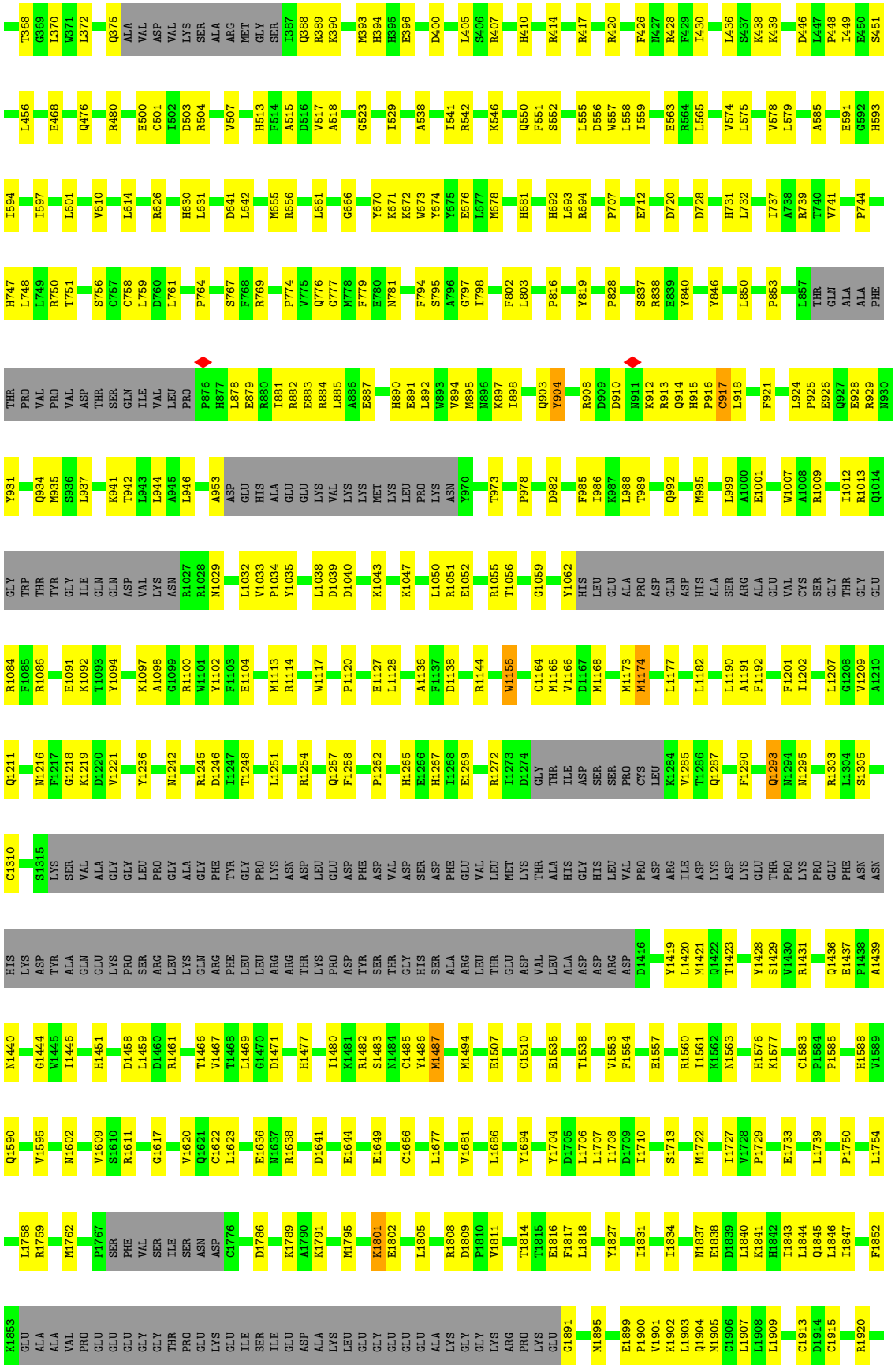


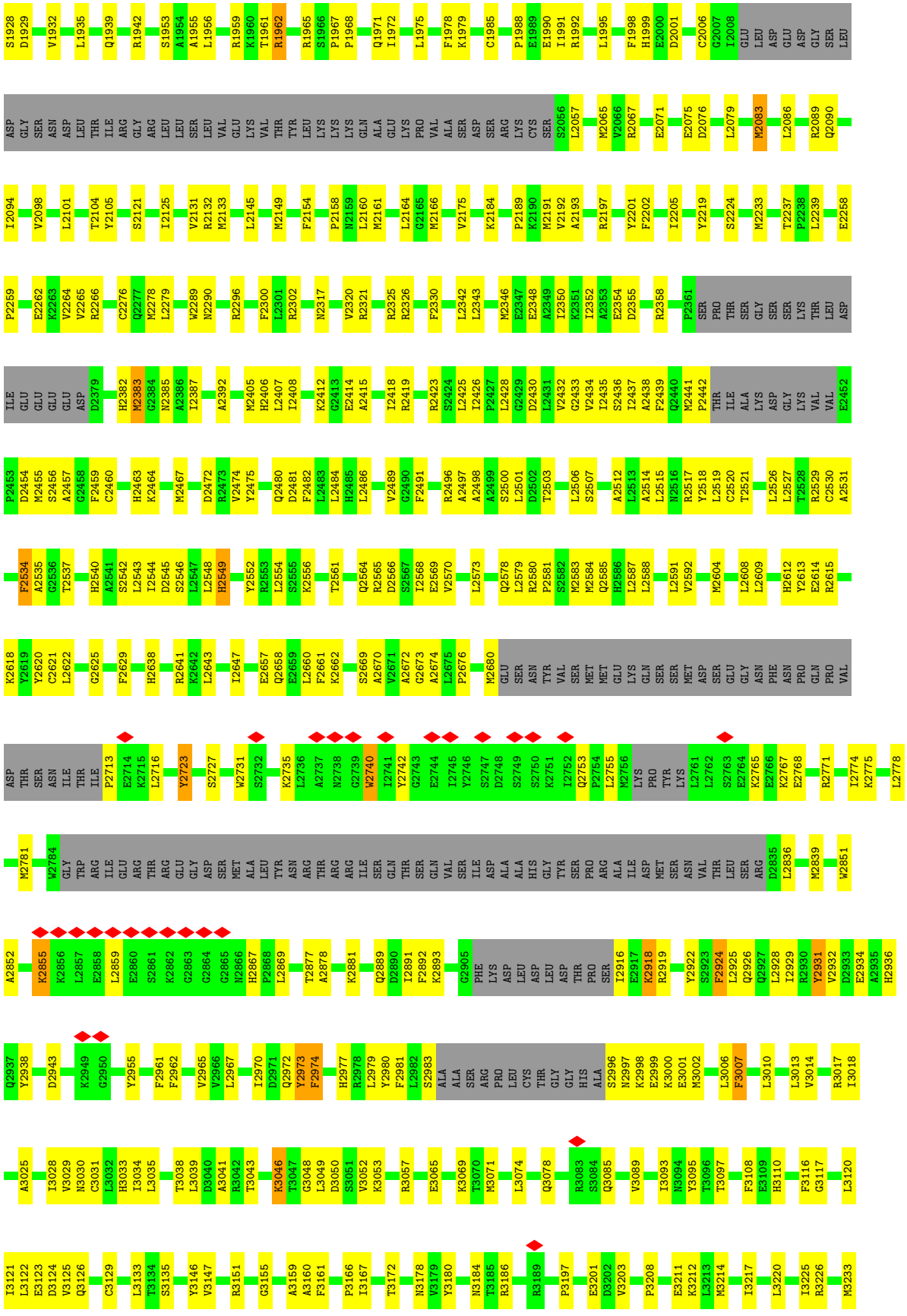


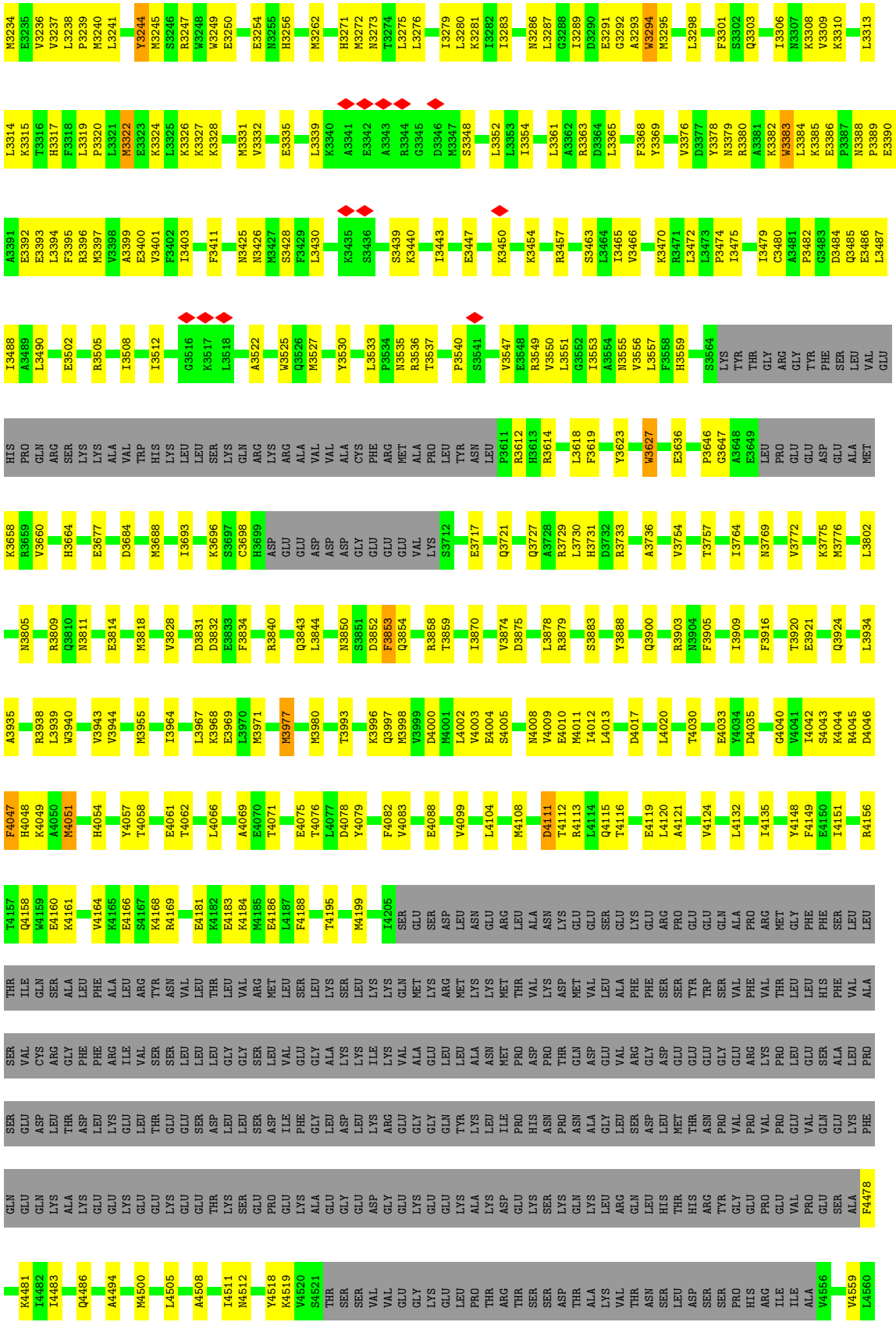
• Molecule 1: Ryanodine receptor 2

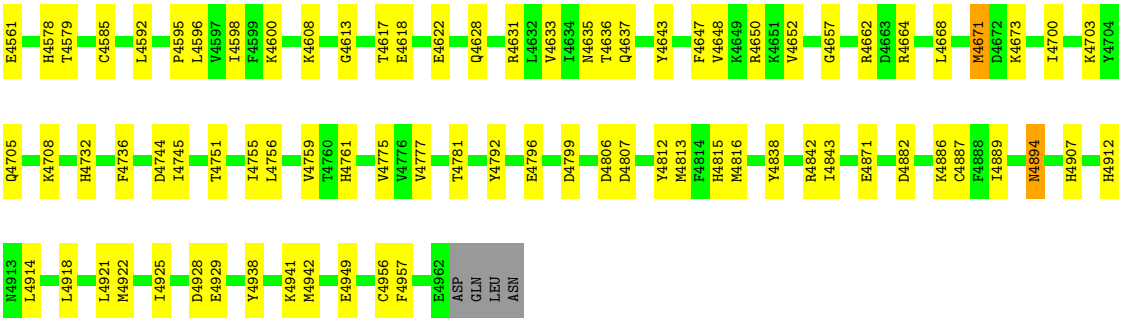
Chain C:





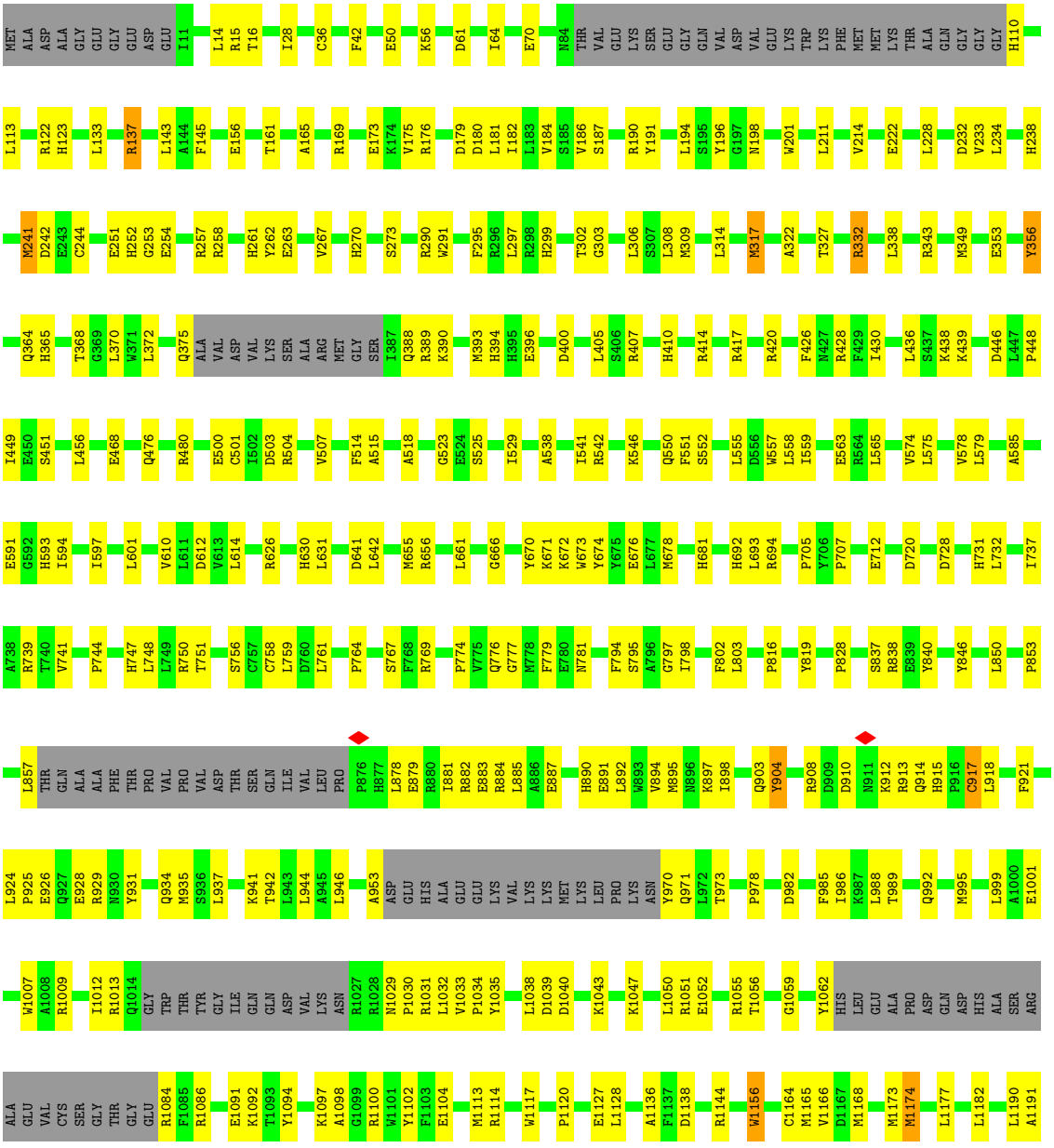


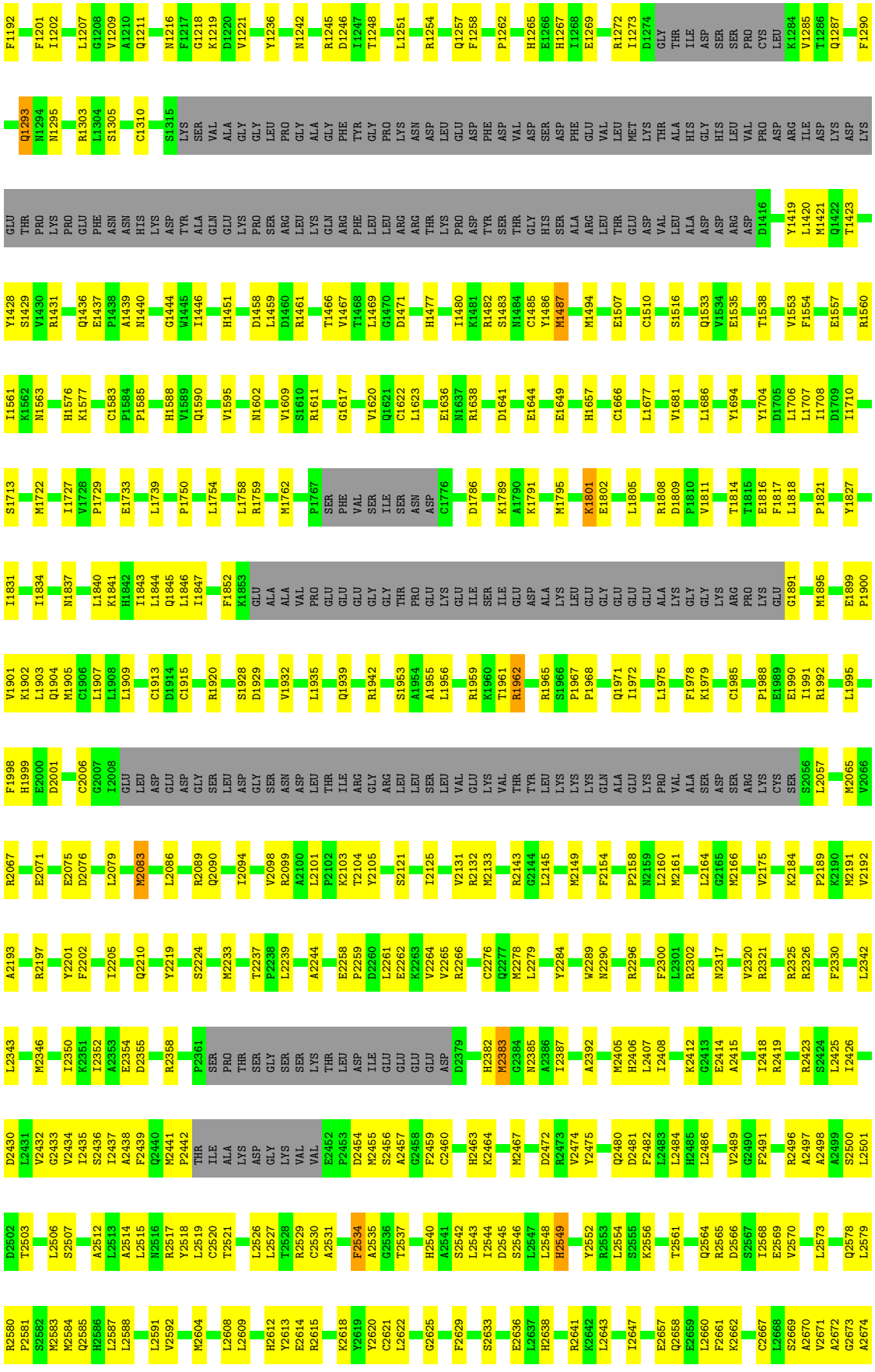


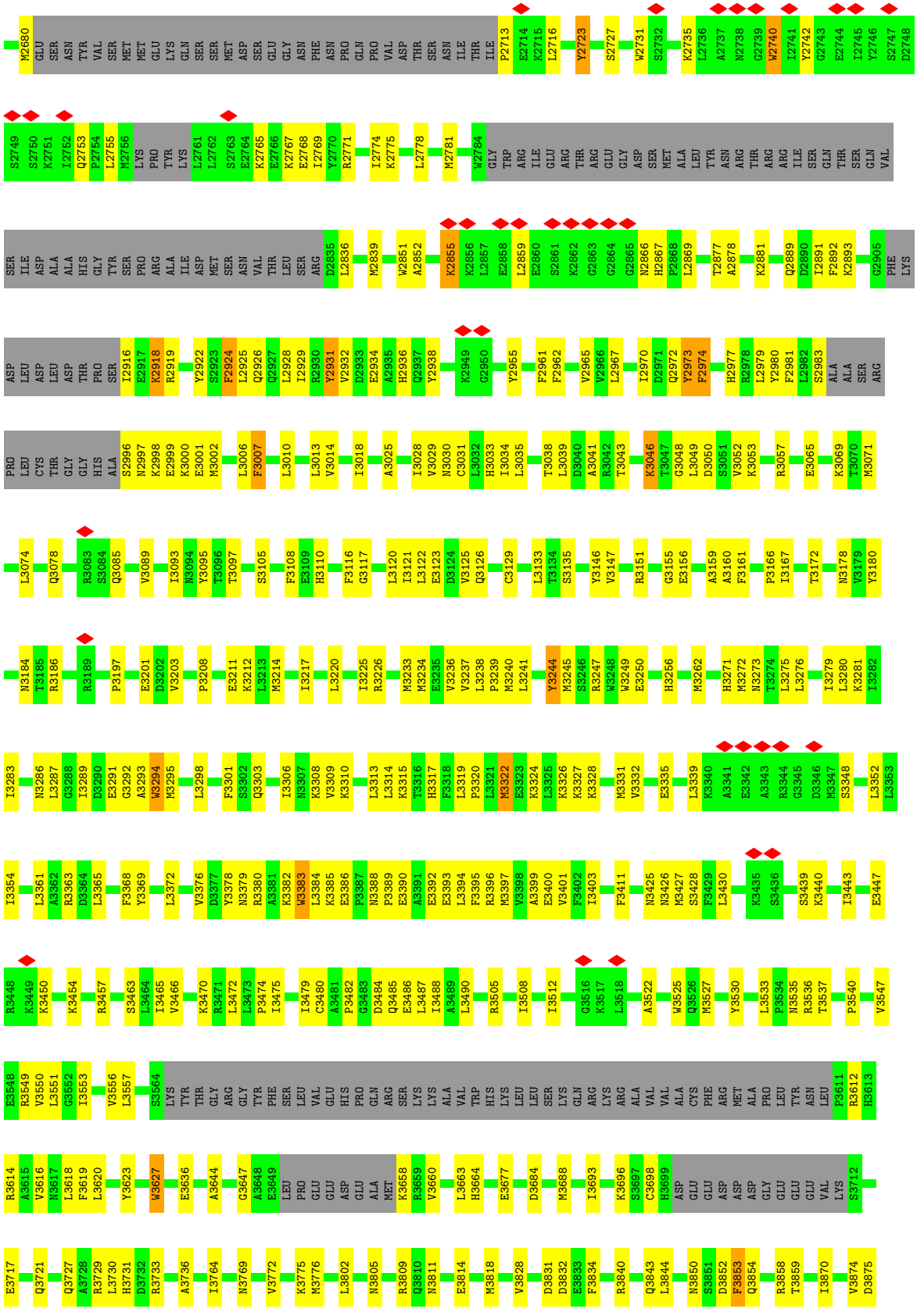


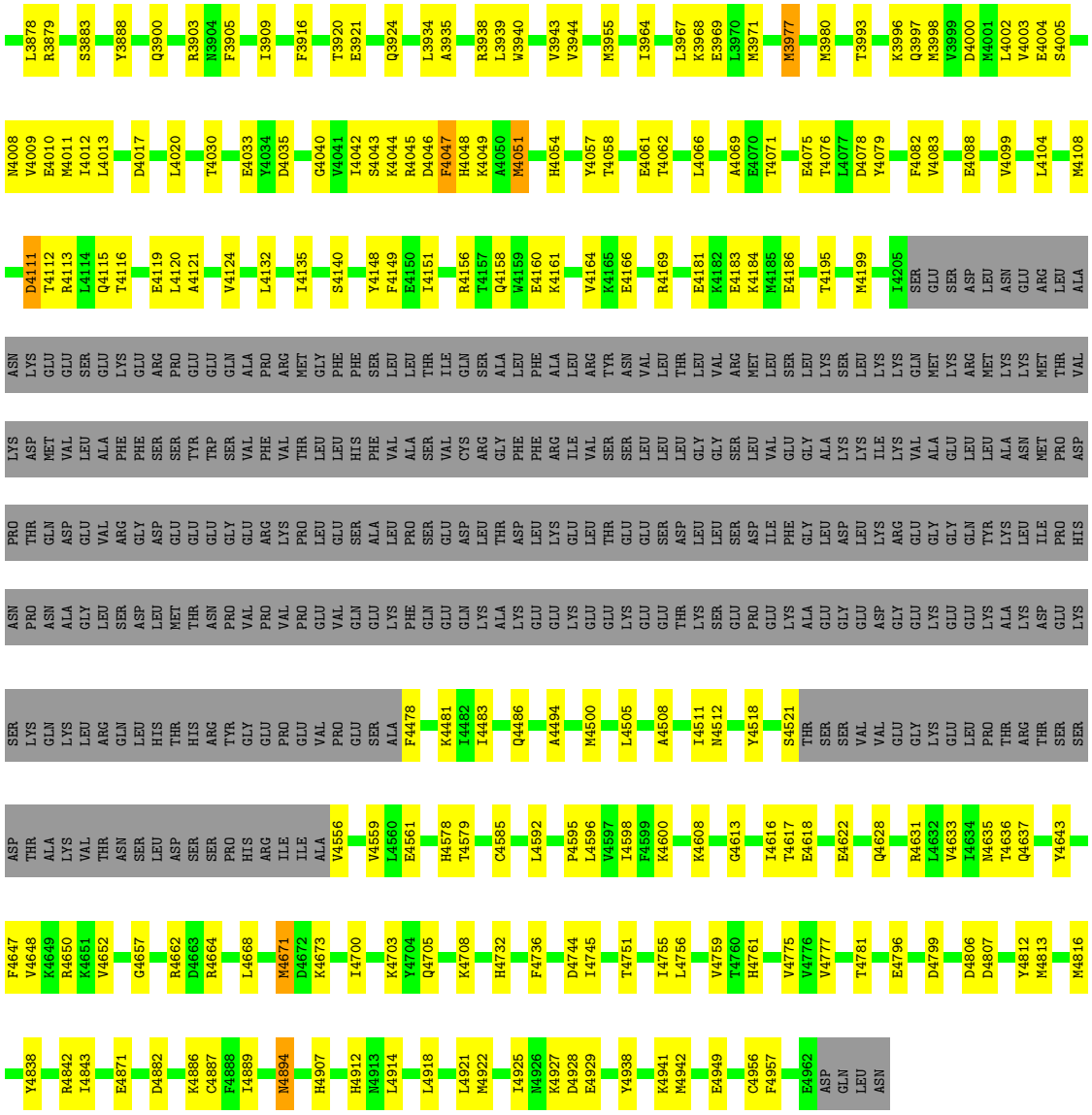
- Molecule 1: Ryanodine receptor 2

Chain E:



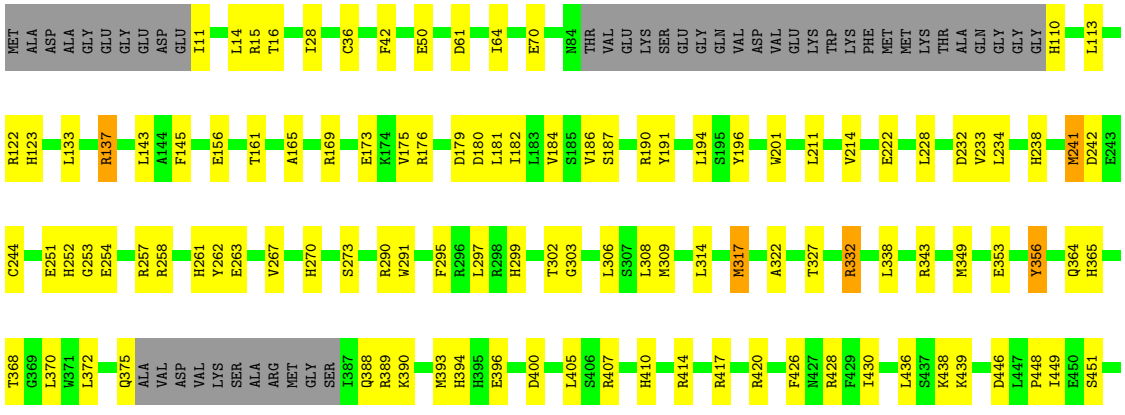

F1192 F1201 I1202 L1207 G1208 V1209 A1210 Q1211 N1216 F1217 G1218 K1219 D1220 V1221 Y1236 N1242 R1245 D1246 I1247 T1248 L1251 R1254 Q1257 F1258 P1262 H1265 E1266 H1267 I1268 E1269 R1272 I1273 D1274 GLY THR THR ILE ASP SER SER PRO CYS LEU K1284 V1285 T1286 Q1287 F1290
Q1293 N1294 N1295 R1303 L1304 S1305 C1310 S1315 LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU ALA ASP ARG ILE ASP LYS ASP LYS
GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ARG ASP D1416 Y1419 L1420 M1421 Q1422 T1423
Y1428 S1429 V1430 R1431 Q1436 E1437 P1438 A1439 N1440 G1444 W1445 I1446 H1451 D1458 L1459 D1460 R1461 T1466 V1467 T1468 L1469 G1470 D1471 H1477 I1480 K1481 R1482 S1483 N1484 C1485 Y1486 M1487 M1494 E1507 C1510 S1516 Q1533 V1534 E1535 T1538 V1553 F1554 E1557 R1560
I1561 K1562 N1563 H1576 K1577 C1583 P1584 P1585 H1588 V1589 Q1590 V1595 N1602 V1609 S1610 R1611 G1617 V1620 Q1621 C1622 L1623 E1636 N1637 R1638 D1641 E1644 E1649 H1657 C1666 L1677 V1681 L1686 Y1694 Y1704 D1705 L1706 L1707 I1708 D1709 I1710
S1713 M1722 I1727 V1728 P1729 E1733 L1739 P1750 L1754 L1758 R1759 M1762 P1767 SER PHE VAL SER ILE SER ASN ASP C1776 D1786 K1789 A1790 K1791 M1795 K1801 E1802 L1805 R1808 D1809 P1810 V1811 T1814 T1815 E1816 F1817 L1818 P1821 Y1827
I1831 I1834 N1837 L1840 K1841 H1842 I1843 L1844 Q1845 L1846 I1847 F1852 K1853 GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU G1891 M1895 E1899 P1900
V1901 K1902 L1903 Q1904 M1905 C1906 L1907 L1908 L1909 C1913 D1914 C1915 R1920 S1928 D1929 V1932 L1935 Q1939 R1942 S1953 A1954 A1955 L1956 R1959 K1960 T1961 R1962 R1965 S1966 P1967 P1968 Q1971 I1972 L1975 F1978 K1979 C1985 P1988 E1989 E1990 I1991 R1992 L1995
F1998 H1999 E2000 D2001 C2006 G2007 I2008 GLU LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 L2057 M2065 V2066
R2067 E2071 E2075 D2076 L2079 M2083 L2086 R2089 Q2090 I2094 V2098 R2099 A2100 L2101 P2102 K2103 T2104 Y2105 S2121 I2125 V2131 R2132 M2133 R2143 G2144 L2145 M2149 F2154 P2158 N2159 L2160 M2161 L2164 G2165 M2166 V2175 K2184 P2189 K2190 M2191 V2192
A2193 R2197 Y2201 F2202 I2205 Q2210 Y2219 S2224 M2233 T2237 P2238 L2239 A2244 E2258 P2259 D2260 L2261 E2262 K2263 V2264 V2265 R2266 C2276 Q2277 M2278 L2279 Y2284 W2289 N2290 R2296 F2300 L2301 R2302 N2317 V2320 R2321 R2325 R2326 F2330 L2342
L2343 M2346 I2350 K2351 I2352 A2353 E2354 D2355 R2358 P2361 SER PRO THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU GLU ASP D2379 H2382 M2383 C2384 N2385 A2386 I2387 A2392 M2405 H2406 L2407 I2408 K2412 G2413 E2414 A2415 I2418 R2419 R2423 S2424 L2425 I2426
D2430 L2431 V2432 G2433 V2434 I2435 S2436 I2437 A2438 F2439 Q2440 M2441 P2442 THR ILE ALA LYS ASP GLY LYS VAL VAL E2452 P2453 D2454 M2455 S2456 A2457 G2458 F2459 C2460 H2463 K2464 M2467 D2472 R2473 V2474 Y2475 Q2480 D2481 F2482 L2483 L2484 H2485 L2486 V2489 G2490 F2491 R2496 A2497 A2498 A2499 S2500 L2501
D2502 T2503 L2506 S2507 A2512 L2513 A2514 L2515 N2516 R2517 Y2518 L2519 C2520 T2521 L2526 L2527 T2528 R2529 C2530 A2531 F2534 A2535 G2536 T2537 H2540 A2541 S2542 L2543 I2544 D2545 S2546 L2547 L2548 H2549 Y2552 R2553 L2554 S2555 K2556 T2561 Q2564 R2565 D2566 S2567 I2568 E2569 V2570 L2573 Q2578 L2579
R2580 P2581 S2582 M2583 M2584 Q2585 H2586 L2587 L2588 L2591 V2592 M2604 L2608 L2609 H2612 Y2613 E2614 R2615 K2618 Y2619 Y2620 C2621 L2622 G2625 F2629 S2633 E2636 L2637 H2638 R2641 K2642 L2643 I2647 E2657 Q2658 E2659 L2660 F2661 K2662 C2667 L2668 S2669 A2670 V2671 A2672 G2673 A2674

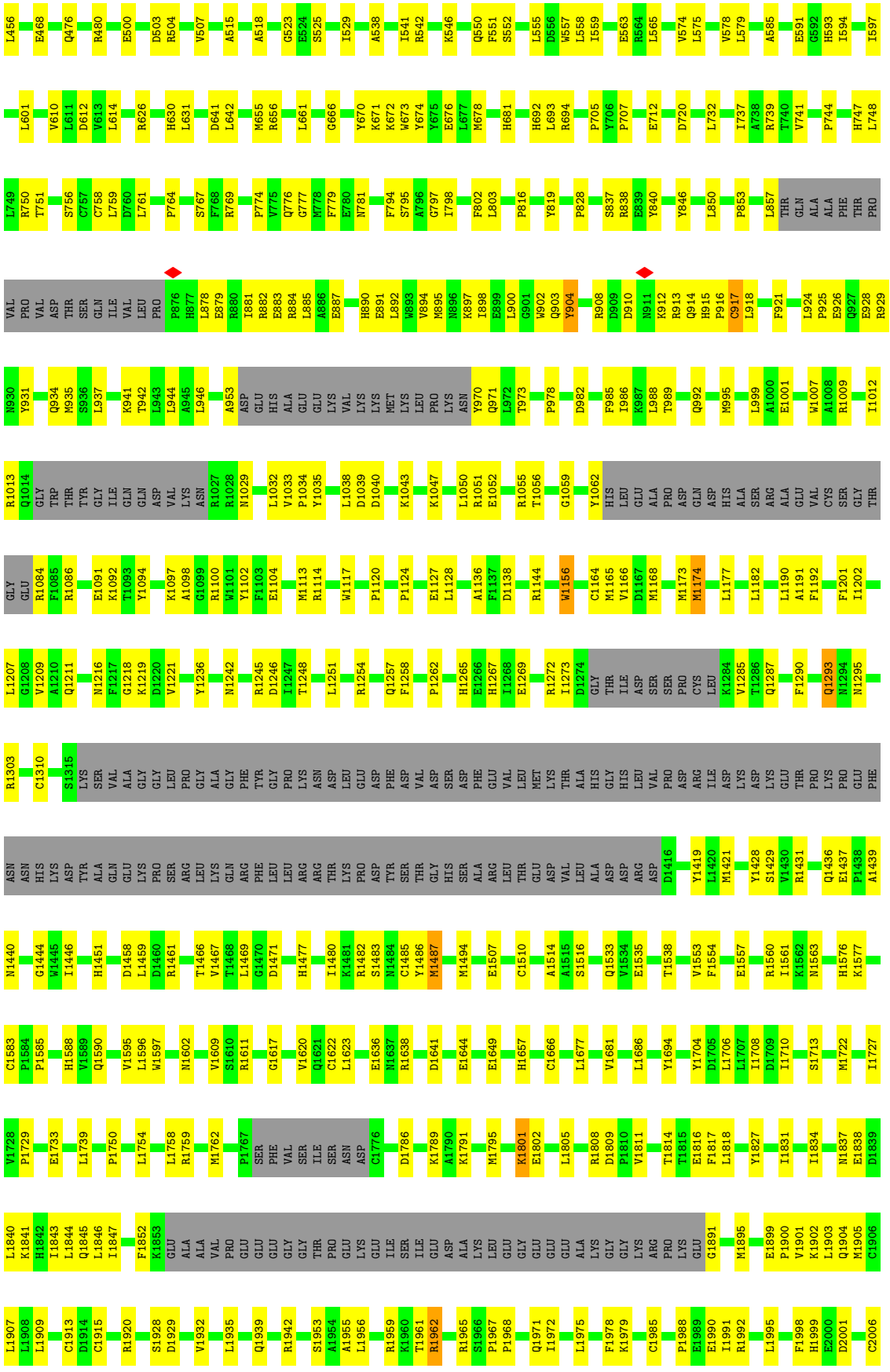


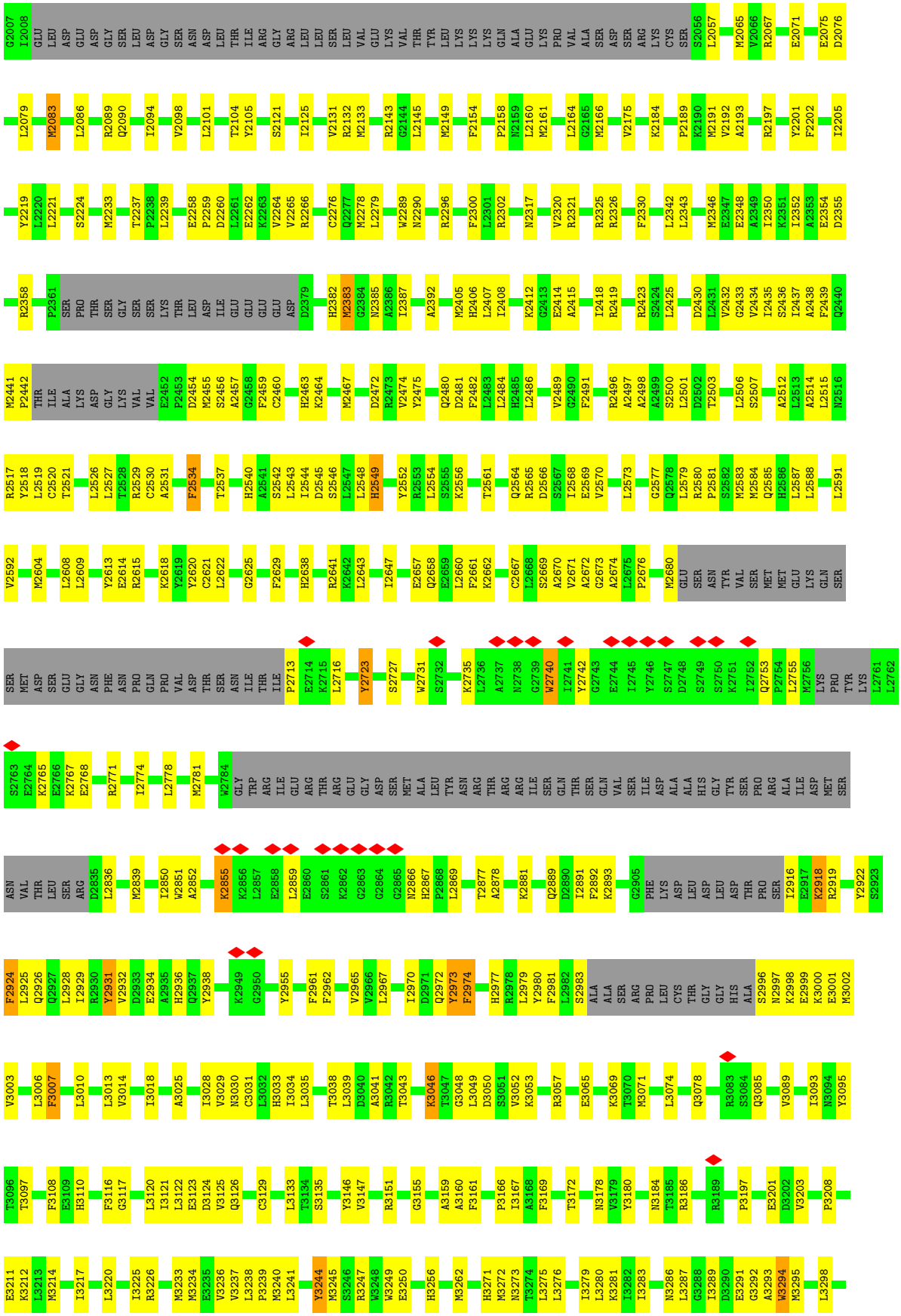


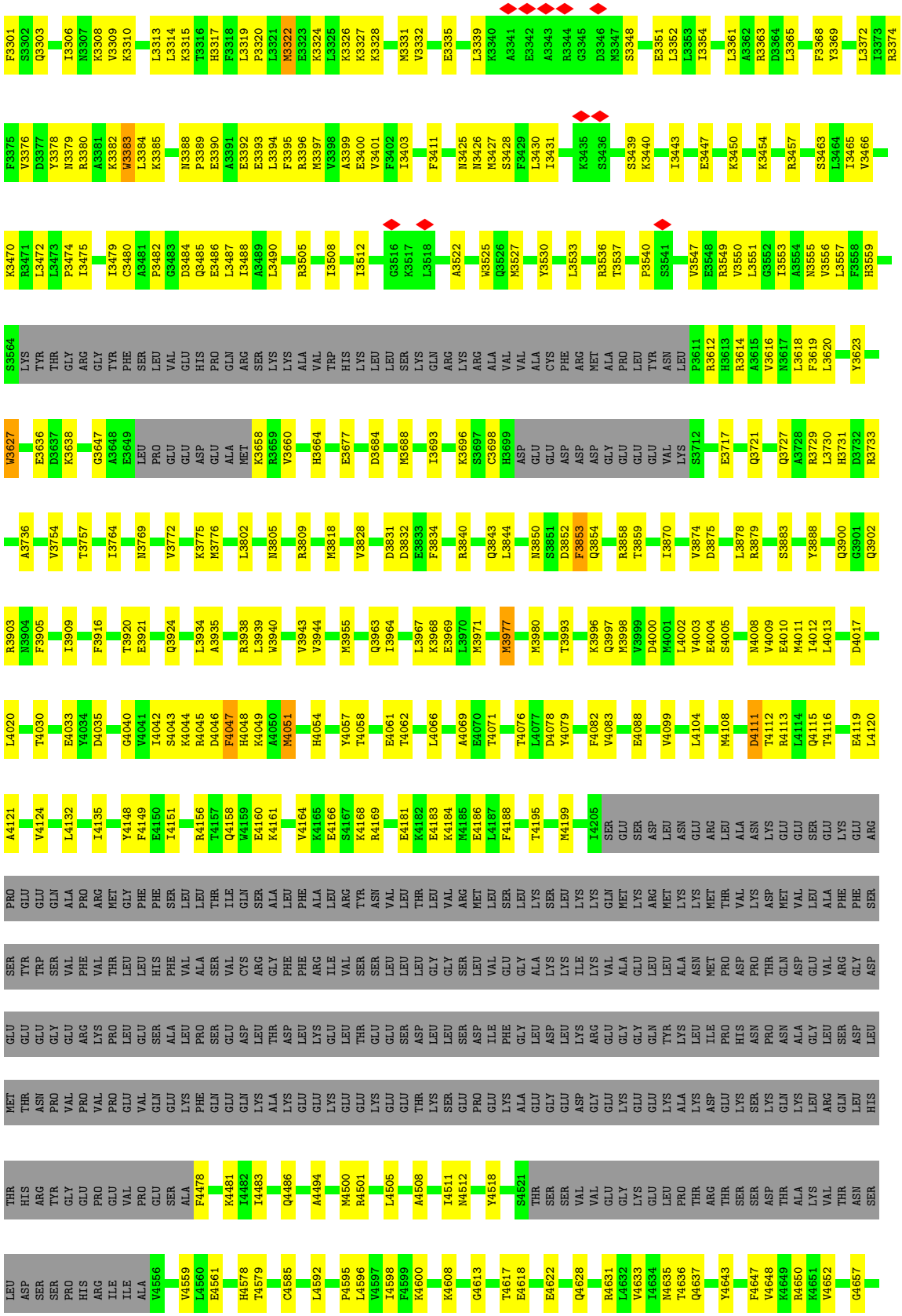
• Molecule 1: Ryanodine receptor 2

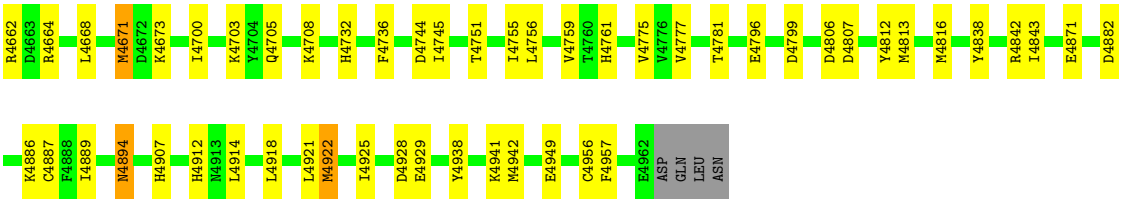
Chain F:




L456 E468 Q476 R480 E500 D503 R504 V507 A515 A518 G523 E524 S525 I529 A538 I541 R542 K546 Q550 F551 S552 L555 D556 W557 L558 I559 E563 R564 L565 V574 L575 V578 L579 A585 E591 G592 H593 I594 I597
L601 V610 L611 D612 V613 L614 R626 H630 L631 D641 L642 M655 R656 L661 G666 Y670 K671 K672 W673 Y674 Y675 E676 L677 M678 H681 H692 L693 R694 P705 Y706 P707 E712 D720 L732 I737 A738 R739 T740 V741 P744 H747 L748
L749 R750 T751 S756 C757 C758 L759 D760 L761 P764 S767 F768 R769 P774 V775 Q776 G777 M778 F779 E780 N781 F794 S795 A796 G797 I798 F802 L803 P816 Y819 P828 S837 R838 E839 Y840 Y846 L850 P853 L857 THR GLN ALA ALA PHE THR PRO
VAL PRO VAL ASP THR SER GLN ILE VAL LEU PRO P876 H877 L878 E879 R880 I881 R882 E883 R884 L885 A886 E887 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 F921 L924 P925 E926 Q927 E928 R929
N930 Y931 Q934 M935 S936 L937 K941 T942 L943 L944 A945 L946 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 P978 D982 F985 I986 K987 L988 T989 Q992 M995 L999 A1000 E1001 W1007 A1008 R1009 I1012
R1013 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 R1028 N1029 L1032 V1033 P1034 Y1035 L1038 D1039 D1040 K1043 K1047 L1050 R1051 E1052 R1055 T1056 G1059 Y1062 HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR
GLY GLU R1084 F1085 R1086 E1091 K1092 T1093 Y1094 K1097 A1098 G1099 R1100 W1101 Y1102 F1103 E1104 M1113 R1114 W1117 P1120 P1124 E1127 L1128 A1136 F1137 D1138 R1144 W1156 C1164 M1165 V1166 D1167 M1168 M1173 M1174 L1177 L1182 L1190 A1191 F1192 F1201 I1202
L1207 G1208 V1209 A1210 Q1211 N1216 F1217 G1218 K1219 D1220 V1221 Y1236 N1242 R1245 D1246 I1247 T1248 L1251 R1254 Q1257 F1258 P1262 H1265 E1266 H1267 I1268 E1269 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU K1284 V1285 T1286 Q1287 F1290 Q1293 N1294 N1295
R1303 C1310 S1315 LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE
ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1419 L1420 M1421 Y1428 S1429 V1430 R1431 Q1436 E1437 P1438 A1439
N1440 G1444 W1445 I1446 H1451 D1458 L1459 D1460 R1461 T1466 V1467 T1468 L1469 G1470 D1471 H1477 I1480 K1481 R1482 S1483 N1484 C1485 Y1486 M1487 M1494 E1507 C1510 A1514 A1515 S1516 Q1533 V1534 E1535 T1538 V1553 F1554 E1557 R1560 I1561 K1562 N1563 H1576 K1577
C1583 P1584 P1585 H1588 V1589 Q1590 V1595 L1596 W1597 N1602 V1609 S1610 R1611 G1617 V1620 Q1621 C1622 L1623 E1636 N1637 R1638 D1641 E1644 E1649 H1657 C1666 L1677 V1681 L1686 Y1694 Y1704 D1705 L1706 L1707 I1708 D1709 I1710 S1713 M1722 I1727
V1728 P1729 E1733 L1739 P1750 L1754 L1758 R1759 M1762 P1767 SER PHE VAL SER ILE SER ASN ASP C1776 D1786 K1789 A1790 K1791 M1795 K1801 E1802 L1805 R1808 D1809 P1810 V1811 T1814 T1815 E1816 F1817 L1818 Y1827 I1831 I1834 N1837 E1838 D1839
L1840 K1841 H1842 I1843 L1844 Q1845 L1846 I1847 F1852 K1853 GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS G1891 M1895 E1899 P1900 V1901 K1902 L1903 Q1904 M1905 C1906
L1907 L1908 L1909 C1913 D1914 C1915 R1920 S1928 D1929 V1932 L1935 Q1939 R1942 S1953 A1954 A1955 L1956 R1959 K1960 T1961 R1962 R1965 S1966 P1967 P1968 Q1971 I1972 L1975 F1978 K1979 C1985 P1988 E1989 E1990 I1991 R1992 L1995 F1998 H1999 E2000 D2001 C2006

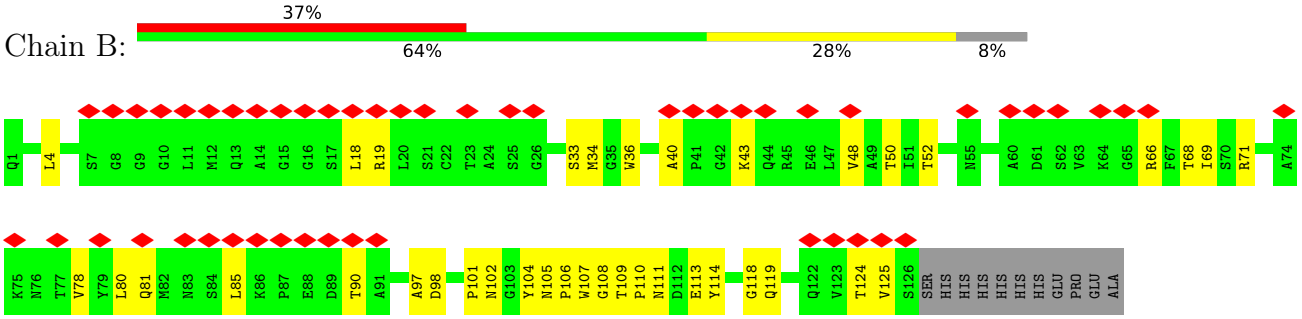






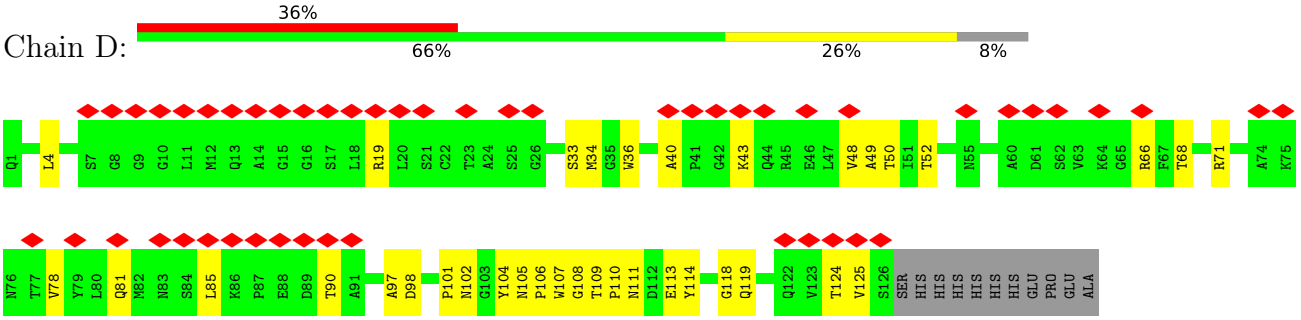
• Molecule 2: Nanobody 9657

Chain B:



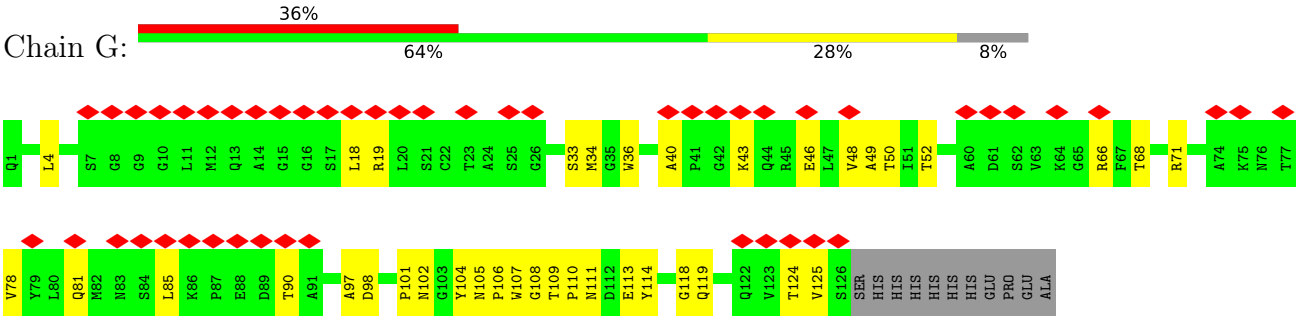
• Molecule 2: Nanobody 9657

Chain D:



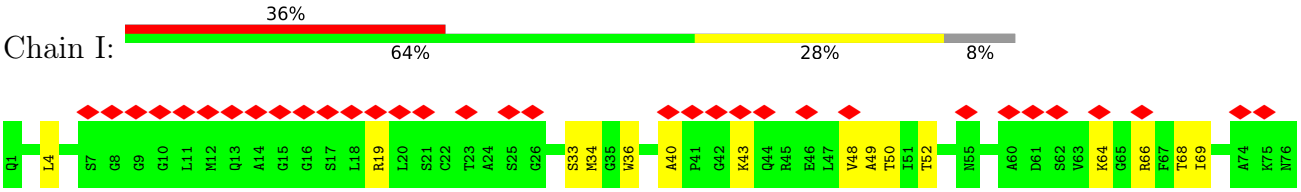
• Molecule 2: Nanobody 9657

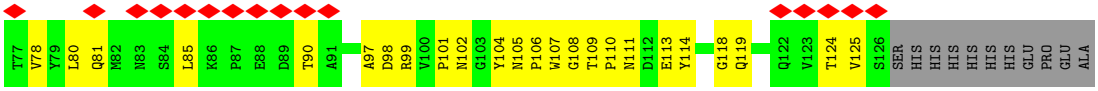
Chain G:



• Molecule 2: Nanobody 9657

Chain I:




T77
V78
Y79
L80
Q81
M82
N83
S84
L85
K86
P87
E88
D89
T90
A91
A97
D98
R99
V100
P101
N102
G103
Y104
N105
P106
W107
G108
T109
P110
N111
D112
E113
Y114
G118
Q119
Q122
V123
T124
V125
S126
SER
HIS
HIS
HIS
HIS
HIS
HIS
GLU
PRO
GLU
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76852	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.181	Depositor
Minimum map value	-0.204	Depositor
Average map value	0.074	Depositor
Map value standard deviation	0.151	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	490.56, 490.56, 490.56	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.46, 1.46, 1.46	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, CFF, CA

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	0.26	0/33802	0.50	1/45653 (0.0%)
1	C	0.26	0/33802	0.50	1/45653 (0.0%)
1	E	0.26	0/33802	0.50	1/45653 (0.0%)
1	F	0.26	0/33802	0.50	1/45653 (0.0%)
2	B	0.26	0/984	0.51	0/1335
2	D	0.26	0/984	0.51	0/1335
2	G	0.26	0/984	0.51	0/1335
2	I	0.26	0/984	0.51	0/1335
All	All	0.26	0/139144	0.50	4/187952 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1494	MET	CA-CB-CG	5.38	122.45	113.30
1	F	1494	MET	CA-CB-CG	5.38	122.44	113.30
1	C	1494	MET	CA-CB-CG	5.37	122.43	113.30
1	A	1494	MET	CA-CB-CG	5.36	122.41	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33088	0	32662	852	0
1	C	33088	0	32662	837	0
1	E	33088	0	32662	853	0
1	F	33088	0	32662	854	0
2	B	965	0	910	28	0
2	D	965	0	910	27	0
2	G	965	0	910	28	0
2	I	965	0	910	27	0
3	A	31	0	12	3	0
3	C	31	0	12	3	0
3	E	31	0	12	3	0
3	F	31	0	12	3	0
4	A	14	0	10	0	0
4	C	14	0	10	0	0
4	E	14	0	10	0	0
4	F	14	0	10	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	136400	0	134376	3465	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 13.

The worst 5 of 3465 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2641:ARG:HH12	1:A:2680:MET:HE3	1.42	0.85
1:C:2641:ARG:HH12	1:C:2680:MET:HE3	1.41	0.84
1:E:2641:ARG:HH12	1:E:2680:MET:HE3	1.41	0.84
1:A:4040:GLY:HA3	1:A:4078:ASP:HA	1.60	0.83
1:F:2641:ARG:HH12	1:F:2680:MET:HE3	1.41	0.83

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4094/4966 (82%)	3987 (97%)	106 (3%)	1 (0%)	100	100
1	C	4094/4966 (82%)	3986 (97%)	107 (3%)	1 (0%)	100	100
1	E	4094/4966 (82%)	3986 (97%)	107 (3%)	1 (0%)	100	100
1	F	4094/4966 (82%)	3983 (97%)	110 (3%)	1 (0%)	100	100
2	B	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
2	D	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
2	G	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
2	I	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
All	All	16872/20412 (83%)	16414 (97%)	454 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2530	CYS
1	C	2530	CYS
1	E	2530	CYS
1	F	2530	CYS

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	3589/4355 (82%)	3516 (98%)	73 (2%)	50	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	3589/4355 (82%)	3517 (98%)	72 (2%)	50 70
1	E	3589/4355 (82%)	3516 (98%)	73 (2%)	50 70
1	F	3589/4355 (82%)	3516 (98%)	73 (2%)	50 70
2	B	103/114 (90%)	102 (99%)	1 (1%)	73 83
2	D	103/114 (90%)	102 (99%)	1 (1%)	73 83
2	G	103/114 (90%)	101 (98%)	2 (2%)	52 71
2	I	103/114 (90%)	102 (99%)	1 (1%)	73 83
All	All	14768/17876 (83%)	14472 (98%)	296 (2%)	50 70

5 of 296 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	913	ARG
1	F	4643	TYR
1	F	1293	GLN
1	F	2924	PHE
1	C	1962	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	238	HIS
1	E	2480	GLN
1	F	3485	GLN
1	E	375	GLN
1	E	1296	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CFF	C	5102	-	8,15,15	1.04	0	8,23,23	2.51	2 (25%)
4	CFF	E	5102	-	8,15,15	1.04	0	8,23,23	2.52	2 (25%)
4	CFF	A	5102	-	8,15,15	1.04	0	8,23,23	2.52	2 (25%)
3	ATP	C	5101	-	26,33,33	0.62	0	31,52,52	0.78	2 (6%)
4	CFF	F	5102	-	8,15,15	1.04	0	8,23,23	2.51	2 (25%)
3	ATP	A	5101	-	26,33,33	0.61	0	31,52,52	0.78	2 (6%)
3	ATP	F	5101	-	26,33,33	0.62	0	31,52,52	0.78	2 (6%)
3	ATP	E	5101	-	26,33,33	0.62	0	31,52,52	0.78	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
4	CFF	C	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	A	5102	-	-	-	0/2/2/2
3	ATP	C	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	F	5102	-	-	-	0/2/2/2
3	ATP	A	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	F	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	5102	CFF	C5-C6-N1	-5.88	111.93	118.20
4	E	5102	CFF	C5-C6-N1	-5.88	111.93	118.20
4	F	5102	CFF	C5-C6-N1	-5.87	111.94	118.20
4	C	5102	CFF	C5-C6-N1	-5.87	111.94	118.20
4	A	5102	CFF	C4-C5-C6	3.73	122.36	119.96

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5101	ATP	C5'-O5'-PA-O1A
3	C	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	F	5101	ATP	C5'-O5'-PA-O1A
3	A	5101	ATP	C4'-C5'-O5'-PA

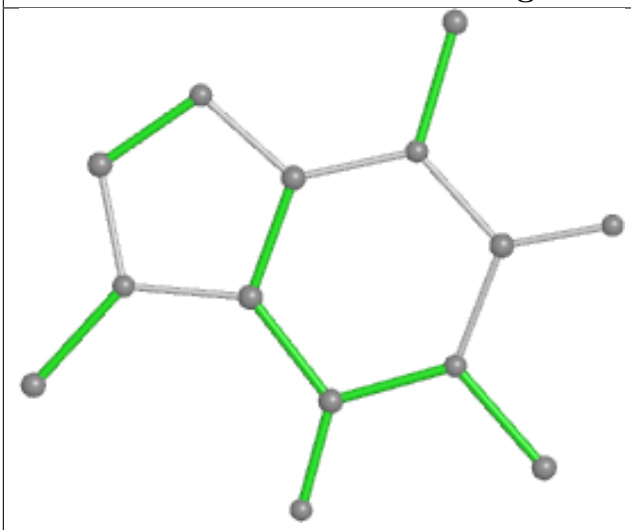
There are no ring outliers.

4 monomers are involved in 12 short contacts:

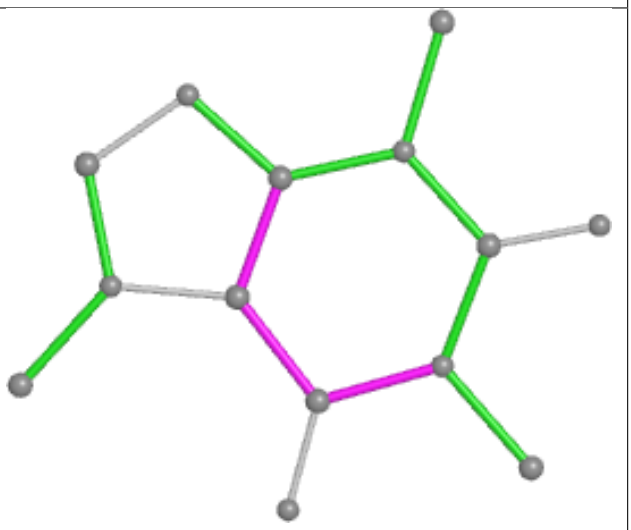
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5101	ATP	3	0
3	A	5101	ATP	3	0
3	F	5101	ATP	3	0
3	E	5101	ATP	3	0

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.

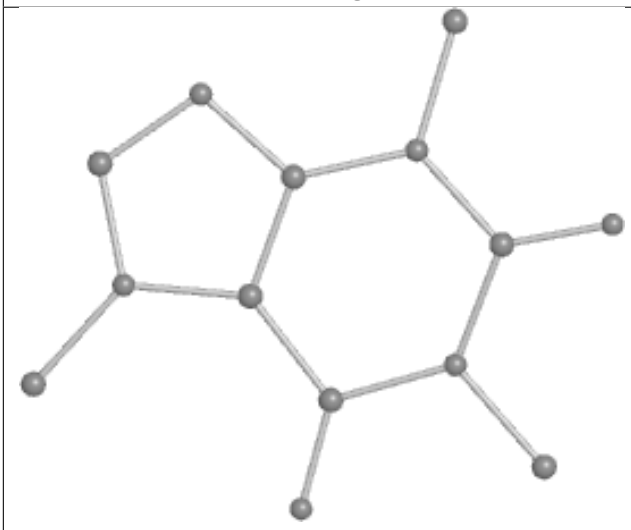
Ligand CFF C 5102



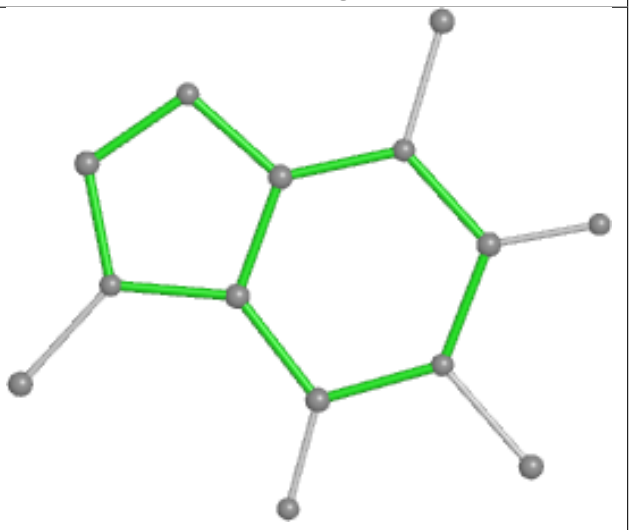
Bond lengths



Bond angles

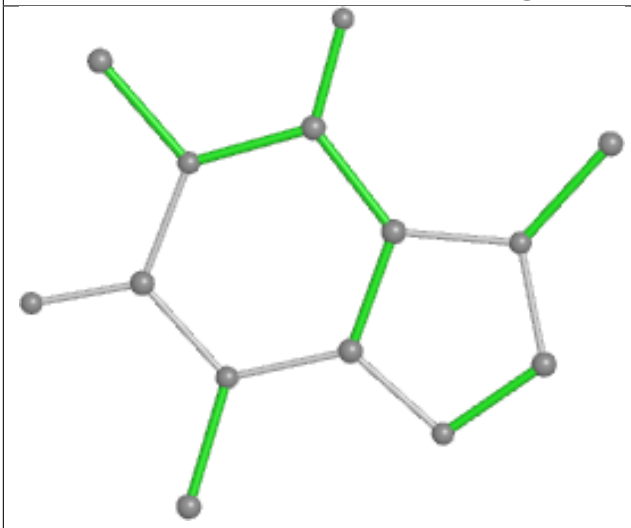


Torsions

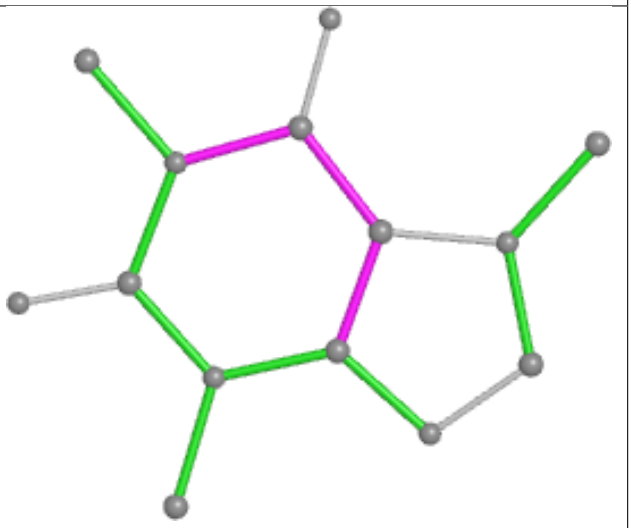


Rings

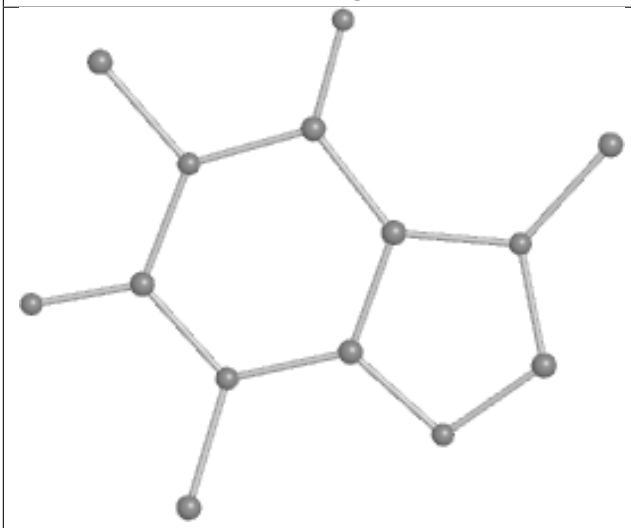
Ligand CFF E 5102



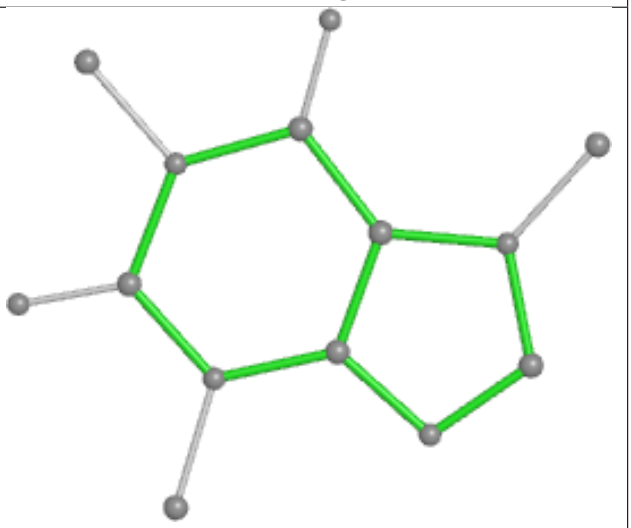
Bond lengths



Bond angles

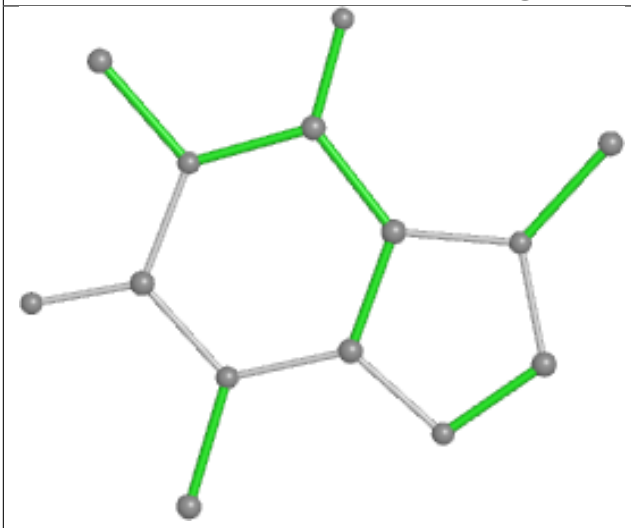


Torsions

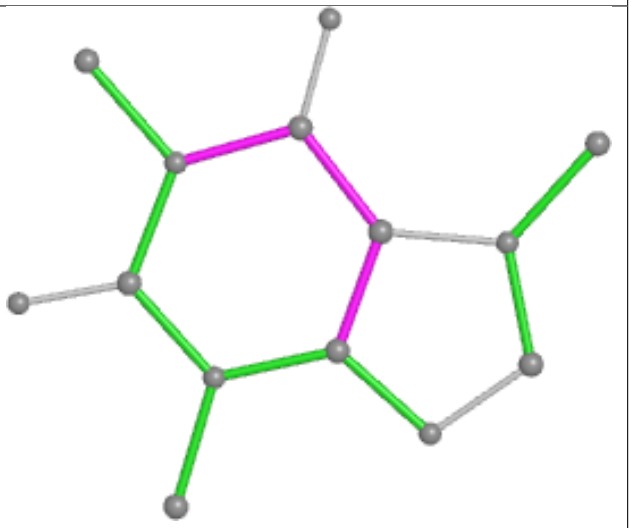


Rings

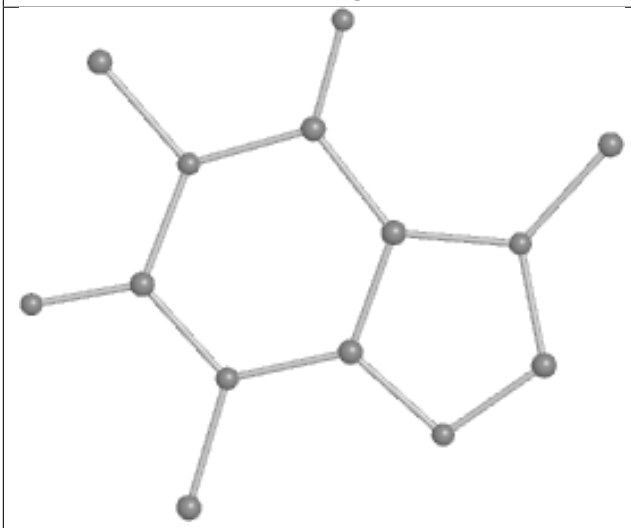
Ligand CFF A 5102



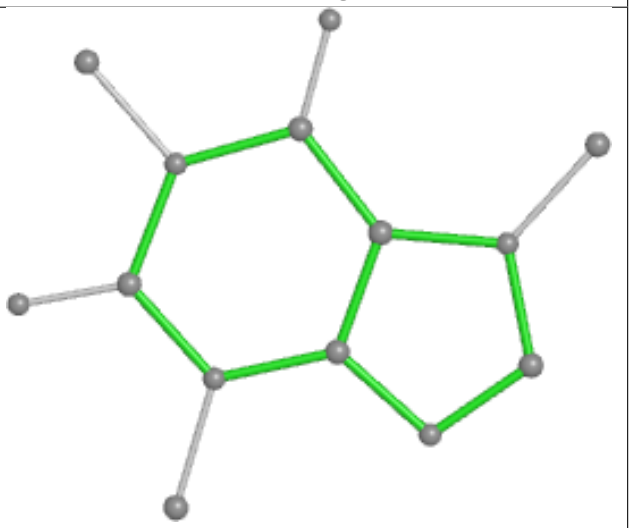
Bond lengths



Bond angles

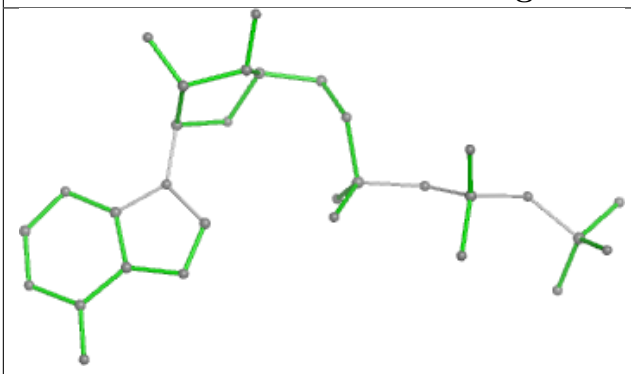


Torsions

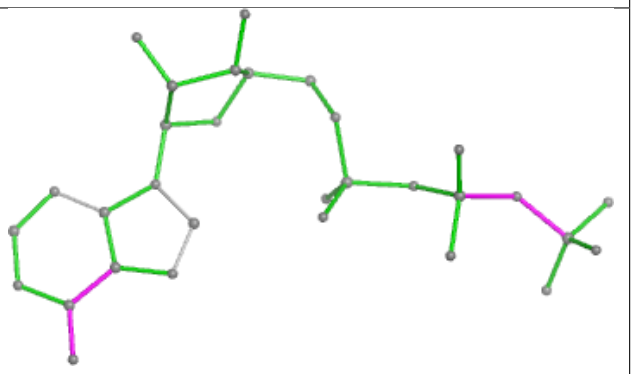


Rings

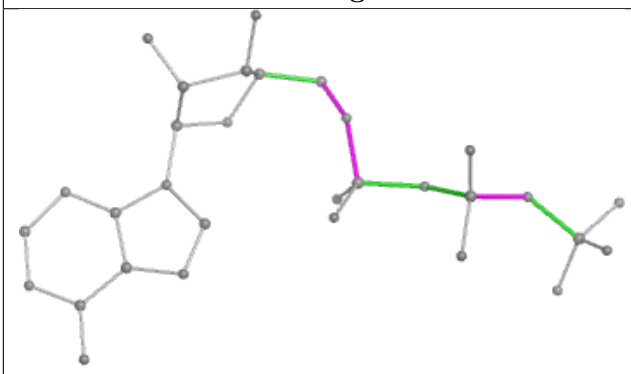
Ligand ATP C 5101



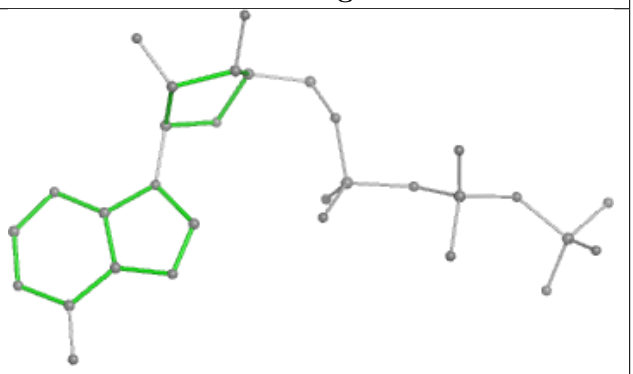
Bond lengths



Bond angles

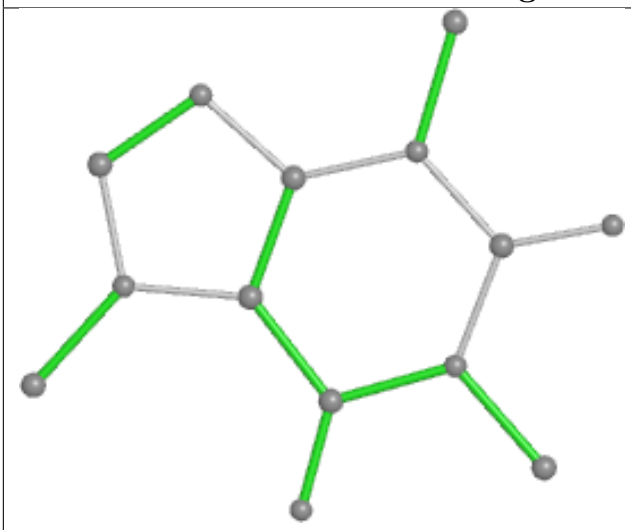


Torsions

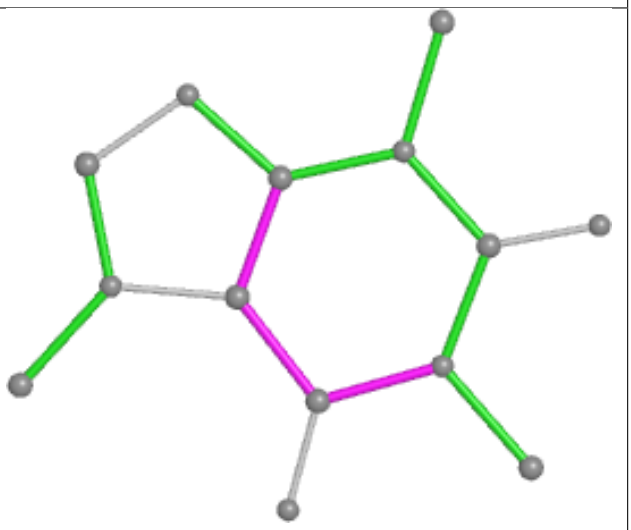


Rings

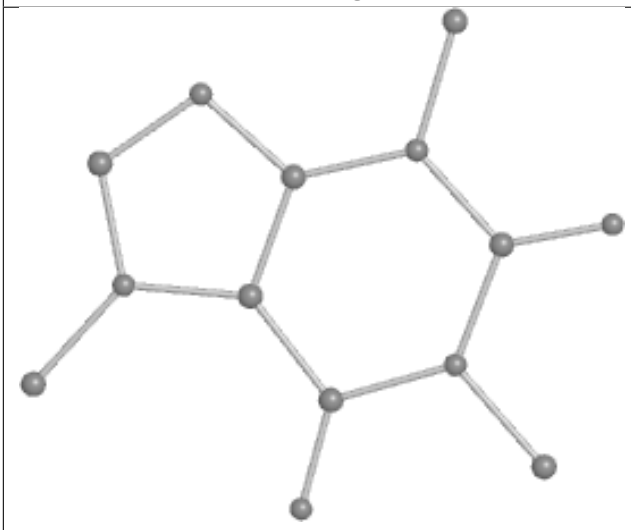
Ligand CFF F 5102



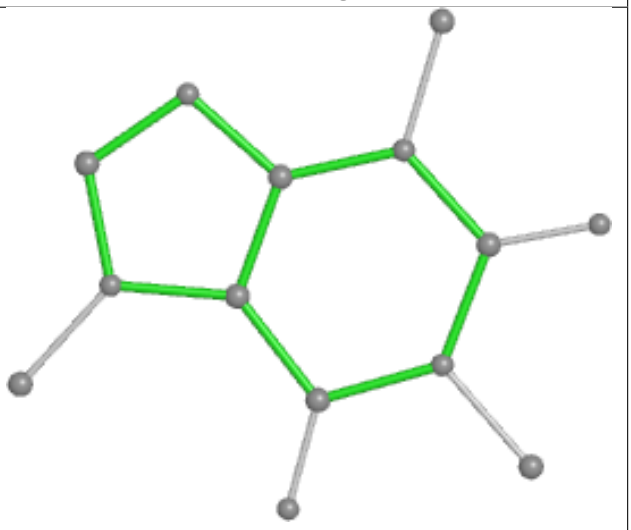
Bond lengths



Bond angles

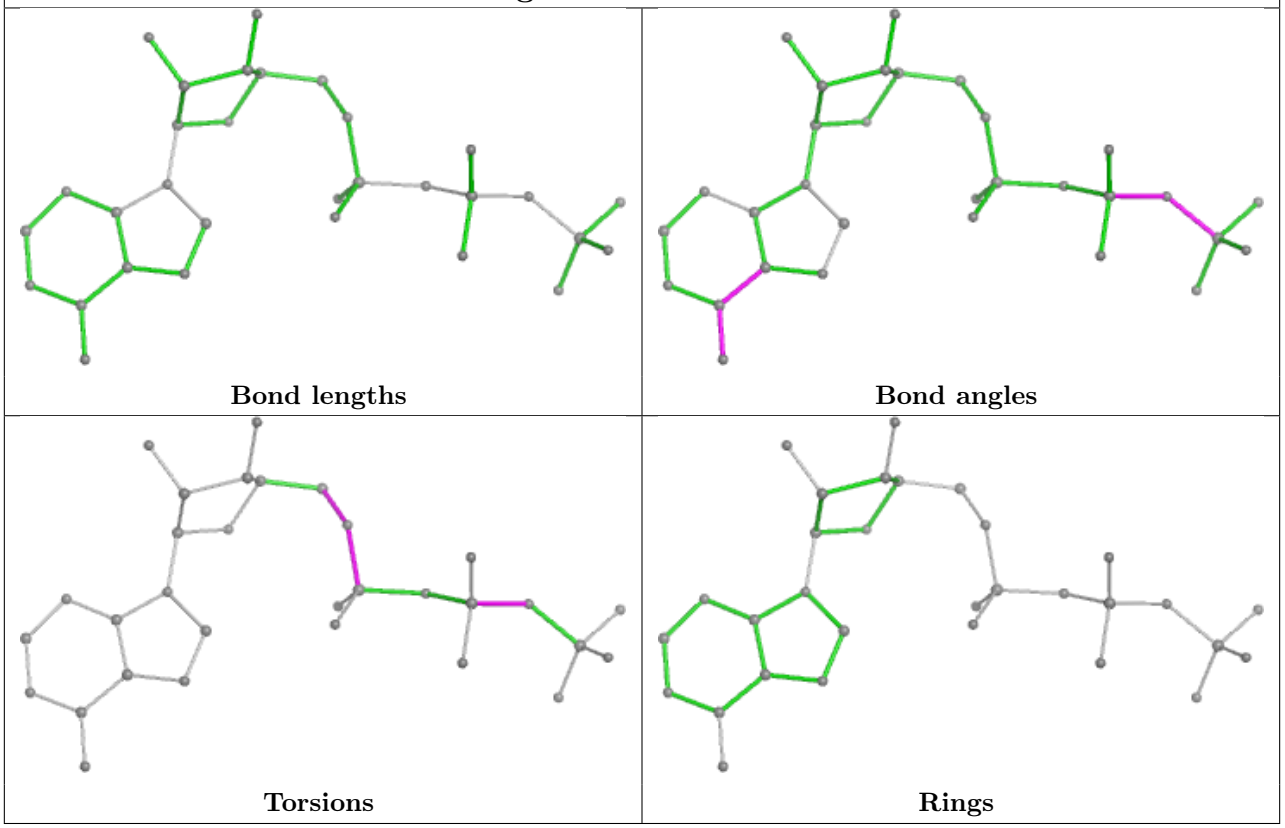


Torsions

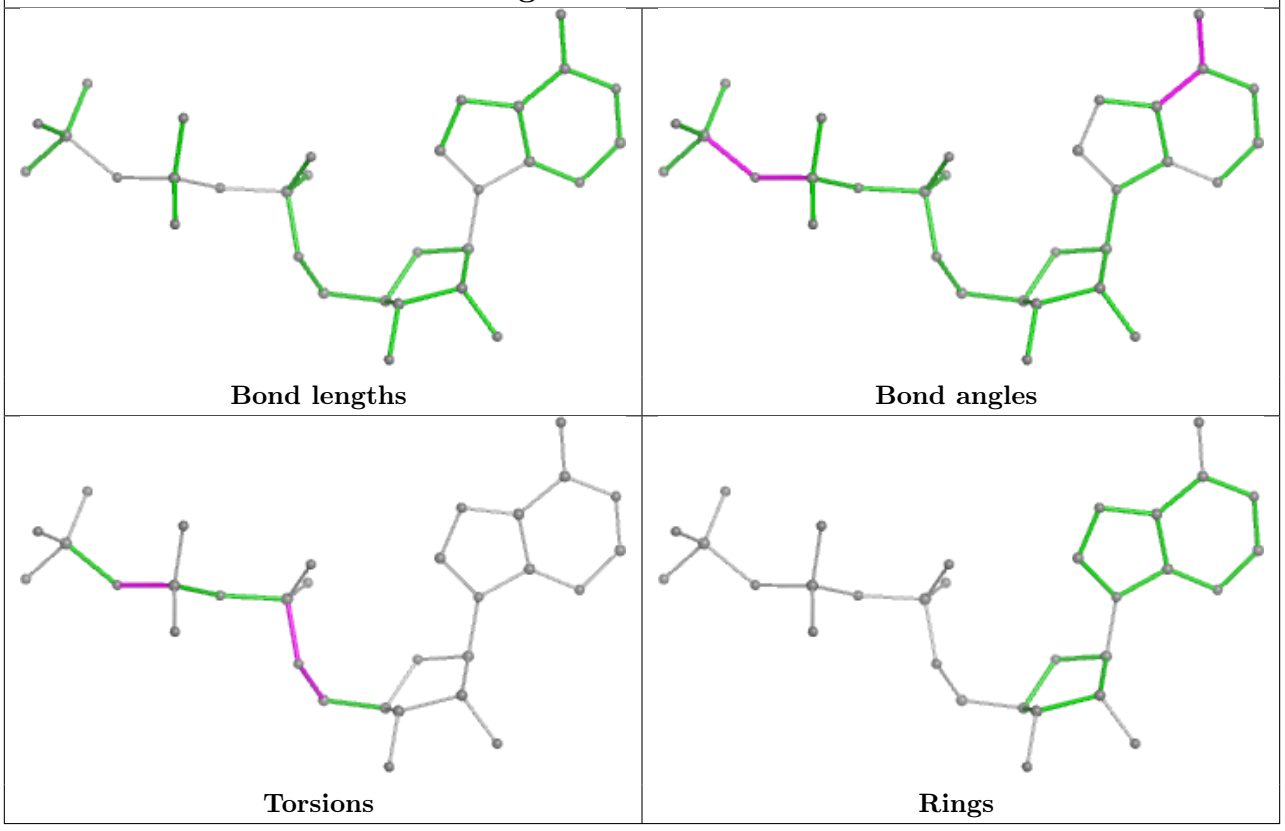


Rings

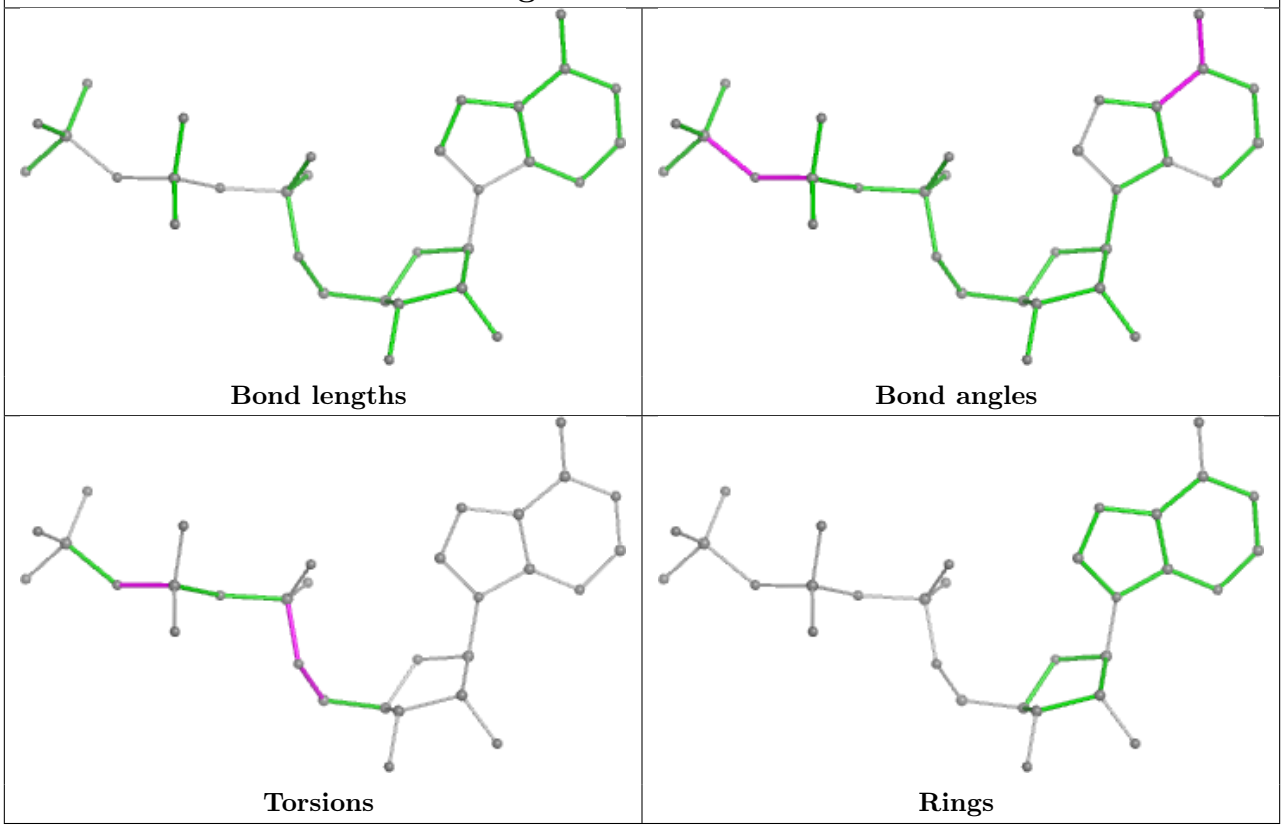
Ligand ATP A 5101



Ligand ATP F 5101



Ligand ATP E 5101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

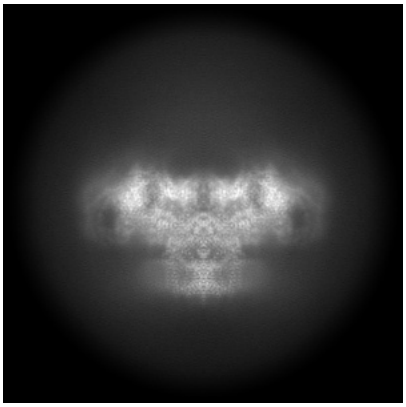
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19463. These allow visual inspection of the internal detail of the map and identification of artifacts.

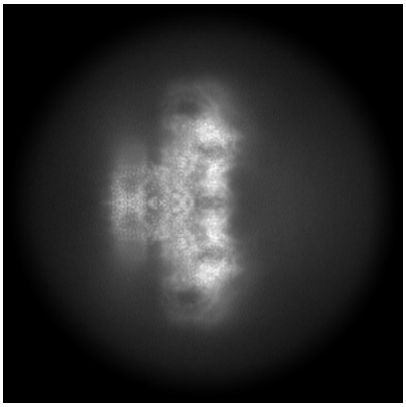
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

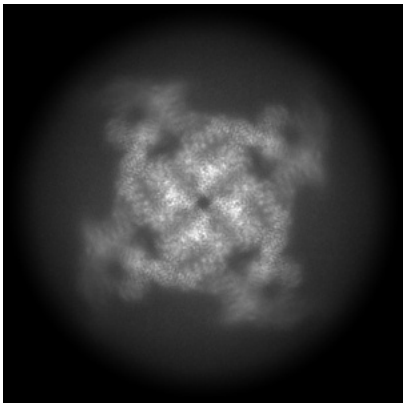
6.1.1 Primary map



X



Y



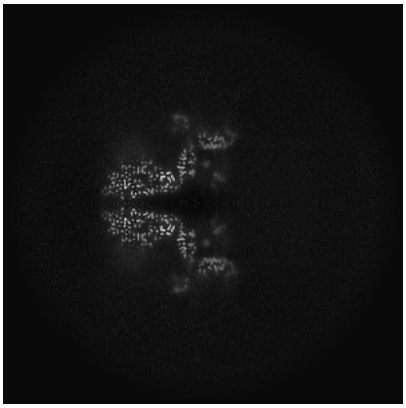
Z

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

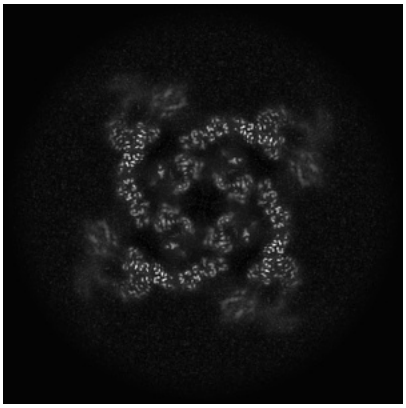
6.2 Central slices

6.2.1 Primary map

X Index: 168



Y Index: 168



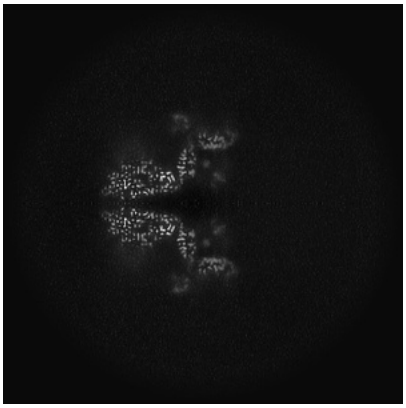
Z Index: 168

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

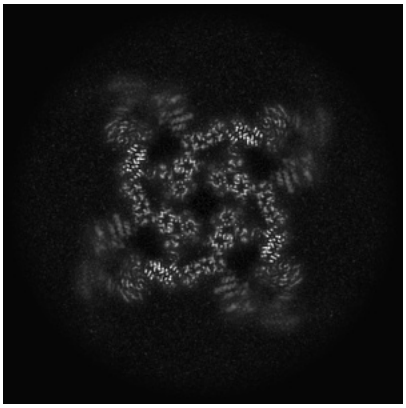
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 168



Y Index: 168

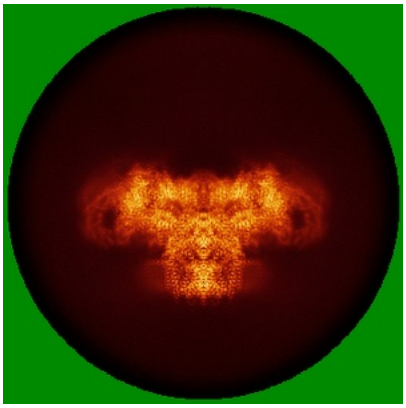


Z Index: 173

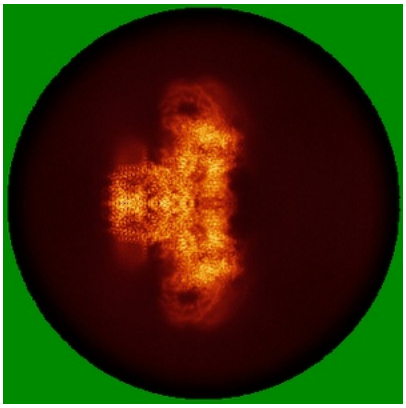
The images above show the largest variance slices of the map in three orthogonal directions.

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

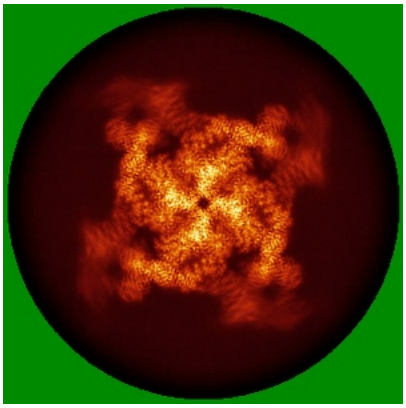
6.4.1 Primary map



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

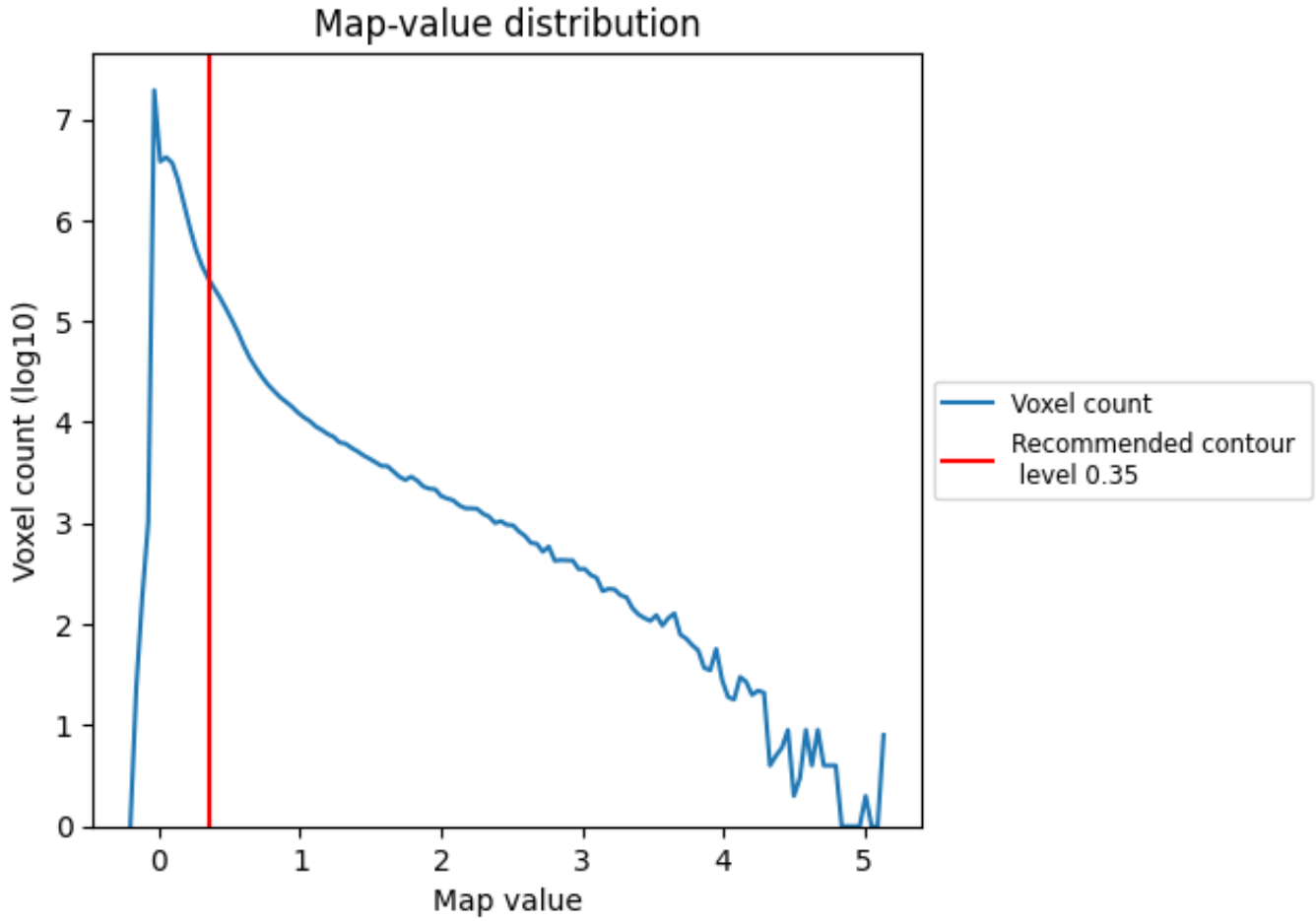
6.6 Mask visualisation (i)

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

7 Map analysis

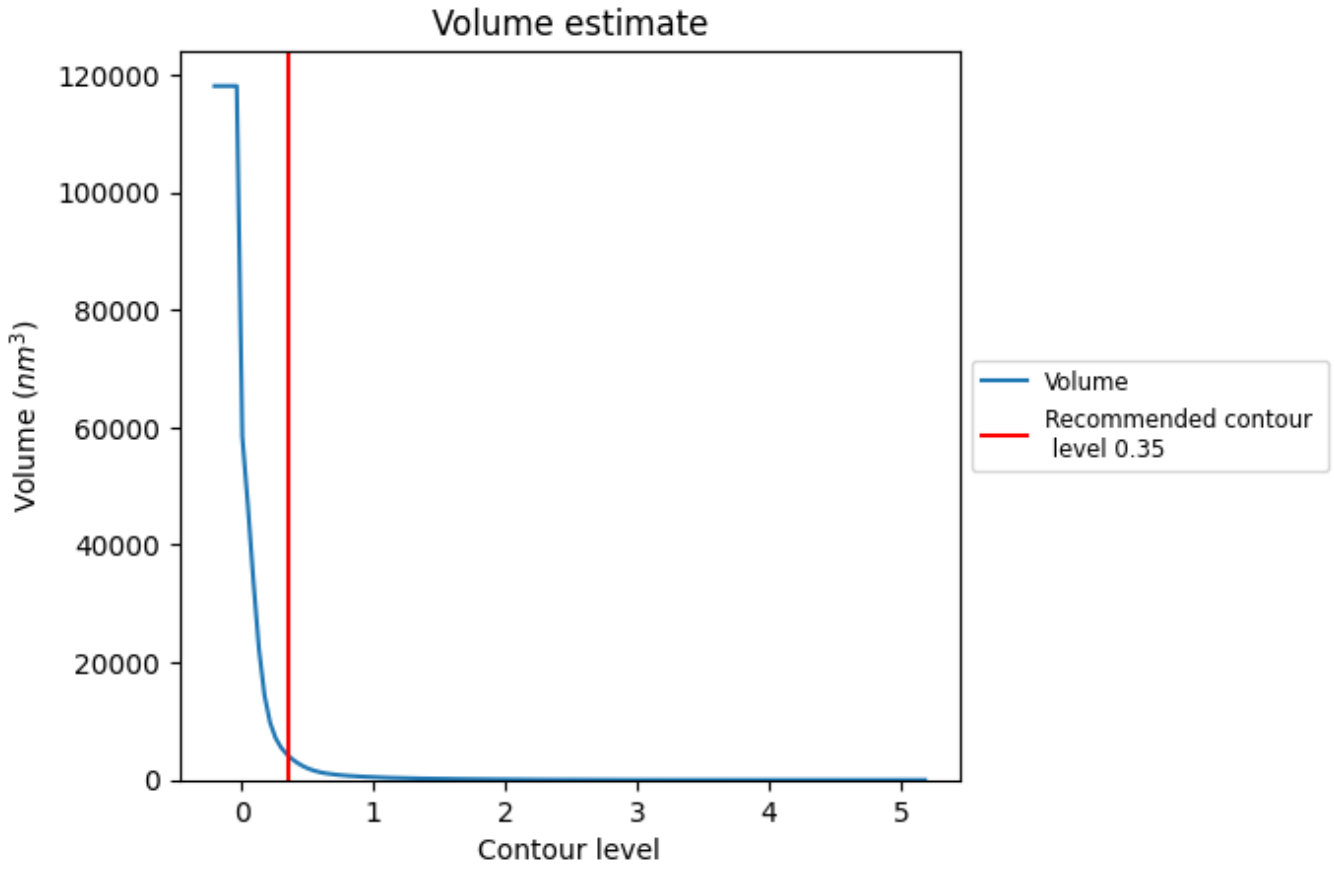
This section contains the results of statistical analysis of the map.

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.

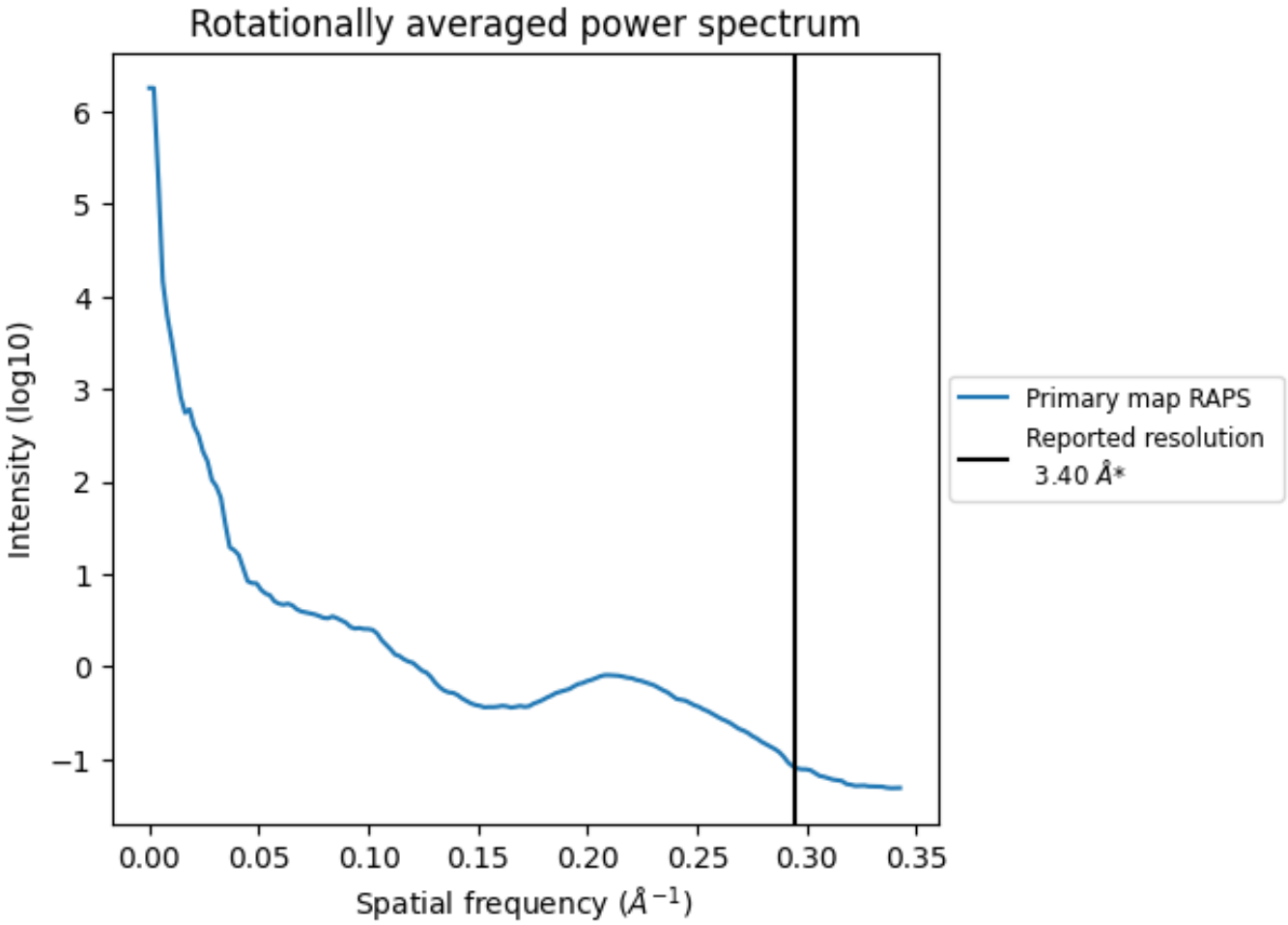
7.2 Volume estimate (i)



The volume at the recommended contour level is 4230 nm^3; this corresponds to an approximate mass of 3821 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

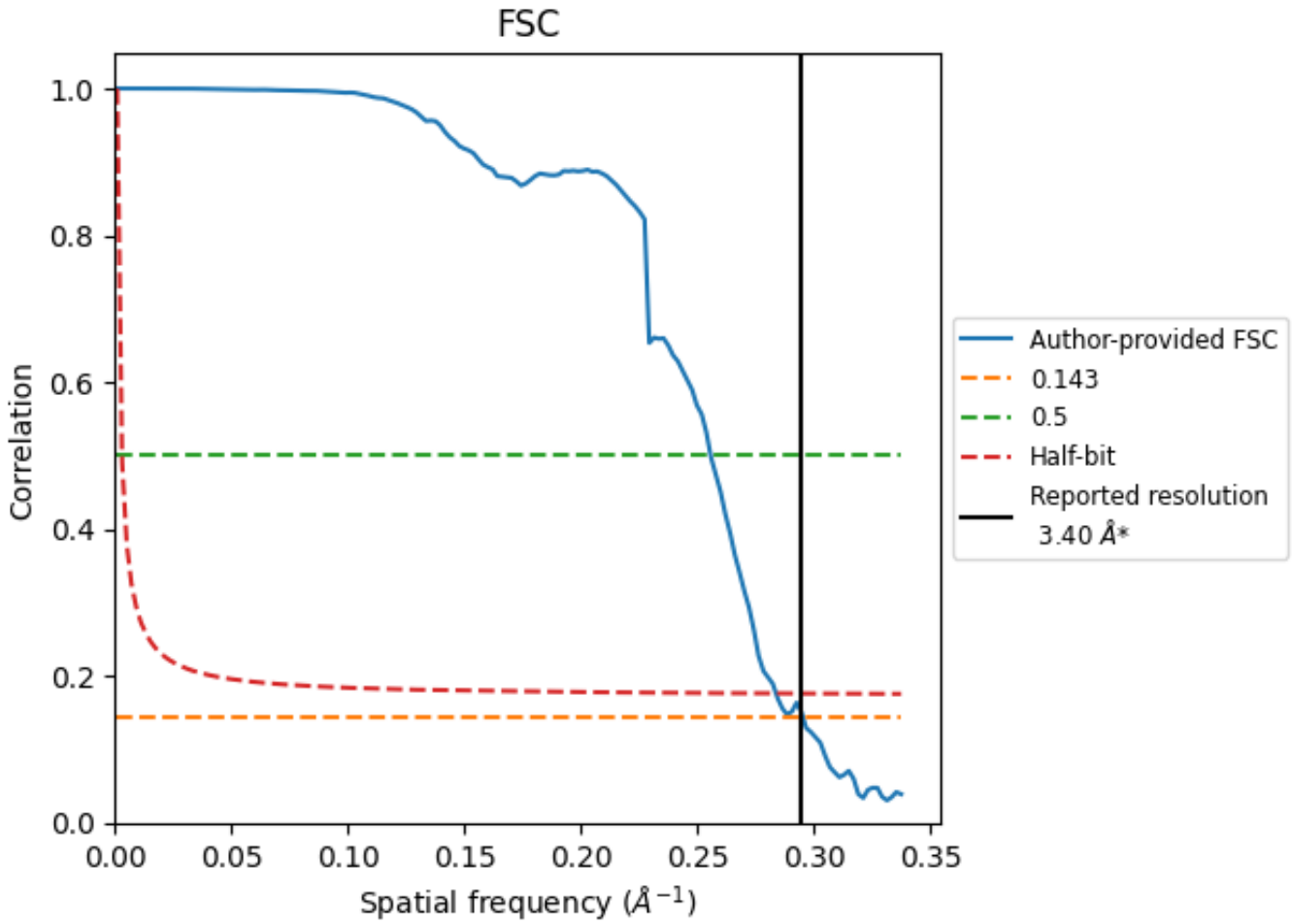


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

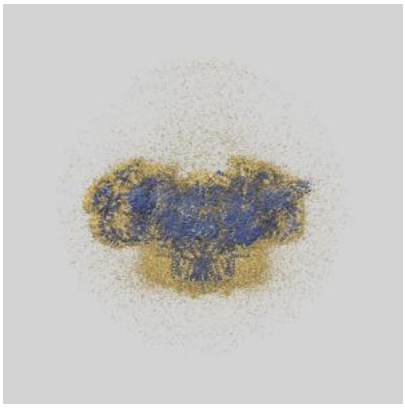
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.91	3.52
Unmasked-calculated*	-	-	-

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

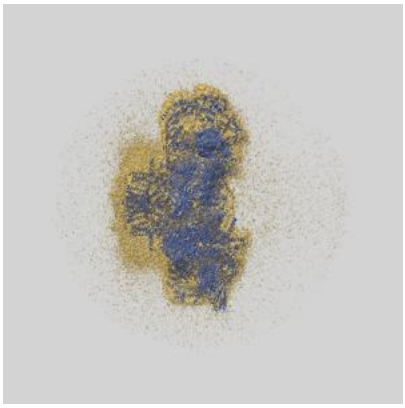
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19463 and PDB model 8RRS. Per-residue inclusion information can be found in section 3 on page 6.

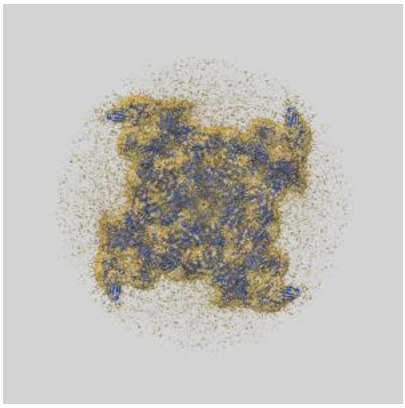
9.1 Map-model overlay



X



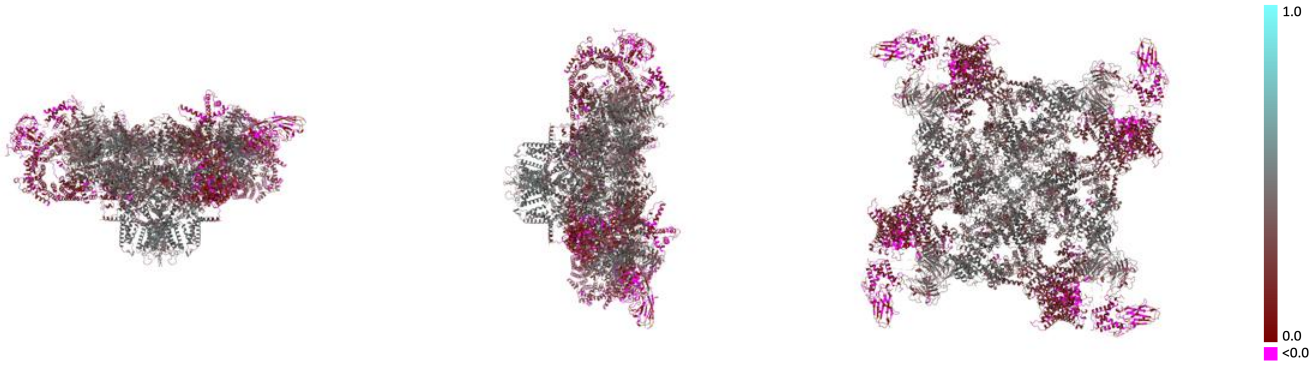
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

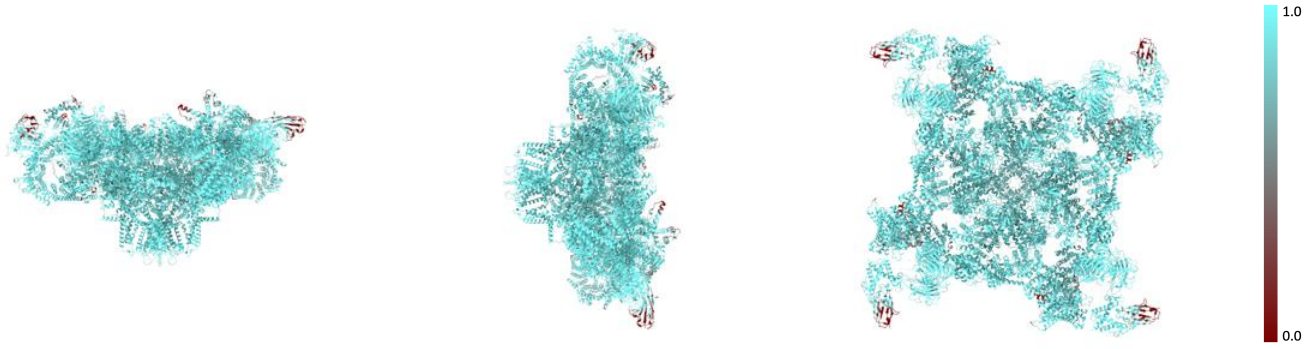
9.2 Q-score mapped to coordinate model (i)



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.

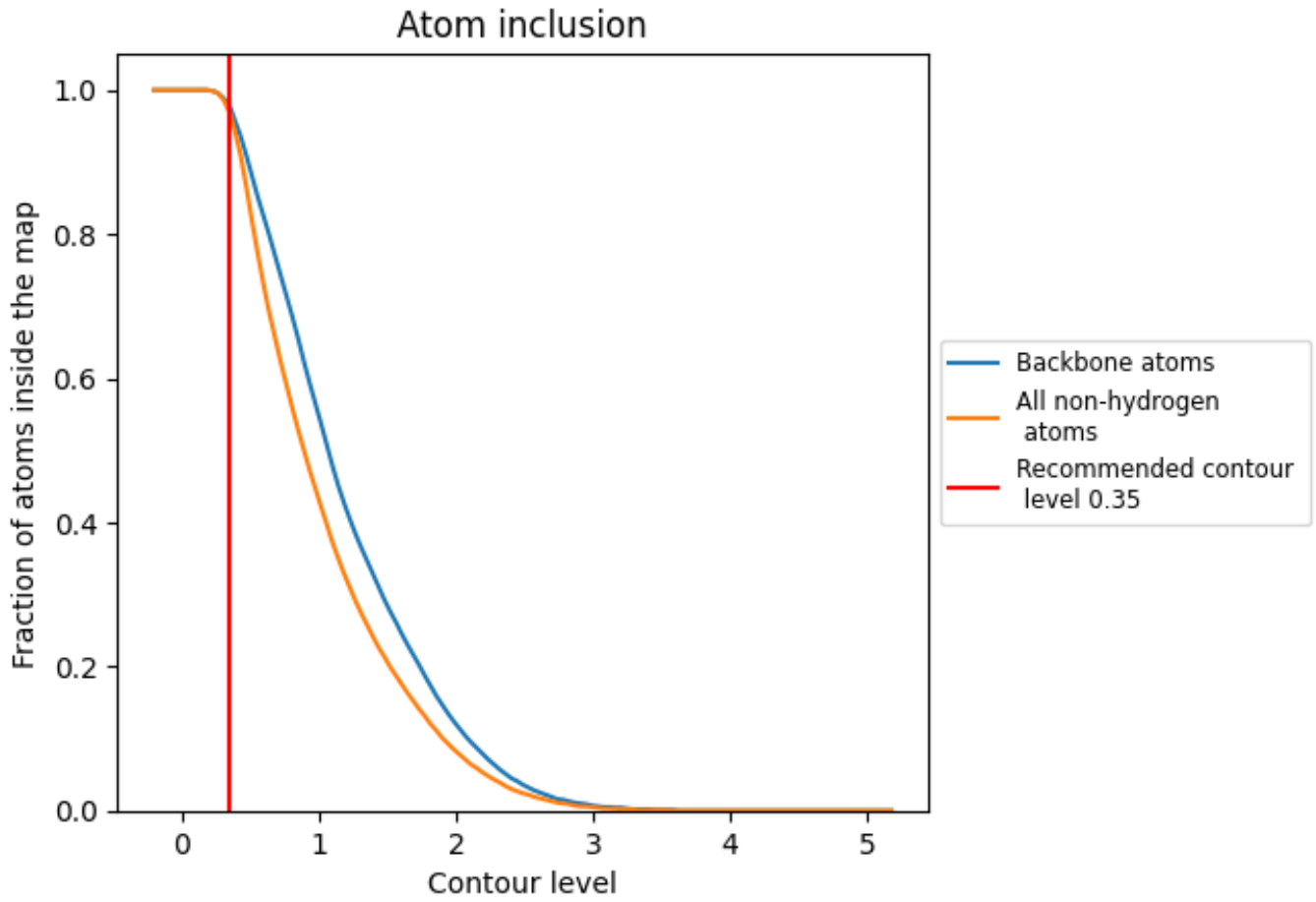
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.3070
A	0.9780	0.3140
B	0.5750	0.0800
C	0.9780	0.3140
D	0.5720	0.0810
E	0.9780	0.3130
F	0.9780	0.3130
G	0.5750	0.0790
I	0.5750	0.0790