wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 03:24 PM EST

PDB ID	:	7U9R
EMDB ID	:	EMD-26407
Title	:	Structure of PKA phosphorylated human RyR2 in the open state
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2022-03-11
Resolution	:	3.69 Å(reported)
Based on initial model	:	7U9Q

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:

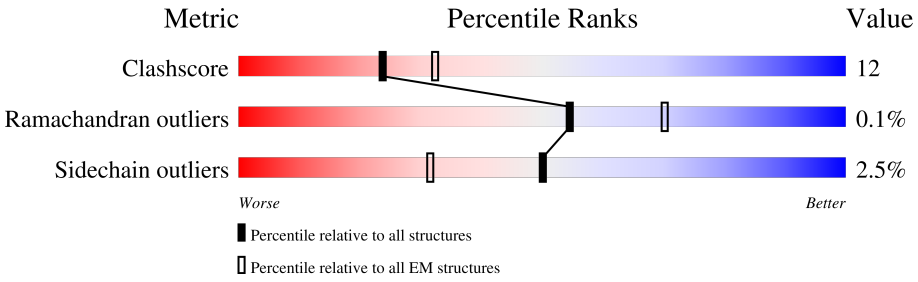
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.69 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	E	108	84% 15%
1	F	108	82% 17%
1	G	108	81% 19%
1	H	108	77% 22%
2	A	4967	8% 60% 23% 15%
2	B	4967	9% 60% 23% 15%
2	C	4967	9% 61% 23% 15%
2	D	4967	9% 61% 23% 15%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 138656 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

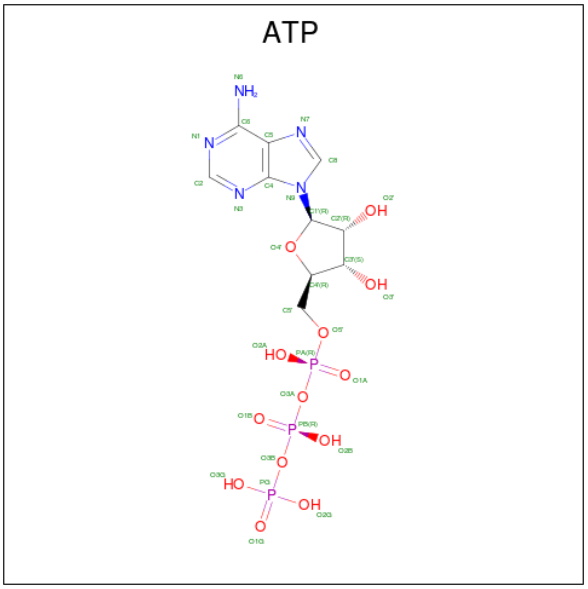
- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
2	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	C	1	Total	C	N	O	P	0
			62	20	10	26	6	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

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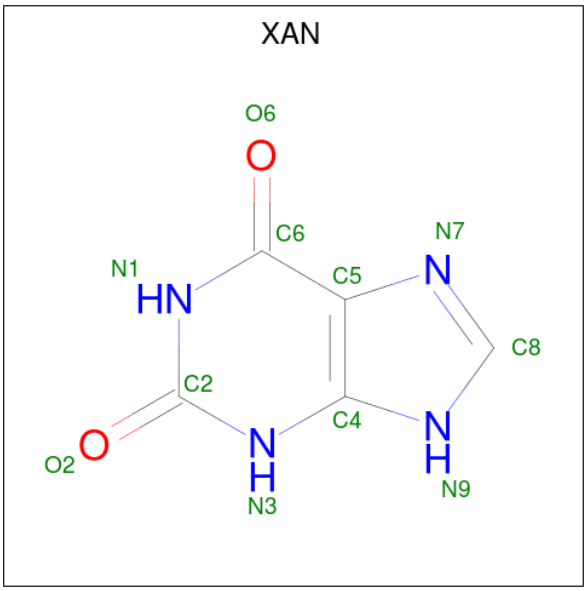
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Ca 1 1	0
5	C	1	Total Ca 1 1	0

- Molecule 6 is XANTHINE (three-letter code: XAN) (formula: $C_5H_4N_4O_2$) (labeled as "Ligand of Interest" by depositor).



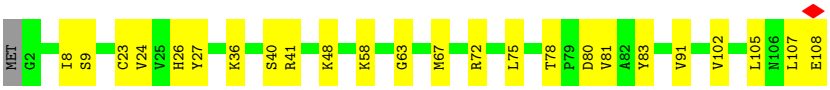
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 11 5 4 2	0
6	D	1	Total C N O 11 5 4 2	0
6	B	1	Total C N O 11 5 4 2	0
6	C	1	Total C N O 11 5 4 2	0

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.

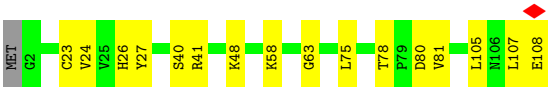
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



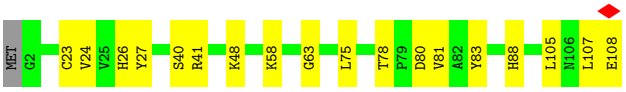
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



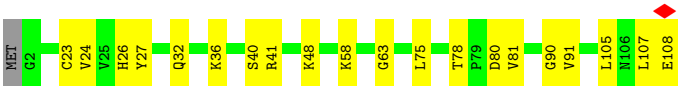
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



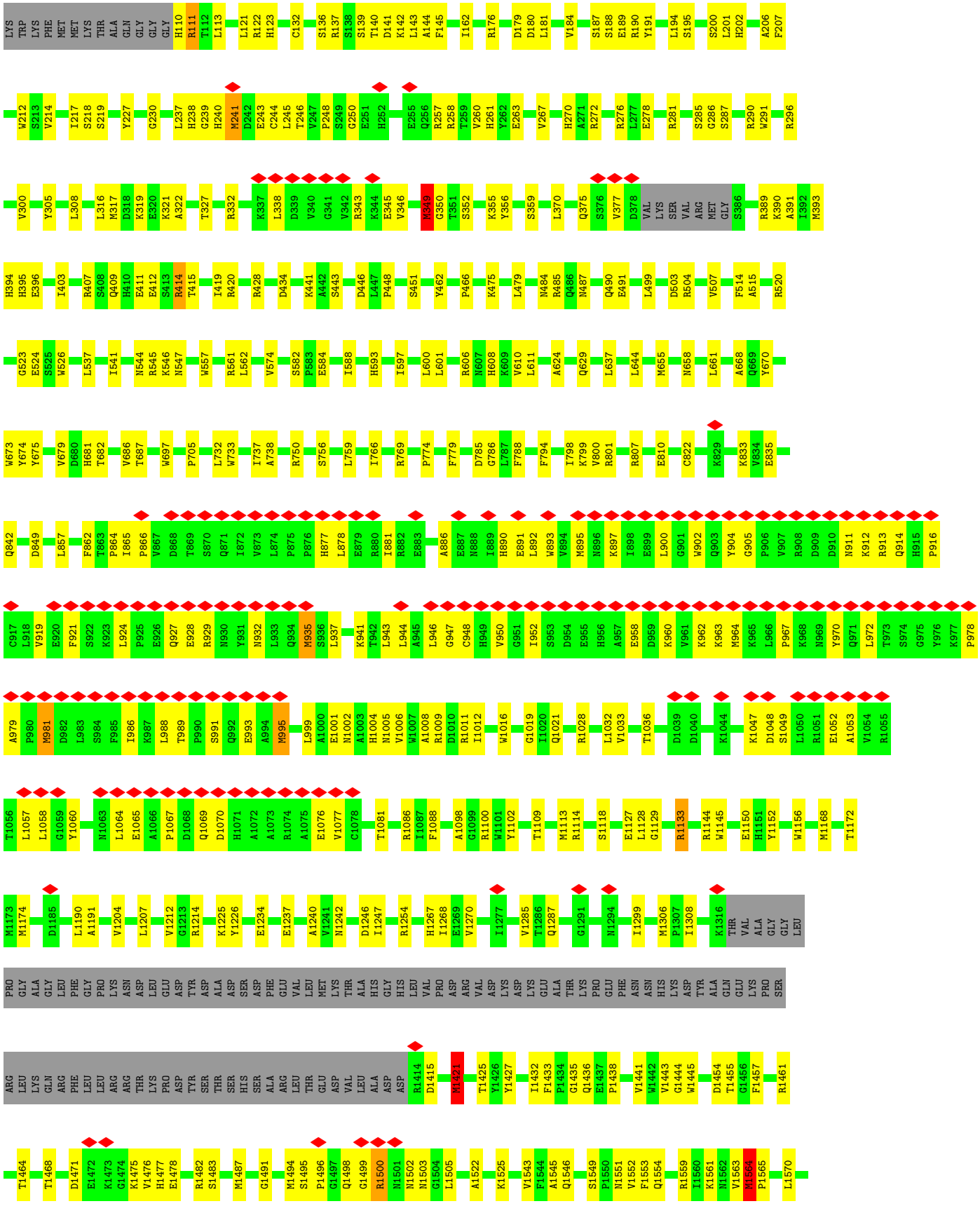
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

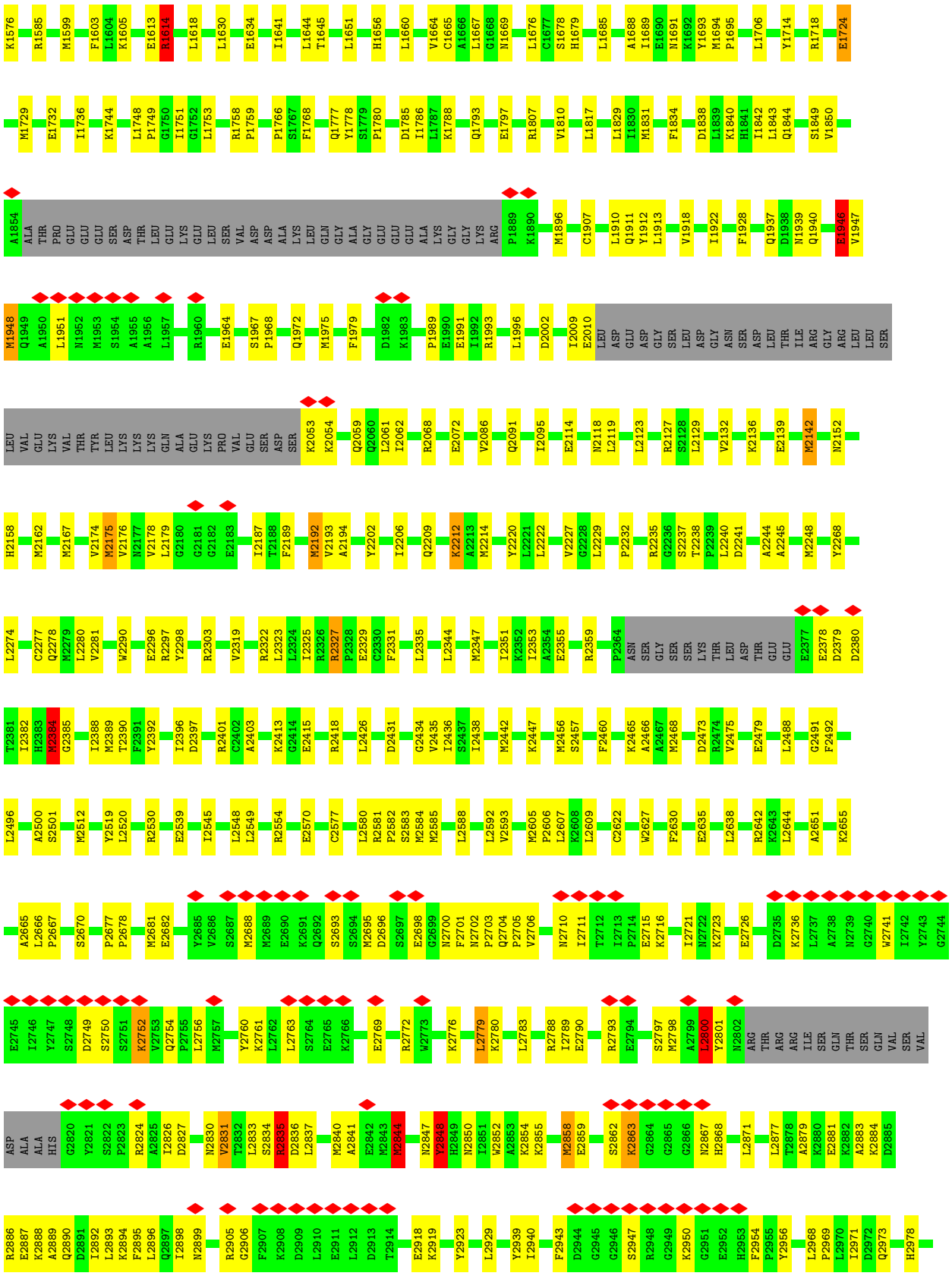
Chain G:

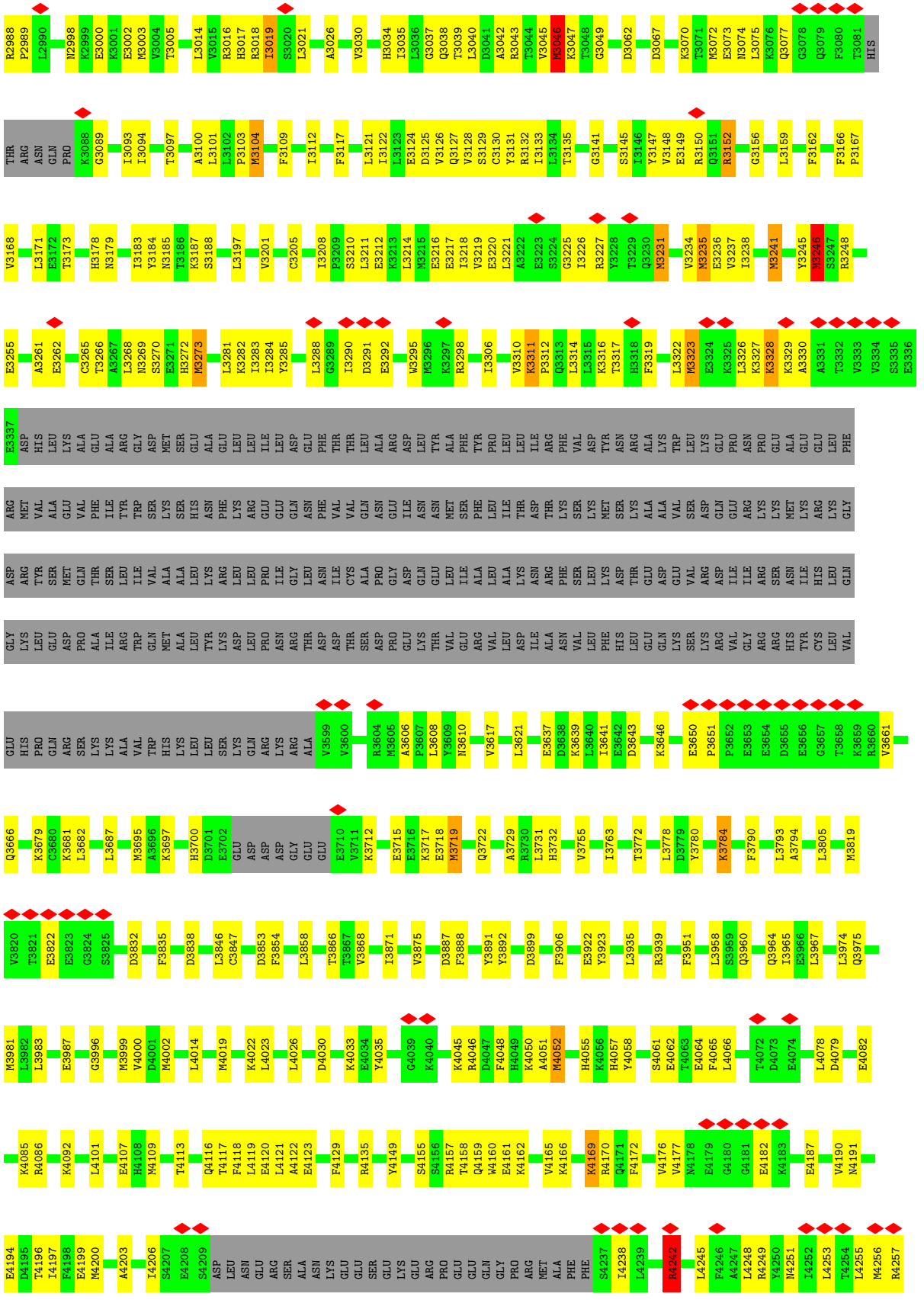


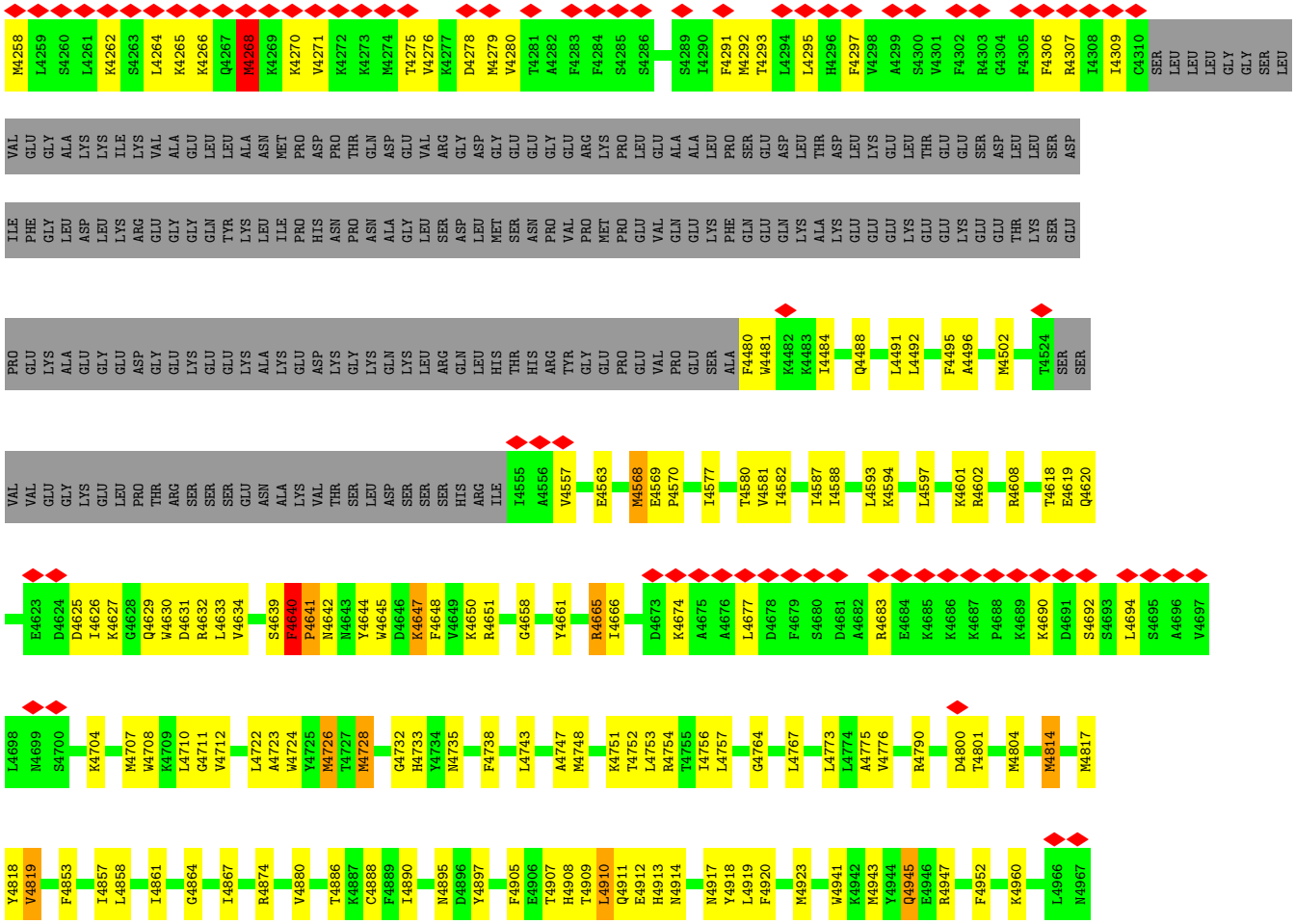
• Molecule 2: Ryanodine receptor 2

Chain A:


LYS TRP LYS PHE MET MET LYS THR ALA GLN GLY GLY GLY H110 R111 T112 L113 L121 R122 H123 C132 S136 R137 S138 S139 T140 D141 K142 L143 A144 F145 I162 R176 D179 D180 L181 V184 S187 S188 E189 R190 Y191 L194 S195 S200 L201 H202 A206 F207
W212 S213 V214 I217 S218 S219 Y227 G230 L237 H238 G239 H240 M241 D242 E243 C244 L245 T246 V247 P248 S249 G250 E251 H252 E255 Q256 R257 R258 T259 V260 H261 Y262 E263 V267 H270 A271 R272 R276 L277 E278 R281 S285 G286 S287 R290 W291 R296
V300 Y305 L308 L316 M317 D318 K319 E320 K321 A322 T327 R332 K337 L338 D339 V340 G341 V342 R343 K344 E345 V346 M349 G350 T351 S352 K355 Y356 S359 L370 Q375 S376 V377 D378 VAL LYS SER VAL ARG MET GLY S386 R389 K390 A391 T392 M393
H394 H395 E396 I403 R407 S408 Q409 H410 E411 E412 S413 R414 T415 I419 R420 R428 D434 K441 A442 S443 D446 L447 P448 S451 Y462 P466 K475 L479 N484 R485 Q486 N487 Q490 E491 L499 D503 R504 V507 F514 A515 R520
G523 E524 S525 W526 L537 I541 N544 R545 K546 N547 W557 R561 L562 V574 S582 P583 E584 I588 H593 I597 L600 L601 R606 W607 H608 K609 V610 L611 A624 Q629 L637 L644 M655 N658 L661 A668 Q669 Y670
W673 Y674 Y675 V679 D680 H681 T682 V686 T687 W697 P705 L732 W733 I737 A738 R750 S756 L759 I766 R769 P774 F779 D785 G786 L787 F788 F794 I798 K799 V800 R801 R807 E810 C822 K829 K833 V834 E835
Q842 D849 L857 F862 T863 P864 I865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916
C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978
A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 L999 A1000 E1001 N1002 A1003 H1004 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 W1016 G1019 I1020 Q1021 R1028 L1032 V1033 T1036 D1039 D1040 K1044 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055
T1056 L1057 L1058 G1059 Y1060 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 T1081 R1086 I1087 F1088 A1098 G1099 R1100 W1101 Y1102 T1109 M1113 R1114 S1118 E1127 L1128 G1129 R1133 R1144 W1145 E1150 H1151 Y1152 W1156 M1168 T1172
M1173 M1174 D1185 L1190 A1191 V1204 L1207 V1212 G1213 R1214 K1225 Y1226 E1234 E1237 A1240 V1241 N1242 D1246 I1247 R1254 H1267 I1268 E1269 V1270 I1277 V1285 T1286 Q1287 G1291 N1294 I1299 M1306 P1307 I1308 K1316 THR VAL ALA GLY GLY LEU
PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR 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 SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 M1421 T1425 Y1426 Y1427 I1432 F1433 P1434 G1435 Q1436 E1437 P1438 V1441 W1442 V1443 G1444 W1445 D1454 T1455 G1456 F1457 R1461
T1464 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 R1482 S1483 M1487 G1491 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 A1522 K1525 V1543 F1544 A1545 Q1546 S1549 P1550 N1551 V1552 F1553 Q1554 R1559 I1560 K1561 N1562 V1563 M1564 P1565 L1570

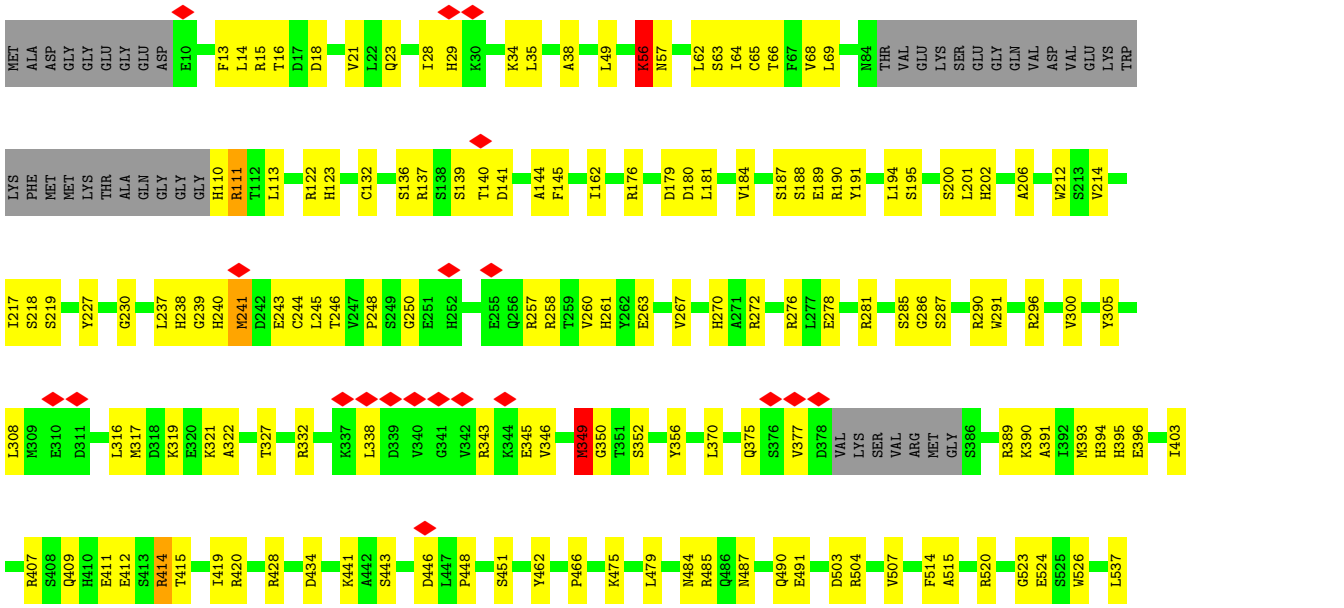


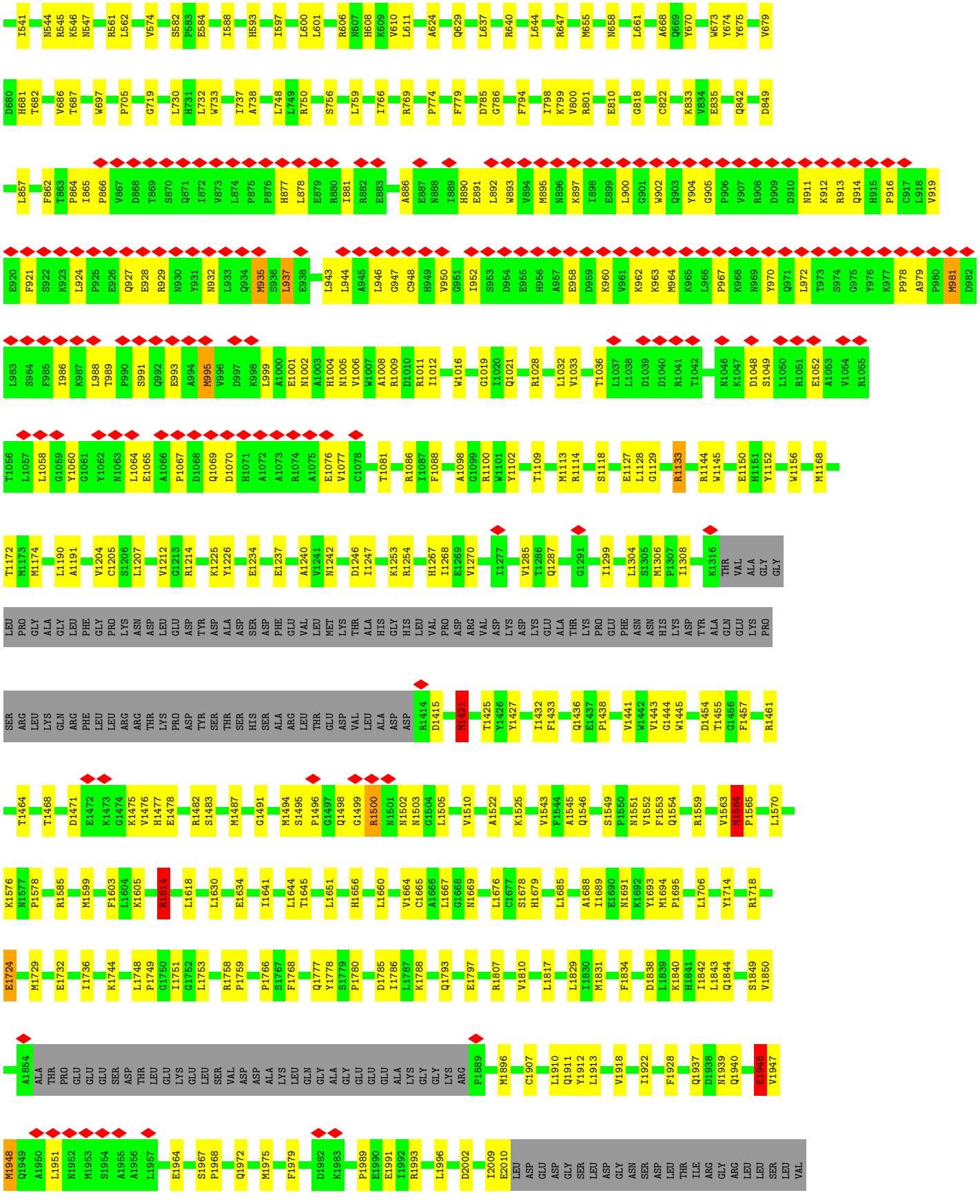


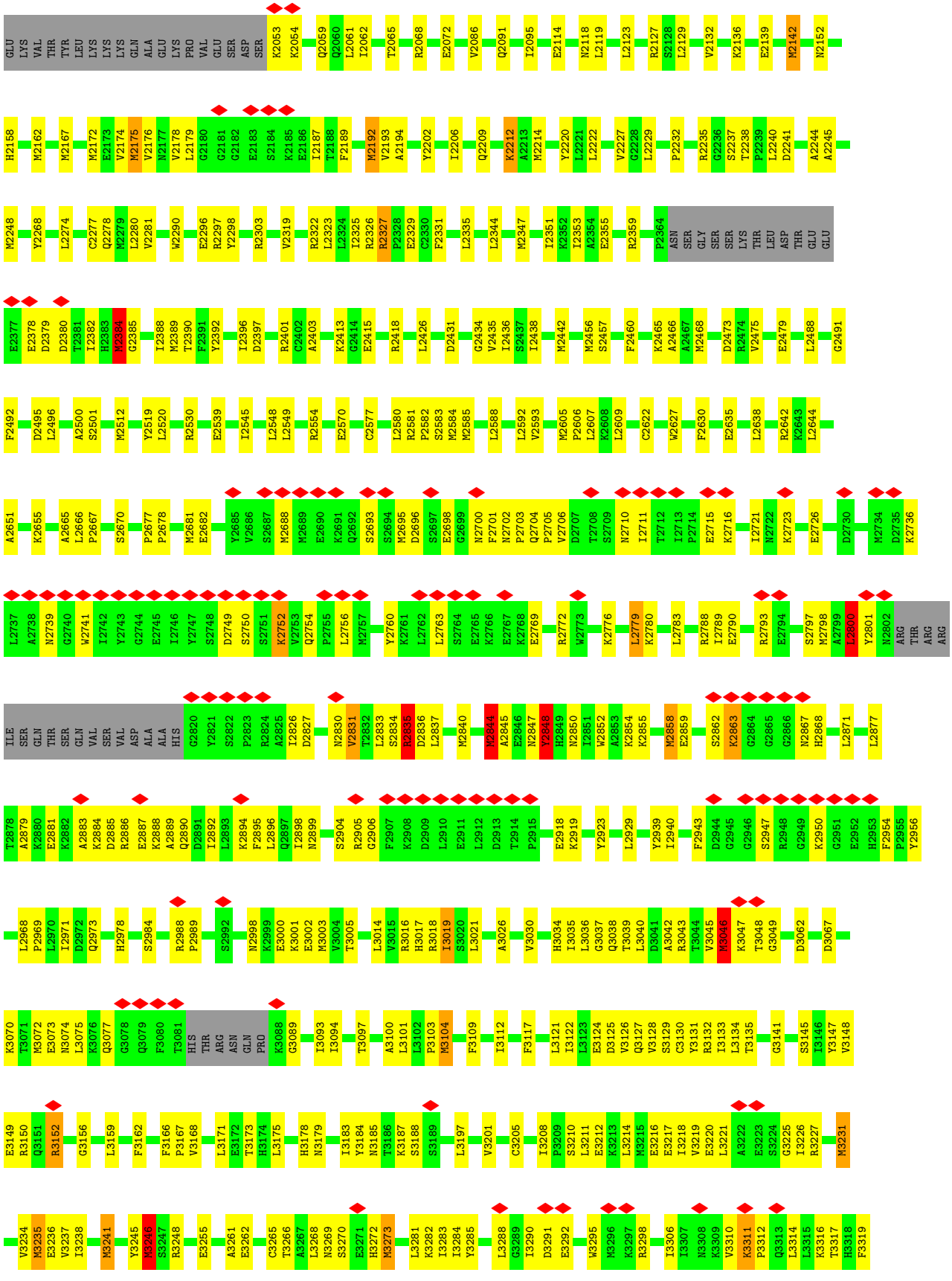


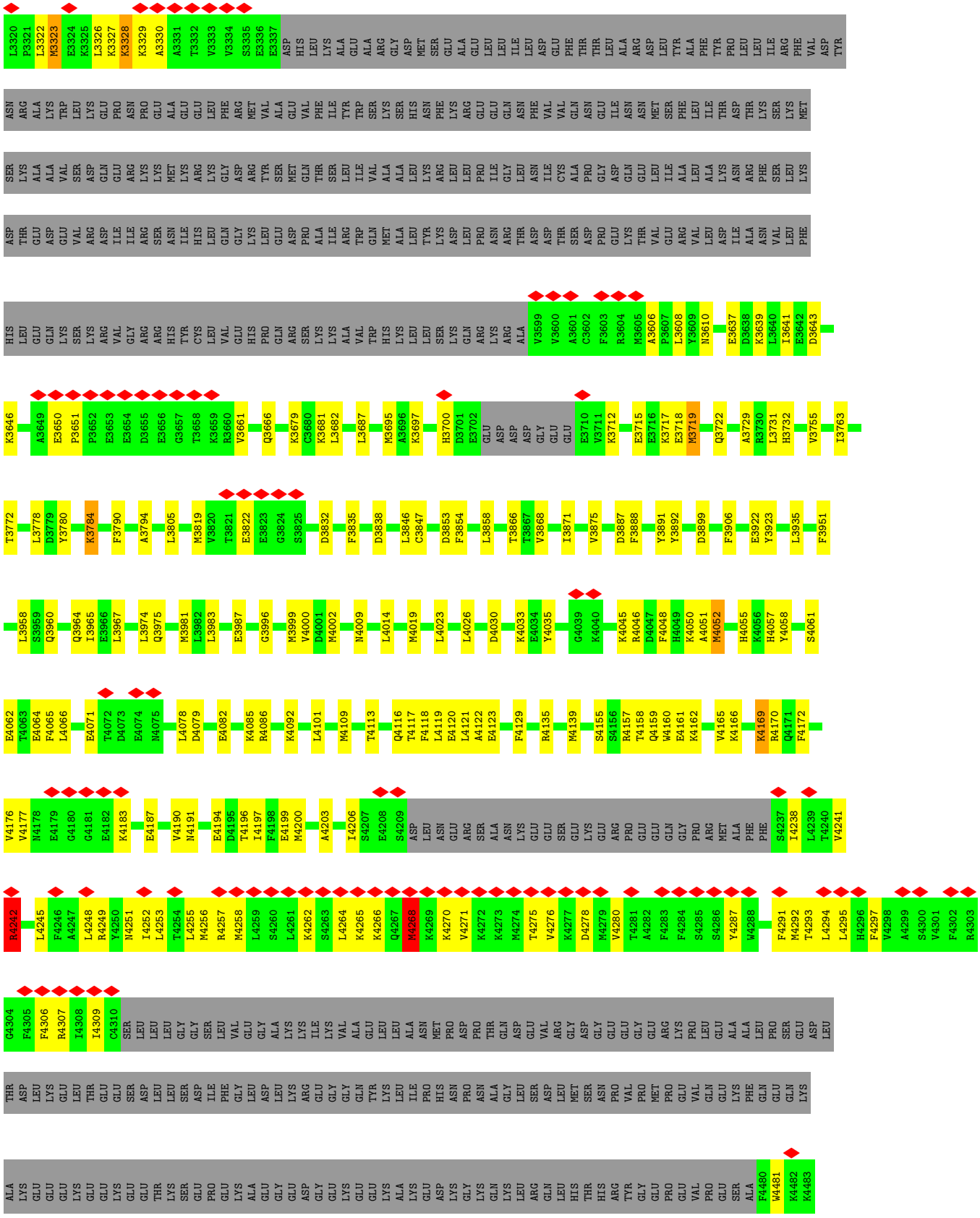
• Molecule 2: Ryanodine receptor 2

Chain D:




I541 N544 R545 K546 N547 R561 L562 V574 S582 P583 E584 I588 H593 I597 L600 L601 R606 N607 H608 K609 V610 L611 A624 Q629 L637 R640 L644 R647 M655 N658 L661 A668 Q669 Y670 W673 Y674 Y675 V679
D680 H681 T682 V686 T687 W697 P705 G719 L730 H731 L732 W733 I737 A738 L748 L749 R750 S756 L759 I766 R769 P774 F779 D785 G786 F794 I798 K799 V800 R801 E810 G818 C822 K833 V834 E835 Q842 D849
L857 F862 T863 P864 I865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919
E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982
L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998 L999 A1000 E1001 N1002 A1003 H1004 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 W1016 G1019 I1020 Q1021 R1028 L1032 V1033 T1036 L1037 L1038 D1039 D1040 R1041 T1042 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055
T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 T1081 R1086 I1087 F1088 A1098 G1099 R1100 W1101 Y1102 T1109 M1113 R1114 S1118 E1127 L1128 G1129 R1133 R1144 W1145 E1150 H1151 Y1152 W1156 M1168
T1172 M1173 M1174 L1190 A1191 V1204 C1205 S1206 L1207 V1212 G1213 R1214 K1225 Y1226 E1234 E1237 A1240 V1241 N1242 D1246 I1247 K1253 R1254 H1267 I1268 E1269 V1270 I1277 V1285 T1286 Q1287 G1291 I1299 L1304 S1305 M1306 P1307 I1308 K1316 THR VAL ALA GLY GLY
LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR 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 ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP R1414 D1415 M1421 T1425 Y1426 Y1427 I1432 F1433 Q1436 E1437 P1438 V1441 W1442 V1443 G1444 W1445 D1454 T1455 G1456 F1457 R1461
T1464 T1468 D1471 E1472 K1473 G1474 K1475 V1476 H1477 E1478 R1482 S1483 M1487 G1491 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 V1510 A1522 K1525 V1543 F1544 A1545 Q1546 S1549 P1550 N1551 V1552 F1553 Q1554 R1559 V1563 M1564 P1565 L1570
K1576 N1577 P1578 R1585 M1599 F1603 L1604 K1605 R1614 L1618 L1630 E1634 I1641 L1644 T1645 L1651 H1656 L1660 V1664 C1665 A1666 L1667 G1668 N1669 L1676 C1677 S1678 H1679 L1685 A1688 I1689 E1690 N1691 K1692 Y1693 M1694 P1695 L1706 Y1714 R1718
E1724 M1729 E1732 I1736 K1744 L1748 P1749 G1750 I1751 G1752 L1753 R1758 P1759 P1766 S1767 F1768 Q1777 Y1778 S1779 P1780 D1785 I1786 L1787 K1788 Q1793 E1797 R1807 V1810 L1817 L1829 I1830 M1831 F1834 D1838 L1839 K1840 H1841 I1842 L1843 Q1844 S1849 V1850
A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 M1896 C1907 L1910 Q1911 Y1912 L1913 V1918 I1922 F1928 Q1937 D1938 N1939 Q1940 E1946 V1947
M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 E1964 S1967 P1968 Q1972 M1975 F1979 D1982 K1983 P1989 E1990 E1991 I1992 R1993 L1996 D2002 I2009 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL

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ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET
SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS
ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG ASP ILE ASP ASN ILE PHE
HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA V3599 V3600 A3601 C3602 F3603 R3604 M3605 A3606 P3607 L3608 Y3609 N3610 E3637 D3638 K3639 L3640 I3641 E3642 D3643
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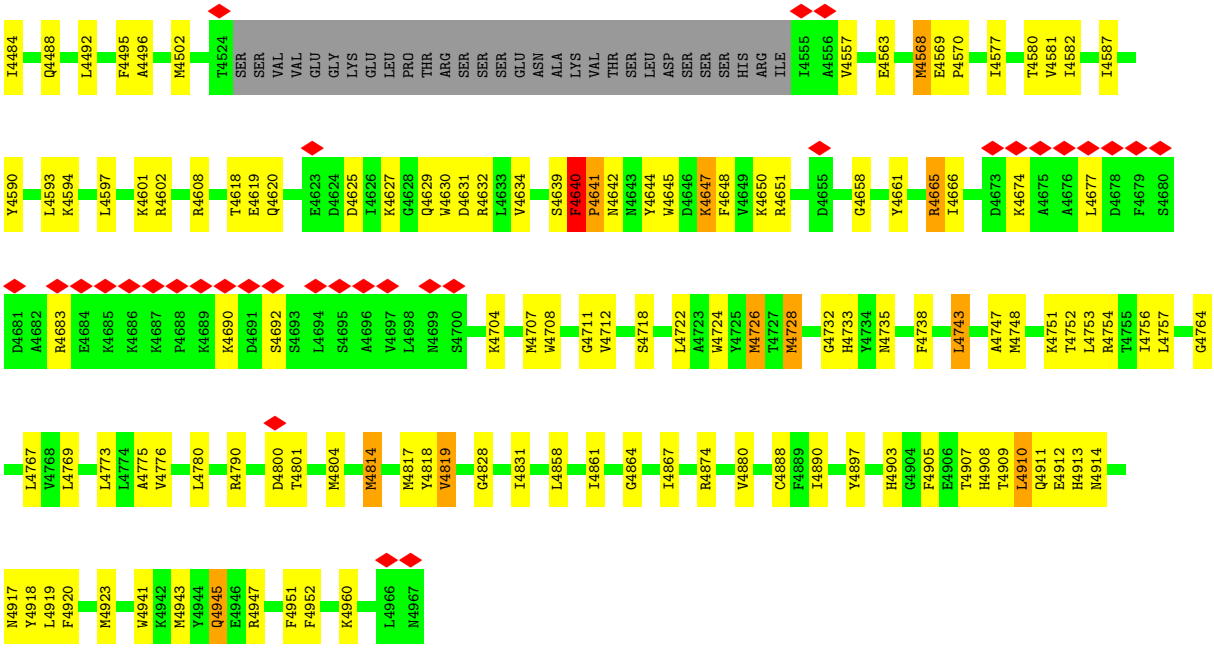
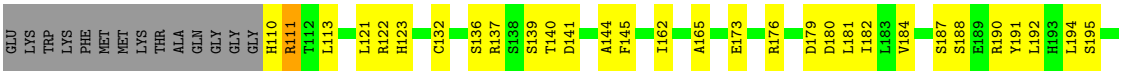
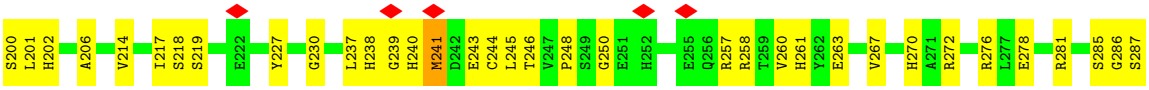
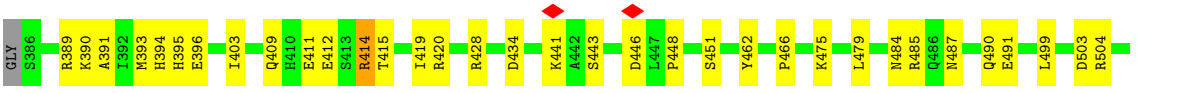
G4304 F4305 F4306 R4307 I4308 I4309 C4310 SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLY GLU GLU GLY GLU GLU ARG LYS PRO LEU GLU GLU ALA ALA LEU PRO SER GLU ASP PRO
THR ASP LEU LYS GLU GLU LEU THR GLU GLU SER ASP LEU LEU SER ILE PHE GLY LEU ASP LEU LYS ARG GLU LEU ASP GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET SER ASN PRO VAL PRO MET PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS
ALA LYS GLU GLU GLU LYS GLU GLU LYS GLU GLU LYS ALA LYS GLY LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA F4480 W4481 K4482 K4483

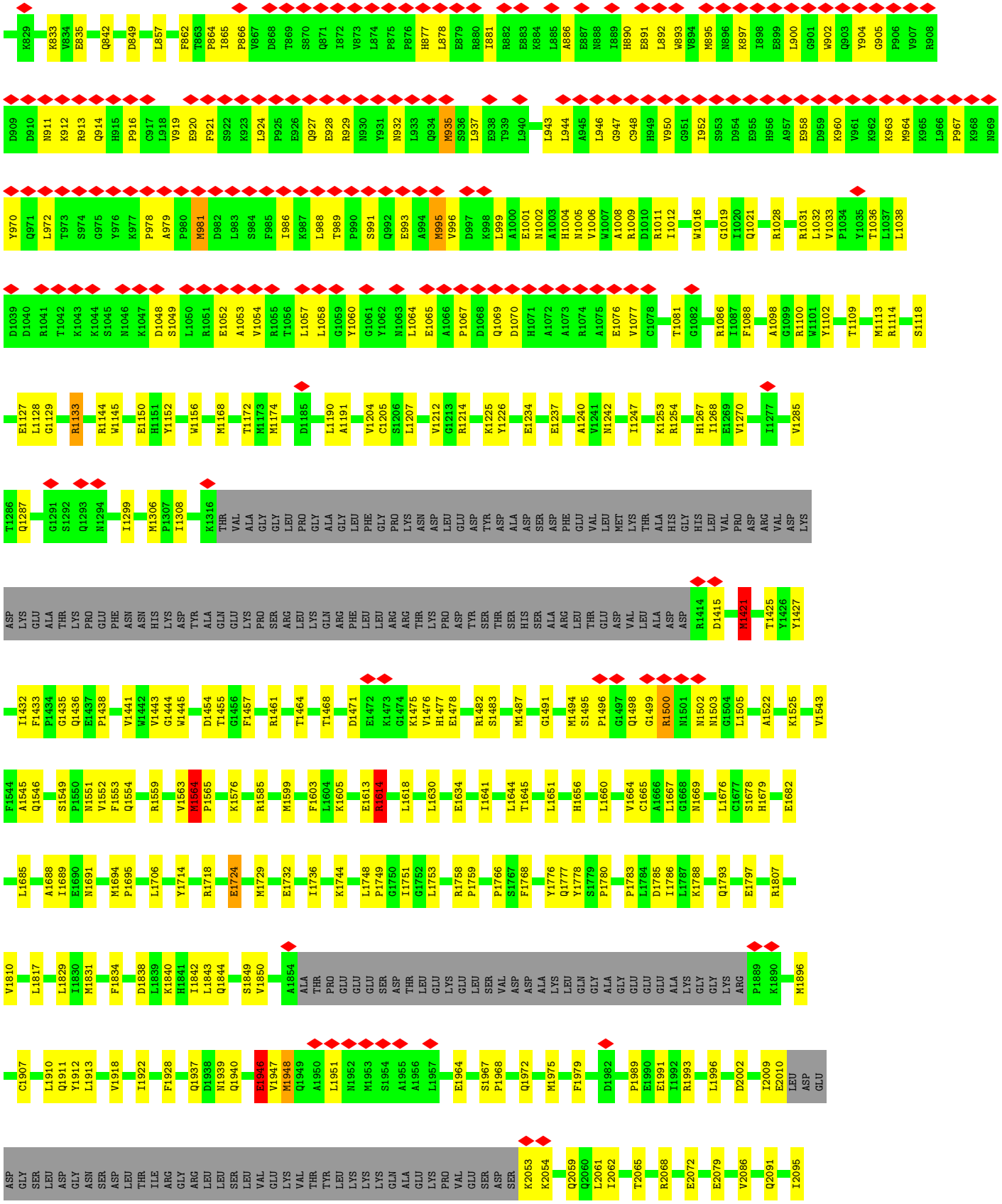


• Molecule 2: Ryanodine receptor 2





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T1286 Q1287 G1291 S1292 Q1293 N1294 I1299 M1306 P1307 I1308 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS
ASP LYS GLU ALA THR 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 SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 N1421 T1425 Y1426 Y1427
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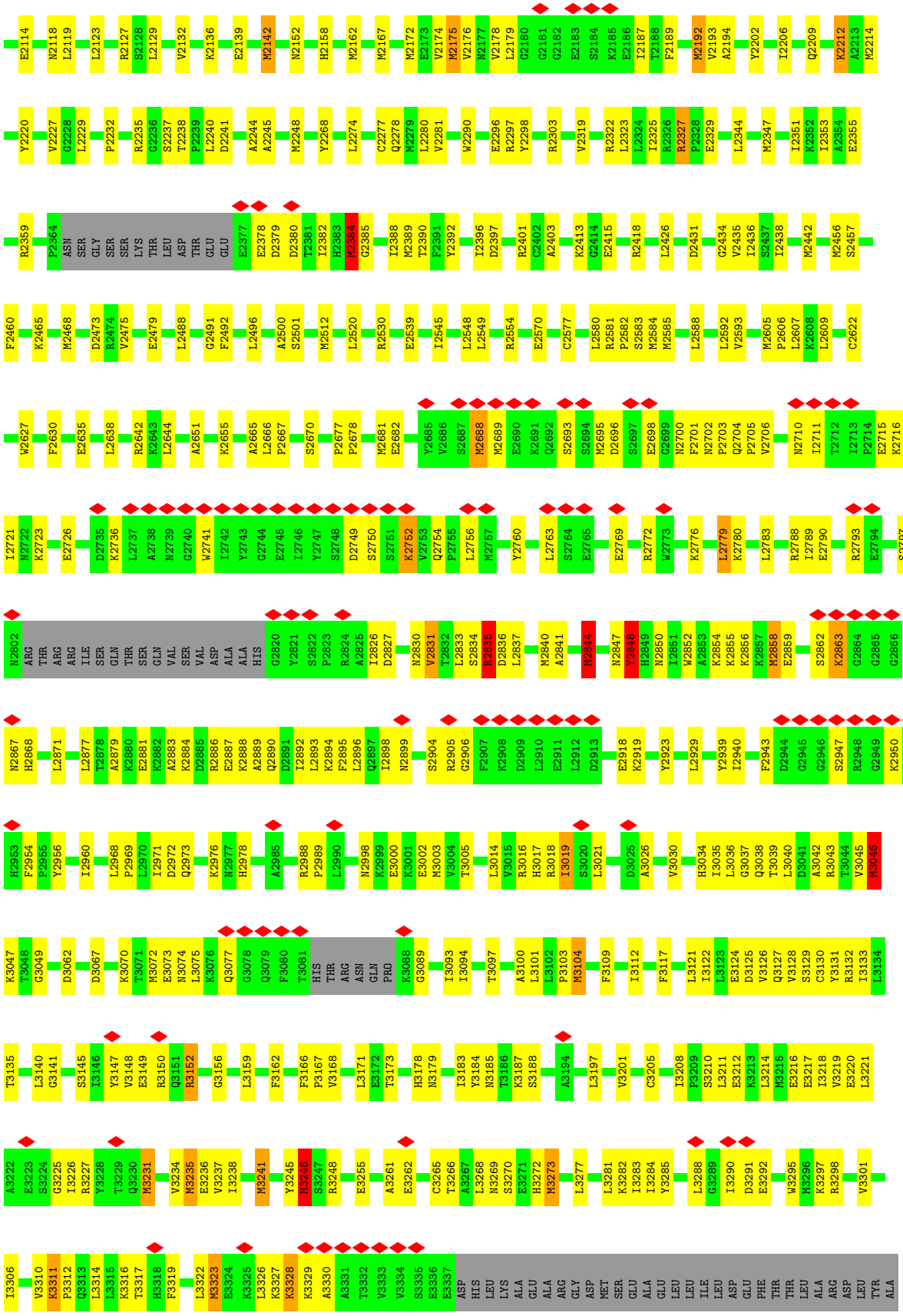
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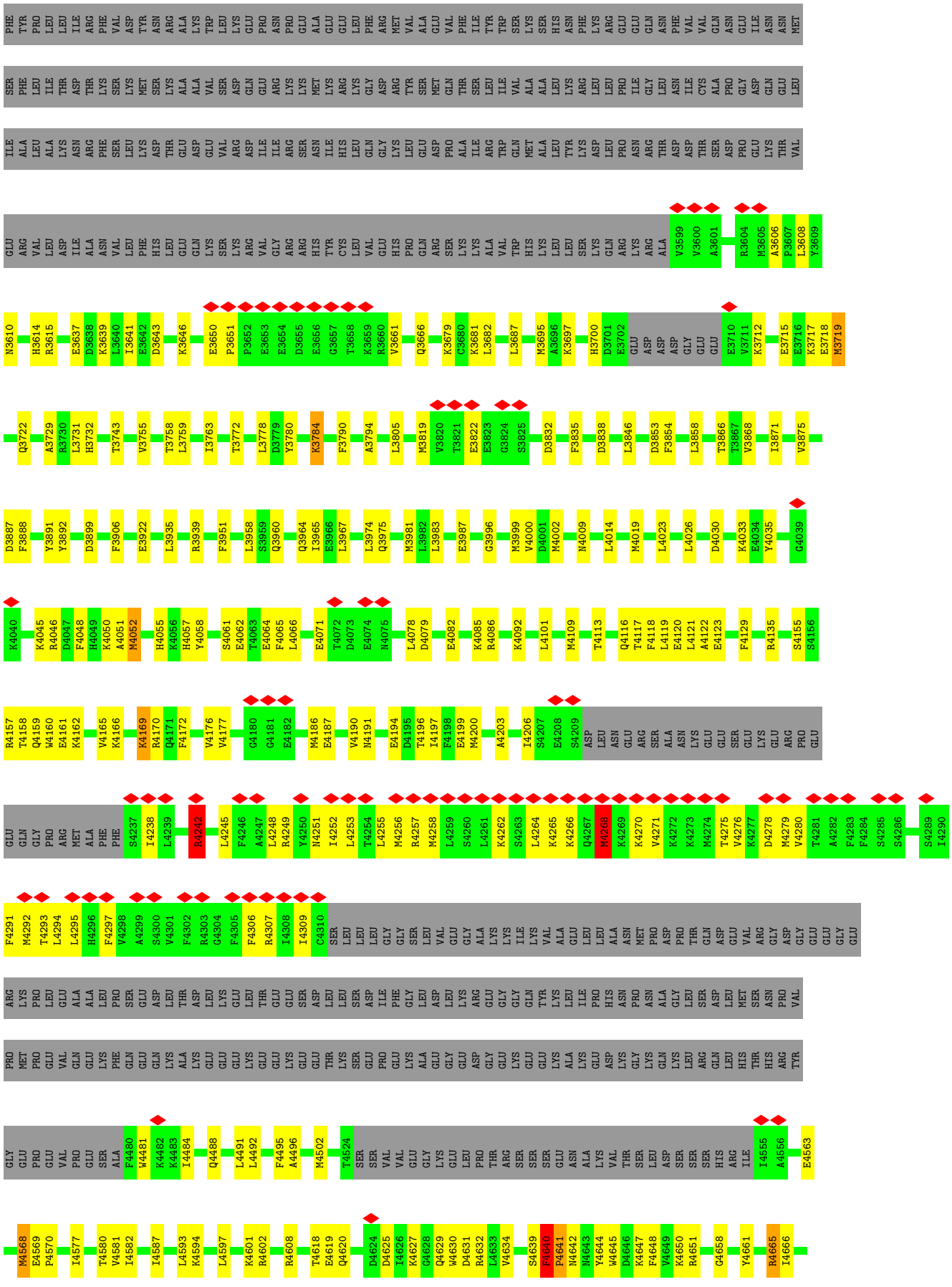
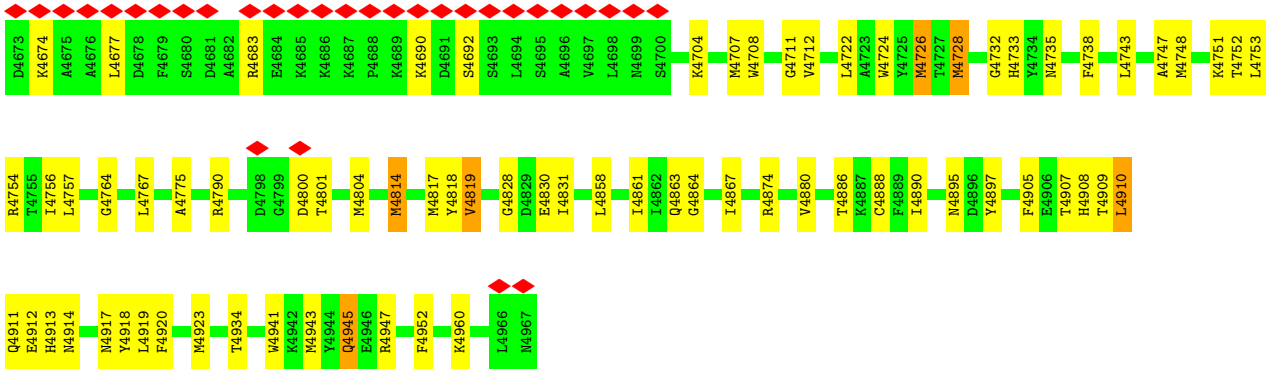
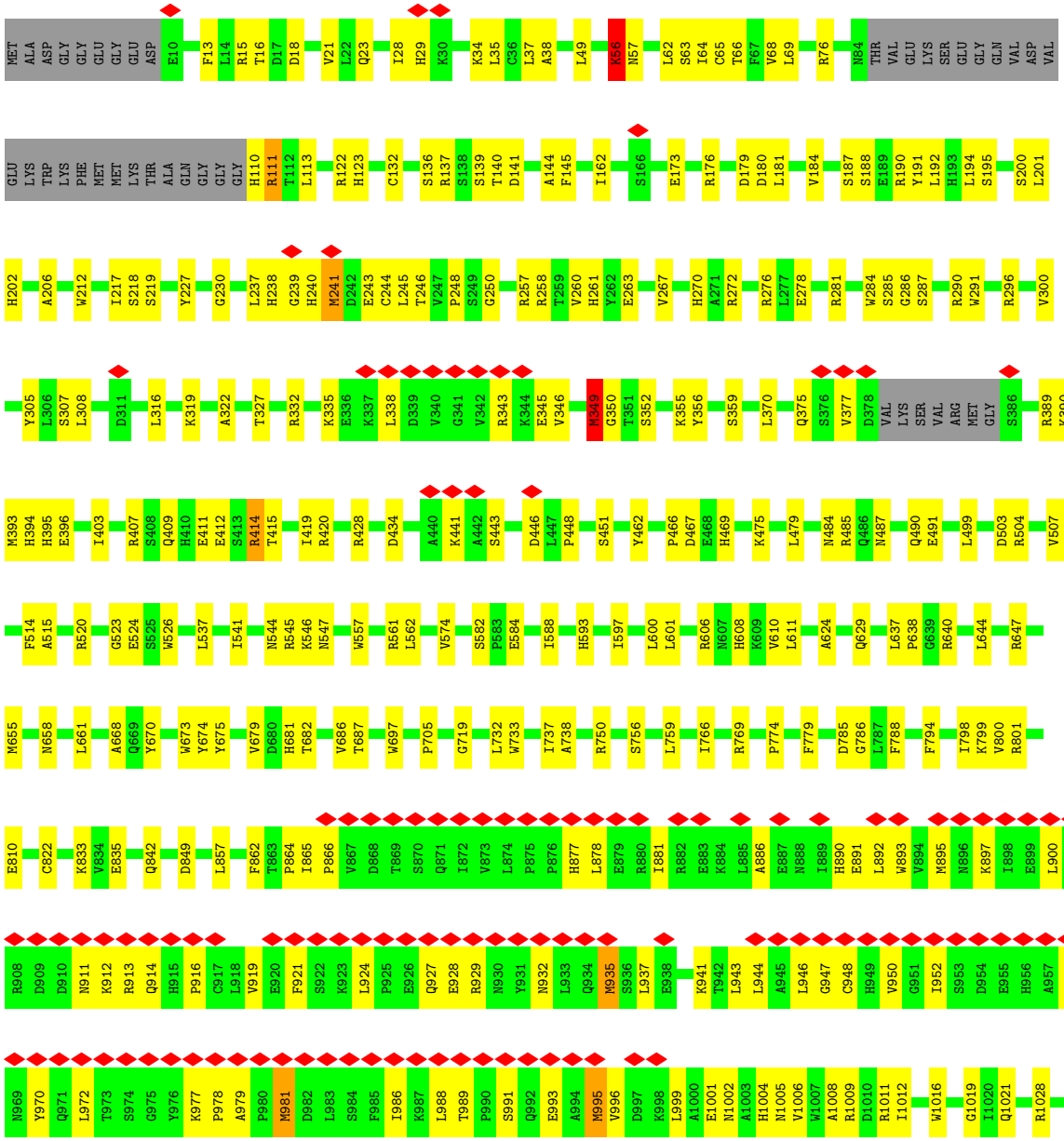
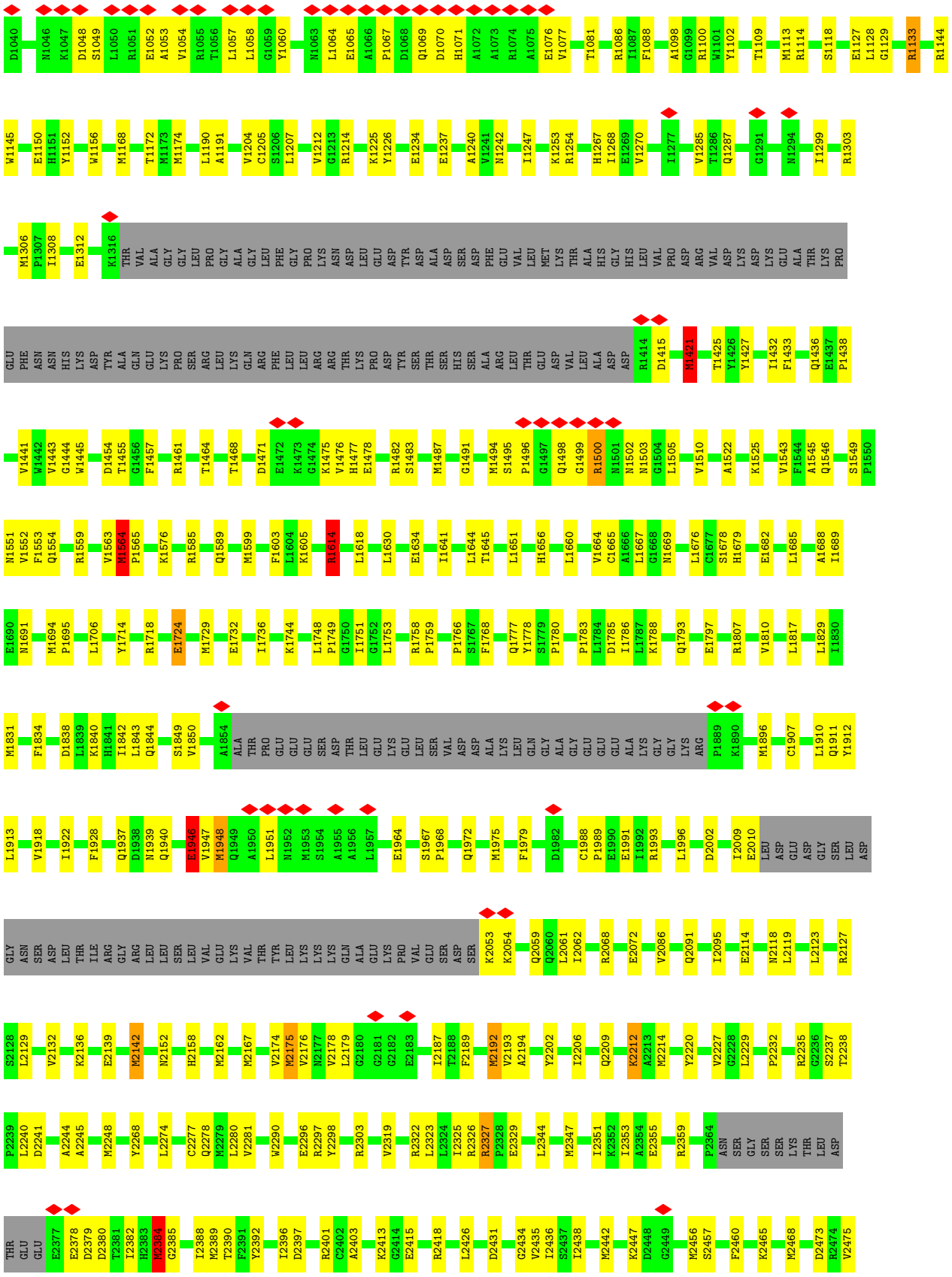




• Molecule 2: Ryanodine receptor 2

Chain C:

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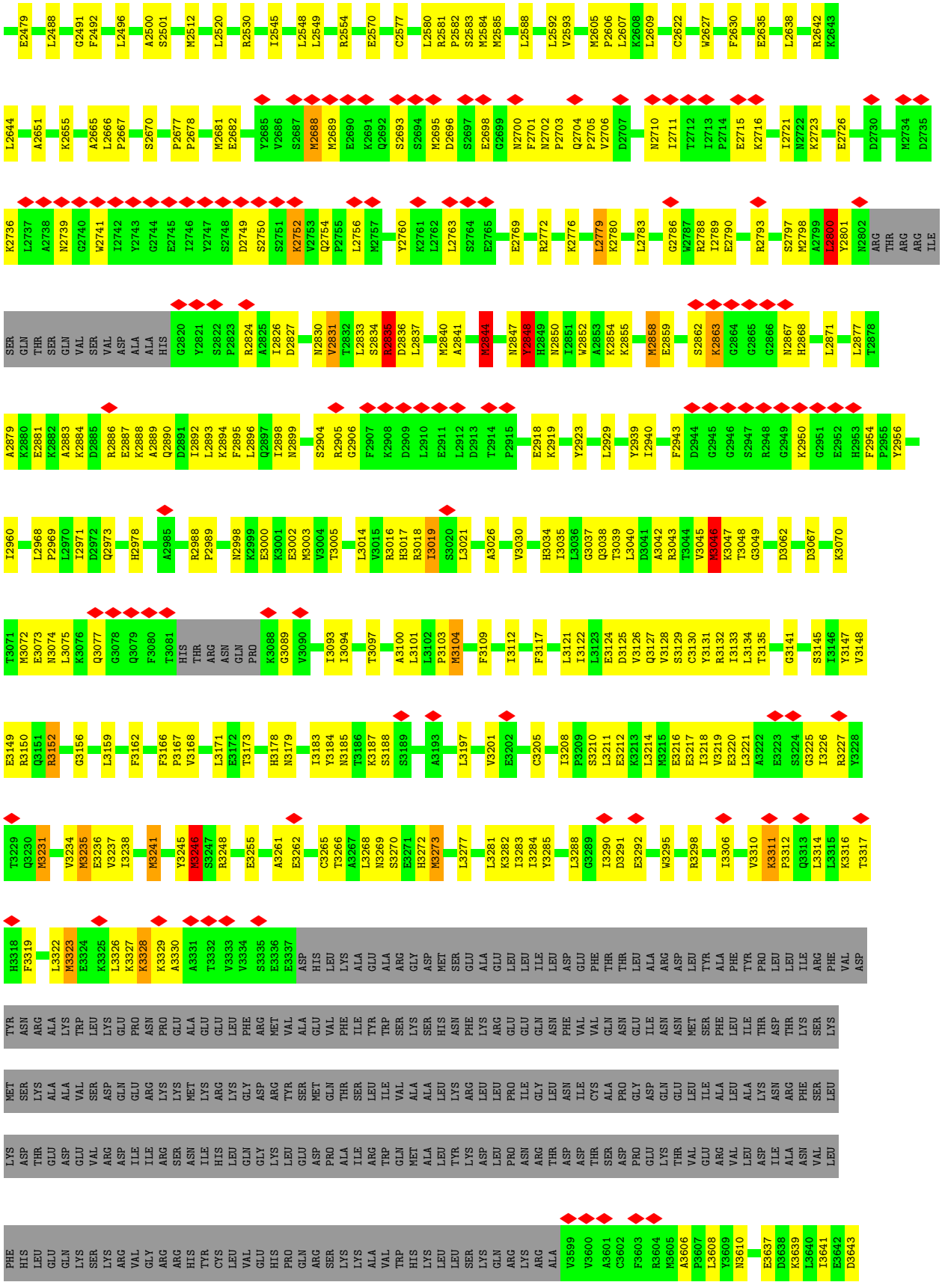

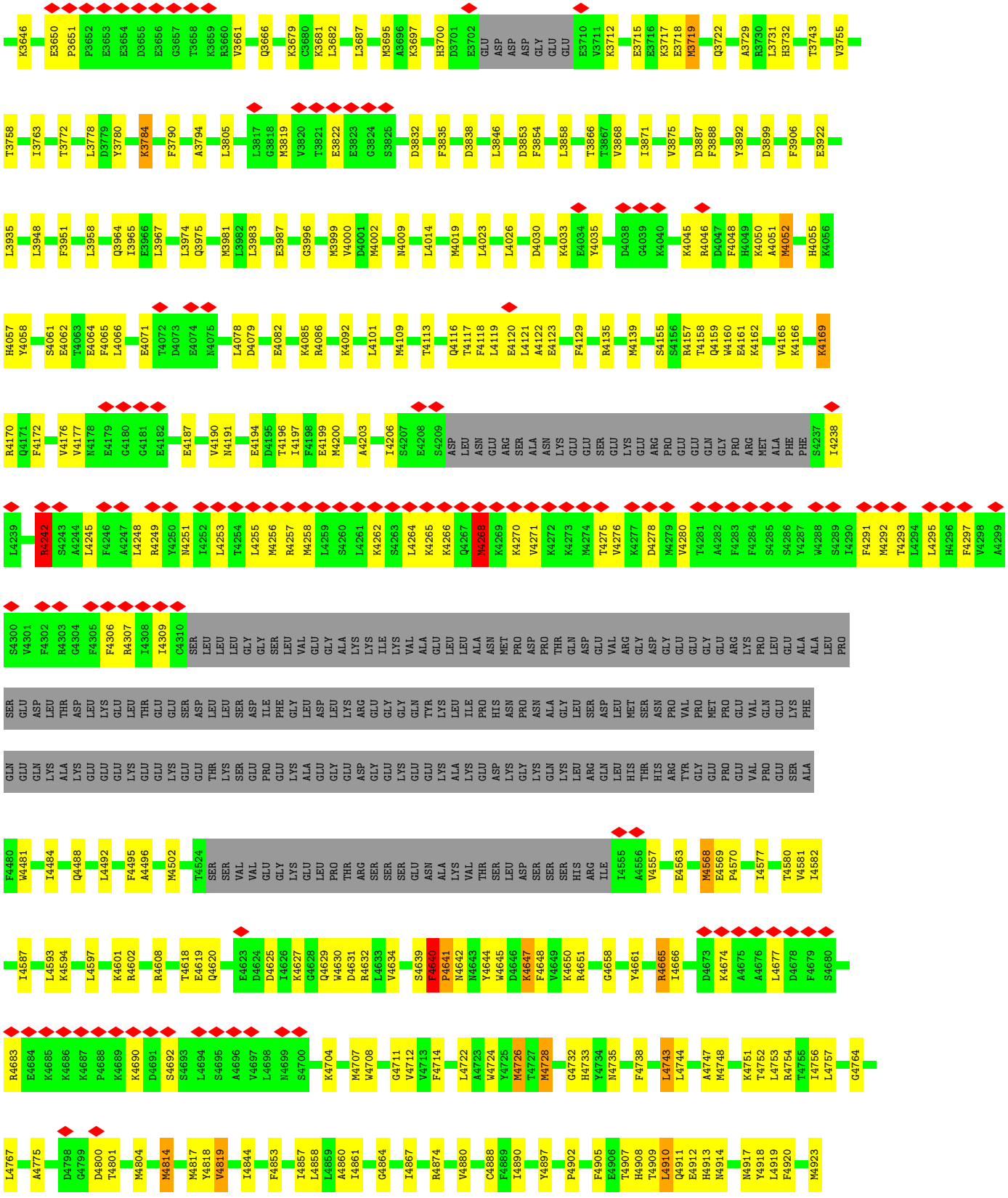

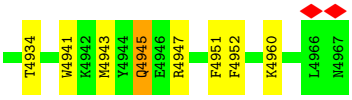
T4934
W4941
K4942
M4943
Y4944
Q4945
E4946
R4947
F4951
F4952
K4960
L4966
N4967

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.629	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

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	E	0.27	0/834	0.50	0/1123
1	F	0.26	0/834	0.50	0/1123
1	G	0.26	0/834	0.50	0/1123
1	H	0.27	0/834	0.50	0/1123
2	A	0.27	0/34511	0.54	30/46614 (0.1%)
2	B	0.27	0/34511	0.54	30/46614 (0.1%)
2	C	0.27	0/34511	0.54	29/46614 (0.1%)
2	D	0.27	0/34511	0.54	30/46614 (0.1%)
All	All	0.27	0/141380	0.54	119/190948 (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
2	A	0	3
2	B	0	3
2	C	0	3
2	D	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2800	LEU	CA-CB-CG	13.22	145.71	115.30
2	D	2800	LEU	CA-CB-CG	13.22	145.71	115.30
2	B	2800	LEU	CA-CB-CG	13.22	145.70	115.30
2	A	2800	LEU	CA-CB-CG	13.21	145.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4242	ARG	CA-CB-CG	9.30	133.86	113.40

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	111	ARG	Sidechain
2	A	1614	ARG	Sidechain
2	A	4640	PHE	Peptide
2	D	111	ARG	Sidechain
2	D	1614	ARG	Sidechain

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	E	818	0	821	12	0
1	F	818	0	821	14	0
1	G	818	0	821	17	0
1	H	818	0	821	20	0
2	A	33771	0	33453	849	0
2	B	33771	0	33453	836	0
2	C	33771	0	33453	823	0
2	D	33771	0	33453	858	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	5	0
4	B	62	0	24	5	0
4	C	62	0	24	5	0
4	D	62	0	24	5	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	D	1	0	0	1	0
6	A	11	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	11	0	4	0	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
All	All	138656	0	137208	3337	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 12.

The worst 5 of 3337 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2844:MET:O	2:C:2848:TYR:HB2	1.61	1.01
2:A:2844:MET:O	2:A:2848:TYR:HB2	1.61	1.00
2:D:2844:MET:O	2:D:2848:TYR:HB2	1.61	0.99
2:B:2844:MET:O	2:B:2848:TYR:HB2	1.61	0.99
2:A:143:LEU:HD21	2:D:2325:ILE:HD11	1.44	0.99

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	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
1	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	A	4198/4967 (84%)	4091 (98%)	103 (2%)	4 (0%)	51	83
2	B	4198/4967 (84%)	4092 (98%)	102 (2%)	4 (0%)	51	83
2	C	4198/4967 (84%)	4091 (98%)	103 (2%)	4 (0%)	51	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	4198/4967 (84%)	4092 (98%)	102 (2%)	4 (0%)	51 83
All	All	17212/20300 (85%)	16778 (98%)	418 (2%)	16 (0%)	54 83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1553	PHE
2	A	4641	PRO
2	A	4819	VAL
2	D	1553	PHE
2	D	4641	PRO

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	E	88/89 (99%)	88 (100%)	0	100 100
1	F	88/89 (99%)	88 (100%)	0	100 100
1	G	88/89 (99%)	88 (100%)	0	100 100
1	H	88/89 (99%)	88 (100%)	0	100 100
2	A	3708/4358 (85%)	3615 (98%)	93 (2%)	47 70
2	B	3708/4358 (85%)	3615 (98%)	93 (2%)	47 70
2	C	3708/4358 (85%)	3615 (98%)	93 (2%)	47 70
2	D	3708/4358 (85%)	3615 (98%)	93 (2%)	47 70
All	All	15184/17788 (85%)	14812 (98%)	372 (2%)	50 71

5 of 372 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2783	LEU
2	C	937	LEU
2	B	2863	LYS
2	B	3981	MET

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Mol	Chain	Res	Type
2	C	1614	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	2118	ASN
2	C	2899	ASN
2	D	544	ASN
2	D	487	ASN
2	C	2978	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
6	XAN	D	5004	-	8,12,12	1.56	1 (12%)	4,17,17	6.59	2 (50%)
6	XAN	A	5004	-	8,12,12	1.56	1 (12%)	4,17,17	6.55	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ATP	C	5002	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
4	ATP	A	5002	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
4	ATP	B	5005	-	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
6	XAN	C	5004	-	8,12,12	1.56	1 (12%)	4,17,17	6.56	2 (50%)
4	ATP	B	5002	-	26,33,33	0.59	0	31,52,52	0.73	2 (6%)
4	ATP	C	5005	-	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
4	ATP	A	5005	-	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
4	ATP	D	5002	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
4	ATP	D	5005	-	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
6	XAN	B	5004	-	8,12,12	1.57	1 (12%)	4,17,17	6.56	2 (50%)

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
6	XAN	D	5004	-	-	-	0/2/2/2
6	XAN	A	5004	-	-	-	0/2/2/2
4	ATP	C	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	B	5005	-	-	8/18/38/38	0/3/3/3
6	XAN	C	5004	-	-	-	0/2/2/2
4	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	C	5005	-	-	8/18/38/38	0/3/3/3
4	ATP	A	5005	-	-	7/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	8/18/38/38	0/3/3/3
4	ATP	D	5005	-	-	8/18/38/38	0/3/3/3
6	XAN	B	5004	-	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5004	XAN	C6-N1	4.05	1.40	1.33
6	D	5004	XAN	C6-N1	4.02	1.40	1.33
6	A	5004	XAN	C6-N1	4.02	1.40	1.33
6	C	5004	XAN	C6-N1	4.01	1.40	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	5004	XAN	C2-N1-C6	11.30	124.68	115.14
6	B	5004	XAN	C2-N1-C6	11.25	124.64	115.14
6	C	5004	XAN	C2-N1-C6	11.23	124.63	115.14
6	A	5004	XAN	C2-N1-C6	11.22	124.61	115.14
6	D	5004	XAN	C5-C6-N1	-6.76	114.18	123.43

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5005	ATP	PB-O3B-PG-O2G
4	A	5005	ATP	C5'-O5'-PA-O1A
4	A	5005	ATP	C5'-O5'-PA-O2A
4	D	5002	ATP	C5'-O5'-PA-O3A

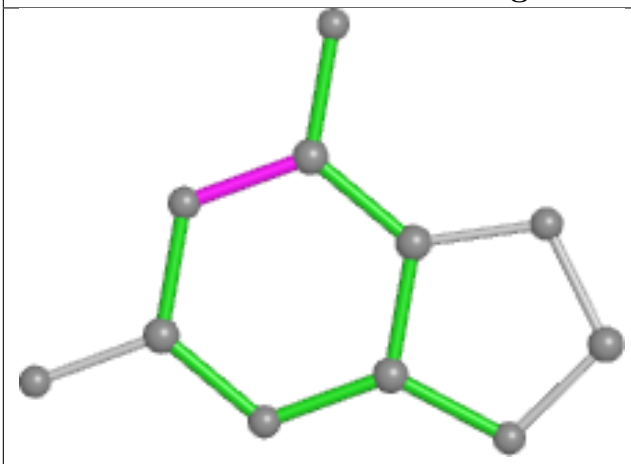
There are no ring outliers.

4 monomers are involved in 20 short contacts:

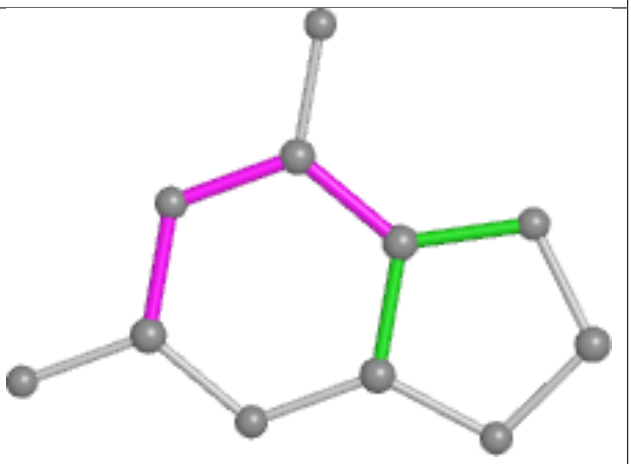
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5002	ATP	5	0
4	A	5002	ATP	5	0
4	B	5002	ATP	5	0
4	D	5002	ATP	5	0

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.

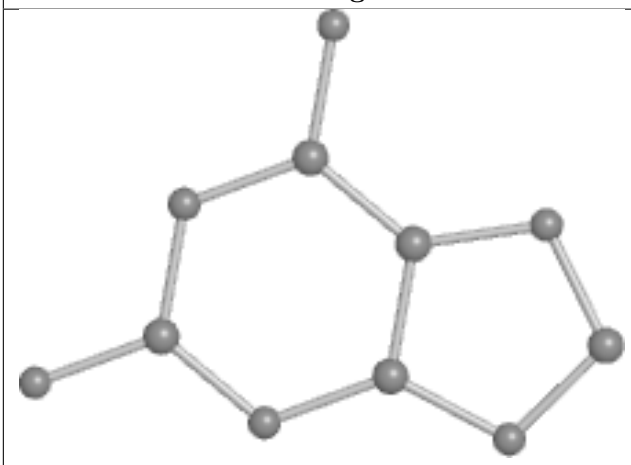
Ligand XAN D 5004



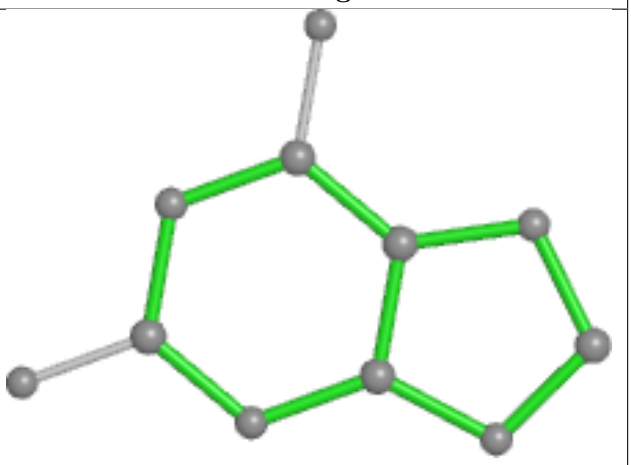
Bond lengths



Bond angles

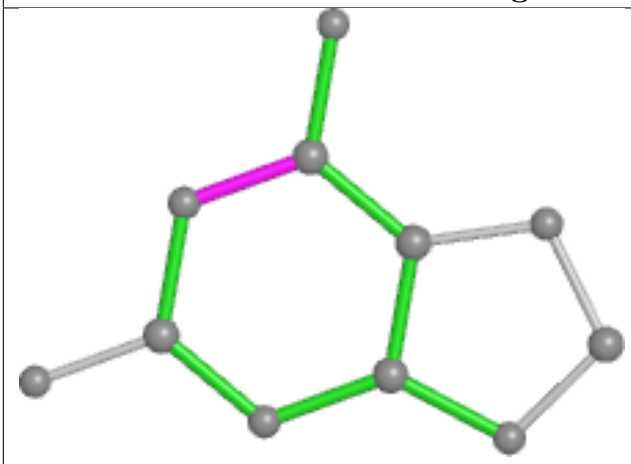


Torsions



Rings

Ligand XAN A 5004



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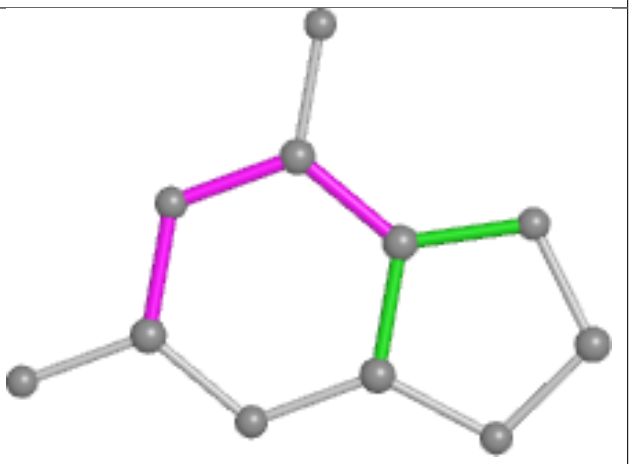

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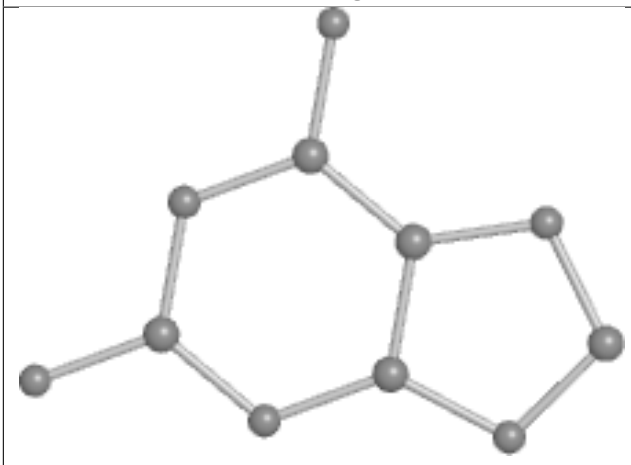

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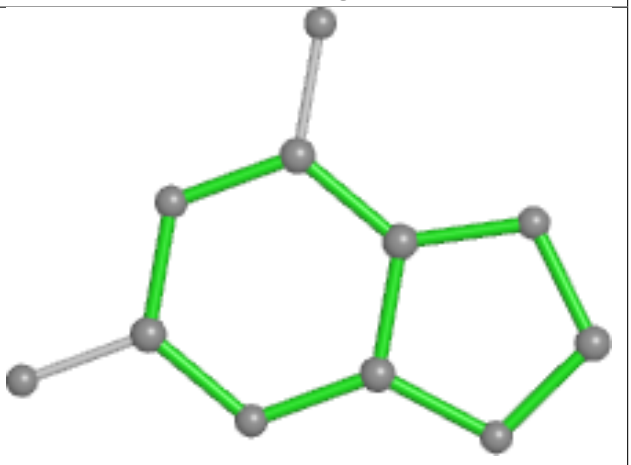
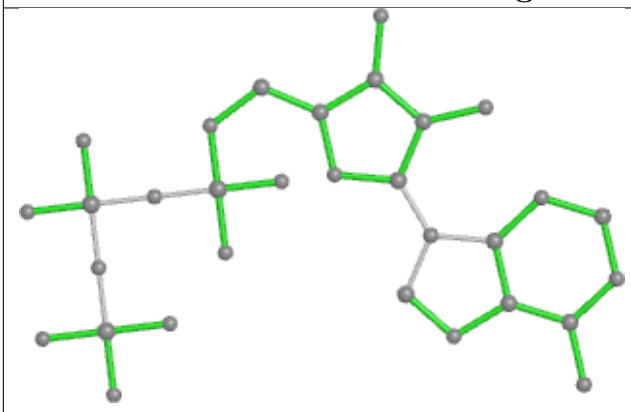
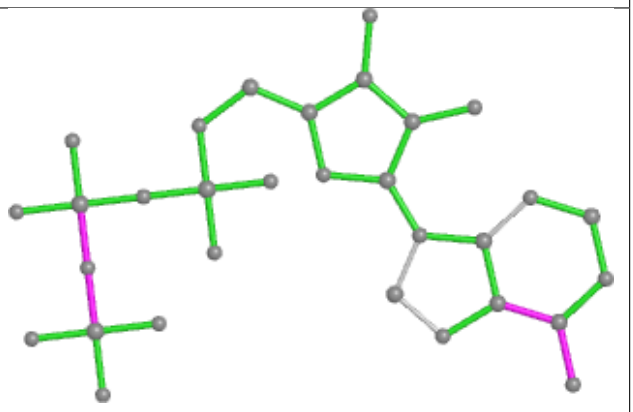


Rings

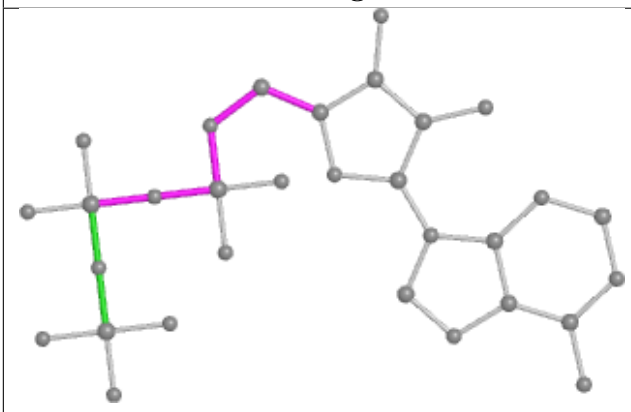
Ligand ATP C 5002



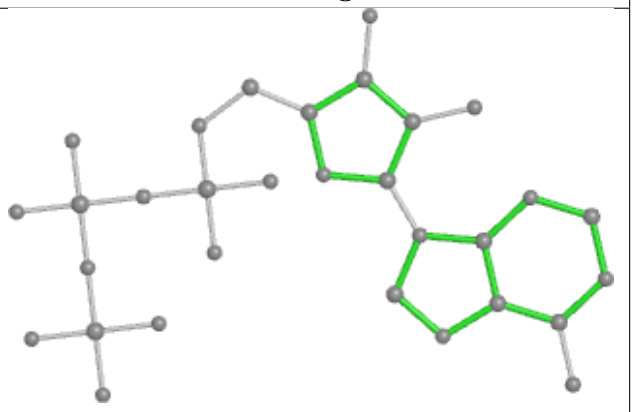
Bond lengths



Bond angles

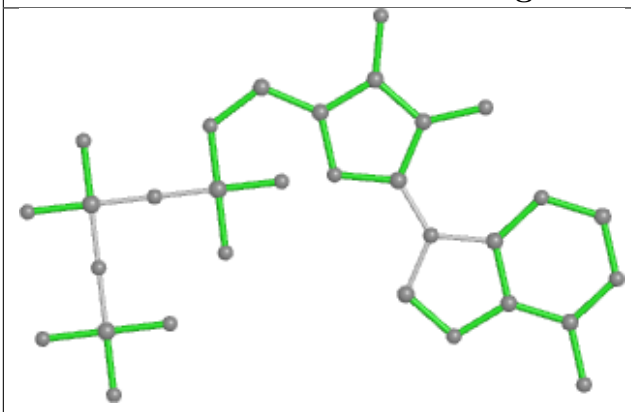


Torsions

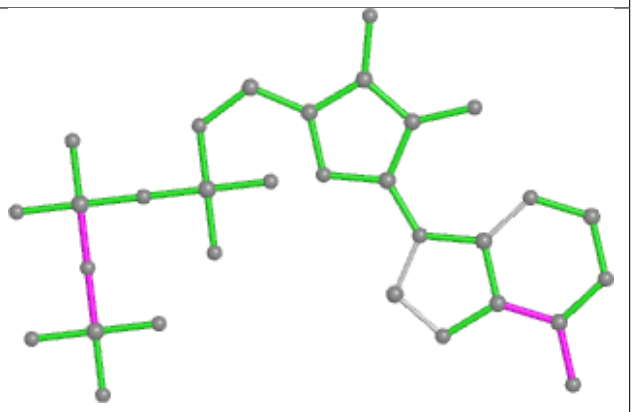


Rings

Ligand ATP A 5002



Bond lengths



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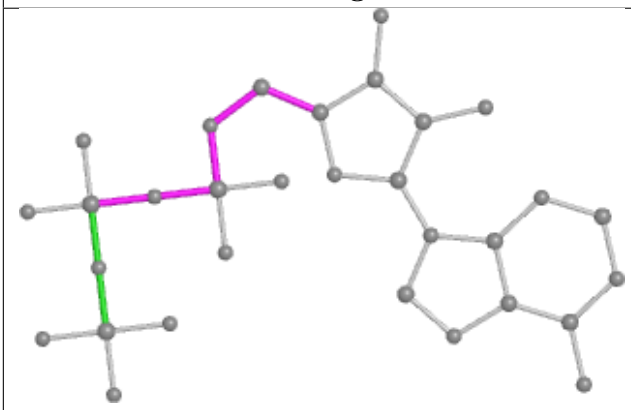

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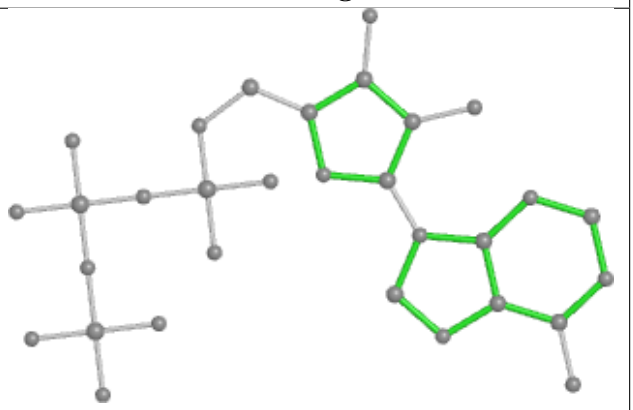
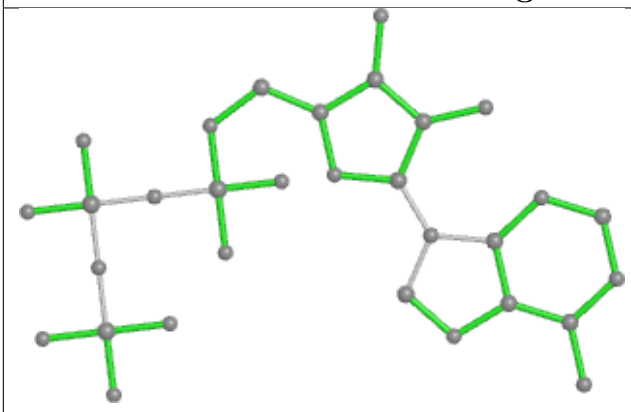
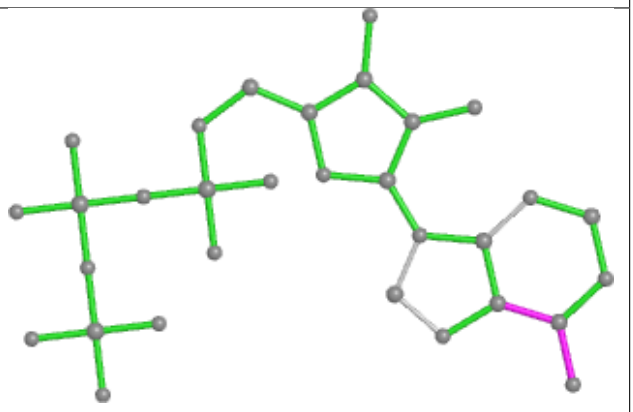


Rings

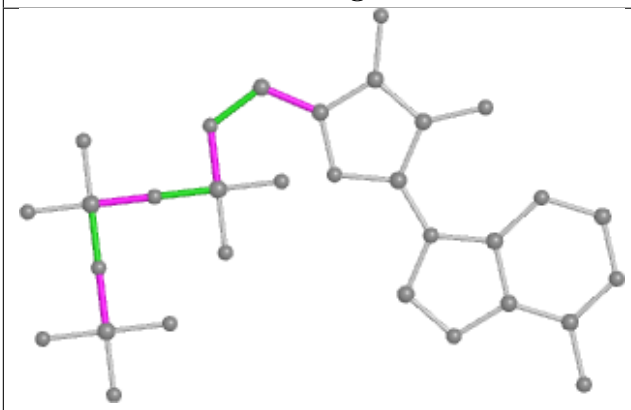
Ligand ATP B 5005



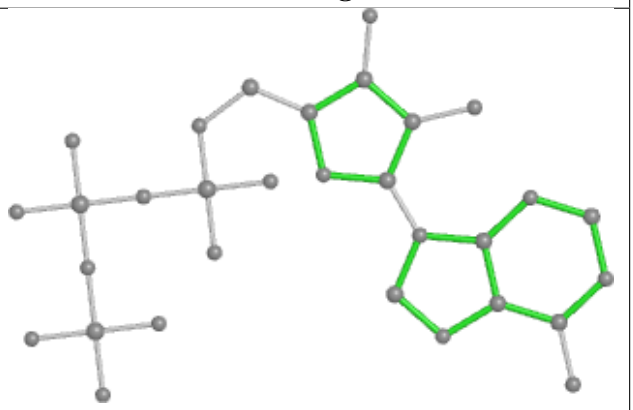
Bond lengths



Bond angles

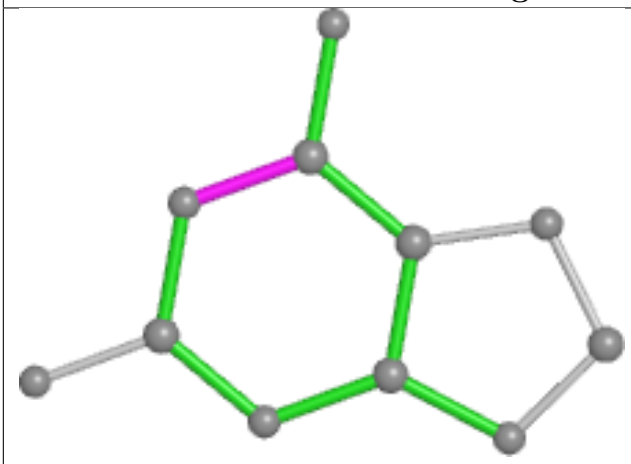


Torsions

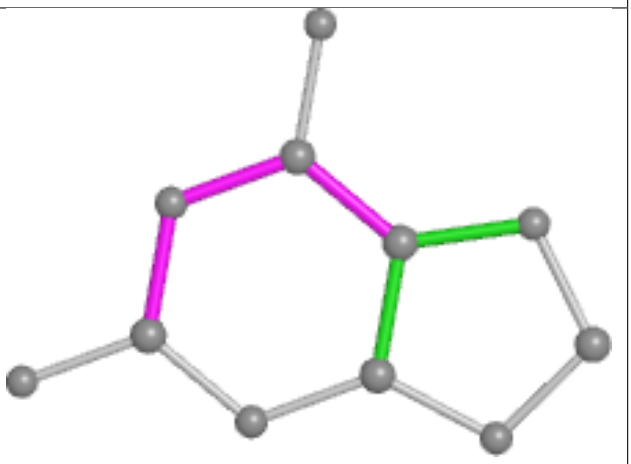


Rings

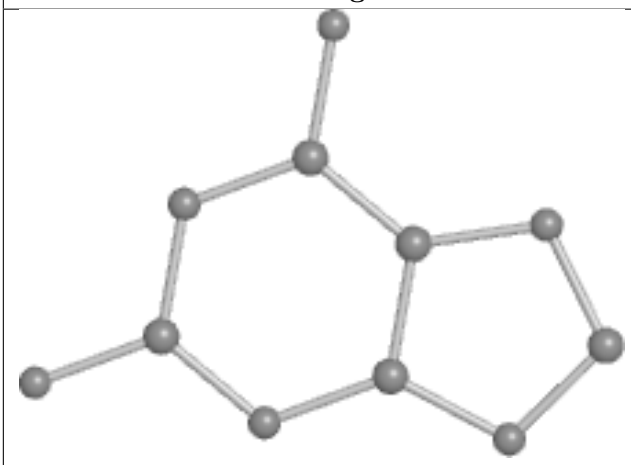
Ligand XAN C 5004



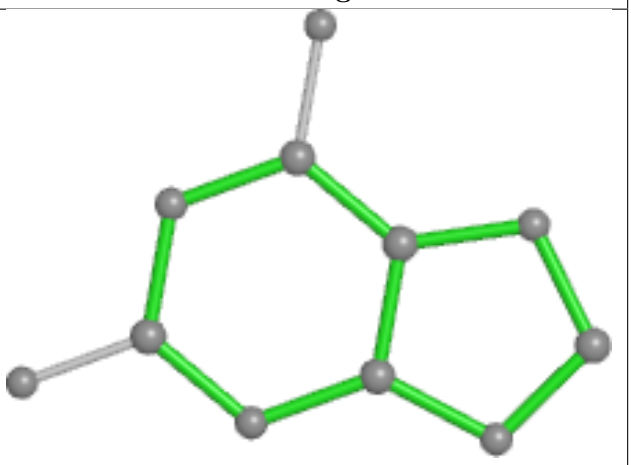
Bond lengths



Bond angles

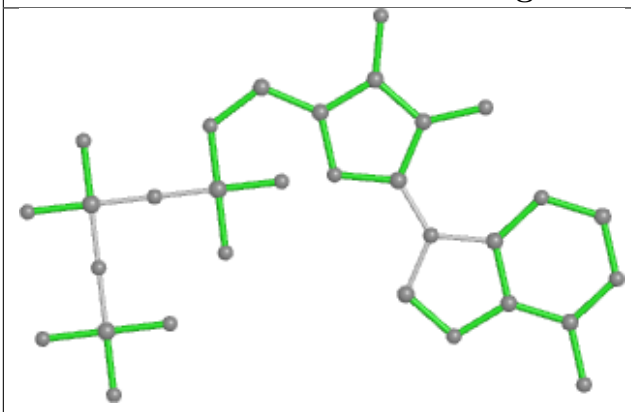


Torsions

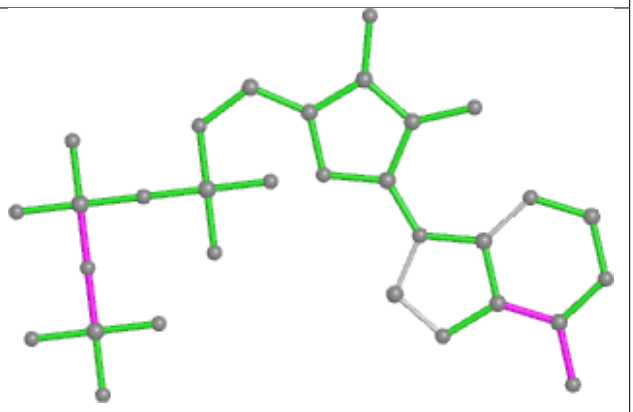


Rings

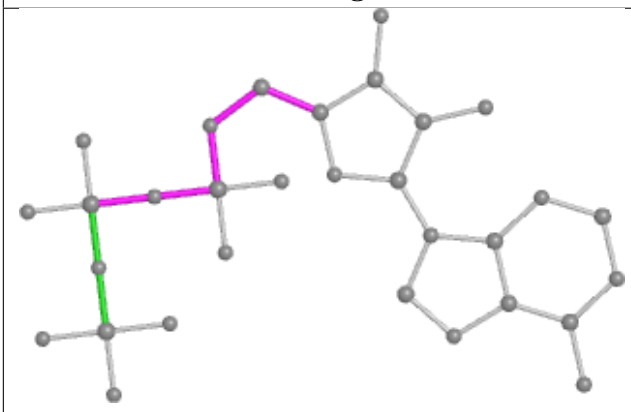
Ligand ATP B 5002



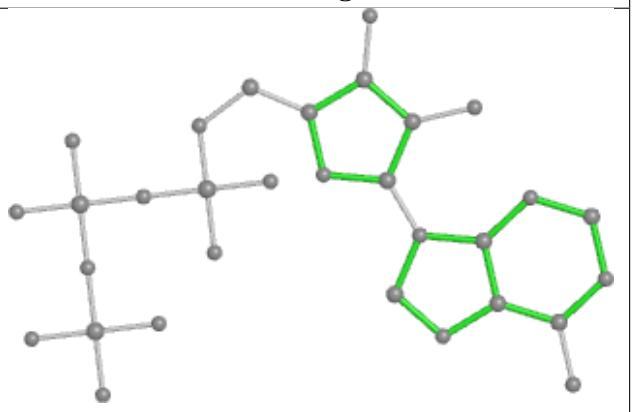
Bond lengths



Bond angles

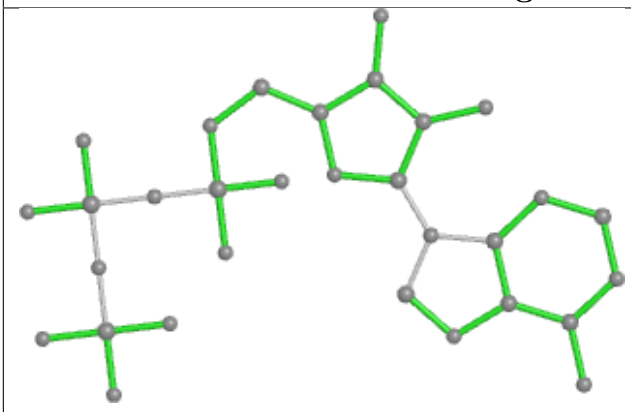


Torsions

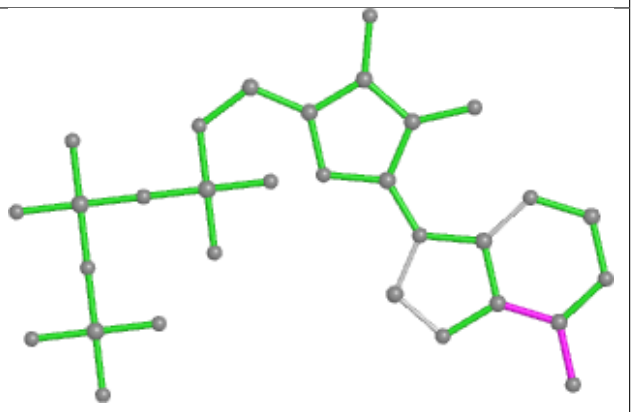


Rings

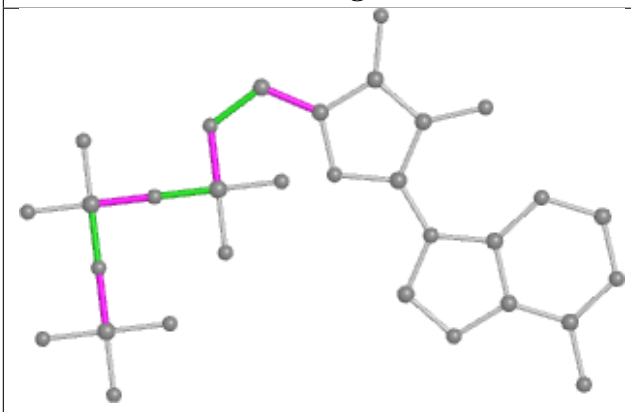
Ligand ATP C 5005



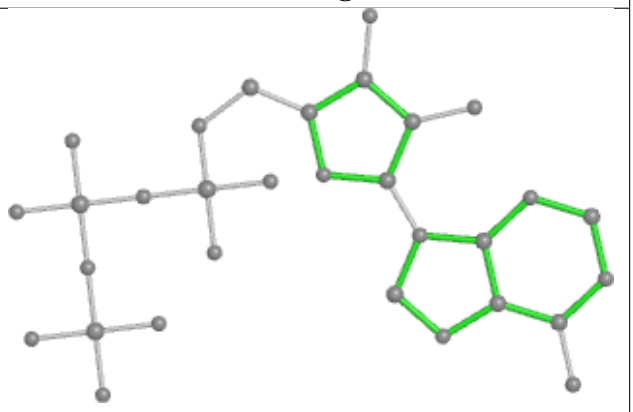
Bond lengths



Bond angles

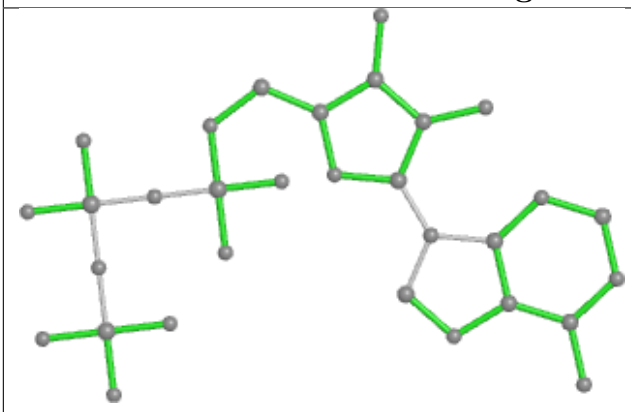


Torsions

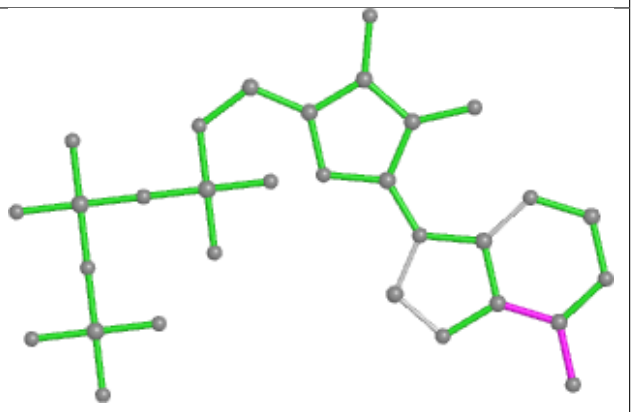


Rings

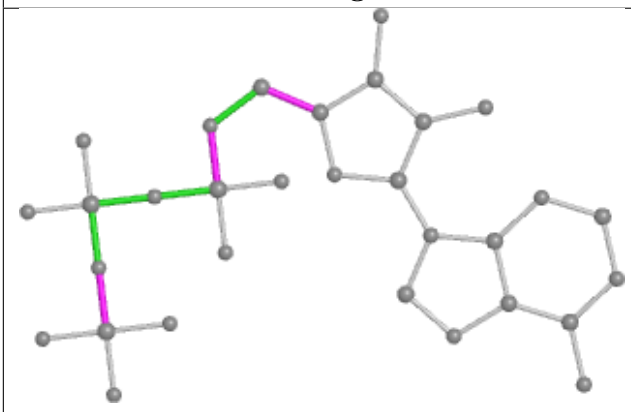
Ligand ATP A 5005



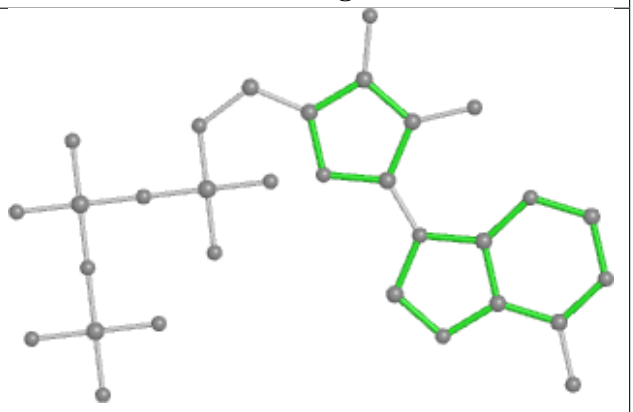
Bond lengths



Bond angles

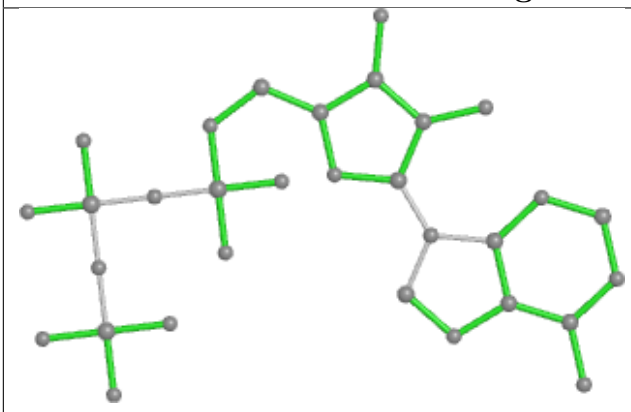


Torsions

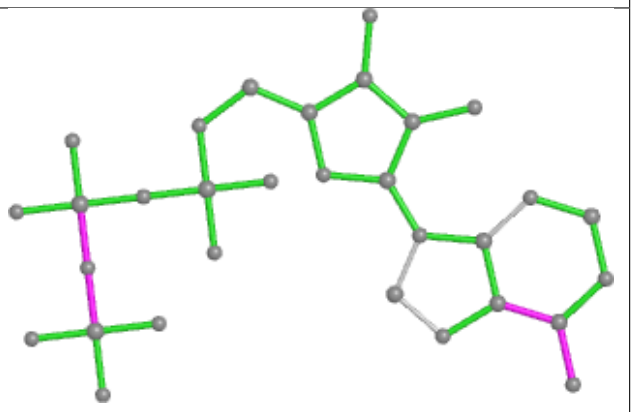


Rings

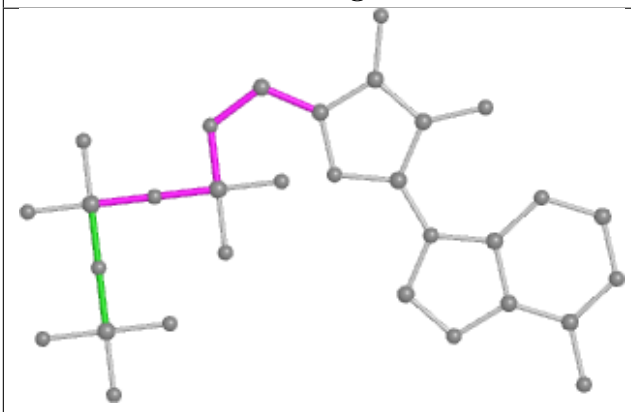
Ligand ATP D 5002



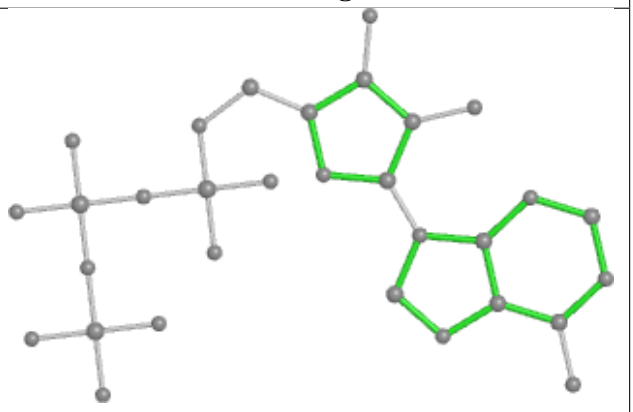
Bond lengths



Bond angles

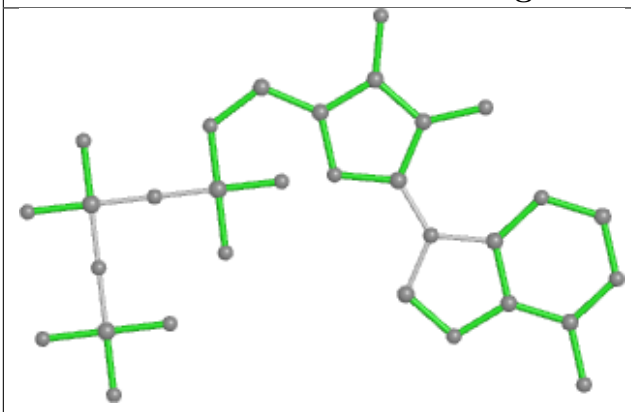


Torsions

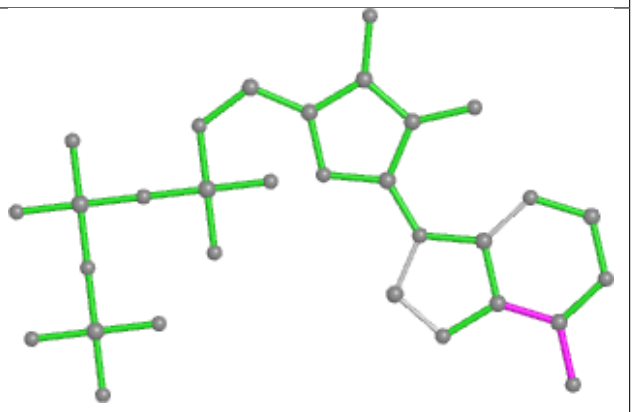


Rings

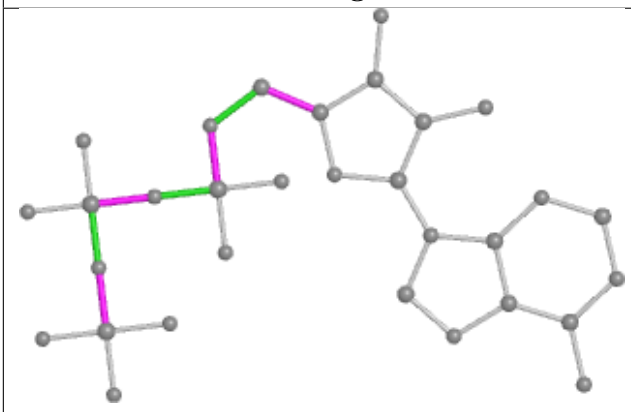
Ligand ATP D 5005



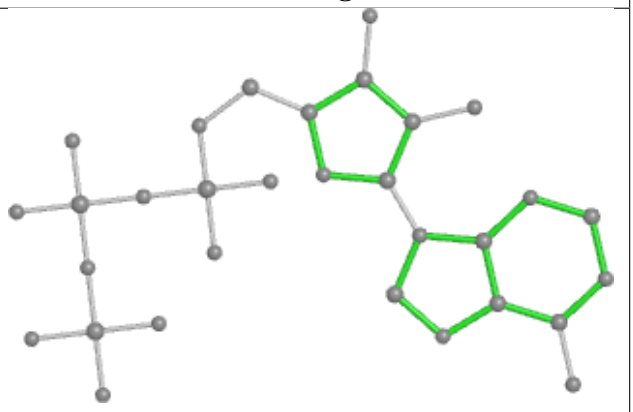
Bond lengths



Bond angles

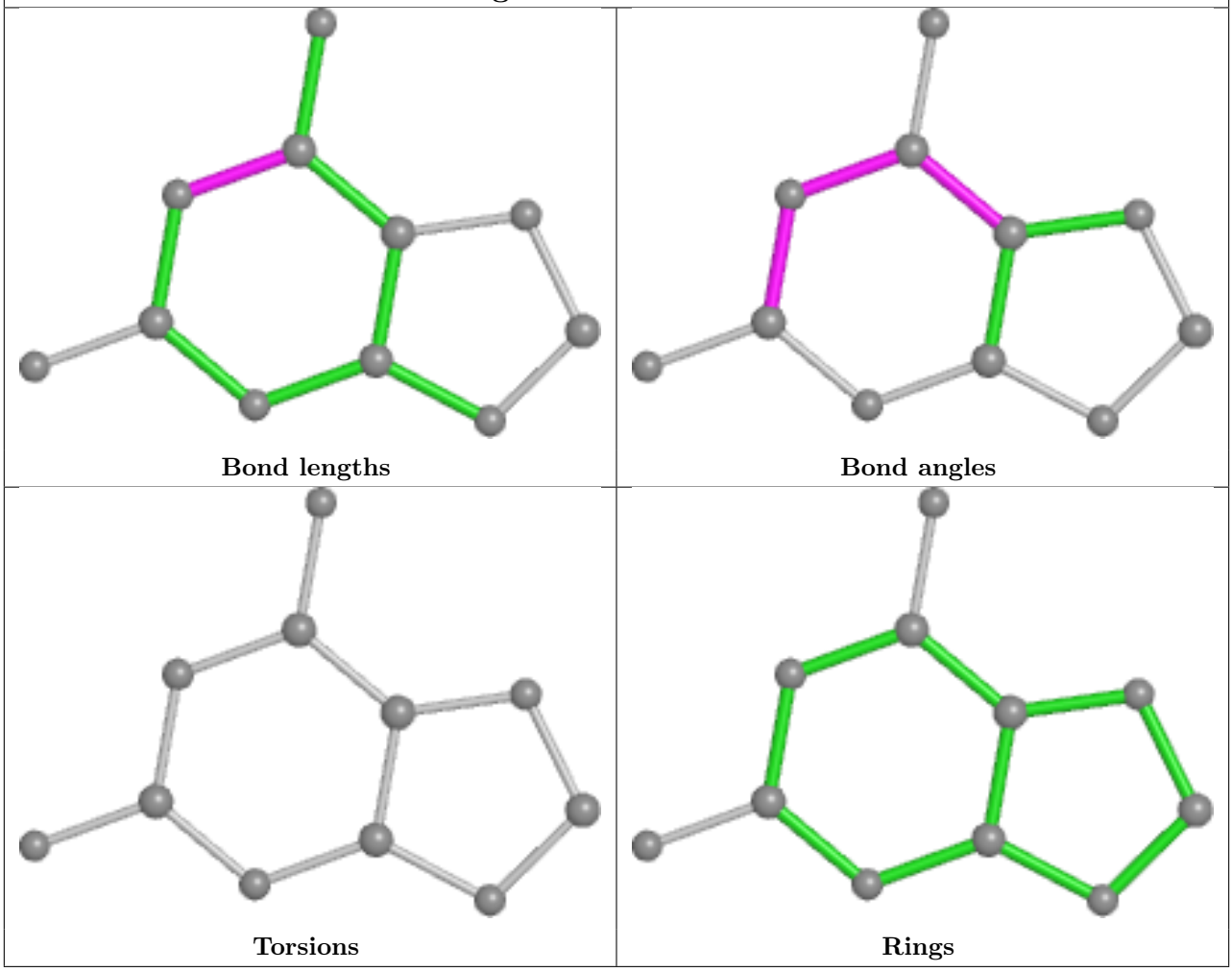


Torsions



Rings

Ligand XAN B 5004



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.

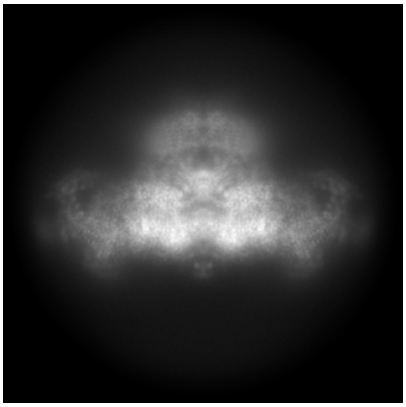
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26407. These allow visual inspection of the internal detail of the map and identification of artifacts.

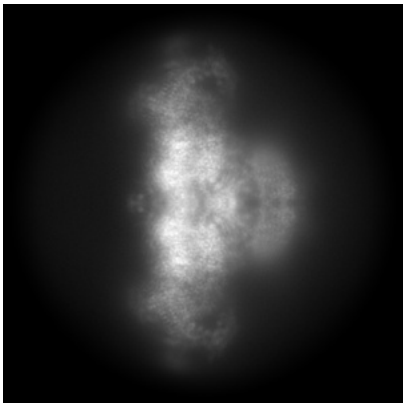
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

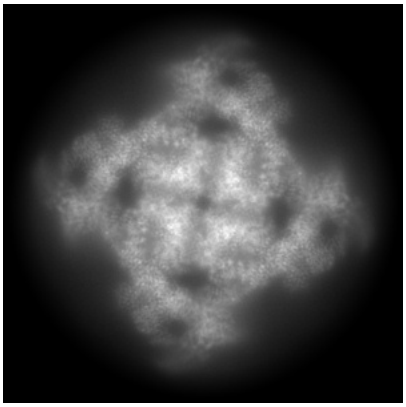
6.1.1 Primary map



X



Y

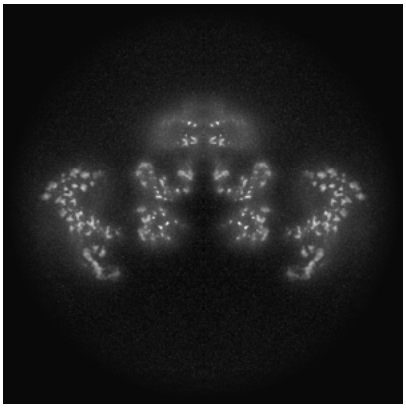


Z

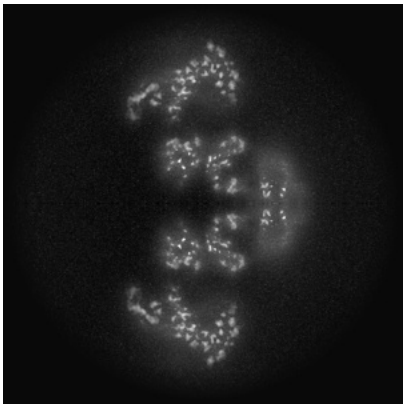
The images above show the map projected in three orthogonal directions.

6.2 Central slices

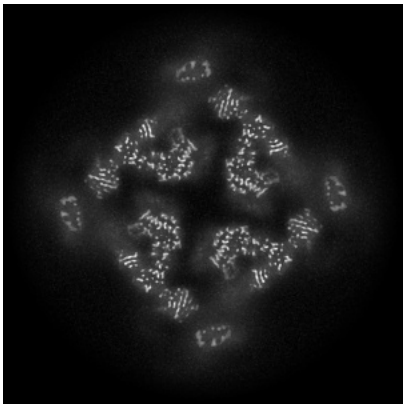
6.2.1 Primary map



X Index: 256



Y Index: 256

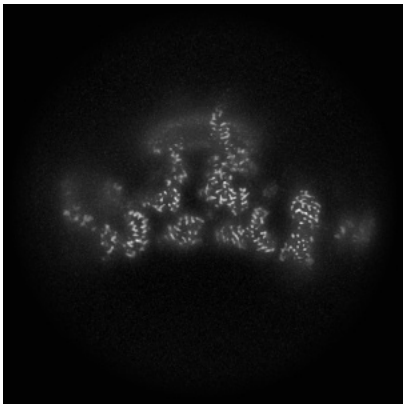


Z Index: 256

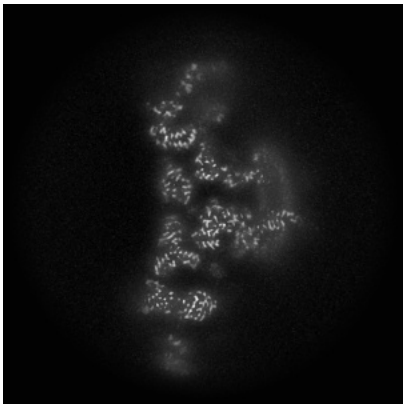
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

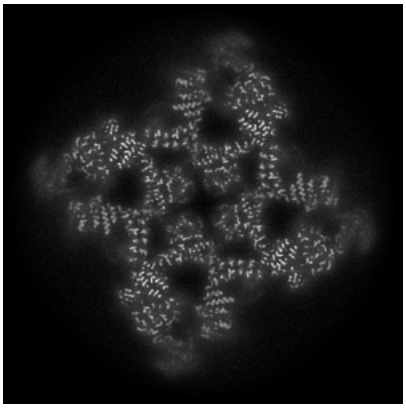
6.3.1 Primary map



X Index: 292



Y Index: 292

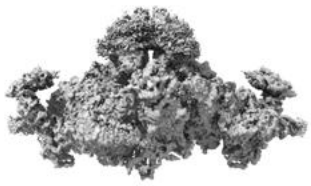


Z Index: 227

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

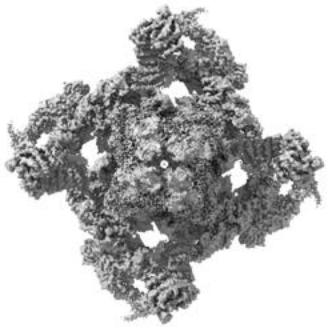
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

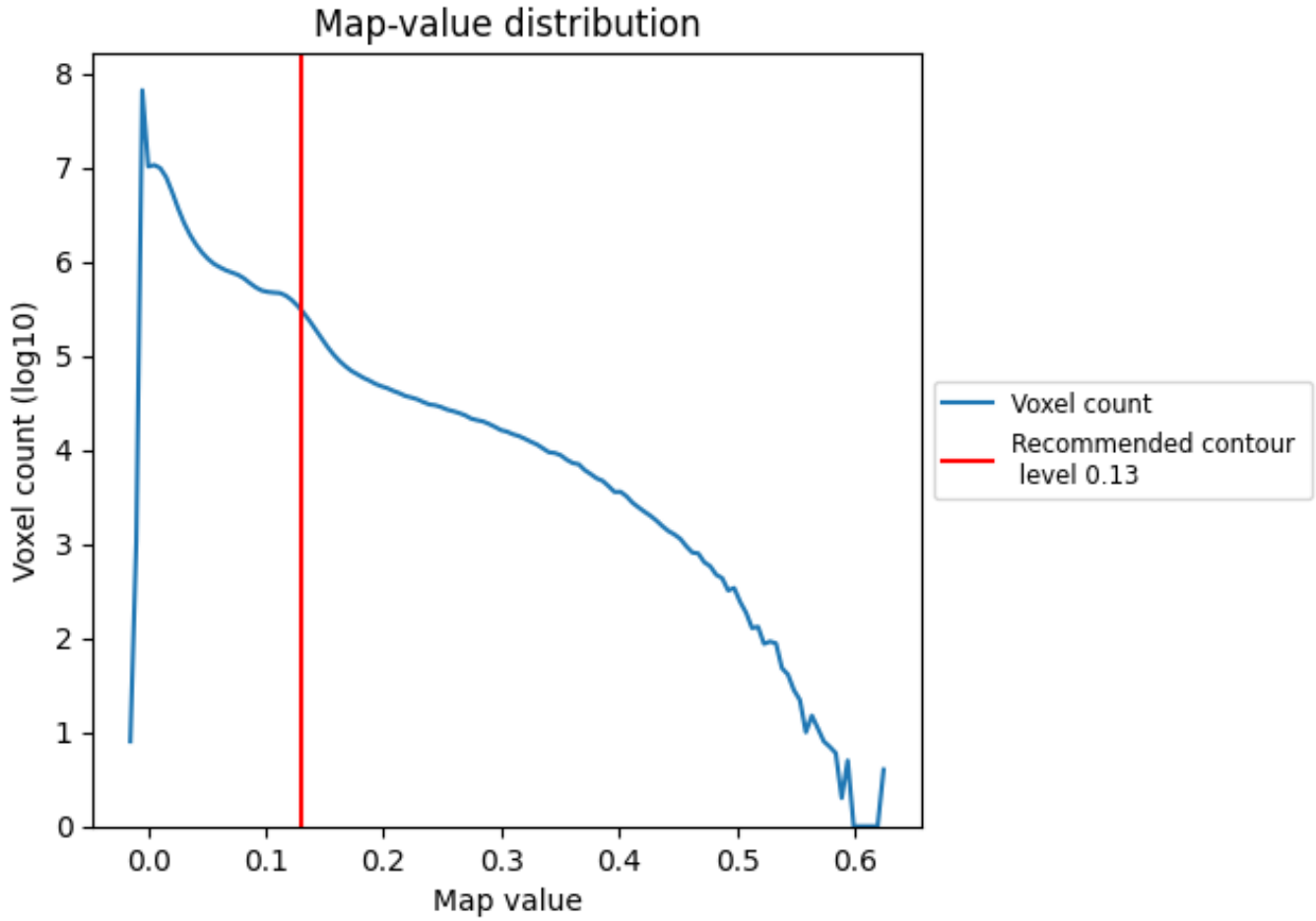
6.5 Mask visualisation (i)

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

7 Map analysis

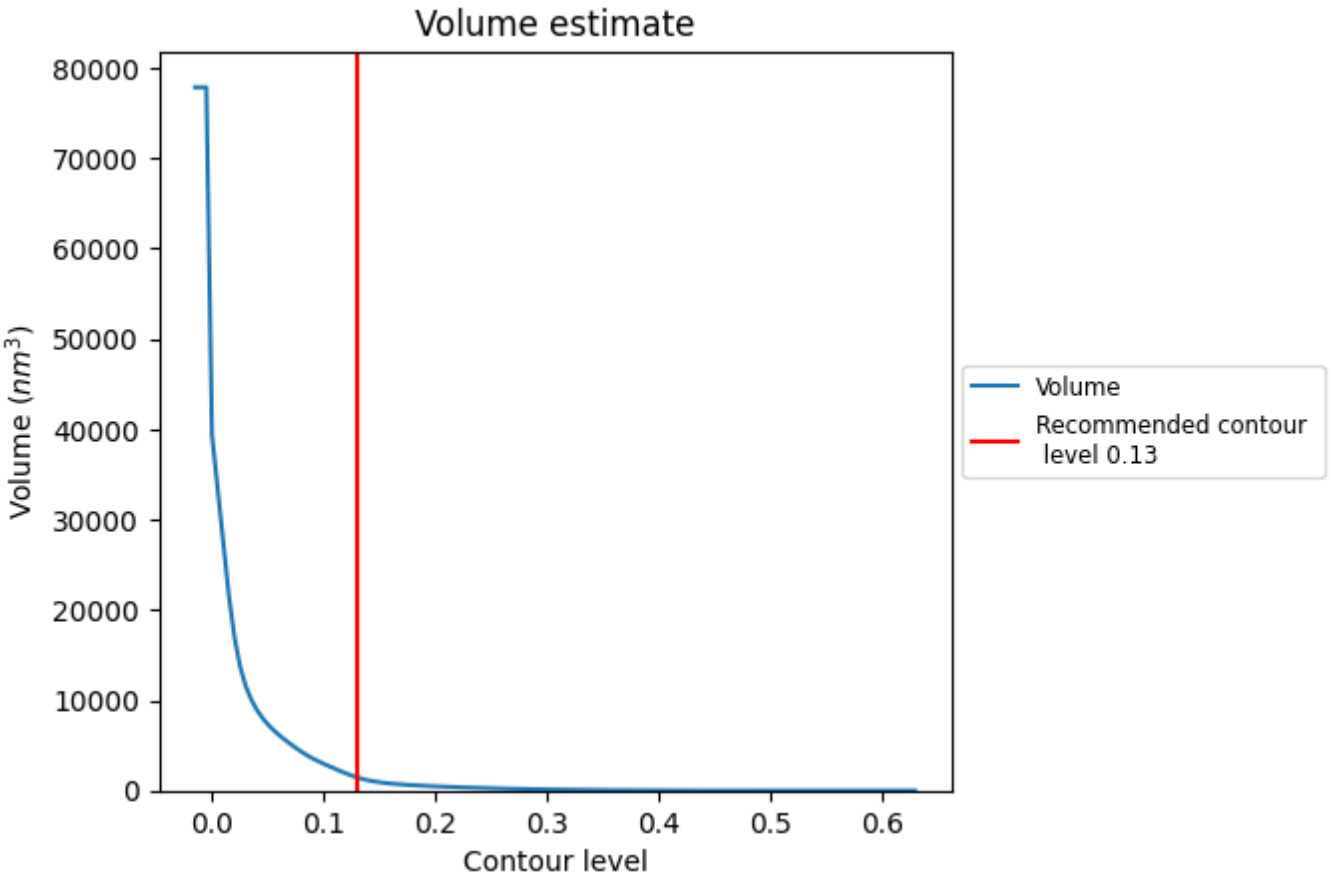
This section contains the results of statistical analysis of the map.

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.

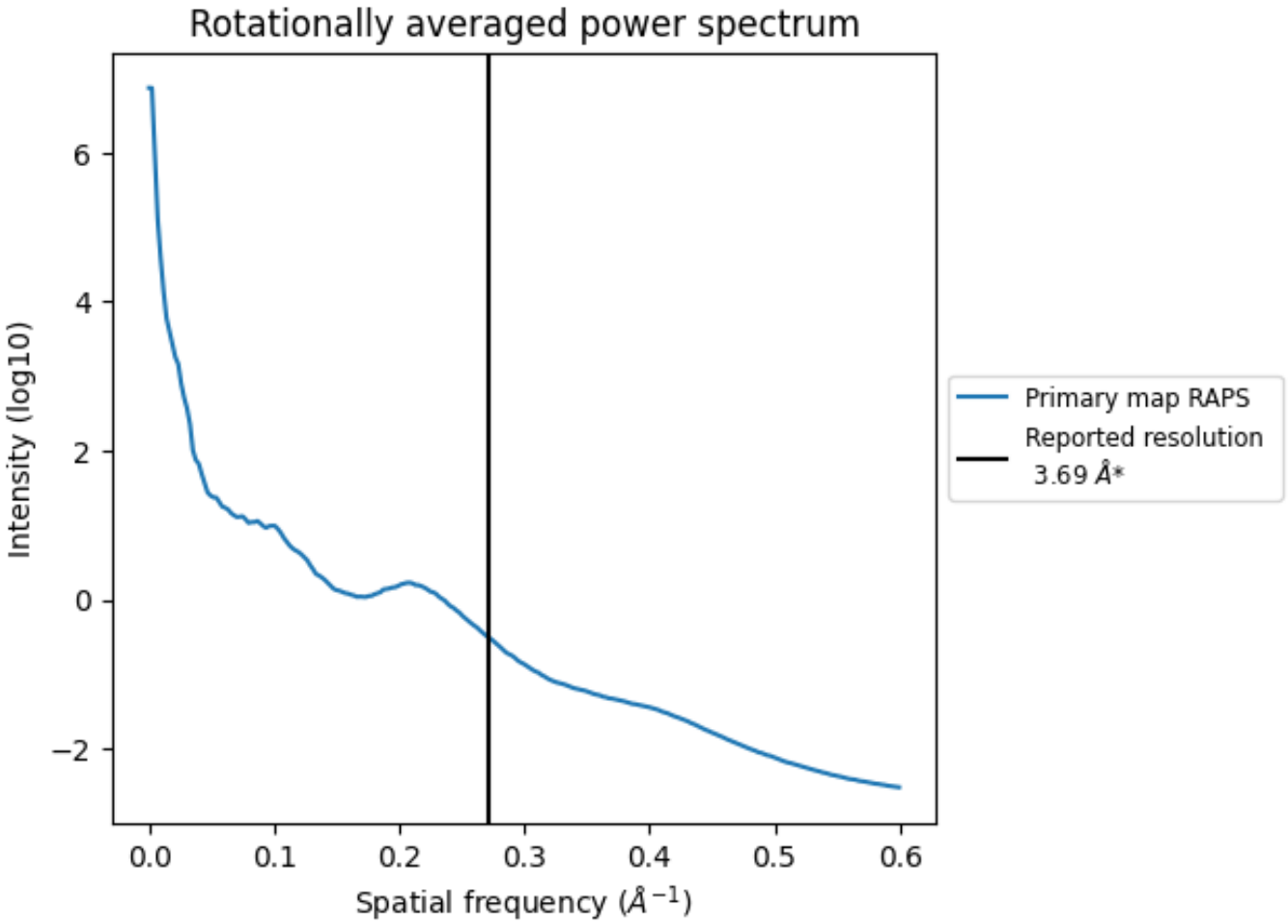
7.2 Volume estimate (i)



The volume at the recommended contour level is 1461 nm^3; this corresponds to an approximate mass of 1320 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 0.271 Å^{-1}

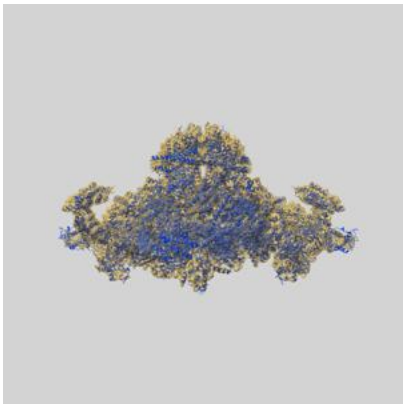
8 Fourier-Shell correlation

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

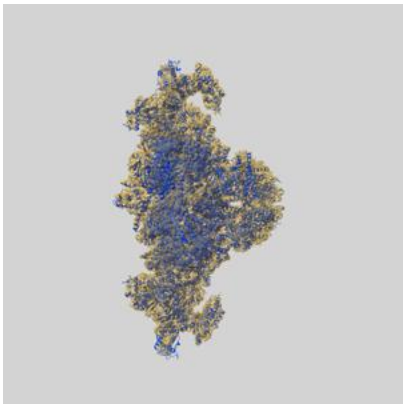
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26407 and PDB model 7U9R. Per-residue inclusion information can be found in section 3 on page 6.

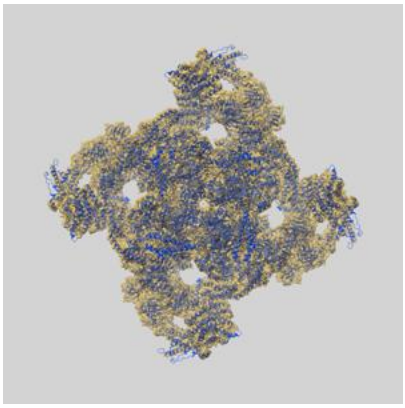
9.1 Map-model overlay



X



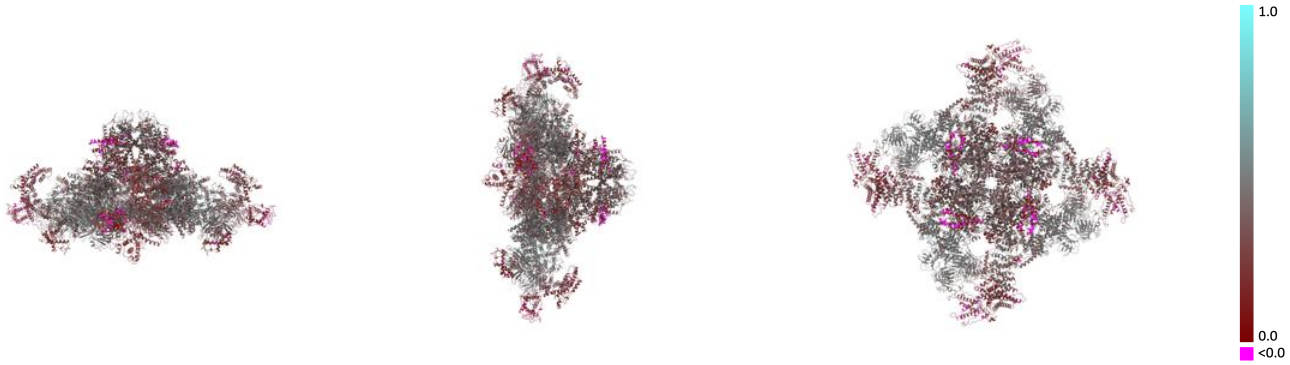
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

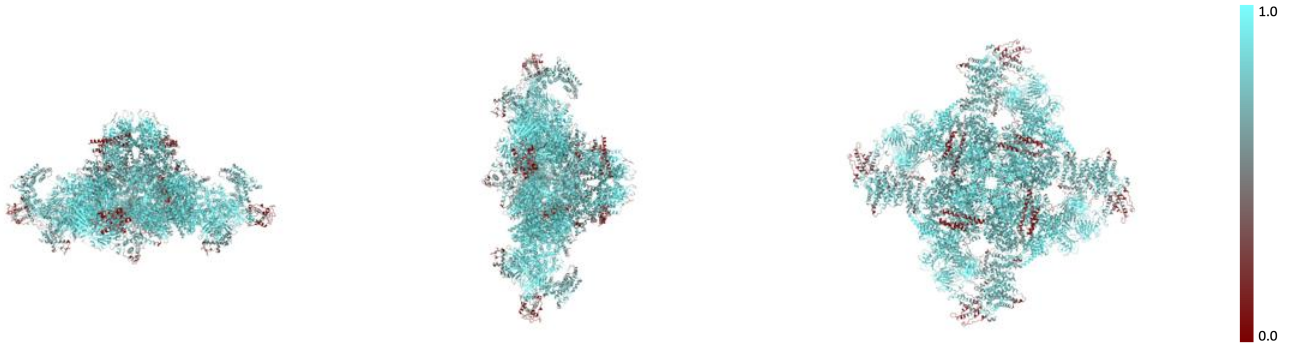
9.2 Q-score mapped to coordinate model (i)



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.

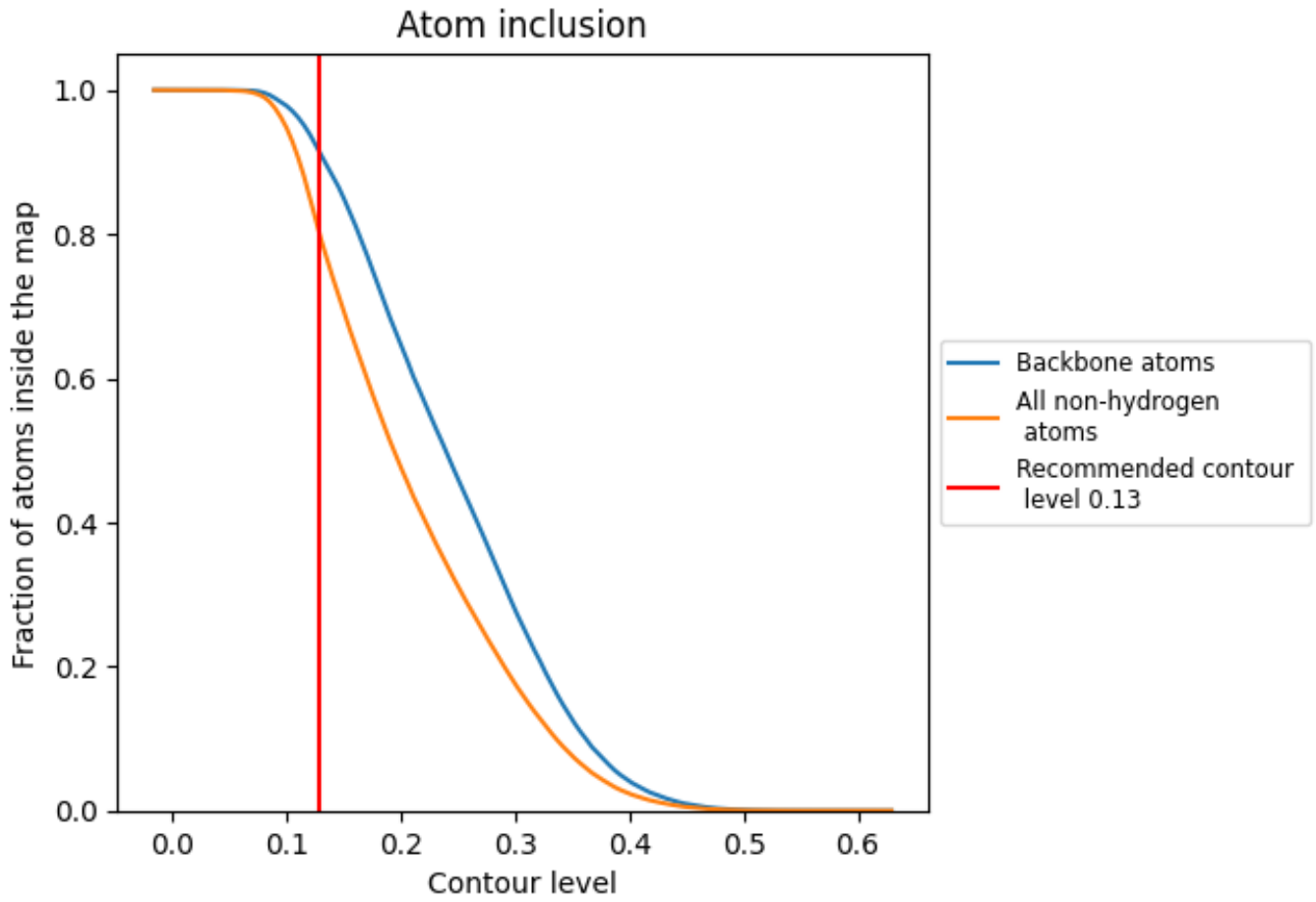
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 80% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7976	0.3530
A	0.7992	0.3650
B	0.7928	0.3440
C	0.7908	0.3410
D	0.7964	0.3510
E	0.9169	0.4860
F	0.9194	0.4720
G	0.9119	0.4770
H	0.9094	0.4720