wwPDB EM Validation Summary Report (i)

Oct 7, 2024 – 02:05 AM EDT

PDB ID	:	8UXM
EMDB ID	:	EMD-42769
Title	:	Structure of PKA phosphorylated human RyR2-R420W in the open state in the presence of calcium and calmodulin
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2023-11-09
Resolution	:	3.56 Å(reported)
Based on initial model	:	7UA5

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

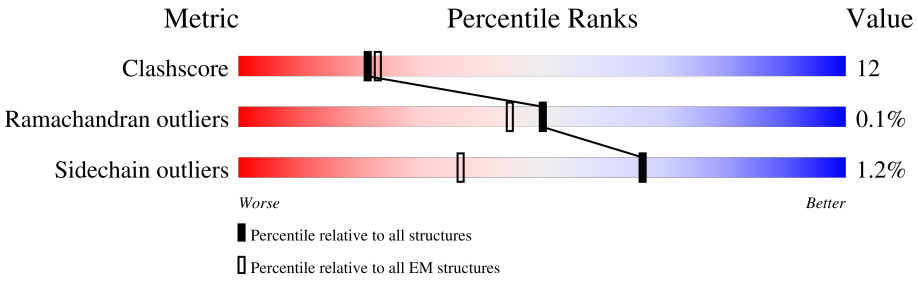
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.56 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	I	149	5% 52% 40%
1	J	149	5% 58% 34%
1	K	149	6% 56% 36%
1	L	149	6% 56% 36%
2	A	4967	10% 63% 21% 15%
2	B	4967	10% 63% 21% 15%
2	C	4967	10% 64% 21% 15%
2	D	4967	10% 63% 21% 15%

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Mol	Chain	Length	Quality of chain
3	E	108	
3	F	108	
3	G	108	
3	H	108	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 143464 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	J	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	L	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		
1	K	143	Total	C	N	O	S	0	0
			1131	694	182	246	9		

- Molecule 2 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	B	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	C	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		
2	D	4231	Total	C	N	O	S	2	0
			33849	21572	5764	6283	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

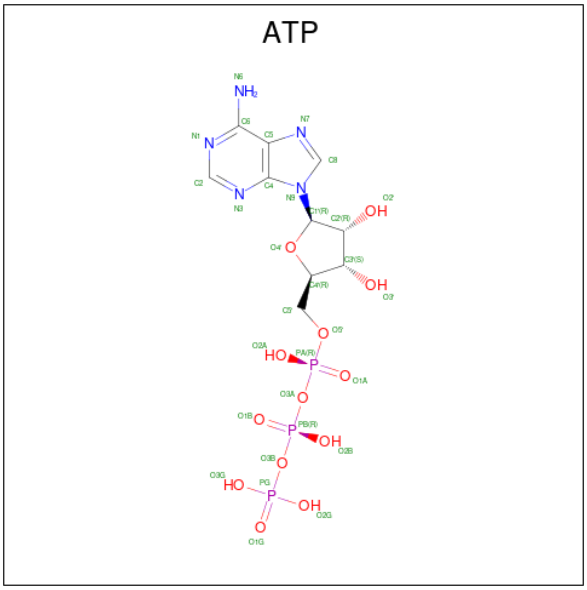
Mol	Chain	Residues	Atoms		AltConf
4	I	4	Total 4	Ca 4	0
4	A	1	Total 1	Ca 1	0
4	J	4	Total 4	Ca 4	0
4	L	4	Total 4	Ca 4	0
4	K	4	Total 4	Ca 4	0
4	B	1	Total 1	Ca 1	0
4	C	1	Total 1	Ca 1	0
4	D	1	Total 1	Ca 1	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 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).



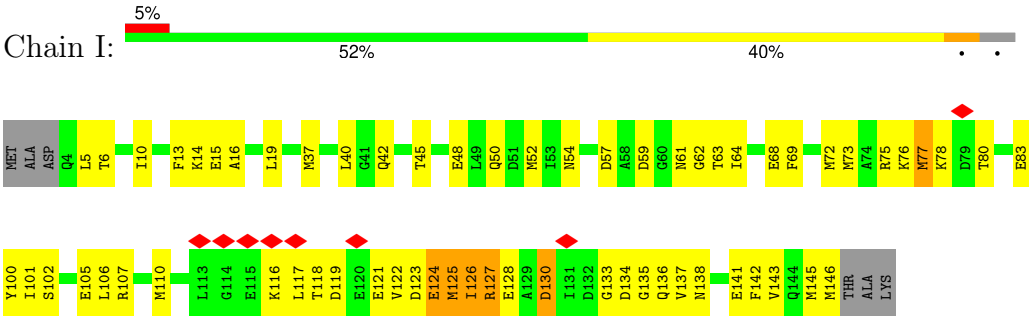
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

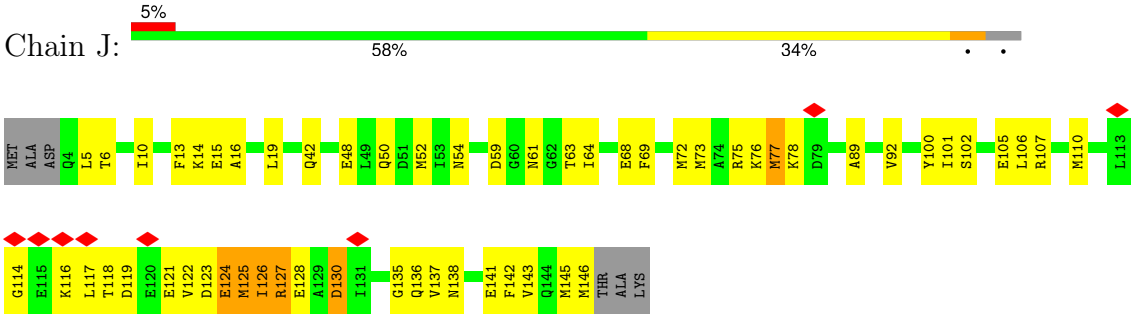
• Molecule 1: Calmodulin-1

Chain I:



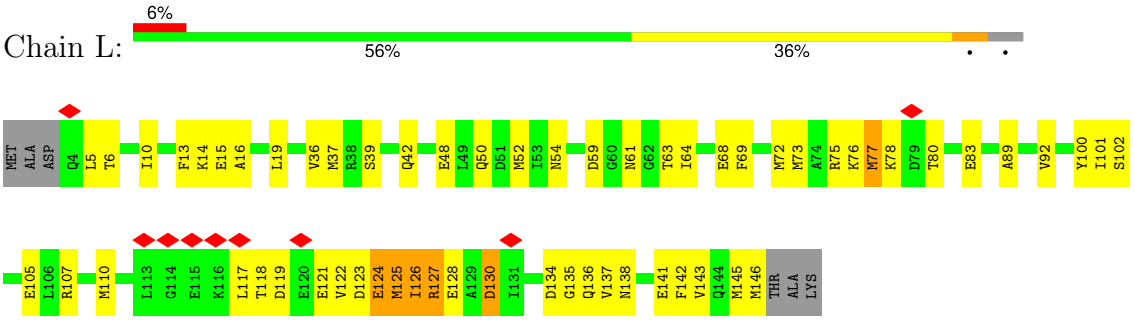
• Molecule 1: Calmodulin-1

Chain J:



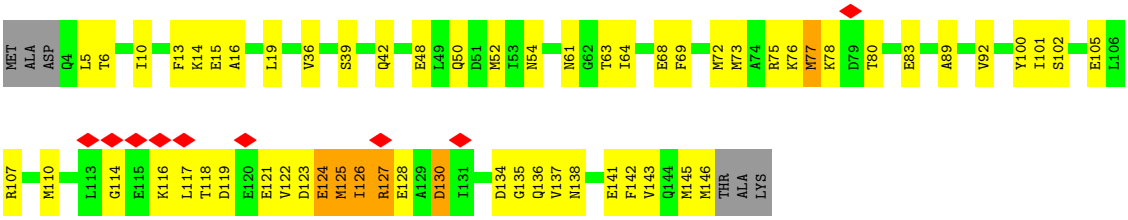
• Molecule 1: Calmodulin-1

Chain L:



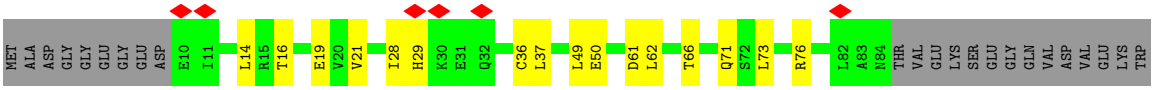
• Molecule 1: Calmodulin-1

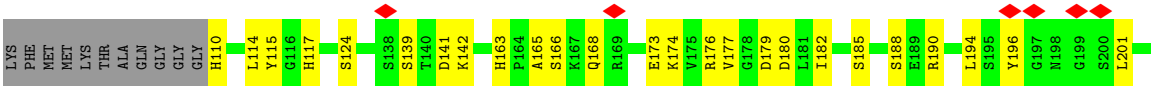
Chain K:

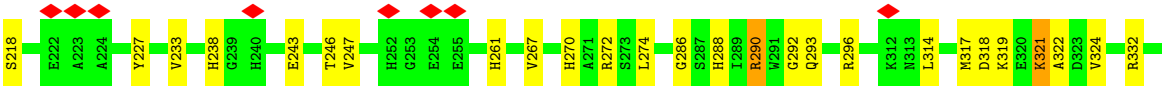


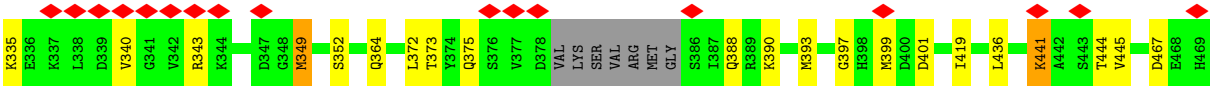
• Molecule 2: Ryanodine receptor 2

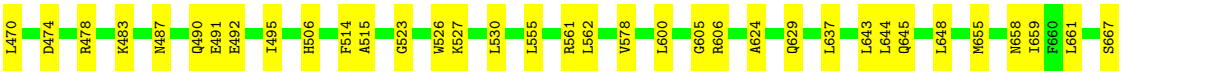
Chain A:

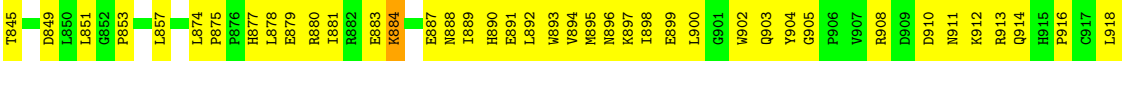


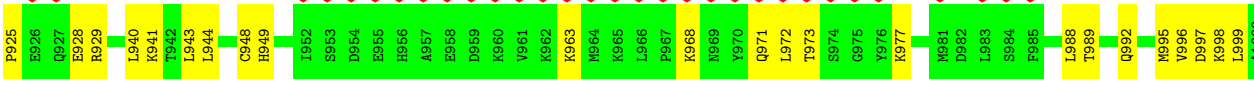


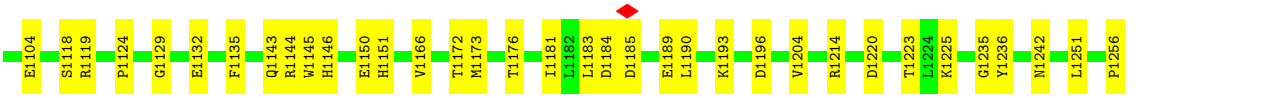


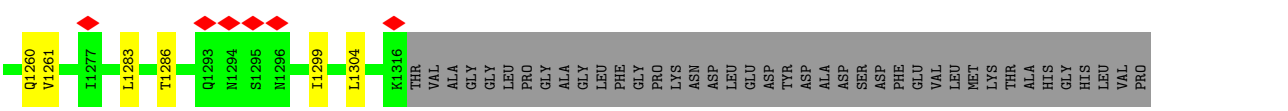


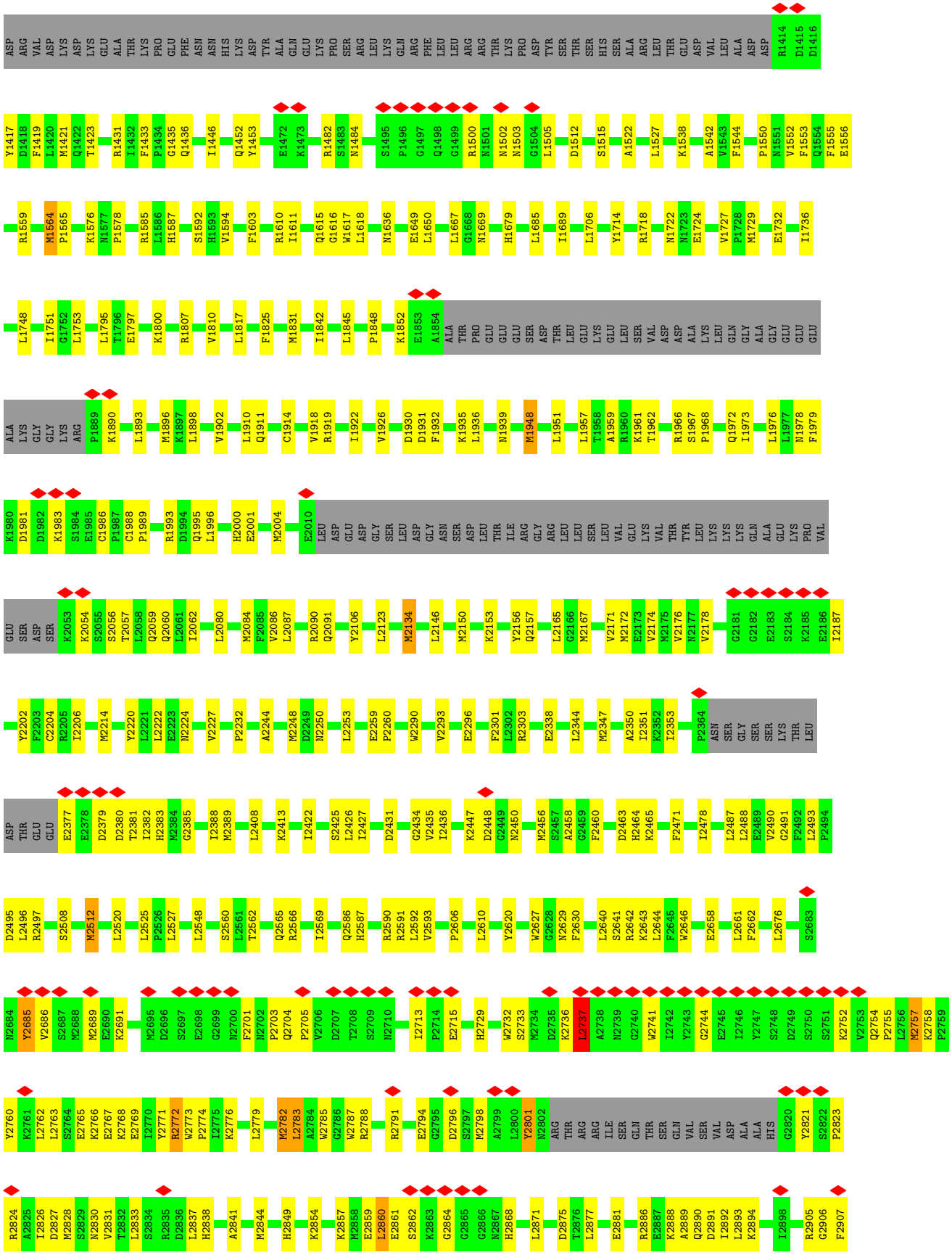


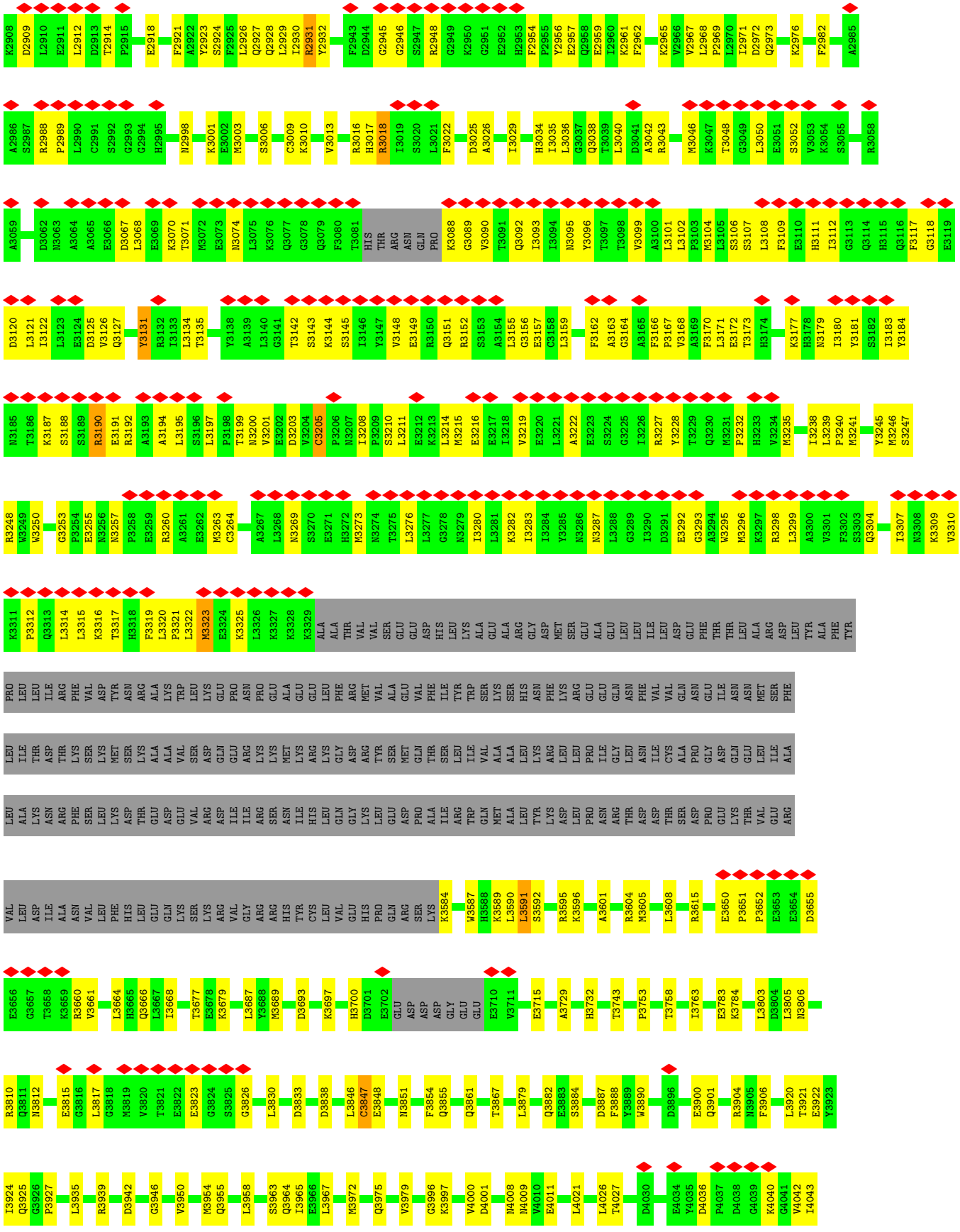








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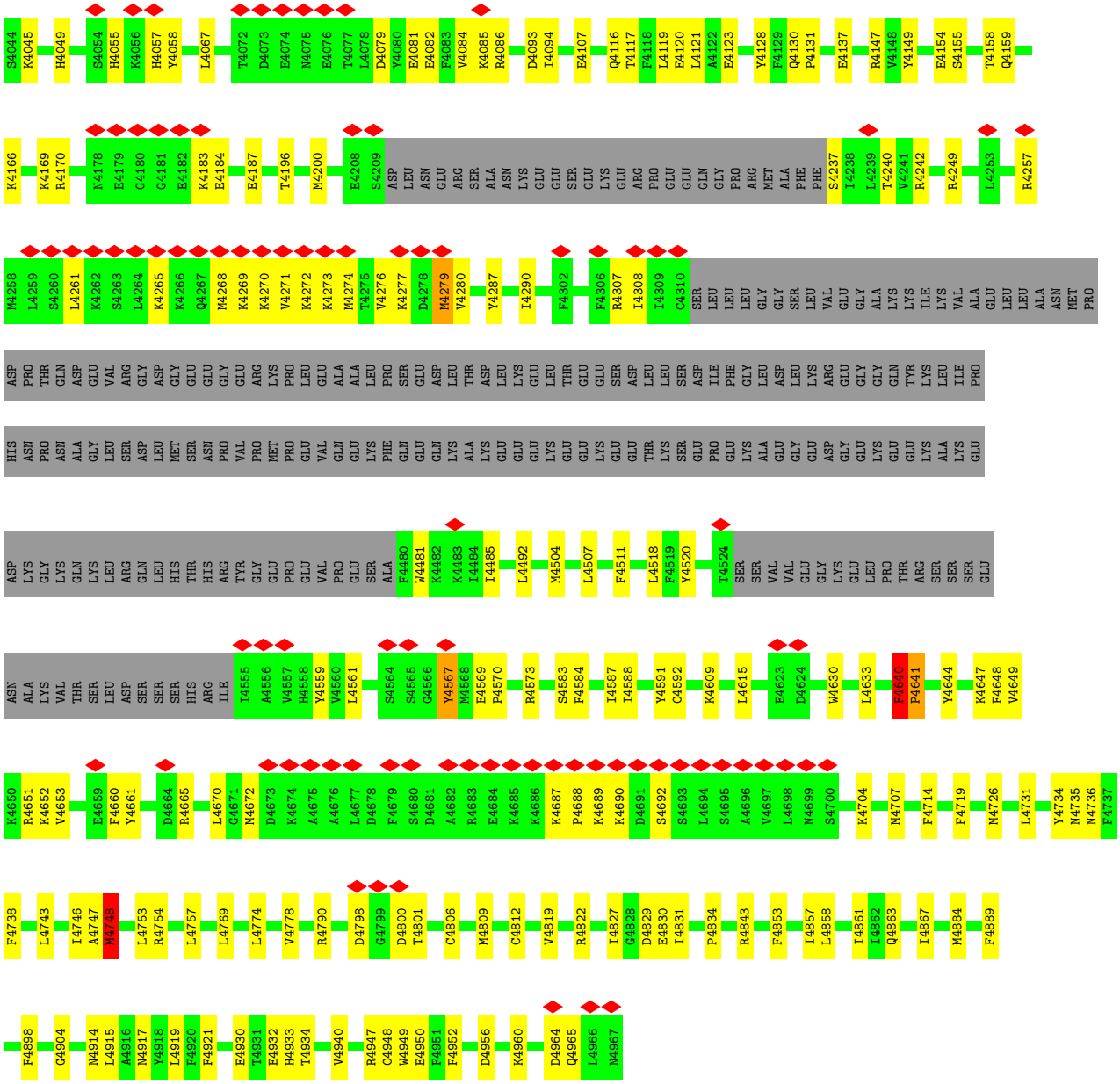
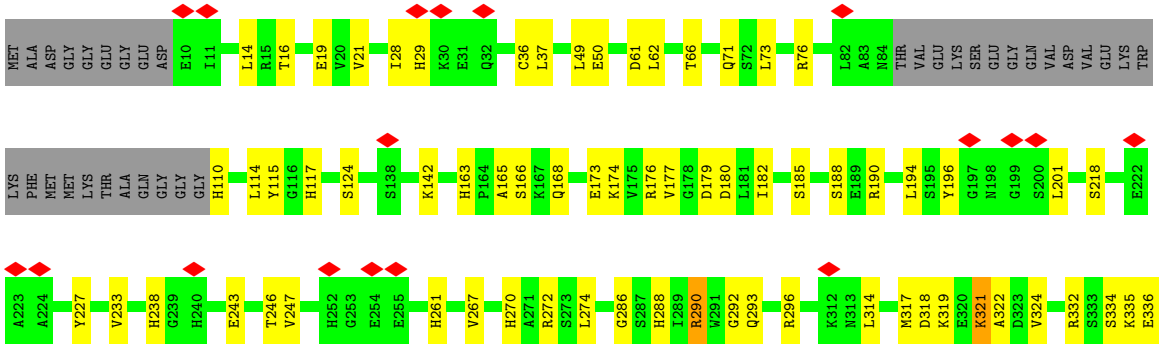
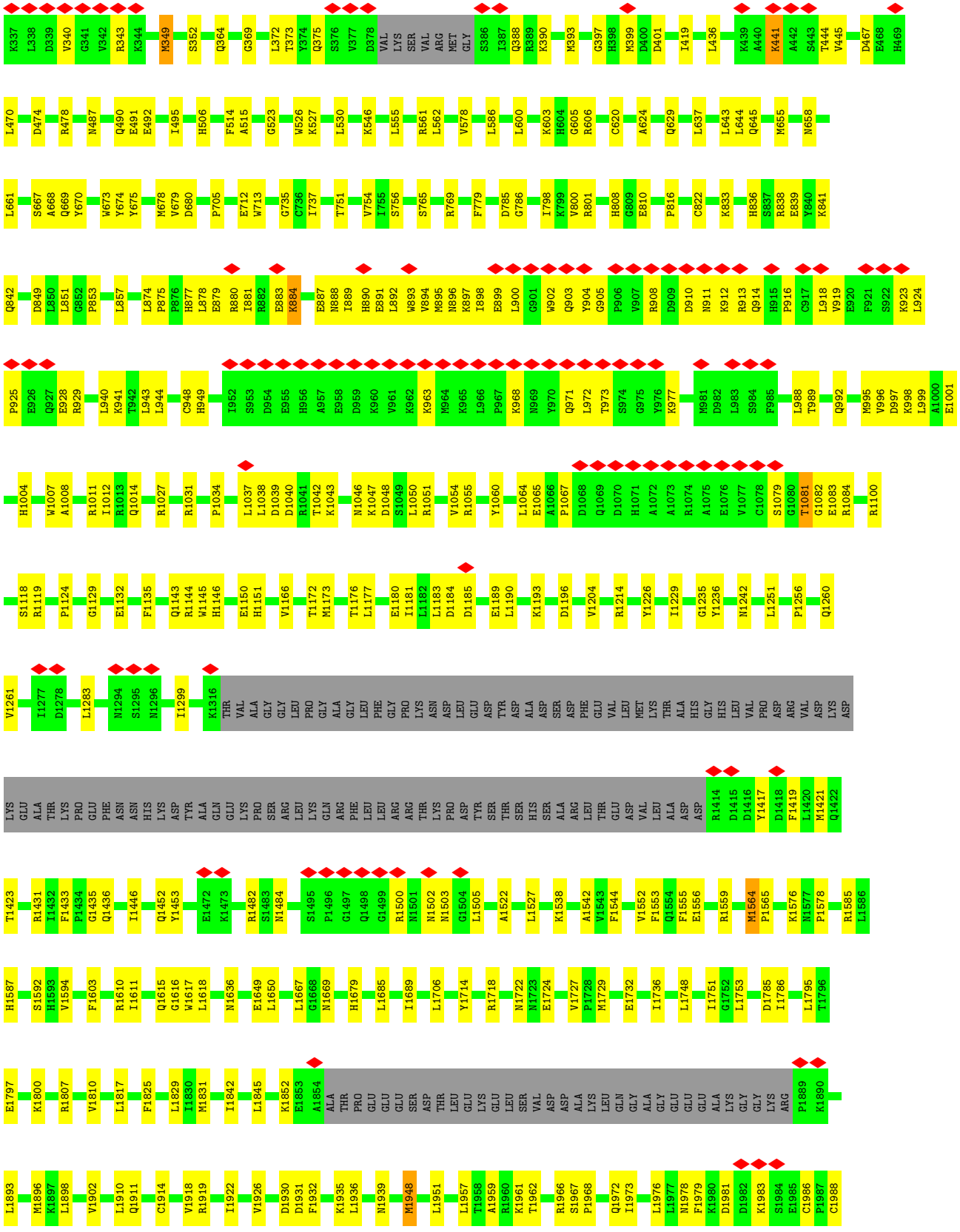
A2986 S2987 R2988 P2989 L2990 C2991 S2992 G2993 G2994 H2995 N2998 K3001 E3002 M3003 S3006 C3009 K3010 V3013 R3016 H3017 R3018 I3019 S3020 L3021 F3022 D3025 A3026 I3029 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 M3046 K3047 T3048 G3049 L3050 E3051 S3052 V3053 K3054 S3055 R3058
A3059 D3062 N3063 A3064 A3065 E3066 D3067 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 V3090 T3091 Q3092 I3093 T3094 N3095 Y3096 T3097 T3098 V3099 A3100 L3101 L3102 P3103 M3104 K3105 S3106 S3107 L3108 F3109 E3110 H3111 I3112 G3113 Q3114 H3115 Q3116 F3117 G3118 E3119
D3120 L3121 I3122 L3123 E3124 D3125 V3126 Q3127 Y3131 R3132 I3133 L3134 T3135 Y3138 A3139 L3140 G3141 T3142 S3143 K3144 S3145 I3146 Y3147 V3148 E3149 R3150 Q3151 R3152 S3153 A3154 L3155 G3156 E3157 C3158 L3159 F3162 A3163 G3164 A3165 F3166 P3167 V3168 A3169 F3170 L3171 E3172 T3173 H3174 K3177 H3178 N3179 I3180 Y3181 S3182 I3183 Y3184
N3185 T3186 K3187 S3188 S3189 R3190 E3191 R3192 A3193 A3194 L3195 S3196 L3197 P3198 T3199 N3200 V3201 E3202 D3203 V3204 C3205 P3206 N3207 I3208 P3209 S3210 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3220 L3221 A3222 E3223 S3224 G3225 I3226 R3227 Y3228 T3229 Q3230 M3231 P3232 H3233 V3234 M3235 I3238 L3239 P3240 M3241 Y3245 M3246 S3247
R3248 W3249 W3250 G3253 P3254 E3255 N3256 N3257 P3258 E3259 R3260 A3261 E3262 M3263 C3264 A3267 L3268 N3269 S3270 E3271 H3272 M3273 N3274 T3275 L3276 L3277 G3278 N3279 I3280 L3281 K3282 I3283 I3284 Y3285 N3286 N3287 L3288 G3289 I3290 D3291 E3292 G3293 A3294 W3295 M3296 K3297 R3298 L3299 A3300 V3301 F3302 S3303 Q3304 I3307 N3308 K3309 V3310
K3311 P3312 Q3313 L3314 L3315 K3316 T3317 H3318 F3319 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 K3328 K3329 ALA ALA THR VAL VAL SER GLU GLU GLY ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR
PRO LEU LEU ILE ARG PHE VAL ASP TYR 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 ASP 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 LYS THR VAL GLU LEU
LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP 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 LEU PRO ASN ARG THR ASP ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG
VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS K3584 W3587 H3588 K3589 L3590 L3591 S3592 R3595 K3596 A3601 R3604 M3605 L3608 R3615 E3650 P3651 P3652 E3653 E3654 D3655
E3656 G3657 T3658 K3659 R3660 V3661 L3664 H3665 Q3666 L3667 I3668 T3677 E3678 K3679 L3687 Y3688 M3689 D3693 K3697 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 V3711 E3715 A3729 H3732 T3743 P3753 T3758 I3763 E3783 K3784 L3803 D3804 L3805 N3806
R3810 Q3811 N3812 E3815 G3816 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 L3830 D3833 D3838 L3846 C3847 E3848 N3851 F3854 Q3855 Q3861 T3867 L3879 Q3882 E3883 S3884 D3887 F3888 Y3889 W3890 D3896 E3900 Q3901 R3904 N3905 F3906 L3920 T3921 E3922 Y3923
I3924 Q3925 G3926 P3927 L3935 R3939 D3942 G3946 V3950 M3954 Q3955 L3958 S3963 Q3964 I3965 E3966 L3967 M3972 Q3975 V3979 G3996 K3997 V4000 D4001 N4008 N4009 V4010 E4011 L4021 L4026 T4027 D4030 E4034 Y4035 D4036 P4037 D4038 G4039 K4040 G4041 V4042 I4043



• Molecule 2: Ryanodine receptor 2

Chain B:

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L470 D474 R478 N487 Q490 E491 E492 I495 H506 F514 A515 G523 W526 K527 L530 K646 L555 R561 L562 V578 L586 L600 K603 H604 G605 R606 C620 A624 Q629 L637 L643 L644 Q645 M655 N658
L661 S667 A668 Q669 Y670 W673 Y674 Y675 M678 V679 D680 P705 E712 W713 G735 C736 I737 T751 V754 I755 S756 S765 R769 F779 D785 G786 I798 K799 V800 R801 H808 G809 E810 P816 C822 K833 H836 S837 R838 E839 Y840 K841
Q842 D849 L850 L851 G852 P853 L857 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 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 L940 K941 T942 L943 L944 C948 H949 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 M981 D982 L983 S984 F985 L988 T989 Q992 M995 V996 D997 K998 L999 A1000 E1001
H1004 W1007 A1008 R1011 I1012 R1013 Q1014 R1027 R1031 P1034 L1037 L1038 D1039 D1040 R1041 T1042 K1043 N1046 K1047 D1048 S1049 L1050 R1051 V1054 R1055 Y1060 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 R1100
S1118 R1119 P1124 G1129 E1132 F1135 Q1143 R1144 W1145 H1146 E1150 H1151 V1166 T1172 M1173 T1176 L1177 E1180 I1181 L1182 L1183 D1184 D1185 E1189 L1190 K1193 D1196 V1204 R1214 Y1226 I1229 G1235 Y1236 N1242 L1251 P1256 Q1260
V1261 I1277 D1278 L1283 N1294 S1295 N1296 I1299 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 R1414 D1415 D1416 Y1417 D1418 F1419 L1420 M1421 Q1422
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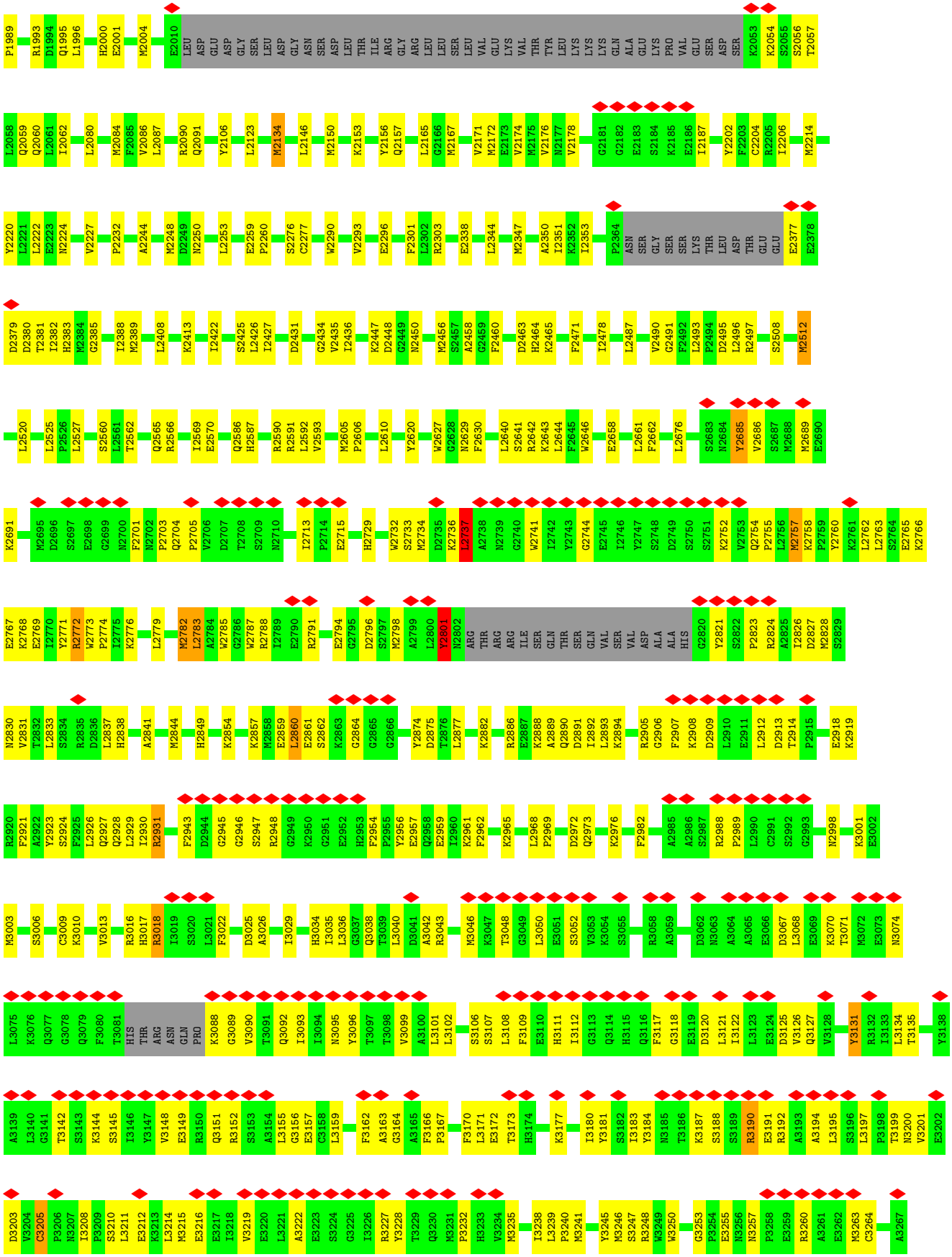
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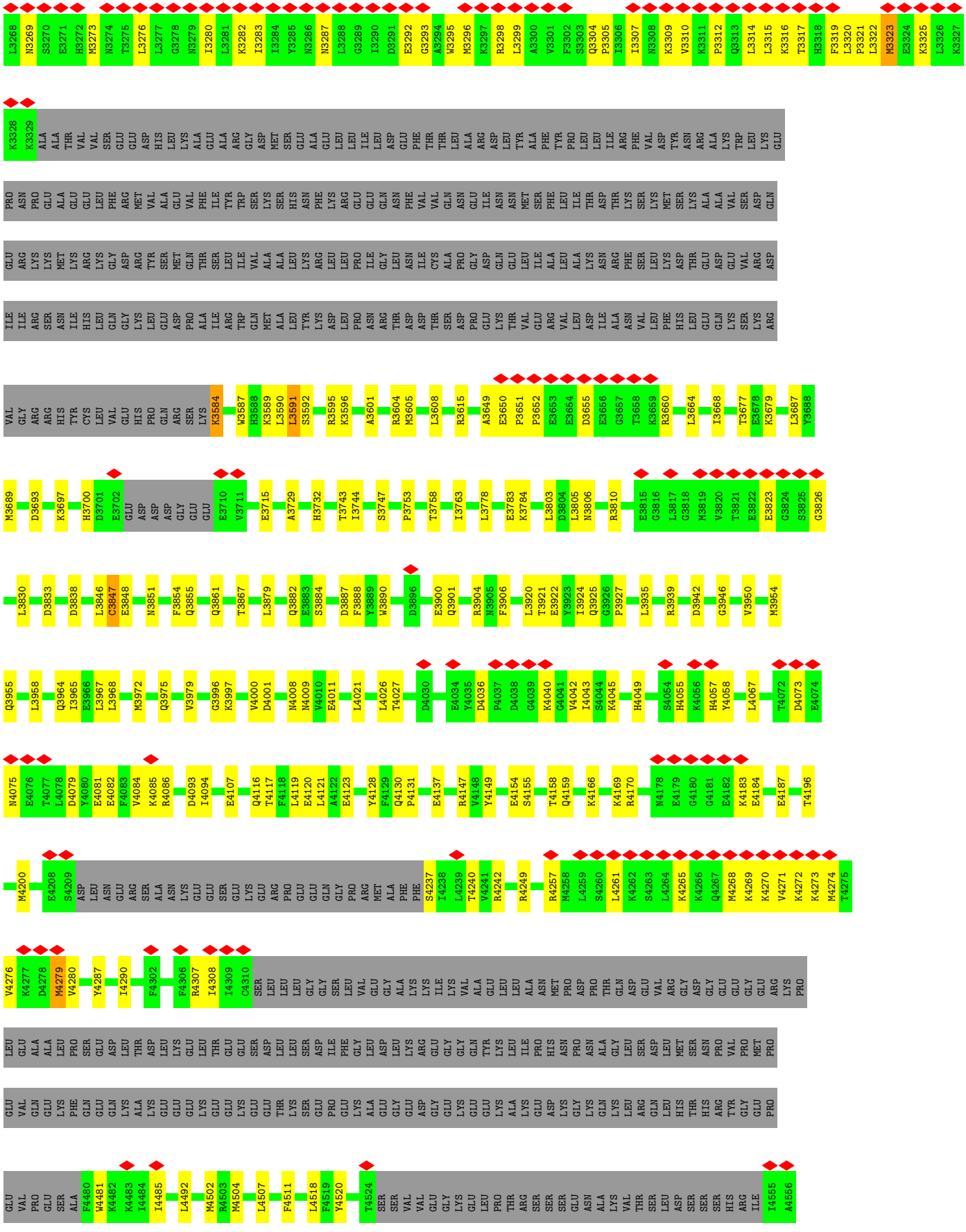
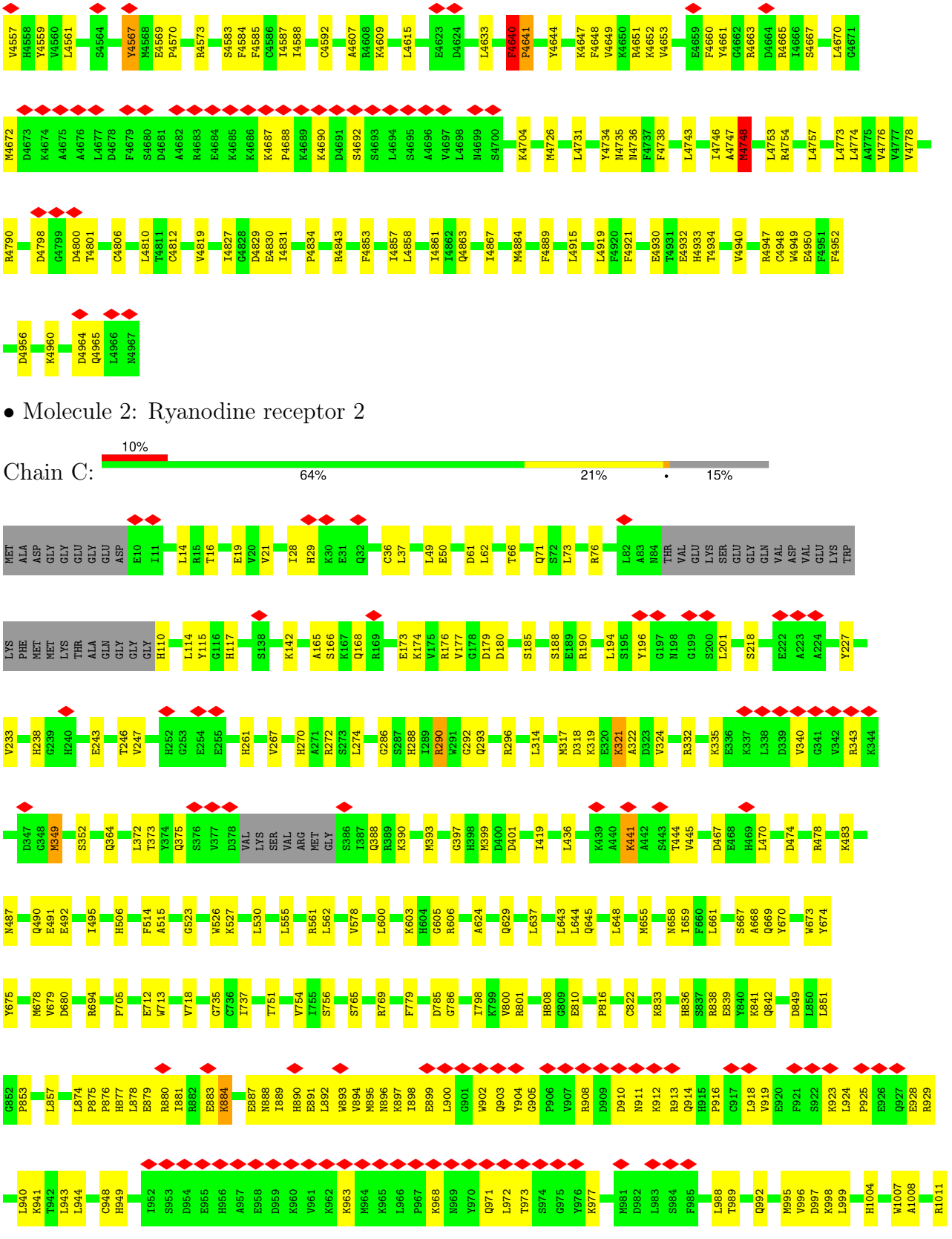
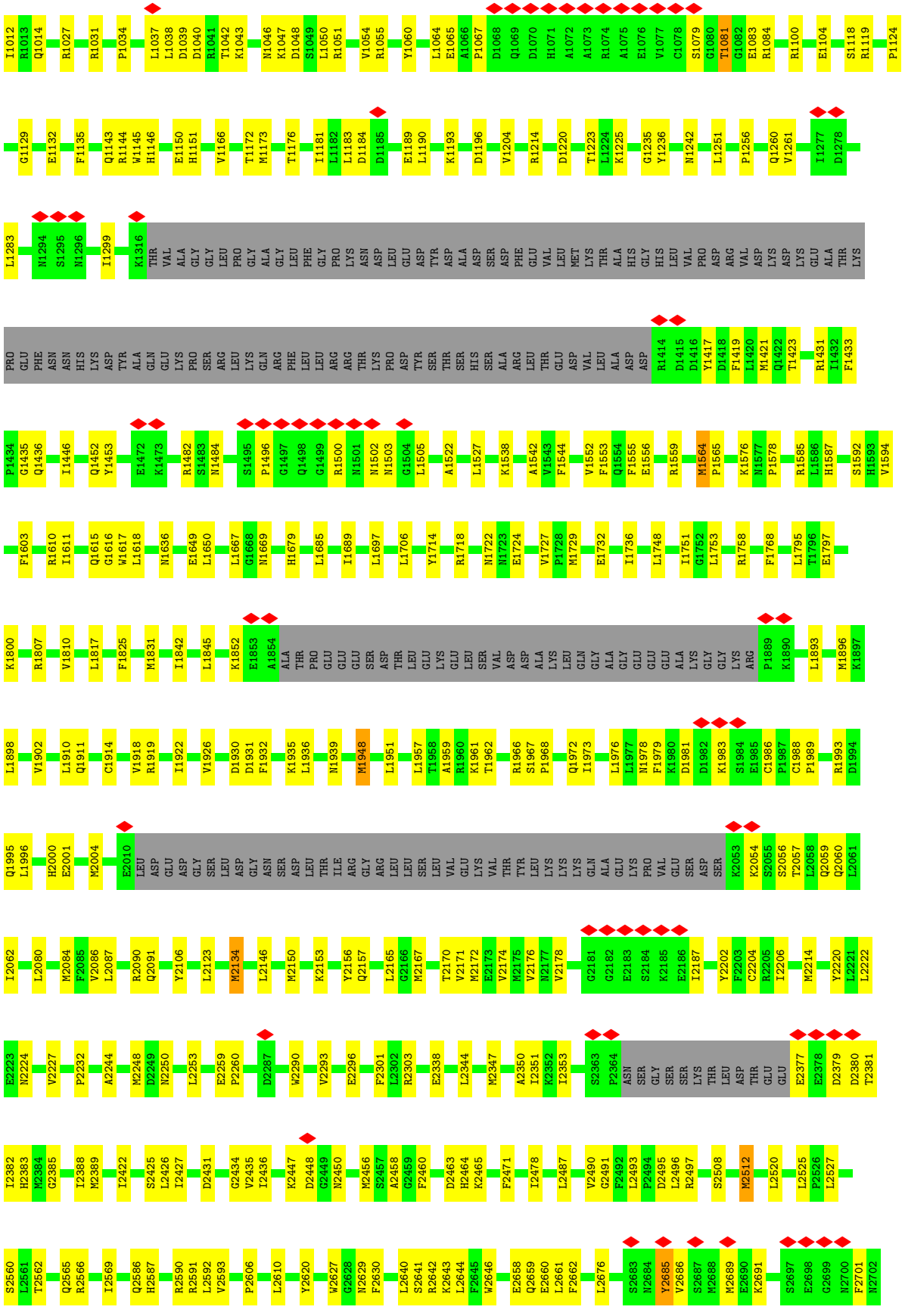




• Molecule 2: Ryanodine receptor 2

Chain C: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PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER THR HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 F1419 L1420 M1421 Q1422 T1423 R1431 I1432 F1433
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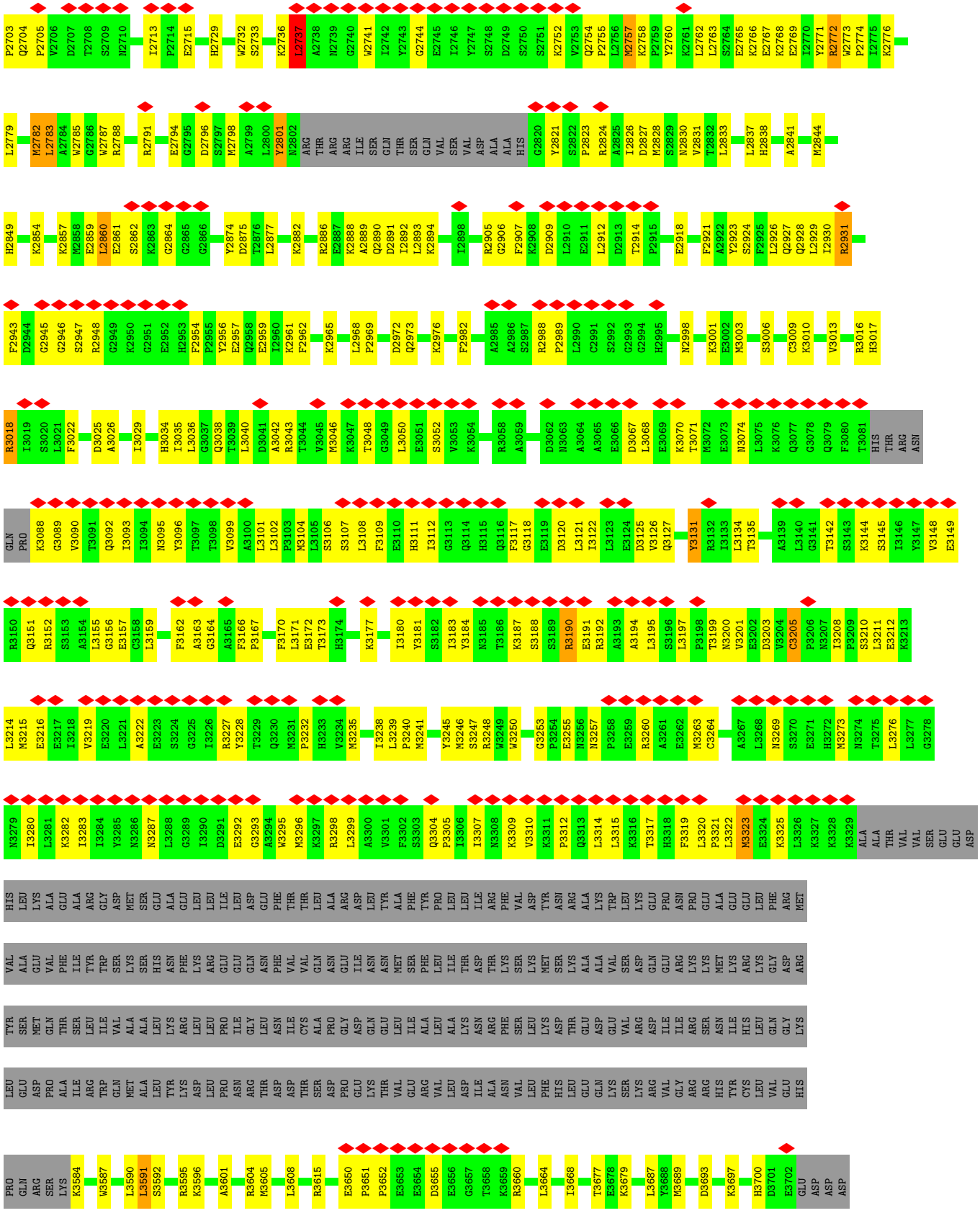
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HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA ALA LYS TRP LEU LYS GLU PRO ASN ARG LYS LYS PRO GLU ALA LYS SER GLU LEU LEU PHE ARG MET
VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN ASN PHE VAL VAL GLN ASN ARG ILE ASN ASN MET SER PHE LEU ILE 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 ARG SER ASN ILE HIS LEU GLU GLN LYS SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU GLY LYS
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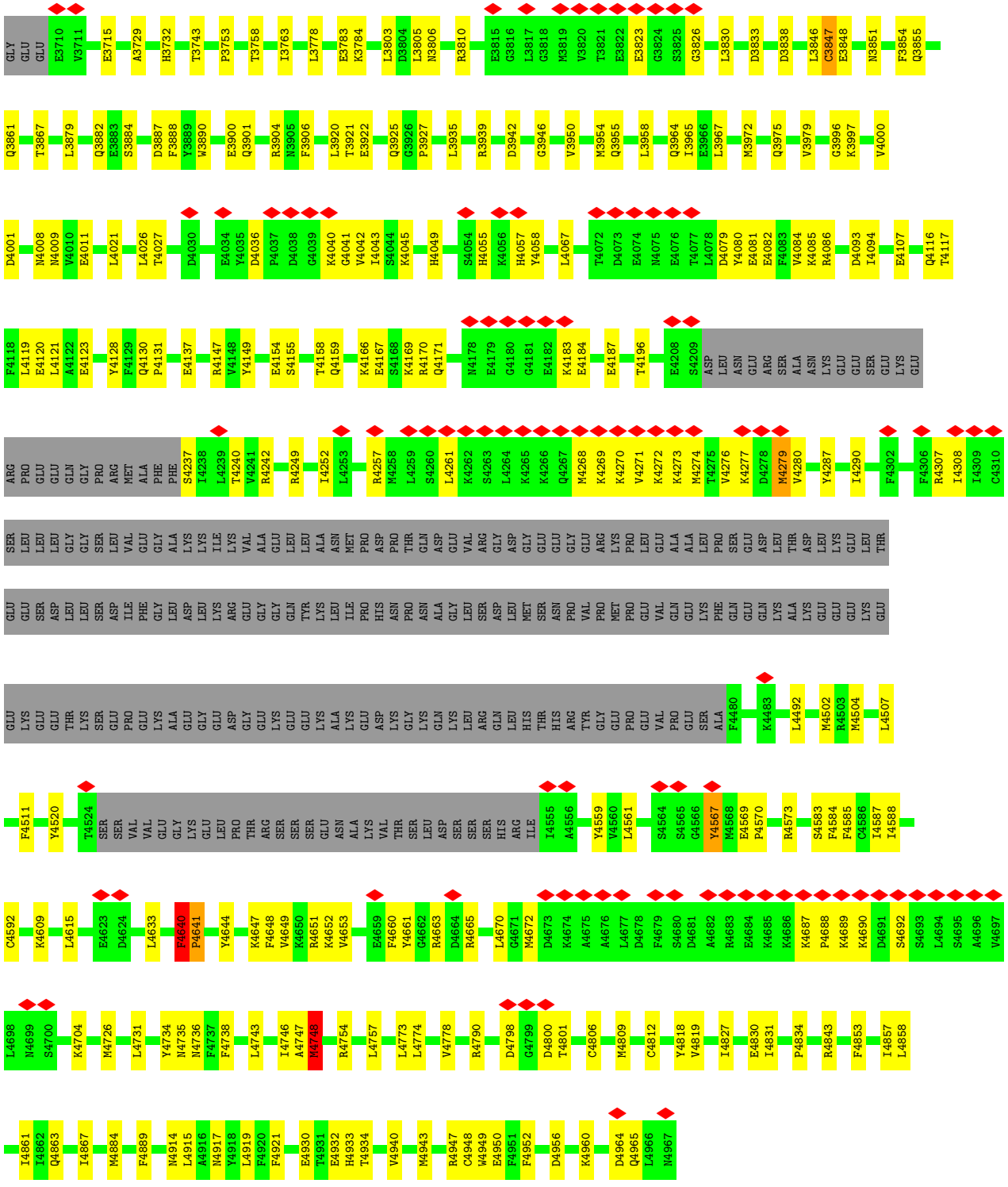
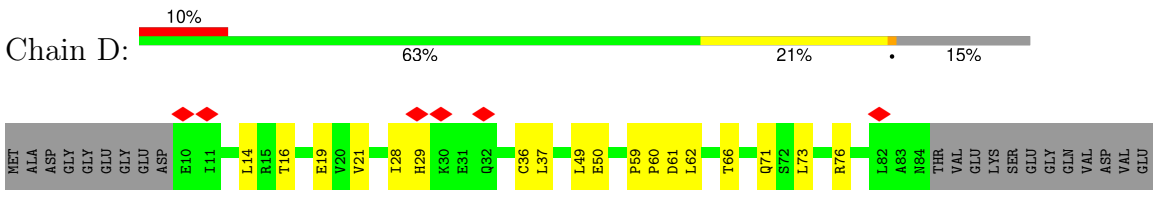
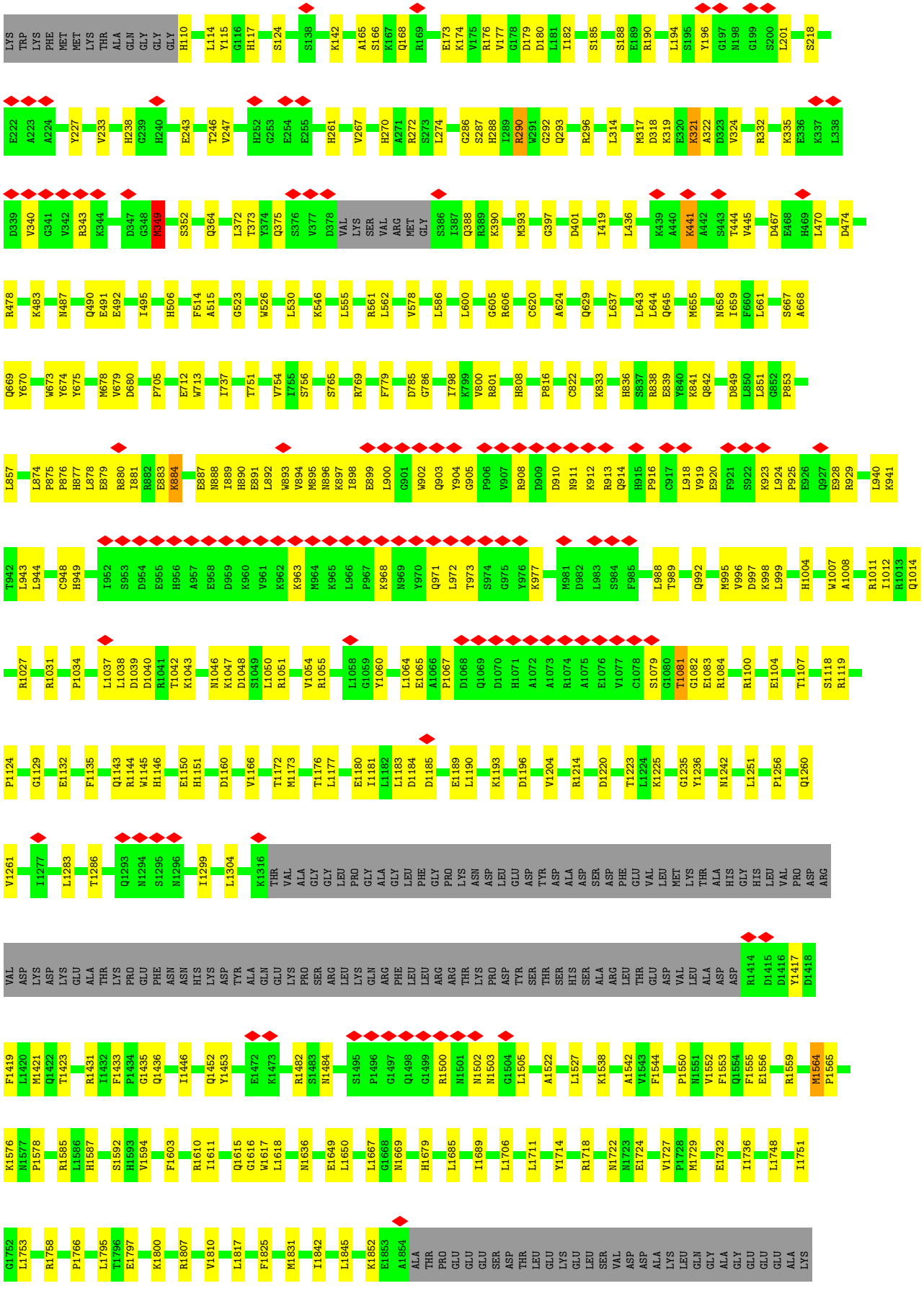


• Molecule 2: Ryanodine receptor 2

Chain D:

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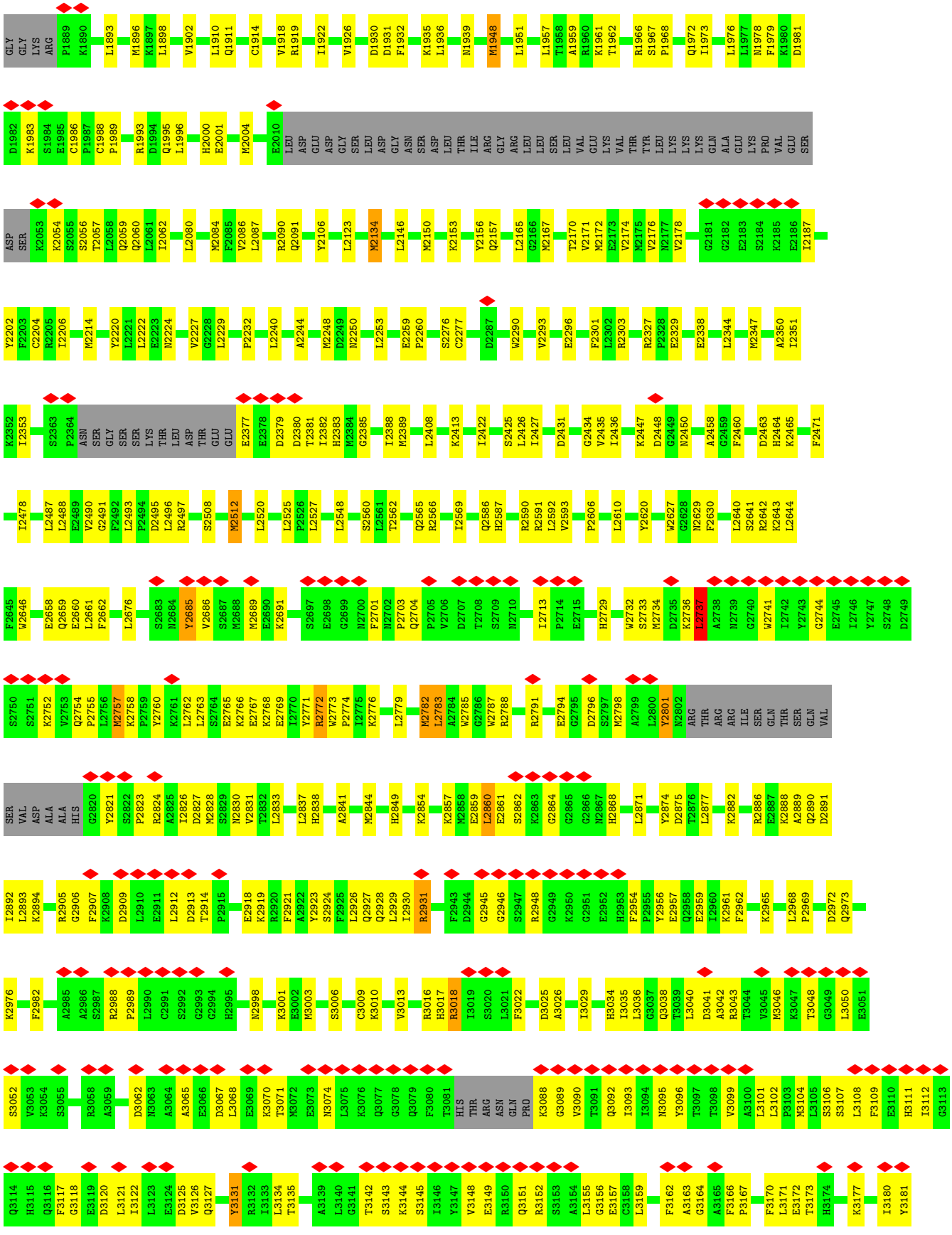
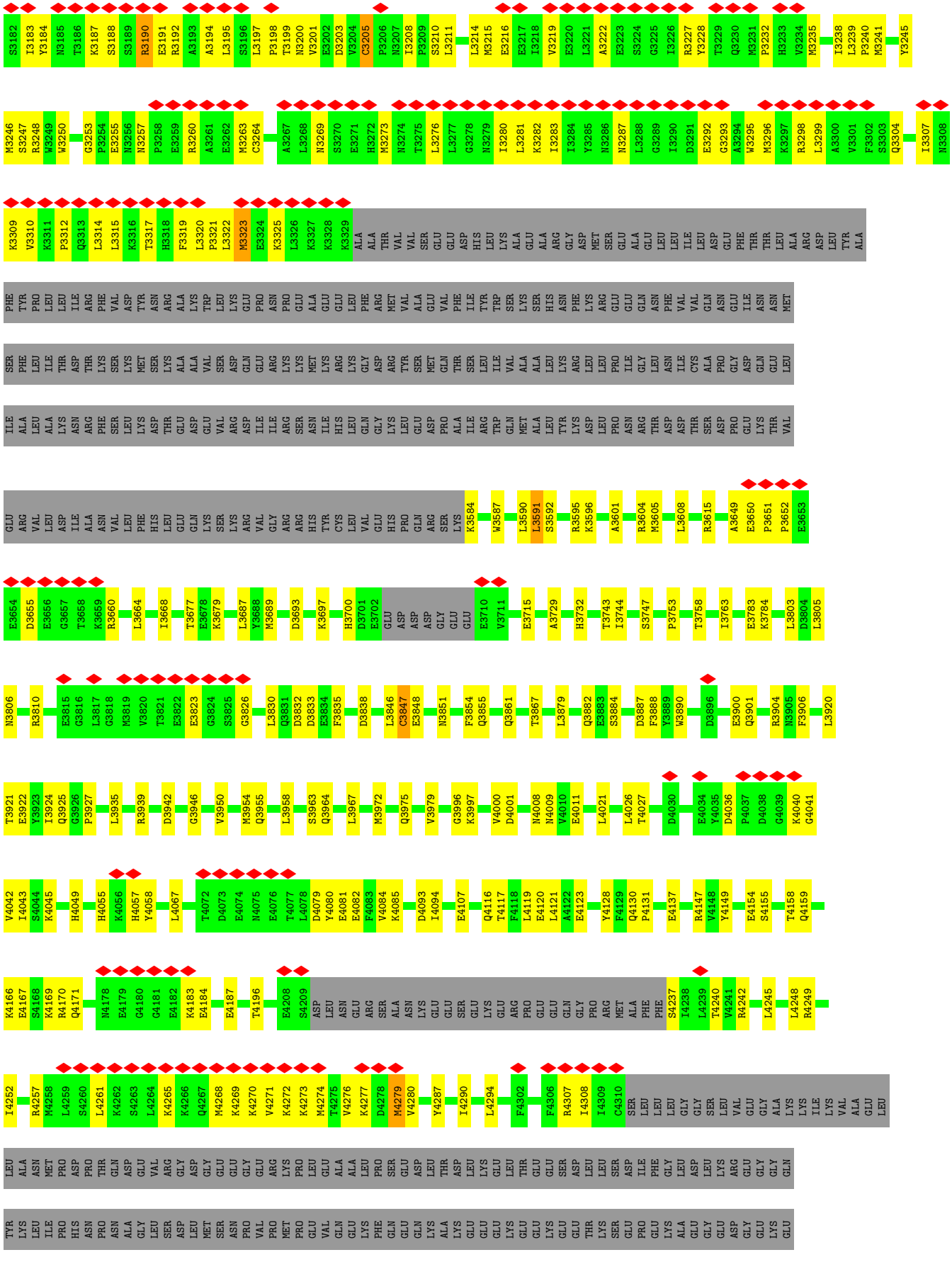
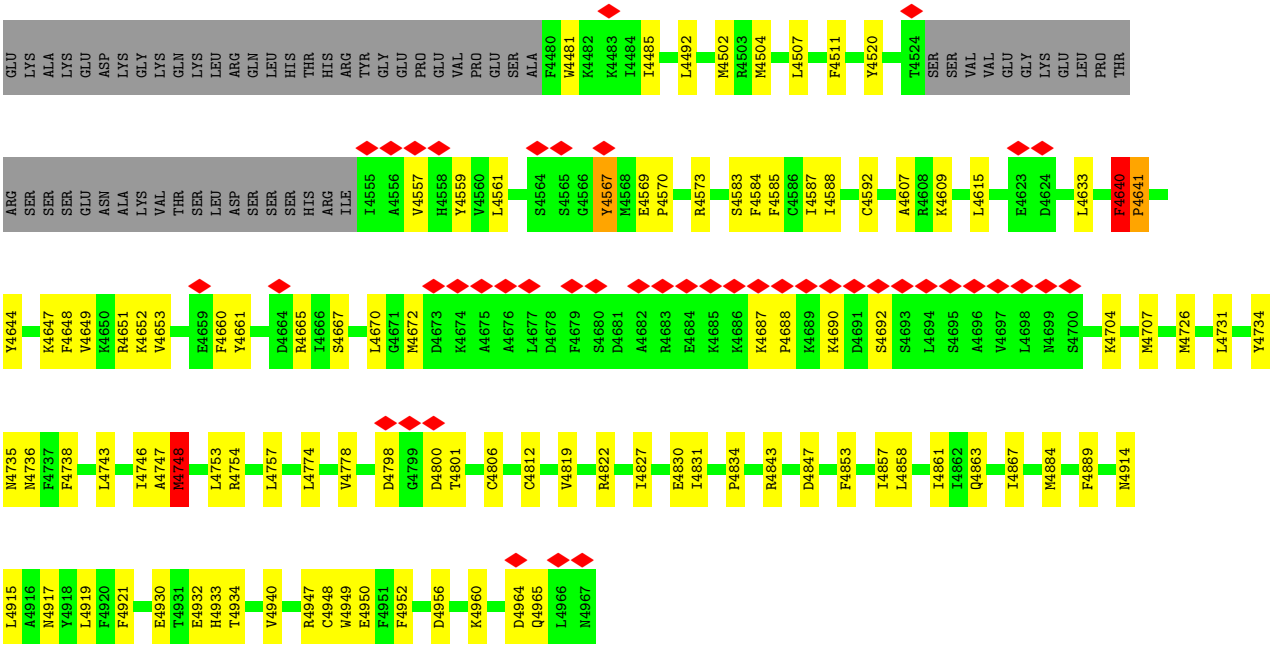
R1027 R1031 P1034 L1037 L1038 D1039 D1040 R1041 T1042 K1043 N1046 K1047 D1048 S1049 L1050 R1051 V1054 R1055 L1058 G1059 Y1060 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 R1100 E1104 T1107 S1118 R1119
P1124 G1129 E1132 F1135 Q1143 R1144 W1145 H1146 E1150 H1151 D1160 V1166 T1172 M1173 T1176 L1177 E1180 I1181 L1182 L1183 D1184 D1185 E1189 L1190 K1193 D1196 V1204 R1214 D1220 T1223 L1224 K1225 G1235 Y1236 N1242 L1251 P1256 Q1260
V1261 I1277 L1283 T1286 Q1293 N1294 S1295 N1296 I1299 L1304 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 D1416 Y1417 D1418
F1419 L1420 M1421 Q1422 T1423 R1431 T1432 F1433 P1434 G1435 Q1436 I1446 Q1452 Y1453 E1472 K1473 R1482 S1483 N1484 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 G1504 L1505 A1522 L1527 K1538 A1542 Y1543 F1544 P1550 N1581 V1552 F1553 Q1584 F1555 E1556 R1559 M1564 P1565
K1576 N1577 P1578 R1585 L1586 H1587 S1592 H1593 V1594 F1603 R1610 I1611 Q1615 G1616 W1617 L1618 N1636 E1649 L1650 L1667 G1668 N1669 H1679 L1685 I1689 L1706 L1711 Y1714 R1718 N1722 N1723 E1724 V1727 P1728 M1729 E1732 I1736 L1748 I1751
G1752 L1753 R1758 P1766 L1795 T1796 E1797 K1800 R1807 V1810 L1817 F1825 M1831 I1842 L1845 K1852 E1853 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







• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

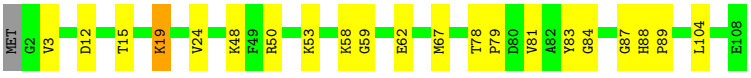
Chain E:

• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:

• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49606	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)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.594	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	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, 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	I	0.30	0/1143	0.58	1/1534 (0.1%)
1	J	0.30	0/1143	0.58	1/1534 (0.1%)
1	K	0.30	0/1143	0.58	1/1534 (0.1%)
1	L	0.30	0/1143	0.58	1/1534 (0.1%)
2	A	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	B	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	C	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
2	D	0.69	7/34594 (0.0%)	0.51	8/46723 (0.0%)
3	E	0.29	0/834	0.54	0/1123
3	F	0.28	0/834	0.53	0/1123
3	G	0.28	0/834	0.54	0/1123
3	H	0.28	0/834	0.54	0/1123
All	All	0.68	28/146284 (0.0%)	0.51	36/197520 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	B	0	2
2	C	0	2
2	D	0	2
All	All	0	8

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3205	CYS	CB-SG	105.30	3.61	1.82
2	B	3205	CYS	CB-SG	105.27	3.61	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3205	CYS	CB-SG	105.27	3.61	1.82
2	C	3205	CYS	CB-SG	105.21	3.61	1.82
2	B	3131	TYR	CD2-CE2	29.66	1.83	1.39

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3205	CYS	CA-CB-SG	12.07	135.73	114.00
2	A	3205	CYS	CA-CB-SG	12.06	135.71	114.00
2	D	3205	CYS	CA-CB-SG	12.05	135.68	114.00
2	B	3205	CYS	CA-CB-SG	12.04	135.68	114.00
2	D	2737	LEU	CA-CB-CG	7.16	131.77	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2801	TYR	Peptide
2	A	4640	PHE	Peptide
2	B	2801	TYR	Peptide
2	B	4640	PHE	Peptide
2	C	2801	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1131	0	1058	50	0
1	J	1131	0	1058	45	0
1	K	1131	0	1058	47	0
1	L	1131	0	1058	46	0
2	A	33849	0	33549	793	0
2	B	33849	0	33549	790	0
2	C	33849	0	33549	767	0
2	D	33849	0	33549	795	0
3	E	818	0	821	11	0
3	F	818	0	821	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	818	0	821	13	0
3	H	818	0	821	11	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	62	0	24	1	0
6	B	62	0	24	1	0
6	C	62	0	24	1	0
6	D	62	0	24	1	0
All	All	143464	0	141808	3297	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 3297 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:D:3131:TYR:CD1	2:D:3131:TYR:CE1	1.82	1.68
2:A:3131:TYR:CD1	2:A:3131:TYR:CE1	1.82	1.63
2:C:3131:TYR:CD2	2:C:3131:TYR:CE2	1.83	1.61
2:C:3131:TYR:CE1	2:C:3131:TYR:CD1	1.82	1.61
2:D:3131:TYR:CE2	2:D:3131:TYR:CD2	1.83	1.61

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	I	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	J	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	K	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	L	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	A	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	48	79
2	B	4205/4967 (85%)	4081 (97%)	119 (3%)	5 (0%)	48	79
2	C	4205/4967 (85%)	4082 (97%)	118 (3%)	5 (0%)	48	79
2	D	4205/4967 (85%)	4080 (97%)	120 (3%)	5 (0%)	48	79
3	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	H	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
All	All	17804/20896 (85%)	17292 (97%)	492 (3%)	20 (0%)	50	79

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3927	PRO
2	A	4641	PRO
2	B	3927	PRO
2	B	4641	PRO
2	C	3927	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	I	123/127 (97%)	112 (91%)	11 (9%)	8	32
1	J	123/127 (97%)	112 (91%)	11 (9%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	123/127 (97%)	112 (91%)	11 (9%)	8 32
1	L	123/127 (97%)	112 (91%)	11 (9%)	8 32
2	A	3715/4358 (85%)	3678 (99%)	37 (1%)	73 85
2	B	3715/4358 (85%)	3678 (99%)	37 (1%)	73 85
2	C	3715/4358 (85%)	3678 (99%)	37 (1%)	73 85
2	D	3715/4358 (85%)	3678 (99%)	37 (1%)	73 85
3	E	88/89 (99%)	87 (99%)	1 (1%)	70 84
3	F	88/89 (99%)	87 (99%)	1 (1%)	70 84
3	G	88/89 (99%)	87 (99%)	1 (1%)	70 84
3	H	88/89 (99%)	87 (99%)	1 (1%)	70 84
All	All	15704/18296 (86%)	15508 (99%)	196 (1%)	66 83

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3847	CYS
2	C	2783	LEU
2	B	4748	MET
2	C	1564	MET
2	C	3591	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	4933	HIS
2	D	3151	GLN
2	D	658	ASN
2	D	2540	HIS
2	D	4933	HIS

5.3.3 RNA

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 32 ligands modelled in this entry, 24 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	$\#\|Z\| > 2$
6	ATP	B	5004	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
6	ATP	B	5002	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)
6	ATP	D	5002	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)
6	ATP	A	5002	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)
6	ATP	D	5004	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
6	ATP	C	5002	-	28,33,33	0.75	0	34,52,52	0.75	1 (2%)
6	ATP	C	5004	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)
6	ATP	A	5004	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)

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	ATP	B	5004	-	-	11/18/38/38	0/3/3/3
6	ATP	B	5002	-	-	8/18/38/38	0/3/3/3
6	ATP	D	5002	-	-	8/18/38/38	0/3/3/3
6	ATP	A	5002	-	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	D	5004	-	-	11/18/38/38	0/3/3/3
6	ATP	C	5002	-	-	8/18/38/38	0/3/3/3
6	ATP	C	5004	-	-	11/18/38/38	0/3/3/3
6	ATP	A	5004	-	-	11/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	5002	ATP	C5-C6-N6	2.35	123.88	120.31
6	B	5002	ATP	C5-C6-N6	2.33	123.86	120.31
6	C	5002	ATP	C5-C6-N6	2.33	123.86	120.31
6	A	5004	ATP	C5-C6-N6	2.32	123.84	120.31
6	C	5004	ATP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	5002	ATP	C5'-O5'-PA-O1A
6	A	5002	ATP	C5'-O5'-PA-O2A
6	A	5002	ATP	C5'-O5'-PA-O3A
6	A	5004	ATP	PB-O3A-PA-O5'
6	A	5004	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

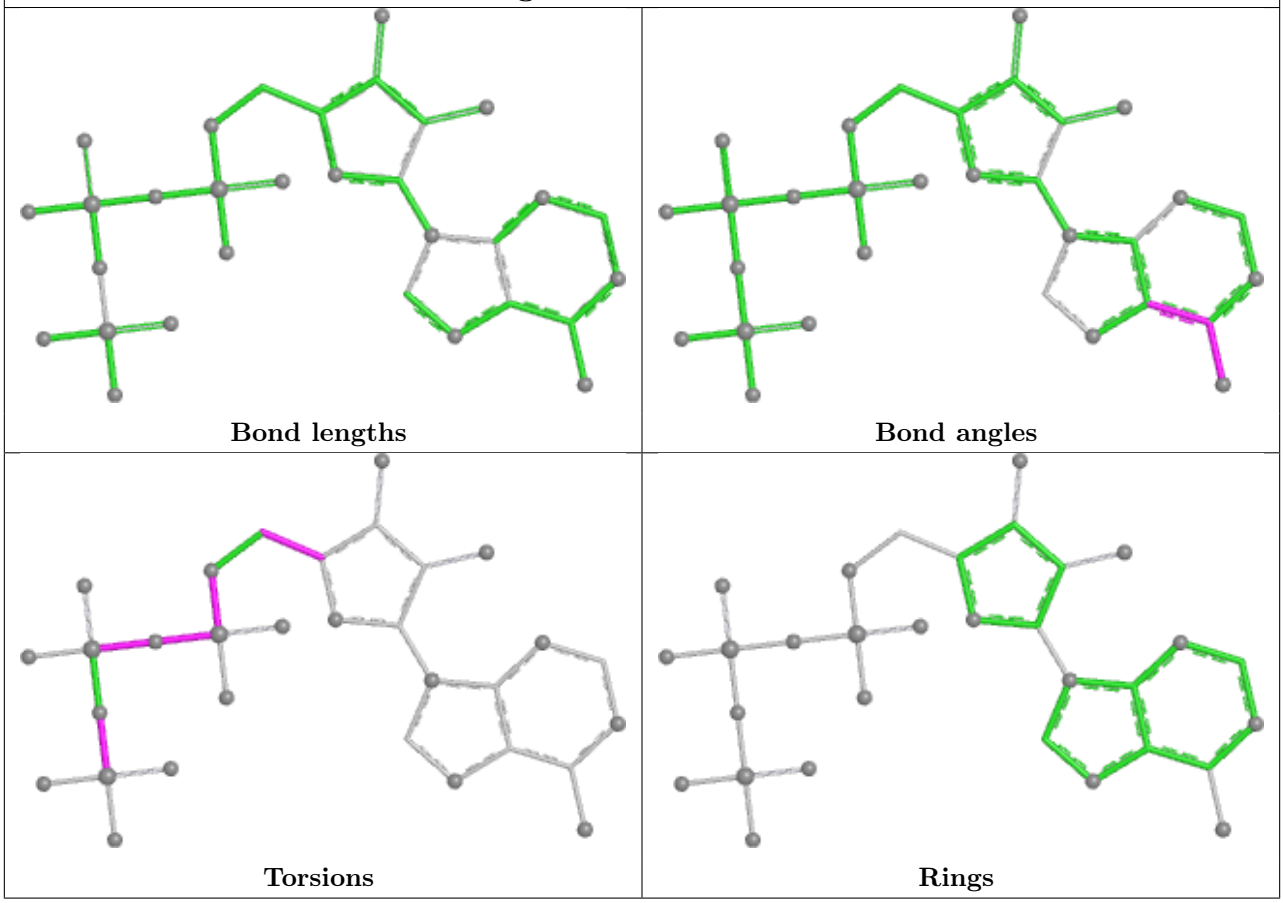
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	5004	ATP	1	0
6	D	5004	ATP	1	0
6	C	5004	ATP	1	0
6	A	5004	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

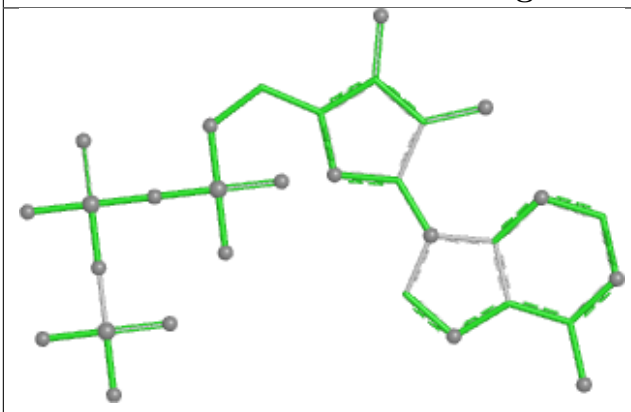
Ligand ATP B 5004



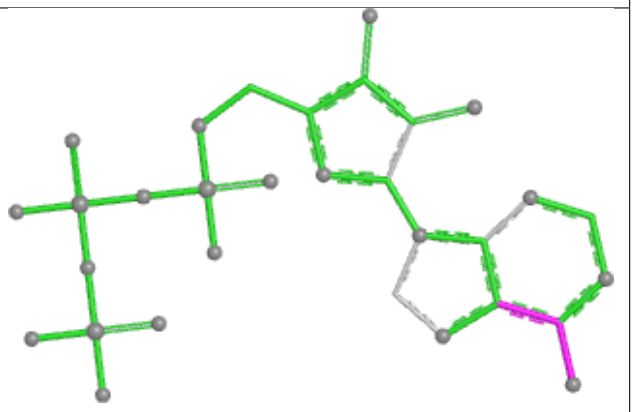
Bond lengths | **Bond angles**

Torsions | **Rings**

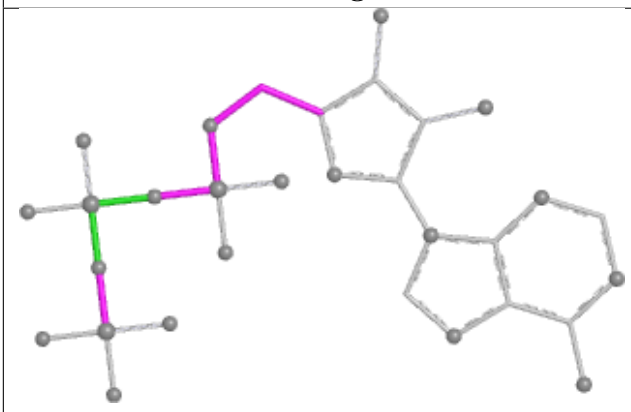
Ligand ATP B 5002



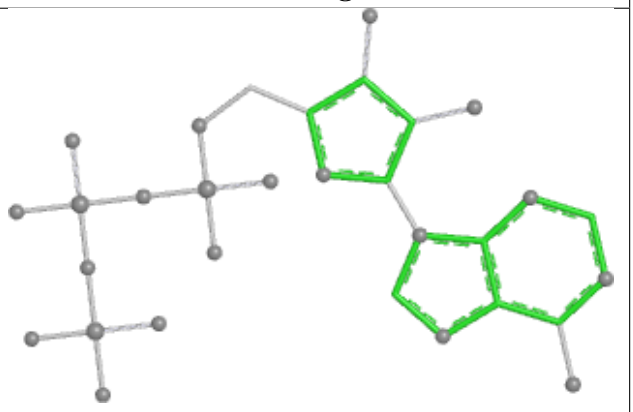
Bond lengths



Bond angles

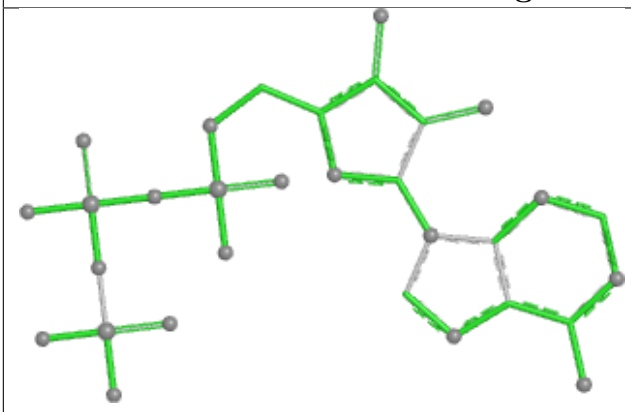


Torsions

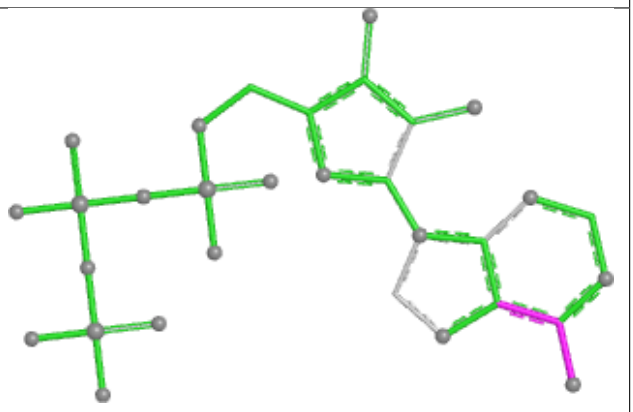


Rings

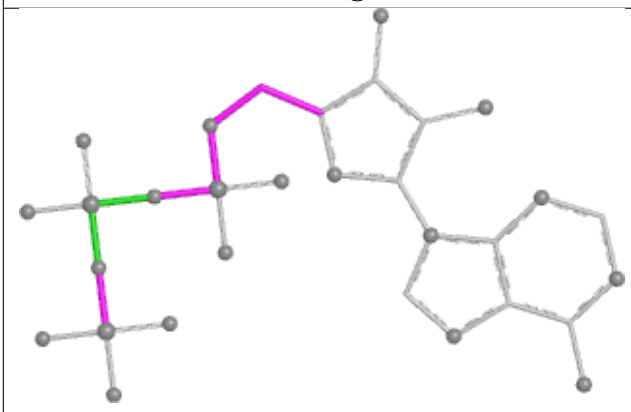
Ligand ATP D 5002



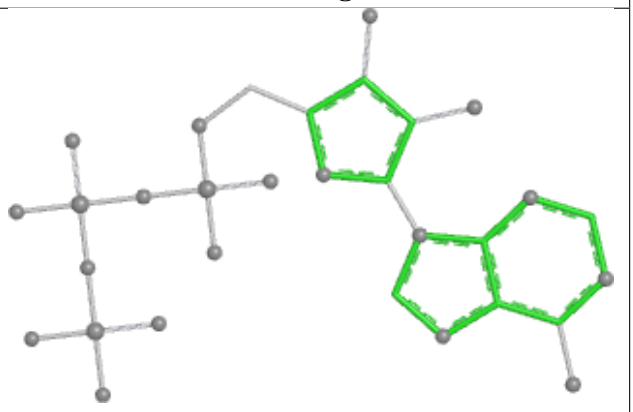
Bond lengths



Bond angles

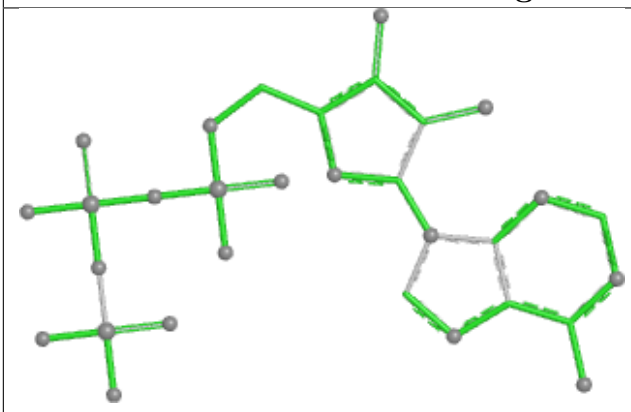


Torsions

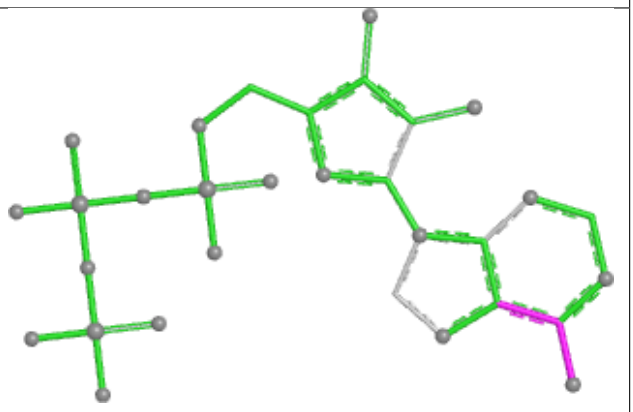


Rings

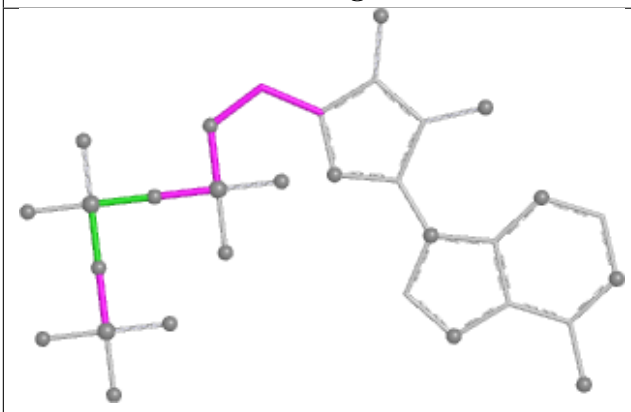
Ligand ATP A 5002



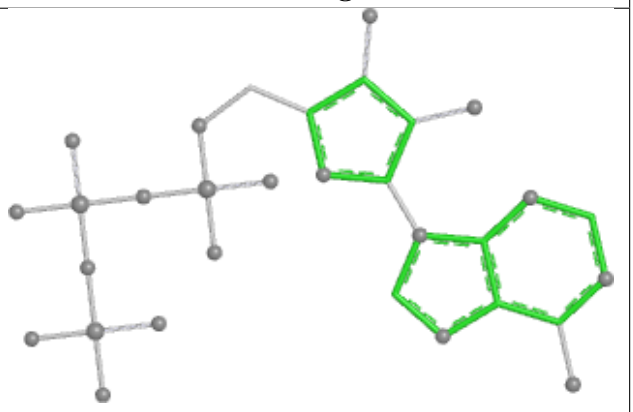
Bond lengths



Bond angles

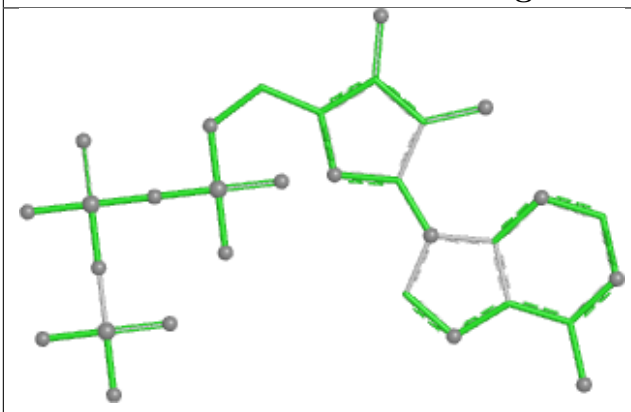


Torsions

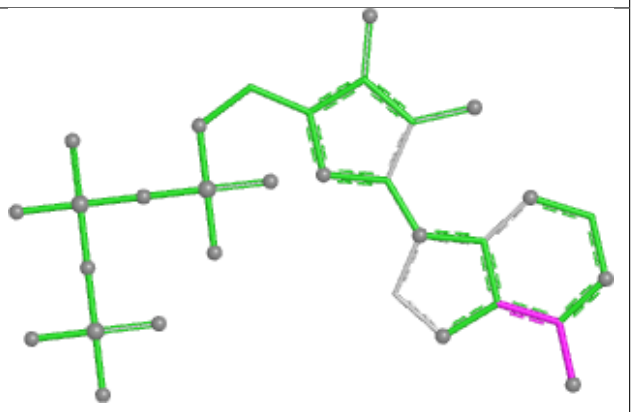


Rings

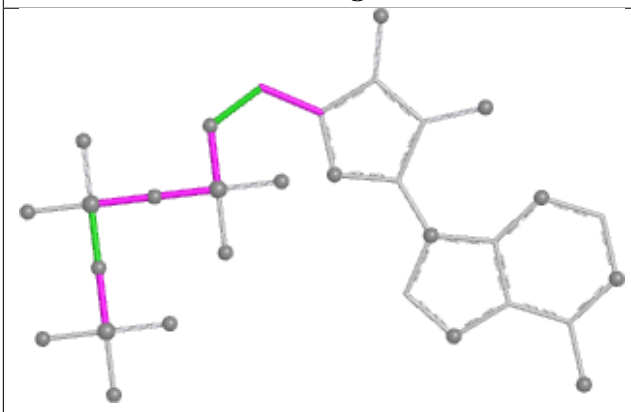
Ligand ATP D 5004



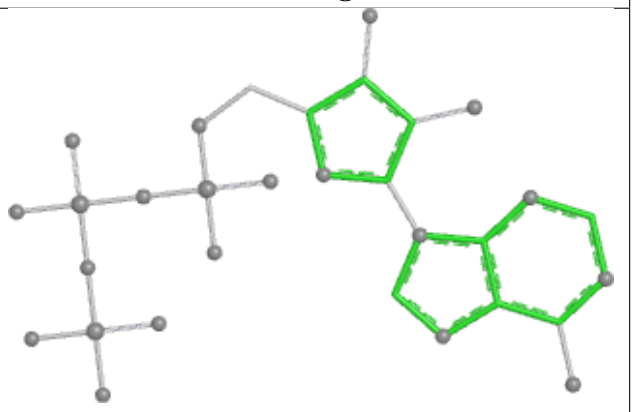
Bond lengths



Bond angles

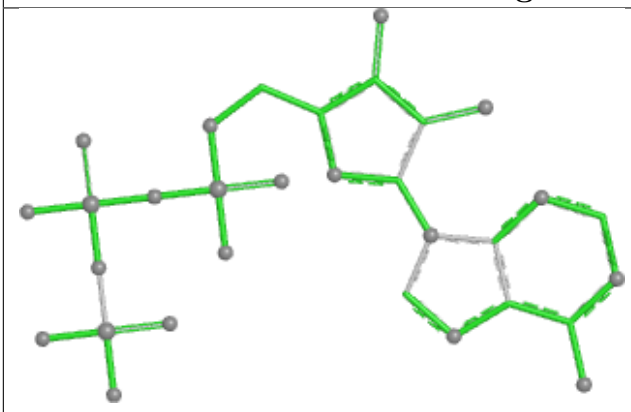


Torsions

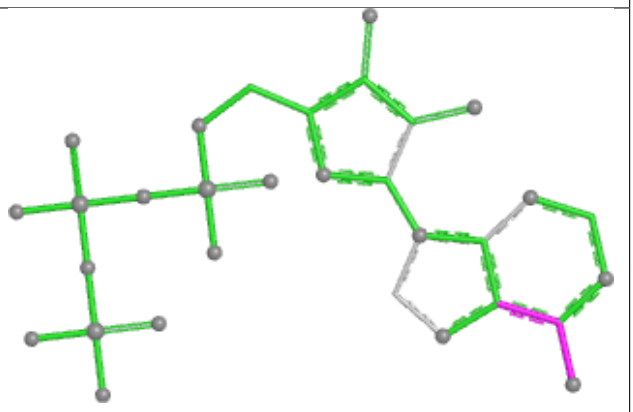


Rings

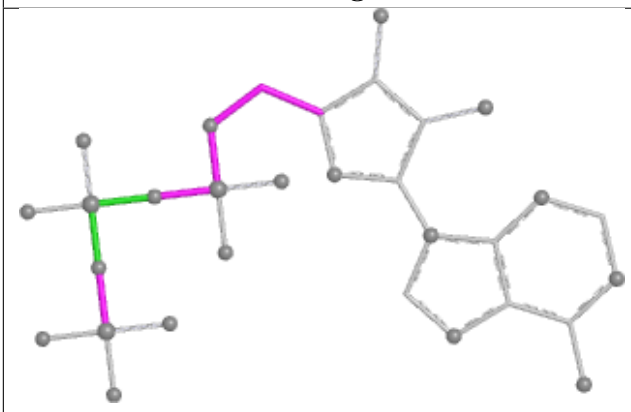
Ligand ATP C 5002



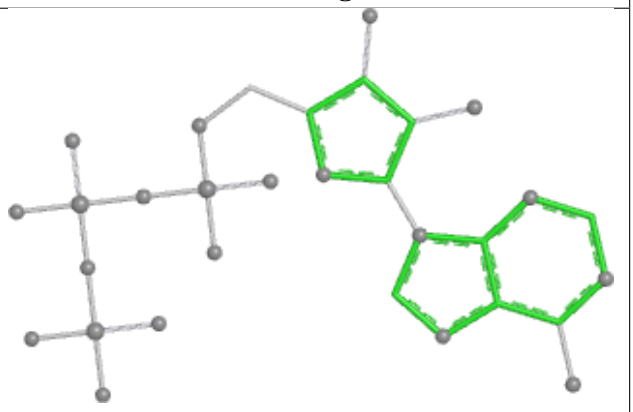
Bond lengths



Bond angles

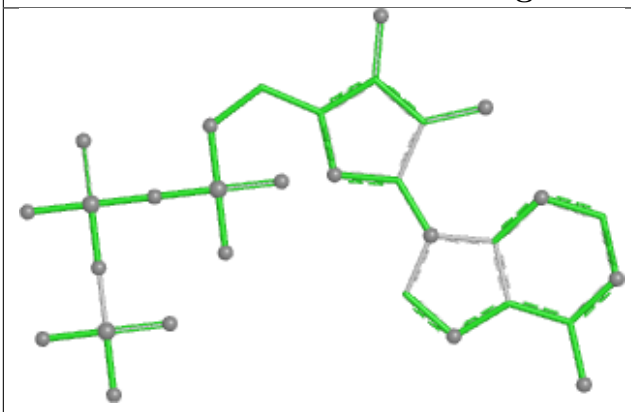


Torsions

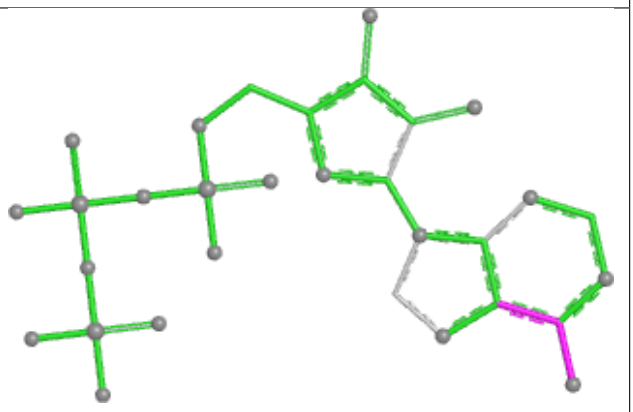


Rings

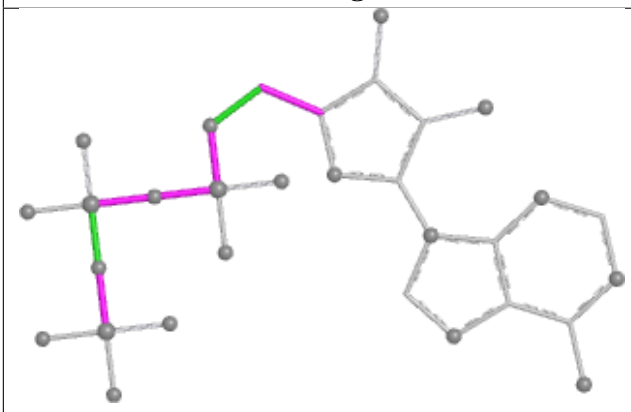
Ligand ATP C 5004



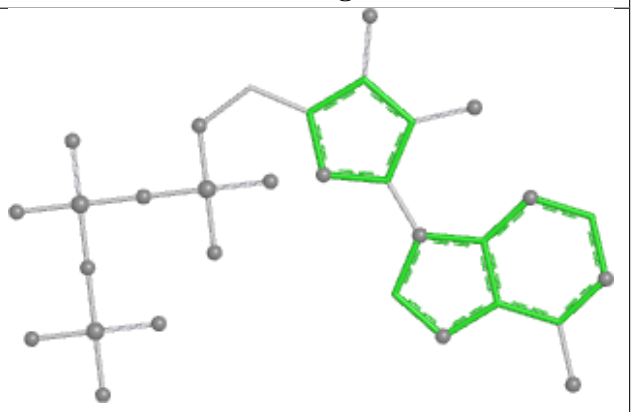
Bond lengths



Bond angles

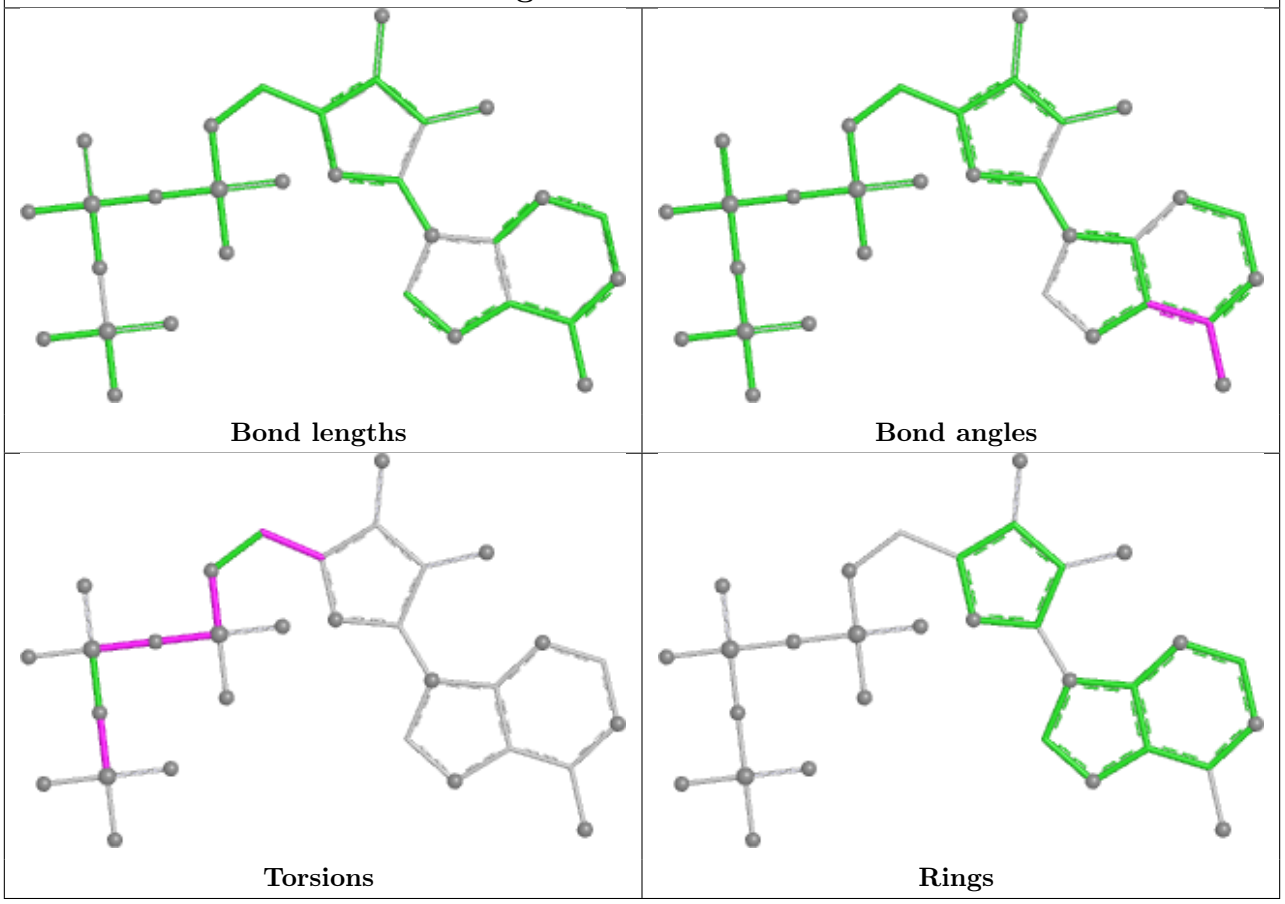


Torsions



Rings

Ligand ATP A 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.

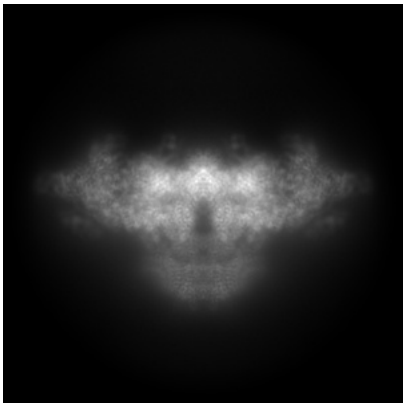
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42769. These allow visual inspection of the internal detail of the map and identification of artifacts.

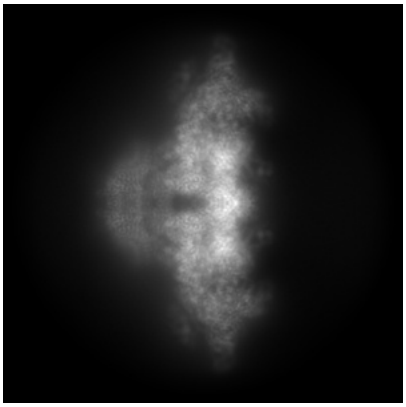
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

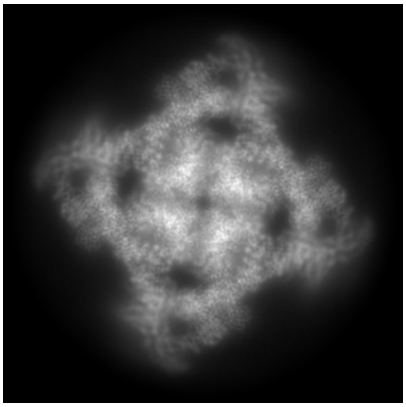
6.1.1 Primary map



X



Y

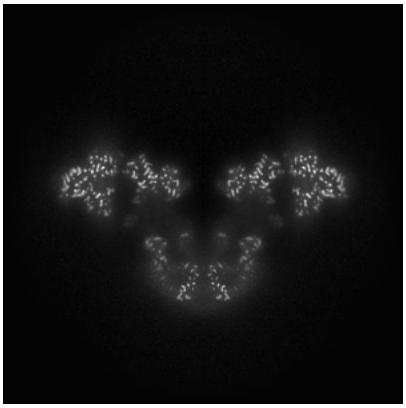


Z

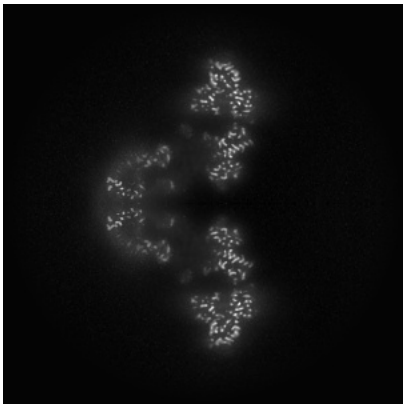
The images above show the map projected in three orthogonal directions.

6.2 Central slices

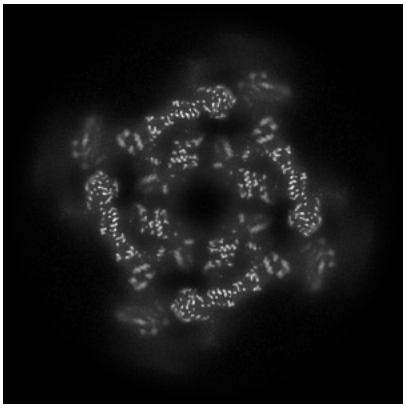
6.2.1 Primary map



X Index: 256



Y Index: 256

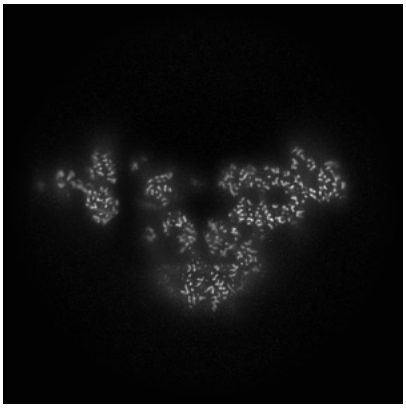


Z Index: 256

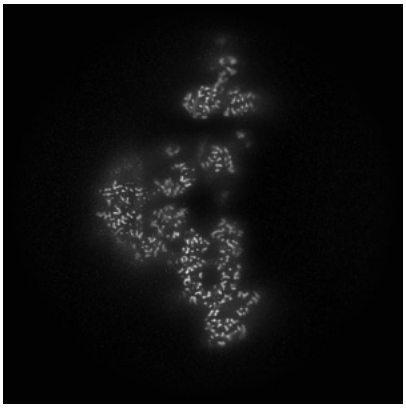
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

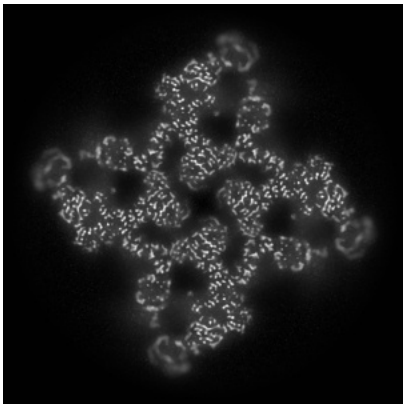
6.3.1 Primary map



X Index: 239



Y Index: 239

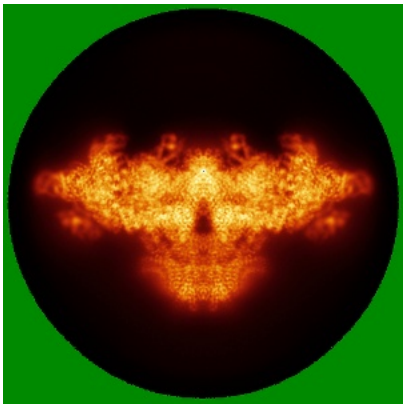


Z Index: 283

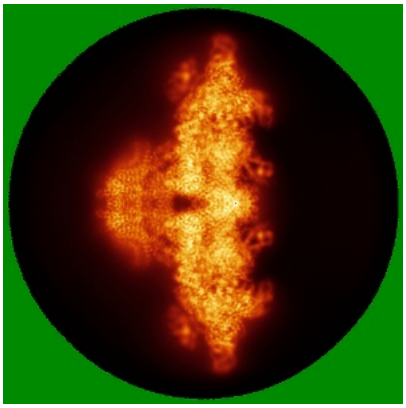
The images above show the largest variance slices of the map in three orthogonal directions.

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

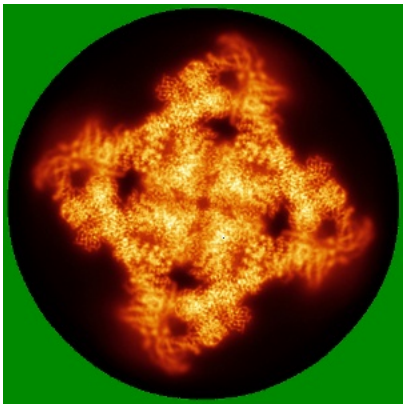
6.4.1 Primary map



X



Y

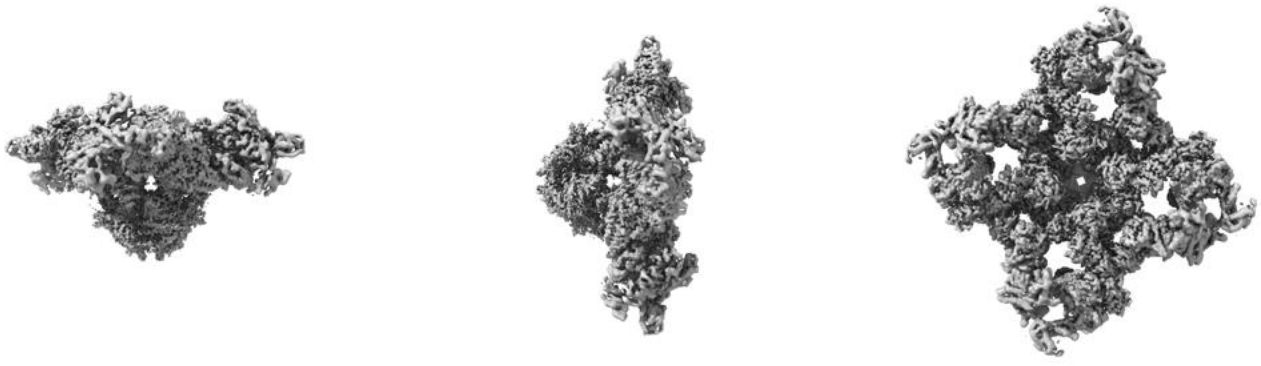


Z

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

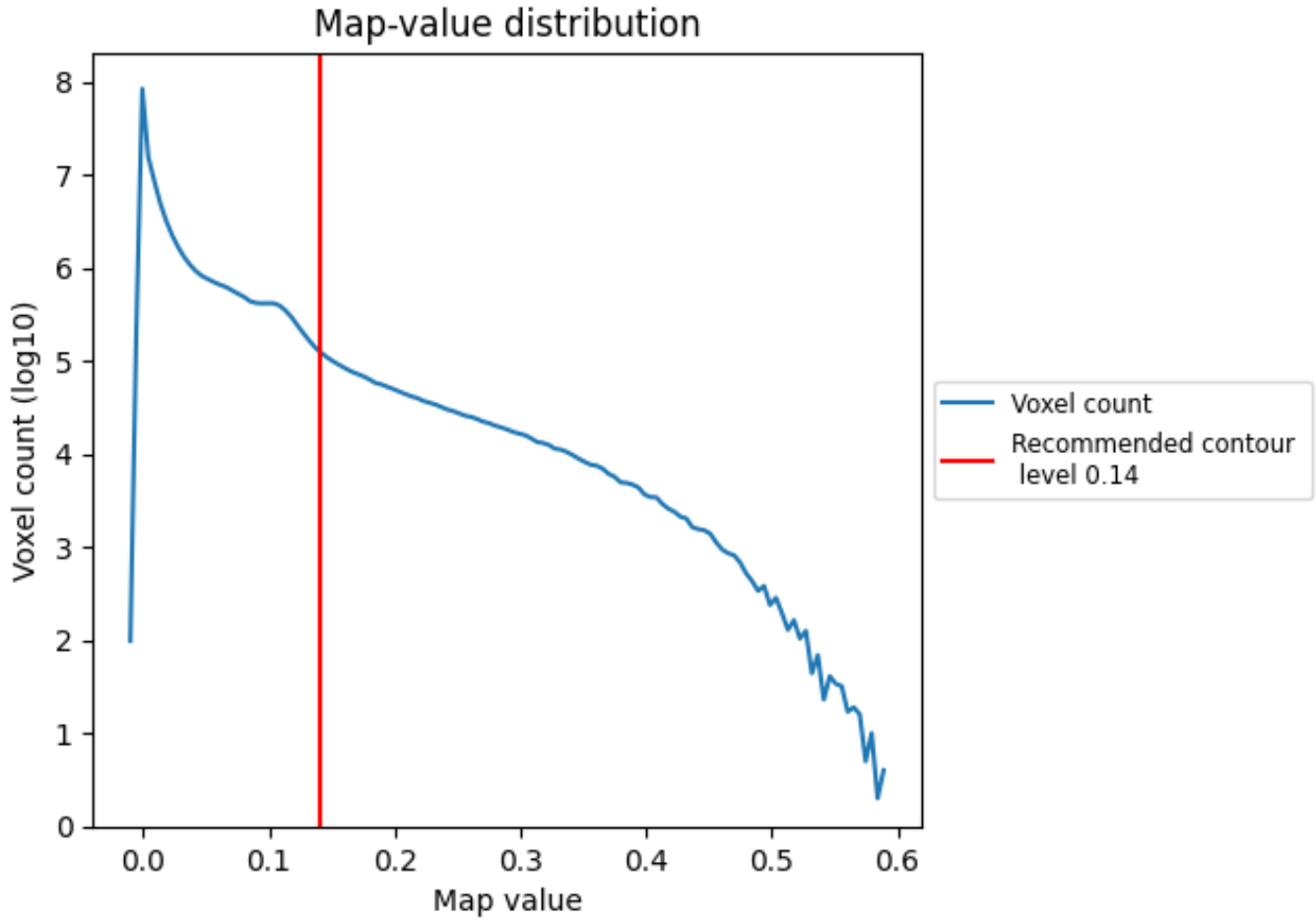
6.6 Mask visualisation (i)

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

7 Map analysis

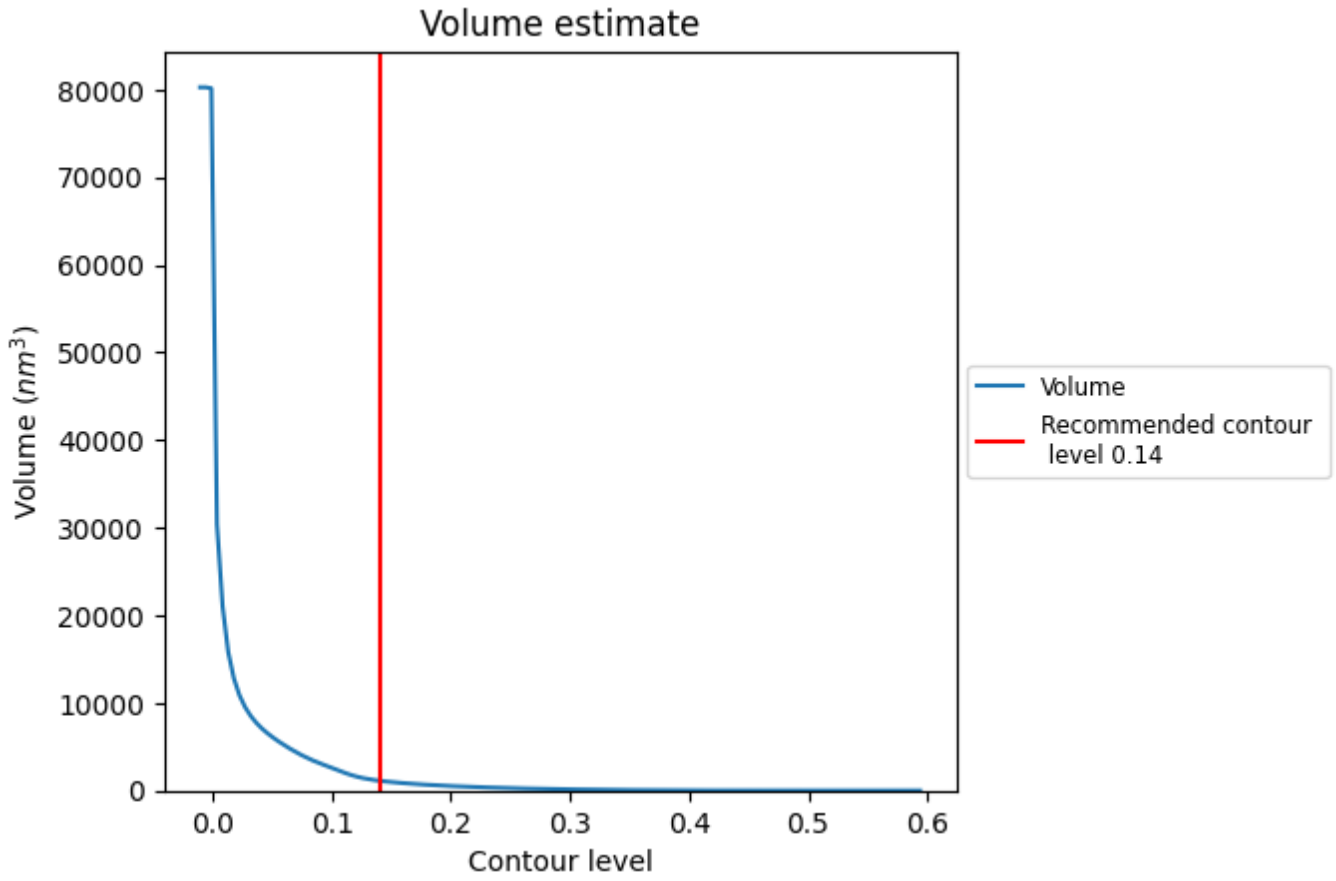
This section contains the results of statistical analysis of the map.

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.

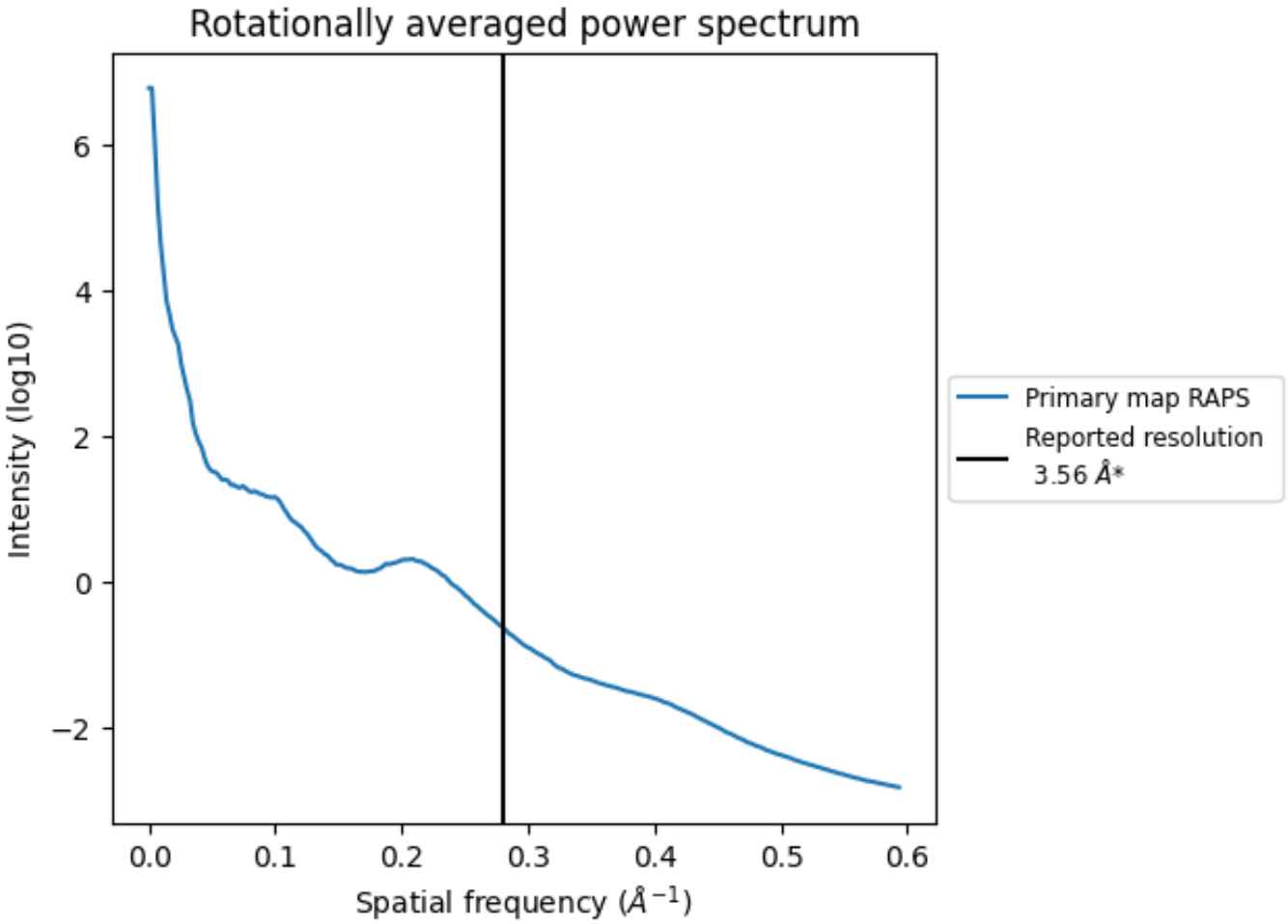
7.2 Volume estimate (i)



The volume at the recommended contour level is 1122 nm^3; this corresponds to an approximate mass of 1014 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 0.281 Å^{-1}

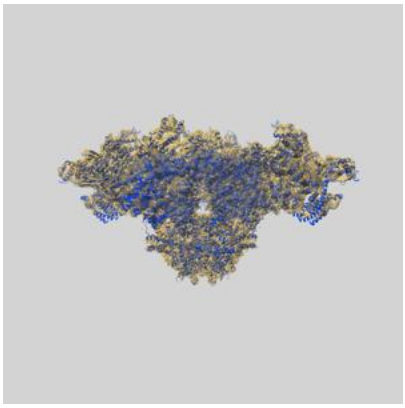
8 Fourier-Shell correlation (i)

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

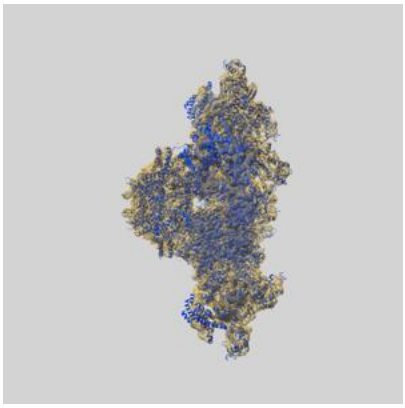
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42769 and PDB model 8UXM. Per-residue inclusion information can be found in section 3 on page 7.

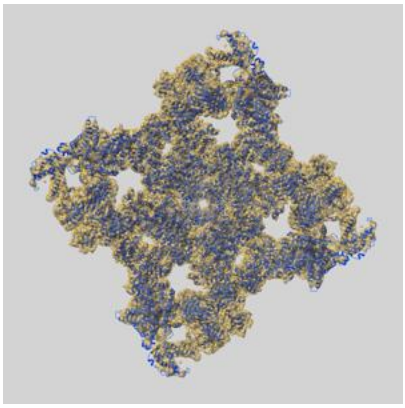
9.1 Map-model overlay



X



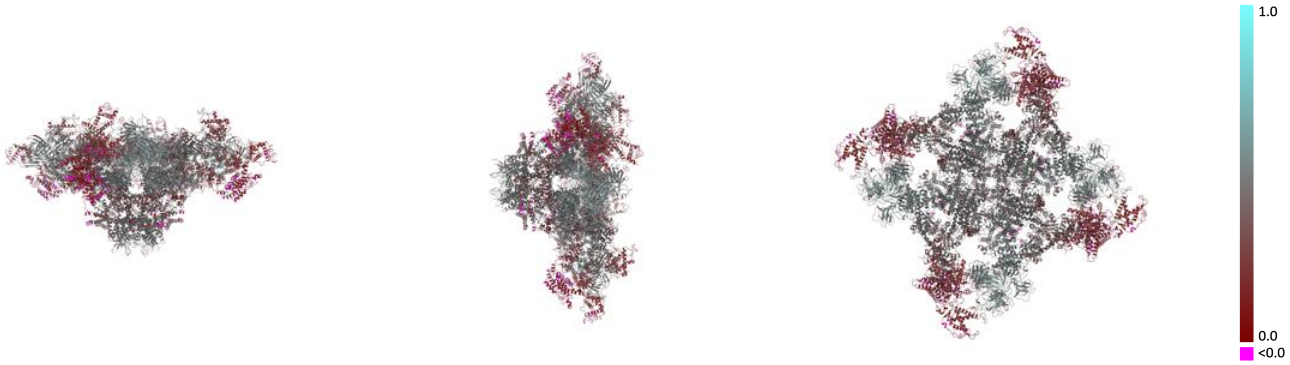
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

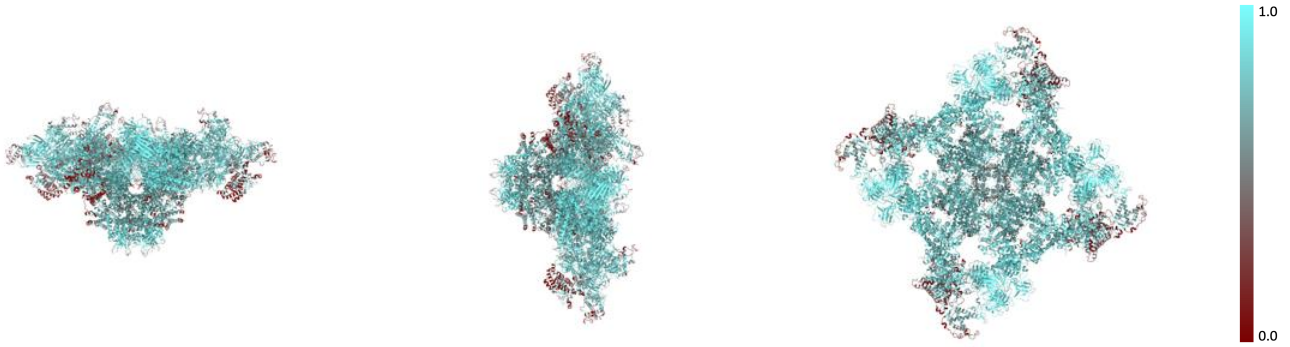
9.2 Q-score mapped to coordinate model



X Y Z

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

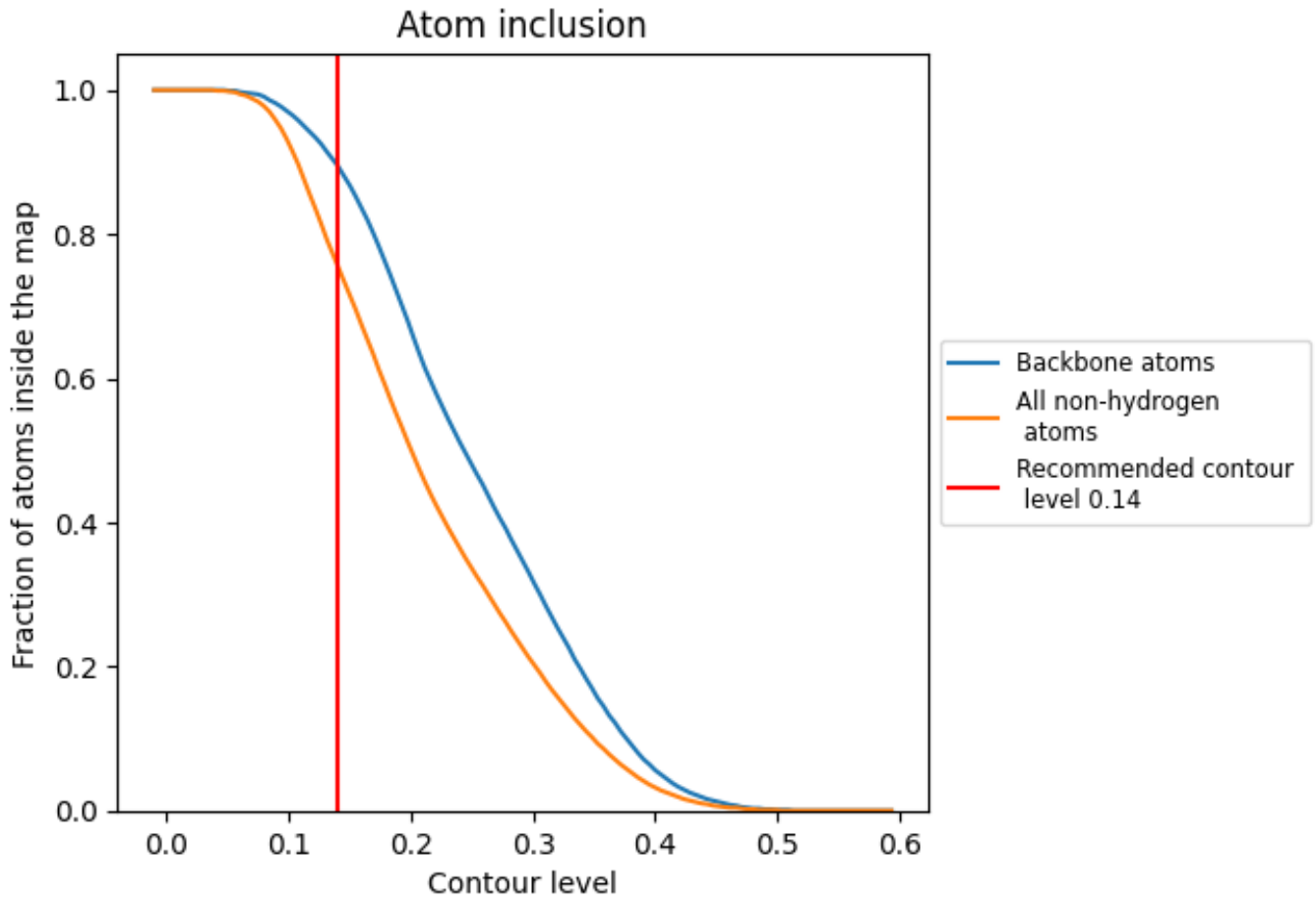
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.3810
A	0.7540	0.3840
B	0.7560	0.3860
C	0.7520	0.3800
D	0.7540	0.3820
E	0.8920	0.5130
F	0.8910	0.5110
G	0.8960	0.5120
H	0.8970	0.5110
I	0.7240	0.2220
J	0.7320	0.2220
K	0.7240	0.2220
L	0.7310	0.2190