Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 11:34 AM EST

PDB ID	:	6WOU
EMDB ID	:	EMD-21861
Title	:	Cryo-EM structure of recombinant mouse Ryanodine Receptor type 2 mutant R176Q in complex with FKBP12.6 in nanodisc
Authors	:	Iyer, K.A.; Hu, Y.; Kurebayashi, N.; Murayama, T.; Samso, M.
Deposited on	:	2020-04-25
Resolution	:	3.27 Å(reported)
Based on initial model	:	5L1D

This is a Full wwPDB EM Validation 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:

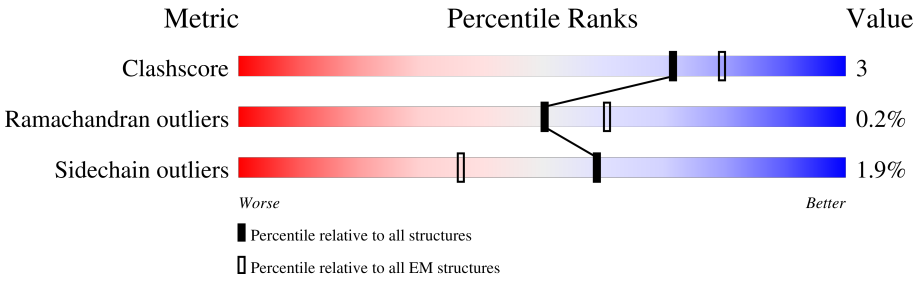
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4966	16% 70% 8% 21%
1	B	4966	16% 70% 8% 21%
1	C	4966	16% 70% 8% 21%
1	D	4966	16% 70% 8% 21%
2	E	107	92% 7%
2	F	107	92% 7%
2	G	107	93% 5%
2	H	107	92% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 245683 atoms, of which 120439 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	3921	Total	C	H	N	O	S	0	0
			59779	19348	29287	5250	5702	192		
1	B	3921	Total	C	H	N	O	S	0	0
			59778	19348	29286	5250	5702	192		
1	C	3921	Total	C	H	N	O	S	0	0
			59778	19348	29286	5250	5702	192		
1	D	3921	Total	C	H	N	O	S	0	0
			59776	19348	29284	5250	5702	192		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	GLN	ARG	engineered mutation	UNP E9Q401
B	176	GLN	ARG	engineered mutation	UNP E9Q401
C	176	GLN	ARG	engineered mutation	UNP E9Q401
D	176	GLN	ARG	engineered mutation	UNP E9Q401

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	107	Total	C	H	N	O	S	0	0
			1642	516	824	144	154	4		
2	F	107	Total	C	H	N	O	S	0	0
			1642	516	824	144	154	4		
2	G	107	Total	C	H	N	O	S	0	0
			1642	516	824	144	154	4		
2	H	107	Total	C	H	N	O	S	0	0
			1642	516	824	144	154	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

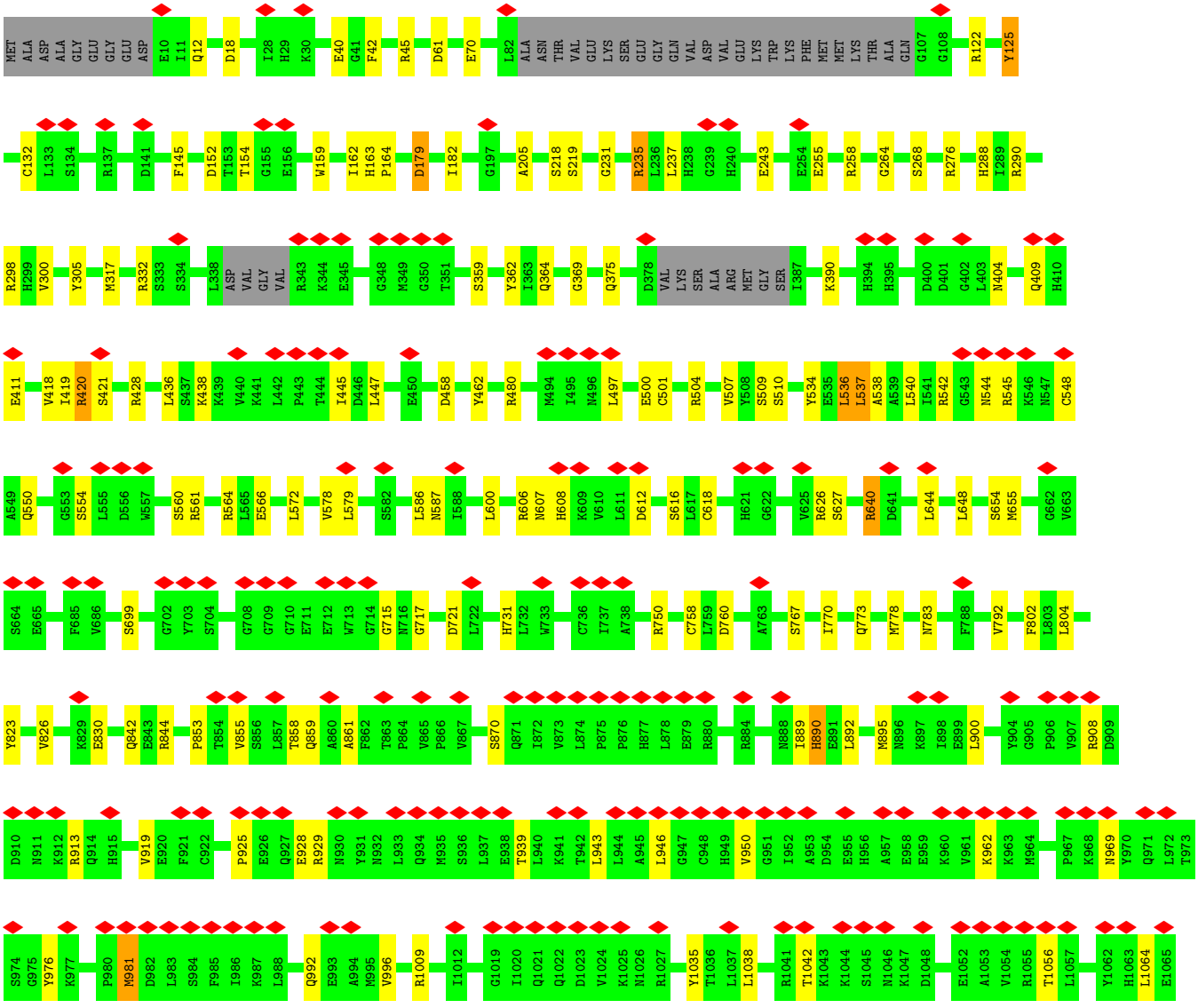
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

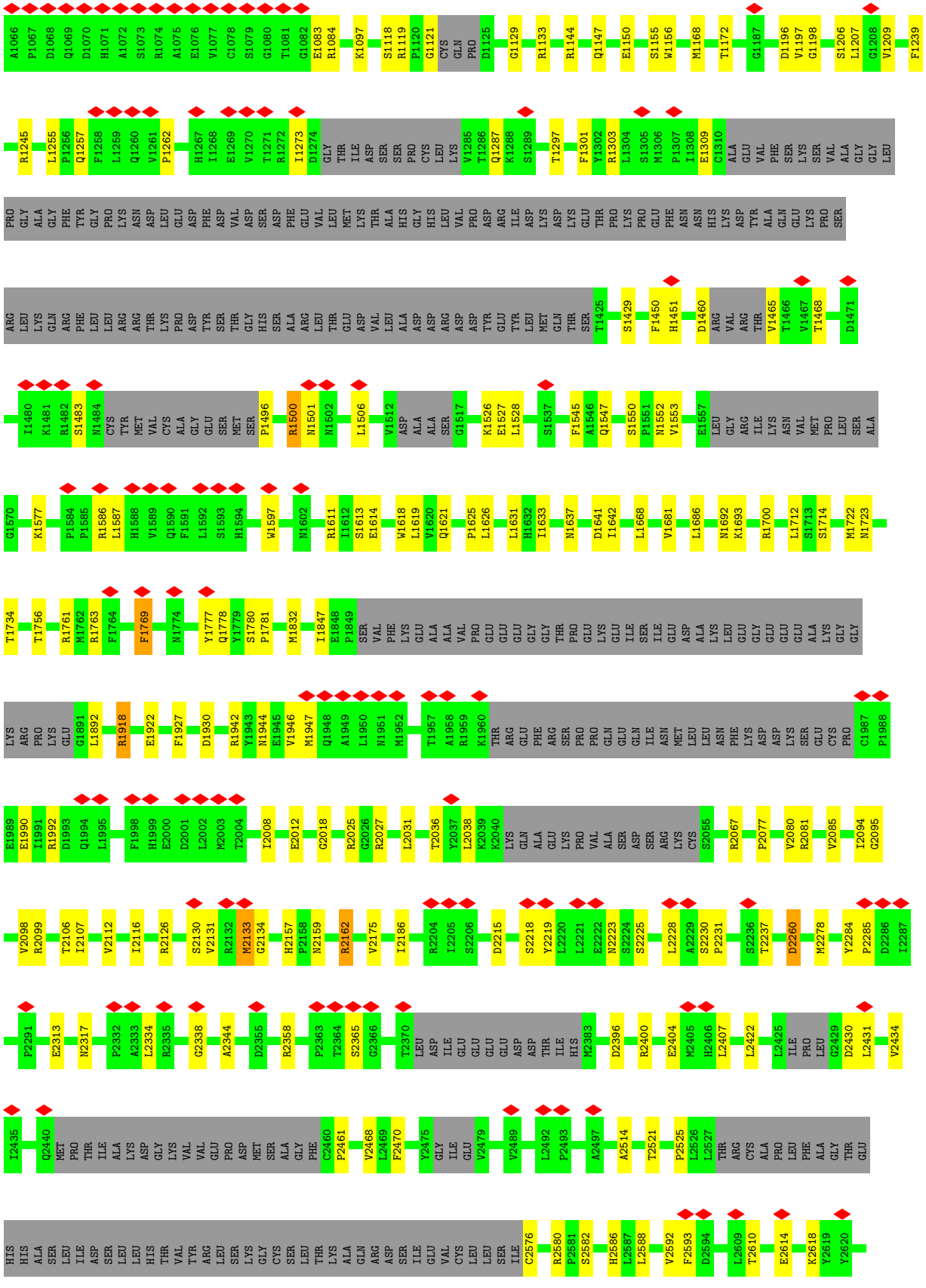
3 Residue-property plots (i)

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: Ryanodine receptor 2

Chain A:

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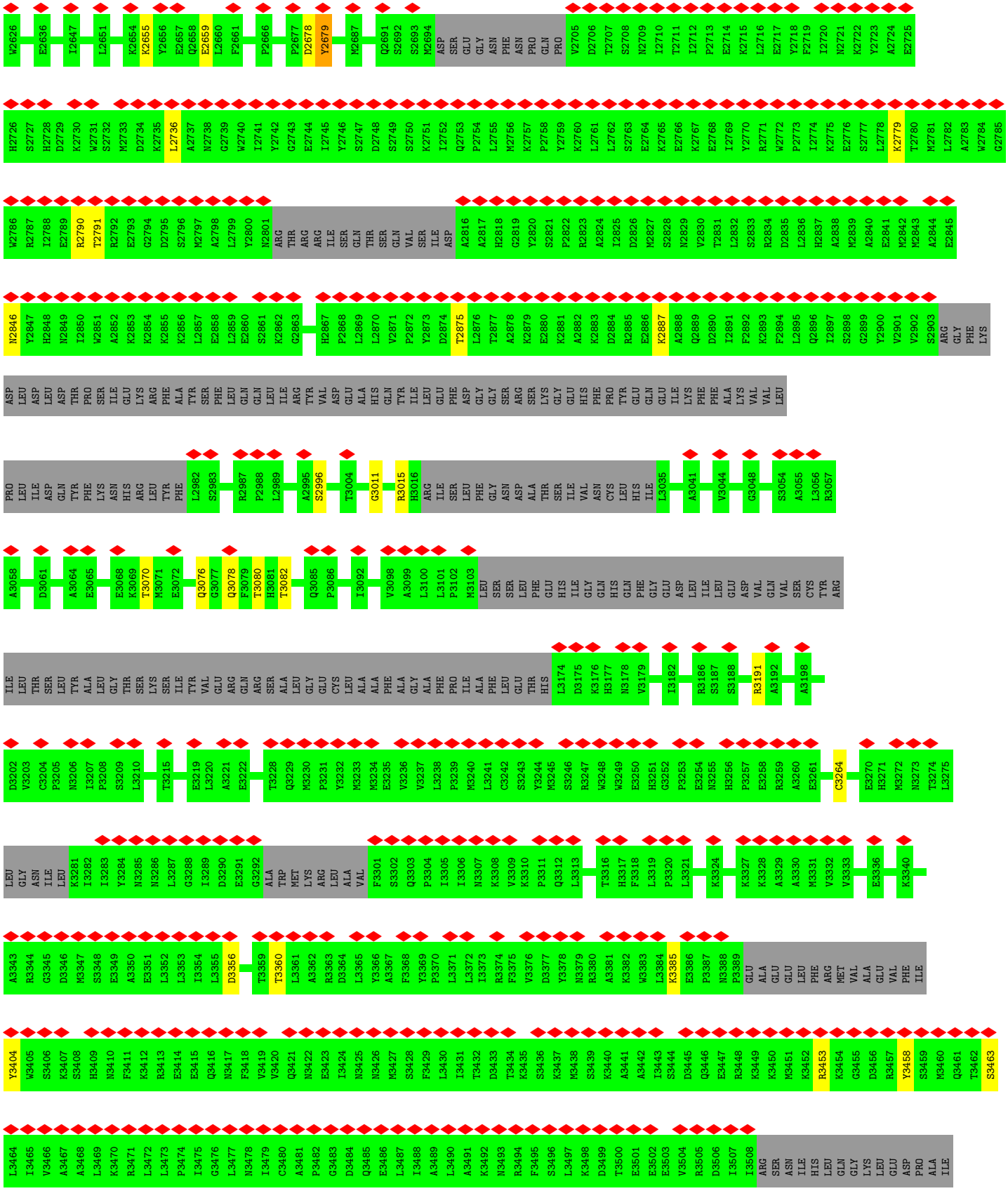
R1245 L1255 P1256 Q1257 F1258 L1259 Q1260 V1261 P1262 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287 K1288 S1289 T1297 F1301 Y1302 R1303 L1304 S1305 M1306 P1307 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS SER VAL ALA GLY GLY LEU
PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER
ARG LEU LYS GLN ARG PHE LEU LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU TYR LEU MET GLN THR SER T1425 S1429 F1450 H1451 D1460 ARG VAL ARG THR V1465 T1466 V1467 T1468 D1471
T1480 K1481 R1482 S1483 N1484 CYS TYR MET VAL CYS ALA GLY GLU SER MET SER P1496 R1500 N1501 N1502 L1506 V1512 ASP ALA ALA SER G1517 K1526 E1527 L1528 S1537 F1545 A1546 Q1547 S1550 P1551 N1552 V1553 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA
G1570 K1577 P1584 P1585 R1586 L1587 H1588 V1589 Q1590 F1591 L1592 S1593 H1594 W1597 N1602 R1611 I1612 S1613 E1614 W1618 L1619 V1620 Q1621 P1625 L1626 L1631 H1632 I1633 N1637 D1641 I1642 L1668 V1681 L1686 N1692 K1693 R1700 L1712 S1713 S1714 M1722 N1723
T1734 T1756 R1761 M1762 R1763 F1764 F1769 N1774 Y1777 Q1778 Y1779 S1780 P1781 M1832 I1847 E1848 P1849 SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY
LYS ARG PRO LYS GLU G1891 L1892 R1918 E1922 F1927 D1930 R1942 Y1943 N1944 E1945 V1946 M1947 Q1948 A1949 L1950 N1951 M1952 T1957 A1958 R1959 K1960 THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO C1987 P1988
E1989 E1990 I1991 R1992 D1993 Q1994 L1995 F1998 H1999 E2000 D2001 L2002 M2003 T2004 I2008 E2012 G2018 R2025 G2026 R2027 L2031 T2036 Y2037 L2038 K2039 K2040 LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS S2055 R2067 P2077 V2080 R2081 V2085 I2094 G2095
V2098 R2099 T2106 I2107 V2112 I2116 R2126 S2130 V2131 R2132 M2133 G2134 H2157 P2158 N2159 R2162 V2175 I2186 R2204 I2205 S2206 D2215 S2218 Y2219 L2220 L2221 E2222 N2223 S2224 S2225 L2228 A2229 S2230 P2231 S2236 T2237 D2260 M2278 Y2284 P2285 D2286 I2287
P2291 E2313 N2317 P2332 A2333 L2334 R2335 G2338 A2344 D2355 R2358 P2363 T2364 S2365 G2366 T2370 LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383 D2396 R2400 E2404 M2405 H2406 L2407 L2422 L2425 ILE PRO LEU G2429 D2430 L2431 V2434
I2435 Q2440 MET PRO THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY PHE C2460 P2461 V2468 L2469 F2470 Y2475 GLY ILE GLU V2479 V2489 L2492 P2493 A2497 A2514 T2521 P2525 L2526 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR GLU
HIS HIS ALA SER LEU ILE ASP SER LEU LEU HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE C2576 R2580 P2581 S2582 H2586 L2587 L2588 V2592 F2593 D2594 L2609 T2610 E2614 K2618 Y2619 Y2620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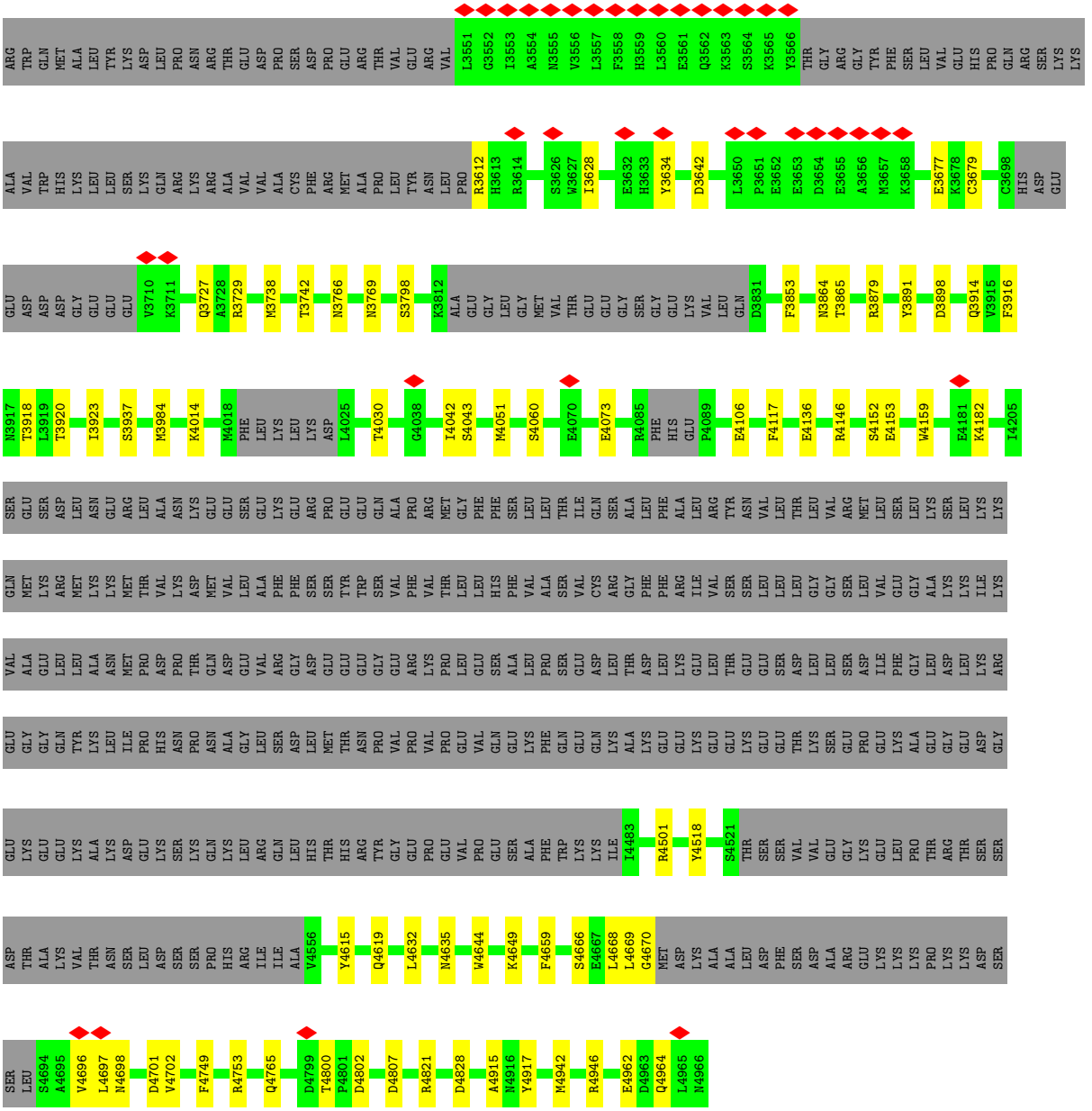
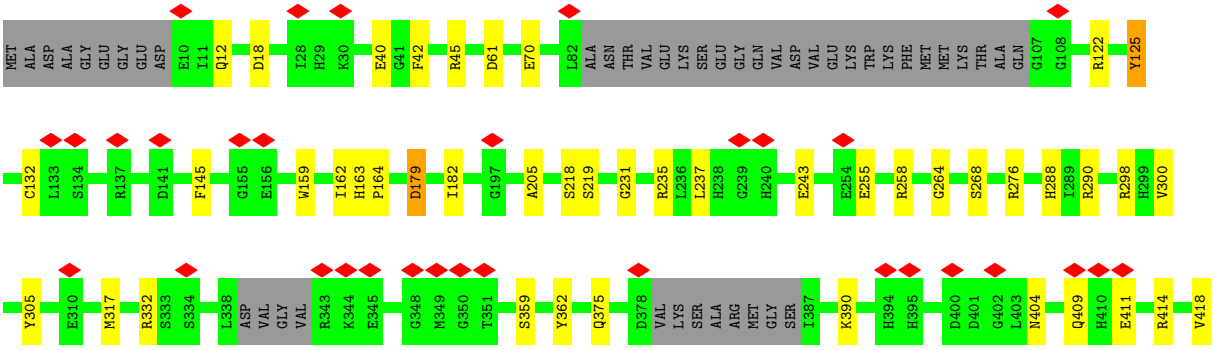
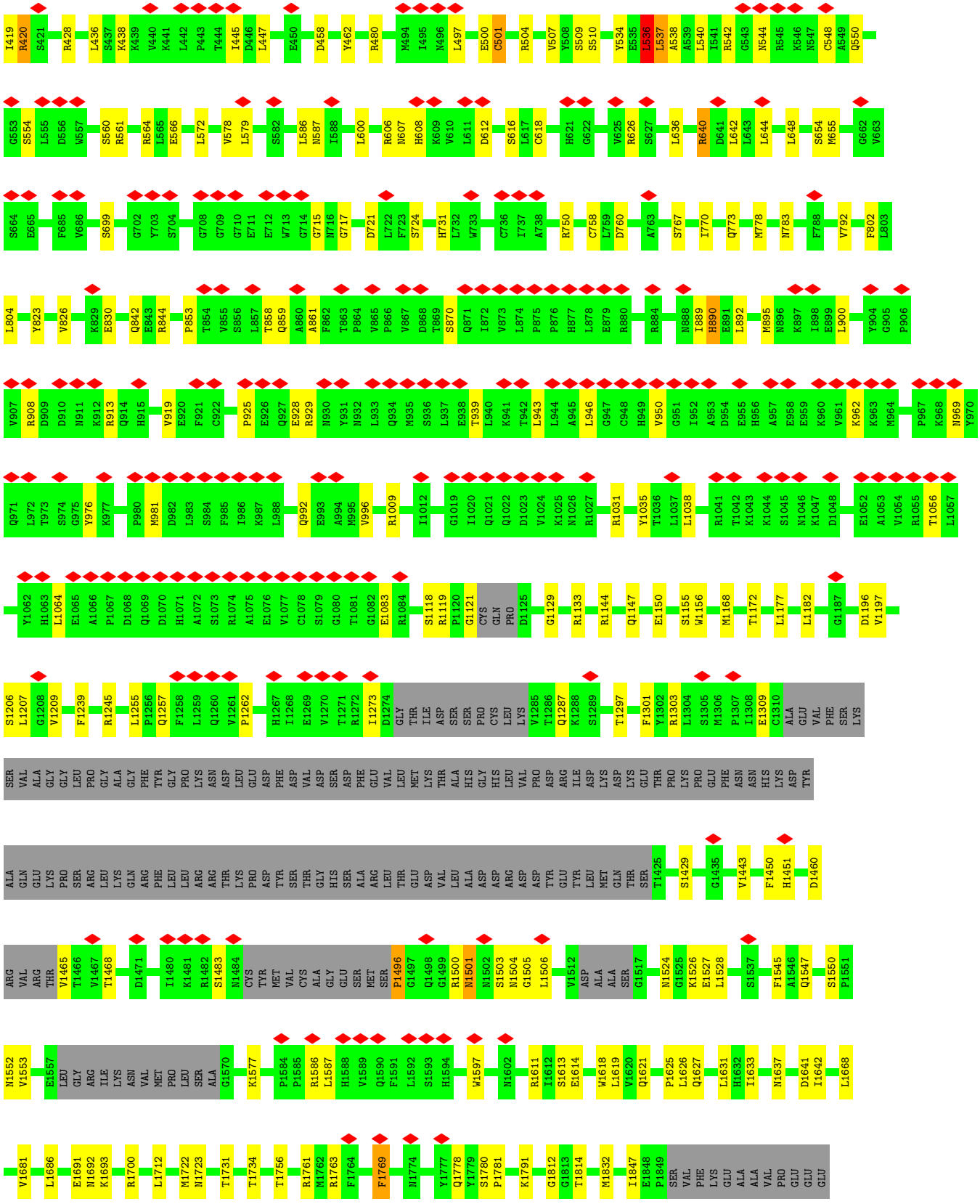
H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785
W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP A2816 A2817 H2818 C2819 Y2820 S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845
N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 ARG GLY PHE LYS
ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU
PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE L2982 S2983 R2987 P2988 L2989 A2995 S2996 T3004 G3011 R3015 H3016 ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE ILE VAL ASN CYS LEU HIS ILE L3035 A3041 V3044 G3048 S3054 A3055 L3056 R3057
A3058 D3061 A3064 E3065 E3068 K3069 T3070 M3071 E3072 Q3076 G3077 Q3078 F3079 T3080 H3081 T3082 Q3085 P3086 I3092 V3098 A3099 L3100 L3101 P3102 M3103 LEU SER SER LEU PHE GLU GLY HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU ILE LEU GLU GLU ASP VAL GLN VAL SER CYS TYR ARG
ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS L3174 D3175 K3176 H3177 N3178 V3179 I3182 R3186 S3187 S3188 R3191 A3192 A3198
D3202 V3203 C3204 P3205 N3206 I3207 P3208 S3209 L3210 T3215 E3219 L3220 A3221 E3222 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 V3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 M3245 S3246 R3247 W3248 W3249 E3250 H3251 G3252 P3253 E3254 N3255 H3256 P3257 E3258 R3259 A3260 E3261 C3264 E3270 H3271 M3272 N3273 T3274 L3275
LEU GLY ASN ILE LEU K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 T3316 H3317 F3318 L3319 P3320 L3321 K3324 K3327 K3328 A3329 A3330 M3331 V3332 V3333 E3336 K3340
A3343 R3344 G3345 D3346 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 T3359 T3360 L3361 A3362 R3363 D3364 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374 F3375 V3376 D3377 Y3378 N3379 R3380 A3381 K3382 W3383 L3384 K3385 E3386 P3387 N3388 P3389 GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE
Y3404 W3405 S3406 K3407 S3408 H3409 N3410 F3411 K3412 R3413 E3414 E3415 Q3416 N3417 F3418 V3419 V3420 Q3421 N3422 E3423 I3424 N3425 N3426 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 K3440 A3441 A3442 I3443 S3444 D3445 Q3446 E3447 R3448 K3449 K3450 M3451 K3452 R3453 K3454 G3455 D3456 R3457 Y3458 S3459 M3460 Q3461 T3462 S3463
L3464 I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 C3480 A3481 P3482 G3483 D3484 Q3485 E3486 L3487 I3488 A3489 L3490 A3491 K3492 N3493 R3494 F3495 S3496 L3497 K3498 D3499 T3500 E3501 E3502 E3503 V3504 R3505 D3506 I3507 I3508 ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE



• Molecule 1: Ryanodine receptor 2

Chain B:

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G553 S554 L555 D556 W557 S560 R561 R564 L565 E566 L572 V578 L579 S582 L586 N587 I588 L600 R606 N607 H608 K609 V610 L611 D612 S616 K617 C618 H621 G622 Y625 R626 S627 L636 R640 D641 L642 L643 L644 L648 S654 M655 G662 V663
S664 E665 F685 V686 S699 G702 Y703 S704 G708 G709 G710 E711 E712 W713 G714 G715 N716 G717 D721 L722 F723 S724 H731 L732 W733 C736 I737 A738 R750 C758 L759 D760 A763 S767 I770 Q773 M778 N783 F788 V792 F802 L803
L804 Y823 V826 K829 E830 Q842 E843 R844 P853 T854 V855 S856 L857 T858 Q859 A860 A861 F862 T863 P864 V865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 R884 N888 I889 H890 E891 L892 M895 N896 K897 I898 E899 L900 Y904 G905 P906
V907 R908 D909 D910 N911 K912 R913 Q914 H915 V919 E920 F921 C922 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953 D954 E955 H956 A957 E958 E959 K960 V961 K962 K963 M964 P967 K968 N969 Y970
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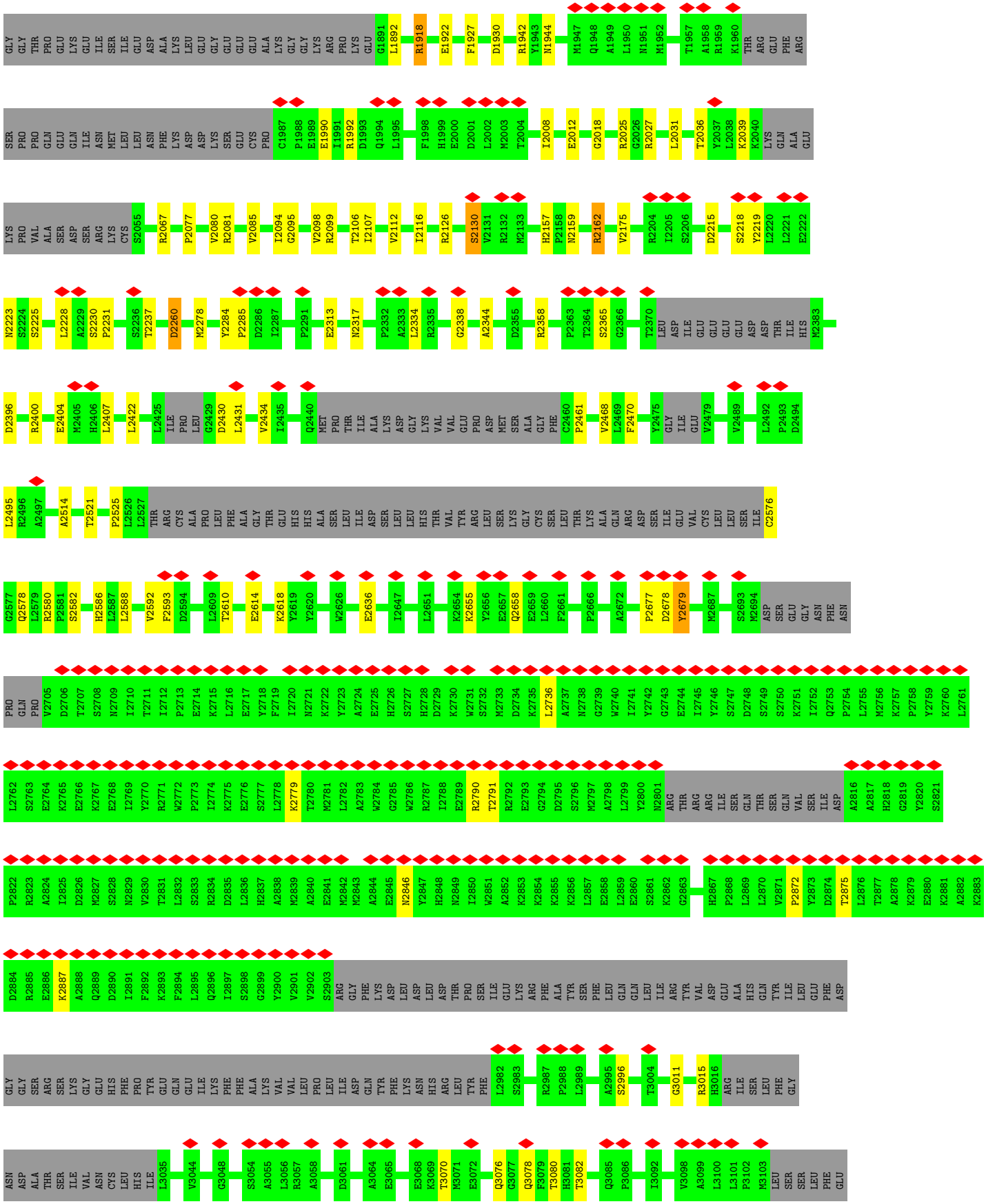
Y1062 H1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 S1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 S1118 R1119 P1120 G1121 CYS GLN PRO D1125 G1129 R1133 R1144 Q1147 E1150 S1155 W1156 M1168 T1172 L1177 L1182 G1187 D1196 V1197
S1206 L1207 G1208 V1209 F1239 R1245 L1255 P1256 Q1257 F1258 L1259 Q1260 V1261 P1262 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER PRO CYS LEU LYS V1285 T1286 Q1287 K1288 S1289 T1297 F1301 Y1302 R1303 L1304 S1305 M1306 P1307 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS
SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR
ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU TYR LEU MET GLN THR SER T1425 S1429 G1435 V1443 F1450 H1451 D1460
ARG VAL ARG THR V1465 T1466 V1467 T1468 D1471 I1480 K1481 R1482 S1483 N1484 CYS TYR MET VAL CYS ALA GLY GLU SER MET SER P1496 G1497 Q1498 G1499 R1500 N1501 N1502 S1503 N1504 G1505 L1506 V1512 ASP ALA ALA SER G1517 N1524 G1525 K1526 E1527 L1528 S1537 F1545 A1546 Q1547 S1550 P1551
N1552 V1553 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU LEU SER ALA G1570 K1577 P1584 P1585 R1586 L1587 H1588 V1589 Q1590 F1591 L1592 S1593 H1594 W1597 N1602 R1611 I1612 S1613 E1614 W1618 L1619 V1620 Q1621 P1625 L1626 Q1627 L1631 H1632 I1633 N1637 D1641 I1642 L1668
V1681 L1686 E1691 N1692 K1693 R1700 L1712 M1722 N1723 T1731 T1734 T1756 R1761 M1762 R1763 F1764 F1769 N1774 Y1777 Q1778 Y1779 S1780 P1781 K1791 G1812 G1813 T1814 M1832 I1847 E1848 P1849 SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU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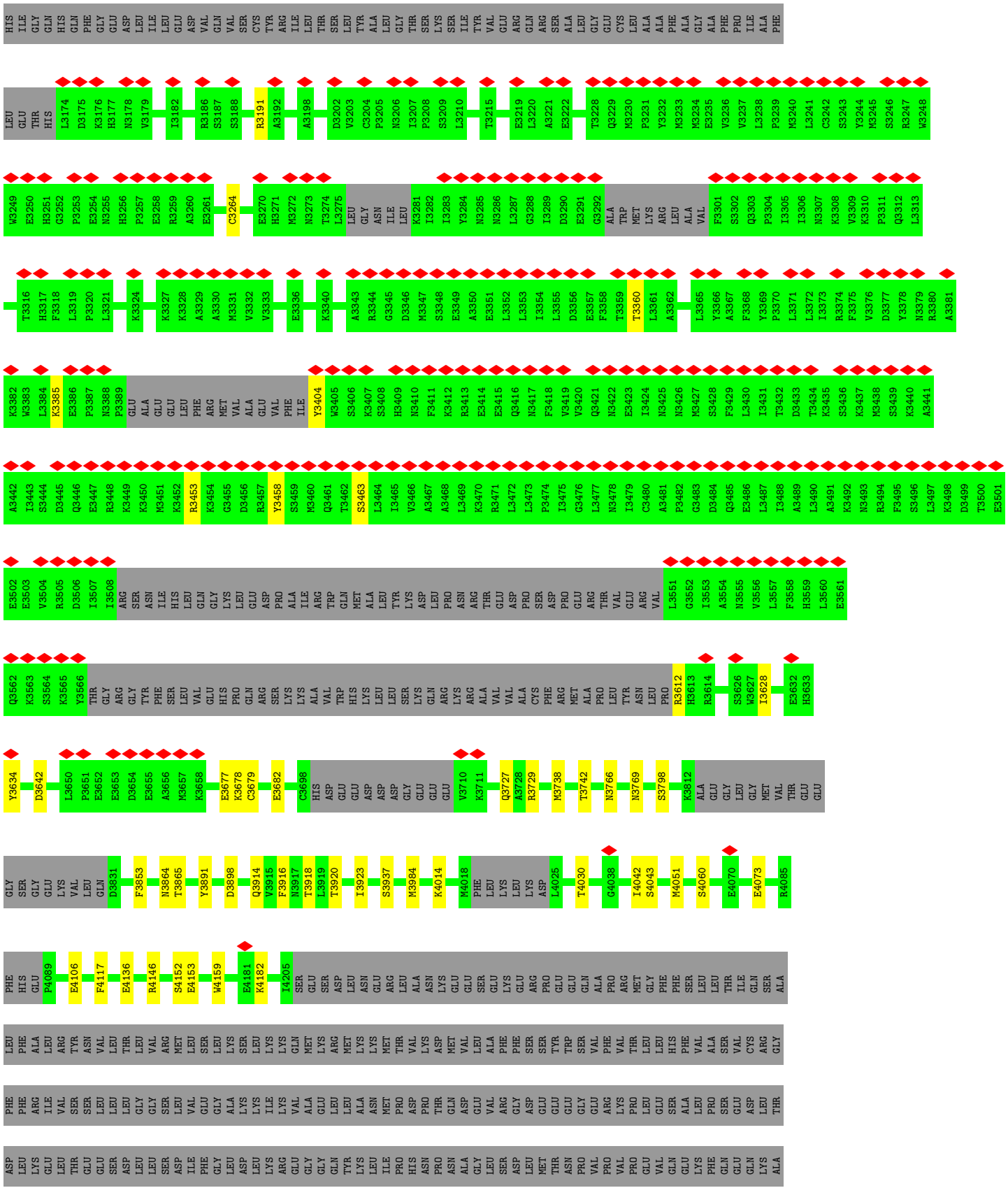
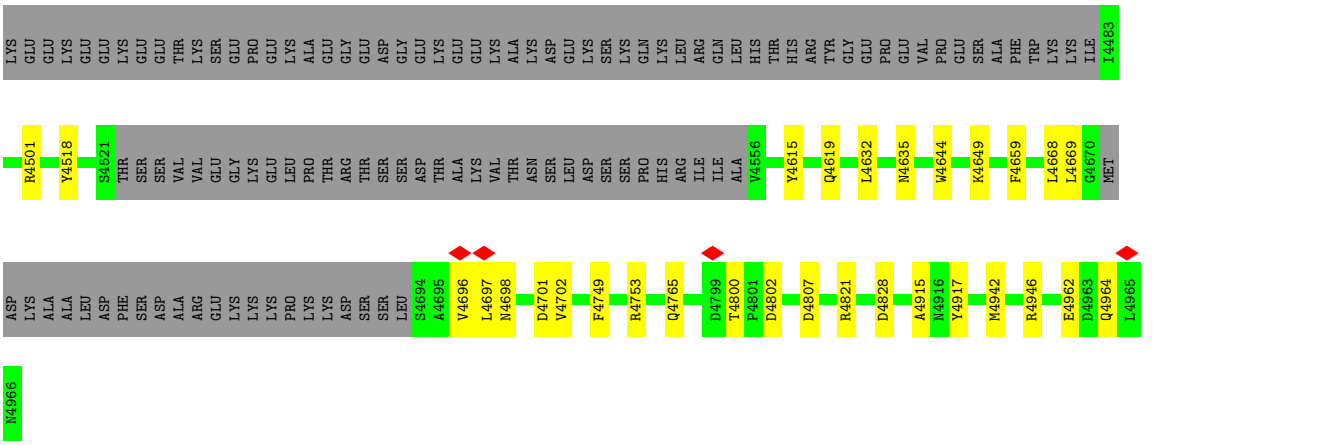
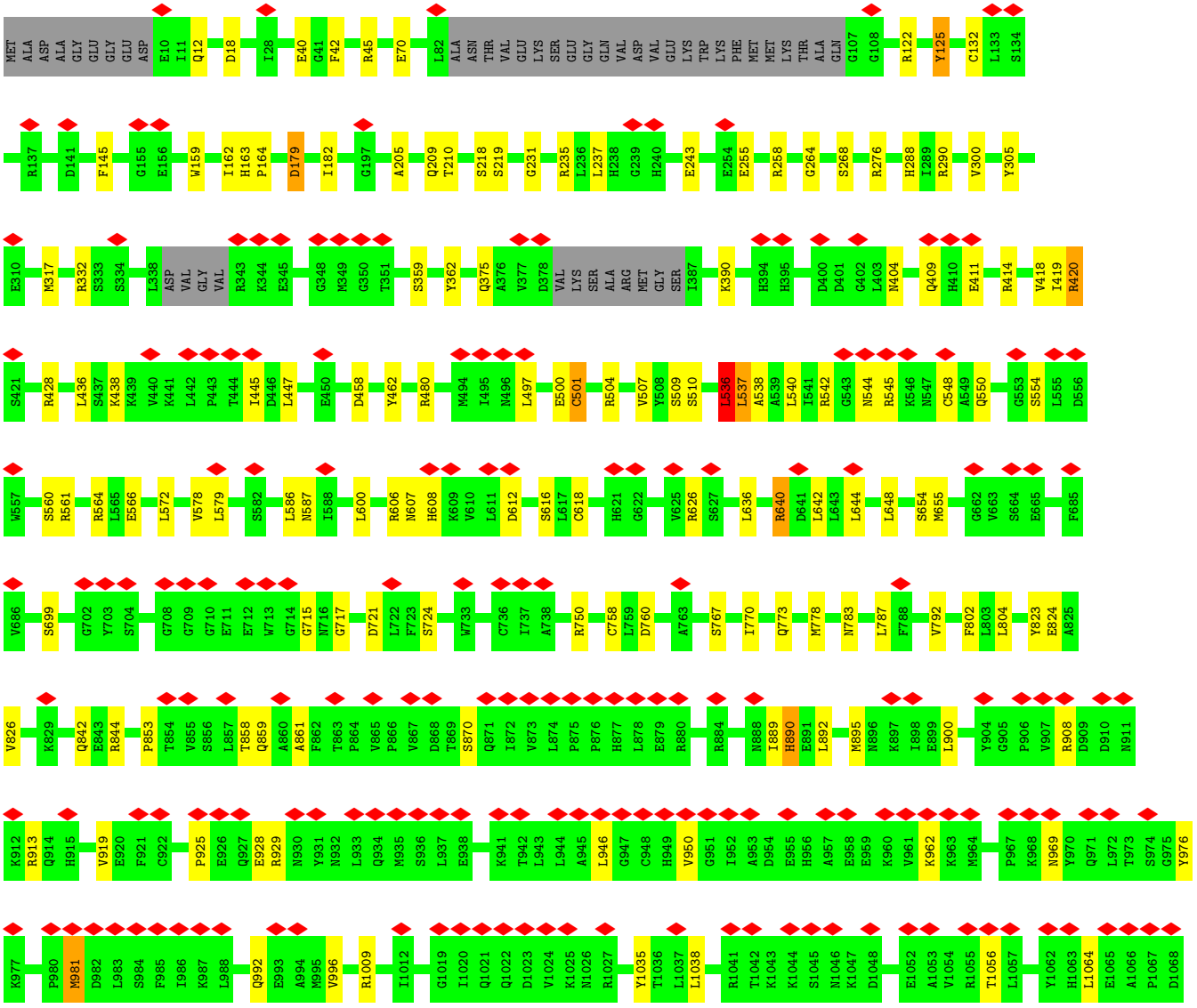
SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS PRO C1987 P1988 E1989 E1990 I1991 R1992 D1993 Q1994 L1996 F1998 H1999 E2000 D2001 L2002 M2003 T2004 I2008 E2012 G2018 R2025 G2026 R2027 L2031 T2036 Y2037 L2038 K2039 K2040 LYS GLN ALA GLU
LYS PRO VAL ALA SER ASP SER ARG LYS CYS S2055 R2067 P2077 V2080 R2081 V2085 I2094 G2095 V2098 R2099 T2106 I2107 V2112 I2116 R2126 S2130 V2131 R2132 M2133 H2157 P2158 N2159 R2162 V2175 R2204 I2205 S2206 D2215 S2218 Y2219 L2220 L2221 E2222
N2223 S2224 S2225 L2228 A2229 S2230 P2231 S2236 T2237 D2260 M2278 Y2284 P2285 D2286 I2287 P2291 E2313 N2317 P2332 A2333 L2334 R2335 G2338 A2344 D2355 R2358 P2363 T2364 S2365 G2366 T2370 LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383
D2396 R2400 E2404 M2405 H2406 L2407 L2422 L2425 ILE PRO LEU G2429 D2430 L2431 V2434 I2435 Q2440 MET PRO THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY PHE C2460 P2461 V2468 L2469 F2470 Y2475 GLY ILE GLU V2479 V2489 L2492 P2493 D2494
L2495 R2496 A2497 A2514 T2521 P2525 L2526 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU ILE ASP SER LEU LEU HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE C2576
G2577 Q2578 L2579 R2580 P2581 S2582 H2586 K2587 L2588 V2592 F2593 D2594 L2609 T2610 E2614 K2618 Y2619 Y2620 W2626 E2636 I2647 L2651 K2654 K2655 Y2656 E2657 Q2658 E2659 L2660 F2661 P2666 A2672 P2677 D2678 Y2679 M2687 S2693 M2694 ASP SER GLU GLY ASN PHE ASN
PRO GLN PRO V2705 D2706 T2707 T2707 S2708 N2709 I2710 T2711 I2712 I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761
L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 N2800 N2801 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821
P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883
D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP
GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE L2982 S2983 R2987 P2988 L2989 A2995 S2996 T3004 G3011 R3015 H3016 ARG ILE SER LEU PHE GLY
ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE L3035 V3044 G3048 S3054 A3055 L3056 R3057 A3058 D3061 A3064 E3065 E3068 K3069 T3070 M3071 E3072 Q3076 G3077 Q3078 F3079 T3080 H3081 T3082 Q3085 P3086 I3092 V3098 A3099 L3100 L3101 P3102 M3103 LEU SER SER LEU PHE GLU

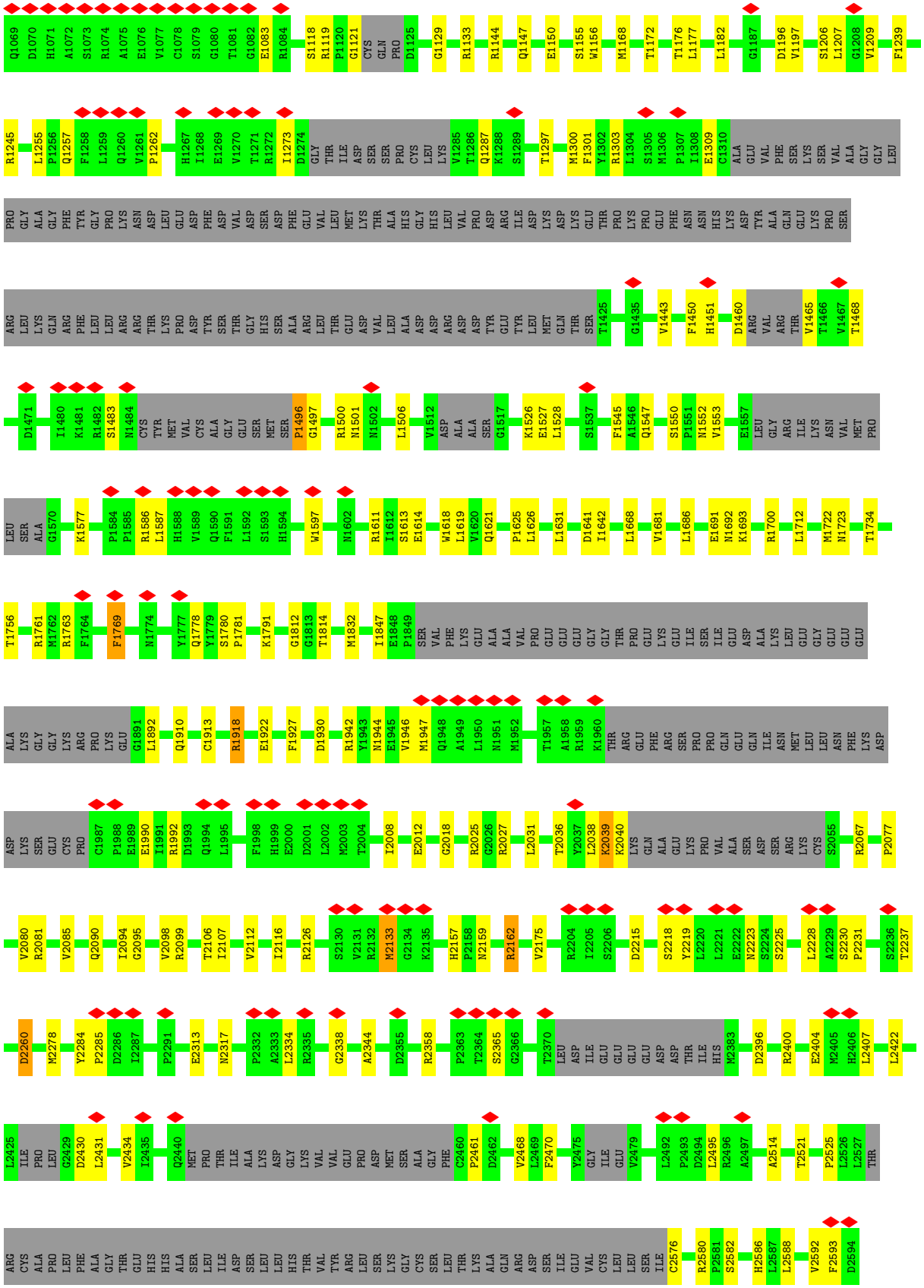

HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE
LEU GLU THR HIS L3174 D3175 K3176 H3177 N3178 V3179 I3182 R3186 S3187 S3188 R3191 A3192 A3198 D3202 V3203 C3204 P3205 N3206 I3207 P3208 S3209 L3210 T3215 E3219 L3220 A3221 E3222 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 V3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 M3245 S3246 R3247 W3248
W3249 E3250 H3251 G3252 P3253 E3254 N3255 H3256 P3257 E3258 R3259 A3260 E3261 C3264 E3270 H3271 M3272 N3273 T3274 L3275 LEU GLY ASN ILE LEU K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313
T3316 H3317 F3318 L3319 P3320 L3321 K3324 K3327 K3328 A3329 A3330 M3331 V3332 V3333 E3336 K3340 A3343 R3344 G3345 D3346 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357 F3358 T3359 T3360 L3361 A3362 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374 F3375 V3376 D3377 Y3378 N3379 R3380 A3381
K3382 W3383 L3384 K3385 E3386 P3387 N3388 P3389 GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE Y3404 W3405 S3406 K3407 S3408 H3409 N3410 F3411 K3412 R3413 E3414 E3415 Q3416 N3417 F3418 V3419 V3420 Q3421 N3422 E3423 I3424 N3425 N3426 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 K3440 A3441
A3442 I3443 S3444 D3445 Q3446 E3447 R3448 K3449 K3450 M3451 K3452 R3453 K3454 G3455 D3456 R3457 Y3458 S3459 M3460 Q3461 T3462 S3463 L3464 I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 C3480 A3481 P3482 G3483 D3484 Q3485 E3486 L3487 I3488 A3489 L3490 A3491 K3492 N3493 R3494 F3495 S3496 L3497 K3498 D3499 T3500 E3501
E3502 E3503 V3504 R3505 D3506 I3507 I3508 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 GLU ASP PRO SER ASP PRO GLU ARG THR VAL GLU ARG VAL L3551 G3552 I3553 A3554 N3555 V3556 L3557 F3558 H3559 L3560 E3561
Q3562 K3563 S3564 K3565 Y3566 THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN LEU PRO R3612 H3613 R3614 S3626 W3627 I3628 E3632 H3633
Y3634 D3642 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 E3677 K3678 C3679 E3682 C3698 HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU V3710 K3711 Q3727 A3728 R3729 M3738 T3742 N3766 N3769 S3798 K3812 ALA GLU GLY LEU GLY MET VAL THR GLU GLU
GLY SER GLY GLU LYS VAL LEU GLN D3831 F3853 N3864 T3865 Y3891 D3898 Q3914 Y3915 F3916 N3917 T3918 L3919 T3920 I3923 S3937 M3984 K4014 M4018 PHE LEU LYS LEU LYS ASP L4025 T4030 G4038 I4042 S4043 M4051 S4060 E4070 E4073 R4085
PHE HIS GLU P4089 E4106 F4117 E4136 R4146 S4152 E4153 W4159 E4181 K4182 I4205 SER GLU SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA
LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU LEU HIS PHE SER VAL ALA SER LEU LEU THR VAL CYS ARG GLY
PHE PHE ARG ILE VAL SER SER LEU LEU LEU LEU GLY GLY SER LEU VAL GLU 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 GLU GLU GLU GLY GLU ARG LYS PRO LEU GLU SER ALA LEU PRO SER GLU ASP LEU THR
ASP LEU LYS GLU LEU LEU LEU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET THR ASN PRO VAL PRO VAL PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA

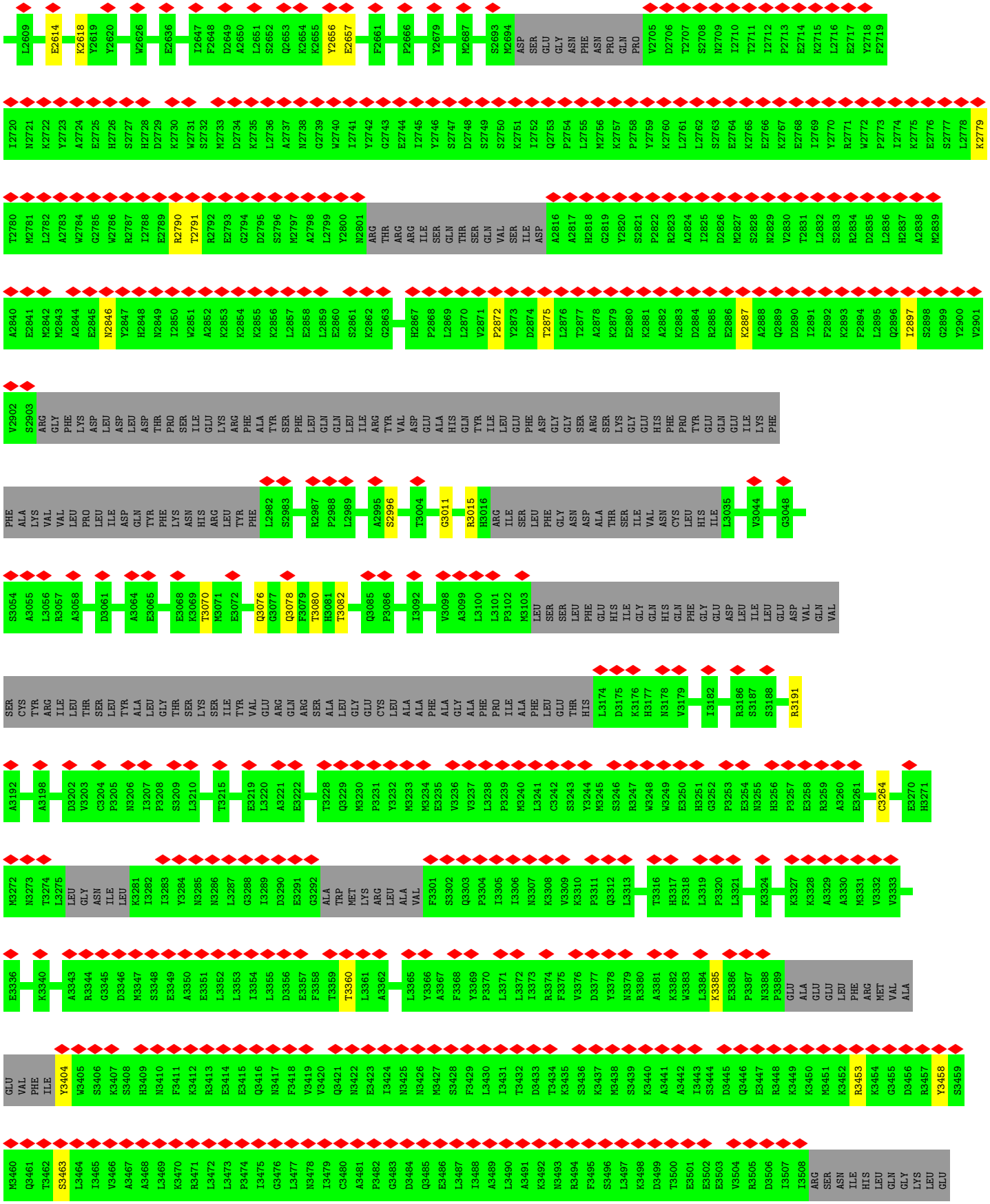


• Molecule 1: Ryanodine receptor 2

Chain C:



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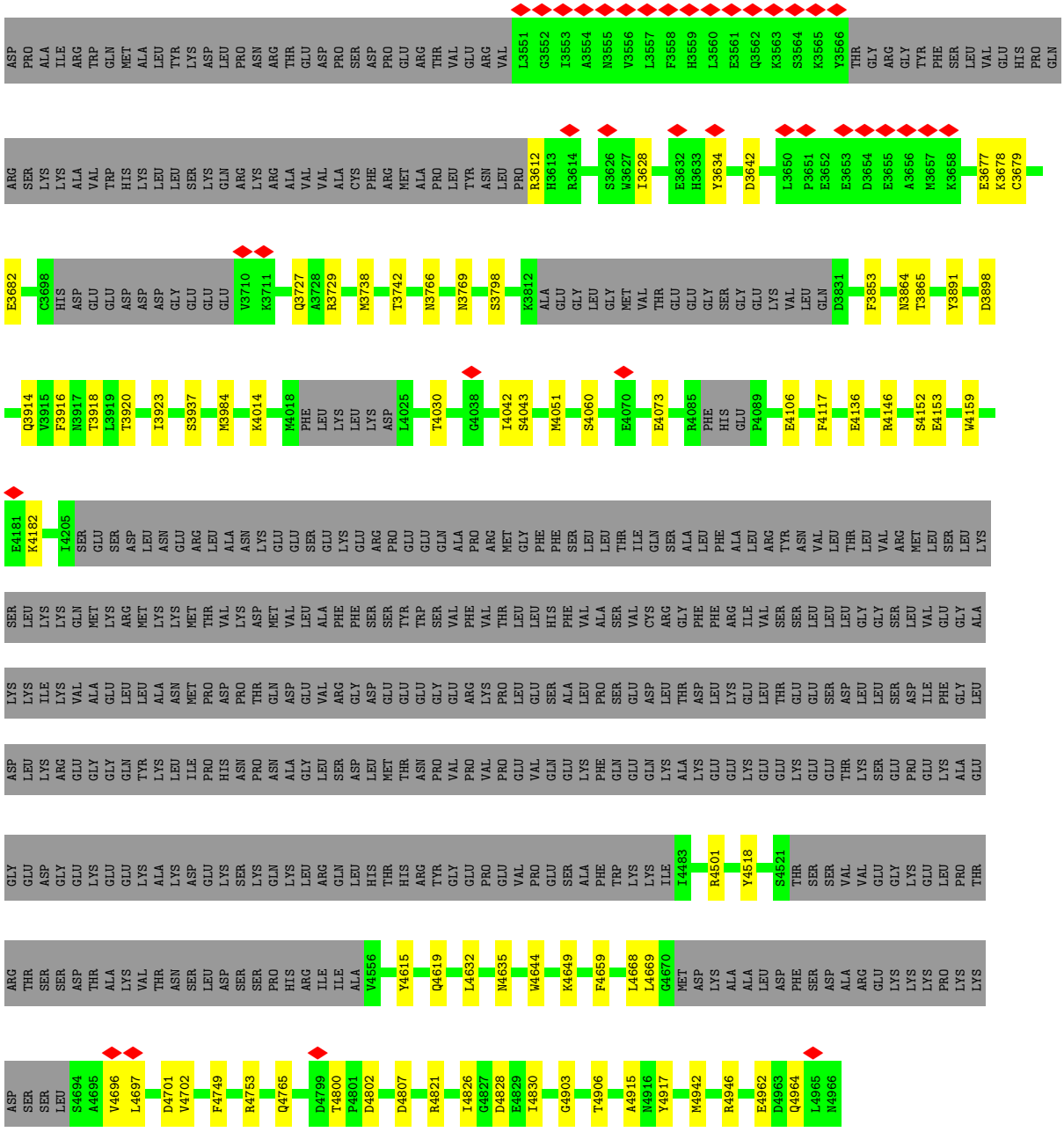
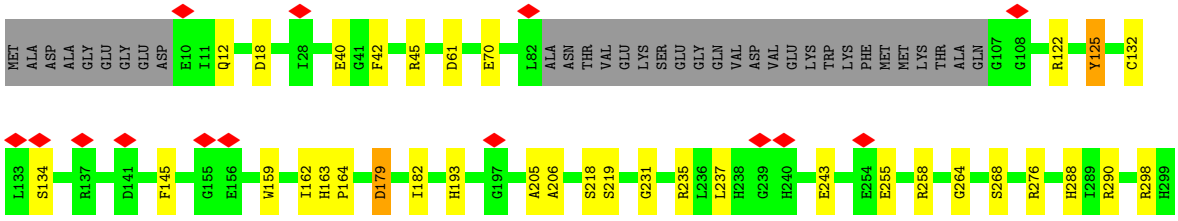
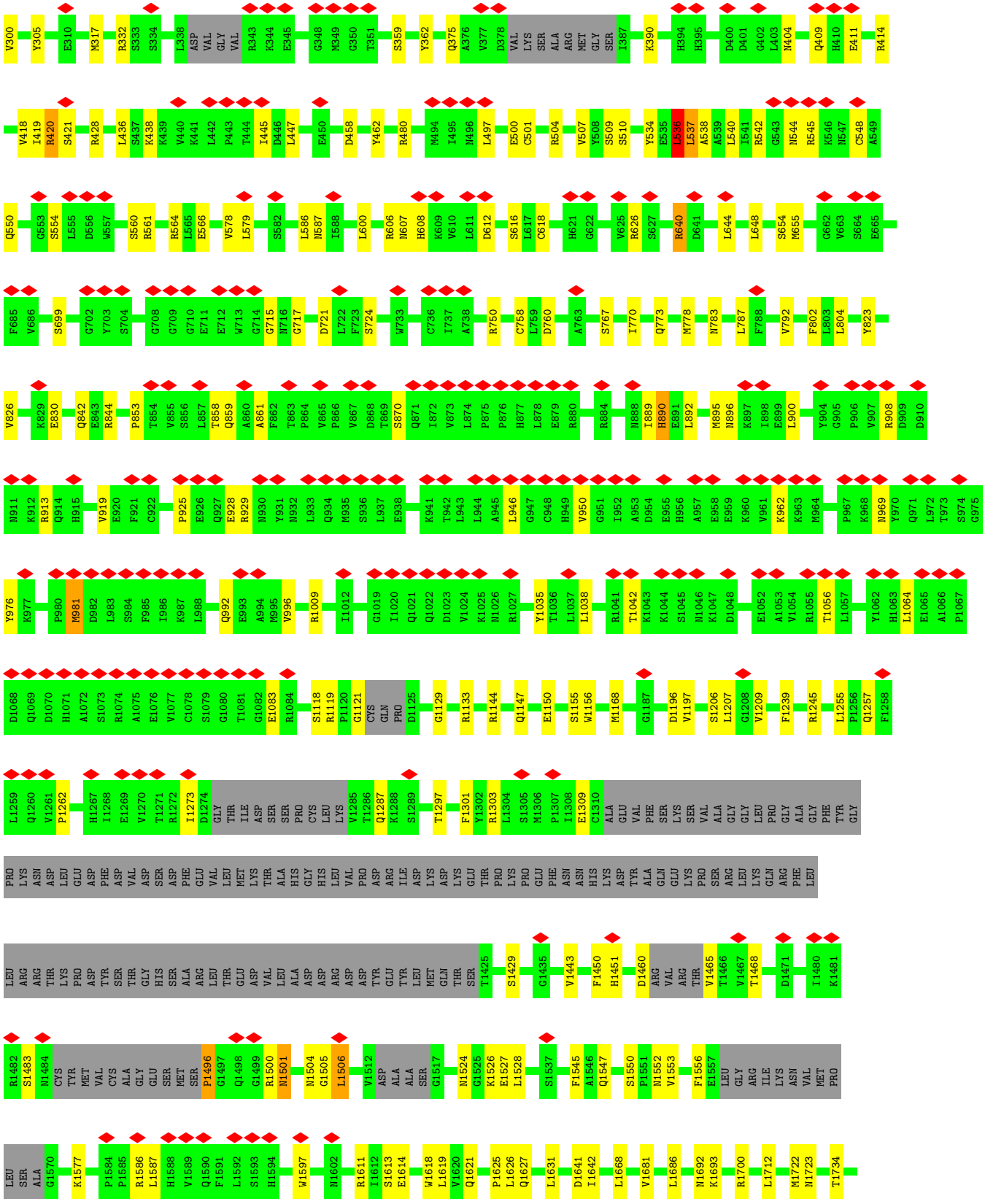
I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779
T2780 M2781 L2782 A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839
A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 K2857 E2858 L2859 E2860 S2861 K2862 G2863 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901
V2902 S2903 ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE
PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE L2982 S2983 R2987 P2988 L2989 A2995 S2996 T3004 G3011 R3015 H3016 ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE L3035 V3044 G3048
S3054 A3055 L3056 R3057 A3058 D3061 A3064 E3065 E3068 K3069 T3070 M3071 E3072 Q3076 G3077 Q3078 F3079 T3080 H3081 T3082 Q3085 P3086 I3092 V3098 A3099 L3100 L3101 P3102 M3103 LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU ILE LEU GLU ASP VAL GLN VAL
SER CYS TYR ARG ILE LEU LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS L3174 D3175 K3176 H3177 N3178 V3179 T3182 R3186 S3187 S3188 R3191
A3192 A3198 D3202 V3203 C3204 P3205 N3206 I3207 P3208 S3209 L3210 T3215 E3219 L3220 A3221 E3222 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 V3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 M3245 S3246 R3247 W3248 W3249 E3250 H3251 G3252 P3253 E3254 N3255 H3256 P3257 E3258 R3259 A3260 E3261 C3264 E3270 H3271
M3272 N3273 T3274 L3275 LEU GLY ASN ILE LEU K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 T3316 H3317 F3318 L3319 P3320 L3321 K3324 K3327 K3328 A3329 A3330 M3331 V3332 V3333
E3336 K3340 A3343 R3344 G3345 D3346 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357 F3358 T3359 T3360 L3361 A3362 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374 F3375 V3376 D3377 Y3378 N3379 R3380 A3381 K3382 W3383 L3384 K3385 E3386 P3387 N3388 P3389 GLU ALA GLU GLU LEU PHE ARG MET VAL ALA
GLU VAL PHE ILE Y3404 W3405 S3406 K3407 S3408 H3409 N3410 F3411 K3412 R3413 E3414 E3415 Q3416 N3417 F3418 V3419 V3420 Q3421 N3422 E3423 I3424 N3425 N3426 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 K3440 A3441 A3442 I3443 S3444 D3445 Q3446 E3447 R3448 K3449 K3450 M3451 K3452 R3453 K3454 G3455 D3456 R3457 Y3458 S3459
M3460 Q3461 T3462 S3463 L3464 I3465 Y3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 C3480 A3481 P3482 G3483 D3484 Q3485 E3486 L3487 I3488 A3489 L3490 A3491 K3492 N3493 R3494 F3495 S3496 L3497 K3498 D3499 T3500 E3501 E3502 E3503 V3504 R3505 D3506 I3507 I3508 ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU



• Molecule 1: Ryanodine receptor 2

Chain D:

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V418 I419 R420 S421 R428 L436 S437 K438 K439 V440 K441 L442 P443 T444 I445 D446 L447 E450 D458 Y462 R480 M494 I495 N496 L497 E500 C501 R504 V507 Y508 S509 S510 Y534 E535 L536 L537 A538 A539 L540 L541 R542 G543 N544 R545 K546 N547 C548 A549
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F685 V686 S699 G702 Y703 S704 G708 G709 G710 E711 E712 W713 G714 G715 N716 G717 D721 L722 F723 S724 W733 C736 I737 A738 R750 C758 L759 D760 A763 S767 I770 Q773 M778 N783 L787 F788 V792 F802 L803 L804 Y823
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N911 K912 R913 Q914 H915 V919 E920 F921 C922 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953 D954 E955 H956 A957 E958 E959 K960 V961 K962 K963 M964 P967 K968 N969 Y970 Q971 L972 T973 S974 G975
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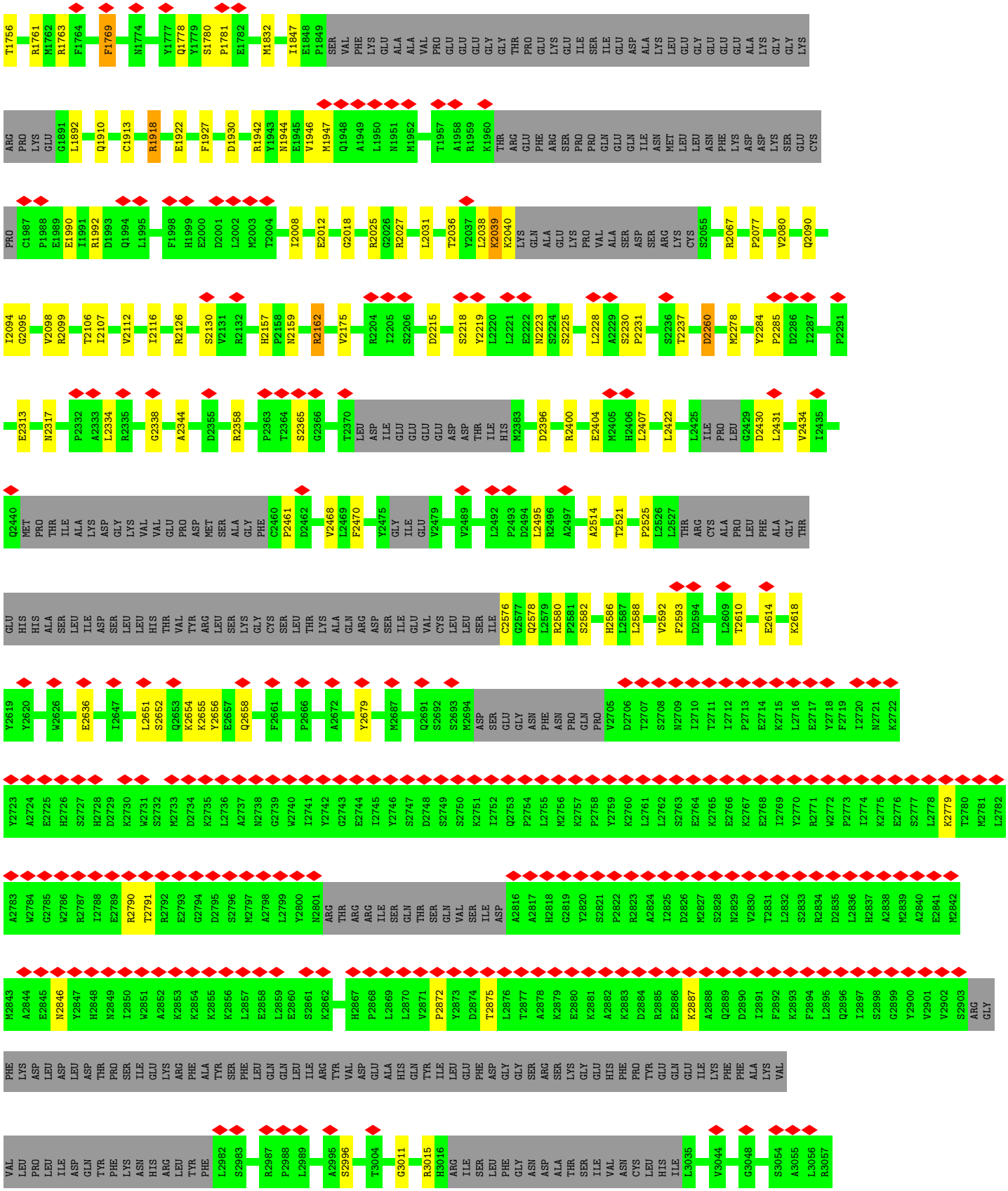
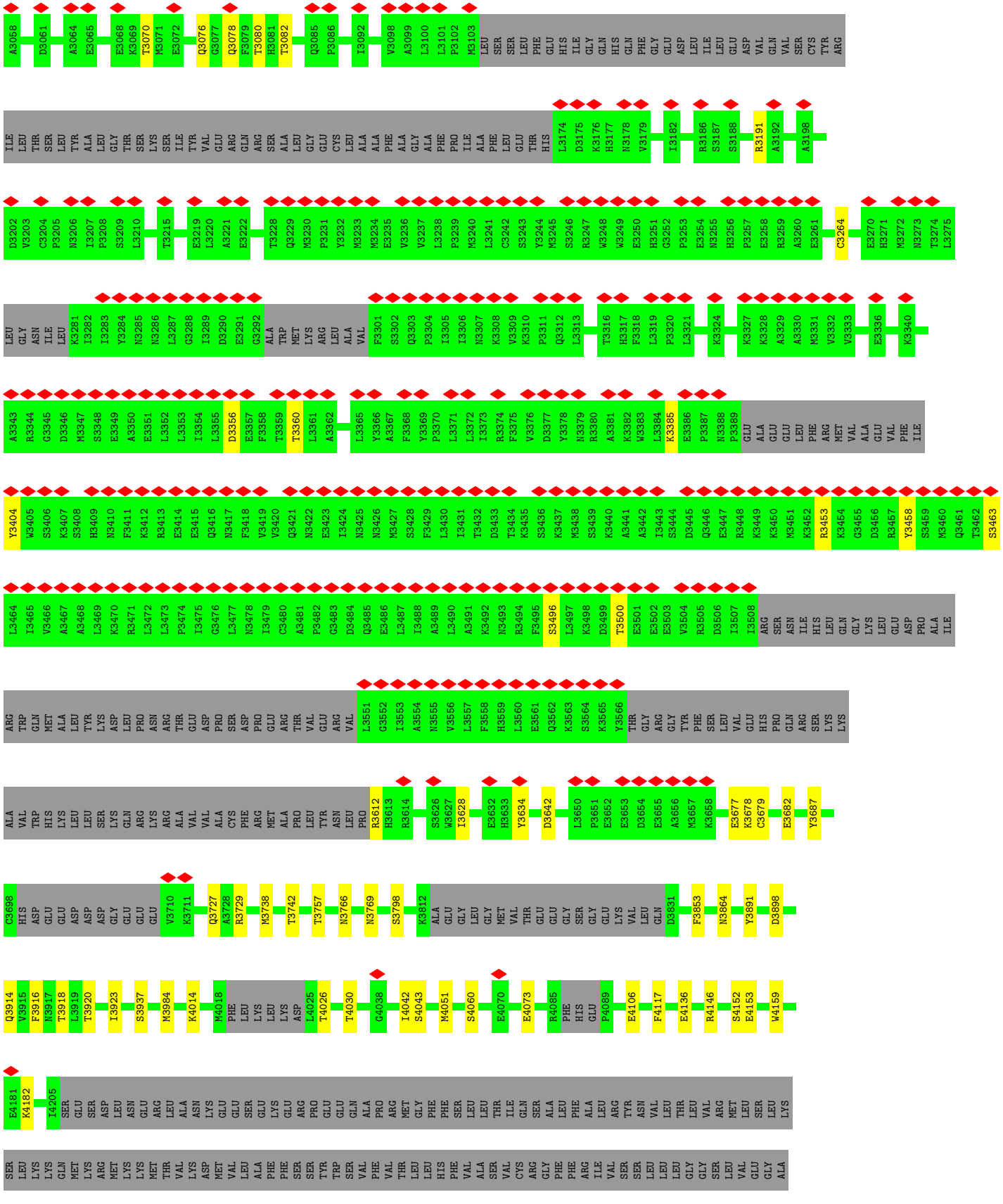
D1068 Q1069 D1070 H1071 A1072 S1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 S1118 R1119 P1120 G1121 CYS GLN PRO D1125 G1129 R1133 R1144 Q1147 E1150 S1155 W1156 M1168 G1187 D1196 V1197 S1206 L1207 G1208 V1209 F1239 R1245 L1255 P1256 Q1257 F1258
L1259 Q1260 V1261 P1262 H1267 I1268 E1269 V1270 T1271 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287 K1288 S1289 T1297 F1301 Y1302 R1303 L1304 S1305 M1306 P1307 I1308 E1309 C1310 ALA GLU VAL PHE SER LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY
PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU
LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU TYR LEU MET GLN THR SER T1425 S1429 G1435 V1443 F1450 H1451 D1460 ARG VAL ARG THR V1465 T1466 V1467 T1468 D1471 I1480 K1481
R1482 S1483 N1484 CYS TYR MET VAL CYS ALA GLY GLU SER MET SER P1496 G1497 Q1498 G1499 R1500 N1501 N1504 G1505 L1506 V1512 ASP ALA ALA SER G1517 N1524 G1525 K1526 E1527 L1528 S1537 F1545 A1546 Q1547 S1550 P1551 N1552 V1553 F1556 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO
LEU SER ALA G1570 K1577 P1584 P1585 R1586 L1587 H1588 V1589 Q1590 F1591 L1592 S1593 H1594 W1597 N1602 R1611 I1612 S1613 E1614 W1618 L1619 V1620 Q1621 P1625 L1626 Q1627 L1631 D1641 I1642 L1668 V1681 L1686 N1692 K1693 R1700 L1712 M1722 N1723 T1734


T1756 R1761 M1762 R1763 F1764 F1769 N1774 Y1777 Q1778 Y1779 S1780 P1781 E1782 M1832 I1847 E1848 P1849 SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS
ARG PRO LYS GLU G1891 L1892 Q1910 C1913 R1918 E1922 F1927 D1930 R1942 Y1943 N1944 E1945 V1946 M1947 Q1948 A1949 L1950 N1951 M1952 T1957 A1958 R1959 K1960 THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU CYS
PRO C1987 P1988 E1989 E1990 I1991 R1992 D1993 Q1994 L1995 F1998 H1999 E2000 D2001 L2002 M2003 T2004 I2008 E2012 G2018 R2025 G2026 R2027 L2031 T2036 Y2037 L2038 K2039 K2040 LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS S2055 R2067 P2077 V2080 Q2090
I2094 G2095 V2098 R2099 T2106 I2107 V2112 I2116 R2126 S2130 V2131 R2132 H2157 P2158 N2159 R2162 V2175 R2204 I2205 S2206 D2215 S2218 Y2219 L2220 L2221 E2222 N2223 S2224 S2225 L2228 A2229 S2230 P2231 S2236 T2237 D2260 M2278 Y2284 P2285 D2286 I2287 P2291
E2313 N2317 P2332 A2333 L2334 R2335 G2338 A2344 D2355 R2358 P2363 T2364 S2365 G2366 T2370 LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383 D2396 R2400 E2404 M2405 H2406 L2407 L2422 L2425 ILE PRO LEU G2429 D2430 L2431 V2434 I2435
Q2440 MET PRO THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY PHE C2460 P2461 D2462 V2468 L2469 F2470 Y2475 GLY ILE GLU V2479 V2489 L2492 P2493 D2494 L2495 R2496 A2497 A2514 T2521 P2525 L2526 L2527 THR ARG CYS ALA PRO LEU PHE ALA GLY THR
GLU HIS HIS ALA SER LEU ILE ASP SER LEU LEU LEU HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER ILE C2576 G2577 Q2578 L2579 R2580 P2581 S2582 H2586 L2587 L2588 V2592 F2593 D2594 L2609 T2610 E2614 K2618
Y2619 Y2620 W2626 E2636 I2647 L2651 S2652 Q2653 K2654 K2655 Y2656 E2657 Q2658 F2661 P2666 A2672 Y2679 M2687 Q2691 S2692 S2693 M2694 ASP SER GLU GLY ASN PHE ASN PRO GLN PRO V2705 D2706 T2707 S2708 N2709 I2710 I2711 I2712 P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722
Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782
A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP A2816 A2817 H2818 G2819 Y2820 S2821 P2822 R2823 A2824 I2825 D2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842
M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 ARG GLY
PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL
VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE L2982 S2983 R2987 P2988 L2989 A2995 S2996 T3004 G3011 R3015 H3016 ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE L3035 V3044 G3048 S3054 A3055 L3056 R3057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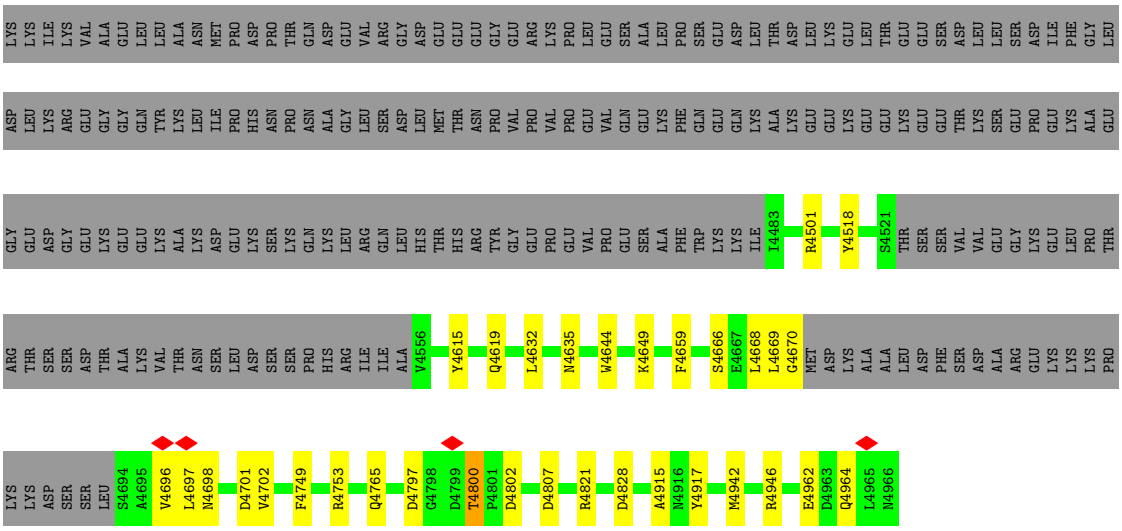
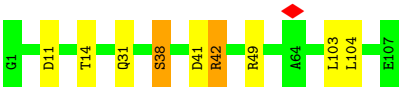
ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS L3174 D3175 K3176 H3177 N3178 V3179 I3182 R3186 S3187 S3188 R3191 A3192 A3198
D3202 V3203 C3204 P3205 N3206 I3207 P3208 S3209 L3210 T3215 E3219 L3220 A3221 E3222 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 V3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 M3245 S3246 R3247 W3248 W3249 E3250 H3251 G3252 P3253 E3254 N3255 H3256 P3257 E3258 R3259 A3260 E3261 C3264 E3270 H3271 M3272 N3273 T3274 L3275
LEU GLY ASN ILE LEU K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 ALA TRP MET LYS ARG LEU ALA VAL F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 T3316 H3317 F3318 L3319 P3320 L3321 K3324 K3327 K3328 A3329 A3330 M3331 V3332 V3333 E3336 K3340
A3343 R3344 G3345 D3346 M3347 S3348 H3349 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357 F3358 T3359 T3360 L3361 A3362 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374 F3375 V3376 D3377 Y3378 N3379 R3380 A3381 K3382 W3383 L3384 K3385 E3386 P3387 N3388 P3389 GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE
Y3404 W3405 S3406 K3407 S3408 H3409 N3410 F3411 K3412 R3413 E3414 E3415 Q3416 N3417 F3418 V3419 V3420 Q3421 N3422 E3423 I3424 N3425 N3426 M3427 S3428 F3429 L3430 I3431 T3432 D3433 T3434 K3435 S3436 K3437 M3438 S3439 K3440 A3441 A3442 I3443 S3444 D3445 Q3446 E3447 R3448 K3449 K3450 M3451 K3452 R3453 K3454 G3455 D3456 R3457 Y3458 S3459 M3460 Q3461 T3462 S3463
L3464 I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 C3480 A3481 P3482 G3483 D3484 Q3485 E3486 L3487 I3488 A3489 L3490 A3491 K3492 N3493 R3494 F3495 S3496 L3497 K3498 D3499 T3500 E3501 E3502 E3503 V3504 R3505 D3506 I3507 I3508 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 GLU ASP PRO SER ASP PRO GLU ARG THR VAL GLU ARG VAL L3551 G3552 I3553 A3554 N3555 V3556 L3557 F3558 H3559 L3560 E3561 Q3562 K3563 S3564 K3565 Y3566 THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS
ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN LEU PRO R3612 H3613 R3614 S3626 W3627 I3628 E3632 H3633 Y3634 D3642 L3650 P3651 E3652 E3653 D3664 E3665 A3666 M3657 K3658 E3677 K3678 C3679 E3682 Y3687
C3698 HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU V3710 K3711 Q3727 A3728 R3729 M3738 T3742 T3757 N3766 N3769 S3798 K3812 ALA GLU GLY LEU GLY MET VAL THR GLU GLU GLY SER GLY GLU LYS VAL LEU GLN D3831 F3853 N3864 Y3891 D3898
Q3914 V3915 F3916 N3917 T3918 L3919 T3920 I3923 S3937 M3984 K4014 M4018 PHE LEU LYS LEU LYS ASP L4025 T4026 T4030 G4038 I4042 S4043 M4051 S4060 E4070 E4073 R4085 PHE HIS GLU P4089 E4106 F4117 E4136 R4146 S4152 E4153 W4159
E4181 K4182 I4205 SER GLU SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER LEU LYS
SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE VAL ALA SER VAL CYS ARG GLY PHE PHE ARG ILE VAL SER SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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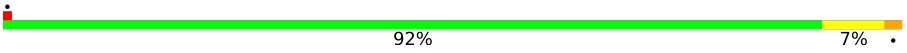
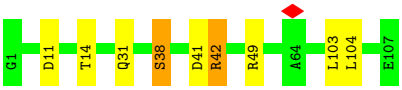
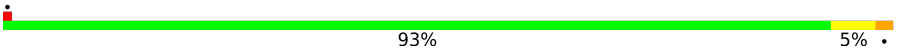
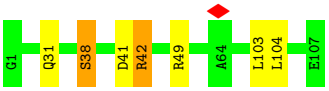




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

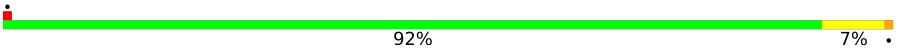
Chain G:

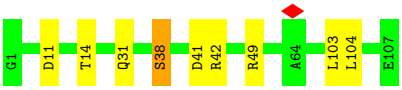




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	282778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50, 50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.715	Depositor
Minimum map value	-0.955	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.38	0/31107	0.67	22/42056 (0.1%)
1	B	0.38	0/31107	0.67	16/42056 (0.0%)
1	C	0.38	0/31107	0.67	17/42056 (0.0%)
1	D	0.38	0/31107	0.67	19/42056 (0.0%)
2	E	0.31	0/834	0.65	1/1123 (0.1%)
2	F	0.31	0/834	0.65	1/1123 (0.1%)
2	G	0.31	0/834	0.64	1/1123 (0.1%)
2	H	0.31	0/834	0.64	0/1123
All	All	0.38	0/127764	0.67	77/172716 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
1	C	0	9
1	D	0	7
All	All	0	34

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	536	LEU	CA-CB-CG	8.00	133.70	115.30
1	A	536	LEU	CA-CB-CG	7.99	133.68	115.30
1	C	536	LEU	CA-CB-CG	7.97	133.64	115.30
1	D	536	LEU	CA-CB-CG	7.96	133.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1303	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	2162	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	2162	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	1303	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	1303	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	2162	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	640	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	640	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	1303	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	2067	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	536	LEU	CB-CG-CD1	6.16	121.48	111.00
1	A	2162	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	1496	PRO	N-CA-CB	6.16	110.69	103.30
1	D	1496	PRO	N-CA-CB	6.15	110.68	103.30
1	A	536	LEU	CB-CG-CD1	6.14	121.45	111.00
1	B	536	LEU	CB-CG-CD1	6.12	121.41	111.00
1	B	2067	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	536	LEU	CB-CG-CD1	6.12	121.41	111.00
1	B	1496	PRO	N-CA-CB	6.11	110.63	103.30
1	C	2067	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	D	2067	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	1942	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	1942	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	1496	PRO	N-CA-CB	5.97	110.47	103.30
1	A	1942	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	1500	ARG	N-CA-C	5.92	126.99	111.00
1	D	1942	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	4501	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	D	1700	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	1700	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	1700	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	4501	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	C	3729	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	1700	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	4501	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	4501	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	1500	ARG	N-CA-C	5.62	126.17	111.00
1	D	3729	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	3729	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	3729	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	640	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	640	ARG	NE-CZ-NH1	5.41	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1918	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	D	4501	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	1918	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	1918	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	428	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	1918	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	750	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	2679	TYR	CB-CG-CD2	5.20	124.12	121.00
1	B	750	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	4501	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	C	1761	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	2679	TYR	CA-CB-CG	5.18	123.24	113.40
1	C	428	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	428	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	4501	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	750	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	428	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	C	4501	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	1761	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	1761	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	F	42	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	750	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	G	42	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	545	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	1556	PHE	CB-CG-CD1	5.06	124.34	120.80
1	A	1761	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	E	42	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	545	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	545	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	235	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	3879	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1552	ASN	Peptide
1	A	159	TRP	Peptide
1	A	1769	PHE	Peptide
1	A	1780	SER	Peptide
1	A	2038	LEU	Peptide
1	A	2131	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	2525	PRO	Peptide
1	A	2655	LYS	Peptide
1	A	618	CYS	Peptide
1	B	1552	ASN	Peptide
1	B	159	TRP	Peptide
1	B	1769	PHE	Peptide
1	B	1780	SER	Peptide
1	B	2130	SER	Peptide
1	B	2525	PRO	Peptide
1	B	2655	LYS	Peptide
1	B	2677	PRO	Peptide
1	B	618	CYS	Peptide
1	C	1552	ASN	Peptide
1	C	159	TRP	Peptide
1	C	1769	PHE	Peptide
1	C	1780	SER	Peptide
1	C	2038	LEU	Peptide
1	C	2133	MET	Peptide
1	C	2525	PRO	Peptide
1	C	2657	GLU	Peptide
1	C	618	CYS	Peptide
1	D	1552	ASN	Peptide
1	D	159	TRP	Peptide
1	D	1769	PHE	Peptide
1	D	1780	SER	Peptide
1	D	2038	LEU	Peptide
1	D	2525	PRO	Peptide
1	D	618	CYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30492	29287	29275	204	0
1	B	30492	29286	29275	212	0
1	C	30492	29286	29275	206	0
1	D	30492	29284	29275	215	0
2	E	818	824	824	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	818	824	824	4	0
2	G	818	824	824	3	0
2	H	818	824	824	4	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
All	All	125244	120439	120396	848	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 3.

All (848) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:ASP:O	1:D:616:SER:OG	2.07	0.72
1:C:612:ASP:O	1:C:616:SER:OG	2.07	0.70
1:B:612:ASP:O	1:B:616:SER:OG	2.07	0.70
1:A:612:ASP:O	1:A:616:SER:OG	2.07	0.69
1:C:2278:MET:SD	1:C:2284:TYR:OH	2.51	0.69
1:A:2278:MET:SD	1:A:2284:TYR:OH	2.51	0.69
1:D:2278:MET:SD	1:D:2284:TYR:OH	2.51	0.69
1:B:2278:MET:SD	1:B:2284:TYR:OH	2.51	0.69
1:D:1586:ARG:NH2	1:D:1587:LEU:O	2.27	0.68
1:A:235:ARG:NE	1:A:268:SER:O	2.27	0.68
1:A:900:LEU:O	1:A:913:ARG:NH2	2.26	0.68
1:B:1586:ARG:NH2	1:B:1587:LEU:O	2.27	0.68
1:D:900:LEU:O	1:D:913:ARG:NH2	2.26	0.68
1:A:1586:ARG:NH2	1:A:1587:LEU:O	2.27	0.68
1:B:235:ARG:NE	1:B:268:SER:O	2.27	0.68
1:C:235:ARG:NE	1:C:268:SER:O	2.27	0.68
1:C:699:SER:OG	1:C:721:ASP:OD2	2.12	0.68
1:B:900:LEU:O	1:B:913:ARG:NH2	2.26	0.67
1:C:1586:ARG:NH2	1:C:1587:LEU:O	2.27	0.67
1:C:900:LEU:O	1:C:913:ARG:NH2	2.26	0.67
1:B:1756:THR:OG1	1:B:1922:GLU:OE2	2.12	0.67
1:C:1756:THR:OG1	1:C:1922:GLU:OE2	2.13	0.67
1:D:1990:GLU:OE1	1:D:1992:ARG:NH1	2.28	0.67
1:A:1245:ARG:NH1	1:A:1693:LYS:O	2.28	0.67
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.28	0.67
1:B:699:SER:OG	1:B:721:ASP:OD2	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4106:GLU:OE2	1:D:4146:ARG:NH1	2.28	0.67
1:B:1245:ARG:NH1	1:B:1693:LYS:O	2.28	0.67
1:D:235:ARG:NE	1:D:268:SER:O	2.27	0.67
1:D:699:SER:OG	1:D:721:ASP:OD2	2.13	0.67
1:B:1990:GLU:OE1	1:B:1992:ARG:NH1	2.28	0.67
1:B:3078:GLN:O	1:B:3082:THR:OG1	2.13	0.67
1:C:1119:ARG:NH2	1:C:1196:ASP:O	2.28	0.67
1:A:1756:THR:OG1	1:A:1922:GLU:OE2	2.13	0.66
1:C:1990:GLU:OE1	1:C:1992:ARG:NH1	2.28	0.66
1:C:4106:GLU:OE2	1:C:4146:ARG:NH1	2.28	0.66
1:D:3891:TYR:OH	1:D:3898:ASP:OD1	2.13	0.66
1:B:4106:GLU:OE2	1:B:4146:ARG:NH1	2.28	0.66
1:D:870:SER:OG	1:D:1009:ARG:NH1	2.28	0.66
1:D:1245:ARG:NH1	1:D:1693:LYS:O	2.28	0.66
1:D:1756:THR:OG1	1:D:1922:GLU:OE2	2.13	0.66
1:A:4106:GLU:OE2	1:A:4146:ARG:NH1	2.28	0.66
1:B:3891:TYR:OH	1:B:3898:ASP:OD1	2.13	0.66
1:C:721:ASP:O	1:C:724:SER:OG	2.12	0.66
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.28	0.66
1:C:778:MET:O	1:C:1468:THR:OG1	2.14	0.66
1:C:870:SER:OG	1:C:1009:ARG:NH1	2.28	0.66
1:C:1245:ARG:NH1	1:C:1693:LYS:O	2.28	0.66
1:A:699:SER:OG	1:A:721:ASP:OD2	2.13	0.66
1:A:778:MET:O	1:A:1468:THR:OG1	2.14	0.66
1:B:300:VAL:HG21	1:B:419:ILE:HD12	1.77	0.66
1:B:870:SER:OG	1:B:1009:ARG:NH1	2.28	0.66
1:B:1119:ARG:NH2	1:B:1196:ASP:O	2.28	0.66
1:B:969:ASN:ND2	1:B:981:MET:SD	2.69	0.66
1:A:1990:GLU:OE1	1:A:1992:ARG:NH1	2.28	0.66
1:A:3078:GLN:O	1:A:3082:THR:OG1	2.13	0.66
1:C:3891:TYR:OH	1:C:3898:ASP:OD1	2.13	0.66
1:A:560:SER:OG	1:A:561:ARG:NH2	2.29	0.66
1:A:3727:GLN:OE1	1:A:3769:ASN:ND2	2.29	0.66
1:B:497:LEU:O	1:B:501:CYS:N	2.29	0.66
1:D:969:ASN:ND2	1:D:981:MET:SD	2.69	0.66
1:D:3727:GLN:OE1	1:D:3769:ASN:ND2	2.29	0.66
1:B:778:MET:O	1:B:1468:THR:OG1	2.14	0.65
1:C:497:LEU:O	1:C:501:CYS:N	2.29	0.65
1:C:560:SER:OG	1:C:561:ARG:NH2	2.29	0.65
1:A:870:SER:OG	1:A:1009:ARG:NH1	2.28	0.65
1:A:1309:GLU:OE1	1:A:1577:LYS:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:969:ASN:ND2	1:C:981:MET:SD	2.69	0.65
1:C:3727:GLN:OE1	1:C:3769:ASN:ND2	2.29	0.65
1:B:3727:GLN:OE1	1:B:3769:ASN:ND2	2.29	0.65
1:C:1443:VAL:O	1:C:1496:PRO:N	2.29	0.65
1:A:969:ASN:ND2	1:A:981:MET:SD	2.69	0.65
1:C:1309:GLU:OE1	1:C:1577:LYS:N	2.30	0.65
1:A:1723:ASN:O	1:A:1918:ARG:NH2	2.30	0.65
1:A:627:SER:OG	1:A:2134:GLY:N	2.30	0.65
1:C:300:VAL:HG21	1:C:419:ILE:HD12	1.77	0.65
1:A:300:VAL:HG21	1:A:419:ILE:HD12	1.77	0.65
1:A:3891:TYR:OH	1:A:3898:ASP:OD1	2.14	0.65
1:B:560:SER:OG	1:B:561:ARG:NH2	2.29	0.65
1:D:300:VAL:HG21	1:D:419:ILE:HD12	1.77	0.65
1:D:3078:GLN:O	1:D:3082:THR:OG1	2.13	0.65
1:B:1309:GLU:OE1	1:B:1577:LYS:N	2.30	0.65
1:B:1443:VAL:O	1:B:1496:PRO:N	2.31	0.65
1:C:2018:GLY:O	1:C:2025:ARG:NH2	2.30	0.65
1:D:1309:GLU:OE1	1:D:1577:LYS:N	2.30	0.65
1:D:1723:ASN:O	1:D:1918:ARG:NH2	2.30	0.65
1:D:778:MET:O	1:D:1468:THR:OG1	2.14	0.64
1:D:4635:ASN:ND2	1:D:4668:LEU:O	2.30	0.64
1:B:1723:ASN:O	1:B:1918:ARG:NH2	2.30	0.64
1:D:497:LEU:O	1:D:501:CYS:N	2.30	0.64
1:A:4749:PHE:O	1:A:4753:ARG:NH1	2.30	0.64
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.31	0.64
1:C:4635:ASN:ND2	1:C:4668:LEU:O	2.30	0.64
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.30	0.64
1:D:4749:PHE:O	1:D:4753:ARG:NH1	2.30	0.64
1:C:1723:ASN:O	1:C:1918:ARG:NH2	2.30	0.64
1:C:4749:PHE:O	1:C:4753:ARG:NH1	2.30	0.64
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.30	0.64
1:B:4749:PHE:O	1:B:4753:ARG:NH1	2.30	0.64
1:A:2018:GLY:O	1:A:2025:ARG:NH2	2.31	0.64
1:B:4635:ASN:ND2	1:B:4668:LEU:O	2.30	0.64
1:D:2018:GLY:O	1:D:2025:ARG:NH2	2.31	0.64
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.30	0.64
1:B:2018:GLY:O	1:B:2025:ARG:NH2	2.31	0.64
1:C:626:ARG:NH1	1:C:1668:LEU:O	2.31	0.64
1:A:497:LEU:O	1:A:501:CYS:N	2.30	0.63
1:A:4635:ASN:ND2	1:A:4668:LEU:O	2.30	0.63
1:B:332:ARG:N	1:B:362:TYR:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:HIS:NE2	1:A:919:VAL:O	2.32	0.63
1:A:626:ARG:NH1	1:A:1668:LEU:O	2.32	0.63
1:D:332:ARG:N	1:D:362:TYR:O	2.32	0.63
1:A:2106:THR:OG1	1:A:3612:ARG:O	2.16	0.62
1:D:890:HIS:NE2	1:D:919:VAL:O	2.32	0.62
1:A:842:GLN:OE1	1:A:844:ARG:NH2	2.32	0.62
1:A:2358:ARG:NH1	1:A:2365:SER:O	2.31	0.62
1:B:3360:THR:O	1:B:3404:TYR:OH	2.17	0.62
1:C:3078:GLN:O	1:C:3082:THR:OG1	2.13	0.62
1:A:332:ARG:N	1:A:362:TYR:O	2.32	0.62
1:B:40:GLU:OE1	1:B:420:ARG:NH1	2.32	0.62
1:B:890:HIS:NE2	1:B:919:VAL:O	2.32	0.62
1:D:842:GLN:OE1	1:D:844:ARG:NH2	2.32	0.62
1:B:2358:ARG:NH1	1:B:2365:SER:O	2.32	0.62
1:A:4136:GLU:O	1:A:4917:TYR:OH	2.18	0.62
1:C:332:ARG:N	1:C:362:TYR:O	2.32	0.62
1:C:2358:ARG:NH1	1:C:2365:SER:O	2.32	0.62
1:D:4014:LYS:NZ	1:D:4060:SER:O	2.33	0.62
1:B:4014:LYS:NZ	1:B:4060:SER:O	2.33	0.62
1:C:890:HIS:NE2	1:C:919:VAL:O	2.32	0.62
1:D:40:GLU:OE1	1:D:420:ARG:NH1	2.32	0.62
1:D:1501:ASN:O	1:D:1505:GLY:N	2.32	0.62
1:C:842:GLN:OE1	1:C:844:ARG:NH2	2.32	0.62
1:D:1443:VAL:O	1:D:1496:PRO:N	2.33	0.62
1:A:2215:ASP:O	1:A:2218:SER:OG	2.15	0.62
1:A:2580:ARG:NH1	1:A:2614:GLU:OE1	2.33	0.62
1:A:4014:LYS:NZ	1:A:4060:SER:O	2.33	0.62
1:C:40:GLU:OE1	1:C:420:ARG:NH1	2.32	0.62
1:C:4014:LYS:NZ	1:C:4060:SER:O	2.33	0.62
1:B:842:GLN:OE1	1:B:844:ARG:NH2	2.32	0.61
1:A:40:GLU:OE1	1:A:420:ARG:NH1	2.32	0.61
1:B:721:ASP:O	1:B:724:SER:OG	2.12	0.61
1:C:480:ARG:NH1	1:C:3677:GLU:OE2	2.33	0.61
1:D:480:ARG:NH1	1:D:3677:GLU:OE2	2.33	0.61
1:D:2215:ASP:O	1:D:2218:SER:OG	2.15	0.61
1:D:2358:ARG:NH1	1:D:2365:SER:O	2.32	0.61
1:D:4136:GLU:O	1:D:4917:TYR:OH	2.18	0.61
1:B:480:ARG:NH1	1:B:3677:GLU:OE2	2.33	0.61
1:C:1614:GLU:O	1:C:1619:LEU:N	2.34	0.61
1:D:560:SER:OG	1:D:561:ARG:NH2	2.34	0.61
1:A:1614:GLU:O	1:A:1619:LEU:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ARG:NH1	1:A:3677:GLU:OE2	2.33	0.61
1:D:1614:GLU:O	1:D:1619:LEU:N	2.34	0.60
1:D:2580:ARG:NH1	1:D:2614:GLU:OE1	2.34	0.60
1:C:859:GLN:NE2	1:C:859:GLN:O	2.34	0.60
1:B:626:ARG:NH1	1:B:1668:LEU:O	2.34	0.60
1:B:1614:GLU:O	1:B:1619:LEU:N	2.34	0.60
1:B:859:GLN:O	1:B:859:GLN:NE2	2.34	0.60
1:B:4136:GLU:O	1:B:4917:TYR:OH	2.18	0.60
1:C:2215:ASP:O	1:C:2218:SER:OG	2.14	0.60
1:A:1631:LEU:HD13	1:A:1642:ILE:HD11	1.83	0.60
1:D:859:GLN:O	1:D:859:GLN:NE2	2.34	0.60
1:A:859:GLN:O	1:A:859:GLN:NE2	2.34	0.60
2:F:38:SER:OG	2:F:41:ASP:OD1	2.20	0.60
2:E:38:SER:OG	2:E:41:ASP:OD1	2.20	0.60
1:C:1631:LEU:HD13	1:C:1642:ILE:HD11	1.82	0.60
2:H:38:SER:OG	2:H:41:ASP:OD1	2.20	0.60
1:A:1465:VAL:O	1:A:1483:SER:N	2.35	0.59
1:C:2580:ARG:NH1	1:C:2614:GLU:OE1	2.34	0.59
1:A:858:THR:OG1	1:A:861:ALA:O	2.17	0.59
2:G:38:SER:OG	2:G:41:ASP:OD1	2.20	0.59
1:B:1631:LEU:HD13	1:B:1642:ILE:HD11	1.83	0.59
1:B:2580:ARG:NH1	1:B:2614:GLU:OE1	2.36	0.59
1:A:1144:ARG:N	1:A:1150:GLU:O	2.36	0.59
1:B:1465:VAL:O	1:B:1483:SER:N	2.35	0.59
1:B:1501:ASN:N	1:B:1505:GLY:O	2.36	0.59
1:B:2106:THR:OG1	1:B:3612:ARG:O	2.16	0.59
1:D:1465:VAL:O	1:D:1483:SER:N	2.35	0.59
1:D:1631:LEU:HD13	1:D:1642:ILE:HD11	1.82	0.59
1:C:3360:THR:O	1:C:3404:TYR:OH	2.17	0.58
1:C:4136:GLU:O	1:C:4917:TYR:OH	2.18	0.58
1:A:3356:ASP:O	1:A:3360:THR:OG1	2.16	0.58
1:B:1144:ARG:N	1:B:1150:GLU:O	2.36	0.58
1:C:1144:ARG:N	1:C:1150:GLU:O	2.36	0.58
1:D:1144:ARG:N	1:D:1150:GLU:O	2.36	0.58
1:A:255:GLU:OE2	1:A:258:ARG:NH1	2.37	0.58
1:A:3385:LYS:O	1:A:3453:ARG:NH1	2.36	0.58
1:C:1465:VAL:O	1:C:1483:SER:N	2.35	0.58
1:D:2576:CYS:O	1:D:2618:LYS:NZ	2.36	0.58
1:B:770:ILE:O	1:B:773:GLN:NE2	2.36	0.58
1:C:255:GLU:OE2	1:C:258:ARG:NH1	2.37	0.58
1:C:770:ILE:O	1:C:773:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:770:ILE:O	1:D:773:GLN:NE2	2.37	0.58
1:A:770:ILE:O	1:A:773:GLN:NE2	2.36	0.58
1:D:3385:LYS:O	1:D:3453:ARG:NH1	2.37	0.58
1:C:2576:CYS:O	1:C:2618:LYS:NZ	2.36	0.58
1:D:3076:GLN:O	1:D:3080:THR:HG23	2.04	0.58
1:B:255:GLU:OE2	1:B:258:ARG:NH1	2.37	0.58
1:B:3385:LYS:O	1:B:3453:ARG:NH1	2.37	0.58
1:B:2576:CYS:O	1:B:2618:LYS:NZ	2.37	0.57
1:C:3385:LYS:O	1:C:3453:ARG:NH1	2.37	0.57
1:D:255:GLU:OE2	1:D:258:ARG:NH1	2.37	0.57
1:B:1504:ASN:O	1:B:1524:ASN:ND2	2.38	0.57
1:A:1763:ARG:O	1:A:1778:GLN:N	2.37	0.57
1:C:1763:ARG:O	1:C:1778:GLN:N	2.37	0.57
1:D:889:ILE:HD12	1:D:892:LEU:HD12	1.86	0.57
1:B:889:ILE:HD12	1:B:892:LEU:HD12	1.86	0.57
1:C:889:ILE:HD12	1:C:892:LEU:HD12	1.86	0.57
1:C:925:PRO:O	1:C:929:ARG:N	2.38	0.57
1:D:3360:THR:O	1:D:3404:TYR:OH	2.17	0.57
1:C:3076:GLN:O	1:C:3080:THR:HG23	2.04	0.57
1:A:3076:GLN:O	1:A:3080:THR:HG23	2.04	0.57
1:D:858:THR:OG1	1:D:861:ALA:O	2.16	0.57
1:A:889:ILE:HD12	1:A:892:LEU:HD12	1.86	0.56
1:A:1550:SER:O	1:A:1550:SER:OG	2.22	0.56
1:A:2036:THR:HG21	1:A:3628:ILE:HG23	1.87	0.56
1:B:3076:GLN:O	1:B:3080:THR:HG23	2.04	0.56
1:C:2159:ASN:OD1	1:C:2162:ARG:NH2	2.38	0.56
1:D:2159:ASN:OD1	1:D:2162:ARG:NH2	2.38	0.56
1:B:2636:GLU:OE1	1:B:2679:TYR:OH	2.16	0.56
1:B:4696:VAL:HG13	1:B:4697:LEU:HG	1.87	0.56
1:C:2396:ASP:OD1	1:C:2400:ARG:NE	2.39	0.56
1:C:2106:THR:OG1	1:C:3612:ARG:O	2.17	0.56
1:B:925:PRO:O	1:B:929:ARG:N	2.38	0.56
1:B:2036:THR:HG21	1:B:3628:ILE:HG23	1.88	0.56
1:B:2215:ASP:O	1:B:2218:SER:OG	2.15	0.56
1:D:2106:THR:OG1	1:D:3612:ARG:O	2.16	0.56
1:C:564:ARG:O	1:C:1586:ARG:NH2	2.39	0.56
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.38	0.56
1:B:858:THR:OG1	1:B:861:ALA:O	2.16	0.56
1:C:2430:ASP:O	1:C:2434:VAL:HG13	2.05	0.56
1:B:2430:ASP:O	1:B:2434:VAL:HG13	2.05	0.56
1:D:218:SER:OG	1:D:219:SER:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2430:ASP:O	1:D:2434:VAL:HG13	2.05	0.56
1:A:2430:ASP:O	1:A:2434:VAL:HG13	2.05	0.55
1:D:4696:VAL:HG13	1:D:4697:LEU:HG	1.87	0.55
1:A:1144:ARG:NH1	1:A:1150:GLU:OE2	2.40	0.55
1:A:4696:VAL:HG13	1:A:4697:LEU:HG	1.87	0.55
1:B:564:ARG:O	1:B:1586:ARG:NH2	2.39	0.55
1:C:2036:THR:HG21	1:C:3628:ILE:HG23	1.88	0.55
1:A:925:PRO:O	1:A:929:ARG:N	2.38	0.55
1:D:3458:TYR:O	1:D:3463:SER:N	2.39	0.55
1:A:2576:CYS:O	1:A:2618:LYS:NZ	2.38	0.55
1:B:2396:ASP:OD1	1:B:2400:ARG:NE	2.39	0.55
1:B:3191:ARG:NE	1:B:3191:ARG:O	2.40	0.55
1:C:2223:ASN:O	1:C:2225:SER:OG	2.22	0.55
1:D:70:GLU:OE1	1:D:122:ARG:NH1	2.40	0.55
1:D:1144:ARG:NH1	1:D:1150:GLU:OE2	2.40	0.55
1:C:4696:VAL:HG13	1:C:4697:LEU:HG	1.88	0.55
1:D:925:PRO:O	1:D:929:ARG:N	2.38	0.55
1:D:3191:ARG:O	1:D:3191:ARG:NE	2.40	0.55
1:A:2077:PRO:HA	1:A:2080:VAL:HG12	1.88	0.55
1:B:218:SER:OG	1:B:219:SER:N	2.39	0.55
1:B:1763:ARG:O	1:B:1778:GLN:N	2.38	0.55
1:A:3191:ARG:O	1:A:3191:ARG:NE	2.39	0.55
1:B:1144:ARG:NH1	1:B:1150:GLU:OE2	2.39	0.55
1:C:3191:ARG:O	1:C:3191:ARG:NE	2.39	0.55
1:A:218:SER:OG	1:A:219:SER:N	2.39	0.55
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.38	0.55
1:A:3360:THR:O	1:A:3404:TYR:OH	2.20	0.55
1:B:3458:TYR:O	1:B:3463:SER:N	2.40	0.55
1:C:1913:CYS:SG	1:C:2090:GLN:NE2	2.80	0.55
1:C:2077:PRO:HA	1:C:2080:VAL:HG12	1.88	0.55
1:C:3458:TYR:O	1:C:3463:SER:N	2.40	0.55
1:D:2396:ASP:OD1	1:D:2400:ARG:NE	2.39	0.55
1:A:70:GLU:OE1	1:A:122:ARG:NH1	2.40	0.54
1:C:237:LEU:O	1:C:404:ASN:N	2.40	0.54
1:D:1763:ARG:O	1:D:1778:GLN:N	2.37	0.54
1:B:2077:PRO:HA	1:B:2080:VAL:HG12	1.88	0.54
1:C:70:GLU:OE1	1:C:122:ARG:NH1	2.40	0.54
1:B:606:ARG:O	1:B:608:HIS:ND1	2.41	0.54
1:B:783:ASN:ND2	1:B:1460:ASP:O	2.41	0.54
1:C:1144:ARG:NH1	1:C:1150:GLU:OE2	2.40	0.54
1:D:2036:THR:HG21	1:D:3628:ILE:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:892:LEU:HD13	1:C:1056:THR:HG21	1.89	0.54
1:A:564:ARG:O	1:A:1586:ARG:NH2	2.39	0.54
1:A:606:ARG:O	1:A:608:HIS:ND1	2.41	0.54
1:A:2396:ASP:OD1	1:A:2400:ARG:NE	2.39	0.54
1:B:892:LEU:HD13	1:B:1056:THR:HG21	1.89	0.54
1:C:218:SER:OG	1:C:219:SER:N	2.40	0.54
1:C:305:TYR:O	1:C:317:MET:N	2.40	0.54
1:D:892:LEU:HD13	1:D:1056:THR:HG21	1.89	0.54
1:B:2223:ASN:O	1:B:2225:SER:OG	2.22	0.54
1:B:70:GLU:OE1	1:B:122:ARG:NH1	2.40	0.54
1:B:237:LEU:O	1:B:404:ASN:N	2.40	0.54
1:D:2077:PRO:HA	1:D:2080:VAL:HG12	1.88	0.54
1:A:305:TYR:O	1:A:317:MET:N	2.40	0.54
1:D:1913:CYS:SG	1:D:2090:GLN:NE2	2.80	0.54
1:A:783:ASN:ND2	1:A:1460:ASP:O	2.41	0.53
1:A:3458:TYR:O	1:A:3463:SER:N	2.40	0.53
1:C:359:SER:O	1:C:404:ASN:ND2	2.41	0.53
1:C:2588:LEU:O	1:C:2592:VAL:HG23	2.08	0.53
1:A:2588:LEU:O	1:A:2592:VAL:HG23	2.08	0.53
1:D:564:ARG:O	1:D:1586:ARG:NH2	2.39	0.53
1:D:654:SER:OG	1:D:655:MET:N	2.42	0.53
1:D:1129:GLY:O	1:D:1147:GLN:N	2.42	0.53
1:A:359:SER:O	1:A:404:ASN:ND2	2.41	0.53
1:A:1129:GLY:O	1:A:1147:GLN:N	2.42	0.53
1:C:654:SER:OG	1:C:655:MET:N	2.42	0.53
1:D:1712:LEU:HD22	1:D:1832:MET:SD	2.49	0.53
1:A:892:LEU:HD13	1:A:1056:THR:HG21	1.89	0.53
1:C:606:ARG:O	1:C:608:HIS:ND1	2.41	0.53
1:D:606:ARG:O	1:D:608:HIS:ND1	2.42	0.53
1:D:783:ASN:ND2	1:D:1460:ASP:O	2.41	0.53
1:A:654:SER:OG	1:A:655:MET:N	2.42	0.53
1:A:2223:ASN:O	1:A:2225:SER:OG	2.22	0.53
1:B:359:SER:O	1:B:404:ASN:ND2	2.41	0.53
1:C:783:ASN:ND2	1:C:1460:ASP:O	2.41	0.53
1:C:1712:LEU:HD22	1:C:1832:MET:SD	2.49	0.53
1:D:2588:LEU:O	1:D:2592:VAL:HG23	2.08	0.53
1:A:237:LEU:O	1:A:404:ASN:N	2.41	0.52
1:B:305:TYR:O	1:B:317:MET:N	2.40	0.52
1:B:2588:LEU:O	1:B:2592:VAL:HG23	2.08	0.52
1:D:305:TYR:O	1:D:317:MET:N	2.40	0.52
1:D:359:SER:O	1:D:404:ASN:ND2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLN:N	1:C:12:GLN:OE1	2.41	0.52
1:C:1692:ASN:OD1	1:C:1693:LYS:N	2.43	0.52
1:D:2112:VAL:O	1:D:2116:ILE:HD12	2.10	0.52
1:A:572:LEU:HD13	1:A:612:ASP:CB	2.40	0.52
1:A:2112:VAL:O	1:A:2116:ILE:HD12	2.10	0.52
1:C:1129:GLY:O	1:C:1147:GLN:N	2.42	0.52
1:C:2112:VAL:O	1:C:2116:ILE:HD12	2.10	0.52
1:B:1712:LEU:HD22	1:B:1832:MET:SD	2.49	0.52
1:C:1930:ASP:OD1	1:C:2027:ARG:NH2	2.43	0.52
1:A:1712:LEU:HD22	1:A:1832:MET:SD	2.49	0.52
1:C:1847:ILE:HG22	1:C:1892:LEU:HB3	1.92	0.52
1:D:1692:ASN:OD1	1:D:1693:LYS:N	2.43	0.52
1:D:1847:ILE:HG22	1:D:1892:LEU:HB3	1.92	0.52
1:D:1930:ASP:OD1	1:D:2027:ARG:NH2	2.43	0.52
1:A:1297:THR:O	1:A:1547:GLN:NE2	2.43	0.52
1:B:1692:ASN:OD1	1:B:1693:LYS:N	2.43	0.52
1:B:2112:VAL:O	1:B:2116:ILE:HD12	2.10	0.52
1:D:1297:THR:O	1:D:1547:GLN:NE2	2.43	0.52
1:B:12:GLN:N	1:B:12:GLN:OE1	2.43	0.52
1:B:1297:THR:O	1:B:1547:GLN:NE2	2.43	0.52
1:B:2334:LEU:N	1:B:2338:GLY:O	2.43	0.52
1:D:237:LEU:O	1:D:404:ASN:N	2.41	0.52
1:C:1172:THR:O	1:C:1172:THR:OG1	2.28	0.52
1:D:1527:GLU:O	1:D:1528:LEU:HD23	2.10	0.52
1:A:12:GLN:OE1	1:A:12:GLN:N	2.43	0.51
1:A:1930:ASP:OD1	1:A:2027:ARG:NH2	2.43	0.51
1:B:654:SER:OG	1:B:655:MET:N	2.42	0.51
1:C:550:GLN:O	1:C:554:SER:N	2.44	0.51
1:D:162:ILE:O	1:D:163:HIS:ND1	2.44	0.51
1:A:162:ILE:O	1:A:163:HIS:ND1	2.44	0.51
1:A:409:GLN:NE2	1:A:3864:ASN:OD1	2.43	0.51
1:C:1297:THR:O	1:C:1547:GLN:NE2	2.43	0.51
1:A:418:VAL:HG12	1:A:462:TYR:HE2	1.76	0.51
1:B:162:ILE:O	1:B:163:HIS:ND1	2.44	0.51
1:C:162:ILE:O	1:C:163:HIS:ND1	2.44	0.51
1:A:1692:ASN:OD1	1:A:1693:LYS:N	2.43	0.51
1:B:1847:ILE:HG22	1:B:1892:LEU:HB3	1.92	0.51
1:D:12:GLN:N	1:D:12:GLN:OE1	2.43	0.51
1:D:946:LEU:HD23	1:D:1064:LEU:HD11	1.93	0.51
1:A:1526:LYS:HG3	1:A:1528:LEU:HD21	1.93	0.51
1:A:2334:LEU:N	1:A:2338:GLY:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:992:GLN:O	1:B:996:VAL:HG23	2.11	0.51
1:B:2334:LEU:HD21	1:B:2344:ALA:CB	2.41	0.51
1:D:1035:TYR:CD1	1:D:1038:LEU:HD12	2.46	0.51
1:A:1035:TYR:CD1	1:A:1038:LEU:HD12	2.46	0.51
1:A:2334:LEU:HD21	1:A:2344:ALA:CB	2.41	0.51
1:B:418:VAL:HG12	1:B:462:TYR:HE2	1.76	0.51
1:D:418:VAL:HG12	1:D:462:TYR:HE2	1.76	0.51
1:D:1501:ASN:O	1:D:1504:ASN:N	2.44	0.51
1:A:992:GLN:O	1:A:996:VAL:HG23	2.11	0.51
1:D:992:GLN:O	1:D:996:VAL:HG23	2.11	0.51
1:D:2334:LEU:HD21	1:D:2344:ALA:CB	2.41	0.51
1:B:1625:PRO:O	1:B:1626:LEU:HD12	2.11	0.51
1:B:2422:LEU:O	1:B:2431:LEU:HD11	2.11	0.51
1:C:436:LEU:HD13	1:C:447:LEU:HB2	1.92	0.51
1:C:992:GLN:O	1:C:996:VAL:HG23	2.11	0.51
1:C:2334:LEU:N	1:C:2338:GLY:O	2.43	0.51
1:B:1035:TYR:CD1	1:B:1038:LEU:HD12	2.46	0.50
1:C:2422:LEU:O	1:C:2431:LEU:HD11	2.11	0.50
1:D:626:ARG:NH1	1:D:1668:LEU:O	2.43	0.50
1:A:946:LEU:HD23	1:A:1064:LEU:HD11	1.94	0.50
1:A:1625:PRO:O	1:A:1626:LEU:HD12	2.12	0.50
1:B:436:LEU:HD13	1:B:447:LEU:HB2	1.92	0.50
1:B:1930:ASP:OD1	1:B:2027:ARG:NH2	2.43	0.50
1:C:418:VAL:HG12	1:C:462:TYR:HE2	1.76	0.50
1:C:2334:LEU:HD21	1:C:2344:ALA:CB	2.41	0.50
1:A:1847:ILE:HG22	1:A:1892:LEU:HB3	1.92	0.50
1:B:1129:GLY:O	1:B:1147:GLN:N	2.42	0.50
1:C:3916:PHE:O	1:C:3920:THR:HG23	2.12	0.50
1:D:2223:ASN:O	1:D:2225:SER:OG	2.22	0.50
1:D:2334:LEU:N	1:D:2338:GLY:O	2.43	0.50
1:C:1722:MET:SD	1:C:2126:ARG:NH1	2.84	0.50
1:D:550:GLN:O	1:D:554:SER:N	2.43	0.50
1:A:804:LEU:HD12	1:A:1618:TRP:CZ3	2.47	0.50
1:B:946:LEU:HD23	1:B:1064:LEU:HD11	1.94	0.50
1:C:946:LEU:HD23	1:C:1064:LEU:HD11	1.94	0.50
1:D:1625:PRO:O	1:D:1626:LEU:HD12	2.12	0.50
1:D:2422:LEU:O	1:D:2431:LEU:HD11	2.11	0.50
1:A:436:LEU:HD13	1:A:447:LEU:HB2	1.92	0.50
1:C:1526:LYS:HG3	1:C:1528:LEU:HD21	1.93	0.50
1:D:4152:SER:OG	1:D:4153:GLU:N	2.45	0.50
1:C:4701:ASP:OD1	1:C:4702:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:LEU:HD13	1:D:447:LEU:HB2	1.92	0.50
1:D:4030:THR:HG21	1:D:4051:MET:SD	2.52	0.50
1:C:804:LEU:HD12	1:C:1618:TRP:CZ3	2.47	0.50
1:C:908:ARG:NH1	1:C:928:GLU:OE2	2.45	0.50
1:D:2996:SER:OG	1:D:3070:THR:HG21	2.12	0.50
1:A:908:ARG:NH1	1:A:928:GLU:OE2	2.45	0.49
1:B:908:ARG:NH1	1:B:928:GLU:OE2	2.45	0.49
1:C:288:HIS:O	1:C:290:ARG:NH1	2.45	0.49
1:C:1035:TYR:CD1	1:C:1038:LEU:HD12	2.46	0.49
1:C:1625:PRO:O	1:C:1626:LEU:HD12	2.12	0.49
1:D:804:LEU:HD12	1:D:1618:TRP:CZ3	2.47	0.49
1:C:2996:SER:OG	1:C:3070:THR:HG21	2.12	0.49
1:A:2422:LEU:O	1:A:2431:LEU:HD11	2.12	0.49
1:A:4152:SER:OG	1:A:4153:GLU:N	2.45	0.49
1:D:243:GLU:OE1	1:D:264:GLY:N	2.46	0.49
1:D:3687:TYR:OH	1:D:3757:THR:OG1	2.19	0.49
1:D:3916:PHE:O	1:D:3920:THR:HG23	2.12	0.49
1:B:4152:SER:OG	1:B:4153:GLU:N	2.45	0.49
1:D:4701:ASP:OD1	1:D:4702:VAL:N	2.45	0.49
1:A:4159:TRP:CZ2	1:A:4915:ALA:HB2	2.48	0.49
1:B:804:LEU:HD12	1:B:1618:TRP:CZ3	2.47	0.49
1:B:1526:LYS:HG3	1:B:1528:LEU:HD21	1.93	0.49
1:B:4030:THR:HG21	1:B:4051:MET:SD	2.52	0.49
1:D:288:HIS:O	1:D:290:ARG:NH1	2.46	0.49
1:B:4701:ASP:OD1	1:B:4702:VAL:N	2.45	0.49
1:C:145:PHE:O	1:C:205:ALA:N	2.43	0.49
1:D:1273:ILE:O	1:D:1287:GLN:N	2.46	0.49
1:A:243:GLU:OE1	1:A:264:GLY:N	2.46	0.49
1:A:550:GLN:O	1:A:554:SER:N	2.44	0.49
1:A:1631:LEU:HD13	1:A:1642:ILE:CD1	2.43	0.49
1:A:2996:SER:OG	1:A:3070:THR:HG21	2.12	0.49
1:A:4030:THR:HG21	1:A:4051:MET:SD	2.52	0.49
1:B:3916:PHE:O	1:B:3920:THR:HG23	2.12	0.49
1:C:243:GLU:OE1	1:C:264:GLY:N	2.45	0.49
1:B:1631:LEU:HD13	1:B:1642:ILE:CD1	2.43	0.49
1:D:2779:LYS:NZ	1:D:2846:ASN:OD1	2.46	0.49
2:E:38:SER:O	2:E:42:ARG:NH2	2.46	0.49
2:F:38:SER:O	2:F:42:ARG:NH2	2.46	0.49
2:H:11:ASP:OD2	2:H:14:THR:OG1	2.16	0.49
1:A:4701:ASP:OD1	1:A:4702:VAL:N	2.45	0.49
1:D:908:ARG:NH1	1:D:928:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:ILE:O	1:A:1287:GLN:N	2.46	0.48
1:A:2008:ILE:HG23	1:A:2012:GLU:HB2	1.95	0.48
1:B:243:GLU:OE1	1:B:264:GLY:N	2.46	0.48
1:B:4159:TRP:CZ2	1:B:4915:ALA:HB2	2.48	0.48
1:D:4159:TRP:CZ2	1:D:4915:ALA:HB2	2.48	0.48
1:A:2582:SER:HB2	1:A:2875:THR:HG22	1.94	0.48
1:B:550:GLN:O	1:B:554:SER:N	2.44	0.48
1:C:4030:THR:HG21	1:C:4051:MET:SD	2.52	0.48
1:D:1631:LEU:HD13	1:D:1642:ILE:CD1	2.43	0.48
1:B:288:HIS:O	1:B:290:ARG:NH1	2.46	0.48
1:B:2582:SER:HB2	1:B:2875:THR:HG22	1.94	0.48
1:D:1526:LYS:HG3	1:D:1528:LEU:HD21	1.95	0.48
1:A:288:HIS:O	1:A:290:ARG:NH1	2.46	0.48
1:A:537:LEU:HD13	1:A:538:ALA:N	2.29	0.48
1:A:1722:MET:SD	1:A:2126:ARG:NH1	2.87	0.48
1:A:3916:PHE:O	1:A:3920:THR:HG23	2.12	0.48
1:B:1527:GLU:O	1:B:1528:LEU:HD23	2.14	0.48
1:B:2996:SER:OG	1:B:3070:THR:HG21	2.12	0.48
1:C:2582:SER:HB2	1:C:2875:THR:HG22	1.95	0.48
1:C:4152:SER:OG	1:C:4153:GLU:N	2.45	0.48
1:D:537:LEU:HD13	1:D:538:ALA:N	2.28	0.48
1:A:2779:LYS:NZ	1:A:2846:ASN:OD1	2.46	0.48
1:B:2228:LEU:HD12	1:B:2237:THR:HB	1.96	0.48
1:C:1527:GLU:O	1:C:1528:LEU:HD23	2.12	0.48
1:C:2228:LEU:HD12	1:C:2237:THR:HB	1.96	0.48
1:C:2779:LYS:NZ	1:C:2846:ASN:OD1	2.45	0.48
1:A:145:PHE:O	1:A:205:ALA:N	2.44	0.48
2:G:38:SER:O	2:G:42:ARG:NH2	2.46	0.48
1:A:2228:LEU:HD12	1:A:2237:THR:HB	1.96	0.48
1:B:2779:LYS:NZ	1:B:2846:ASN:OD1	2.46	0.48
1:C:1273:ILE:O	1:C:1287:GLN:N	2.46	0.48
1:C:4159:TRP:CZ2	1:C:4915:ALA:HB2	2.48	0.48
1:C:4649:LYS:HG2	1:C:4669:LEU:HD23	1.96	0.48
1:D:305:TYR:N	1:D:317:MET:O	2.46	0.48
1:D:1550:SER:O	1:D:1550:SER:OG	2.25	0.48
1:D:1722:MET:SD	1:D:2126:ARG:NH1	2.87	0.48
1:D:2582:SER:HB2	1:D:2875:THR:HG22	1.94	0.48
1:D:4649:LYS:HG2	1:D:4669:LEU:HD23	1.96	0.48
1:C:1206:SER:O	1:C:1207:LEU:HD23	2.14	0.48
1:C:4807:ASP:OD1	1:C:4807:ASP:N	2.47	0.48
1:B:537:LEU:HD13	1:B:538:ALA:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4807:ASP:N	1:B:4807:ASP:OD1	2.47	0.48
2:H:38:SER:O	2:H:42:ARG:NH2	2.46	0.48
1:D:2228:LEU:HD12	1:D:2237:THR:HB	1.96	0.47
1:D:4807:ASP:OD1	1:D:4807:ASP:N	2.47	0.47
1:A:1613:SER:O	1:A:1613:SER:OG	2.32	0.47
1:B:2008:ILE:HG23	1:B:2012:GLU:HB2	1.95	0.47
1:C:1691:GLU:OE1	1:C:1791:LYS:NZ	2.33	0.47
1:D:4797:ASP:O	1:D:4800:THR:OG1	2.22	0.47
1:A:4802:ASP:OD1	1:A:4802:ASP:N	2.48	0.47
1:C:18:ASP:OD1	1:C:18:ASP:N	2.47	0.47
1:C:537:LEU:HD13	1:C:538:ALA:N	2.28	0.47
1:D:2008:ILE:HG23	1:D:2012:GLU:HB2	1.95	0.47
1:A:1206:SER:O	1:A:1207:LEU:HD23	2.14	0.47
1:B:409:GLN:NE2	1:B:3864:ASN:OD1	2.48	0.47
1:C:3914:GLN:O	1:C:3918:THR:HG23	2.14	0.47
2:G:103:LEU:HD23	2:G:104:LEU:N	2.30	0.47
1:A:853:PRO:HB2	1:A:1209:VAL:HG22	1.96	0.47
1:A:1527:GLU:O	1:A:1528:LEU:HD23	2.15	0.47
1:A:4042:ILE:HD12	1:A:4043:SER:O	2.14	0.47
1:B:1273:ILE:O	1:B:1287:GLN:N	2.46	0.47
1:D:853:PRO:HB2	1:D:1209:VAL:HG22	1.97	0.47
1:D:1206:SER:O	1:D:1207:LEU:HD23	2.14	0.47
1:C:1631:LEU:HD13	1:C:1642:ILE:CD1	2.43	0.47
2:E:11:ASP:OD2	2:E:14:THR:OG1	2.16	0.47
1:A:4649:LYS:HG2	1:A:4669:LEU:HD23	1.96	0.47
2:H:103:LEU:HD23	2:H:104:LEU:N	2.29	0.47
1:B:4042:ILE:HD12	1:B:4043:SER:O	2.15	0.47
1:C:305:TYR:N	1:C:317:MET:O	2.46	0.47
1:C:853:PRO:HB2	1:C:1209:VAL:HG22	1.97	0.47
1:D:655:MET:N	1:D:792:VAL:O	2.48	0.47
1:D:4042:ILE:HD12	1:D:4043:SER:O	2.15	0.47
1:B:1722:MET:SD	1:B:2126:ARG:NH1	2.87	0.47
1:C:2008:ILE:HG23	1:C:2012:GLU:HB2	1.95	0.47
2:F:103:LEU:HD23	2:F:104:LEU:N	2.30	0.47
1:B:1206:SER:O	1:B:1207:LEU:HD23	2.14	0.47
1:B:4649:LYS:HG2	1:B:4669:LEU:HD23	1.96	0.47
1:B:4802:ASP:OD1	1:B:4802:ASP:N	2.48	0.47
1:D:18:ASP:N	1:D:18:ASP:OD1	2.47	0.47
1:D:145:PHE:O	1:D:205:ALA:N	2.44	0.47
1:A:4807:ASP:OD1	1:A:4807:ASP:N	2.48	0.46
1:B:305:TYR:N	1:B:317:MET:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4042:ILE:HD12	1:C:4043:SER:O	2.14	0.46
1:D:409:GLN:NE2	1:D:3864:ASN:OD1	2.48	0.46
1:D:1257:GLN:O	1:D:1597:TRP:N	2.48	0.46
2:E:103:LEU:HD23	2:E:104:LEU:N	2.29	0.46
1:B:18:ASP:N	1:B:18:ASP:OD1	2.47	0.46
1:C:4802:ASP:N	1:C:4802:ASP:OD1	2.47	0.46
1:D:2790:ARG:NH1	1:D:2791:THR:O	2.48	0.46
1:B:3864:ASN:OD1	1:B:3865:THR:OG1	2.15	0.46
1:B:3914:GLN:O	1:B:3918:THR:HG23	2.16	0.46
1:A:2586:HIS:NE2	1:A:2875:THR:HG21	2.31	0.46
1:B:853:PRO:HB2	1:B:1209:VAL:HG22	1.96	0.46
1:B:1257:GLN:O	1:B:1597:TRP:N	2.49	0.46
1:C:655:MET:N	1:C:792:VAL:O	2.48	0.46
1:C:2586:HIS:NE2	1:C:2875:THR:HG21	2.31	0.46
1:A:438:LYS:NZ	1:A:507:VAL:HG11	2.31	0.46
1:A:3914:GLN:O	1:A:3918:THR:HG23	2.15	0.46
1:B:612:ASP:O	1:B:616:SER:CB	2.64	0.46
1:B:655:MET:N	1:B:792:VAL:O	2.48	0.46
1:D:4802:ASP:OD1	1:D:4802:ASP:N	2.48	0.46
1:A:830:GLU:OE2	1:A:830:GLU:N	2.49	0.46
1:A:1257:GLN:O	1:A:1597:TRP:N	2.49	0.46
1:B:438:LYS:NZ	1:B:507:VAL:HG11	2.31	0.46
1:B:2586:HIS:NE2	1:B:2875:THR:HG21	2.31	0.46
1:A:231:GLY:O	1:A:276:ARG:NH1	2.48	0.46
1:D:2586:HIS:NE2	1:D:2875:THR:HG21	2.31	0.46
1:D:3914:GLN:O	1:D:3918:THR:HG23	2.15	0.46
1:B:231:GLY:O	1:B:276:ARG:NH1	2.49	0.46
1:C:950:VAL:CG1	1:C:1064:LEU:HD13	2.46	0.46
1:D:438:LYS:NZ	1:D:507:VAL:HG11	2.31	0.46
1:D:950:VAL:CG1	1:D:1064:LEU:HD13	2.46	0.46
1:A:655:MET:N	1:A:792:VAL:O	2.48	0.46
1:B:2175:VAL:HG11	1:B:2219:TYR:OH	2.16	0.46
1:A:2133:MET:SD	1:A:2186:ILE:HD13	2.55	0.46
1:C:1257:GLN:O	1:C:1597:TRP:N	2.49	0.46
1:A:612:ASP:O	1:A:616:SER:CB	2.65	0.45
1:B:572:LEU:HD13	1:B:612:ASP:CB	2.46	0.45
1:A:950:VAL:CG1	1:A:1064:LEU:HD13	2.46	0.45
1:C:4942:MET:O	1:C:4946:ARG:N	2.49	0.45
1:A:1155:SER:OG	1:A:1156:TRP:N	2.50	0.45
1:D:231:GLY:O	1:D:276:ARG:NH1	2.48	0.45
1:A:411:GLU:OE1	1:A:411:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:LYS:NZ	1:A:1198:GLY:O	2.33	0.45
1:C:231:GLY:O	1:C:276:ARG:NH1	2.48	0.45
1:C:548:CYS:SG	1:C:578:VAL:HG22	2.56	0.45
1:D:1155:SER:OG	1:D:1156:TRP:N	2.50	0.45
1:D:3678:LYS:NZ	1:D:3682:GLU:OE1	2.48	0.45
1:A:548:CYS:SG	1:A:578:VAL:HG22	2.57	0.45
1:A:1172:THR:O	1:A:1172:THR:OG1	2.34	0.45
1:B:830:GLU:N	1:B:830:GLU:OE1	2.49	0.45
1:C:572:LEU:HD13	1:C:612:ASP:CB	2.47	0.45
1:C:612:ASP:O	1:C:616:SER:CB	2.64	0.45
1:C:858:THR:OG1	1:C:861:ALA:O	2.16	0.45
1:C:1155:SER:OG	1:C:1156:TRP:N	2.50	0.45
1:D:3923:ILE:HD13	1:D:3984:MET:SD	2.57	0.45
1:A:305:TYR:N	1:A:317:MET:O	2.46	0.45
1:C:438:LYS:NZ	1:C:507:VAL:HG11	2.31	0.45
1:D:4026:THR:O	1:D:4026:THR:OG1	2.32	0.45
1:B:1155:SER:OG	1:B:1156:TRP:N	2.49	0.45
1:B:3923:ILE:HD13	1:B:3984:MET:SD	2.57	0.45
1:B:4942:MET:O	1:B:4946:ARG:N	2.49	0.45
1:D:548:CYS:SG	1:D:578:VAL:HG22	2.57	0.45
1:A:18:ASP:OD1	1:A:18:ASP:N	2.47	0.45
1:A:1550:SER:HA	1:A:1553:VAL:HG12	1.99	0.45
1:A:4942:MET:O	1:A:4946:ARG:N	2.50	0.45
1:B:950:VAL:CG1	1:B:1064:LEU:HD13	2.46	0.45
1:D:830:GLU:OE1	1:D:830:GLU:N	2.49	0.45
1:D:2468:VAL:HG11	1:D:2521:THR:HG22	1.99	0.45
1:B:2461:PRO:HG3	1:B:2514:ALA:HB1	1.99	0.45
1:A:2468:VAL:HG11	1:A:2521:THR:HG22	1.99	0.44
1:A:2790:ARG:NH1	1:A:2791:THR:O	2.50	0.44
1:B:145:PHE:O	1:B:205:ALA:N	2.44	0.44
1:B:179:ASP:N	1:B:179:ASP:OD1	2.50	0.44
1:B:2468:VAL:HG11	1:B:2521:THR:HG22	1.99	0.44
1:D:612:ASP:O	1:D:616:SER:CB	2.65	0.44
1:D:721:ASP:O	1:D:724:SER:OG	2.12	0.44
1:B:411:GLU:OE1	1:B:411:GLU:N	2.50	0.44
1:C:409:GLN:NE2	1:C:3864:ASN:OD1	2.50	0.44
1:D:1504:ASN:OD1	1:D:1526:LYS:NZ	2.50	0.44
1:A:1681:VAL:HG12	1:A:1686:LEU:HD21	2.00	0.44
1:B:548:CYS:SG	1:B:578:VAL:HG22	2.57	0.44
1:B:1172:THR:O	1:B:1172:THR:OG1	2.33	0.44
1:C:179:ASP:OD1	1:C:179:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2175:VAL:HG11	1:C:2219:TYR:OH	2.17	0.44
1:A:3923:ILE:HD13	1:A:3984:MET:SD	2.57	0.44
1:B:579:LEU:HD11	1:B:616:SER:O	2.17	0.44
1:C:579:LEU:HD11	1:C:616:SER:O	2.18	0.44
1:D:179:ASP:OD1	1:D:179:ASP:N	2.50	0.44
1:D:509:SER:OG	1:D:510:SER:N	2.51	0.44
1:A:4821:ARG:NH1	1:D:4828:ASP:OD1	2.50	0.44
1:B:164:PRO:O	1:B:182:ILE:HD12	2.18	0.44
1:C:3923:ILE:HD13	1:C:3984:MET:SD	2.57	0.44
1:B:1550:SER:HA	1:B:1553:VAL:HG12	1.99	0.44
1:C:164:PRO:O	1:C:182:ILE:HD12	2.17	0.44
1:B:2790:ARG:NH1	1:B:2791:THR:O	2.51	0.44
1:C:1614:GLU:N	1:C:1619:LEU:O	2.50	0.44
1:C:2468:VAL:HG11	1:C:2521:THR:HG22	1.99	0.44
1:C:4828:ASP:OD1	1:D:4821:ARG:NH1	2.50	0.44
1:A:2461:PRO:HG3	1:A:2514:ALA:HB1	1.99	0.44
1:A:4828:ASP:OD1	1:B:4821:ARG:NH1	2.51	0.44
1:B:237:LEU:N	1:B:404:ASN:O	2.51	0.44
1:B:4828:ASP:OD1	1:C:4821:ARG:NH1	2.51	0.44
1:D:45:ARG:NH2	1:D:458:ASP:OD2	2.50	0.44
1:D:164:PRO:O	1:D:182:ILE:HD12	2.18	0.44
1:D:1506:LEU:N	1:D:1524:ASN:OD1	2.47	0.44
1:D:1614:GLU:N	1:D:1619:LEU:O	2.50	0.44
1:B:509:SER:OG	1:B:510:SER:N	2.51	0.44
1:A:509:SER:OG	1:A:510:SER:N	2.51	0.43
1:B:40:GLU:OE2	1:B:125:TYR:OH	2.36	0.43
1:B:1927:PHE:CG	1:B:2031:LEU:HD22	2.53	0.43
1:B:4962:GLU:O	1:B:4964:GLN:N	2.51	0.43
1:D:4962:GLU:O	1:D:4964:GLN:N	2.51	0.43
1:B:1681:VAL:HG12	1:B:1686:LEU:HD21	2.00	0.43
1:C:1613:SER:O	1:C:1613:SER:OG	2.32	0.43
1:C:2461:PRO:HG3	1:C:2514:ALA:HB1	2.01	0.43
1:B:3678:LYS:NZ	1:B:3682:GLU:OE1	2.48	0.43
1:C:237:LEU:N	1:C:404:ASN:O	2.51	0.43
1:C:1550:SER:O	1:C:1550:SER:OG	2.25	0.43
1:C:1927:PHE:CG	1:C:2031:LEU:HD22	2.53	0.43
1:C:2094:ILE:O	1:C:2098:VAL:HG13	2.18	0.43
1:C:4962:GLU:O	1:C:4964:GLN:N	2.51	0.43
1:D:1681:VAL:HG12	1:D:1686:LEU:HD21	2.00	0.43
1:D:2094:ILE:O	1:D:2098:VAL:HG13	2.18	0.43
1:D:2404:GLU:CB	1:D:2407:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2461:PRO:HG3	1:D:2514:ALA:HB1	2.00	0.43
1:D:4615:TYR:O	1:D:4619:GLN:NE2	2.52	0.43
1:A:164:PRO:O	1:A:182:ILE:HD12	2.18	0.43
1:C:2790:ARG:NH1	1:C:2791:THR:O	2.51	0.43
1:C:4073:GLU:OE1	1:C:4073:GLU:N	2.51	0.43
1:D:3496:SER:O	1:D:3500:THR:OG1	2.30	0.43
1:A:579:LEU:HD11	1:A:616:SER:O	2.17	0.43
1:A:4073:GLU:N	1:A:4073:GLU:OE1	2.51	0.43
1:B:600:LEU:HD12	1:B:600:LEU:O	2.18	0.43
1:B:1691:GLU:OE1	1:B:1791:LYS:NZ	2.33	0.43
1:B:2636:GLU:OE1	1:B:2636:GLU:N	2.48	0.43
1:B:3011:GLY:O	1:B:3015:ARG:NE	2.52	0.43
1:B:4073:GLU:OE1	1:B:4073:GLU:N	2.51	0.43
1:B:4615:TYR:O	1:B:4619:GLN:NE2	2.52	0.43
1:C:45:ARG:NH2	1:C:458:ASP:OD2	2.50	0.43
1:C:600:LEU:O	1:C:600:LEU:HD12	2.18	0.43
1:D:40:GLU:OE2	1:D:125:TYR:OH	2.36	0.43
1:D:411:GLU:OE1	1:D:411:GLU:N	2.50	0.43
1:D:1613:SER:O	1:D:1613:SER:OG	2.32	0.43
1:D:1927:PHE:CG	1:D:2031:LEU:HD22	2.53	0.43
1:D:2636:GLU:OE1	1:D:2636:GLU:N	2.49	0.43
1:A:758:CYS:SG	1:A:767:SER:OG	2.77	0.43
1:A:2175:VAL:HG11	1:A:2219:TYR:OH	2.18	0.43
1:B:1500:ARG:HA	1:B:1505:GLY:C	2.39	0.43
1:B:2404:GLU:CB	1:B:2407:LEU:HD13	2.48	0.43
1:C:509:SER:OG	1:C:510:SER:N	2.51	0.43
1:C:1550:SER:HA	1:C:1553:VAL:HG12	2.00	0.43
1:C:2404:GLU:CB	1:C:2407:LEU:HD13	2.48	0.43
1:C:4615:TYR:O	1:C:4619:GLN:NE2	2.51	0.43
1:A:179:ASP:OD1	1:A:179:ASP:N	2.50	0.43
1:B:1504:ASN:OD1	1:B:1524:ASN:ND2	2.51	0.43
1:C:758:CYS:SG	1:C:767:SER:OG	2.76	0.43
1:C:1734:THR:HG22	1:C:1756:THR:OG1	2.19	0.43
1:C:3011:GLY:O	1:C:3015:ARG:NE	2.52	0.43
1:D:3738:MET:O	1:D:3742:THR:HG23	2.19	0.43
1:A:2094:ILE:O	1:A:2098:VAL:HG13	2.18	0.43
1:A:2404:GLU:CB	1:A:2407:LEU:HD13	2.48	0.43
1:A:3738:MET:O	1:A:3742:THR:HG23	2.19	0.43
1:B:375:GLN:N	1:B:390:LYS:O	2.52	0.43
1:C:3678:LYS:NZ	1:C:3682:GLU:OE1	2.48	0.43
1:D:1734:THR:HG22	1:D:1756:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4962:GLU:O	1:A:4964:GLN:N	2.51	0.43
1:B:2094:ILE:O	1:B:2098:VAL:HG13	2.18	0.43
1:D:237:LEU:N	1:D:404:ASN:O	2.51	0.43
1:D:600:LEU:HD12	1:D:600:LEU:O	2.18	0.43
1:D:1255:LEU:HD13	1:D:1451:HIS:CE1	2.54	0.43
1:B:436:LEU:HD11	1:B:445:ILE:HG23	2.01	0.42
1:C:587:ASN:N	1:C:587:ASN:OD1	2.52	0.42
1:D:579:LEU:HD21	1:D:586:LEU:CD1	2.49	0.42
1:D:587:ASN:OD1	1:D:587:ASN:N	2.52	0.42
1:D:1550:SER:HA	1:D:1553:VAL:HG12	1.99	0.42
1:A:1168:MET:HE3	1:A:1197:VAL:HG22	2.01	0.42
1:C:636:LEU:O	1:C:642:LEU:HD21	2.19	0.42
1:C:3738:MET:O	1:C:3742:THR:HG23	2.18	0.42
1:A:40:GLU:OE2	1:A:125:TYR:OH	2.36	0.42
1:A:579:LEU:HD21	1:A:586:LEU:CD1	2.49	0.42
1:A:1255:LEU:HD13	1:A:1451:HIS:CE1	2.55	0.42
1:D:579:LEU:HD11	1:D:616:SER:O	2.18	0.42
1:D:2175:VAL:HG11	1:D:2219:TYR:OH	2.18	0.42
1:A:855:VAL:HG12	1:A:1084:ARG:HD3	2.01	0.42
1:A:1927:PHE:CG	1:A:2031:LEU:HD22	2.53	0.42
1:D:436:LEU:HD11	1:D:445:ILE:HG23	2.01	0.42
1:D:3011:GLY:O	1:D:3015:ARG:NE	2.51	0.42
1:A:600:LEU:HD12	1:A:600:LEU:O	2.18	0.42
1:B:636:LEU:O	1:B:642:LEU:HD21	2.20	0.42
1:B:1255:LEU:HD13	1:B:1451:HIS:CE1	2.54	0.42
1:B:1734:THR:HG22	1:B:1756:THR:OG1	2.19	0.42
1:B:3738:MET:O	1:B:3742:THR:HG23	2.19	0.42
1:C:1255:LEU:HD13	1:C:1451:HIS:CE1	2.54	0.42
1:C:2313:GLU:O	1:C:2317:ASN:ND2	2.52	0.42
1:D:1168:MET:HE3	1:D:1197:VAL:HG22	2.01	0.42
1:A:237:LEU:N	1:A:404:ASN:O	2.51	0.42
1:A:823:TYR:O	1:A:826:VAL:HG23	2.20	0.42
1:B:823:TYR:O	1:B:826:VAL:HG23	2.20	0.42
1:C:436:LEU:HD11	1:C:445:ILE:HG23	2.01	0.42
1:C:2095:GLY:O	1:C:2099:ARG:NH1	2.53	0.42
1:D:4765:GLN:OE1	1:D:4765:GLN:N	2.52	0.42
1:A:3011:GLY:O	1:A:3015:ARG:NE	2.52	0.42
1:B:61:ASP:OD2	1:B:298:ARG:NH1	2.53	0.42
1:B:579:LEU:HD21	1:B:586:LEU:CD1	2.50	0.42
1:D:375:GLN:N	1:D:390:LYS:O	2.52	0.42
1:A:45:ARG:NH2	1:A:458:ASP:OD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:LEU:O	1:B:537:LEU:HD22	2.20	0.42
1:C:1681:VAL:HG12	1:C:1686:LEU:HD21	2.01	0.42
1:C:1812:GLY:O	1:C:1814:THR:N	2.53	0.42
1:D:2313:GLU:O	1:D:2317:ASN:ND2	2.53	0.42
1:A:2095:GLY:O	1:A:2099:ARG:NH1	2.53	0.42
1:B:45:ARG:NH2	1:B:458:ASP:OD2	2.50	0.42
1:B:1168:MET:HE3	1:B:1197:VAL:HG22	2.01	0.42
1:C:579:LEU:HD21	1:C:586:LEU:CD1	2.49	0.42
1:A:61:ASP:OD2	1:A:298:ARG:NH1	2.53	0.42
1:A:1614:GLU:N	1:A:1619:LEU:O	2.50	0.42
1:B:504:ARG:O	1:B:507:VAL:HG13	2.20	0.42
1:C:40:GLU:OE2	1:C:125:TYR:OH	2.37	0.42
1:C:537:LEU:HD22	1:C:537:LEU:O	2.20	0.42
1:D:4942:MET:O	1:D:4946:ARG:N	2.50	0.42
1:A:504:ARG:O	1:A:507:VAL:HG13	2.20	0.41
1:B:587:ASN:OD1	1:B:587:ASN:N	2.52	0.41
1:C:1168:MET:HE3	1:C:1197:VAL:HG22	2.01	0.41
1:D:823:TYR:O	1:D:826:VAL:HG23	2.20	0.41
2:F:11:ASP:OD2	2:F:14:THR:OG1	2.16	0.41
1:A:2107:ILE:HG22	1:A:2157:HIS:CE1	2.55	0.41
1:B:1731:THR:O	1:B:1734:THR:OG1	2.37	0.41
1:B:2495:LEU:HD13	1:B:2872:PRO:HD2	2.02	0.41
1:C:566:GLU:HG2	1:C:1587:LEU:HD21	2.02	0.41
1:C:2495:LEU:HD13	1:C:2872:PRO:HD2	2.02	0.41
1:D:2260:ASP:OD1	1:D:2260:ASP:N	2.53	0.41
1:A:1083:GLU:O	1:A:1209:VAL:HG23	2.20	0.41
1:A:1734:THR:HG22	1:A:1756:THR:OG1	2.19	0.41
1:A:2260:ASP:OD1	1:A:2260:ASP:N	2.53	0.41
1:B:2107:ILE:HG22	1:B:2157:HIS:CE1	2.55	0.41
1:D:504:ARG:O	1:D:507:VAL:HG13	2.20	0.41
1:B:1083:GLU:O	1:B:1209:VAL:HG23	2.20	0.41
1:B:1550:SER:O	1:B:1550:SER:OG	2.24	0.41
1:B:1633:ILE:N	1:B:1637:ASN:OD1	2.53	0.41
1:C:414:ARG:O	1:C:418:VAL:HG13	2.21	0.41
1:C:823:TYR:O	1:C:826:VAL:HG23	2.20	0.41
1:D:2495:LEU:HD13	1:D:2872:PRO:HD2	2.02	0.41
1:D:4073:GLU:N	1:D:4073:GLU:OE1	2.51	0.41
1:A:566:GLU:HG2	1:A:1587:LEU:HD21	2.03	0.41
1:A:1118:SER:OG	1:A:1119:ARG:N	2.53	0.41
1:B:414:ARG:O	1:B:418:VAL:HG13	2.21	0.41
1:B:1118:SER:OG	1:B:1119:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1614:GLU:N	1:B:1619:LEU:O	2.50	0.41
1:B:2313:GLU:O	1:B:2317:ASN:ND2	2.52	0.41
1:D:414:ARG:O	1:D:418:VAL:HG13	2.21	0.41
1:D:2095:GLY:O	1:D:2099:ARG:NH1	2.53	0.41
1:A:537:LEU:HD22	1:A:537:LEU:O	2.20	0.41
1:A:2313:GLU:O	1:A:2317:ASN:ND2	2.53	0.41
1:B:1613:SER:O	1:B:1613:SER:OG	2.32	0.41
1:B:1641:ASP:OD1	1:B:1642:ILE:N	2.54	0.41
1:C:1118:SER:OG	1:C:1119:ARG:N	2.53	0.41
1:C:1641:ASP:OD1	1:C:1642:ILE:N	2.54	0.41
1:C:2260:ASP:N	1:C:2260:ASP:OD1	2.53	0.41
1:C:4903:GLY:O	1:C:4906:THR:OG1	2.35	0.41
1:D:1641:ASP:OD1	1:D:1642:ILE:N	2.54	0.41
1:A:1038:LEU:HD13	1:A:1042:THR:HG21	2.03	0.41
1:A:1714:SER:HG	1:A:1777:TYR:HD1	1.65	0.41
1:A:2081:ARG:O	1:A:2085:VAL:HG23	2.21	0.41
1:B:566:GLU:HG2	1:B:1587:LEU:HD21	2.03	0.41
1:C:209:GLN:OE1	1:C:210:THR:N	2.54	0.41
1:C:1083:GLU:O	1:C:1209:VAL:HG23	2.20	0.41
1:D:537:LEU:HD22	1:D:537:LEU:O	2.20	0.41
1:D:579:LEU:HD21	1:D:586:LEU:HD12	2.03	0.41
1:D:4666:SER:O	1:D:4670:GLY:N	2.54	0.41
1:B:2095:GLY:O	1:B:2099:ARG:NH1	2.53	0.41
1:C:504:ARG:O	1:C:507:VAL:HG13	2.20	0.41
1:C:1946:VAL:HG12	1:C:1947:MET:H	1.86	0.41
1:A:436:LEU:HD11	1:A:445:ILE:HG23	2.01	0.41
1:A:4666:SER:O	1:A:4670:GLY:N	2.54	0.41
1:B:536:LEU:HD12	1:B:537:LEU:N	2.36	0.41
1:B:758:CYS:SG	1:B:767:SER:OG	2.79	0.41
1:B:2260:ASP:OD1	1:B:2260:ASP:N	2.53	0.41
1:B:2576:CYS:N	1:B:2578:GLN:OE1	2.54	0.41
1:B:4765:GLN:OE1	1:B:4765:GLN:N	2.52	0.41
1:C:2039:LYS:NZ	1:C:2040:LYS:O	2.42	0.41
1:C:4765:GLN:OE1	1:C:4765:GLN:N	2.52	0.41
1:C:4826:ILE:HG13	1:C:4830:ILE:HD12	2.03	0.41
1:D:536:LEU:HD12	1:D:537:LEU:N	2.36	0.41
1:D:758:CYS:SG	1:D:767:SER:OG	2.76	0.41
1:D:1038:LEU:HD13	1:D:1042:THR:HG21	2.02	0.41
1:D:2107:ILE:HG22	1:D:2157:HIS:CE1	2.55	0.41
1:D:3356:ASP:O	1:D:3360:THR:OG1	2.16	0.41
1:A:4615:TYR:O	1:A:4619:GLN:NE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:GLY:O	1:B:717:GLY:N	2.54	0.41
1:C:2081:ARG:O	1:C:2085:VAL:HG23	2.21	0.41
1:C:3864:ASN:OD1	1:C:3865:THR:OG1	2.15	0.41
1:D:1118:SER:OG	1:D:1119:ARG:N	2.54	0.41
1:D:1946:VAL:HG12	1:D:1947:MET:H	1.86	0.41
1:D:2039:LYS:NZ	1:D:2040:LYS:O	2.43	0.41
1:B:534:TYR:CD1	1:B:537:LEU:HD12	2.56	0.40
1:B:939:THR:O	1:B:943:LEU:HD22	2.22	0.40
1:B:2081:ARG:O	1:B:2085:VAL:HG23	2.21	0.40
1:C:2107:ILE:HG22	1:C:2157:HIS:CE1	2.55	0.40
1:D:534:TYR:CD1	1:D:537:LEU:HD12	2.56	0.40
1:D:2576:CYS:N	1:D:2578:GLN:OE1	2.54	0.40
1:A:375:GLN:N	1:A:390:LYS:O	2.52	0.40
1:A:587:ASN:OD1	1:A:587:ASN:N	2.53	0.40
1:A:715:GLY:O	1:A:717:GLY:N	2.54	0.40
1:A:939:THR:O	1:A:943:LEU:HD22	2.22	0.40
1:A:1633:ILE:N	1:A:1637:ASN:OD1	2.54	0.40
1:A:1641:ASP:OD1	1:A:1642:ILE:N	2.54	0.40
1:C:375:GLN:N	1:C:390:LYS:O	2.52	0.40
1:C:411:GLU:OE1	1:C:411:GLU:N	2.50	0.40
1:C:579:LEU:HD21	1:C:586:LEU:HD12	2.03	0.40
1:C:1176:THR:O	1:C:1176:THR:OG1	2.39	0.40
1:D:61:ASP:OD2	1:D:298:ARG:NH1	2.53	0.40
1:A:152:ASP:O	1:A:154:THR:HG23	2.22	0.40
1:A:4765:GLN:OE1	1:A:4765:GLN:N	2.52	0.40
1:B:1177:LEU:HD12	1:B:1182:LEU:HD11	2.03	0.40
1:D:715:GLY:O	1:D:717:GLY:N	2.54	0.40
1:D:2008:ILE:HG23	1:D:2012:GLU:CB	2.51	0.40
1:A:364:GLN:NE2	1:A:369:GLY:O	2.54	0.40
1:A:534:TYR:CD1	1:A:537:LEU:HD12	2.56	0.40
1:A:3864:ASN:OD1	1:A:3865:THR:OG1	2.15	0.40
1:C:536:LEU:HD12	1:C:537:LEU:N	2.36	0.40
1:D:134:SER:O	1:D:134:SER:OG	2.35	0.40
1:D:1083:GLU:O	1:D:1209:VAL:HG23	2.20	0.40
1:A:1946:VAL:HG12	1:A:1947:MET:H	1.86	0.40
1:B:1031:ARG:HG2	1:B:1038:LEU:HD11	2.04	0.40
1:B:1812:GLY:O	1:B:1814:THR:N	2.53	0.40
1:C:715:GLY:O	1:C:717:GLY:N	2.54	0.40
1:C:1177:LEU:HD12	1:C:1182:LEU:HD11	2.04	0.40
1:D:193:HIS:CG	1:D:206:ALA:HB3	2.57	0.40
1:D:566:GLU:HG2	1:D:1587:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:896:ASN:OD1	1:D:896:ASN:N	2.55	0.40
1:D:2468:VAL:HG11	1:D:2521:THR:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3849/4966 (78%)	3318 (86%)	523 (14%)	8 (0%)	47	77
1	B	3849/4966 (78%)	3325 (86%)	517 (13%)	7 (0%)	47	77
1	C	3849/4966 (78%)	3323 (86%)	516 (13%)	10 (0%)	41	72
1	D	3849/4966 (78%)	3329 (86%)	512 (13%)	8 (0%)	47	77
2	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	F	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	G	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	H	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
All	All	15816/20292 (78%)	13687 (86%)	2096 (13%)	33 (0%)	50	77

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	ASN
1	B	607	ASN
1	B	1501	ASN
1	C	607	ASN
1	C	1497	GLY
1	C	2133	MET
1	D	607	ASN
1	D	1501	ASN

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Mol	Chain	Res	Type
1	A	1501	ASN
1	A	2230	SER
1	B	2230	SER
1	C	1500	ARG
1	C	1501	ASN
1	C	2230	SER
1	D	2230	SER
1	A	1262	PRO
1	A	1500	ARG
1	B	1262	PRO
1	C	1262	PRO
1	D	1262	PRO
1	D	2658	GLN
1	A	1781	PRO
1	B	1781	PRO
1	C	1781	PRO
1	D	1781	PRO
1	A	2231	PRO
1	B	2231	PRO
1	B	2285	PRO
1	C	2231	PRO
1	D	2231	PRO
1	A	2285	PRO
1	C	2285	PRO
1	D	2285	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	A	3181/4355 (73%)	3121 (98%)	60 (2%)	57 77
1	B	3181/4355 (73%)	3120 (98%)	61 (2%)	57 77
1	C	3181/4355 (73%)	3124 (98%)	57 (2%)	59 78
1	D	3181/4355 (73%)	3117 (98%)	64 (2%)	55 76
2	E	88/88 (100%)	85 (97%)	3 (3%)	37 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	88/88 (100%)	85 (97%)	3 (3%)	37 65
2	G	88/88 (100%)	85 (97%)	3 (3%)	37 65
2	H	88/88 (100%)	85 (97%)	3 (3%)	37 65
All	All	13076/17772 (74%)	12822 (98%)	254 (2%)	59 77

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	PHE
1	A	125	TYR
1	A	132	CYS
1	A	179	ASP
1	A	420	ARG
1	A	421	SER
1	A	500	GLU
1	A	536	LEU
1	A	537	LEU
1	A	540	LEU
1	A	542	ARG
1	A	544	ASN
1	A	640	ARG
1	A	644	LEU
1	A	648	LEU
1	A	731	HIS
1	A	760	ASP
1	A	802	PHE
1	A	890	HIS
1	A	895	MET
1	A	962	LYS
1	A	976	TYR
1	A	981	MET
1	A	1239	PHE
1	A	1301	PHE
1	A	1429	SER
1	A	1450	PHE
1	A	1506	LEU
1	A	1545	PHE
1	A	1611	ARG
1	A	1621	GLN
1	A	1769	PHE
1	A	1944	ASN

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Mol	Chain	Res	Type
1	A	2130	SER
1	A	2133	MET
1	A	2260	ASP
1	A	2470	PHE
1	A	2593	PHE
1	A	2610	THR
1	A	2659	GLU
1	A	2678	ASP
1	A	2679	TYR
1	A	2736	LEU
1	A	2887	LYS
1	A	3264	CYS
1	A	3634	TYR
1	A	3642	ASP
1	A	3679	CYS
1	A	3766	ASN
1	A	3798	SER
1	A	3853	PHE
1	A	3937	SER
1	A	4117	PHE
1	A	4182	LYS
1	A	4518	TYR
1	A	4632	LEU
1	A	4644	TRP
1	A	4659	PHE
1	A	4698	ASN
1	A	4800	THR
1	B	42	PHE
1	B	125	TYR
1	B	132	CYS
1	B	179	ASP
1	B	420	ARG
1	B	500	GLU
1	B	501	CYS
1	B	536	LEU
1	B	537	LEU
1	B	540	LEU
1	B	542	ARG
1	B	544	ASN
1	B	640	ARG
1	B	644	LEU
1	B	648	LEU

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Mol	Chain	Res	Type
1	B	731	HIS
1	B	760	ASP
1	B	802	PHE
1	B	890	HIS
1	B	895	MET
1	B	962	LYS
1	B	976	TYR
1	B	1239	PHE
1	B	1301	PHE
1	B	1429	SER
1	B	1450	PHE
1	B	1503	SER
1	B	1506	LEU
1	B	1545	PHE
1	B	1611	ARG
1	B	1621	GLN
1	B	1627	GLN
1	B	1769	PHE
1	B	1944	ASN
1	B	2039	LYS
1	B	2130	SER
1	B	2260	ASP
1	B	2470	PHE
1	B	2593	PHE
1	B	2610	THR
1	B	2658	GLN
1	B	2678	ASP
1	B	2679	TYR
1	B	2736	LEU
1	B	2887	LYS
1	B	3264	CYS
1	B	3634	TYR
1	B	3642	ASP
1	B	3679	CYS
1	B	3766	ASN
1	B	3798	SER
1	B	3853	PHE
1	B	3937	SER
1	B	4117	PHE
1	B	4182	LYS
1	B	4518	TYR
1	B	4632	LEU

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Mol	Chain	Res	Type
1	B	4644	TRP
1	B	4659	PHE
1	B	4698	ASN
1	B	4800	THR
1	C	42	PHE
1	C	125	TYR
1	C	132	CYS
1	C	179	ASP
1	C	420	ARG
1	C	500	GLU
1	C	501	CYS
1	C	536	LEU
1	C	537	LEU
1	C	540	LEU
1	C	542	ARG
1	C	544	ASN
1	C	640	ARG
1	C	644	LEU
1	C	648	LEU
1	C	760	ASP
1	C	787	LEU
1	C	802	PHE
1	C	824	GLU
1	C	890	HIS
1	C	895	MET
1	C	962	LYS
1	C	976	TYR
1	C	981	MET
1	C	1239	PHE
1	C	1300	MET
1	C	1301	PHE
1	C	1450	PHE
1	C	1506	LEU
1	C	1545	PHE
1	C	1611	ARG
1	C	1621	GLN
1	C	1769	PHE
1	C	1910	GLN
1	C	1944	ASN
1	C	2039	LYS
1	C	2260	ASP
1	C	2470	PHE

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Mol	Chain	Res	Type
1	C	2593	PHE
1	C	2656	TYR
1	C	2887	LYS
1	C	2897	ILE
1	C	3264	CYS
1	C	3634	TYR
1	C	3642	ASP
1	C	3679	CYS
1	C	3766	ASN
1	C	3798	SER
1	C	3853	PHE
1	C	3937	SER
1	C	4117	PHE
1	C	4182	LYS
1	C	4518	TYR
1	C	4632	LEU
1	C	4644	TRP
1	C	4659	PHE
1	C	4800	THR
1	D	42	PHE
1	D	125	TYR
1	D	132	CYS
1	D	179	ASP
1	D	420	ARG
1	D	421	SER
1	D	500	GLU
1	D	536	LEU
1	D	537	LEU
1	D	540	LEU
1	D	542	ARG
1	D	544	ASN
1	D	640	ARG
1	D	644	LEU
1	D	648	LEU
1	D	760	ASP
1	D	787	LEU
1	D	802	PHE
1	D	890	HIS
1	D	895	MET
1	D	962	LYS
1	D	976	TYR
1	D	981	MET

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Mol	Chain	Res	Type
1	D	1239	PHE
1	D	1301	PHE
1	D	1429	SER
1	D	1450	PHE
1	D	1506	LEU
1	D	1545	PHE
1	D	1611	ARG
1	D	1621	GLN
1	D	1627	GLN
1	D	1769	PHE
1	D	1910	GLN
1	D	1944	ASN
1	D	2039	LYS
1	D	2130	SER
1	D	2260	ASP
1	D	2470	PHE
1	D	2593	PHE
1	D	2610	THR
1	D	2651	LEU
1	D	2652	SER
1	D	2654	LYS
1	D	2655	LYS
1	D	2656	TYR
1	D	2679	TYR
1	D	2887	LYS
1	D	3264	CYS
1	D	3634	TYR
1	D	3642	ASP
1	D	3679	CYS
1	D	3766	ASN
1	D	3798	SER
1	D	3853	PHE
1	D	3937	SER
1	D	4117	PHE
1	D	4182	LYS
1	D	4518	TYR
1	D	4632	LEU
1	D	4644	TRP
1	D	4659	PHE
1	D	4698	ASN
1	D	4800	THR
2	E	31	GLN

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Mol	Chain	Res	Type
2	E	38	SER
2	E	49	ARG
2	F	31	GLN
2	F	38	SER
2	F	49	ARG
2	G	31	GLN
2	G	38	SER
2	G	49	ARG
2	H	31	GLN
2	H	38	SER
2	H	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	GLN
1	A	658	ASN
1	A	781	ASN
1	A	930	ASN
1	A	1440	ASN
1	A	1547	GLN
1	A	4056	HIS
1	B	409	GLN
1	B	658	ASN
1	B	781	ASN
1	B	930	ASN
1	B	1440	ASN
1	B	4056	HIS
1	C	409	GLN
1	C	658	ASN
1	C	781	ASN
1	C	930	ASN
1	C	1440	ASN
1	C	1451	HIS
1	C	1547	GLN
1	C	2090	GLN
1	C	4056	HIS
1	D	409	GLN
1	D	658	ASN
1	D	781	ASN
1	D	930	ASN
1	D	1440	ASN

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Mol	Chain	Res	Type
1	D	2090	GLN
1	D	4056	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

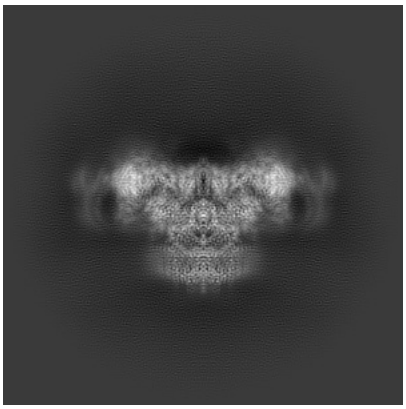
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21861. These allow visual inspection of the internal detail of the map and identification of artifacts.

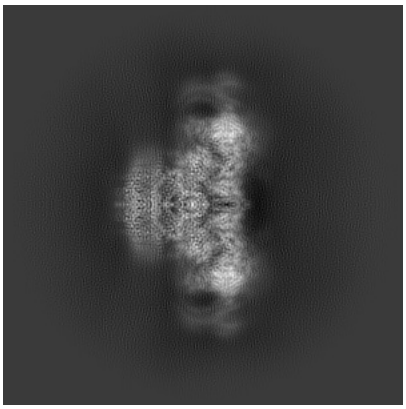
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

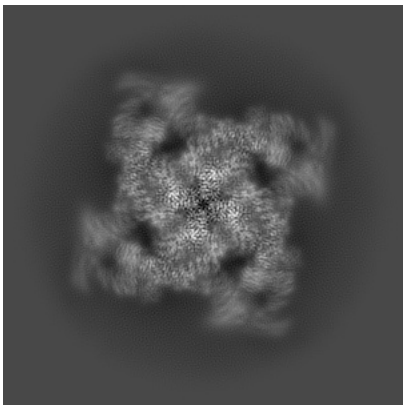
6.1.1 Primary map



X

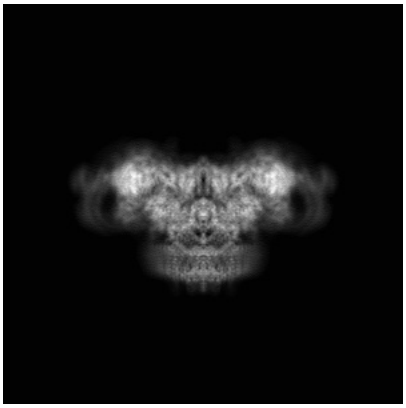


Y

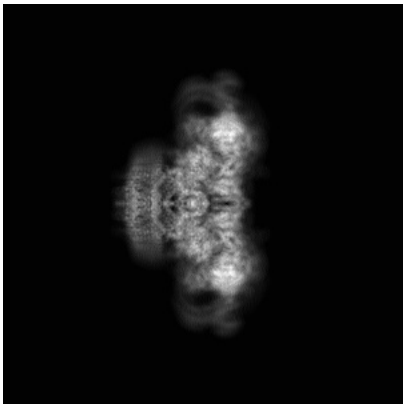


Z

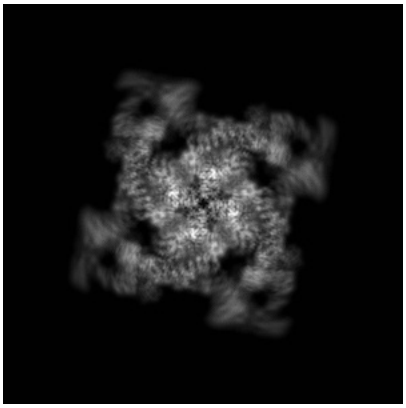
6.1.2 Raw map



X



Y

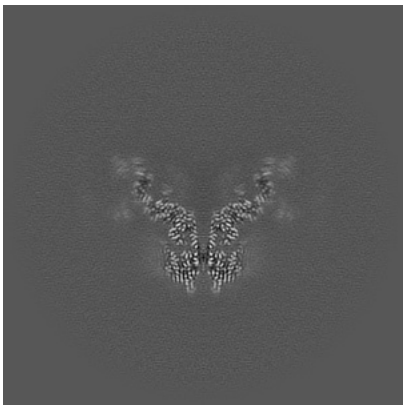


Z

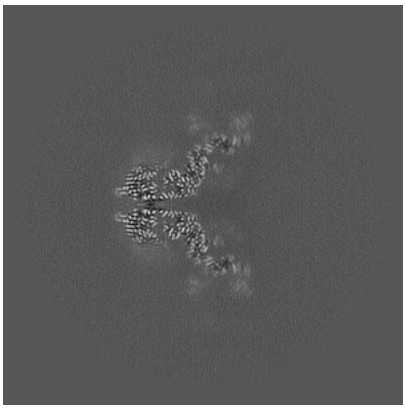
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

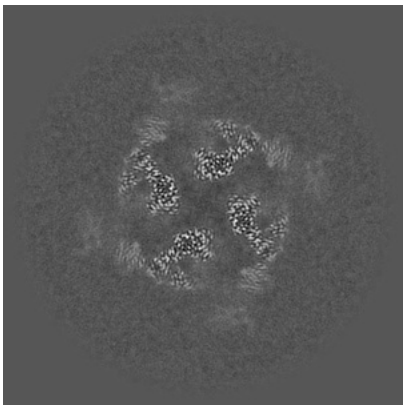
6.2.1 Primary map



X Index: 232

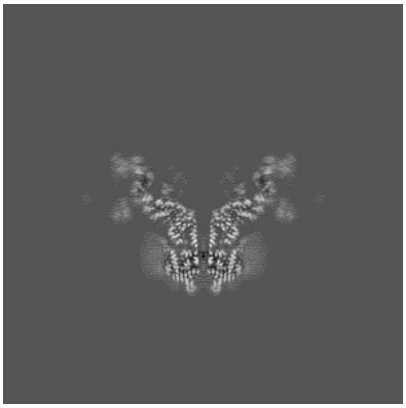


Y Index: 232

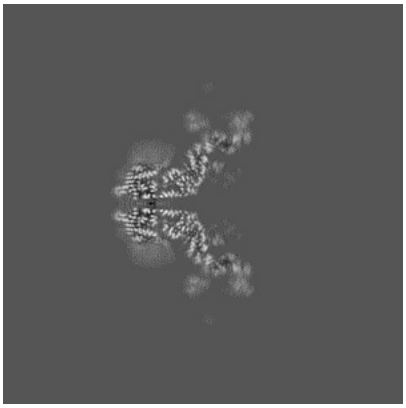


Z Index: 232

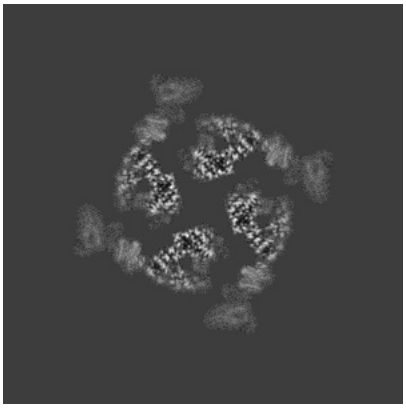
6.2.2 Raw map



X Index: 232



Y Index: 232

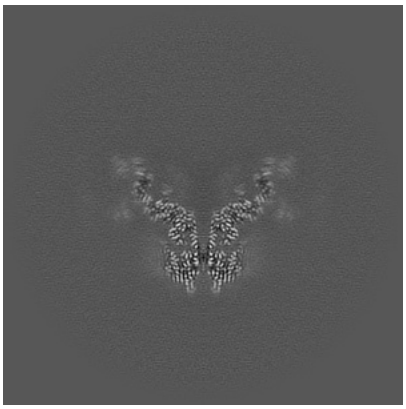


Z Index: 232

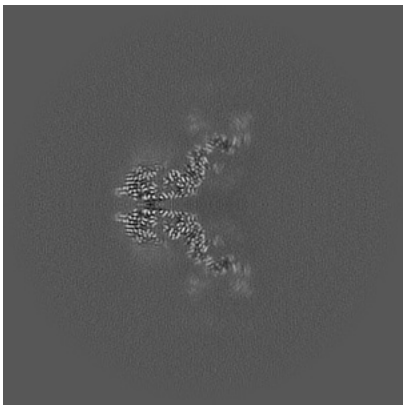
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

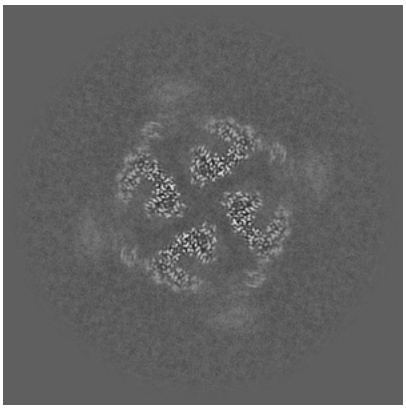
6.3.1 Primary map



X Index: 232

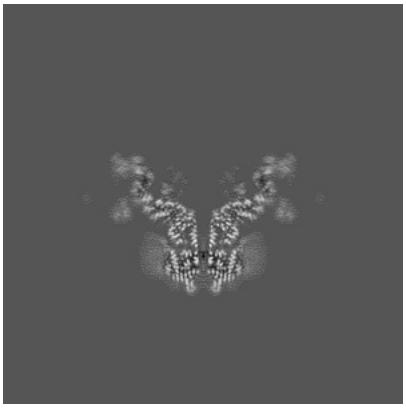


Y Index: 232

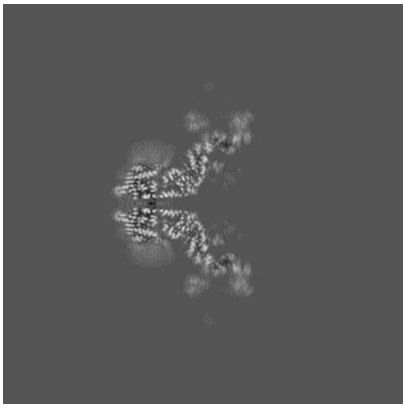


Z Index: 227

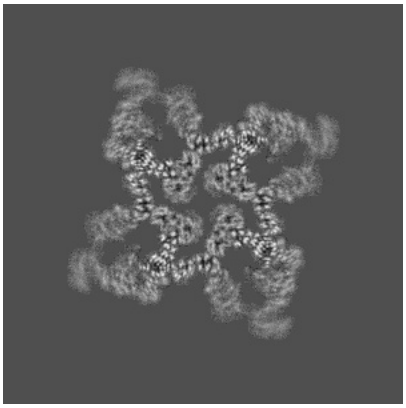
6.3.2 Raw map



X Index: 232



Y Index: 232

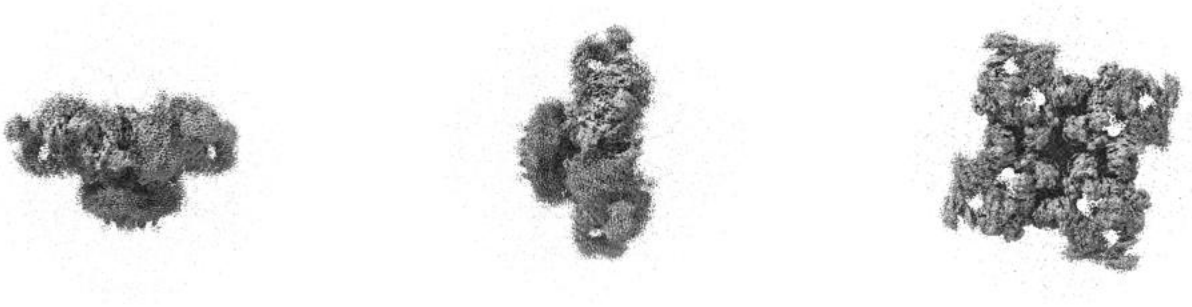


Z Index: 259

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

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

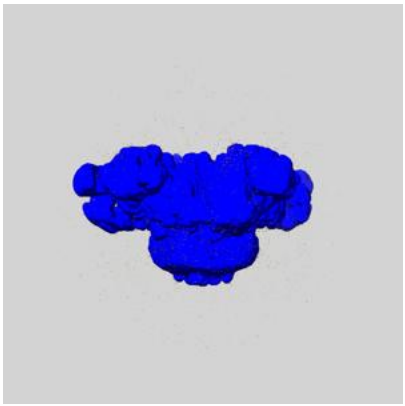
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

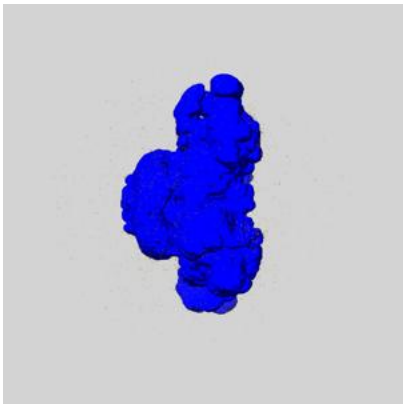
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

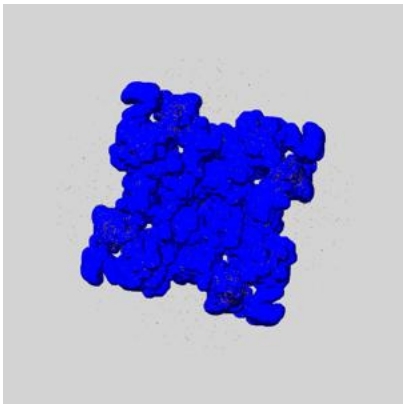
6.5.1 emd_21861_msk_1.map (i)



X



Y

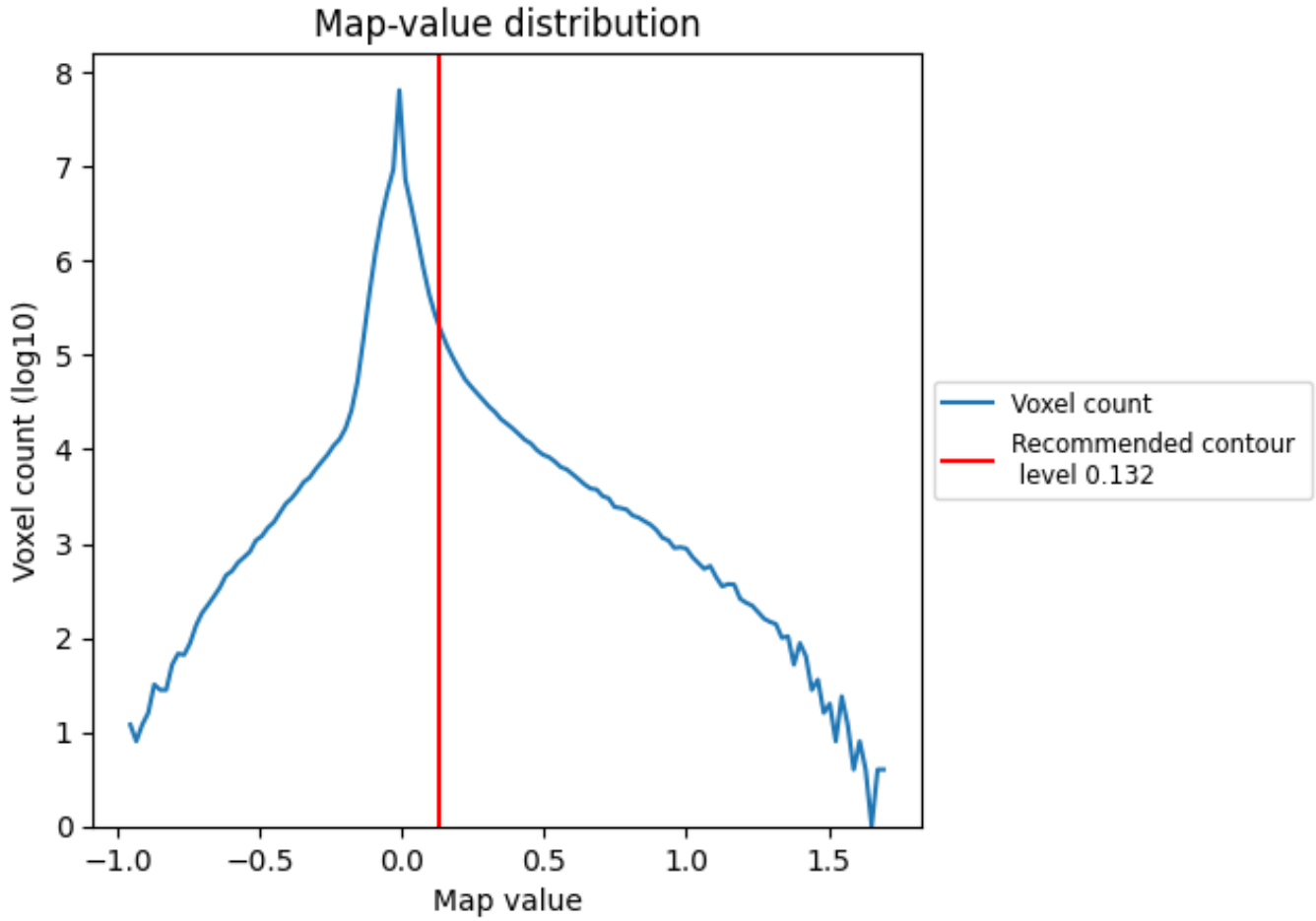


Z

7 Map analysis

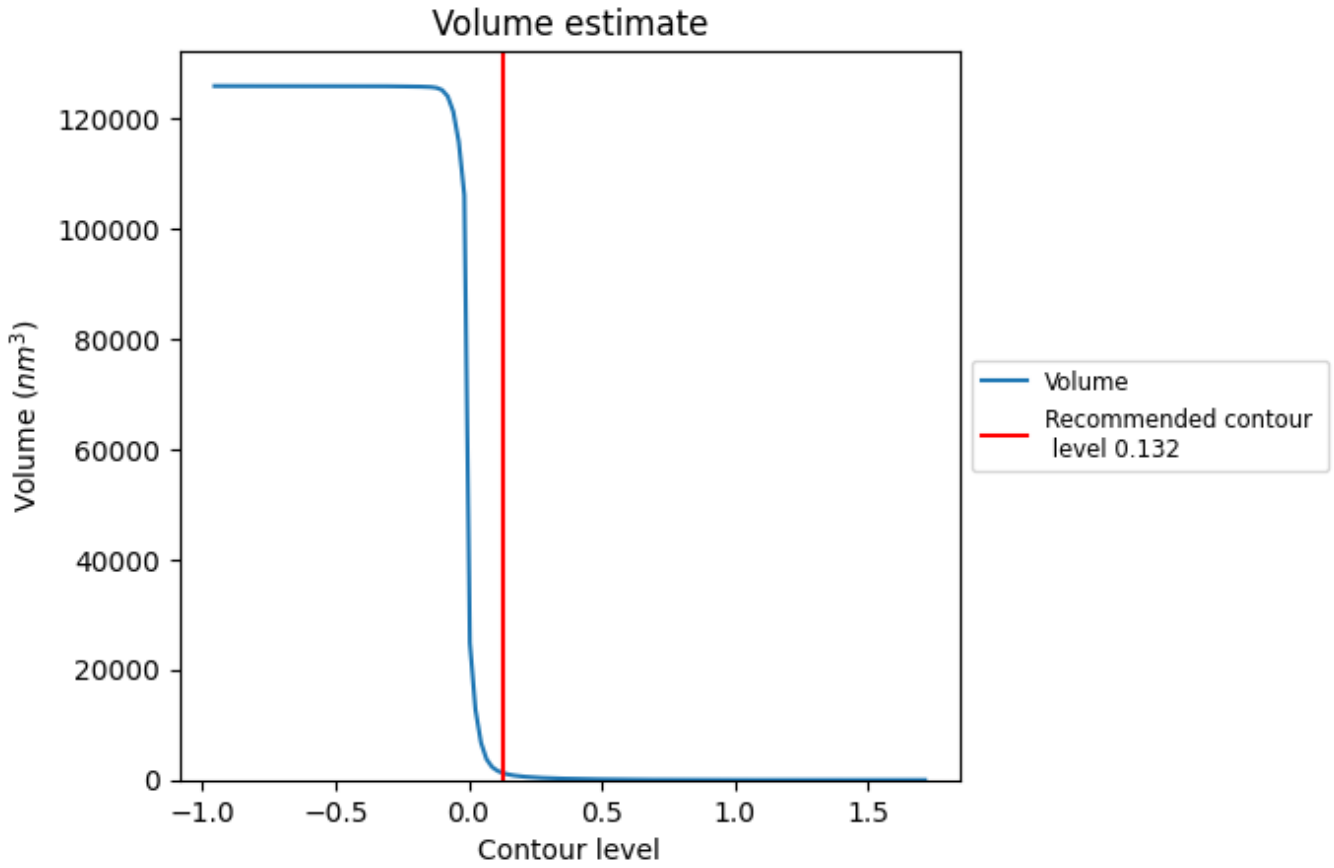
This section contains the results of statistical analysis of the map.

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.

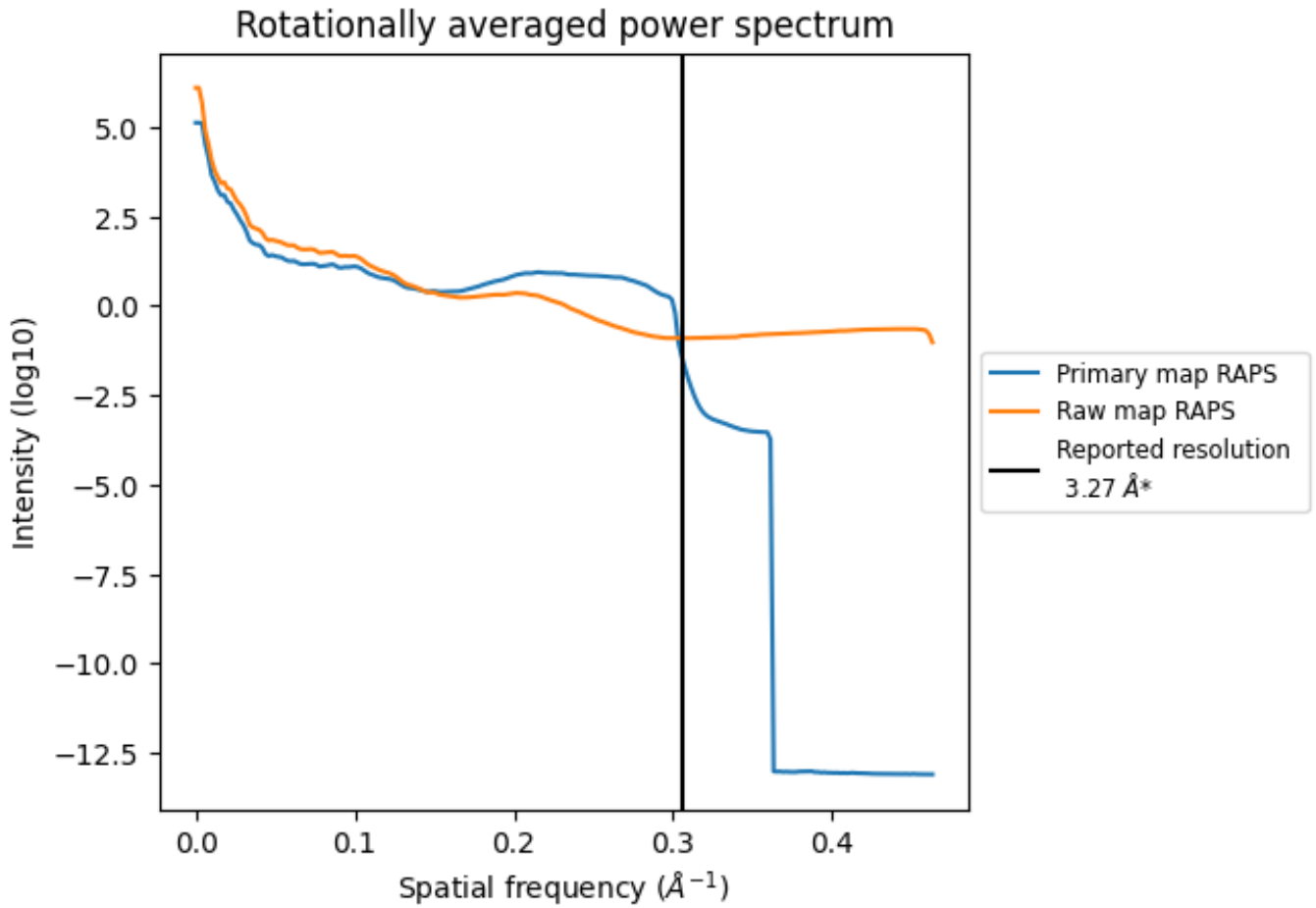
7.2 Volume estimate



The volume at the recommended contour level is 1213 nm^3; this corresponds to an approximate mass of 1096 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)

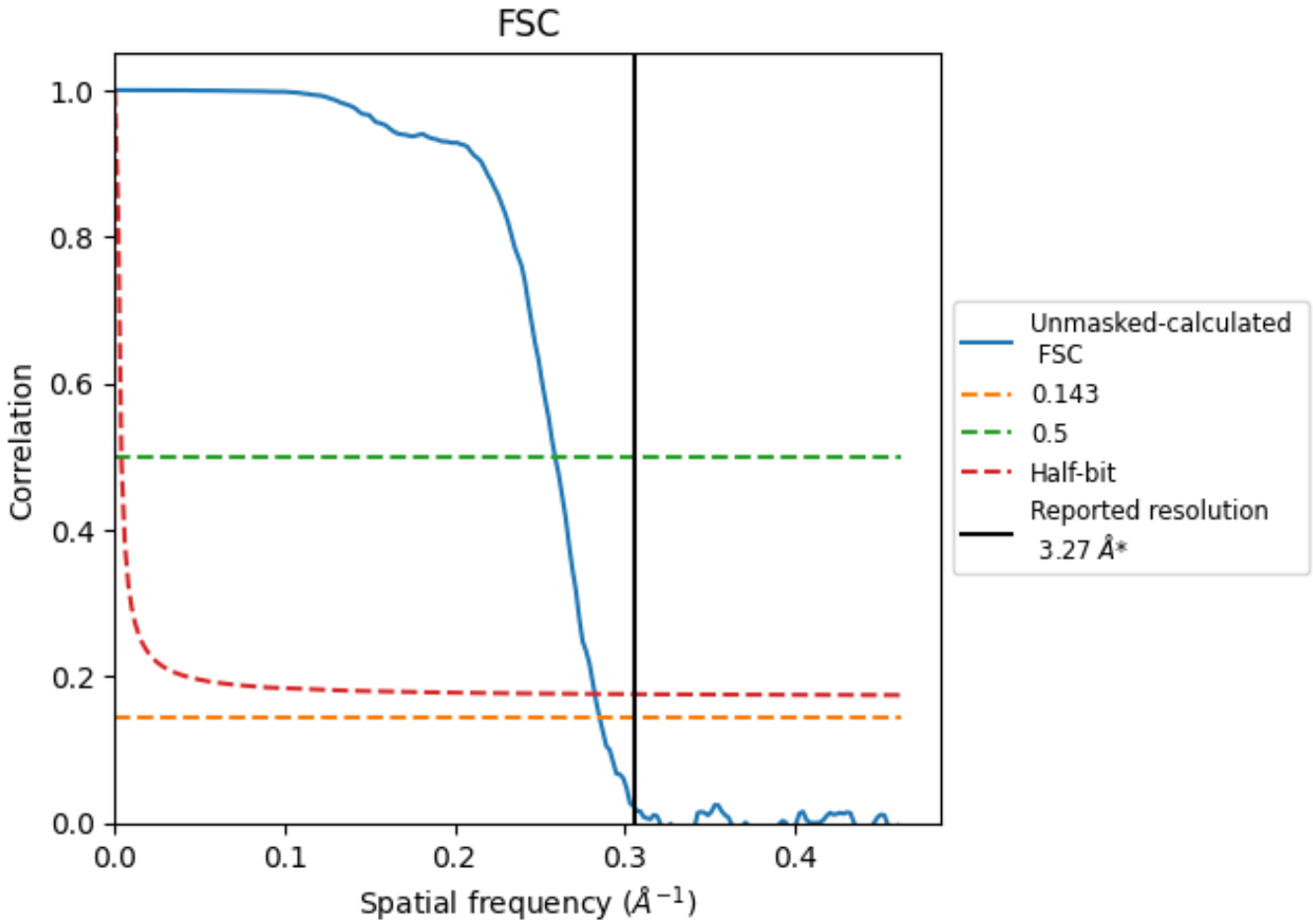


*Reported resolution corresponds to spatial frequency of 0.306 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.306 Å^{-1}

8.2 Resolution estimates (i)

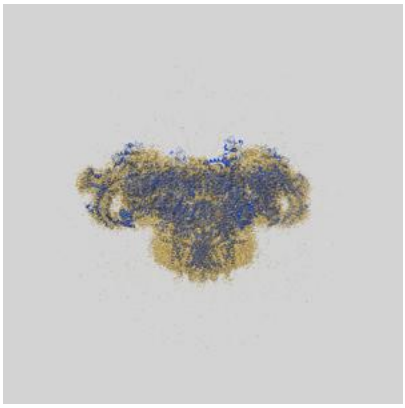
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	3.86	3.54

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

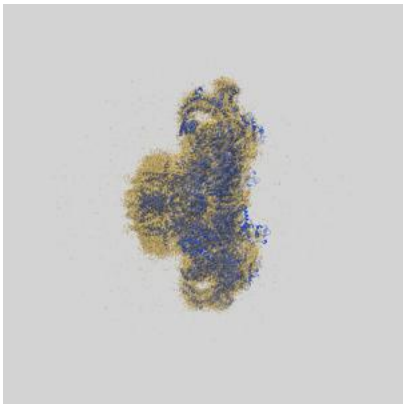
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21861 and PDB model 6WOU. Per-residue inclusion information can be found in section 3 on page 5.

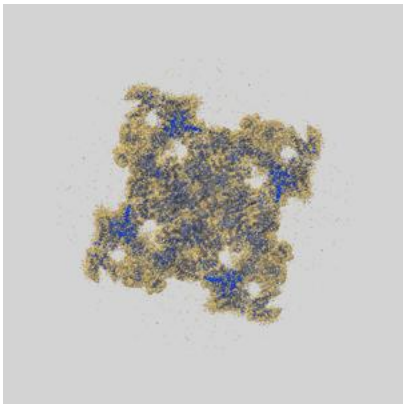
9.1 Map-model overlay



X



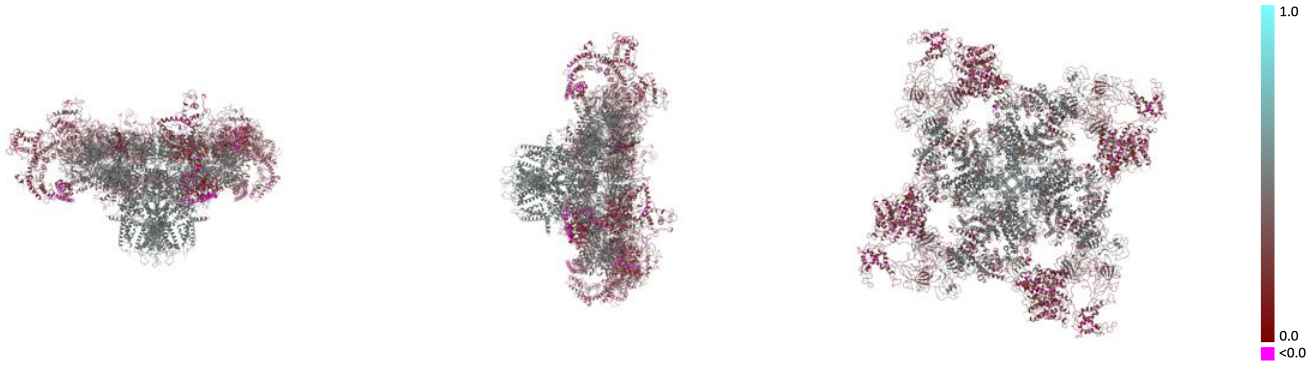
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.132 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.

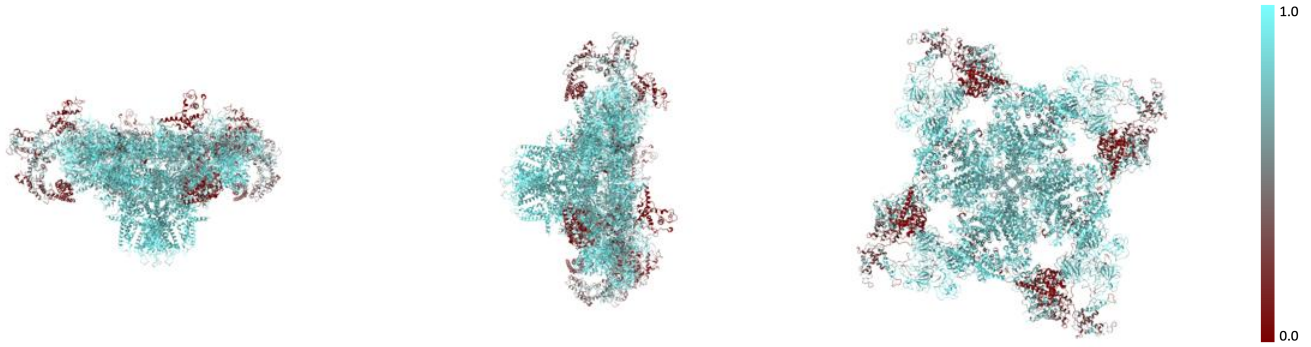
9.2 Q-score mapped to coordinate model (i)



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.

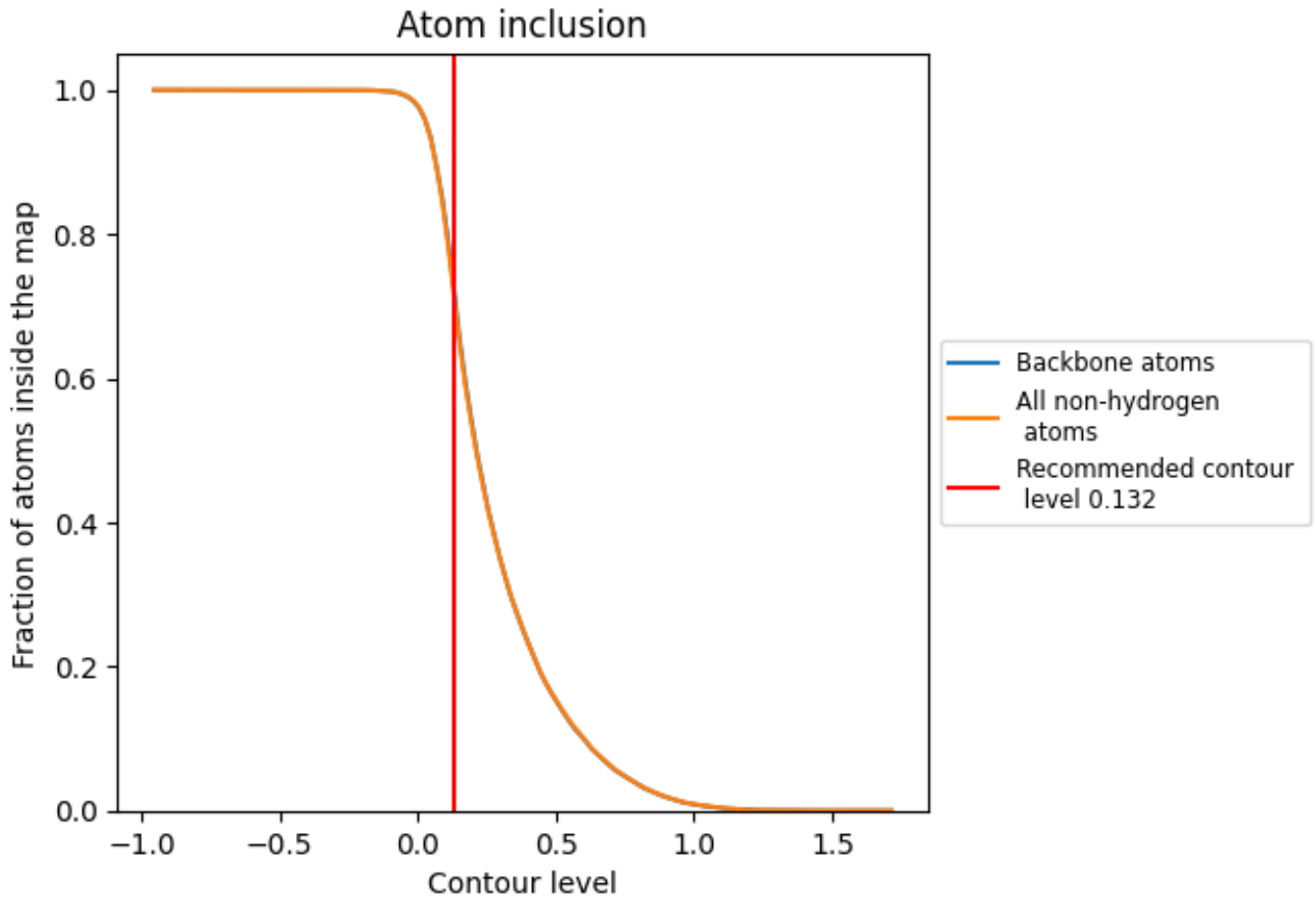
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.132).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7117	0.3760
A	0.7107	0.3740
B	0.7107	0.3730
C	0.7110	0.3740
D	0.7109	0.3740
E	0.8710	0.4550
F	0.8722	0.4560
G	0.8672	0.4560
H	0.8685	0.4580