Full wwPDB EM Validation Report ⓘ

Jan 25, 2024 – 01:41 PM EST

PDB ID	:	8DTZ
EMDB ID	:	EMD-27712
Title	:	Recombinant mouse RyR2 triple phosphonull mutant S2807A/S2813A/S2030A in complex with FKBP12.6 and nanodisc under closed-state conditions
Authors	:	Iyer, K.A.; Hu, Y.; Murayama, T.; Samso, M.
Deposited on	:	2022-07-26
Resolution	:	3.60 Å(reported)
Based on initial model	:	6WOU

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:

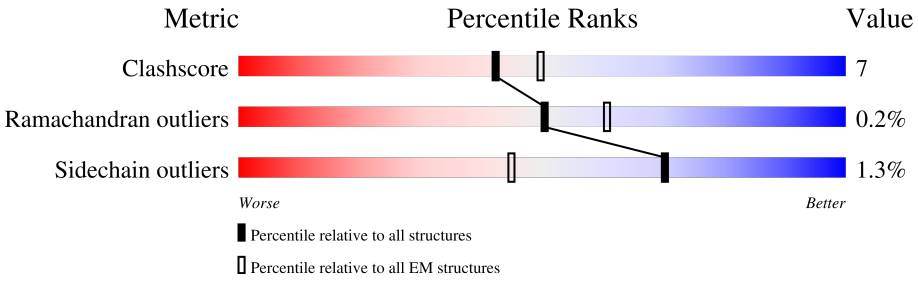
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	9% 67% 15% 18%
1	B	4966	9% 67% 15% 18%
1	C	4966	9% 67% 15% 18%
1	D	4966	9% 67% 14% 18%
2	E	107	77% 22%
2	F	107	73% 26%
2	G	107	76% 23%
2	H	107	76% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 129524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4061	Total	C	N	O	S	0	0
			31562	20044	5390	5931	197		
1	B	4061	Total	C	N	O	S	0	0
			31562	20044	5390	5931	197		
1	C	4061	Total	C	N	O	S	0	0
			31562	20044	5390	5931	197		
1	D	4061	Total	C	N	O	S	0	0
			31562	20044	5390	5931	197		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2030	ALA	SER	engineered mutation	UNP E9Q401
A	2807	ALA	SER	engineered mutation	UNP E9Q401
A	2813	ALA	SER	engineered mutation	UNP E9Q401
B	2030	ALA	SER	engineered mutation	UNP E9Q401
B	2807	ALA	SER	engineered mutation	UNP E9Q401
B	2813	ALA	SER	engineered mutation	UNP E9Q401
C	2030	ALA	SER	engineered mutation	UNP E9Q401
C	2807	ALA	SER	engineered mutation	UNP E9Q401
C	2813	ALA	SER	engineered mutation	UNP E9Q401
D	2030	ALA	SER	engineered mutation	UNP E9Q401
D	2807	ALA	SER	engineered mutation	UNP E9Q401
D	2813	ALA	SER	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	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

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

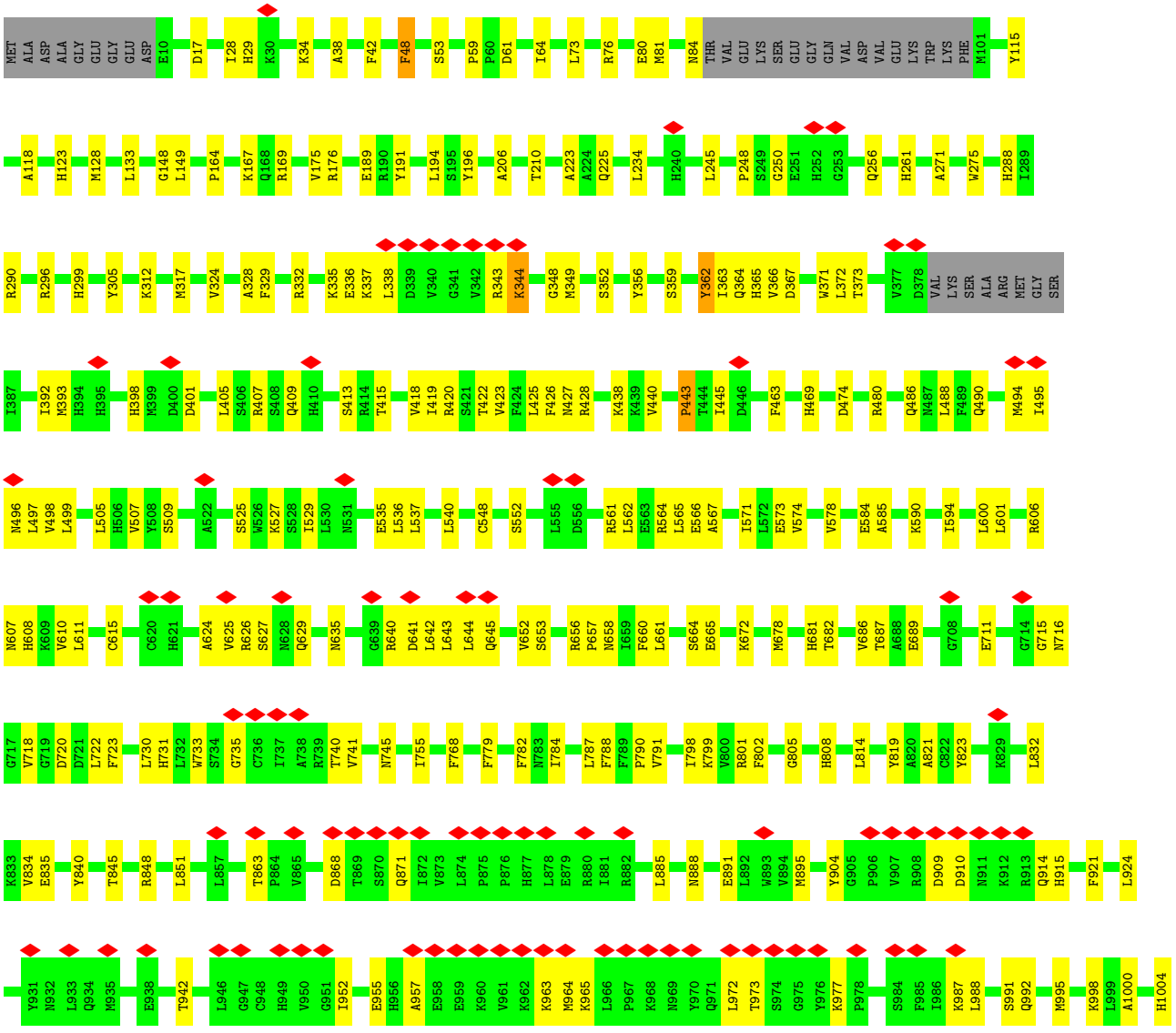
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

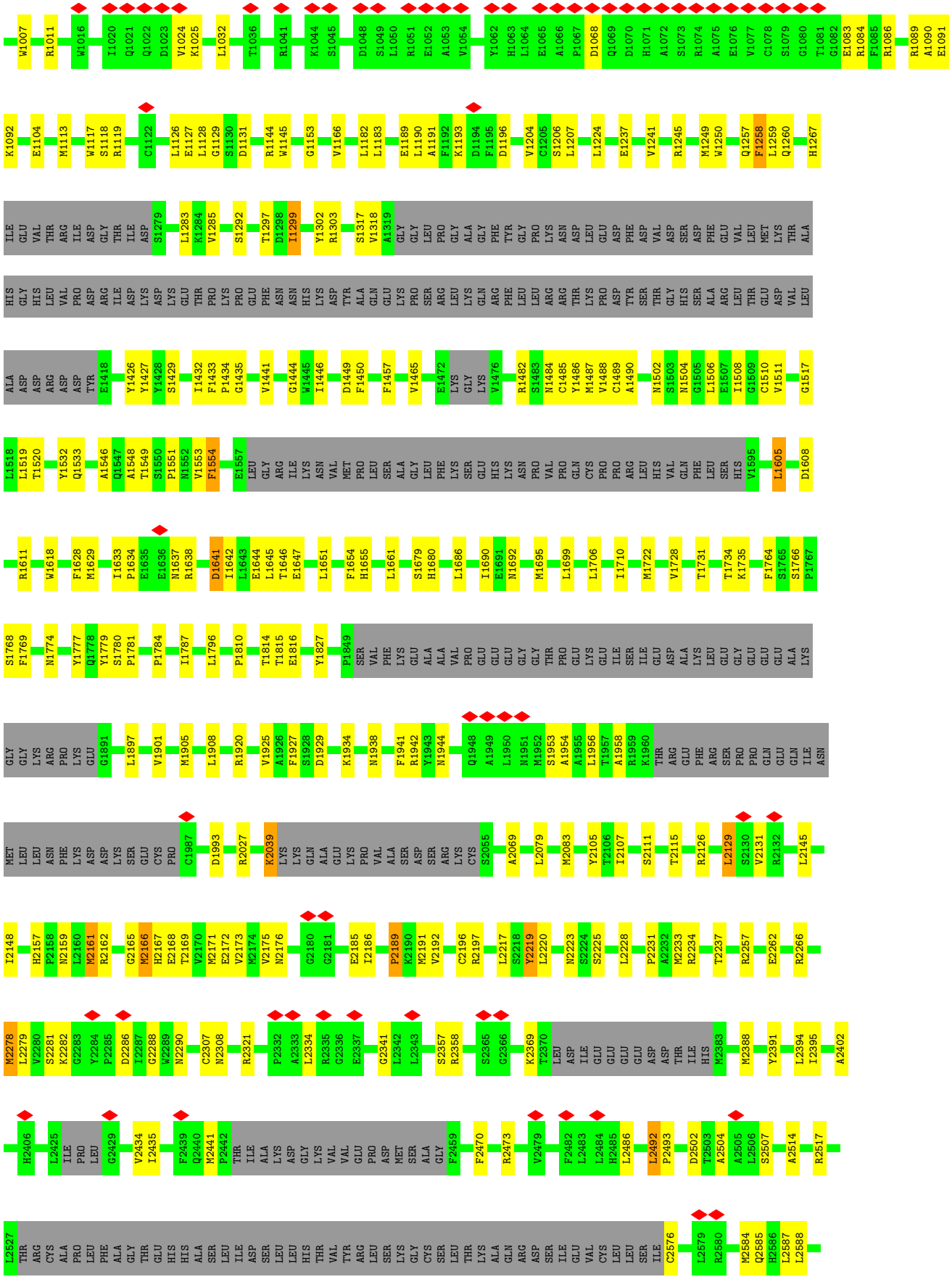
3 Residue-property plots (i)

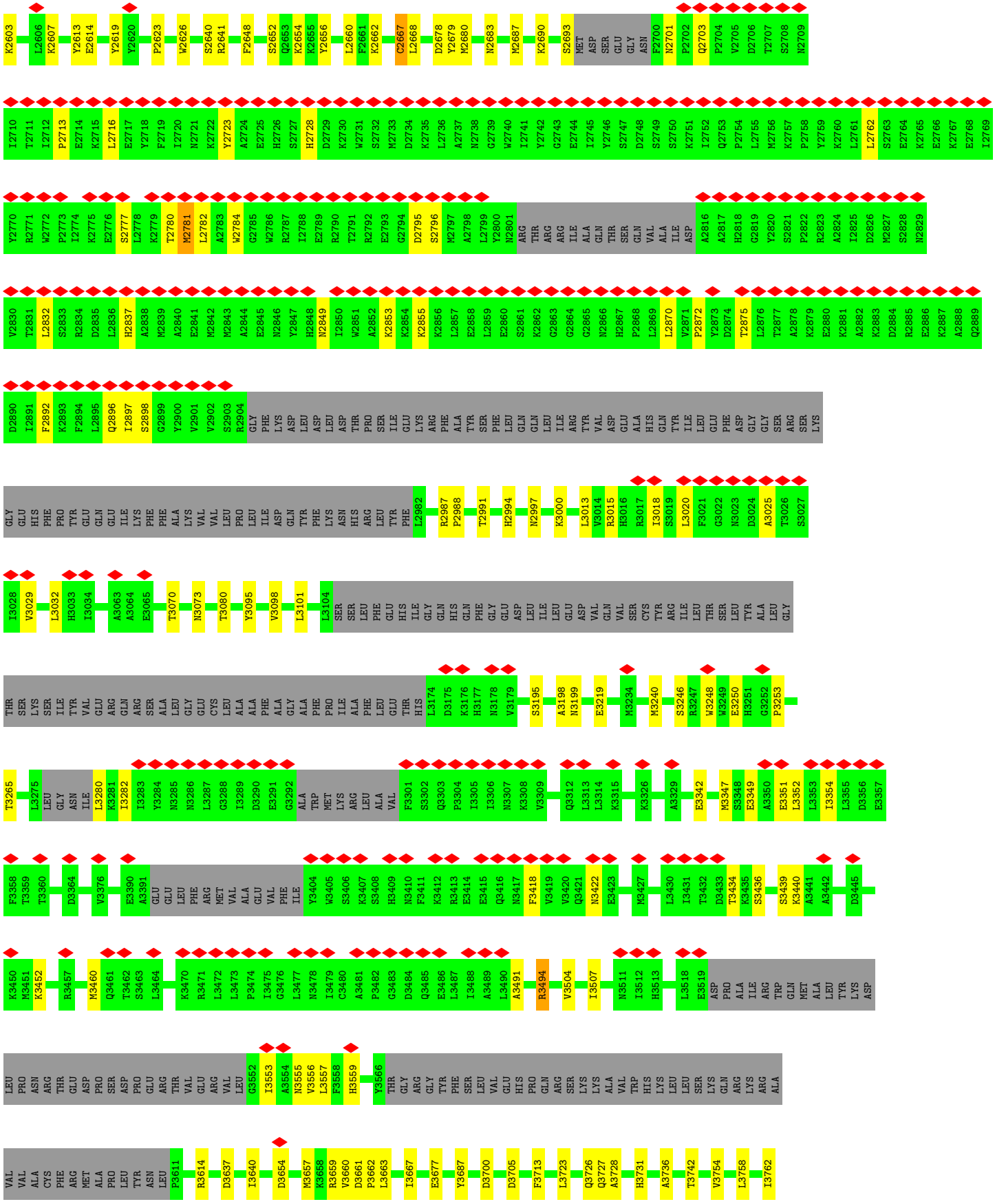
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

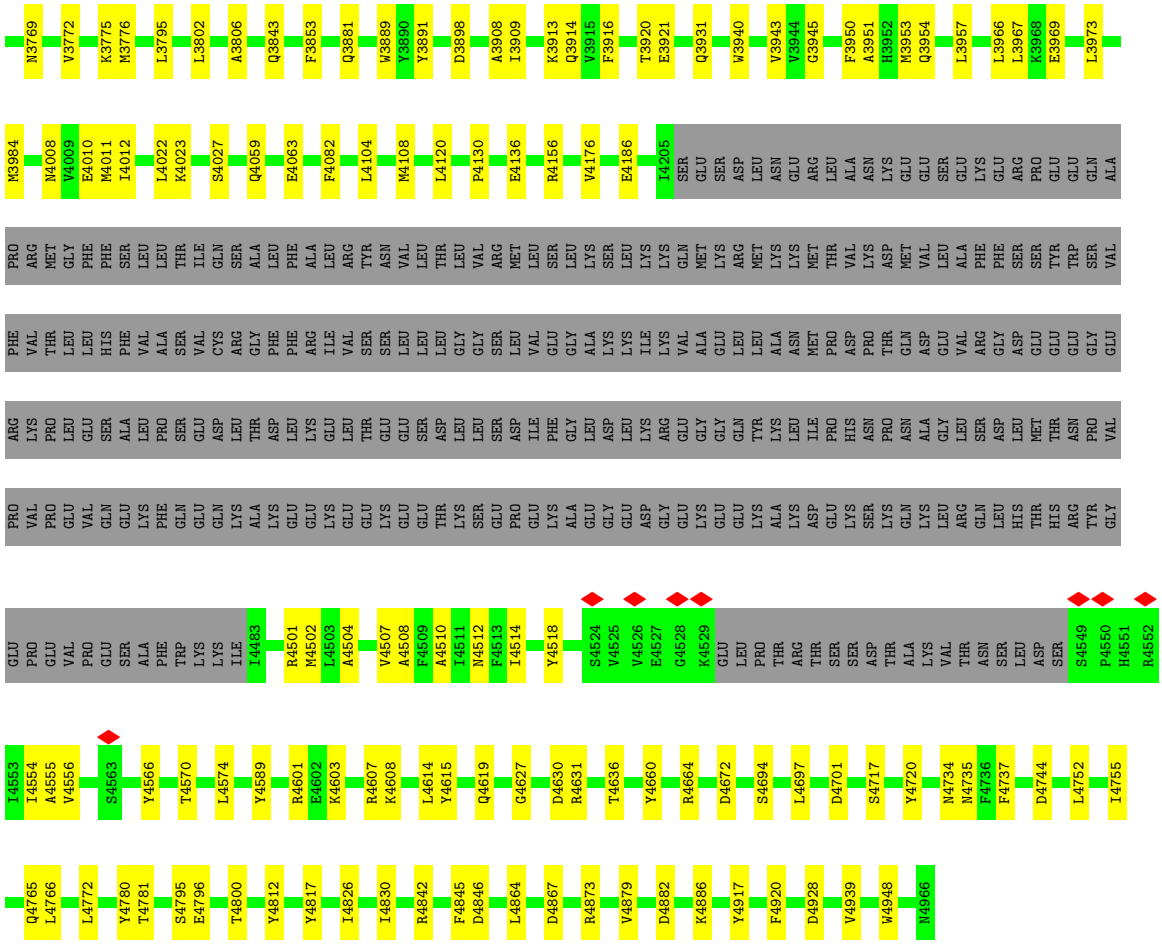
• Molecule 1: Ryanodine receptor 2

Chain A:



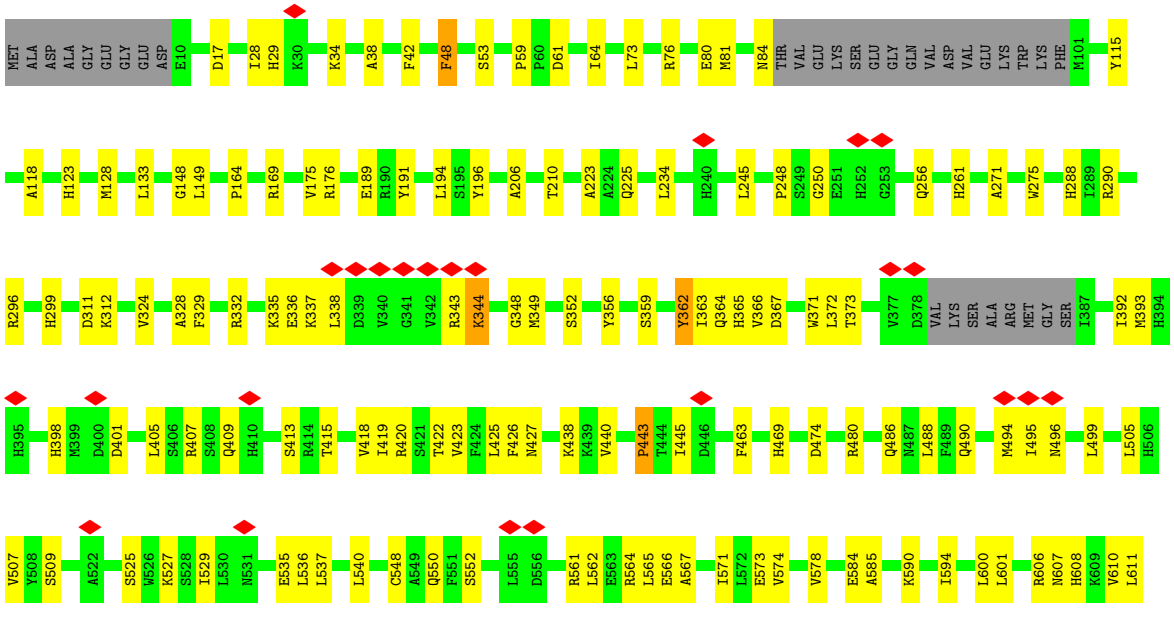


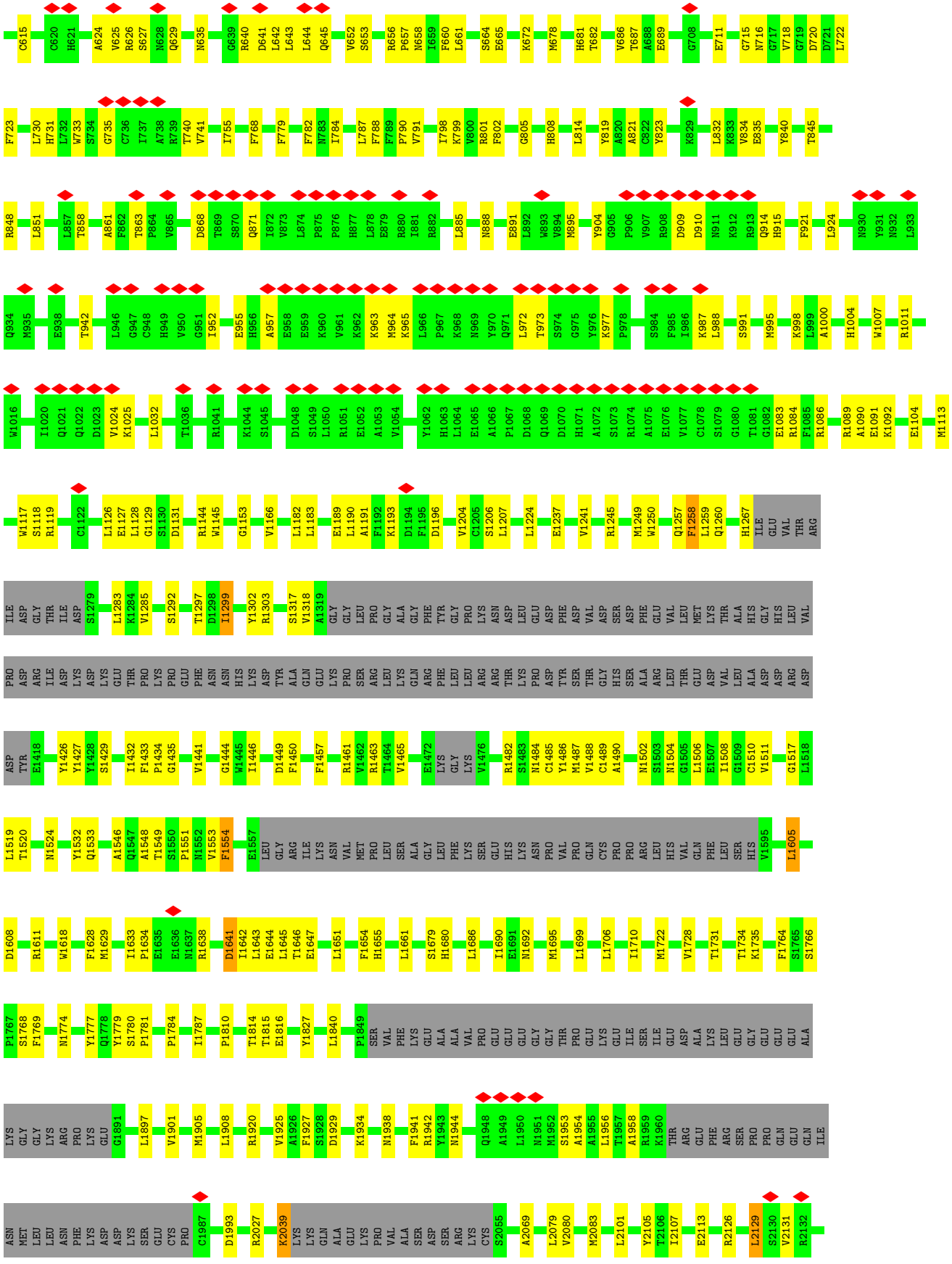

K2603 L2606 K2607 Y2613 E2614 Y2619 Y2620 P2623 W2626 S2640 R2641 F2648 S2652 Q2653 K2654 K2655 Y2656 L2660 F2661 K2662 C2667 L2668 D2678 Y2679 M2680 N2683 M2687 K2690 S2693 MET ASP SER GLU GLY ASN P2700 N2701 P2702 Q2703 P2704 V2705 D2706 T2707 S2708 N2709
I2710 T2711 I2712 P2713 E2714 K2715 L2716 E2717 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 ALA GLN THR SER GLN VAL ALA 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 G2864 G2865 N2866 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 R2904 GLY PHE LYS ASP LEU ASP LEU ILE 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 R2987 P2988 T2991 H2994 N2997 K3000 L3013 V3014 R3015 H3016 R3017 I3018 S3019 L3020 F3021 G3022 N3023 D3024 A3025 T3026 S3027
I3028 V3029 L3032 H3033 I3034 A3063 A3064 E3065 T3070 N3073 T3080 Y3095 V3098 L3101 L3104 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 S3195 A3198 N3199 E3219 M3234 M3240 S3246 R3247 W3248 W3249 E3250 H3251 G3252 P3253
T3265 L3275 LEU GLY ASN ILE L3280 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 Q3312 L3313 L3314 K3315 K3326 A3329 E3342 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357
F3358 T3359 T3360 D3364 V3376 E3390 A3391 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 M3427 L3430 I3431 T3432 D3433 T3434 K3435 S3436 S3439 K3440 A3441 A3442 D3445
K3450 M3451 K3452 R3457 M3460 Q3461 T3462 S3463 L3464 K3470 R3471 L3472 L3473 P3474 I3475 G3476 L3477 N3478 I3479 C3480 A3481 P3482 G3483 D3484 Q3485 E3486 L3487 I3488 A3489 L3490 A3491 R3494 V3504 I3507 N3511 I3512 H3513 L3518 E3519 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 LEU G3552 I3553 A3554 N3555 V3556 L3557 F3558 H3559 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 LEU SER LYS GLN ARG LYS ARG ALA
VAL VAL ALA CYS PHE ARG MET ALA PRO LEU TYR ASN LEU P3611 R3614 D3637 I3640 D3654 M3657 K3658 R3659 V3660 D3661 P3662 L3663 I3667 E3677 Y3687 D3700 D3705 F3713 L3723 Q3726 Q3727 A3728 H3731 A3736 T3742 V3754 L3758 I3762



• Molecule 1: Ryanodine receptor 2

Chain B:

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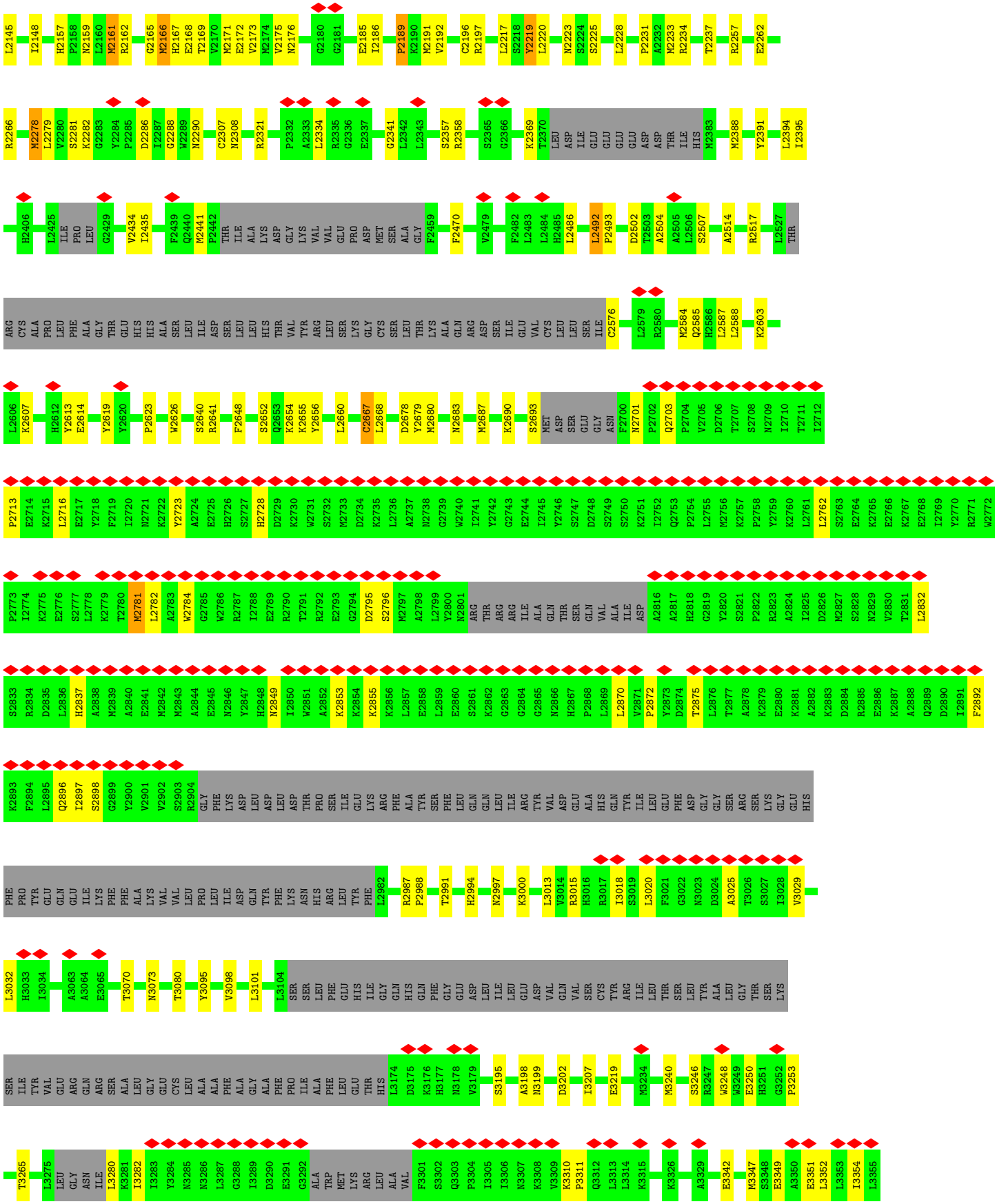
F723 L730 H731 L732 W733 S734 G735 C736 I737 A738 R739 T740 V741 I755 F768 F779 F782 N783 I784 L787 F788 F789 P790 V791 I798 K799 V800 R801 F802 G805 H808 L814 Y819 A820 A821 C822 Y823 K829 L832 K833 V834 E835 Y840 T845
R848 L851 L857 T858 A861 F862 T863 P864 V865 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 L885 N888 E891 L892 W893 V894 M895 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 F921 L924 N930 Y931 N932 L933
Q934 M935 E938 T942 L946 G947 C948 H949 V950 G951 I952 E955 H956 A957 E958 E959 K960 V961 K962 K963 N964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 S984 F985 I986 K987 L988 S991 M995 K998 L999 A1000 H1004 W1007 R1011
W1016 I1020 Q1021 Q1022 D1023 V1024 K1025 L1032 T1036 R1041 K1044 S1045 D1048 S1049 L1050 R1051 E1052 A1053 V1054 Y1062 H1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 S1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 F1085 R1086 R1089 A1090 E1091 K1092 E1104 M1113
W1117 S1118 R1119 C1122 L1126 E1127 L1128 G1129 S1130 D1131 R1144 W1145 G1153 V1166 L1182 L1183 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1204 C1205 S1206 L1207 L1224 E1237 V1241 R1245 M1249 W1250 Q1257 F1258 L1259 Q1260 H1267 ILE GLU VAL THR ARG
ILE ASP GLY THR ILE ASP S1279 L1283 K1284 V1285 S1292 T1297 D1298 I1299 Y1302 R1303 S1317 V1318 A1319 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 E1418 Y1426 Y1427 Y1428 S1429 I1432 F1433 P1434 G1435 V1441 G1444 W1445 I1446 D1449 F1450 F1457 R1461 V1462 R1463 T1464 V1465 E1472 LYS GLY LYS V1476 R1482 S1483 N1484 C1485 Y1486 M1487 V1488 C1489 A1490 N1502 S1503 N1504 G1505 L1506 E1507 I1508 G1509 C1510 V1511 G1517 L1518
L1519 T1520 N1524 Y1532 Q1533 A1546 Q1547 A1548 T1549 S1550 P1551 N1552 V1553 F1554 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA GLY LEU PHE LYS SER GLU HIS LYS ASN PRO VAL PRO GLN CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER HIS V1595 L1605
D1608 R1611 W1618 F1628 M1629 I1633 P1634 E1635 E1636 N1637 R1638 D1641 I1642 L1643 E1644 L1645 T1646 E1647 L1651 F1654 H1655 L1661 S1679 H1680 L1686 I1690 E1691 N1692 M1695 L1699 L1706 I1710 M1722 V1728 T1731 T1734 K1735 F1764 S1765 S1766
P1767 S1768 F1769 N1774 Y1777 Q1778 Y1779 S1780 P1781 P1784 I1787 P1810 T1814 T1815 E1816 Y1827 L1840 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 L1897 V1901 M1905 L1908 R1920 V1925 A1926 F1927 S1928 D1929 K1934 N1938 F1941 R1942 Y1943 N1944 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 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 D1993 R2027 K2039 LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS S2055 A2069 L2079 V2080 M2083 L2101 Y2105 T2106 I2107 E2113 R2126 L2129 S2130 V2131 R2132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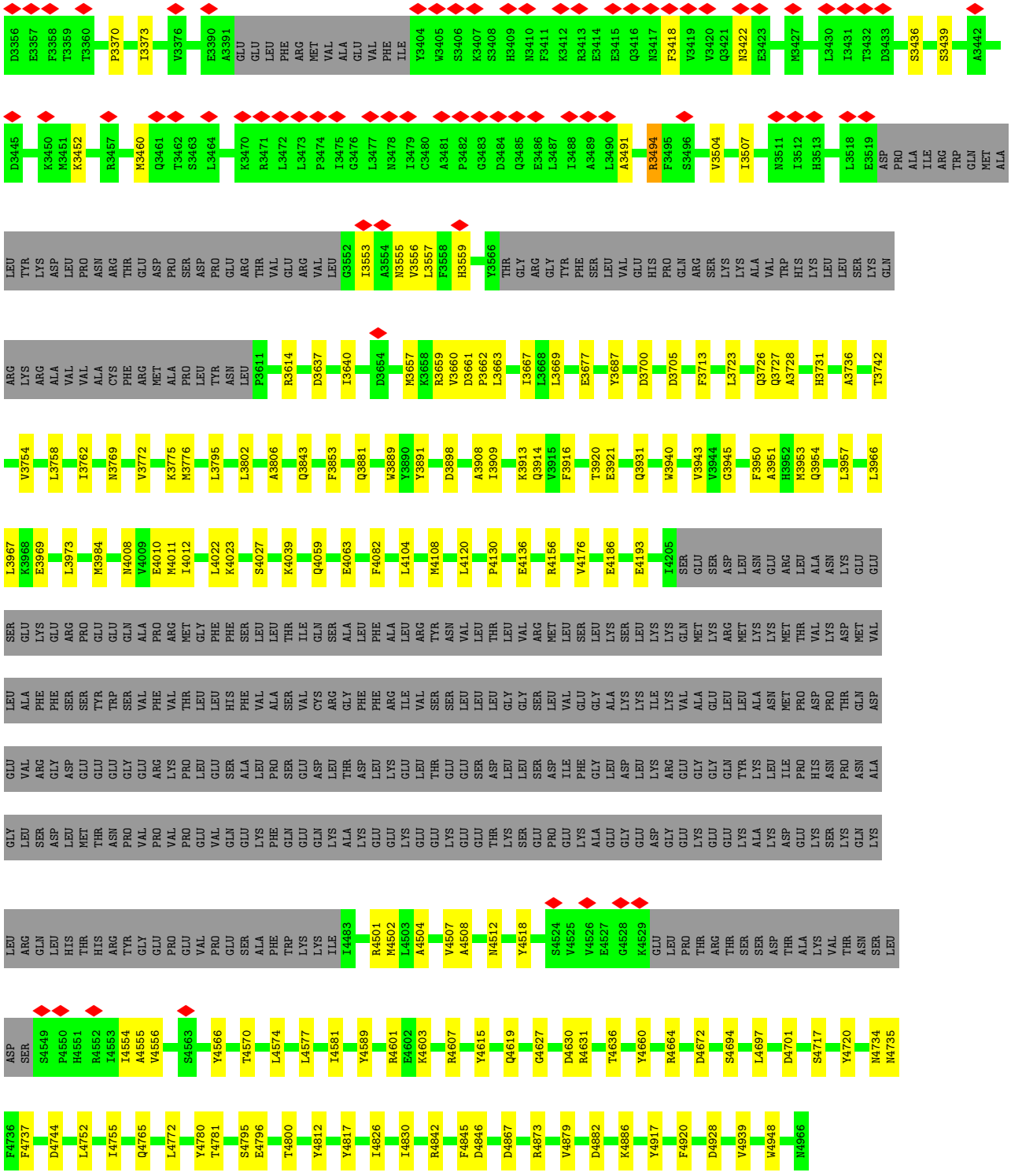
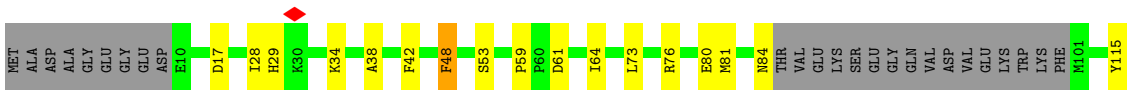
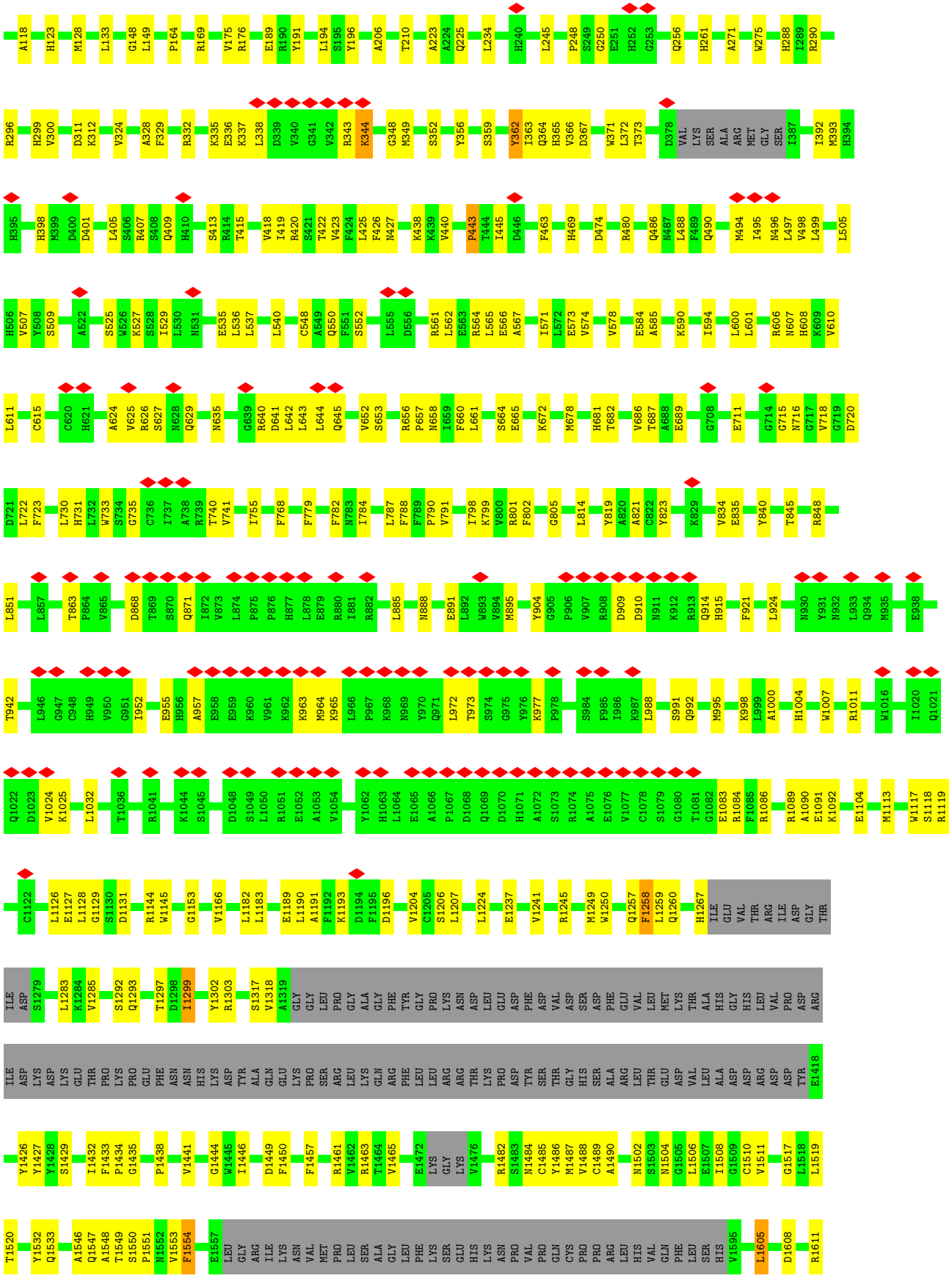
R2266 M2278 L2279 V2280 S2281 K2282 G2283 Y2284 P2285 D2286 I2287 G2288 W2289 N2290 C2307 N2308 R2321 P2332 A2333 L2334 R2335 G2336 E2337 G2341 L2342 L2343 S2357 R2358 S2365 G2366 K2369 T2370 LEU ASP ILE GLU GLU GLU ASP ASP THR ILE HIS M2383 M2388 Y2391 L2394 I2395
H2406 L2425 ILE PRO LEU G2429 V2434 I2435 F2439 Q2440 M2441 P2442 THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY F2459 F2470 V2479 F2482 L2483 L2484 H2485 L2486 L2492 P2493 D2502 T2503 A2504 A2505 L2506 S2507 A2514 R2517 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 LEU SER LYS GLY GLY CYS SER LEU LEU THR LYS ALA ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU LEU SER ILE C2576 L2579 R2580 M2584 Q2585 H2586 L2587 L2588 K2603
L2606 K2607 H2612 Y2613 E2614 Y2619 Y2620 P2623 W2626 S2640 R2641 F2648 S2652 Q2653 K2654 K2655 Y2656 L2660 C2667 L2668 D2678 Y2679 M2680 N2683 M2687 K2690 S2693 MET ASP SER GLU GLY ASN F2700 N2701 P2702 Q2703 P2704 V2705 D2706 T2707 S2708 N2709 I2710 T2711 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 ALA GLN THR SER GLN VAL ALA 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 G2864 G2865 N2866 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 R2904 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 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 R2987 P2988 T2991 H2994 N2997 K3000 L3013 V3014 R3015 H3016 R3017 I3018 S3019 L3020 F3021 G3022 N3023 D3024 A3025 T3026 S3027 I3028 V3029
L3032 H3033 I3034 A3063 A3064 E3065 T3070 N3073 T3080 Y3095 V3098 L3101 L3104 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 PHE ALA GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS L3174 D3175 K3176 H3177 N3178 V3179 S3195 A3198 N3199 D3202 I3207 E3219 M3234 M3240 S3246 R3247 W3248 W3249 E3250 H3251 G3252 P3253
T3265 L3275 LEU GLY ASN ILE L3280 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 L3314 K3315 K3326 A3329 E3342 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355



• Molecule 1: Ryanodine receptor 2

Chain C:

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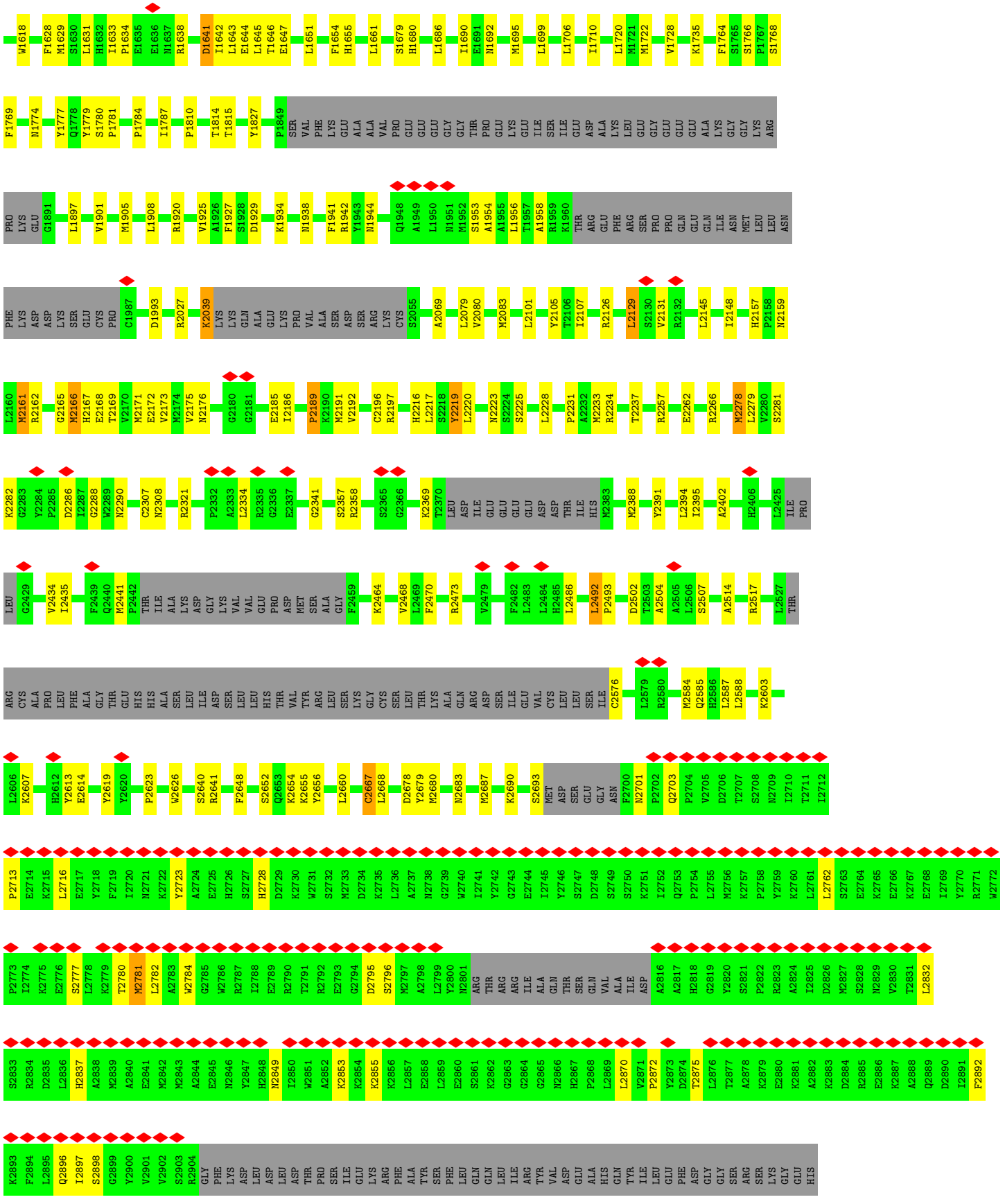
R296 H299 V300 D311 K312 V324 A328 F329 R332 K335 E336 K337 L338 D339 V340 G341 V342 R343 K344 G348 M349 S352 Y356 S359 Y362 I363 Q364 H365 V366 D367 W371 L372 T373 D378 VAL LYS SER ALA ARG MET GLY SER I387 I392 M393 H394
H395 H398 M399 D400 D401 L405 S406 R407 S408 Q409 H410 S413 R414 T415 V418 I419 R420 S421 T422 V423 F424 L425 F426 N427 K438 K439 V440 P443 T444 I445 D446 F463 H469 D474 R480 Q486 N487 L488 F489 Q490 N494 I495 N496 L497 V498 L499 L505
H506 V507 Y508 S509 A522 S525 W526 K527 S528 I529 L530 N531 E535 L536 L537 L540 C548 A549 Q550 F551 S552 L555 D556 R561 L562 E563 R564 L565 E566 A567 I571 L572 E573 V574 V578 E584 A585 K590 I594 L600 L601 R606 N607 H608 K609 V610
L611 C615 C620 H621 A624 V625 R626 S627 N628 Q629 N635 G639 R640 D641 L642 L643 L644 Q645 V652 S653 R656 P657 N658 I659 F660 L661 S664 E665 K672 M678 H681 T682 V686 T687 A688 E689 G708 E711 G714 G715 N716 G717 V718 G719 D720
D721 L722 F723 L730 H731 L732 W733 S734 G735 C736 I737 A738 R739 T740 V741 I755 F768 F779 F782 N783 I784 L787 F788 F789 P790 V791 I798 K799 V800 R801 F802 G805 L814 Y819 A820 A821 C822 Y823 K829 V834 E835 Y840 T845 R848
L851 L857 T863 P864 V865 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 L885 N888 E891 L892 W893 V894 M895 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 F921 L924 N930 Y931 N932 L933 Q934 M935 E938
T942 L946 G947 C948 H949 V950 Q951 I952 E955 H956 A957 E958 E959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 S984 F985 I986 K987 L988 S991 Q992 M995 K998 L999 A1000 H1004 W1007 R1011 W1016 I1020 Q1021
Q1022 D1023 V1024 K1025 L1032 T1036 R1041 K1044 S1045 D1048 S1049 L1050 R1051 E1052 A1053 V1054 Y1062 H1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 S1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 R1084 F1085 R1086 R1089 A1090 E1091 K1092 E1104 M1113 W1117 S1118 R1119
C1122 L1126 E1127 L1128 G1129 S1130 D1131 R1144 W1145 G1153 V1166 L1182 L1183 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1204 C1205 S1206 L1207 L1224 E1237 V1241 R1245 M1249 W1250 Q1257 F1258 L1259 Q1260 H1267 ILE GLU VAL THR ARG ILE ASP GLY THR
ILE ASP S1279 L1283 K1284 V1285 S1292 Q1293 T1297 D1298 I1299 Y1302 R1303 S1317 V1318 A1319 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 ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ASP ALA ARG LEU THR GLU ASP VAL LEU LEU ALA ASP ASP ARG ASP ASP TYR E1418
Y1426 Y1427 Y1428 S1429 I1432 F1433 P1434 G1435 P1438 V1441 G1444 W1445 I1446 D1449 F1450 F1457 R1461 V1462 R1463 T1464 V1465 E1472 LYS GLY LYS V1476 R1482 S1483 N1484 C1485 Y1486 M1487 V1488 C1489 A1490 N1502 S1503 N1504 G1505 L1506 E1507 I1508 G1509 C1510 V1511 G1517 L1518 L1519
T1520 Y1532 Q1533 A1546 Q1547 A1548 T1549 S1550 P1551 N1552 V1553 F1554 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA GLY LEU PHE LYS SER GLU HIS LYS ASN PRO VAL PRO GLN CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER HIS V1595 L1605 D1608 R1611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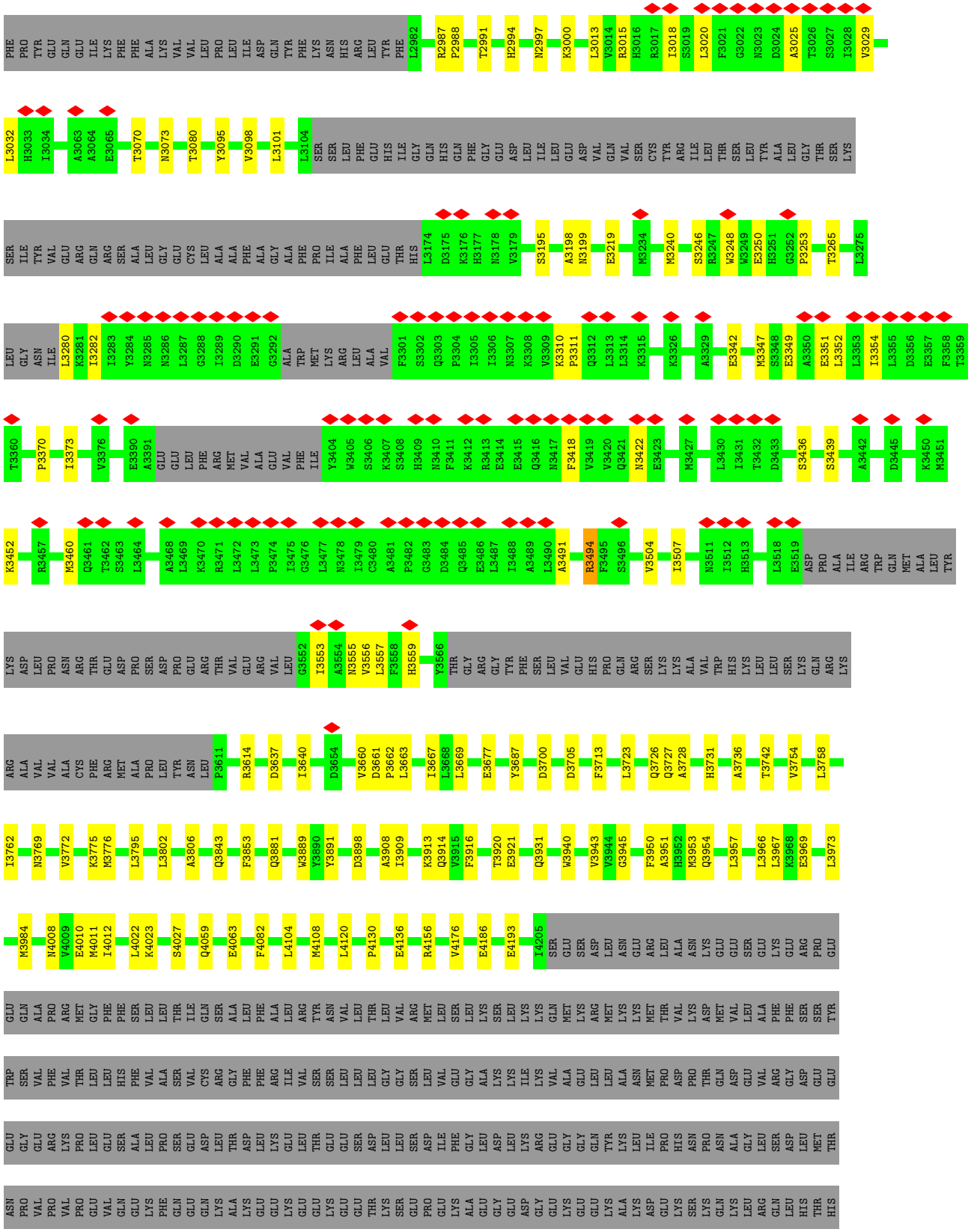
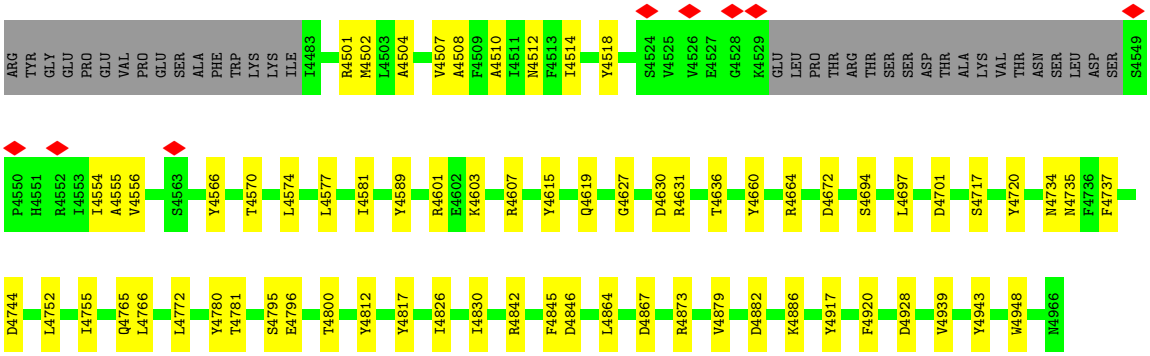
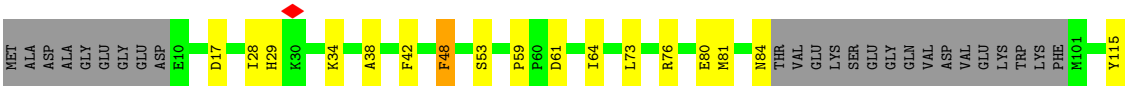
F1769 N1774 Y1777 Q1778 Y1779 S1780 P1781 P1784 I1787 P1810 T1814 T1815 Y1827 P1849 SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG
PRO LYS GLU G1891 L1897 V1901 M1905 L1908 R1920 V1925 A1926 F1927 S1928 D1929 K1934 N1938 F1941 R1942 Y1943 N1944 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 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 D1993 R2027 K2039 LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS S2055 A2069 L2079 V2080 M2083 L2101 Y2105 T2106 I2107 R2126 L2129 S2130 V2131 R2132 L2145 I2148 H2157 P2158 N2159
L2160 M2161 R2162 G2165 M2166 H2167 E2168 T2169 V2170 M2171 E2172 V2173 M2174 V2175 N2176 G2180 G2181 E2185 I2186 P2189 K2190 M2191 V2192 C2196 R2197 H2216 L2217 S2218 Y2219 L2220 N2223 S2224 S2225 L2228 P2231 A2232 M2233 R2234 T2237 R2257 E2262 R2266 M2278 L2279 V2280 S2281
K2282 G2283 Y2284 P2285 D2286 I2287 G2288 W2289 N2290 C2307 N2308 R2321 P2332 A2333 L2334 R2335 G2336 E2337 G2341 S2357 R2358 S2365 G2366 K2369 T2370 LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383 M2388 Y2391 L2394 I2395 A2402 H2406 L2425 ILE PRO
LEU G2429 V2434 T2435 F2439 Q2440 M2441 P2442 THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY F2459 K2464 V2468 L2469 F2470 R2473 V2479 F2482 L2483 L2484 H2485 L2486 L2492 P2493 D2502 T2503 A2504 A2505 L2506 S2507 A2514 R2517 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 VAL TYR ARG LEU LEU SER LYS GLY GLY CYS SER LEU LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU LEU SER ILE C2576 L2579 R2580 M2584 Q2585 H2586 L2587 L2588 K2603
L2606 K2607 H2612 Y2613 E2614 Y2619 Y2620 P2623 W2626 S2640 R2641 F2648 S2652 Q2653 K2654 K2655 Y2656 L2660 C2667 L2668 D2678 Y2679 M2680 N2683 M2687 K2690 S2693 MET ASP SER GLU GLY ASN F2700 N2701 P2702 Q2703 P2704 V2705 D2706 T2707 S2708 N2709 I2710 T2711 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 ALA GLN THR SER GLN VAL ALA 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 G2864 G2865 N2866 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 R2904 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

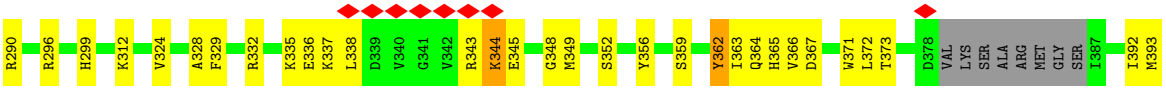


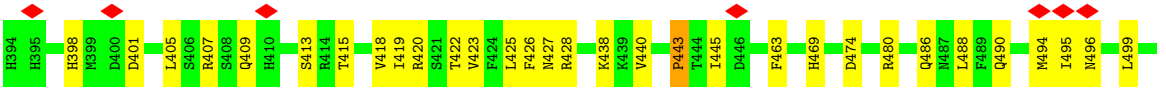


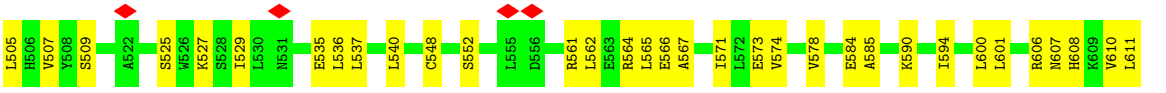
• Molecule 1: Ryanodine receptor 2

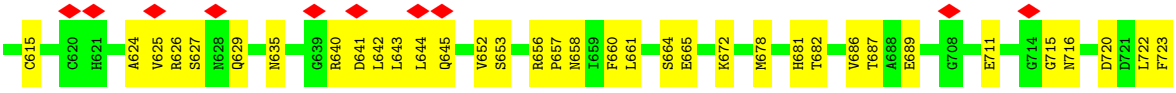
Chain D:

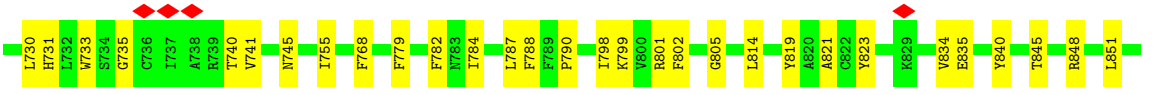


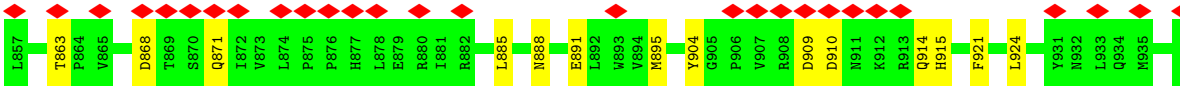


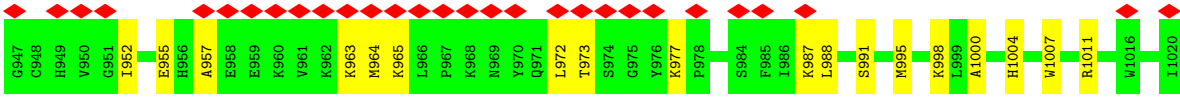


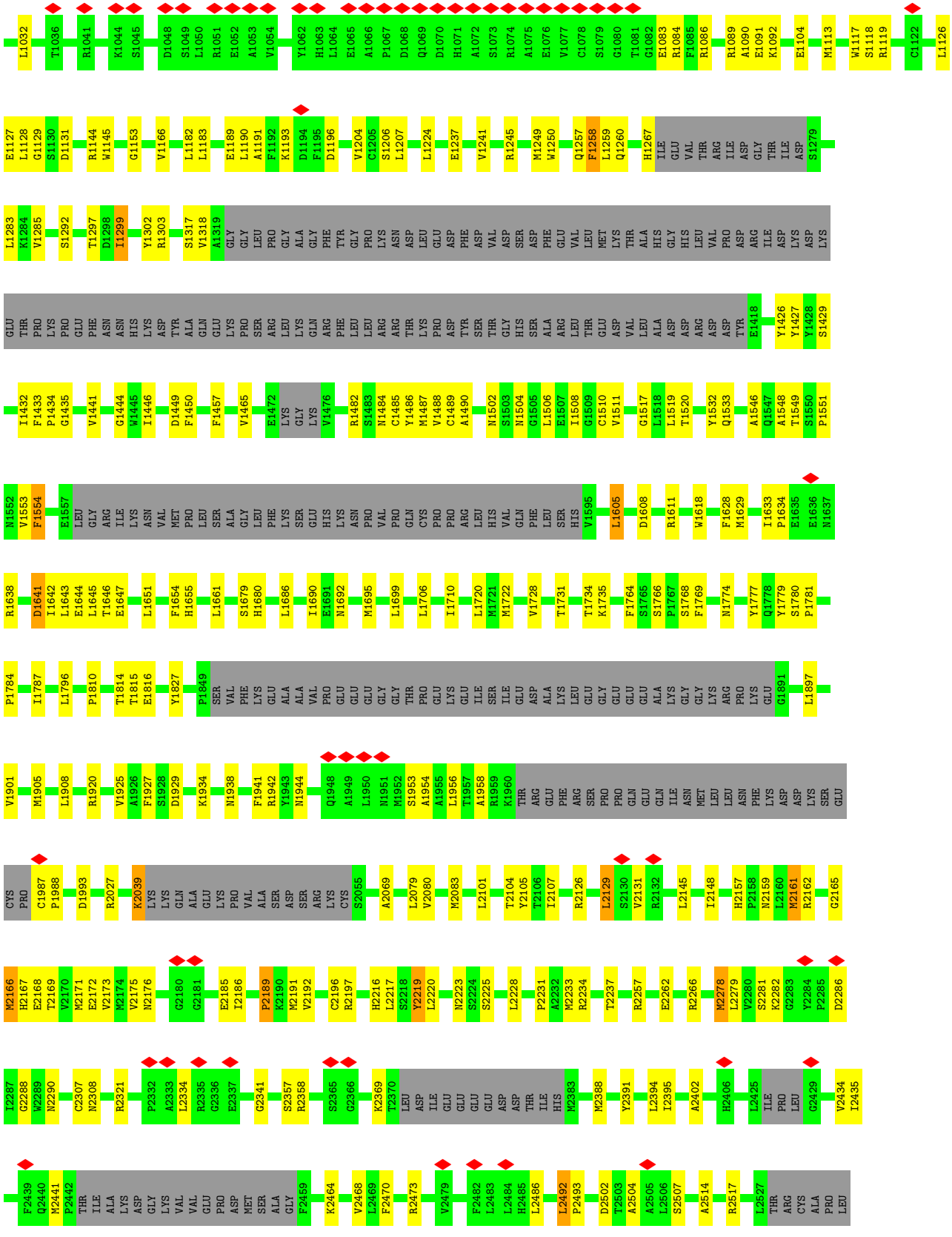








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E1127 L1128 G1129 S1130 D1131 R1144 W1145 G1153 V1166 L1182 L1183 E1189 L1190 A1191 F1192 K1193 D1194 F1195 D1196 V1204 C1205 S1206 L1207 L1224 E1237 V1241 R1245 M1249 W1250 Q1257 F1258 L1259 Q1260 H1267 ILE GLU VAL THR ARG ILE ASP GLY THR ILE ASP S1279
L1283 K1284 V1285 S1292 T1297 D1298 I1299 Y1302 R1303 S1317 V1318 A1319 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 E1418 Y1426 Y1427 Y1428 S1429
I1432 F1433 P1434 G1435 V1441 G1444 W1445 I1446 D1449 F1450 F1457 V1465 E1472 LYS GLY LYS V1476 R1482 S1483 N1484 C1485 Y1486 M1487 V1488 C1489 A1490 N1502 S1503 N1504 G1505 L1506 E1507 I1508 G1509 C1510 V1511 G1517 L1518 L1519 T1520 Y1532 Q1533 A1546 Q1547 A1548 T1549 S1550 P1551
N1552 V1553 F1554 E1557 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER ALA GLY LEU PHE LYS SER GLU HIS LYS ASN PRO VAL PRO GLN CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER HIS V1595 L1605 D1608 R1611 W1618 F1628 M1629 I1633 P1634 E1635 E1636 N1637
R1638 D1641 I1642 L1643 E1644 L1645 T1646 E1647 L1651 F1654 H1655 L1661 S1679 H1680 L1686 I1690 E1691 N1692 M1695 L1699 L1706 I1710 L1720 M1721 M1722 V1728 T1731 T1734 K1735 F1764 S1765 S1766 P1767 S1768 F1769 N1774 Y1777 Q1778 Y1779 S1780 P1781
P1784 I1787 L1796 P1810 T1814 T1815 E1816 Y1827 P1849 SER VAL PHE LYS GLU GLU ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU GLU ASP ALA LYS LEU GLU GLU GLY GLU GLU GLU GLU ALA LYS GLY GLY GLY LYS ARG PRO LYS GLU G1891 L1897
V1901 M1905 L1908 R1920 V1925 A1926 F1927 S1928 D1929 K1934 N1938 F1941 R1942 Y1943 N1944 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 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 D1993 R2027 K2039 LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS S2055 A2069 L2079 V2080 M2083 L2101 T2104 Y2105 T2106 I2107 R2126 L2129 S2130 V2131 R2132 L2145 I2148 H2157 P2158 N2159 L2160 M2161 R2162 G2165
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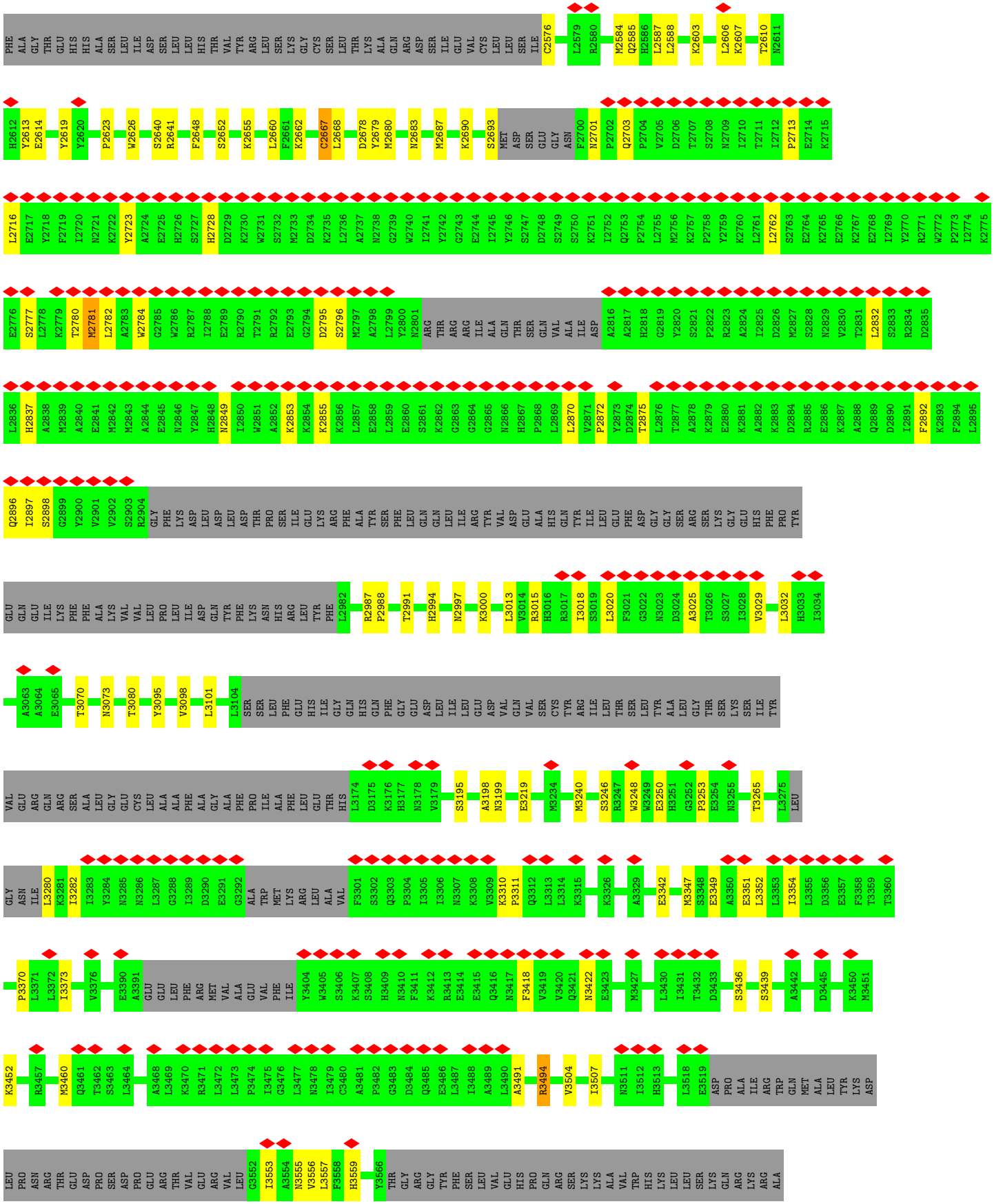
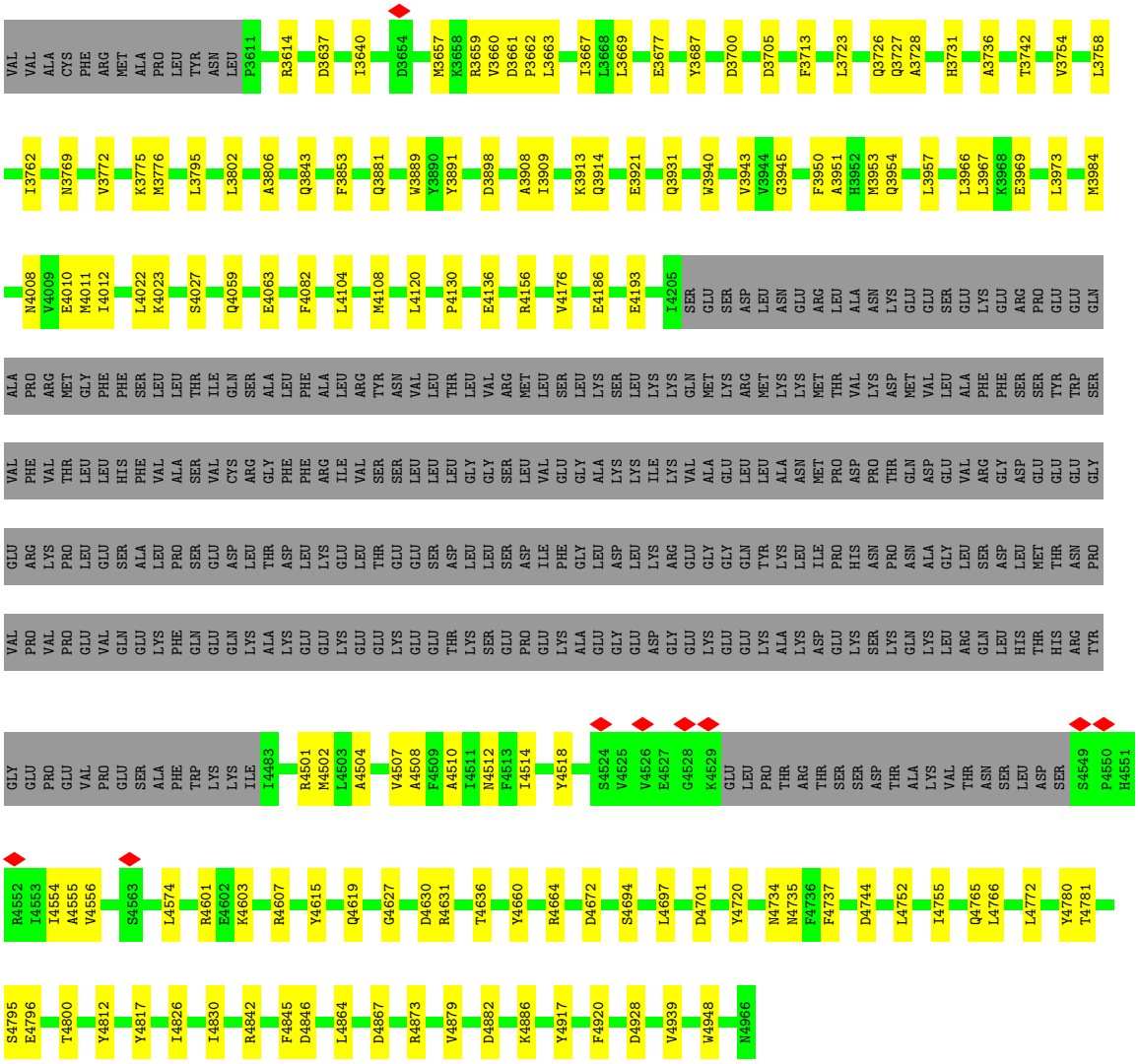
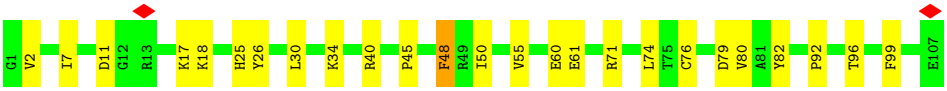
I2287 G2288 W2289 N2290 C2307 N2308 R2321 P2332 A2333 L2334 R2335 G2336 E2337 G2341 S2357 R2358 S2365 G2366 K2369 T2370 LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS M2383 M2388 Y2391 L2394 I2395 A2402 H2406 L2425 ILE PRO LEU G2429 V2434 I2435
F2439 Q2440 M2441 P2442 THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY F2459 K2464 V2468 L2469 F2470 R2473 V2479 F2482 L2483 L2484 H2485 L2486 L2492 P2493 D2502 T2503 A2504 A2505 L2506 S2507 A2514 R2517 L2527 THR ARG CYS ALA PRO LEU





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

Chain E:

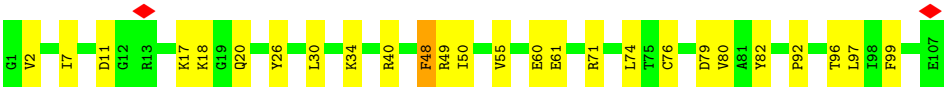


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:

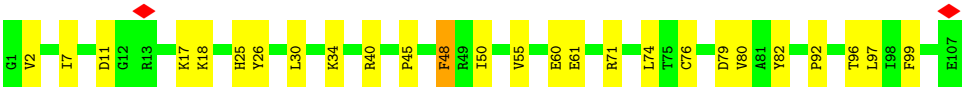
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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	136874	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 ($e^-/Å^2$)	52.95	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.288	Depositor
Minimum map value	-1.682	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	496.79996, 496.79996, 496.79996	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0799999, 1.0799999, 1.0799999	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	0.25	0/32214	0.52	8/43602 (0.0%)
1	B	0.25	0/32214	0.52	8/43602 (0.0%)
1	C	0.25	0/32214	0.52	8/43602 (0.0%)
1	D	0.25	0/32214	0.52	8/43602 (0.0%)
2	E	0.27	0/834	0.54	0/1123
2	F	0.27	0/834	0.54	0/1123
2	G	0.27	0/834	0.54	0/1123
2	H	0.27	0/834	0.54	0/1123
All	All	0.25	0/132192	0.52	32/178900 (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	4
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	16

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4022	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	4022	LEU	CA-CB-CG	6.16	129.46	115.30
1	C	4022	LEU	CA-CB-CG	6.16	129.46	115.30
1	D	4022	LEU	CA-CB-CG	6.16	129.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	562	LEU	CA-CB-CG	6.11	129.35	115.30
1	B	562	LEU	CA-CB-CG	6.11	129.35	115.30
1	C	562	LEU	CA-CB-CG	6.11	129.35	115.30
1	D	562	LEU	CA-CB-CG	6.11	129.35	115.30
1	A	2781	MET	CA-CB-CG	5.93	123.37	113.30
1	B	2781	MET	CA-CB-CG	5.93	123.37	113.30
1	C	2781	MET	CA-CB-CG	5.93	123.37	113.30
1	D	2781	MET	CA-CB-CG	5.93	123.37	113.30
1	A	2129	LEU	CA-CB-CG	5.72	128.45	115.30
1	B	2129	LEU	CA-CB-CG	5.72	128.45	115.30
1	C	2129	LEU	CA-CB-CG	5.72	128.45	115.30
1	D	2129	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	2278	MET	CA-CB-CG	5.70	122.99	113.30
1	B	2278	MET	CA-CB-CG	5.70	122.99	113.30
1	C	2278	MET	CA-CB-CG	5.70	122.99	113.30
1	D	2278	MET	CA-CB-CG	5.70	122.99	113.30
1	A	2189	PRO	CA-N-CD	-5.66	103.58	111.50
1	B	2189	PRO	CA-N-CD	-5.66	103.58	111.50
1	C	2189	PRO	CA-N-CD	-5.66	103.58	111.50
1	D	2189	PRO	CA-N-CD	-5.66	103.58	111.50
1	A	1605	LEU	CA-CB-CG	5.21	127.28	115.30
1	B	1605	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	1605	LEU	CA-CB-CG	5.21	127.28	115.30
1	D	1605	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	505	LEU	CA-CB-CG	5.21	127.28	115.30
1	B	505	LEU	CA-CB-CG	5.21	127.28	115.30
1	C	505	LEU	CA-CB-CG	5.21	127.28	115.30
1	D	505	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1777	TYR	Peptide
1	A	4023	LYS	Peptide
1	A	443	PRO	Peptide
1	A	4555	ALA	Peptide
1	B	1777	TYR	Peptide
1	B	4023	LYS	Peptide
1	B	443	PRO	Peptide
1	B	4555	ALA	Peptide
1	C	1777	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	C	4023	LYS	Peptide
1	C	443	PRO	Peptide
1	C	4555	ALA	Peptide
1	D	1777	TYR	Peptide
1	D	4023	LYS	Peptide
1	D	443	PRO	Peptide
1	D	4555	ALA	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	31562	0	30401	448	0
1	B	31562	0	30401	448	0
1	C	31562	0	30401	452	0
1	D	31562	0	30401	449	0
2	E	818	0	824	19	0
2	F	818	0	824	22	0
2	G	818	0	824	20	0
2	H	818	0	824	20	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	129524	0	124900	1834	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 7.

All (1834) 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:B:329:PHE:HB3	1:B:363:ILE:HD11	1.67	0.76
1:D:329:PHE:HB3	1:D:363:ILE:HD11	1.67	0.76
1:A:329:PHE:HB3	1:A:363:ILE:HD11	1.67	0.75
1:C:329:PHE:HB3	1:C:363:ILE:HD11	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1954:ALA:HA	1:C:1958:ALA:HB3	1.69	0.75
1:D:1954:ALA:HA	1:D:1958:ALA:HB3	1.69	0.74
1:B:2626:TRP:HE1	1:B:2641:ARG:HE	1.36	0.74
1:A:1954:ALA:HA	1:A:1958:ALA:HB3	1.69	0.73
1:B:1954:ALA:HA	1:B:1958:ALA:HB3	1.69	0.73
1:D:2626:TRP:HE1	1:D:2641:ARG:HE	1.36	0.73
1:A:2626:TRP:HE1	1:A:2641:ARG:HE	1.36	0.73
1:B:731:HIS:HB2	1:B:740:THR:HA	1.70	0.73
1:B:2987:ARG:HH11	1:B:2997:ASN:HB3	1.54	0.72
1:C:2626:TRP:HE1	1:C:2641:ARG:HE	1.36	0.72
1:A:2987:ARG:HH11	1:A:2997:ASN:HB3	1.54	0.72
1:D:731:HIS:HB2	1:D:740:THR:HA	1.70	0.72
1:A:731:HIS:HB2	1:A:740:THR:HA	1.70	0.71
1:C:731:HIS:HB2	1:C:740:THR:HA	1.70	0.71
1:C:2987:ARG:HH11	1:C:2997:ASN:HB3	1.54	0.71
1:B:672:LYS:HB3	1:B:819:TYR:HA	1.72	0.71
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.72	0.71
1:D:2987:ARG:HH11	1:D:2997:ASN:HB3	1.54	0.71
1:B:3843:GLN:HG3	1:B:3921:GLU:HG3	1.72	0.71
1:C:3843:GLN:HG3	1:C:3921:GLU:HG3	1.72	0.71
1:D:3843:GLN:HG3	1:D:3921:GLU:HG3	1.72	0.70
1:A:672:LYS:HB3	1:A:819:TYR:HA	1.72	0.70
1:D:672:LYS:HB3	1:D:819:TYR:HA	1.72	0.70
1:C:672:LYS:HB3	1:C:819:TYR:HA	1.72	0.70
2:F:50:ILE:HD12	2:F:60:GLU:HG3	1.74	0.70
2:E:50:ILE:HD12	2:E:60:GLU:HG3	1.74	0.69
1:A:957:ALA:HB1	1:A:963:LYS:H	1.57	0.69
1:B:1655:HIS:HD2	1:B:1699:LEU:HD11	1.58	0.69
1:C:3769:ASN:HB3	1:C:3772:VAL:HG12	1.75	0.69
1:C:1655:HIS:HD2	1:C:1699:LEU:HD11	1.58	0.69
2:G:50:ILE:HD12	2:G:60:GLU:HG3	1.74	0.69
2:H:50:ILE:HD12	2:H:60:GLU:HG3	1.74	0.69
1:C:957:ALA:HB1	1:C:963:LYS:H	1.57	0.69
1:B:722:LEU:HD13	1:B:735:GLY:HA3	1.75	0.68
1:D:957:ALA:HB1	1:D:963:LYS:H	1.57	0.68
1:A:3280:LEU:HG	1:A:3282:ILE:HG22	1.75	0.68
1:B:957:ALA:HB1	1:B:963:LYS:H	1.57	0.68
1:B:3280:LEU:HG	1:B:3282:ILE:HG22	1.75	0.68
1:C:722:LEU:HD13	1:C:735:GLY:HA3	1.75	0.68
1:D:3769:ASN:HB3	1:D:3772:VAL:HG12	1.75	0.68
1:A:3769:ASN:HB3	1:A:3772:VAL:HG12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3769:ASN:HB3	1:B:3772:VAL:HG12	1.75	0.67
1:D:1655:HIS:HD2	1:D:1699:LEU:HD11	1.58	0.67
1:D:3280:LEU:HG	1:D:3282:ILE:HG22	1.75	0.67
1:A:2514:ALA:HA	1:A:2517:ARG:HE	1.60	0.67
1:A:1655:HIS:HD2	1:A:1699:LEU:HD11	1.58	0.67
1:C:3280:LEU:HG	1:C:3282:ILE:HG22	1.75	0.67
1:B:418:VAL:O	1:B:422:THR:OG1	2.12	0.66
2:F:17:LYS:HE3	2:F:18:LYS:H	1.60	0.66
1:D:722:LEU:HD13	1:D:735:GLY:HA3	1.75	0.66
2:E:17:LYS:HE3	2:E:18:LYS:H	1.60	0.66
2:G:17:LYS:HE3	2:G:18:LYS:H	1.60	0.66
1:A:722:LEU:HD13	1:A:735:GLY:HA3	1.75	0.66
1:D:645:GLN:HE22	2:H:34:LYS:HB3	1.60	0.66
1:D:1117:TRP:HE1	1:D:1166:VAL:HG22	1.61	0.66
1:D:2514:ALA:HA	1:D:2517:ARG:HE	1.60	0.66
2:H:17:LYS:HE3	2:H:18:LYS:H	1.60	0.66
1:C:1117:TRP:HE1	1:C:1166:VAL:HG22	1.61	0.66
1:D:1090:ALA:HA	1:D:1249:MET:HA	1.78	0.66
1:A:1090:ALA:HA	1:A:1249:MET:HA	1.78	0.66
1:C:645:GLN:HE22	2:G:34:LYS:HB3	1.60	0.66
1:C:1090:ALA:HA	1:C:1249:MET:HA	1.78	0.65
1:D:1267:HIS:HB3	1:D:1292:SER:HA	1.79	0.65
1:A:645:GLN:HE22	2:E:34:LYS:HB3	1.60	0.65
1:A:1267:HIS:HB3	1:A:1292:SER:HA	1.79	0.65
1:B:645:GLN:HE22	2:F:34:LYS:HB3	1.60	0.65
1:C:1267:HIS:HB3	1:C:1292:SER:HA	1.79	0.65
1:C:2514:ALA:HA	1:C:2517:ARG:HE	1.60	0.65
1:D:644:LEU:O	1:D:1680:HIS:ND1	2.30	0.65
1:B:1090:ALA:HA	1:B:1249:MET:HA	1.78	0.65
1:B:2514:ALA:HA	1:B:2517:ARG:HE	1.60	0.65
1:B:1117:TRP:HE1	1:B:1166:VAL:HG22	1.61	0.65
1:B:1267:HIS:HB3	1:B:1292:SER:HA	1.79	0.65
1:C:715:GLY:HA3	1:C:720:ASP:HB3	1.78	0.65
1:A:1117:TRP:HE1	1:A:1166:VAL:HG22	1.61	0.65
1:B:715:GLY:HA3	1:B:720:ASP:HB3	1.78	0.65
1:C:644:LEU:O	1:C:1680:HIS:ND1	2.30	0.65
1:D:1434:PRO:HG2	1:D:1504:ASN:HB3	1.79	0.65
1:D:2441:MET:HB3	1:D:2492:LEU:HD13	1.79	0.65
1:A:1434:PRO:HG2	1:A:1504:ASN:HB3	1.79	0.65
1:C:2441:MET:HB3	1:C:2492:LEU:HD13	1.79	0.65
1:D:715:GLY:HA3	1:D:720:ASP:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3931:GLN:NE2	1:D:3984:MET:O	2.30	0.64
1:A:715:GLY:HA3	1:A:720:ASP:HB3	1.78	0.64
1:A:4830:ILE:HB	1:A:4842:ARG:HH21	1.62	0.64
1:B:2678:ASP:OD2	1:B:2679:TYR:N	2.31	0.64
1:C:3931:GLN:NE2	1:C:3984:MET:O	2.30	0.64
1:A:418:VAL:O	1:A:422:THR:OG1	2.12	0.64
1:A:3931:GLN:NE2	1:A:3984:MET:O	2.30	0.64
1:B:4830:ILE:HB	1:B:4842:ARG:HH21	1.62	0.64
1:C:4518:TYR:OH	1:C:4735:ASN:ND2	2.31	0.64
1:A:4518:TYR:OH	1:A:4735:ASN:ND2	2.31	0.64
1:B:1434:PRO:HG2	1:B:1504:ASN:HB3	1.79	0.64
1:B:2441:MET:HB3	1:B:2492:LEU:HD13	1.79	0.64
1:C:2678:ASP:OD2	1:C:2679:TYR:N	2.31	0.64
1:C:2196:CYS:SG	1:C:2197:ARG:N	2.71	0.64
1:C:3018:ILE:HG22	1:C:3020:LEU:H	1.63	0.64
1:C:4830:ILE:HB	1:C:4842:ARG:HH21	1.62	0.64
1:B:644:LEU:O	1:B:1680:HIS:ND1	2.30	0.64
1:A:3018:ILE:HG22	1:A:3020:LEU:H	1.63	0.64
1:C:2576:CYS:N	1:C:2613:TYR:O	2.31	0.64
1:D:2576:CYS:N	1:D:2613:TYR:O	2.31	0.64
1:A:2441:MET:HB3	1:A:2492:LEU:HD13	1.79	0.63
1:A:2678:ASP:OD2	1:A:2679:TYR:N	2.31	0.63
1:B:2576:CYS:N	1:B:2613:TYR:O	2.31	0.63
1:B:3931:GLN:NE2	1:B:3984:MET:O	2.30	0.63
1:B:4518:TYR:OH	1:B:4735:ASN:ND2	2.31	0.63
1:C:1434:PRO:HG2	1:C:1504:ASN:HB3	1.79	0.63
1:A:324:VAL:O	1:A:328:ALA:HB2	1.99	0.63
1:D:2678:ASP:OD2	1:D:2679:TYR:N	2.31	0.63
1:D:3018:ILE:HG22	1:D:3020:LEU:H	1.63	0.63
1:D:4830:ILE:HB	1:D:4842:ARG:HH21	1.62	0.63
1:A:644:LEU:O	1:A:1680:HIS:ND1	2.30	0.63
1:B:419:ILE:O	1:B:423:VAL:HG22	1.99	0.63
1:D:4518:TYR:OH	1:D:4735:ASN:ND2	2.31	0.63
1:A:419:ILE:O	1:A:423:VAL:HG22	1.99	0.63
1:A:2196:CYS:SG	1:A:2197:ARG:N	2.71	0.63
1:A:2576:CYS:N	1:A:2613:TYR:O	2.31	0.63
1:C:419:ILE:O	1:C:423:VAL:HG22	1.99	0.63
1:C:2587:LEU:HD11	1:C:2603:LYS:HB3	1.81	0.63
1:C:3349:GLU:HA	1:C:3352:LEU:HD23	1.81	0.63
1:B:2196:CYS:SG	1:B:2197:ARG:N	2.71	0.63
1:D:1104:GLU:HG3	1:D:1224:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2587:LEU:HD11	1:D:2603:LYS:HB3	1.81	0.63
1:C:1104:GLU:HG3	1:C:1224:LEU:HD22	1.81	0.63
1:D:2196:CYS:SG	1:D:2197:ARG:N	2.71	0.63
1:B:3018:ILE:HG22	1:B:3020:LEU:H	1.63	0.62
1:B:3349:GLU:HA	1:B:3352:LEU:HD23	1.81	0.62
1:C:802:PHE:HB2	1:C:1618:TRP:HB2	1.81	0.62
1:D:537:LEU:HD23	1:D:540:LEU:HD13	1.82	0.62
1:D:324:VAL:O	1:D:328:ALA:HB2	1.99	0.62
1:D:802:PHE:HB2	1:D:1618:TRP:HB2	1.81	0.62
1:A:363:ILE:HG23	1:A:372:LEU:HD13	1.82	0.62
1:A:802:PHE:HB2	1:A:1618:TRP:HB2	1.81	0.62
1:A:3349:GLU:HA	1:A:3352:LEU:HD23	1.81	0.62
1:B:802:PHE:HB2	1:B:1618:TRP:HB2	1.81	0.62
1:B:1091:GLU:HG2	1:B:1250:TRP:HE1	1.65	0.62
1:C:1091:GLU:HG2	1:C:1250:TRP:HE1	1.65	0.62
1:D:419:ILE:O	1:D:423:VAL:HG22	1.99	0.62
1:B:324:VAL:O	1:B:328:ALA:HB2	1.99	0.62
1:D:3349:GLU:HA	1:D:3352:LEU:HD23	1.81	0.62
1:C:324:VAL:O	1:C:328:ALA:HB2	1.99	0.62
1:D:3891:TYR:HE2	1:D:3898:ASP:H	1.48	0.62
1:B:2587:LEU:HD11	1:B:2603:LYS:HB3	1.81	0.62
1:C:537:LEU:HD23	1:C:540:LEU:HD13	1.82	0.62
1:A:2587:LEU:HD11	1:A:2603:LYS:HB3	1.81	0.62
1:B:1432:ILE:HD13	1:B:1546:ALA:HB2	1.82	0.62
1:C:3000:LYS:HG2	1:C:3070:THR:HG22	1.82	0.62
1:D:1432:ILE:HD13	1:D:1546:ALA:HB2	1.82	0.62
1:A:2185:GLU:HG2	1:A:2186:ILE:HG12	1.82	0.61
1:A:3891:TYR:HE2	1:A:3898:ASP:H	1.48	0.61
1:D:1091:GLU:HG2	1:D:1250:TRP:HE1	1.65	0.61
1:A:1091:GLU:HG2	1:A:1250:TRP:HE1	1.65	0.61
1:B:537:LEU:HD23	1:B:540:LEU:HD13	1.82	0.61
1:A:653:SER:HB2	1:A:1611:ARG:HH12	1.65	0.61
1:A:1104:GLU:HG3	1:A:1224:LEU:HD22	1.81	0.61
1:C:2185:GLU:HG2	1:C:2186:ILE:HG12	1.82	0.61
1:D:2307:CYS:SG	1:D:2308:ASN:N	2.73	0.61
1:D:2185:GLU:HG2	1:D:2186:ILE:HG12	1.82	0.61
1:A:3025:ALA:HB3	1:A:3029:VAL:HB	1.82	0.61
1:B:1104:GLU:HG3	1:B:1224:LEU:HD22	1.81	0.61
1:C:1432:ILE:HG12	1:C:1554:PHE:HB2	1.83	0.61
1:D:653:SER:HB2	1:D:1611:ARG:HH12	1.65	0.61
1:D:363:ILE:HG23	1:D:372:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE1	1:D:2321:ARG:NH1	2.34	0.61
1:C:678:MET:HB3	1:C:801:ARG:HB2	1.83	0.61
1:D:3000:LYS:HG2	1:D:3070:THR:HG22	1.82	0.61
1:B:363:ILE:HG23	1:B:372:LEU:HD13	1.82	0.61
1:B:653:SER:HB2	1:B:1611:ARG:HH12	1.65	0.61
1:B:1432:ILE:HG12	1:B:1554:PHE:HB2	1.83	0.61
1:B:3000:LYS:HG2	1:B:3070:THR:HG22	1.82	0.61
1:C:271:ALA:HB2	1:C:488:LEU:HD11	1.83	0.61
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.82	0.61
1:D:3025:ALA:HB3	1:D:3029:VAL:HB	1.82	0.61
1:D:4781:THR:HG21	1:D:4812:TYR:HA	1.83	0.61
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.82	0.61
1:B:271:ALA:HB2	1:B:488:LEU:HD11	1.83	0.61
1:A:271:ALA:HB2	1:A:488:LEU:HD11	1.83	0.60
1:A:537:LEU:HD23	1:A:540:LEU:HD13	1.82	0.60
1:B:678:MET:HB3	1:B:801:ARG:HB2	1.83	0.60
1:A:644:LEU:HD11	1:A:1634:PRO:HG3	1.84	0.60
1:C:644:LEU:HD11	1:C:1634:PRO:HG3	1.84	0.60
1:A:4781:THR:HG21	1:A:4812:TYR:HA	1.83	0.60
1:B:2648:PHE:O	1:B:2652:SER:CB	2.50	0.60
1:D:271:ALA:HB2	1:D:488:LEU:HD11	1.83	0.60
1:A:1633:ILE:HG13	1:A:1651:LEU:HD11	1.83	0.60
1:A:3000:LYS:HG2	1:A:3070:THR:HG22	1.82	0.60
1:B:2185:GLU:HG2	1:B:2186:ILE:HG12	1.82	0.60
1:C:653:SER:HB2	1:C:1611:ARG:HH12	1.65	0.60
1:D:678:MET:HB3	1:D:801:ARG:HB2	1.83	0.60
1:C:1920:ARG:NH2	1:C:2039:LYS:O	2.34	0.60
1:A:678:MET:HB3	1:A:801:ARG:HB2	1.83	0.60
1:A:1432:ILE:HG12	1:A:1554:PHE:HB2	1.83	0.60
1:B:644:LEU:HD11	1:B:1634:PRO:HG3	1.84	0.60
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.82	0.60
1:A:1432:ILE:HD13	1:A:1546:ALA:HB2	1.82	0.60
1:A:2648:PHE:O	1:A:2652:SER:CB	2.50	0.60
1:B:1633:ILE:HG13	1:B:1651:LEU:HD11	1.83	0.60
1:C:1432:ILE:HD13	1:C:1546:ALA:HB2	1.82	0.60
1:C:2281:SER:OG	1:C:2282:LYS:NZ	2.35	0.60
1:C:3891:TYR:HE2	1:C:3898:ASP:H	1.48	0.60
1:C:4781:THR:HG21	1:C:4812:TYR:HA	1.83	0.60
1:D:1920:ARG:NH2	1:D:2039:LYS:O	2.34	0.60
1:C:438:LYS:HG3	1:C:440:VAL:HG23	1.84	0.60
1:D:2281:SER:OG	1:D:2282:LYS:NZ	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3195:SER:O	1:D:3199:ASN:N	2.35	0.60
1:B:3025:ALA:HB3	1:B:3029:VAL:HB	1.82	0.60
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.82	0.59
1:C:2648:PHE:O	1:C:2652:SER:CB	2.50	0.59
1:C:3951:ALA:HB1	1:C:4011:MET:HE1	1.84	0.59
1:D:644:LEU:HD11	1:D:1634:PRO:HG3	1.84	0.59
1:D:2648:PHE:O	1:D:2652:SER:CB	2.50	0.59
1:A:1444:GLY:HA3	1:A:1488:VAL:HA	1.84	0.59
1:B:34:LYS:H	1:B:53:SER:HB3	1.67	0.59
1:B:2321:ARG:NH1	1:C:189:GLU:OE1	2.34	0.59
1:B:3891:TYR:HE2	1:B:3898:ASP:H	1.48	0.59
1:C:363:ILE:HG23	1:C:372:LEU:HD13	1.82	0.59
1:C:1245:ARG:NH1	1:C:1810:PRO:O	2.36	0.59
1:C:3025:ALA:HB3	1:C:3029:VAL:HB	1.82	0.59
1:C:3195:SER:O	1:C:3199:ASN:N	2.35	0.59
1:A:1920:ARG:NH2	1:A:2039:LYS:O	2.34	0.59
1:C:1633:ILE:HG13	1:C:1651:LEU:HD11	1.83	0.59
1:A:1190:LEU:HD21	1:A:1193:LYS:HB2	1.85	0.59
1:A:2307:CYS:SG	1:A:2308:ASN:N	2.73	0.59
1:B:438:LYS:HG3	1:B:440:VAL:HG23	1.84	0.59
1:C:1441:VAL:HG21	1:C:1546:ALA:HA	1.85	0.59
1:C:1444:GLY:HA3	1:C:1488:VAL:HA	1.84	0.59
1:B:4781:THR:HG21	1:B:4812:TYR:HA	1.83	0.59
1:C:2648:PHE:O	1:C:2652:SER:HB2	2.03	0.59
1:D:438:LYS:HG3	1:D:440:VAL:HG23	1.84	0.59
1:B:607:ASN:O	1:B:608:HIS:ND1	2.36	0.59
1:A:34:LYS:H	1:A:53:SER:HB3	1.67	0.59
1:B:1441:VAL:HG21	1:B:1546:ALA:HA	1.85	0.59
1:C:4601:ARG:NH1	1:C:4630:ASP:OD1	2.35	0.59
1:D:1432:ILE:HG12	1:D:1554:PHE:HB2	1.83	0.59
1:D:1633:ILE:HG13	1:D:1651:LEU:HD11	1.83	0.59
1:D:3700:ASP:OD2	1:D:3726:GLN:NE2	2.36	0.59
1:A:438:LYS:HG3	1:A:440:VAL:HG23	1.84	0.59
1:B:1258:PHE:O	1:B:1303:ARG:NH1	2.36	0.59
1:B:2281:SER:OG	1:B:2282:LYS:NZ	2.35	0.59
1:B:2648:PHE:O	1:B:2652:SER:HB2	2.03	0.59
1:C:1258:PHE:O	1:C:1303:ARG:NH1	2.36	0.59
1:C:2307:CYS:SG	1:C:2308:ASN:N	2.73	0.59
1:C:2321:ARG:NH1	1:D:189:GLU:OE1	2.34	0.59
1:C:3957:LEU:HB3	1:C:3967:LEU:HD12	1.85	0.59
1:D:1444:GLY:HA3	1:D:1488:VAL:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1444:GLY:HA3	1:B:1488:VAL:HA	1.84	0.59
1:C:34:LYS:H	1:C:53:SER:HB3	1.67	0.59
1:C:607:ASN:O	1:C:608:HIS:ND1	2.36	0.59
1:C:942:THR:O	1:C:998:LYS:NZ	2.36	0.59
1:A:2281:SER:OG	1:A:2282:LYS:NZ	2.35	0.58
1:D:463:PHE:HB3	1:D:536:LEU:HD12	1.85	0.58
1:A:942:THR:O	1:A:998:LYS:NZ	2.36	0.58
1:A:1258:PHE:O	1:A:1303:ARG:NH1	2.36	0.58
1:A:2321:ARG:NH1	1:B:189:GLU:OE1	2.34	0.58
1:A:2334:LEU:HD12	1:A:2341:GLY:HA3	1.85	0.58
1:B:1920:ARG:NH2	1:B:2039:LYS:O	2.34	0.58
1:B:2334:LEU:HD12	1:B:2341:GLY:HA3	1.85	0.58
1:C:2334:LEU:HD12	1:C:2341:GLY:HA3	1.85	0.58
1:D:418:VAL:O	1:D:422:THR:OG1	2.12	0.58
1:D:2334:LEU:HD12	1:D:2341:GLY:HA3	1.85	0.58
1:A:1245:ARG:NH1	1:A:1810:PRO:O	2.36	0.58
1:B:1190:LEU:HD21	1:B:1193:LYS:HB2	1.85	0.58
1:A:4010:GLU:HG2	1:A:4120:LEU:HD13	1.86	0.58
1:C:245:LEU:HB2	1:C:275:TRP:HH2	1.68	0.58
1:D:4010:GLU:HG2	1:D:4120:LEU:HD13	1.86	0.58
1:A:607:ASN:O	1:A:608:HIS:ND1	2.36	0.58
1:A:2648:PHE:O	1:A:2652:SER:HB2	2.03	0.58
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.37	0.58
1:B:1245:ARG:NH1	1:B:1810:PRO:O	2.36	0.58
1:B:1780:SER:HB2	1:B:1781:PRO:HD3	1.85	0.58
1:B:4619:GLN:OE1	1:B:4631:ARG:NH1	2.36	0.58
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.37	0.58
1:D:1190:LEU:HD21	1:D:1193:LYS:HB2	1.85	0.58
1:D:1441:VAL:HG21	1:D:1546:ALA:HA	1.85	0.58
1:A:3195:SER:O	1:A:3199:ASN:N	2.35	0.58
1:A:3700:ASP:OD2	1:A:3726:GLN:NE2	2.36	0.58
1:A:4601:ARG:NH1	1:A:4630:ASP:OD1	2.35	0.58
1:C:3700:ASP:OD2	1:C:3726:GLN:NE2	2.36	0.58
1:D:34:LYS:H	1:D:53:SER:HB3	1.67	0.58
1:A:245:LEU:HB2	1:A:275:TRP:HH2	1.68	0.58
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.37	0.58
1:B:463:PHE:HB3	1:B:536:LEU:HD12	1.85	0.58
1:D:3957:LEU:HB3	1:D:3967:LEU:HD12	1.85	0.58
1:A:463:PHE:HB3	1:A:536:LEU:HD12	1.85	0.58
1:A:1780:SER:HB2	1:A:1781:PRO:HD3	1.85	0.58
1:A:4619:GLN:OE1	1:A:4631:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:THR:O	1:B:998:LYS:NZ	2.36	0.58
1:B:3700:ASP:OD2	1:B:3726:GLN:NE2	2.36	0.58
1:D:607:ASN:O	1:D:608:HIS:ND1	2.36	0.58
1:D:942:THR:O	1:D:998:LYS:NZ	2.36	0.58
2:F:30:LEU:HB3	2:F:34:LYS:HB2	1.86	0.58
1:A:1441:VAL:HG21	1:A:1546:ALA:HA	1.85	0.58
1:B:3195:SER:O	1:B:3199:ASN:N	2.35	0.58
1:D:4601:ARG:NH1	1:D:4630:ASP:OD1	2.35	0.58
1:B:1119:ARG:NH2	1:B:1196:ASP:O	2.37	0.57
1:B:4601:ARG:NH1	1:B:4630:ASP:OD1	2.35	0.57
1:D:1258:PHE:O	1:D:1303:ARG:NH1	2.36	0.57
1:D:1780:SER:HB2	1:D:1781:PRO:HD3	1.85	0.57
1:B:245:LEU:HB2	1:B:275:TRP:HH2	1.68	0.57
1:C:463:PHE:HB3	1:C:536:LEU:HD12	1.85	0.57
1:C:1083:GLU:OE1	1:C:1084:ARG:NH1	2.38	0.57
1:D:548:CYS:O	1:D:552:SER:OG	2.22	0.57
1:D:904:TYR:O	1:D:914:GLN:NE2	2.37	0.57
1:C:904:TYR:O	1:C:914:GLN:NE2	2.37	0.57
1:D:711:GLU:HG3	1:D:1259:LEU:HD21	1.86	0.57
1:D:1245:ARG:NH1	1:D:1810:PRO:O	2.36	0.57
1:D:2648:PHE:O	1:D:2652:SER:HB2	2.03	0.57
1:A:4589:TYR:OH	1:A:4717:SER:OG	2.22	0.57
1:B:904:TYR:O	1:B:914:GLN:NE2	2.37	0.57
1:B:3957:LEU:HB3	1:B:3967:LEU:HD12	1.85	0.57
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.37	0.57
1:C:1190:LEU:HD21	1:C:1193:LYS:HB2	1.85	0.57
2:E:30:LEU:HB3	2:E:34:LYS:HB2	1.86	0.57
1:B:527:LYS:NZ	1:B:566:GLU:OE1	2.32	0.57
1:A:1119:ARG:NH2	1:A:1196:ASP:O	2.37	0.57
1:C:711:GLU:HG3	1:C:1259:LEU:HD21	1.86	0.57
1:C:1780:SER:HB2	1:C:1781:PRO:HD3	1.85	0.57
1:C:3913:LYS:HG3	1:C:3973:LEU:HD13	1.86	0.57
1:D:245:LEU:HB2	1:D:275:TRP:HH2	1.68	0.57
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.37	0.57
1:A:3957:LEU:HB3	1:A:3967:LEU:HD12	1.85	0.57
1:D:3754:VAL:HG11	1:D:3795:LEU:HD21	1.86	0.57
1:A:1735:LYS:NZ	1:A:1929:ASP:OD2	2.38	0.57
1:B:4010:GLU:HG2	1:B:4120:LEU:HD13	1.86	0.57
2:G:30:LEU:HB3	2:G:34:LYS:HB2	1.86	0.57
1:A:711:GLU:HG3	1:A:1259:LEU:HD21	1.86	0.57
1:A:904:TYR:O	1:A:914:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1119:ARG:NH2	1:C:1196:ASP:O	2.37	0.57
1:B:1299:ILE:HG12	1:B:1457:PHE:HE1	1.70	0.57
1:B:3913:LYS:HG3	1:B:3973:LEU:HD13	1.86	0.57
1:D:81:MET:N	1:D:81:MET:SD	2.78	0.57
1:B:2307:CYS:SG	1:B:2308:ASN:N	2.73	0.56
1:B:3754:VAL:HG11	1:B:3795:LEU:HD21	1.86	0.56
1:B:3950:PHE:HZ	1:B:3973:LEU:HG	1.69	0.56
1:C:527:LYS:NZ	1:C:566:GLU:OE1	2.32	0.56
1:C:4010:GLU:HG2	1:C:4120:LEU:HD13	1.86	0.56
1:B:4130:PRO:O	1:B:4156:ARG:NH2	2.39	0.56
1:C:81:MET:N	1:C:81:MET:SD	2.78	0.56
1:C:3754:VAL:HG11	1:C:3795:LEU:HD21	1.86	0.56
1:C:3950:PHE:HZ	1:C:3973:LEU:HG	1.69	0.56
1:D:2219:TYR:O	1:D:2223:ASN:ND2	2.39	0.56
1:D:4130:PRO:O	1:D:4156:ARG:NH2	2.39	0.56
2:H:30:LEU:HB3	2:H:34:LYS:HB2	1.86	0.56
1:A:3754:VAL:HG11	1:A:3795:LEU:HD21	1.86	0.56
1:B:1083:GLU:OE1	1:B:1084:ARG:NH1	2.38	0.56
1:B:3013:LEU:HD13	1:B:3032:LEU:H	1.71	0.56
1:C:4589:TYR:OH	1:C:4717:SER:OG	2.22	0.56
1:D:3950:PHE:HZ	1:D:3973:LEU:HG	1.69	0.56
1:A:527:LYS:NZ	1:A:566:GLU:OE1	2.32	0.56
1:A:2219:TYR:O	1:A:2223:ASN:ND2	2.39	0.56
1:A:3913:LYS:HG3	1:A:3973:LEU:HD13	1.86	0.56
1:D:1299:ILE:HG12	1:D:1457:PHE:HE1	1.70	0.56
1:B:711:GLU:HG3	1:B:1259:LEU:HD21	1.86	0.56
1:C:1283:LEU:HD21	1:C:1427:TYR:HB3	1.88	0.56
1:A:2680:MET:HB3	1:A:2683:ASN:HB2	1.88	0.56
1:D:527:LYS:NZ	1:D:566:GLU:OE1	2.32	0.56
1:D:3913:LYS:HG3	1:D:3973:LEU:HD13	1.86	0.56
1:A:81:MET:N	1:A:81:MET:SD	2.78	0.56
1:A:871:GLN:HE22	1:A:998:LYS:HD3	1.71	0.56
1:A:1299:ILE:HG12	1:A:1457:PHE:HE1	1.70	0.56
1:A:4130:PRO:O	1:A:4156:ARG:NH2	2.39	0.56
1:C:871:GLN:HE22	1:C:998:LYS:HD3	1.71	0.56
1:C:4619:GLN:OE1	1:C:4631:ARG:NH1	2.36	0.56
1:B:81:MET:SD	1:B:81:MET:N	2.78	0.56
1:B:689:GLU:OE2	2:F:71:ARG:NH1	2.39	0.56
1:B:910:ASP:OD2	1:B:915:HIS:NE2	2.39	0.56
1:B:2219:TYR:O	1:B:2223:ASN:ND2	2.39	0.56
1:C:548:CYS:O	1:C:552:SER:OG	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1299:ILE:HG12	1:C:1457:PHE:HE1	1.70	0.56
1:C:2357:SER:OG	1:C:2358:ARG:N	2.39	0.56
1:C:4130:PRO:O	1:C:4156:ARG:NH2	2.39	0.56
1:D:2680:MET:HB3	1:D:2683:ASN:HB2	1.88	0.56
1:A:3013:LEU:HD13	1:A:3032:LEU:H	1.71	0.56
1:A:3950:PHE:HZ	1:A:3973:LEU:HG	1.69	0.56
1:C:3013:LEU:HD13	1:C:3032:LEU:H	1.71	0.56
1:A:1283:LEU:HD21	1:A:1427:TYR:HB3	1.88	0.55
1:B:2286:ASP:OD1	1:B:2286:ASP:N	2.39	0.55
1:C:3015:ARG:HH22	1:C:3080:THR:HB	1.71	0.55
1:D:1283:LEU:HD21	1:D:1427:TYR:HB3	1.88	0.55
2:G:74:LEU:HB3	2:G:99:PHE:HB2	1.88	0.55
1:A:910:ASP:OD2	1:A:915:HIS:NE2	2.39	0.55
1:A:1429:SER:HB2	1:A:1508:ILE:HA	1.88	0.55
1:B:1283:LEU:HD21	1:B:1427:TYR:HB3	1.88	0.55
1:D:784:ILE:HA	1:D:788:PHE:HZ	1.72	0.55
1:D:3015:ARG:HH22	1:D:3080:THR:HB	1.71	0.55
1:A:2286:ASP:OD1	1:A:2286:ASP:N	2.39	0.55
1:A:3015:ARG:HH22	1:A:3080:THR:HB	1.71	0.55
1:C:910:ASP:OD2	1:C:915:HIS:NE2	2.39	0.55
1:C:2219:TYR:O	1:C:2223:ASN:ND2	2.39	0.55
1:D:910:ASP:OD2	1:D:915:HIS:NE2	2.39	0.55
1:D:1083:GLU:OE1	1:D:1084:ARG:NH1	2.38	0.55
1:B:474:ASP:OD2	1:B:474:ASP:N	2.39	0.55
1:B:548:CYS:O	1:B:552:SER:OG	2.22	0.55
1:B:784:ILE:HA	1:B:788:PHE:HZ	1.72	0.55
1:C:418:VAL:O	1:C:422:THR:OG1	2.12	0.55
1:D:1735:LYS:NZ	1:D:1929:ASP:OD2	2.38	0.55
1:A:784:ILE:HA	1:A:788:PHE:HZ	1.72	0.55
1:D:871:GLN:HE22	1:D:998:LYS:HD3	1.71	0.55
1:D:4619:GLN:OE1	1:D:4631:ARG:NH1	2.36	0.55
2:F:48:PHE:HD1	2:F:55:VAL:HG11	1.72	0.55
1:C:343:ARG:HG2	1:C:344:LYS:H	1.72	0.55
1:C:2680:MET:HB3	1:C:2683:ASN:HB2	1.88	0.55
1:D:343:ARG:HG2	1:D:344:LYS:H	1.72	0.55
1:D:689:GLU:OE2	2:H:71:ARG:NH1	2.39	0.55
2:E:74:LEU:HB3	2:E:99:PHE:HB2	1.88	0.55
1:C:689:GLU:OE2	2:G:71:ARG:NH1	2.39	0.55
1:C:1429:SER:HB2	1:C:1508:ILE:HA	1.88	0.55
1:C:3504:VAL:HA	1:C:3507:ILE:HD12	1.89	0.55
2:F:74:LEU:HB3	2:F:99:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:48:PHE:HD1	2:G:55:VAL:HG11	1.72	0.55
1:B:343:ARG:HG2	1:B:344:LYS:H	1.72	0.55
1:B:4755:ILE:HD11	1:C:4765:GLN:HB3	1.89	0.55
1:D:2357:SER:OG	1:D:2358:ARG:N	2.39	0.55
1:A:343:ARG:HG2	1:A:344:LYS:H	1.72	0.54
2:E:48:PHE:HD1	2:E:55:VAL:HG11	1.72	0.54
1:B:3015:ARG:HH22	1:B:3080:THR:HB	1.71	0.54
1:C:2286:ASP:OD1	1:C:2286:ASP:N	2.39	0.54
1:C:4755:ILE:HD11	1:D:4765:GLN:HB3	1.89	0.54
1:A:3265:THR:HB	1:A:3342:GLU:HG3	1.90	0.54
1:A:4765:GLN:HB3	1:D:4755:ILE:HD11	1.89	0.54
1:B:2357:SER:OG	1:B:2358:ARG:N	2.39	0.54
1:B:2680:MET:HB3	1:B:2683:ASN:HB2	1.88	0.54
1:B:3265:THR:HB	1:B:3342:GLU:HG3	1.90	0.54
1:C:2391:TYR:O	1:C:2395:ILE:HD12	2.07	0.54
1:D:3013:LEU:HD13	1:D:3032:LEU:H	1.71	0.54
1:A:2441:MET:HG2	1:A:2493:PRO:HD3	1.90	0.54
1:B:3504:VAL:HA	1:B:3507:ILE:HD12	1.89	0.54
1:C:784:ILE:HA	1:C:788:PHE:HZ	1.72	0.54
1:D:1429:SER:HB2	1:D:1508:ILE:HA	1.88	0.54
1:A:4672:ASP:OD1	1:A:4672:ASP:N	2.41	0.54
1:C:1000:ALA:O	1:C:1004:HIS:ND1	2.37	0.54
1:C:1735:LYS:NZ	1:C:1929:ASP:OD2	2.38	0.54
1:D:3265:THR:HB	1:D:3342:GLU:HG3	1.90	0.54
2:H:74:LEU:HB3	2:H:99:PHE:HB2	1.88	0.54
1:A:1083:GLU:OE1	1:A:1084:ARG:NH1	2.38	0.54
1:A:2391:TYR:O	1:A:2395:ILE:HD12	2.07	0.54
1:A:4615:TYR:OH	1:A:4627:GLY:O	2.24	0.54
1:B:2391:TYR:O	1:B:2395:ILE:HD12	2.07	0.54
1:B:2441:MET:HG2	1:B:2493:PRO:HD3	1.90	0.54
1:A:2357:SER:OG	1:A:2358:ARG:N	2.39	0.54
1:C:991:SER:O	1:C:995:MET:HG2	2.08	0.54
1:C:1510:CYS:O	1:C:1520:THR:OG1	2.26	0.54
1:C:4615:TYR:OH	1:C:4627:GLY:O	2.24	0.54
1:D:1000:ALA:O	1:D:1004:HIS:ND1	2.37	0.54
1:D:2391:TYR:O	1:D:2395:ILE:HD12	2.07	0.54
1:A:689:GLU:OE2	2:E:71:ARG:NH1	2.39	0.54
1:A:2701:ASN:O	1:A:2849:ASN:ND2	2.41	0.54
1:A:4755:ILE:HD11	1:B:4765:GLN:HB3	1.89	0.54
1:B:871:GLN:HE22	1:B:998:LYS:HD3	1.71	0.54
1:B:991:SER:O	1:B:995:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1993:ASP:OD1	1:D:1993:ASP:N	2.41	0.54
1:D:3909:ILE:HG21	1:D:3969:GLU:HG2	1.90	0.54
1:A:3909:ILE:HG21	1:A:3969:GLU:HG2	1.90	0.54
1:C:2991:THR:HA	1:C:2994:HIS:HB3	1.90	0.54
1:D:1722:MET:SD	1:D:2126:ARG:NH2	2.81	0.54
1:D:2701:ASN:O	1:D:2849:ASN:ND2	2.41	0.54
1:D:3504:VAL:HA	1:D:3507:ILE:HD12	1.89	0.54
2:H:48:PHE:HD1	2:H:55:VAL:HG11	1.72	0.54
1:A:548:CYS:O	1:A:552:SER:OG	2.22	0.54
1:A:1722:MET:SD	1:A:2126:ARG:NH2	2.81	0.54
1:A:3504:VAL:HA	1:A:3507:ILE:HD12	1.89	0.54
1:B:1429:SER:OG	1:B:1506:LEU:O	2.24	0.54
1:C:3265:THR:HB	1:C:3342:GLU:HG3	1.90	0.54
1:D:2872:PRO:O	1:D:2875:THR:OG1	2.26	0.54
1:B:1722:MET:SD	1:B:2126:ARG:NH2	2.81	0.53
1:D:4672:ASP:OD1	1:D:4672:ASP:N	2.41	0.53
1:C:2872:PRO:O	1:C:2875:THR:OG1	2.26	0.53
1:D:1429:SER:OG	1:D:1506:LEU:O	2.24	0.53
1:D:2619:TYR:HB3	1:D:2623:PRO:HG3	1.90	0.53
1:D:3951:ALA:HB1	1:D:4011:MET:HE1	1.90	0.53
1:B:1735:LYS:NZ	1:B:1929:ASP:OD2	2.38	0.53
1:B:2159:ASN:OD1	1:B:2162:ARG:NH2	2.41	0.53
1:B:2872:PRO:O	1:B:2875:THR:OG1	2.26	0.53
1:D:2286:ASP:OD1	1:D:2286:ASP:N	2.39	0.53
1:A:1000:ALA:O	1:A:1004:HIS:ND1	2.37	0.53
1:A:4660:TYR:O	1:A:4664:ARG:NH2	2.42	0.53
1:D:2159:ASN:OD1	1:D:2162:ARG:NH2	2.41	0.53
1:D:3843:GLN:OE1	1:D:3914:GLN:NE2	2.41	0.53
1:A:2619:TYR:HB3	1:A:2623:PRO:HG3	1.90	0.53
1:B:1429:SER:HB2	1:B:1508:ILE:HA	1.88	0.53
1:B:2145:LEU:HD23	1:B:2148:ILE:HD11	1.91	0.53
1:C:1722:MET:SD	1:C:2126:ARG:NH2	2.81	0.53
1:C:3843:GLN:OE1	1:C:3914:GLN:NE2	2.41	0.53
1:C:3909:ILE:HG21	1:C:3969:GLU:HG2	1.90	0.53
1:C:4672:ASP:N	1:C:4672:ASP:OD1	2.41	0.53
1:A:2145:LEU:HD23	1:A:2148:ILE:HD11	1.91	0.53
1:A:2159:ASN:OD1	1:A:2162:ARG:NH2	2.41	0.53
1:A:2262:GLU:O	1:A:2266:ARG:HG2	2.09	0.53
1:A:2872:PRO:O	1:A:2875:THR:OG1	2.26	0.53
1:B:535:GLU:HG2	1:B:573:GLU:HG3	1.91	0.53
1:B:4059:GLN:HA	1:B:4063:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4615:TYR:OH	1:B:4627:GLY:O	2.24	0.53
1:C:2159:ASN:OD1	1:C:2162:ARG:NH2	2.41	0.53
1:C:2441:MET:HG2	1:C:2493:PRO:HD3	1.90	0.53
1:D:474:ASP:OD2	1:D:474:ASP:N	2.39	0.53
1:D:2262:GLU:O	1:D:2266:ARG:HG2	2.09	0.53
1:A:474:ASP:OD2	1:A:474:ASP:N	2.39	0.53
1:B:2217:LEU:HA	1:B:2220:LEU:HB2	1.91	0.53
1:D:2991:THR:HA	1:D:2994:HIS:HB3	1.90	0.53
1:D:3418:PHE:O	1:D:3422:ASN:ND2	2.35	0.53
1:D:4660:TYR:O	1:D:4664:ARG:NH2	2.42	0.53
1:A:3687:TYR:HE2	1:A:3742:THR:HG21	1.74	0.53
1:A:4507:VAL:HG23	1:A:4574:LEU:HD22	1.91	0.53
1:B:1510:CYS:O	1:B:1520:THR:OG1	2.26	0.53
1:B:4660:TYR:O	1:B:4664:ARG:NH2	2.42	0.53
1:C:2703:GLN:HE22	1:C:2853:LYS:HD3	1.74	0.53
1:C:4507:VAL:HG23	1:C:4574:LEU:HD22	1.91	0.53
1:D:2703:GLN:HE22	1:D:2853:LYS:HD3	1.74	0.53
1:A:1450:PHE:HD1	1:A:1485:CYS:HB3	1.74	0.53
1:B:3909:ILE:HG21	1:B:3969:GLU:HG2	1.90	0.53
1:C:535:GLU:HG2	1:C:573:GLU:HG3	1.91	0.53
1:C:4660:TYR:O	1:C:4664:ARG:NH2	2.42	0.53
1:D:2217:LEU:HA	1:D:2220:LEU:HB2	1.91	0.53
1:D:3687:TYR:HE2	1:D:3742:THR:HG21	1.74	0.53
1:A:1429:SER:OG	1:A:1506:LEU:O	2.24	0.53
1:A:2991:THR:HA	1:A:2994:HIS:HB3	1.90	0.53
1:B:1450:PHE:HD1	1:B:1485:CYS:HB3	1.74	0.53
1:C:3452:LYS:NZ	1:C:3553:ILE:O	2.42	0.53
1:A:535:GLU:HG2	1:A:573:GLU:HG3	1.91	0.52
1:A:4554:ILE:HG12	1:A:4556:VAL:HA	1.91	0.52
1:B:288:HIS:CD2	1:B:352:SER:H	2.28	0.52
1:B:2619:TYR:HB3	1:B:2623:PRO:HG3	1.90	0.52
1:B:3687:TYR:HE2	1:B:3742:THR:HG21	1.74	0.52
1:B:4554:ILE:HG12	1:B:4556:VAL:HA	1.91	0.52
1:C:1784:PRO:HB2	1:C:1787:ILE:HG12	1.91	0.52
1:D:2441:MET:HG2	1:D:2493:PRO:HD3	1.90	0.52
1:D:2892:PHE:O	1:D:2896:GLN:HB2	2.10	0.52
1:D:3095:TYR:OH	1:D:3219:GLU:OE1	2.27	0.52
1:A:288:HIS:CD2	1:A:352:SER:H	2.28	0.52
1:A:991:SER:O	1:A:995:MET:HG2	2.08	0.52
1:B:2069:ALA:HB1	1:B:3662:PRO:HB3	1.92	0.52
1:B:2991:THR:HA	1:B:2994:HIS:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2145:LEU:HD23	1:C:2148:ILE:HD11	1.91	0.52
1:C:2892:PHE:O	1:C:2896:GLN:HB2	2.10	0.52
1:C:4059:GLN:HA	1:C:4063:GLU:HB2	1.91	0.52
1:D:991:SER:O	1:D:995:MET:HG2	2.08	0.52
1:B:3843:GLN:OE1	1:B:3914:GLN:NE2	2.41	0.52
1:C:1429:SER:OG	1:C:1506:LEU:O	2.24	0.52
1:C:1450:PHE:HD1	1:C:1485:CYS:HB3	1.74	0.52
1:D:288:HIS:CD2	1:D:352:SER:H	2.28	0.52
1:C:730:LEU:HG	2:G:7:ILE:HG22	1.92	0.52
1:C:2619:TYR:HB3	1:C:2623:PRO:HG3	1.90	0.52
1:B:640:ARG:H	1:B:643:LEU:HD12	1.75	0.52
1:B:1000:ALA:O	1:B:1004:HIS:ND1	2.37	0.52
1:B:4672:ASP:N	1:B:4672:ASP:OD1	2.41	0.52
1:B:4694:SER:HA	1:B:4697:LEU:HD13	1.91	0.52
1:C:288:HIS:CD2	1:C:352:SER:H	2.28	0.52
1:C:2069:ALA:HB1	1:C:3662:PRO:HB3	1.92	0.52
1:C:2217:LEU:HA	1:C:2220:LEU:HB2	1.91	0.52
1:C:2262:GLU:O	1:C:2266:ARG:HG2	2.09	0.52
1:D:1784:PRO:HB2	1:D:1787:ILE:HG12	1.91	0.52
1:B:1126:LEU:HD12	1:B:1127:GLU:H	1.75	0.52
1:B:2262:GLU:O	1:B:2266:ARG:HG2	2.09	0.52
1:D:1450:PHE:HD1	1:D:1485:CYS:HB3	1.74	0.52
1:D:2069:ALA:HB1	1:D:3662:PRO:HB3	1.92	0.52
1:C:3663:LEU:O	1:C:3667:ILE:HG12	2.10	0.52
1:A:1128:LEU:HD23	1:A:1206:SER:HB2	1.92	0.52
1:A:3843:GLN:OE1	1:A:3914:GLN:NE2	2.41	0.52
1:A:4694:SER:HA	1:A:4697:LEU:HD13	1.91	0.52
1:B:61:ASP:OD1	1:B:61:ASP:N	2.42	0.52
1:C:1126:LEU:HD12	1:C:1127:GLU:H	1.75	0.52
1:C:4694:SER:HA	1:C:4697:LEU:HD13	1.91	0.52
1:D:730:LEU:HG	2:H:7:ILE:HG22	1.92	0.52
1:A:1784:PRO:HB2	1:A:1787:ILE:HG12	1.91	0.52
1:B:2148:ILE:HD12	1:B:2166:MET:SD	2.50	0.52
1:B:2892:PHE:O	1:B:2896:GLN:HB2	2.10	0.52
1:C:3095:TYR:OH	1:C:3219:GLU:OE1	2.27	0.52
1:C:3687:TYR:HE2	1:C:3742:THR:HG21	1.74	0.52
1:D:1126:LEU:HD12	1:D:1127:GLU:H	1.75	0.52
1:A:656:ARG:HG3	1:A:835:GLU:HB3	1.92	0.52
1:A:2069:ALA:HB1	1:A:3662:PRO:HB3	1.92	0.52
1:B:656:ARG:HG3	1:B:835:GLU:HB3	1.92	0.52
1:B:4501:ARG:NH2	1:B:4744:ASP:OD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4501:ARG:NH2	1:D:4744:ASP:OD1	2.43	0.52
1:A:194:LEU:HD13	1:A:210:THR:HG21	1.92	0.51
1:A:2217:LEU:HA	1:A:2220:LEU:HB2	1.91	0.51
1:A:3555:ASN:O	1:A:3559:HIS:NE2	2.44	0.51
1:B:1953:SER:HA	1:B:1956:LEU:HD12	1.92	0.51
1:B:2701:ASN:O	1:B:2849:ASN:ND2	2.41	0.51
1:D:535:GLU:HG2	1:D:573:GLU:HG3	1.91	0.51
1:D:2145:LEU:HD23	1:D:2148:ILE:HD11	1.91	0.51
1:D:2148:ILE:HD12	1:D:2166:MET:SD	2.50	0.51
1:D:4059:GLN:HA	1:D:4063:GLU:HB2	1.91	0.51
1:D:4554:ILE:HG12	1:D:4556:VAL:HA	1.91	0.51
1:A:606:ARG:HE	1:A:1633:ILE:HG21	1.75	0.51
1:A:1766:SER:O	1:A:1774:ASN:ND2	2.44	0.51
1:A:2148:ILE:HD12	1:A:2166:MET:SD	2.50	0.51
1:A:2892:PHE:O	1:A:2896:GLN:HB2	2.10	0.51
1:B:1489:CYS:SG	1:B:1490:ALA:N	2.84	0.51
1:B:2703:GLN:HE22	1:B:2853:LYS:HD3	1.74	0.51
1:B:3951:ALA:HB1	1:B:4011:MET:HE1	1.91	0.51
1:B:4507:VAL:HG23	1:B:4574:LEU:HD22	1.91	0.51
1:C:194:LEU:HD13	1:C:210:THR:HG21	1.92	0.51
1:C:640:ARG:H	1:C:643:LEU:HD12	1.75	0.51
1:C:2148:ILE:HD12	1:C:2166:MET:SD	2.50	0.51
1:D:1128:LEU:HD23	1:D:1206:SER:HB2	1.92	0.51
1:D:1953:SER:HA	1:D:1956:LEU:HD12	1.92	0.51
1:A:730:LEU:HG	2:E:7:ILE:HG22	1.92	0.51
1:A:1489:CYS:SG	1:A:1490:ALA:N	2.84	0.51
1:D:606:ARG:HE	1:D:1633:ILE:HG21	1.75	0.51
1:B:3095:TYR:OH	1:B:3219:GLU:OE1	2.27	0.51
1:A:1510:CYS:O	1:A:1520:THR:OG1	2.26	0.51
1:A:4501:ARG:NH2	1:A:4744:ASP:OD1	2.43	0.51
1:B:3555:ASN:O	1:B:3559:HIS:NE2	2.44	0.51
1:C:606:ARG:HE	1:C:1633:ILE:HG21	1.75	0.51
1:C:972:LEU:HD12	1:C:977:LYS:HB2	1.92	0.51
1:C:1766:SER:O	1:C:1774:ASN:ND2	2.44	0.51
1:C:4501:ARG:NH2	1:C:4744:ASP:OD1	2.43	0.51
1:D:1489:CYS:SG	1:D:1490:ALA:N	2.84	0.51
1:A:3434:THR:O	1:A:3440:LYS:NZ	2.31	0.51
1:B:1449:ASP:OD1	1:B:1449:ASP:N	2.44	0.51
1:B:1766:SER:O	1:B:1774:ASN:ND2	2.44	0.51
1:D:2234:ARG:NH2	1:D:2281:SER:OG	2.44	0.51
1:A:640:ARG:H	1:A:643:LEU:HD12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1302:TYR:HE2	1:A:1546:ALA:HB3	1.76	0.51
1:A:2234:ARG:NH2	1:A:2281:SER:OG	2.44	0.51
1:A:2703:GLN:HE22	1:A:2853:LYS:HD3	1.74	0.51
1:A:4059:GLN:HA	1:A:4063:GLU:HB2	1.91	0.51
1:B:1784:PRO:HB2	1:B:1787:ILE:HG12	1.91	0.51
1:B:1905:MET:SD	1:B:1905:MET:N	2.81	0.51
1:B:2161:MET:HE1	1:B:2161:MET:H	1.75	0.51
1:C:4554:ILE:HG12	1:C:4556:VAL:HA	1.91	0.51
1:D:640:ARG:H	1:D:643:LEU:HD12	1.75	0.51
1:D:3452:LYS:NZ	1:D:3553:ILE:O	2.42	0.51
1:D:4507:VAL:HG23	1:D:4574:LEU:HD22	1.91	0.51
1:D:4636:THR:OG1	1:D:4701:ASP:OD2	2.29	0.51
1:B:606:ARG:HE	1:B:1633:ILE:HG21	1.75	0.51
1:B:730:LEU:HG	2:F:7:ILE:HG22	1.92	0.51
1:C:656:ARG:HG3	1:C:835:GLU:HB3	1.92	0.51
1:C:1489:CYS:SG	1:C:1490:ALA:N	2.84	0.51
1:C:1897:LEU:HD22	1:C:1901:VAL:HG11	1.93	0.51
1:C:1905:MET:SD	1:C:1905:MET:N	2.81	0.51
1:D:656:ARG:HG3	1:D:835:GLU:HB3	1.92	0.51
1:D:1302:TYR:HE2	1:D:1546:ALA:HB3	1.76	0.51
1:D:2587:LEU:HD23	1:D:2607:LYS:HB2	1.92	0.51
1:D:4694:SER:HA	1:D:4697:LEU:HD13	1.91	0.51
1:A:1126:LEU:HD12	1:A:1127:GLU:H	1.75	0.51
1:D:194:LEU:HD13	1:D:210:THR:HG21	1.92	0.51
1:D:3555:ASN:O	1:D:3559:HIS:NE2	2.44	0.51
1:D:3663:LEU:O	1:D:3667:ILE:HG12	2.10	0.51
1:A:1905:MET:SD	1:A:1905:MET:N	2.81	0.51
1:B:1128:LEU:HD23	1:B:1206:SER:HB2	1.92	0.51
1:B:3452:LYS:NZ	1:B:3553:ILE:O	2.42	0.51
1:B:3663:LEU:O	1:B:3667:ILE:HG12	2.10	0.51
1:C:3555:ASN:O	1:C:3559:HIS:NE2	2.44	0.51
1:D:731:HIS:CE1	1:D:733:TRP:HB3	2.46	0.51
1:D:4882:ASP:OD1	1:D:4886:LYS:NZ	2.44	0.51
1:A:245:LEU:HB2	1:A:275:TRP:CH2	2.47	0.50
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.44	0.50
1:A:3802:LEU:HD21	1:A:3908:ALA:HB2	1.93	0.50
1:A:4882:ASP:OD1	1:A:4886:LYS:NZ	2.44	0.50
1:B:245:LEU:HB2	1:B:275:TRP:CH2	2.47	0.50
1:B:1302:TYR:HE2	1:B:1546:ALA:HB3	1.76	0.50
1:B:1769:PHE:O	2:F:82:TYR:OH	2.29	0.50
1:B:1897:LEU:HD22	1:B:1901:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2648:PHE:O	1:B:2652:SER:OG	2.29	0.50
1:C:1302:TYR:HE2	1:C:1546:ALA:HB3	1.76	0.50
1:C:2587:LEU:HD23	1:C:2607:LYS:HB2	1.92	0.50
1:C:2648:PHE:O	1:C:2652:SER:OG	2.29	0.50
1:D:1766:SER:O	1:D:1774:ASN:ND2	2.44	0.50
1:D:1897:LEU:HD22	1:D:1901:VAL:HG11	1.93	0.50
1:D:972:LEU:HD12	1:D:977:LYS:HB2	1.92	0.50
1:A:972:LEU:HD12	1:A:977:LYS:HB2	1.92	0.50
1:A:4636:THR:OG1	1:A:4701:ASP:OD2	2.29	0.50
1:B:972:LEU:HD12	1:B:977:LYS:HB2	1.92	0.50
1:C:61:ASP:OD1	1:C:61:ASP:N	2.42	0.50
1:C:686:VAL:HG13	1:C:687:THR:HG23	1.94	0.50
1:C:1953:SER:HA	1:C:1956:LEU:HD12	1.92	0.50
1:D:1769:PHE:O	2:H:82:TYR:OH	2.29	0.50
1:A:3663:LEU:O	1:A:3667:ILE:HG12	2.10	0.50
1:C:1128:LEU:HD23	1:C:1206:SER:HB2	1.92	0.50
1:D:723:PHE:HB3	1:D:1465:VAL:HG21	1.94	0.50
1:A:2587:LEU:HD23	1:A:2607:LYS:HB2	1.92	0.50
1:B:4636:THR:OG1	1:B:4701:ASP:OD2	2.29	0.50
1:C:731:HIS:CE1	1:C:733:TRP:HB3	2.46	0.50
1:D:4720:TYR:OH	1:D:4744:ASP:OD1	2.26	0.50
1:A:723:PHE:HB3	1:A:1465:VAL:HG21	1.94	0.50
1:A:731:HIS:CE1	1:A:733:TRP:HB3	2.46	0.50
1:A:1953:SER:HA	1:A:1956:LEU:HD12	1.92	0.50
1:A:2585:GLN:HA	1:A:2588:LEU:HD12	1.93	0.50
1:C:4636:THR:OG1	1:C:4701:ASP:OD2	2.29	0.50
1:A:1897:LEU:HD22	1:A:1901:VAL:HG11	1.93	0.50
1:A:3418:PHE:O	1:A:3422:ASN:ND2	2.35	0.50
1:B:191:TYR:N	1:B:206:ALA:O	2.38	0.50
1:C:245:LEU:HB2	1:C:275:TRP:CH2	2.47	0.50
1:C:3802:LEU:HD21	1:C:3908:ALA:HB2	1.93	0.50
1:D:1510:CYS:O	1:D:1520:THR:OG1	2.26	0.50
1:A:419:ILE:HG13	1:A:420:ARG:N	2.27	0.50
1:B:194:LEU:HD13	1:B:210:THR:HG21	1.92	0.50
1:B:723:PHE:HB3	1:B:1465:VAL:HG21	1.94	0.50
1:B:2587:LEU:HD23	1:B:2607:LYS:HB2	1.92	0.50
1:C:723:PHE:HB3	1:C:1465:VAL:HG21	1.94	0.50
1:C:2585:GLN:HA	1:C:2588:LEU:HD12	1.93	0.50
1:B:332:ARG:NE	1:B:364:GLN:OE1	2.44	0.50
1:B:686:VAL:HG13	1:B:687:THR:HG23	1.94	0.50
1:B:2234:ARG:NH2	1:B:2281:SER:OG	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3731:HIS:O	1:B:3775:LYS:NZ	2.41	0.50
1:B:4795:SER:OG	1:B:4800:THR:OG1	2.30	0.50
1:C:288:HIS:HD2	1:C:352:SER:H	1.58	0.50
1:C:474:ASP:OD2	1:C:474:ASP:N	2.39	0.50
1:C:1449:ASP:OD1	1:C:1449:ASP:N	2.44	0.50
1:C:2105:TYR:HE1	1:C:2159:ASN:HB2	1.76	0.50
1:C:2701:ASN:O	1:C:2849:ASN:ND2	2.41	0.50
1:A:288:HIS:HD2	1:A:352:SER:H	1.58	0.49
1:A:4795:SER:OG	1:A:4800:THR:OG1	2.30	0.49
1:B:288:HIS:HD2	1:B:352:SER:H	1.58	0.49
1:B:2105:TYR:HE1	1:B:2159:ASN:HB2	1.76	0.49
1:C:2234:ARG:NH2	1:C:2281:SER:OG	2.44	0.49
1:D:245:LEU:HB2	1:D:275:TRP:CH2	2.47	0.49
1:D:419:ILE:HG13	1:D:420:ARG:N	2.27	0.49
1:D:3731:HIS:O	1:D:3775:LYS:NZ	2.41	0.49
1:D:4615:TYR:OH	1:D:4627:GLY:O	2.24	0.49
1:A:1024:VAL:HG13	1:A:1025:LYS:HG2	1.94	0.49
1:A:1769:PHE:O	2:E:82:TYR:OH	2.29	0.49
1:D:288:HIS:HD2	1:D:352:SER:H	1.58	0.49
1:C:1769:PHE:O	2:G:82:TYR:OH	2.29	0.49
1:D:681:HIS:HB3	1:D:799:LYS:HG2	1.95	0.49
1:D:2585:GLN:HA	1:D:2588:LEU:HD12	1.93	0.49
1:A:80:GLU:OE1	1:A:84:ASN:ND2	2.42	0.49
1:A:952:ILE:HD11	1:A:955:GLU:HA	1.95	0.49
1:A:2231:PRO:HG2	1:A:2233:MET:HG2	1.94	0.49
1:B:419:ILE:HG13	1:B:420:ARG:N	2.27	0.49
1:B:731:HIS:CE1	1:B:733:TRP:HB3	2.46	0.49
1:B:868:ASP:OD1	1:B:868:ASP:N	2.46	0.49
1:C:480:ARG:NH1	1:C:3677:GLU:OE2	2.45	0.49
1:C:681:HIS:HB3	1:C:799:LYS:HG2	1.95	0.49
1:D:419:ILE:HG13	1:D:420:ARG:H	1.76	0.49
1:A:3452:LYS:NZ	1:A:3553:ILE:O	2.42	0.49
1:D:1905:MET:HA	1:D:1908:LEU:HB2	1.94	0.49
1:D:2231:PRO:HG2	1:D:2233:MET:HG2	1.94	0.49
1:D:2648:PHE:O	1:D:2652:SER:OG	2.29	0.49
1:D:3727:GLN:O	1:D:3731:HIS:ND1	2.44	0.49
1:A:288:HIS:CD2	1:A:349:MET:HB3	2.47	0.49
1:A:480:ARG:NH1	1:A:3677:GLU:OE2	2.45	0.49
1:B:480:ARG:NH1	1:B:3677:GLU:OE2	2.45	0.49
1:B:681:HIS:HB3	1:B:799:LYS:HG2	1.95	0.49
1:B:2585:GLN:HA	1:B:2588:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4882:ASP:OD1	1:B:4886:LYS:NZ	2.44	0.49
1:C:419:ILE:HG13	1:C:420:ARG:N	2.27	0.49
1:C:561:ARG:HH22	1:C:567:ALA:H	1.61	0.49
1:D:288:HIS:CD2	1:D:349:MET:HB3	2.47	0.49
1:D:480:ARG:NH1	1:D:3677:GLU:OE2	2.45	0.49
1:D:868:ASP:N	1:D:868:ASP:OD1	2.46	0.49
1:A:419:ILE:HG13	1:A:420:ARG:H	1.76	0.49
1:A:681:HIS:HB3	1:A:799:LYS:HG2	1.95	0.49
1:A:686:VAL:HG13	1:A:687:THR:HG23	1.94	0.49
1:B:332:ARG:N	1:B:362:TYR:O	2.44	0.49
1:B:952:ILE:HD11	1:B:955:GLU:HA	1.95	0.49
1:B:3436:SER:O	1:B:3439:SER:N	2.45	0.49
1:C:1905:MET:HA	1:C:1908:LEU:HB2	1.94	0.49
1:D:61:ASP:OD1	1:D:61:ASP:N	2.42	0.49
1:D:2105:TYR:HE1	1:D:2159:ASN:HB2	1.76	0.49
1:A:1993:ASP:OD1	1:A:1993:ASP:N	2.41	0.49
1:A:4720:TYR:OH	1:A:4744:ASP:OD1	2.26	0.49
1:B:80:GLU:OE1	1:B:84:ASN:ND2	2.42	0.49
1:B:419:ILE:HG13	1:B:420:ARG:H	1.76	0.49
1:B:821:ALA:HB3	1:B:823:TYR:HE1	1.78	0.49
1:B:2795:ASP:N	1:B:2795:ASP:OD1	2.46	0.49
1:B:4104:LEU:O	1:B:4108:MET:HB2	2.13	0.49
1:C:288:HIS:CD2	1:C:349:MET:HB3	2.47	0.49
1:C:1944:ASN:OD1	1:C:1944:ASN:N	2.46	0.49
1:C:2231:PRO:HG2	1:C:2233:MET:HG2	1.94	0.49
1:D:191:TYR:N	1:D:206:ALA:O	2.38	0.49
1:D:686:VAL:HG13	1:D:687:THR:HG23	1.94	0.49
1:D:3436:SER:O	1:D:3439:SER:N	2.45	0.49
1:A:372:LEU:H	1:A:372:LEU:HD12	1.78	0.49
1:A:868:ASP:N	1:A:868:ASP:OD1	2.46	0.49
1:A:1944:ASN:OD1	1:A:1944:ASN:N	2.46	0.49
1:C:1024:VAL:HG13	1:C:1025:LYS:HG2	1.94	0.49
1:D:1024:VAL:HG13	1:D:1025:LYS:HG2	1.94	0.49
1:A:1434:PRO:HD3	1:A:1506:LEU:HD23	1.95	0.49
1:A:1728:VAL:HG11	1:A:1925:VAL:HG11	1.95	0.49
1:B:234:LEU:HD12	1:B:405:LEU:HD22	1.95	0.49
1:B:288:HIS:CD2	1:B:349:MET:HB3	2.47	0.49
1:B:1517:GLY:O	1:B:1533:GLN:NE2	2.46	0.49
1:B:3802:LEU:HD21	1:B:3908:ALA:HB2	1.93	0.49
1:C:1153:GLY:HA2	1:C:1182:LEU:HD12	1.95	0.49
1:C:2713:PRO:HD2	1:C:2782:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1153:GLY:HA2	1:D:1182:LEU:HD12	1.95	0.49
1:D:3802:LEU:HD21	1:D:3908:ALA:HB2	1.93	0.49
1:B:372:LEU:HD12	1:B:372:LEU:H	1.78	0.48
1:C:3727:GLN:O	1:C:3731:HIS:ND1	2.44	0.48
1:D:561:ARG:HH22	1:D:567:ALA:H	1.61	0.48
1:A:234:LEU:HD12	1:A:405:LEU:HD22	1.95	0.48
1:A:921:PHE:HA	1:A:924:LEU:HD12	1.96	0.48
1:A:2105:TYR:HE1	1:A:2159:ASN:HB2	1.76	0.48
1:A:3731:HIS:O	1:A:3775:LYS:NZ	2.41	0.48
1:C:419:ILE:HG13	1:C:420:ARG:H	1.76	0.48
1:C:486:GLN:HG2	1:C:540:LEU:HG	1.96	0.48
1:C:4104:LEU:O	1:C:4108:MET:HB2	2.13	0.48
1:D:578:VAL:HG11	1:D:585:ALA:H	1.79	0.48
1:D:4104:LEU:O	1:D:4108:MET:HB2	2.13	0.48
1:A:191:TYR:N	1:A:206:ALA:O	2.38	0.48
1:A:332:ARG:N	1:A:362:TYR:O	2.44	0.48
1:B:561:ARG:HH22	1:B:567:ALA:H	1.61	0.48
1:B:578:VAL:HG11	1:B:585:ALA:H	1.79	0.48
1:B:1317:SER:OG	1:B:1318:VAL:N	2.46	0.48
1:B:1993:ASP:OD1	1:B:1993:ASP:N	2.41	0.48
1:C:578:VAL:HG11	1:C:585:ALA:H	1.79	0.48
1:D:2713:PRO:HD2	1:D:2782:LEU:HD13	1.95	0.48
1:A:1938:ASN:HB3	1:A:1942:ARG:HH12	1.79	0.48
1:A:2713:PRO:HD2	1:A:2782:LEU:HD13	1.95	0.48
1:A:3951:ALA:HB1	1:A:4011:MET:HE1	1.94	0.48
1:B:921:PHE:HA	1:B:924:LEU:HD12	1.96	0.48
1:B:1605:LEU:HD21	1:B:1608:ASP:HA	1.96	0.48
1:C:290:ARG:HH22	1:C:349:MET:HA	1.79	0.48
1:C:3436:SER:O	1:C:3439:SER:N	2.45	0.48
1:C:3460:MET:SD	1:C:3460:MET:N	2.87	0.48
1:C:3731:HIS:O	1:C:3775:LYS:NZ	2.41	0.48
1:C:4186:GLU:OE1	1:C:4948:TRP:NE1	2.42	0.48
1:D:1517:GLY:O	1:D:1533:GLN:NE2	2.46	0.48
1:D:1605:LEU:HD21	1:D:1608:ASP:HA	1.96	0.48
1:D:1728:VAL:HG11	1:D:1925:VAL:HG11	1.95	0.48
2:G:2:VAL:HG11	2:G:61:GLU:HB3	1.95	0.48
1:A:578:VAL:HG11	1:A:585:ALA:H	1.79	0.48
1:A:1153:GLY:HA2	1:A:1182:LEU:HD12	1.95	0.48
1:A:1905:MET:HA	1:A:1908:LEU:HB2	1.94	0.48
1:A:2168:GLU:O	1:A:2172:GLU:HG3	2.14	0.48
1:A:2648:PHE:O	1:A:2652:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:VAL:HG13	1:B:1025:LYS:HG2	1.94	0.48
1:B:2168:GLU:O	1:B:2172:GLU:HG3	2.14	0.48
1:B:2191:MET:SD	1:B:2191:MET:N	2.85	0.48
1:C:1605:LEU:HD21	1:C:1608:ASP:HA	1.96	0.48
1:D:1938:ASN:HB3	1:D:1942:ARG:HH12	1.79	0.48
1:A:561:ARG:HH22	1:A:567:ALA:H	1.61	0.48
1:A:1487:MET:HG2	1:A:1487:MET:O	2.14	0.48
1:A:3436:SER:O	1:A:3439:SER:N	2.45	0.48
1:A:4104:LEU:O	1:A:4108:MET:HB2	2.13	0.48
1:B:1938:ASN:HB3	1:B:1942:ARG:HH12	1.79	0.48
1:B:2713:PRO:HD2	1:B:2782:LEU:HD13	1.95	0.48
1:C:3198:ALA:HB2	1:C:3248:TRP:CE2	2.49	0.48
1:C:4882:ASP:OD1	1:C:4886:LYS:NZ	2.44	0.48
1:D:290:ARG:HH22	1:D:349:MET:HA	1.79	0.48
1:D:372:LEU:H	1:D:372:LEU:HD12	1.78	0.48
1:D:952:ILE:HD11	1:D:955:GLU:HA	1.95	0.48
2:H:2:VAL:HG11	2:H:61:GLU:HB3	1.95	0.48
1:A:1605:LEU:HD21	1:A:1608:ASP:HA	1.96	0.48
1:A:3095:TYR:OH	1:A:3219:GLU:OE1	2.27	0.48
1:A:4752:LEU:HD11	1:B:4772:LEU:HD11	1.96	0.48
1:A:4846:ASP:OD2	1:D:4817:TYR:OH	2.27	0.48
1:B:1434:PRO:HD3	1:B:1506:LEU:HD23	1.95	0.48
1:C:290:ARG:NH1	1:C:349:MET:O	2.38	0.48
1:C:821:ALA:HB3	1:C:823:TYR:HE1	1.78	0.48
1:C:2161:MET:HE1	1:C:2161:MET:H	1.79	0.48
1:D:234:LEU:HD12	1:D:405:LEU:HD22	1.95	0.48
1:D:821:ALA:HB3	1:D:823:TYR:HE1	1.78	0.48
1:A:64:ILE:O	1:A:123:HIS:NE2	2.47	0.48
1:B:486:GLN:HG2	1:B:540:LEU:HG	1.96	0.48
1:B:1153:GLY:HA2	1:B:1182:LEU:HD12	1.95	0.48
1:C:234:LEU:HD12	1:C:405:LEU:HD22	1.95	0.48
1:C:3556:VAL:O	1:C:3557:LEU:HD13	2.14	0.48
1:D:1434:PRO:HD3	1:D:1506:LEU:HD23	1.95	0.48
2:E:11:ASP:OD1	2:E:11:ASP:N	2.47	0.48
1:A:73:LEU:O	1:A:118:ALA:N	2.46	0.48
1:A:248:PRO:HD3	1:A:261:HIS:CD2	2.49	0.48
1:A:821:ALA:HB3	1:A:823:TYR:HE1	1.78	0.48
1:A:2660:LEU:HD13	1:A:2693:SER:H	1.79	0.48
1:B:1487:MET:O	1:B:1487:MET:HG2	2.14	0.48
1:B:4752:LEU:HD11	1:C:4772:LEU:HD11	1.96	0.48
1:C:952:ILE:HD11	1:C:955:GLU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:PRO:HD3	1:D:261:HIS:CD2	2.49	0.48
1:D:1944:ASN:N	1:D:1944:ASN:OD1	2.46	0.48
1:A:290:ARG:HH22	1:A:349:MET:HA	1.79	0.48
1:A:1317:SER:OG	1:A:1318:VAL:N	2.46	0.48
1:A:3025:ALA:N	1:A:3029:VAL:O	2.46	0.48
1:A:4734:ASN:HB3	1:A:4737:PHE:HD2	1.79	0.48
1:B:73:LEU:O	1:B:118:ALA:N	2.46	0.48
1:B:248:PRO:HD3	1:B:261:HIS:CD2	2.49	0.48
1:B:490:GLN:HG3	1:B:540:LEU:CD2	2.44	0.48
1:B:1905:MET:HA	1:B:1908:LEU:HB2	1.94	0.48
1:B:1944:ASN:N	1:B:1944:ASN:OD1	2.46	0.48
1:B:3198:ALA:HB2	1:B:3248:TRP:CE2	2.49	0.48
1:C:248:PRO:HD3	1:C:261:HIS:CD2	2.49	0.48
1:C:2660:LEU:HD13	1:C:2693:SER:H	1.79	0.48
1:C:3418:PHE:O	1:C:3422:ASN:ND2	2.35	0.48
1:D:486:GLN:HG2	1:D:540:LEU:HG	1.96	0.48
1:C:1487:MET:O	1:C:1487:MET:HG2	2.14	0.47
1:D:490:GLN:HG3	1:D:540:LEU:CD2	2.44	0.47
1:D:921:PHE:HA	1:D:924:LEU:HD12	1.96	0.47
1:A:490:GLN:HG3	1:A:540:LEU:CD2	2.44	0.47
1:B:1728:VAL:HG11	1:B:1925:VAL:HG11	1.95	0.47
1:B:2231:PRO:HG2	1:B:2233:MET:HG2	1.94	0.47
1:B:3418:PHE:O	1:B:3422:ASN:ND2	2.35	0.47
1:C:921:PHE:HA	1:C:924:LEU:HD12	1.96	0.47
1:C:4566:TYR:O	1:C:4570:THR:OG1	2.26	0.47
1:C:4752:LEU:HD11	1:D:4772:LEU:HD11	1.96	0.47
1:D:1433:PHE:HB2	1:D:1553:VAL:HA	1.96	0.47
1:A:845:THR:O	1:A:848:ARG:NH2	2.47	0.47
1:A:1517:GLY:O	1:A:1533:GLN:NE2	2.46	0.47
1:A:3460:MET:N	1:A:3460:MET:SD	2.87	0.47
1:A:3556:VAL:O	1:A:3557:LEU:HD13	2.14	0.47
1:B:3460:MET:N	1:B:3460:MET:SD	2.87	0.47
1:C:372:LEU:H	1:C:372:LEU:HD12	1.78	0.47
1:C:490:GLN:HG2	1:C:494:MET:HE1	1.96	0.47
1:D:332:ARG:N	1:D:362:TYR:O	2.44	0.47
1:D:3556:VAL:O	1:D:3557:LEU:HD13	2.14	0.47
1:A:2278:MET:SD	1:A:2279:LEU:N	2.88	0.47
1:B:164:PRO:HB3	1:B:169:ARG:HB2	1.96	0.47
1:B:336:GLU:HG3	1:B:338:LEU:HD22	1.97	0.47
1:B:840:TYR:OH	1:B:1086:ARG:NH1	2.37	0.47
1:B:909:ASP:OD1	1:B:909:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2278:MET:SD	1:B:2279:LEU:HB2	2.55	0.47
1:C:332:ARG:N	1:C:362:TYR:O	2.44	0.47
1:C:490:GLN:HG3	1:C:540:LEU:CD2	2.44	0.47
1:C:1434:PRO:HD3	1:C:1506:LEU:HD23	1.95	0.47
1:C:2168:GLU:O	1:C:2172:GLU:HG3	2.14	0.47
1:D:490:GLN:HG2	1:D:494:MET:HE1	1.96	0.47
1:D:2168:GLU:O	1:D:2172:GLU:HG3	2.14	0.47
1:D:2655:LYS:HB3	1:D:2655:LYS:HE3	1.77	0.47
1:D:2660:LEU:HD13	1:D:2693:SER:H	1.79	0.47
1:D:3460:MET:N	1:D:3460:MET:SD	2.87	0.47
1:D:4734:ASN:HB3	1:D:4737:PHE:HD2	1.79	0.47
1:D:4795:SER:OG	1:D:4800:THR:OG1	2.30	0.47
2:E:2:VAL:HG11	2:E:61:GLU:HB3	1.95	0.47
2:F:2:VAL:HG11	2:F:61:GLU:HB3	1.95	0.47
1:A:640:ARG:HB3	2:E:92:PRO:HB3	1.97	0.47
1:A:909:ASP:N	1:A:909:ASP:OD1	2.48	0.47
1:B:290:ARG:HH22	1:B:349:MET:HA	1.79	0.47
1:B:787:LEU:HD11	1:B:863:THR:H	1.80	0.47
1:B:1433:PHE:HB2	1:B:1553:VAL:HA	1.96	0.47
1:B:4720:TYR:OH	1:B:4744:ASP:OD1	2.26	0.47
1:C:73:LEU:O	1:C:118:ALA:N	2.46	0.47
1:C:332:ARG:NE	1:C:364:GLN:OE1	2.44	0.47
1:D:1646:THR:HG23	1:D:1647:GLU:HG3	1.97	0.47
1:D:2504:ALA:HB3	1:D:2507:SER:HB2	1.96	0.47
1:D:3025:ALA:N	1:D:3029:VAL:O	2.46	0.47
2:E:60:GLU:OE1	2:E:60:GLU:N	2.45	0.47
1:A:336:GLU:HG3	1:A:338:LEU:HD22	1.97	0.47
1:A:499:LEU:HD21	1:A:537:LEU:HD22	1.97	0.47
1:C:164:PRO:HB3	1:C:169:ARG:HB2	1.96	0.47
1:C:640:ARG:HB3	2:G:92:PRO:HB3	1.97	0.47
1:C:787:LEU:HD11	1:C:863:THR:H	1.80	0.47
1:C:1433:PHE:HB2	1:C:1553:VAL:HA	1.96	0.47
1:C:1728:VAL:HG11	1:C:1925:VAL:HG11	1.95	0.47
1:C:2402:ALA:O	1:C:2473:ARG:NH2	2.44	0.47
1:C:2504:ALA:HB3	1:C:2507:SER:HB2	1.96	0.47
1:D:2278:MET:SD	1:D:2279:LEU:N	2.88	0.47
2:G:76:CYS:O	2:G:96:THR:OG1	2.29	0.47
1:A:486:GLN:HG2	1:A:540:LEU:HG	1.96	0.47
1:A:787:LEU:HD11	1:A:863:THR:H	1.80	0.47
1:A:2228:LEU:HG	1:A:2231:PRO:HD2	1.97	0.47
1:A:3198:ALA:HB2	1:A:3248:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4176:VAL:HG11	1:A:4879:VAL:HA	1.96	0.47
1:A:4186:GLU:OE1	1:A:4948:TRP:NE1	2.42	0.47
1:A:4772:LEU:HD11	1:D:4752:LEU:HD11	1.96	0.47
1:B:490:GLN:HG2	1:B:494:MET:HE1	1.96	0.47
1:B:499:LEU:HD21	1:B:537:LEU:HD22	1.97	0.47
1:B:845:THR:O	1:B:848:ARG:NH2	2.47	0.47
1:C:845:THR:O	1:C:848:ARG:NH2	2.47	0.47
1:C:868:ASP:OD1	1:C:868:ASP:N	2.46	0.47
1:C:1938:ASN:HB3	1:C:1942:ARG:HH12	1.79	0.47
1:D:73:LEU:O	1:D:118:ALA:N	2.46	0.47
1:D:644:LEU:HD21	1:D:1634:PRO:HD3	1.97	0.47
1:D:787:LEU:HD11	1:D:863:THR:H	1.80	0.47
1:D:1487:MET:HG2	1:D:1487:MET:O	2.14	0.47
1:D:3881:GLN:NE2	1:D:3945:GLY:HA3	2.30	0.47
1:A:2504:ALA:HB3	1:A:2507:SER:HB2	1.96	0.47
1:B:660:PHE:HZ	1:B:787:LEU:HD23	1.80	0.47
1:C:644:LEU:HD21	1:C:1634:PRO:HD3	1.97	0.47
1:C:4817:TYR:OH	1:D:4846:ASP:OD2	2.27	0.47
1:D:640:ARG:HB3	2:H:92:PRO:HB3	1.97	0.47
1:D:2228:LEU:HG	1:D:2231:PRO:HD2	1.97	0.47
1:B:2504:ALA:HB3	1:B:2507:SER:HB2	1.96	0.47
1:C:191:TYR:N	1:C:206:ALA:O	2.38	0.47
1:C:1317:SER:OG	1:C:1318:VAL:N	2.46	0.47
1:C:2278:MET:SD	1:C:2279:LEU:HB2	2.55	0.47
1:D:290:ARG:NH1	1:D:349:MET:O	2.38	0.47
1:D:332:ARG:NE	1:D:364:GLN:OE1	2.44	0.47
1:D:845:THR:O	1:D:848:ARG:NH2	2.47	0.47
1:D:909:ASP:OD1	1:D:909:ASP:N	2.48	0.47
1:D:1449:ASP:OD1	1:D:1449:ASP:N	2.44	0.47
1:D:3198:ALA:HB2	1:D:3248:TRP:CE2	2.49	0.47
2:F:11:ASP:N	2:F:11:ASP:OD1	2.47	0.47
1:A:644:LEU:HD21	1:A:1634:PRO:HD3	1.97	0.47
1:B:2228:LEU:HG	1:B:2231:PRO:HD2	1.97	0.47
1:B:3556:VAL:O	1:B:3557:LEU:HD13	2.14	0.47
1:C:1549:THR:C	1:C:1551:PRO:HD3	2.36	0.47
1:C:2228:LEU:HG	1:C:2231:PRO:HD2	1.97	0.47
1:C:2278:MET:SD	1:C:2279:LEU:N	2.88	0.47
1:C:4734:ASN:HB3	1:C:4737:PHE:HD2	1.79	0.47
1:D:4176:VAL:HG11	1:D:4879:VAL:HA	1.96	0.47
1:A:3881:GLN:NE2	1:A:3945:GLY:HA3	2.30	0.46
1:B:1113:MET:HG2	1:B:1207:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLU:HG3	1:C:338:LEU:HD22	1.97	0.46
1:C:499:LEU:HD21	1:C:537:LEU:HD22	1.97	0.46
1:C:1646:THR:HG23	1:C:1647:GLU:HG3	1.97	0.46
1:D:336:GLU:HG3	1:D:338:LEU:HD22	1.97	0.46
1:D:2278:MET:SD	1:D:2279:LEU:HB2	2.55	0.46
2:H:60:GLU:OE1	2:H:60:GLU:N	2.45	0.46
1:A:61:ASP:OD1	1:A:61:ASP:N	2.42	0.46
1:A:1646:THR:HG23	1:A:1647:GLU:HG3	1.97	0.46
1:A:2278:MET:SD	1:A:2279:LEU:HB2	2.55	0.46
1:B:644:LEU:HD21	1:B:1634:PRO:HD3	1.97	0.46
1:B:657:PRO:HA	1:B:834:VAL:HA	1.97	0.46
1:B:2660:LEU:HD13	1:B:2693:SER:H	1.79	0.46
1:B:4136:GLU:O	1:B:4917:TYR:OH	2.31	0.46
1:C:2171:MET:O	1:C:2175:VAL:HG23	2.15	0.46
1:C:4176:VAL:HG11	1:C:4879:VAL:HA	1.96	0.46
1:D:499:LEU:HD21	1:D:537:LEU:HD22	1.97	0.46
1:D:1113:MET:HG2	1:D:1207:LEU:HD23	1.97	0.46
2:F:60:GLU:OE1	2:F:60:GLU:N	2.45	0.46
1:A:164:PRO:HB3	1:A:169:ARG:HB2	1.96	0.46
1:A:657:PRO:HA	1:A:834:VAL:HA	1.97	0.46
1:C:3954:GLN:H	1:C:3954:GLN:HG2	1.57	0.46
1:A:1113:MET:HG2	1:A:1207:LEU:HD23	1.97	0.46
1:A:1433:PHE:HB2	1:A:1553:VAL:HA	1.96	0.46
1:B:611:LEU:HD22	1:B:1661:LEU:HD22	1.97	0.46
1:B:640:ARG:HB3	2:F:92:PRO:HB3	1.97	0.46
1:B:2171:MET:O	1:B:2175:VAL:HG23	2.15	0.46
1:B:4176:VAL:HG11	1:B:4879:VAL:HA	1.96	0.46
1:B:4734:ASN:HB3	1:B:4737:PHE:HD2	1.79	0.46
1:C:2687:MET:HB3	1:C:2690:LYS:HE2	1.97	0.46
1:C:3881:GLN:NE2	1:C:3945:GLY:HA3	2.30	0.46
1:D:164:PRO:HB3	1:D:169:ARG:HB2	1.96	0.46
1:D:1905:MET:N	1:D:1905:MET:SD	2.81	0.46
1:B:3727:GLN:O	1:B:3731:HIS:ND1	2.44	0.46
1:D:1549:THR:C	1:D:1551:PRO:HD3	2.36	0.46
1:D:2171:MET:O	1:D:2175:VAL:HG23	2.15	0.46
1:D:3351:GLU:HG2	1:D:3354:ILE:HB	1.98	0.46
1:D:4186:GLU:OE1	1:D:4948:TRP:NE1	2.42	0.46
2:H:48:PHE:CD1	2:H:55:VAL:HG11	2.50	0.46
1:B:1646:THR:HG23	1:B:1647:GLU:HG3	1.97	0.46
1:B:2278:MET:SD	1:B:2279:LEU:N	2.88	0.46
1:B:4781:THR:HG21	1:B:4812:TYR:HD1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1257:GLN:HB2	1:C:1260:GLN:HE22	1.81	0.46
1:C:1645:LEU:HD11	1:C:1651:LEU:HD23	1.98	0.46
2:G:11:ASP:OD1	2:G:11:ASP:N	2.47	0.46
2:H:11:ASP:OD1	2:H:11:ASP:N	2.47	0.46
1:A:490:GLN:HG2	1:A:494:MET:HE1	1.97	0.46
1:A:3351:GLU:HG2	1:A:3354:ILE:HB	1.98	0.46
1:B:2189:PRO:O	1:B:2192:VAL:HG12	2.16	0.46
1:B:3881:GLN:NE2	1:B:3945:GLY:HA3	2.30	0.46
1:D:344:LYS:HB3	1:D:345:GLU:H	1.55	0.46
2:E:48:PHE:CD1	2:E:55:VAL:HG11	2.50	0.46
2:G:60:GLU:OE1	2:G:60:GLU:N	2.45	0.46
1:A:973:THR:HG22	1:A:977:LYS:HG3	1.98	0.46
1:B:356:TYR:CZ	1:B:407:ARG:HB3	2.51	0.46
1:B:973:THR:HG22	1:B:977:LYS:HG3	1.98	0.46
1:B:4566:TYR:O	1:B:4570:THR:OG1	2.26	0.46
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.81	0.46
1:C:356:TYR:CZ	1:C:407:ARG:HB3	2.51	0.46
1:C:4781:THR:HG21	1:C:4812:TYR:HD1	1.81	0.46
1:A:625:VAL:HG12	1:A:627:SER:H	1.81	0.46
1:A:660:PHE:HZ	1:A:787:LEU:HD23	1.80	0.46
1:A:1257:GLN:HB2	1:A:1260:GLN:HE22	1.81	0.46
1:A:1638:ARG:NH2	1:A:1651:LEU:HD22	2.31	0.46
1:A:2189:PRO:O	1:A:2192:VAL:HG12	2.16	0.46
1:A:4566:TYR:O	1:A:4570:THR:OG1	2.26	0.46
1:B:1257:GLN:HB2	1:B:1260:GLN:HE22	1.81	0.46
1:C:1113:MET:HG2	1:C:1207:LEU:HD23	1.97	0.46
1:D:657:PRO:HA	1:D:834:VAL:HA	1.97	0.46
1:D:2502:ASP:N	1:D:2502:ASP:OD1	2.49	0.46
1:D:3660:VAL:HG13	1:D:3661:ASP:H	1.81	0.46
1:A:611:LEU:HD22	1:A:1661:LEU:HD22	1.97	0.46
1:A:840:TYR:OH	1:A:1086:ARG:NH1	2.37	0.46
1:A:2687:MET:HB3	1:A:2690:LYS:HE2	1.97	0.46
1:A:3657:MET:SD	1:A:3659:ARG:N	2.83	0.46
1:B:2502:ASP:N	1:B:2502:ASP:OD1	2.49	0.46
1:B:3351:GLU:HG2	1:B:3354:ILE:HB	1.98	0.46
1:C:660:PHE:HZ	1:C:787:LEU:HD23	1.80	0.46
1:C:2079:LEU:O	1:C:2083:MET:HG3	2.16	0.46
1:C:4795:SER:OG	1:C:4800:THR:OG1	2.30	0.46
1:D:64:ILE:O	1:D:123:HIS:NE2	2.47	0.46
1:D:2079:LEU:O	1:D:2083:MET:HG3	2.16	0.46
1:D:2402:ALA:O	1:D:2473:ARG:NH2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4781:THR:HG21	1:A:4812:TYR:HD1	1.81	0.45
1:D:973:THR:HG22	1:D:977:LYS:HG3	1.98	0.45
1:D:4781:THR:HG21	1:D:4812:TYR:HD1	1.81	0.45
1:A:1089:ARG:HE	1:A:1092:LYS:NZ	2.14	0.45
1:A:1237:GLU:HB3	1:A:1241:VAL:HG11	1.98	0.45
1:A:1549:THR:C	1:A:1551:PRO:HD3	2.36	0.45
1:A:2171:MET:O	1:A:2175:VAL:HG23	2.15	0.45
1:B:1237:GLU:HB3	1:B:1241:VAL:HG11	1.98	0.45
1:C:657:PRO:HA	1:C:834:VAL:HA	1.97	0.45
1:D:660:PHE:HZ	1:D:787:LEU:HD23	1.80	0.45
1:D:2189:PRO:O	1:D:2192:VAL:HG12	2.16	0.45
1:A:3660:VAL:HG13	1:A:3661:ASP:H	1.81	0.45
1:A:4867:ASP:OD1	1:D:4873:ARG:NE	2.43	0.45
1:B:1549:THR:C	1:B:1551:PRO:HD3	2.36	0.45
1:B:1638:ARG:NH2	1:B:1651:LEU:HD22	2.31	0.45
1:B:2655:LYS:HE3	1:B:2655:LYS:HB3	1.77	0.45
1:B:3015:ARG:NH2	1:B:3080:THR:O	2.50	0.45
1:B:3660:VAL:HG13	1:B:3661:ASP:H	1.81	0.45
1:C:373:THR:OG1	1:C:392:ILE:O	2.34	0.45
1:C:611:LEU:HD22	1:C:1661:LEU:HD22	1.97	0.45
1:C:1237:GLU:HB3	1:C:1241:VAL:HG11	1.98	0.45
1:C:2189:PRO:O	1:C:2192:VAL:HG12	2.16	0.45
1:C:3025:ALA:N	1:C:3029:VAL:O	2.46	0.45
1:C:3728:ALA:HA	1:C:3731:HIS:CE1	2.51	0.45
1:D:1257:GLN:HB2	1:D:1260:GLN:HE22	1.81	0.45
1:D:3015:ARG:NH2	1:D:3080:THR:O	2.50	0.45
2:F:48:PHE:CD1	2:F:55:VAL:HG11	2.50	0.45
1:A:1645:LEU:HD11	1:A:1651:LEU:HD23	1.98	0.45
1:A:3015:ARG:NH2	1:A:3080:THR:O	2.50	0.45
1:B:2492:LEU:H	1:B:2492:LEU:HD12	1.81	0.45
1:B:3728:ALA:HA	1:B:3731:HIS:CE1	2.51	0.45
1:C:2502:ASP:OD1	1:C:2502:ASP:N	2.49	0.45
1:D:2492:LEU:H	1:D:2492:LEU:HD12	1.81	0.45
1:A:332:ARG:NE	1:A:364:GLN:OE1	2.44	0.45
1:A:2502:ASP:N	1:A:2502:ASP:OD1	2.49	0.45
1:A:4826:ILE:HG13	1:A:4830:ILE:HD11	1.99	0.45
1:C:3015:ARG:NH2	1:C:3080:THR:O	2.50	0.45
1:C:4826:ILE:HG13	1:C:4830:ILE:HD11	1.99	0.45
1:D:1317:SER:OG	1:D:1318:VAL:N	2.46	0.45
2:E:76:CYS:O	2:E:96:THR:OG1	2.29	0.45
1:A:290:ARG:NH2	1:A:348:GLY:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3954:GLN:H	1:A:3954:GLN:HG2	1.57	0.45
1:B:2687:MET:HB3	1:B:2690:LYS:HE2	1.97	0.45
1:B:3025:ALA:N	1:B:3029:VAL:O	2.46	0.45
1:C:1293:GLN:O	1:C:1550:SER:OG	2.27	0.45
1:C:2492:LEU:HD12	1:C:2492:LEU:H	1.81	0.45
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.81	0.45
1:D:611:LEU:HD22	1:D:1661:LEU:HD22	1.97	0.45
1:D:1118:SER:OG	1:D:1119:ARG:N	2.50	0.45
1:D:1638:ARG:NH2	1:D:1651:LEU:HD22	2.31	0.45
1:A:1118:SER:OG	1:A:1119:ARG:N	2.50	0.45
1:B:1645:LEU:HD11	1:B:1651:LEU:HD23	1.98	0.45
1:C:1089:ARG:HE	1:C:1092:LYS:NZ	2.14	0.45
1:C:2435:ILE:HG12	1:C:2486:LEU:HD11	1.99	0.45
1:D:373:THR:OG1	1:D:392:ILE:O	2.34	0.45
1:D:1089:ARG:HE	1:D:1092:LYS:NZ	2.14	0.45
1:D:1641:ASP:OD1	1:D:1644:GLU:N	2.47	0.45
2:H:76:CYS:O	2:H:96:THR:OG1	2.29	0.45
1:A:1731:THR:O	1:A:1734:THR:OG1	2.33	0.45
1:A:2777:SER:O	1:A:2780:THR:OG1	2.29	0.45
1:B:290:ARG:NH2	1:B:348:GLY:O	2.50	0.45
1:B:625:VAL:HG12	1:B:627:SER:H	1.81	0.45
1:C:1686:LEU:O	1:C:1690:ILE:HG12	2.17	0.45
1:C:3660:VAL:HG13	1:C:3661:ASP:H	1.81	0.45
1:C:4734:ASN:HB3	1:C:4737:PHE:CD2	2.52	0.45
1:A:2228:LEU:HA	1:A:2237:THR:HB	1.99	0.45
1:A:4734:ASN:HB3	1:A:4737:PHE:CD2	2.52	0.45
1:B:1089:ARG:HE	1:B:1092:LYS:NZ	2.14	0.45
1:B:1641:ASP:OD1	1:B:1644:GLU:N	2.47	0.45
1:B:1686:LEU:O	1:B:1690:ILE:HG12	2.17	0.45
1:B:4186:GLU:OE1	1:B:4948:TRP:NE1	2.42	0.45
1:C:625:VAL:HG12	1:C:627:SER:H	1.81	0.45
1:C:909:ASP:OD1	1:C:909:ASP:N	2.48	0.45
1:C:1634:PRO:HD2	1:C:1654:PHE:HE2	1.82	0.45
1:C:3351:GLU:HG2	1:C:3354:ILE:HB	1.98	0.45
1:D:356:TYR:CZ	1:D:407:ARG:HB3	2.51	0.45
1:D:1645:LEU:HD11	1:D:1651:LEU:HD23	1.98	0.45
1:D:1692:ASN:HB3	1:D:1695:MET:HG2	1.99	0.45
1:A:731:HIS:HA	1:A:741:VAL:HG12	1.99	0.45
1:A:2079:LEU:O	1:A:2083:MET:HG3	2.16	0.45
1:B:1634:PRO:HD2	1:B:1654:PHE:HE2	1.82	0.45
1:B:1810:PRO:HG2	1:B:1814:THR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:973:THR:HG22	1:C:977:LYS:HG3	1.98	0.45
1:C:1810:PRO:HG2	1:C:1814:THR:HA	1.99	0.45
1:D:625:VAL:HG12	1:D:627:SER:H	1.81	0.45
1:D:755:ILE:HD11	1:D:768:PHE:HB3	1.99	0.45
1:D:3728:ALA:HA	1:D:3731:HIS:CE1	2.51	0.45
1:D:4826:ILE:HG13	1:D:4830:ILE:HD11	1.99	0.45
1:A:373:THR:OG1	1:A:392:ILE:O	2.34	0.44
1:A:1089:ARG:HB3	1:A:1204:VAL:HG23	2.00	0.44
1:A:1487:MET:HG3	1:A:1532:TYR:HB2	1.99	0.44
1:A:2492:LEU:H	1:A:2492:LEU:HD12	1.81	0.44
1:A:3728:ALA:HA	1:A:3731:HIS:CE1	2.51	0.44
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.81	0.44
1:B:2079:LEU:O	1:B:2083:MET:HG3	2.16	0.44
1:B:3954:GLN:H	1:B:3954:GLN:HG2	1.57	0.44
1:B:4734:ASN:HB3	1:B:4737:PHE:CD2	2.52	0.44
1:C:64:ILE:O	1:C:123:HIS:NE2	2.47	0.44
1:C:324:VAL:O	1:C:328:ALA:CB	2.65	0.44
1:C:641:ASP:OD1	1:C:642:LEU:N	2.49	0.44
1:C:840:TYR:OH	1:C:1086:ARG:NH1	2.37	0.44
1:C:1638:ARG:NH2	1:C:1651:LEU:HD22	2.31	0.44
1:C:4873:ARG:NE	1:D:4867:ASP:OD1	2.43	0.44
1:D:324:VAL:O	1:D:328:ALA:CB	2.65	0.44
1:D:1237:GLU:HB3	1:D:1241:VAL:HG11	1.98	0.44
1:D:2435:ILE:HG12	1:D:2486:LEU:HD11	1.99	0.44
1:D:4734:ASN:HB3	1:D:4737:PHE:CD2	2.52	0.44
1:A:324:VAL:O	1:A:328:ALA:CB	2.65	0.44
1:A:1686:LEU:O	1:A:1690:ILE:HG12	2.17	0.44
1:A:3250:GLU:OE1	1:A:3280:LEU:N	2.51	0.44
1:B:1089:ARG:HB3	1:B:1204:VAL:HG23	2.00	0.44
1:B:4826:ILE:HG13	1:B:4830:ILE:HD11	1.99	0.44
1:C:290:ARG:NH2	1:C:348:GLY:O	2.50	0.44
1:C:805:GLY:HA3	1:C:823:TYR:CD1	2.53	0.44
1:C:1118:SER:OG	1:C:1119:ARG:N	2.50	0.44
1:C:1641:ASP:OD1	1:C:1644:GLU:N	2.47	0.44
1:C:2619:TYR:HB3	1:C:2623:PRO:CG	2.48	0.44
1:C:2795:ASP:OD1	1:C:2795:ASP:N	2.46	0.44
1:D:805:GLY:HA3	1:D:823:TYR:CD1	2.53	0.44
1:D:840:TYR:OH	1:D:1086:ARG:NH1	2.37	0.44
1:D:2228:LEU:HA	1:D:2237:THR:HB	1.99	0.44
1:A:805:GLY:HA3	1:A:823:TYR:CD1	2.53	0.44
1:A:1692:ASN:HB3	1:A:1695:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:HB1	1:B:225:GLN:HE22	1.83	0.44
1:B:805:GLY:HA3	1:B:823:TYR:CD1	2.53	0.44
1:B:3246:SER:HB2	1:B:3280:LEU:HD22	1.99	0.44
1:C:332:ARG:HH22	1:C:366:VAL:HG22	1.82	0.44
1:C:1517:GLY:O	1:C:1533:GLN:NE2	2.46	0.44
1:C:4136:GLU:O	1:C:4917:TYR:OH	2.31	0.44
1:C:4720:TYR:OH	1:C:4744:ASP:OD1	2.26	0.44
1:D:2687:MET:HB3	1:D:2690:LYS:HE2	1.97	0.44
1:A:133:LEU:HD22	1:A:148:GLY:HA3	2.00	0.44
1:A:682:THR:HA	1:A:798:ILE:HD13	1.99	0.44
1:A:755:ILE:HD11	1:A:768:PHE:HB3	1.99	0.44
1:A:1634:PRO:HD2	1:A:1654:PHE:HE2	1.82	0.44
1:A:1641:ASP:OD1	1:A:1644:GLU:N	2.47	0.44
1:A:2619:TYR:HB3	1:A:2623:PRO:CG	2.48	0.44
1:B:28:ILE:HG12	1:B:29:HIS:CE1	2.53	0.44
1:B:133:LEU:HD22	1:B:148:GLY:HA3	2.00	0.44
1:B:682:THR:HA	1:B:798:ILE:HD13	1.99	0.44
1:B:2107:ILE:HG13	1:B:2157:HIS:CE1	2.53	0.44
1:B:2619:TYR:HB3	1:B:2623:PRO:CG	2.48	0.44
1:C:223:ALA:HB1	1:C:225:GLN:HE22	1.83	0.44
1:C:1993:ASP:OD1	1:C:1993:ASP:N	2.41	0.44
1:C:2107:ILE:HG13	1:C:2157:HIS:CE1	2.53	0.44
1:C:2228:LEU:HA	1:C:2237:THR:HB	1.99	0.44
1:D:1487:MET:HG3	1:D:1532:TYR:HB2	1.99	0.44
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.81	0.44
1:A:356:TYR:CZ	1:A:407:ARG:HB3	2.51	0.44
1:A:2584:MET:N	1:A:2584:MET:SD	2.91	0.44
1:A:3727:GLN:O	1:A:3731:HIS:ND1	2.44	0.44
1:A:4873:ARG:NE	1:B:4867:ASP:OD1	2.43	0.44
1:B:409:GLN:O	1:B:413:SER:N	2.51	0.44
1:B:1692:ASN:HB3	1:B:1695:MET:HG2	1.99	0.44
1:B:1731:THR:O	1:B:1734:THR:OG1	2.33	0.44
1:C:28:ILE:HG12	1:C:29:HIS:CE1	2.53	0.44
1:C:2279:LEU:HD22	1:C:2288:GLY:HA2	2.00	0.44
1:D:731:HIS:HA	1:D:741:VAL:HG12	1.99	0.44
2:G:20:GLN:O	2:G:49:ARG:NH2	2.40	0.44
2:G:48:PHE:CD1	2:G:55:VAL:HG11	2.50	0.44
2:H:79:ASP:OD1	2:H:80:VAL:N	2.50	0.44
1:A:4008:ASN:O	1:A:4012:ILE:HG12	2.18	0.44
1:A:4136:GLU:O	1:A:4917:TYR:OH	2.31	0.44
1:A:4796:GLU:HG2	1:A:4800:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:THR:OG1	1:B:392:ILE:O	2.34	0.44
1:B:2584:MET:N	1:B:2584:MET:SD	2.91	0.44
1:C:1089:ARG:HB3	1:C:1204:VAL:HG23	2.00	0.44
1:C:2223:ASN:O	1:C:2225:SER:N	2.51	0.44
1:D:290:ARG:NH2	1:D:348:GLY:O	2.50	0.44
1:D:2107:ILE:HG13	1:D:2157:HIS:CE1	2.53	0.44
1:D:2584:MET:N	1:D:2584:MET:SD	2.91	0.44
1:D:2619:TYR:HB3	1:D:2623:PRO:CG	2.48	0.44
1:D:4008:ASN:O	1:D:4012:ILE:HG12	2.18	0.44
1:B:332:ARG:HH22	1:B:366:VAL:HG22	1.82	0.44
1:B:1779:TYR:CE2	1:B:1781:PRO:HD2	2.53	0.44
1:B:3250:GLU:OE1	1:B:3280:LEU:N	2.51	0.44
1:C:250:GLY:HA3	1:C:256:GLN:OE1	2.18	0.44
1:C:2584:MET:SD	1:C:2584:MET:N	2.91	0.44
1:C:3250:GLU:OE1	1:C:3280:LEU:N	2.51	0.44
1:C:4008:ASN:O	1:C:4012:ILE:HG12	2.18	0.44
1:D:133:LEU:HD22	1:D:148:GLY:HA3	2.00	0.44
1:D:288:HIS:CG	1:D:349:MET:HB3	2.53	0.44
1:D:332:ARG:HH22	1:D:366:VAL:HG22	1.82	0.44
1:D:409:GLN:O	1:D:413:SER:N	2.51	0.44
1:D:664:SER:OG	1:D:665:GLU:N	2.50	0.44
1:D:885:LEU:HA	1:D:888:ASN:HD21	1.83	0.44
2:F:79:ASP:OD1	2:F:80:VAL:N	2.50	0.44
2:G:79:ASP:OD1	2:G:80:VAL:N	2.50	0.44
1:A:223:ALA:HB1	1:A:225:GLN:HE22	1.83	0.44
1:A:661:LEU:HD13	1:A:790:PRO:HD3	2.00	0.44
1:A:885:LEU:HA	1:A:888:ASN:HD21	1.83	0.44
1:A:2223:ASN:O	1:A:2225:SER:N	2.51	0.44
1:A:2290:ASN:OD1	1:A:2290:ASN:N	2.51	0.44
1:B:2228:LEU:HA	1:B:2237:THR:HB	1.99	0.44
1:C:2728:HIS:CD2	1:C:2762:LEU:HD11	2.53	0.44
1:C:3246:SER:HB2	1:C:3280:LEU:HD22	1.99	0.44
1:D:495:ILE:HG23	1:D:496:ASN:H	1.83	0.44
1:D:1089:ARG:HB3	1:D:1204:VAL:HG23	2.00	0.44
1:D:3250:GLU:OE1	1:D:3280:LEU:N	2.51	0.44
1:A:28:ILE:HG12	1:A:29:HIS:CE1	2.53	0.44
1:A:1779:TYR:CE2	1:A:1781:PRO:HD2	2.53	0.44
1:A:2435:ILE:HG12	1:A:2486:LEU:HD11	1.99	0.44
1:A:3246:SER:HB2	1:A:3280:LEU:HD22	1.99	0.44
1:B:661:LEU:HD13	1:B:790:PRO:HD3	2.00	0.44
1:B:664:SER:OG	1:B:665:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4008:ASN:O	1:B:4012:ILE:HG12	2.18	0.44
1:B:4589:TYR:OH	1:B:4717:SER:OG	2.22	0.44
1:C:664:SER:OG	1:C:665:GLU:N	2.50	0.44
1:C:2781:MET:HA	1:C:2784:TRP:HE3	1.83	0.44
1:C:4504:ALA:HA	1:C:4507:VAL:HG12	2.00	0.44
1:D:1686:LEU:O	1:D:1690:ILE:HG12	2.17	0.44
1:A:332:ARG:HH22	1:A:366:VAL:HG22	1.82	0.43
1:B:324:VAL:O	1:B:328:ALA:CB	2.65	0.43
1:B:885:LEU:HA	1:B:888:ASN:HD21	1.83	0.43
1:B:2279:LEU:HD22	1:B:2288:GLY:HA2	2.00	0.43
1:B:4508:ALA:O	1:B:4512:ASN:ND2	2.51	0.43
1:C:755:ILE:HD11	1:C:768:PHE:HB3	1.99	0.43
1:C:1779:TYR:CE2	1:C:1781:PRO:HD2	2.53	0.43
1:D:1810:PRO:HG2	1:D:1814:THR:HA	1.99	0.43
1:D:2223:ASN:O	1:D:2225:SER:N	2.51	0.43
1:D:2279:LEU:HD22	1:D:2288:GLY:HA2	2.00	0.43
1:D:2795:ASP:N	1:D:2795:ASP:OD1	2.46	0.43
1:D:4504:ALA:HA	1:D:4507:VAL:HG12	2.00	0.43
1:A:1810:PRO:HG2	1:A:1814:THR:HA	1.99	0.43
1:A:2107:ILE:HG13	1:A:2157:HIS:CE1	2.53	0.43
1:A:4508:ALA:O	1:A:4512:ASN:ND2	2.51	0.43
1:B:288:HIS:CG	1:B:349:MET:HB3	2.53	0.43
1:B:335:LYS:HD3	1:B:362:TYR:CE2	2.54	0.43
1:B:987:LYS:NZ	1:B:988:LEU:O	2.42	0.43
1:B:2435:ILE:HG12	1:B:2486:LEU:HD11	1.99	0.43
1:B:3951:ALA:HB1	1:B:4011:MET:CE	2.48	0.43
1:C:335:LYS:HD3	1:C:362:TYR:CE2	2.54	0.43
1:C:1487:MET:HG3	1:C:1532:TYR:HB2	1.99	0.43
1:C:2165:GLY:O	1:C:2169:THR:HG23	2.19	0.43
1:D:1634:PRO:HD2	1:D:1654:PHE:HE2	1.82	0.43
1:D:2728:HIS:CD2	1:D:2762:LEU:HD11	2.53	0.43
1:D:2781:MET:HA	1:D:2784:TRP:HE3	1.83	0.43
2:G:97:LEU:HD23	2:G:97:LEU:HA	1.83	0.43
2:H:17:LYS:HE3	2:H:18:LYS:N	2.32	0.43
1:A:290:ARG:NH1	1:A:349:MET:O	2.38	0.43
1:A:2662:LYS:HA	1:A:2662:LYS:HD2	1.82	0.43
1:A:4752:LEU:HD12	1:A:4752:LEU:HA	1.80	0.43
1:A:4817:TYR:OH	1:B:4846:ASP:OD2	2.27	0.43
1:B:38:ALA:HB1	1:B:64:ILE:HD12	2.00	0.43
1:B:64:ILE:O	1:B:123:HIS:NE2	2.47	0.43
1:B:2223:ASN:O	1:B:2225:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3736:ALA:HB1	1:B:3776:MET:HG2	2.00	0.43
1:C:133:LEU:HD22	1:C:148:GLY:HA3	2.00	0.43
1:C:409:GLN:O	1:C:413:SER:N	2.51	0.43
1:C:4508:ALA:O	1:C:4512:ASN:ND2	2.51	0.43
1:D:28:ILE:HG12	1:D:29:HIS:CE1	2.53	0.43
1:D:223:ALA:HB1	1:D:225:GLN:HE22	1.83	0.43
1:D:250:GLY:HA3	1:D:256:GLN:OE1	2.18	0.43
1:D:2191:MET:SD	1:D:2191:MET:N	2.85	0.43
2:F:76:CYS:O	2:F:96:THR:OG1	2.29	0.43
1:A:288:HIS:CG	1:A:349:MET:HB3	2.53	0.43
1:A:409:GLN:O	1:A:413:SER:N	2.51	0.43
1:A:664:SER:OG	1:A:665:GLU:N	2.50	0.43
1:A:2728:HIS:CD2	1:A:2762:LEU:HD11	2.53	0.43
1:B:2165:GLY:O	1:B:2169:THR:HG23	2.19	0.43
1:B:2290:ASN:OD1	1:B:2290:ASN:N	2.51	0.43
1:B:4796:GLU:HG2	1:B:4800:THR:HG21	2.00	0.43
1:C:42:PHE:HB2	1:C:425:LEU:HD12	2.01	0.43
1:C:288:HIS:CG	1:C:349:MET:HB3	2.53	0.43
1:C:311:ASP:OD1	1:C:311:ASP:N	2.47	0.43
1:D:661:LEU:HD13	1:D:790:PRO:HD3	2.00	0.43
1:D:1629:MET:HG3	1:D:1642:ILE:HG12	2.01	0.43
1:D:3736:ALA:HB1	1:D:3776:MET:HG2	2.00	0.43
1:A:250:GLY:HA3	1:A:256:GLN:OE1	2.18	0.43
1:A:2716:LEU:HD23	1:A:2716:LEU:H	1.83	0.43
1:B:311:ASP:OD1	1:B:311:ASP:N	2.47	0.43
1:B:755:ILE:HD11	1:B:768:PHE:HB3	1.99	0.43
1:B:1118:SER:OG	1:B:1119:ARG:N	2.50	0.43
1:B:4504:ALA:HA	1:B:4507:VAL:HG12	2.00	0.43
1:C:415:THR:O	1:C:419:ILE:HG12	2.19	0.43
1:C:682:THR:HA	1:C:798:ILE:HD13	1.99	0.43
1:C:1692:ASN:HB3	1:C:1695:MET:HG2	1.99	0.43
1:C:4796:GLU:HG2	1:C:4800:THR:HG21	2.00	0.43
1:D:2640:SER:OG	1:D:2641:ARG:NH1	2.52	0.43
1:D:4508:ALA:O	1:D:4512:ASN:ND2	2.51	0.43
1:D:4796:GLU:HG2	1:D:4800:THR:HG21	2.00	0.43
2:H:26:TYR:N	2:H:40:ARG:HH12	2.17	0.43
1:A:495:ILE:HG23	1:A:496:ASN:H	1.83	0.43
1:A:1706:LEU:O	1:A:1710:ILE:HG13	2.19	0.43
1:B:1487:MET:HG3	1:B:1532:TYR:HB2	1.99	0.43
1:B:1706:LEU:O	1:B:1710:ILE:HG13	2.19	0.43
1:C:495:ILE:HG23	1:C:496:ASN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3246:SER:HB2	1:D:3280:LEU:HD22	1.99	0.43
1:D:3637:ASP:HA	1:D:3640:ILE:HG22	2.01	0.43
1:D:4752:LEU:HD12	1:D:4752:LEU:HA	1.80	0.43
2:G:26:TYR:N	2:G:40:ARG:HH12	2.17	0.43
1:A:38:ALA:HB1	1:A:64:ILE:HD12	2.00	0.43
1:A:335:LYS:HD3	1:A:362:TYR:CE2	2.54	0.43
1:A:2165:GLY:O	1:A:2169:THR:HG23	2.19	0.43
1:A:2257:ARG:HH21	1:A:3806:ALA:HB1	1.84	0.43
1:A:2640:SER:OG	1:A:2641:ARG:NH1	2.52	0.43
1:B:2161:MET:HG3	1:B:2166:MET:HE3	2.01	0.43
1:B:4873:ARG:NE	1:C:4867:ASP:OD1	2.43	0.43
1:C:3736:ALA:HB1	1:C:3776:MET:HG2	2.00	0.43
1:D:624:ALA:HB3	1:D:2131:VAL:HG12	2.01	0.43
1:D:1779:TYR:CE2	1:D:1781:PRO:HD2	2.53	0.43
1:D:4027:SER:HB2	1:D:4082:PHE:HD1	1.83	0.43
2:F:97:LEU:HD23	2:F:97:LEU:HA	1.83	0.43
1:A:3736:ALA:HB1	1:A:3776:MET:HG2	2.00	0.43
1:A:3951:ALA:HB1	1:A:4011:MET:CE	2.48	0.43
1:B:2781:MET:HA	1:B:2784:TRP:HE3	1.83	0.43
1:B:4027:SER:HB2	1:B:4082:PHE:HD1	1.83	0.43
1:C:1131:ASP:N	1:C:1131:ASP:OD1	2.52	0.43
1:C:2171:MET:SD	1:C:2216:HIS:ND1	2.88	0.43
1:C:3637:ASP:HA	1:C:3640:ILE:HG22	2.01	0.43
1:D:48:PHE:H	1:D:48:PHE:HD2	1.67	0.43
1:D:365:HIS:HE1	1:D:367:ASP:HB2	1.84	0.43
1:D:682:THR:HA	1:D:798:ILE:HD13	1.99	0.43
1:D:1435:GLY:HA3	1:D:1502:ASN:HA	2.01	0.43
1:D:2395:ILE:HD12	1:D:2395:ILE:H	1.84	0.43
2:E:79:ASP:OD1	2:E:80:VAL:N	2.50	0.43
1:A:365:HIS:HE1	1:A:367:ASP:HB2	1.84	0.43
1:A:4928:ASP:OD1	1:A:4928:ASP:N	2.52	0.43
1:B:275:TRP:HE1	1:B:299:HIS:HD2	1.67	0.43
1:B:495:ILE:HG23	1:B:496:ASN:H	1.83	0.43
1:B:731:HIS:HA	1:B:741:VAL:HG12	1.99	0.43
1:B:1435:GLY:HA3	1:B:1502:ASN:HA	2.01	0.43
1:B:1934:LYS:HD2	1:B:2027:ARG:HH21	1.84	0.43
1:B:3637:ASP:HA	1:B:3640:ILE:HG22	2.01	0.43
1:C:2716:LEU:HD23	1:C:2716:LEU:H	1.83	0.43
1:C:4928:ASP:N	1:C:4928:ASP:OD1	2.52	0.43
1:D:2161:MET:HG3	1:D:2166:MET:HE3	2.01	0.43
1:D:2290:ASN:OD1	1:D:2290:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2855:LYS:HE3	1:D:2870:LEU:HB2	2.01	0.43
1:A:1629:MET:HG3	1:A:1642:ILE:HG12	2.01	0.43
1:A:1934:LYS:HD2	1:A:2027:ARG:HH21	1.84	0.43
1:A:2279:LEU:HD22	1:A:2288:GLY:HA2	2.00	0.43
1:A:3940:TRP:HA	1:A:3943:VAL:HG12	2.01	0.43
1:A:4504:ALA:HA	1:A:4507:VAL:HG12	2.00	0.43
1:B:250:GLY:HA3	1:B:256:GLN:OE1	2.18	0.43
1:B:3940:TRP:HA	1:B:3943:VAL:HG12	2.01	0.43
1:C:1641:ASP:OD1	1:C:1642:ILE:N	2.52	0.43
1:C:1706:LEU:O	1:C:1710:ILE:HG13	2.19	0.43
1:C:2257:ARG:HH21	1:C:3806:ALA:HB1	1.84	0.43
1:C:2855:LYS:HE3	1:C:2870:LEU:HB2	2.01	0.43
1:C:3957:LEU:HD11	1:C:3966:LEU:HD22	2.01	0.43
1:C:4027:SER:HB2	1:C:4082:PHE:HD1	1.83	0.43
1:D:2662:LYS:HA	1:D:2662:LYS:HD2	1.82	0.43
1:A:1641:ASP:OD1	1:A:1642:ILE:N	2.52	0.42
1:C:275:TRP:HE1	1:C:299:HIS:HD2	1.67	0.42
1:C:624:ALA:HB3	1:C:2131:VAL:HG12	2.01	0.42
1:C:624:ALA:HB1	1:C:629:GLN:OE1	2.19	0.42
1:C:661:LEU:HD13	1:C:790:PRO:HD3	2.00	0.42
1:C:731:HIS:HA	1:C:741:VAL:HG12	1.99	0.42
1:C:2655:LYS:HE3	1:C:2655:LYS:HB3	1.77	0.42
1:D:275:TRP:HE1	1:D:299:HIS:HD2	1.67	0.42
1:D:415:THR:O	1:D:419:ILE:HG12	2.19	0.42
1:D:2161:MET:H	1:D:2161:MET:HE1	1.84	0.42
1:D:3940:TRP:HA	1:D:3943:VAL:HG12	2.01	0.42
1:A:415:THR:O	1:A:419:ILE:HG12	2.19	0.42
1:A:490:GLN:NE2	1:A:540:LEU:O	2.52	0.42
1:A:624:ALA:HB3	1:A:2131:VAL:HG12	2.01	0.42
1:A:1131:ASP:N	1:A:1131:ASP:OD1	2.52	0.42
1:A:1435:GLY:HA3	1:A:1502:ASN:HA	2.01	0.42
1:A:2278:MET:O	1:A:2279:LEU:HD12	2.20	0.42
1:A:2781:MET:HA	1:A:2784:TRP:HE3	1.83	0.42
1:B:2716:LEU:H	1:B:2716:LEU:HD23	1.83	0.42
1:B:2728:HIS:CD2	1:B:2762:LEU:HD11	2.53	0.42
1:B:3723:LEU:O	1:B:3727:GLN:HG2	2.19	0.42
1:C:48:PHE:H	1:C:48:PHE:HD2	1.67	0.42
1:C:490:GLN:NE2	1:C:540:LEU:O	2.52	0.42
1:D:1641:ASP:OD1	1:D:1642:ILE:N	2.52	0.42
1:D:2257:ARG:HH21	1:D:3806:ALA:HB1	1.84	0.42
1:D:3957:LEU:HD11	1:D:3966:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:LEU:HD23	2:H:97:LEU:HA	1.83	0.42
1:A:626:ARG:HG2	1:A:2131:VAL:HB	2.01	0.42
1:B:42:PHE:HB2	1:B:425:LEU:HD12	2.01	0.42
1:B:731:HIS:NE2	1:B:733:TRP:HB3	2.35	0.42
1:B:3657:MET:SD	1:B:3659:ARG:N	2.83	0.42
1:C:38:ALA:HB1	1:C:64:ILE:HD12	2.00	0.42
1:C:571:ILE:HA	1:C:574:VAL:HG12	2.01	0.42
1:C:731:HIS:NE2	1:C:733:TRP:HB3	2.35	0.42
1:C:1435:GLY:HA3	1:C:1502:ASN:HA	2.01	0.42
1:C:1633:ILE:HD13	1:C:1633:ILE:HA	1.84	0.42
1:C:2667:CYS:SG	1:C:2668:LEU:N	2.93	0.42
1:D:42:PHE:HB2	1:D:425:LEU:HD12	2.01	0.42
1:D:641:ASP:OD1	1:D:642:LEU:N	2.49	0.42
1:D:1706:LEU:O	1:D:1710:ILE:HG13	2.19	0.42
1:D:4928:ASP:OD1	1:D:4928:ASP:N	2.52	0.42
2:F:26:TYR:N	2:F:40:ARG:HH12	2.17	0.42
1:A:2111:SER:O	1:A:2115:THR:OG1	2.33	0.42
1:A:2173:VAL:HA	1:A:2176:ASN:HD21	1.85	0.42
1:A:2391:TYR:O	1:A:2394:LEU:N	2.53	0.42
1:A:2395:ILE:HD12	1:A:2395:ILE:H	1.84	0.42
1:A:4027:SER:HB2	1:A:4082:PHE:HD1	1.83	0.42
1:B:658:ASN:HA	1:B:835:GLU:HB2	2.02	0.42
1:B:1641:ASP:OD1	1:B:1642:ILE:N	2.52	0.42
1:B:1840:LEU:HD12	1:B:1840:LEU:HA	1.91	0.42
1:B:3705:ASP:N	1:B:3705:ASP:OD1	2.53	0.42
1:B:3957:LEU:HD11	1:B:3966:LEU:HD22	2.01	0.42
1:C:885:LEU:HA	1:C:888:ASN:HD21	1.83	0.42
1:C:1629:MET:HG3	1:C:1642:ILE:HG12	2.01	0.42
1:D:335:LYS:HD3	1:D:362:TYR:CE2	2.54	0.42
1:D:422:THR:O	1:D:426:PHE:HB3	2.20	0.42
1:D:658:ASN:HA	1:D:835:GLU:HB2	2.02	0.42
1:D:1827:TYR:HD1	1:D:1908:LEU:HD23	1.85	0.42
1:D:1934:LYS:HD2	1:D:2027:ARG:HH21	1.84	0.42
2:E:26:TYR:N	2:E:40:ARG:HH12	2.17	0.42
1:A:624:ALA:HB1	1:A:629:GLN:OE1	2.19	0.42
1:A:779:PHE:CZ	1:A:782:PHE:HB3	2.54	0.42
1:A:1511:VAL:HG23	1:A:1519:LEU:HD12	2.01	0.42
1:A:2614:GLU:HG2	1:A:2619:TYR:HE1	1.85	0.42
1:B:490:GLN:NE2	1:B:540:LEU:O	2.52	0.42
1:B:1297:THR:HA	1:B:1548:ALA:HB3	2.02	0.42
1:B:2257:ARG:HH21	1:B:3806:ALA:HB1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:VAL:HG22	1:C:716:ASN:HB3	2.02	0.42
1:C:1934:LYS:HD2	1:C:2027:ARG:HH21	1.84	0.42
1:C:2278:MET:O	1:C:2279:LEU:HD12	2.20	0.42
1:D:891:GLU:O	1:D:895:MET:HG2	2.20	0.42
1:D:2165:GLY:O	1:D:2169:THR:HG23	2.19	0.42
1:D:2667:CYS:SG	1:D:2668:LEU:N	2.93	0.42
1:D:3951:ALA:HB1	1:D:4011:MET:CE	2.48	0.42
1:A:275:TRP:HE1	1:A:299:HIS:HD2	1.67	0.42
1:A:565:LEU:HB3	1:A:600:LEU:HD12	2.02	0.42
1:A:658:ASN:HA	1:A:835:GLU:HB2	2.02	0.42
1:A:731:HIS:NE2	1:A:733:TRP:HB3	2.35	0.42
1:A:987:LYS:NZ	1:A:988:LEU:O	2.42	0.42
1:A:1679:SER:HB2	1:A:1769:PHE:CE2	2.55	0.42
1:A:3637:ASP:HA	1:A:3640:ILE:HG22	2.01	0.42
1:B:415:THR:HA	1:B:418:VAL:HG12	2.02	0.42
1:B:415:THR:O	1:B:419:ILE:HG12	2.19	0.42
1:B:652:VAL:HG22	1:B:716:ASN:HB3	2.02	0.42
1:B:2278:MET:O	1:B:2279:LEU:HD12	2.20	0.42
1:C:1297:THR:HA	1:C:1548:ALA:HB3	2.02	0.42
1:C:1511:VAL:HG23	1:C:1519:LEU:HD12	2.01	0.42
1:C:2234:ARG:HH21	1:C:2281:SER:HG	1.68	0.42
1:C:2640:SER:OG	1:C:2641:ARG:NH1	2.52	0.42
1:C:4104:LEU:HD12	1:C:4104:LEU:HA	1.92	0.42
1:C:4176:VAL:HG21	1:C:4879:VAL:HG23	2.02	0.42
1:C:4603:LYS:O	1:C:4607:ARG:HG3	2.20	0.42
1:D:565:LEU:HB3	1:D:600:LEU:HD12	2.02	0.42
1:D:1297:THR:HA	1:D:1548:ALA:HB3	2.02	0.42
1:D:2716:LEU:HD23	1:D:2716:LEU:H	1.83	0.42
1:A:891:GLU:O	1:A:895:MET:HG2	2.20	0.42
1:A:1297:THR:HA	1:A:1548:ALA:HB3	2.02	0.42
1:B:1679:SER:HB2	1:B:1769:PHE:CE2	2.55	0.42
1:B:2173:VAL:HA	1:B:2176:ASN:HD21	1.85	0.42
1:C:422:THR:O	1:C:426:PHE:HB3	2.20	0.42
1:C:1679:SER:HB2	1:C:1769:PHE:CE2	2.55	0.42
1:C:2391:TYR:O	1:C:2394:LEU:N	2.53	0.42
1:C:4193:GLU:OE2	1:C:4943:TYR:OH	2.28	0.42
1:D:490:GLN:NE2	1:D:540:LEU:O	2.52	0.42
1:D:779:PHE:CZ	1:D:782:PHE:HB3	2.54	0.42
1:D:2434:VAL:HG21	1:D:2470:PHE:HD2	1.85	0.42
1:A:415:THR:HA	1:A:418:VAL:HG12	2.02	0.42
1:A:3705:ASP:OD1	1:A:3705:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:THR:O	1:B:426:PHE:HB3	2.20	0.42
1:B:2667:CYS:SG	1:B:2668:LEU:N	2.93	0.42
1:C:1827:TYR:HD1	1:C:1908:LEU:HD23	1.85	0.42
1:C:2161:MET:HG3	1:C:2166:MET:HE3	2.01	0.42
1:C:2395:ILE:HD12	1:C:2395:ILE:H	1.84	0.42
1:D:626:ARG:HG2	1:D:2131:VAL:HB	2.01	0.42
1:D:731:HIS:NE2	1:D:733:TRP:HB3	2.35	0.42
1:D:3723:LEU:O	1:D:3727:GLN:HG2	2.19	0.42
1:D:4136:GLU:O	1:D:4917:TYR:OH	2.31	0.42
1:D:4176:VAL:HG21	1:D:4879:VAL:HG23	2.02	0.42
1:D:4603:LYS:O	1:D:4607:ARG:HG3	2.20	0.42
1:A:422:THR:O	1:A:426:PHE:HB3	2.20	0.42
1:A:2795:ASP:N	1:A:2795:ASP:OD1	2.46	0.42
1:A:3654:ASP:OD1	1:A:3654:ASP:N	2.48	0.42
1:A:3957:LEU:HD11	1:A:3966:LEU:HD22	2.01	0.42
1:B:779:PHE:CZ	1:B:782:PHE:HB3	2.54	0.42
1:B:891:GLU:O	1:B:895:MET:HG2	2.20	0.42
1:B:2391:TYR:O	1:B:2394:LEU:N	2.53	0.42
1:B:2614:GLU:HG2	1:B:2619:TYR:HE1	1.85	0.42
1:B:4176:VAL:HG21	1:B:4879:VAL:HG23	2.02	0.42
1:C:2290:ASN:N	1:C:2290:ASN:OD1	2.51	0.42
1:C:3723:LEU:O	1:C:3727:GLN:HG2	2.19	0.42
1:D:652:VAL:HG22	1:D:716:ASN:HB3	2.02	0.42
1:D:1731:THR:O	1:D:1734:THR:OG1	2.33	0.42
1:D:2171:MET:SD	1:D:2216:HIS:ND1	2.88	0.42
1:D:2173:VAL:HA	1:D:2176:ASN:HD21	1.85	0.42
1:D:2278:MET:O	1:D:2279:LEU:HD12	2.20	0.42
1:D:3000:LYS:HE3	1:D:3070:THR:HA	2.02	0.42
1:A:42:PHE:HB2	1:A:425:LEU:HD12	2.01	0.42
1:A:571:ILE:HA	1:A:574:VAL:HG12	2.01	0.42
1:A:1827:TYR:HD1	1:A:1908:LEU:HD23	1.85	0.42
1:A:2667:CYS:SG	1:A:2668:LEU:N	2.93	0.42
1:A:3000:LYS:HE3	1:A:3070:THR:HA	2.02	0.42
1:B:624:ALA:HB3	1:B:2131:VAL:HG12	2.01	0.42
1:B:4603:LYS:O	1:B:4607:ARG:HG3	2.20	0.42
1:B:4928:ASP:N	1:B:4928:ASP:OD1	2.52	0.42
1:C:80:GLU:OE1	1:C:84:ASN:ND2	2.42	0.42
1:C:312:LYS:HG2	1:C:393:MET:HB2	2.02	0.42
1:C:1011:ARG:HH12	1:C:1032:LEU:N	2.18	0.42
1:D:80:GLU:OE1	1:D:84:ASN:ND2	2.42	0.42
1:D:2777:SER:O	1:D:2780:THR:OG1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:MET:HE2	2:F:72:ALA:HB3	2.02	0.42
1:A:652:VAL:HG22	1:A:716:ASN:HB3	2.02	0.41
1:A:2402:ALA:O	1:A:2473:ARG:NH2	2.44	0.41
1:A:4603:LYS:O	1:A:4607:ARG:HG3	2.20	0.41
1:B:312:LYS:HG2	1:B:393:MET:HB2	2.02	0.41
1:B:571:ILE:HA	1:B:574:VAL:HG12	2.01	0.41
1:B:626:ARG:HG2	1:B:2131:VAL:HB	2.01	0.41
1:B:1629:MET:HG3	1:B:1642:ILE:HG12	2.01	0.41
1:B:4039:LYS:HE2	1:B:4039:LYS:HB2	1.91	0.41
1:C:365:HIS:HE1	1:C:367:ASP:HB2	1.84	0.41
1:C:2173:VAL:HA	1:C:2176:ASN:HD21	1.85	0.41
1:D:128:MET:HB3	1:D:149:LEU:HB3	2.02	0.41
1:D:601:LEU:HG	1:D:610:VAL:HG11	2.02	0.41
1:D:1679:SER:HB2	1:D:1769:PHE:CE2	2.55	0.41
1:A:525:SER:O	1:A:529:ILE:HG22	2.20	0.41
1:A:590:LYS:O	1:A:594:ILE:HG12	2.20	0.41
1:A:601:LEU:HG	1:A:610:VAL:HG11	2.02	0.41
1:A:2855:LYS:HE3	1:A:2870:LEU:HB2	2.01	0.41
1:A:3723:LEU:O	1:A:3727:GLN:HG2	2.19	0.41
1:B:59:PRO:HB3	1:B:296:ARG:CZ	2.50	0.41
1:B:507:VAL:O	1:B:509:SER:N	2.53	0.41
1:B:624:ALA:HB1	1:B:629:GLN:OE1	2.19	0.41
1:B:2855:LYS:HE3	1:B:2870:LEU:HB2	2.01	0.41
1:B:4817:TYR:OH	1:C:4846:ASP:OD2	2.27	0.41
1:C:115:TYR:CZ	1:C:175:VAL:HG22	2.55	0.41
1:C:128:MET:HB3	1:C:149:LEU:HB3	2.02	0.41
1:C:590:LYS:O	1:C:594:ILE:HG12	2.20	0.41
1:C:658:ASN:HA	1:C:835:GLU:HB2	2.02	0.41
1:C:779:PHE:CZ	1:C:782:PHE:HB3	2.54	0.41
1:D:38:ALA:HB1	1:D:64:ILE:HD12	2.00	0.41
1:D:2614:GLU:HG2	1:D:2619:TYR:HE1	1.85	0.41
1:D:3705:ASP:OD1	1:D:3705:ASP:N	2.53	0.41
1:D:4780:TYR:HD1	1:D:4845:PHE:CE1	2.38	0.41
2:F:17:LYS:HE3	2:F:18:LYS:N	2.32	0.41
1:A:48:PHE:H	1:A:48:PHE:HD2	1.67	0.41
1:A:59:PRO:HB3	1:A:296:ARG:CZ	2.50	0.41
1:A:463:PHE:HB3	1:A:536:LEU:CD1	2.50	0.41
1:B:48:PHE:H	1:B:48:PHE:HD2	1.67	0.41
1:B:365:HIS:HE1	1:B:367:ASP:HB2	1.84	0.41
1:B:463:PHE:HB3	1:B:536:LEU:CD1	2.50	0.41
1:B:601:LEU:HG	1:B:610:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4780:TYR:HD1	1:B:4845:PHE:CE1	2.38	0.41
1:C:59:PRO:HB3	1:C:296:ARG:CZ	2.50	0.41
1:C:565:LEU:HB3	1:C:600:LEU:HD12	2.02	0.41
1:C:1720:LEU:HD12	1:C:1720:LEU:HA	1.96	0.41
1:C:3940:TRP:HA	1:C:3943:VAL:HG12	2.01	0.41
1:D:1987:CYS:HA	1:D:1988:PRO:HD3	1.94	0.41
1:A:537:LEU:HD23	1:A:540:LEU:CD1	2.49	0.41
1:A:2161:MET:HE1	1:A:2161:MET:H	1.84	0.41
1:A:2434:VAL:HG21	1:A:2470:PHE:HD2	1.85	0.41
1:A:3758:LEU:O	1:A:3762:ILE:HG23	2.21	0.41
1:A:3889:TRP:HB2	1:B:76:ARG:HE	1.85	0.41
1:B:290:ARG:NH1	1:B:349:MET:O	2.38	0.41
1:B:590:LYS:O	1:B:594:ILE:HG12	2.20	0.41
1:B:1131:ASP:N	1:B:1131:ASP:OD1	2.52	0.41
1:B:1302:TYR:CE2	1:B:1546:ALA:HB3	2.56	0.41
1:B:2832:LEU:HB3	1:B:2837:HIS:CE1	2.56	0.41
1:B:4193:GLU:OE2	1:B:4607:ARG:NH2	2.52	0.41
1:C:891:GLU:O	1:C:895:MET:HG2	2.20	0.41
1:C:1183:LEU:HD11	1:C:1189:GLU:HG2	2.03	0.41
1:C:1642:ILE:HG23	1:C:1643:LEU:HD22	2.03	0.41
1:C:2434:VAL:HG21	1:C:2470:PHE:HD2	1.85	0.41
1:C:4752:LEU:HD12	1:C:4752:LEU:HA	1.80	0.41
1:D:312:LYS:HG2	1:D:393:MET:HB2	2.02	0.41
1:D:1131:ASP:OD1	1:D:1131:ASP:N	2.52	0.41
1:D:2391:TYR:O	1:D:2394:LEU:N	2.53	0.41
2:G:17:LYS:HE3	2:G:18:LYS:N	2.32	0.41
1:A:133:LEU:HB2	1:A:148:GLY:H	1.86	0.41
1:B:115:TYR:CZ	1:B:175:VAL:HG22	2.55	0.41
1:B:1446:ILE:HA	1:B:1486:TYR:HA	2.02	0.41
1:B:3000:LYS:HE3	1:B:3070:THR:HA	2.02	0.41
1:B:3758:LEU:O	1:B:3762:ILE:HG23	2.21	0.41
1:C:507:VAL:O	1:C:509:SER:N	2.53	0.41
1:C:601:LEU:HG	1:C:610:VAL:HG11	2.02	0.41
1:C:1446:ILE:HA	1:C:1486:TYR:HA	2.02	0.41
1:C:2101:LEU:HD23	1:C:2101:LEU:HA	1.89	0.41
1:C:3705:ASP:OD1	1:C:3705:ASP:N	2.53	0.41
1:D:571:ILE:HA	1:D:574:VAL:HG12	2.01	0.41
1:D:2832:LEU:HB3	1:D:2837:HIS:CE1	2.56	0.41
1:D:4735:ASN:OD1	1:D:4735:ASN:N	2.53	0.41
1:A:115:TYR:CZ	1:A:175:VAL:HG22	2.55	0.41
1:A:167:LYS:HA	1:A:167:LYS:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:ARG:HH12	1:A:1032:LEU:N	2.18	0.41
1:A:1426:TYR:HB2	1:A:1511:VAL:HG12	2.03	0.41
1:A:2167:HIS:CE1	1:A:2168:GLU:HG2	2.56	0.41
1:A:3015:ARG:NH2	1:A:3080:THR:HB	2.35	0.41
1:A:4176:VAL:HG21	1:A:4879:VAL:HG23	2.02	0.41
1:B:525:SER:O	1:B:529:ILE:HG22	2.20	0.41
1:B:1511:VAL:HG23	1:B:1519:LEU:HD12	2.01	0.41
1:B:1814:THR:OG1	1:B:1815:THR:N	2.54	0.41
1:B:2395:ILE:HD12	1:B:2395:ILE:H	1.84	0.41
1:B:2434:VAL:HG21	1:B:2470:PHE:HD2	1.85	0.41
1:B:2640:SER:OG	1:B:2641:ARG:NH1	2.52	0.41
1:B:3310:LYS:HG3	1:B:3311:PRO:HD3	2.02	0.41
1:C:626:ARG:HG2	1:C:2131:VAL:HB	2.01	0.41
1:C:2080:VAL:HG13	1:C:3669:LEU:HD22	2.03	0.41
1:C:3310:LYS:HG3	1:C:3311:PRO:HD3	2.02	0.41
1:C:3916:PHE:O	1:C:3920:THR:HG23	2.21	0.41
1:D:507:VAL:O	1:D:509:SER:N	2.53	0.41
1:D:1011:ARG:HH12	1:D:1032:LEU:N	2.18	0.41
1:D:1183:LEU:HD11	1:D:1189:GLU:HG2	2.03	0.41
1:D:2101:LEU:HD23	1:D:2101:LEU:HA	1.89	0.41
1:D:3657:MET:SD	1:D:3659:ARG:N	2.83	0.41
1:A:443:PRO:HA	1:A:445:ILE:HG22	2.02	0.41
1:A:507:VAL:O	1:A:509:SER:N	2.53	0.41
1:A:2832:LEU:HB3	1:A:2837:HIS:CE1	2.56	0.41
1:A:4510:ALA:O	1:A:4514:ILE:HG12	2.21	0.41
1:B:443:PRO:HA	1:B:445:ILE:HG22	2.02	0.41
1:B:1011:ARG:HH12	1:B:1032:LEU:N	2.18	0.41
1:B:1183:LEU:HD11	1:B:1189:GLU:HG2	2.03	0.41
1:B:1633:ILE:HD13	1:B:1633:ILE:HA	1.84	0.41
1:B:2101:LEU:HD23	1:B:2101:LEU:HA	1.89	0.41
1:C:337:LYS:NZ	1:C:371:TRP:HE1	2.18	0.41
1:C:497:LEU:HB3	1:C:498:VAL:H	1.63	0.41
1:C:718:VAL:HG11	1:C:791:VAL:HG11	2.02	0.41
1:C:2614:GLU:HG2	1:C:2619:TYR:HE1	1.85	0.41
1:C:3758:LEU:O	1:C:3762:ILE:HG23	2.21	0.41
1:C:3951:ALA:HB1	1:C:4011:MET:CE	2.48	0.41
1:D:115:TYR:CZ	1:D:175:VAL:HG22	2.55	0.41
1:D:133:LEU:HB2	1:D:148:GLY:H	1.86	0.41
1:D:624:ALA:HB1	1:D:629:GLN:OE1	2.19	0.41
1:D:1511:VAL:HG23	1:D:1519:LEU:HD12	2.01	0.41
1:D:3758:LEU:O	1:D:3762:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:17:LYS:HE3	2:E:18:LYS:N	2.32	0.41
1:A:337:LYS:NZ	1:A:371:TRP:HE1	2.18	0.41
1:A:497:LEU:HB3	1:A:498:VAL:H	1.63	0.41
1:A:641:ASP:OD1	1:A:642:LEU:N	2.49	0.41
1:A:3916:PHE:O	1:A:3920:THR:HG23	2.21	0.41
1:B:537:LEU:HD23	1:B:540:LEU:CD1	2.49	0.41
1:B:1642:ILE:HG23	1:B:1643:LEU:HD22	2.03	0.41
1:B:3916:PHE:O	1:B:3920:THR:HG23	2.21	0.41
1:C:525:SER:O	1:C:529:ILE:HG22	2.20	0.41
1:C:1814:THR:OG1	1:C:1815:THR:N	2.54	0.41
1:C:2777:SER:O	1:C:2780:THR:OG1	2.29	0.41
1:C:3491:ALA:HA	1:C:3494:ARG:HD2	2.03	0.41
1:C:4577:LEU:HG	1:C:4581:ILE:HD11	2.02	0.41
1:D:415:THR:HA	1:D:418:VAL:HG12	2.02	0.41
1:D:525:SER:O	1:D:529:ILE:HG22	2.20	0.41
1:D:1426:TYR:HB2	1:D:1511:VAL:HG12	2.03	0.41
1:D:1720:LEU:HD12	1:D:1720:LEU:HA	1.96	0.41
1:D:2189:PRO:HA	1:D:2191:MET:SD	2.61	0.41
1:D:3491:ALA:HA	1:D:3494:ARG:HD2	2.03	0.41
1:D:4510:ALA:O	1:D:4514:ILE:HG12	2.21	0.41
1:A:76:ARG:HE	1:D:3889:TRP:HB2	1.85	0.41
1:A:128:MET:HB3	1:A:149:LEU:HB3	2.02	0.41
1:A:256:GLN:H	1:A:256:GLN:CD	2.24	0.41
1:A:312:LYS:HG2	1:A:393:MET:HB2	2.02	0.41
1:A:362:TYR:OH	1:A:401:ASP:HB3	2.21	0.41
1:A:1068:ASP:OD1	1:A:1068:ASP:N	2.50	0.41
1:A:4735:ASN:OD1	1:A:4735:ASN:N	2.53	0.41
1:B:1814:THR:HG23	1:B:1816:GLU:HG2	2.03	0.41
1:B:1827:TYR:HD1	1:B:1908:LEU:HD23	1.85	0.41
1:B:2189:PRO:HA	1:B:2191:MET:SD	2.61	0.41
1:B:2796:SER:HB3	1:B:2897:ILE:HG22	2.03	0.41
1:B:3889:TRP:HB2	1:C:76:ARG:HE	1.85	0.41
1:B:4735:ASN:OD1	1:B:4735:ASN:N	2.53	0.41
1:C:133:LEU:HB2	1:C:148:GLY:H	1.86	0.41
1:C:300:VAL:HG21	1:C:419:ILE:HD12	2.03	0.41
1:C:362:TYR:OH	1:C:401:ASP:HB3	2.21	0.41
1:C:1302:TYR:CE2	1:C:1546:ALA:HB3	2.56	0.41
1:C:2189:PRO:HA	1:C:2191:MET:SD	2.61	0.41
1:C:2654:LYS:HG3	1:C:2656:TYR:H	1.86	0.41
1:C:3000:LYS:HE3	1:C:3070:THR:HA	2.02	0.41
1:C:3015:ARG:NH2	1:C:3080:THR:HB	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3098:VAL:HA	1:C:3101:LEU:HD13	2.03	0.41
1:C:3370:PRO:HA	1:C:3373:ILE:HB	2.03	0.41
1:C:3889:TRP:HB2	1:D:76:ARG:HE	1.85	0.41
1:C:4780:TYR:HD1	1:C:4845:PHE:CE1	2.38	0.41
1:D:59:PRO:HB3	1:D:296:ARG:CZ	2.50	0.41
1:D:590:LYS:O	1:D:594:ILE:HG12	2.20	0.41
1:D:1302:TYR:CE2	1:D:1546:ALA:HB3	2.56	0.41
1:D:1796:LEU:HD23	1:D:1796:LEU:HA	1.90	0.41
1:D:1814:THR:HG23	1:D:1816:GLU:HG2	2.03	0.41
1:D:2167:HIS:CE1	1:D:2168:GLU:HG2	2.56	0.41
1:D:2606:LEU:O	1:D:2610:THR:OG1	2.31	0.41
1:D:2796:SER:HB3	1:D:2897:ILE:HG22	2.03	0.41
1:D:3098:VAL:HA	1:D:3101:LEU:HD13	2.03	0.41
1:A:718:VAL:HG11	1:A:791:VAL:HG11	2.02	0.41
1:A:723:PHE:HE1	1:A:1482:ARG:HB3	1.86	0.41
1:A:988:LEU:HD11	1:A:992:GLN:HG2	2.03	0.41
1:A:1446:ILE:HA	1:A:1486:TYR:HA	2.02	0.41
1:B:133:LEU:HB2	1:B:148:GLY:H	1.86	0.41
1:B:256:GLN:H	1:B:256:GLN:CD	2.24	0.41
1:B:362:TYR:OH	1:B:401:ASP:HB3	2.21	0.41
1:B:565:LEU:HB3	1:B:600:LEU:HD12	2.02	0.41
1:C:443:PRO:HA	1:C:445:ILE:HG22	2.02	0.41
1:C:723:PHE:HE1	1:C:1482:ARG:HB3	1.86	0.41
1:C:1461:ARG:O	1:C:1463:ARG:N	2.51	0.41
1:D:337:LYS:NZ	1:D:371:TRP:HE1	2.18	0.41
1:D:362:TYR:OH	1:D:401:ASP:HB3	2.21	0.41
1:D:3954:GLN:H	1:D:3954:GLN:HG2	1.57	0.41
1:D:4766:LEU:HD12	1:D:4864:LEU:HD13	2.03	0.41
1:A:1814:THR:HG23	1:A:1816:GLU:HG2	2.03	0.40
1:A:3098:VAL:HA	1:A:3101:LEU:HD13	2.03	0.40
1:A:4766:LEU:HD12	1:A:4864:LEU:HD13	2.03	0.40
1:B:337:LYS:NZ	1:B:371:TRP:HE1	2.18	0.40
1:B:723:PHE:HE1	1:B:1482:ARG:HB3	1.86	0.40
1:B:858:THR:OG1	1:B:861:ALA:O	2.32	0.40
1:B:1524:ASN:OD1	1:B:1524:ASN:N	2.54	0.40
1:B:2080:VAL:HG13	1:B:3669:LEU:HD22	2.03	0.40
1:B:2654:LYS:HG3	1:B:2656:TYR:H	1.86	0.40
1:B:3491:ALA:HA	1:B:3494:ARG:HD2	2.03	0.40
1:B:4577:LEU:HG	1:B:4581:ILE:HD11	2.02	0.40
1:C:256:GLN:H	1:C:256:GLN:CD	2.24	0.40
1:C:2832:LEU:HB3	1:C:2837:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:745:ASN:O	1:D:745:ASN:ND2	2.55	0.40
1:D:1814:THR:OG1	1:D:1815:THR:N	2.54	0.40
1:B:2113:GLU:OE2	1:B:2113:GLU:N	2.54	0.40
1:B:3098:VAL:HA	1:B:3101:LEU:HD13	2.03	0.40
1:B:3370:PRO:HA	1:B:3373:ILE:HB	2.03	0.40
1:C:988:LEU:HD11	1:C:992:GLN:HG2	2.03	0.40
1:C:4510:ALA:O	1:C:4514:ILE:HG12	2.21	0.40
1:C:4766:LEU:HD12	1:C:4864:LEU:HD13	2.03	0.40
1:D:256:GLN:H	1:D:256:GLN:CD	2.24	0.40
1:D:428:ARG:NH1	1:D:428:ARG:O	2.54	0.40
1:D:537:LEU:HD23	1:D:540:LEU:CD1	2.49	0.40
1:D:1446:ILE:HA	1:D:1486:TYR:HA	2.02	0.40
1:A:745:ASN:O	1:A:745:ASN:ND2	2.55	0.40
1:A:808:HIS:CE1	1:A:832:LEU:HD11	2.57	0.40
1:A:4608:LYS:HD3	1:A:4614:LEU:HD22	2.03	0.40
1:B:2167:HIS:CE1	1:B:2168:GLU:HG2	2.56	0.40
1:B:3202:ASP:HA	1:B:3207:ILE:HD13	2.04	0.40
1:C:405:LEU:HD23	1:C:405:LEU:HA	1.86	0.40
1:C:415:THR:HA	1:C:418:VAL:HG12	2.02	0.40
1:C:537:LEU:HD23	1:C:540:LEU:CD1	2.49	0.40
1:C:1426:TYR:HB2	1:C:1511:VAL:HG12	2.03	0.40
1:C:1438:PRO:HG2	1:C:1547:GLN:HB3	2.04	0.40
1:C:2167:HIS:CE1	1:C:2168:GLU:HG2	2.56	0.40
1:C:2464:LYS:O	1:C:2468:VAL:HG13	2.22	0.40
1:D:405:LEU:HD23	1:D:405:LEU:HA	1.86	0.40
1:D:443:PRO:HA	1:D:445:ILE:HG22	2.02	0.40
1:D:723:PHE:HE1	1:D:1482:ARG:HB3	1.86	0.40
1:D:987:LYS:NZ	1:D:988:LEU:O	2.42	0.40
1:D:2080:VAL:HG13	1:D:3669:LEU:HD22	2.03	0.40
1:D:2101:LEU:O	1:D:2104:THR:HG22	2.22	0.40
1:A:428:ARG:NH1	1:A:428:ARG:O	2.54	0.40
1:A:1183:LEU:HD11	1:A:1189:GLU:HG2	2.03	0.40
1:A:1796:LEU:HD23	1:A:1796:LEU:HA	1.90	0.40
1:A:1814:THR:OG1	1:A:1815:THR:N	2.54	0.40
1:A:2654:LYS:HG3	1:A:2656:TYR:H	1.86	0.40
1:A:2796:SER:HB3	1:A:2897:ILE:HG22	2.03	0.40
1:A:4780:TYR:HD1	1:A:4845:PHE:CE1	2.38	0.40
1:B:128:MET:HB3	1:B:149:LEU:HB3	2.02	0.40
1:B:494:MET:HB3	1:B:550:GLN:HB3	2.04	0.40
1:B:641:ASP:OD1	1:B:642:LEU:N	2.49	0.40
1:B:808:HIS:CE1	1:B:832:LEU:HD11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2723:TYR:CE2	1:B:2898:SER:HB3	2.57	0.40
1:C:1631:LEU:HD12	1:C:1633:ILE:HG12	2.04	0.40
1:D:167:LYS:HD3	1:D:167:LYS:HA	1.89	0.40
1:D:2464:LYS:O	1:D:2468:VAL:HG13	2.22	0.40
1:D:2723:TYR:CE2	1:D:2898:SER:HB3	2.57	0.40
1:D:4193:GLU:OE2	1:D:4607:ARG:NH2	2.52	0.40
2:E:25:HIS:CD2	2:E:45:PRO:HB3	2.56	0.40
2:F:25:HIS:CD2	2:F:45:PRO:HB3	2.56	0.40
1:A:305:TYR:N	1:A:317:MET:O	2.42	0.40
1:A:1637:ASN:OD1	1:A:1637:ASN:N	2.55	0.40
1:A:2191:MET:SD	1:A:2191:MET:N	2.85	0.40
1:A:2307:CYS:HG	1:A:2308:ASN:H	1.68	0.40
1:A:2723:TYR:CE2	1:A:2898:SER:HB3	2.57	0.40
1:A:3491:ALA:HA	1:A:3494:ARG:HD2	2.03	0.40
1:B:718:VAL:HG11	1:B:791:VAL:HG11	2.02	0.40
1:B:1426:TYR:HB2	1:B:1511:VAL:HG12	2.03	0.40
1:B:1461:ARG:O	1:B:1463:ARG:N	2.51	0.40
1:C:494:MET:HB3	1:C:550:GLN:HB3	2.04	0.40
1:C:2723:TYR:CE2	1:C:2898:SER:HB3	2.57	0.40
1:C:2796:SER:HB3	1:C:2897:ILE:HG22	2.03	0.40
1:D:1642:ILE:HG23	1:D:1643:LEU:HD22	2.03	0.40
1:D:2307:CYS:HG	1:D:2308:ASN:H	1.66	0.40
1:D:3310:LYS:HG3	1:D:3311:PRO:HD3	2.02	0.40
1:D:3370:PRO:HA	1:D:3373:ILE:HB	2.03	0.40
2:F:57:LYS:H	2:F:57:LYS:HG2	1.70	0.40
2:H:25:HIS:CD2	2:H:45:PRO:HB3	2.56	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	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	47	79
1	B	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	47	79
1	C	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	47	79
1	D	4011/4966 (81%)	3600 (90%)	404 (10%)	7 (0%)	47	79
2	E	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	F	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	G	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
All	All	16464/20292 (81%)	14804 (90%)	1632 (10%)	28 (0%)	50	79

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	LYS
1	A	1484	ASN
1	A	3253	PRO
1	B	344	LYS
1	B	1484	ASN
1	B	3253	PRO
1	C	344	LYS
1	C	1484	ASN
1	C	3253	PRO
1	D	344	LYS
1	D	1484	ASN
1	D	3253	PRO
1	A	1768	SER
1	B	1768	SER
1	C	1768	SER
1	D	1768	SER
1	A	1285	VAL
1	B	1285	VAL
1	C	1285	VAL
1	D	1285	VAL
1	A	1299	ILE
1	A	2988	PRO
1	B	1299	ILE
1	B	2988	PRO
1	C	1299	ILE
1	C	2988	PRO
1	D	1299	ILE

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Mol	Chain	Res	Type
1	D	2988	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	3319/4352 (76%)	3276 (99%)	43 (1%)	69	86
1	B	3319/4352 (76%)	3276 (99%)	43 (1%)	69	86
1	C	3319/4352 (76%)	3276 (99%)	43 (1%)	69	86
1	D	3319/4352 (76%)	3276 (99%)	43 (1%)	69	86
2	E	88/88 (100%)	87 (99%)	1 (1%)	73	88
2	F	88/88 (100%)	87 (99%)	1 (1%)	73	88
2	G	88/88 (100%)	87 (99%)	1 (1%)	73	88
2	H	88/88 (100%)	87 (99%)	1 (1%)	73	88
All	All	13628/17760 (77%)	13452 (99%)	176 (1%)	70	86

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	48	PHE
1	A	176	ARG
1	A	196	TYR
1	A	359	SER
1	A	362	TYR
1	A	398	HIS
1	A	427	ASN
1	A	469	HIS
1	A	564	ARG
1	A	584	GLU
1	A	615	CYS
1	A	635	ASN
1	A	814	LEU

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Mol	Chain	Res	Type
1	A	851	LEU
1	A	964	MET
1	A	965	LYS
1	A	1007	TRP
1	A	1258	PHE
1	A	1554	PHE
1	A	1628	PHE
1	A	1641	ASP
1	A	1764	PHE
1	A	1927	PHE
1	A	1941	PHE
1	A	2039	LYS
1	A	2129	LEU
1	A	2161	MET
1	A	2166	MET
1	A	2219	TYR
1	A	2369	LYS
1	A	2388	MET
1	A	2492	LEU
1	A	2667	CYS
1	A	3073	ASN
1	A	3240	MET
1	A	3347	MET
1	A	3494	ARG
1	A	3614	ARG
1	A	3713	PHE
1	A	3853	PHE
1	A	3953	MET
1	A	4502	MET
1	B	17	ASP
1	B	48	PHE
1	B	176	ARG
1	B	196	TYR
1	B	359	SER
1	B	362	TYR
1	B	398	HIS
1	B	427	ASN
1	B	469	HIS
1	B	564	ARG
1	B	584	GLU
1	B	615	CYS
1	B	635	ASN

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Mol	Chain	Res	Type
1	B	814	LEU
1	B	851	LEU
1	B	964	MET
1	B	965	LYS
1	B	1007	TRP
1	B	1258	PHE
1	B	1554	PHE
1	B	1628	PHE
1	B	1641	ASP
1	B	1764	PHE
1	B	1927	PHE
1	B	1941	PHE
1	B	2039	LYS
1	B	2129	LEU
1	B	2161	MET
1	B	2166	MET
1	B	2219	TYR
1	B	2369	LYS
1	B	2388	MET
1	B	2492	LEU
1	B	2667	CYS
1	B	3073	ASN
1	B	3240	MET
1	B	3347	MET
1	B	3494	ARG
1	B	3614	ARG
1	B	3713	PHE
1	B	3853	PHE
1	B	3953	MET
1	B	4502	MET
1	C	17	ASP
1	C	48	PHE
1	C	176	ARG
1	C	196	TYR
1	C	359	SER
1	C	362	TYR
1	C	398	HIS
1	C	427	ASN
1	C	469	HIS
1	C	564	ARG
1	C	584	GLU
1	C	615	CYS

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Mol	Chain	Res	Type
1	C	635	ASN
1	C	814	LEU
1	C	851	LEU
1	C	964	MET
1	C	965	LYS
1	C	1007	TRP
1	C	1258	PHE
1	C	1554	PHE
1	C	1628	PHE
1	C	1641	ASP
1	C	1764	PHE
1	C	1927	PHE
1	C	1941	PHE
1	C	2039	LYS
1	C	2129	LEU
1	C	2161	MET
1	C	2166	MET
1	C	2219	TYR
1	C	2369	LYS
1	C	2388	MET
1	C	2492	LEU
1	C	2667	CYS
1	C	3073	ASN
1	C	3240	MET
1	C	3347	MET
1	C	3494	ARG
1	C	3614	ARG
1	C	3713	PHE
1	C	3853	PHE
1	C	3953	MET
1	C	4502	MET
1	D	17	ASP
1	D	48	PHE
1	D	176	ARG
1	D	196	TYR
1	D	359	SER
1	D	362	TYR
1	D	398	HIS
1	D	427	ASN
1	D	469	HIS
1	D	564	ARG
1	D	584	GLU

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Mol	Chain	Res	Type
1	D	615	CYS
1	D	635	ASN
1	D	814	LEU
1	D	851	LEU
1	D	964	MET
1	D	965	LYS
1	D	1007	TRP
1	D	1258	PHE
1	D	1554	PHE
1	D	1628	PHE
1	D	1641	ASP
1	D	1764	PHE
1	D	1927	PHE
1	D	1941	PHE
1	D	2039	LYS
1	D	2129	LEU
1	D	2161	MET
1	D	2166	MET
1	D	2219	TYR
1	D	2369	LYS
1	D	2388	MET
1	D	2492	LEU
1	D	2667	CYS
1	D	3073	ASN
1	D	3240	MET
1	D	3347	MET
1	D	3494	ARG
1	D	3614	ARG
1	D	3713	PHE
1	D	3853	PHE
1	D	3953	MET
1	D	4502	MET
2	E	48	PHE
2	F	48	PHE
2	G	48	PHE
2	H	48	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	288	HIS

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Mol	Chain	Res	Type
1	A	645	GLN
1	A	890	HIS
1	A	2223	ASN
1	A	3948	HIS
1	A	4735	ASN
1	B	261	HIS
1	B	288	HIS
1	B	645	GLN
1	B	2176	ASN
1	B	2223	ASN
1	B	3930	ASN
1	B	3948	HIS
1	B	4735	ASN
1	C	261	HIS
1	C	288	HIS
1	C	645	GLN
1	C	2176	ASN
1	C	2223	ASN
1	C	3930	ASN
1	C	3931	GLN
1	C	3948	HIS
1	C	4735	ASN
1	D	261	HIS
1	D	288	HIS
1	D	645	GLN
1	D	2176	ASN
1	D	2223	ASN
1	D	3930	ASN
1	D	3948	HIS
1	D	4735	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.

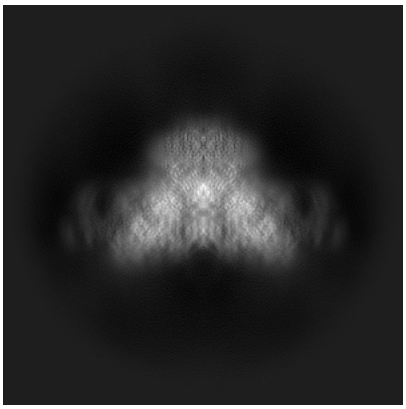
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27712. These allow visual inspection of the internal detail of the map and identification of artifacts.

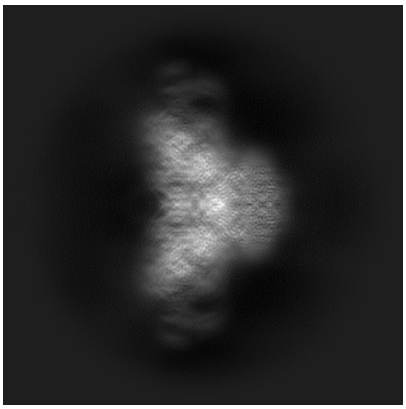
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

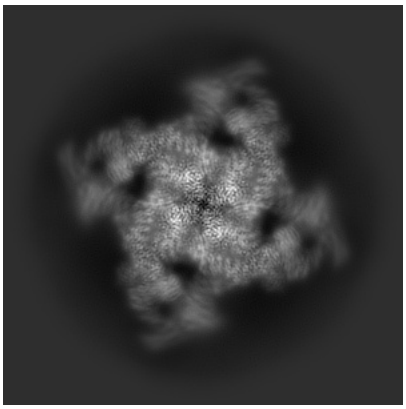
6.1.1 Primary map



X

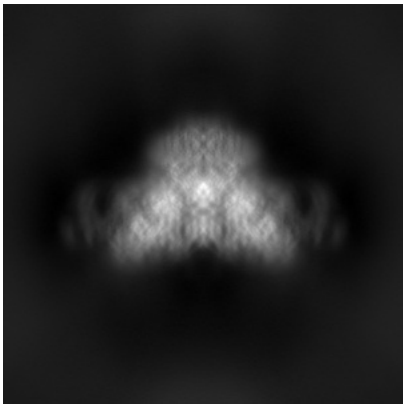


Y

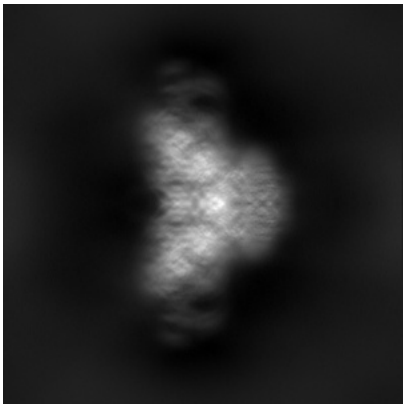


Z

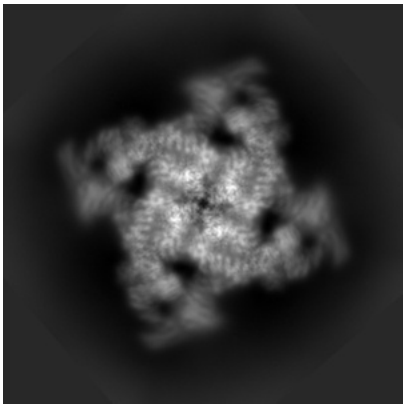
6.1.2 Raw map



X



Y

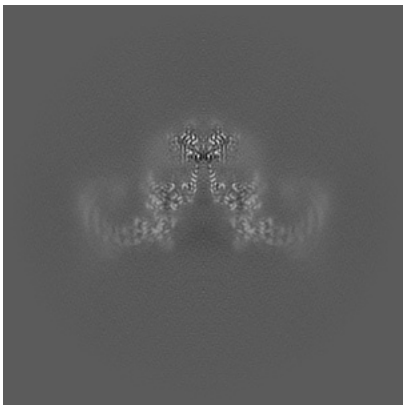


Z

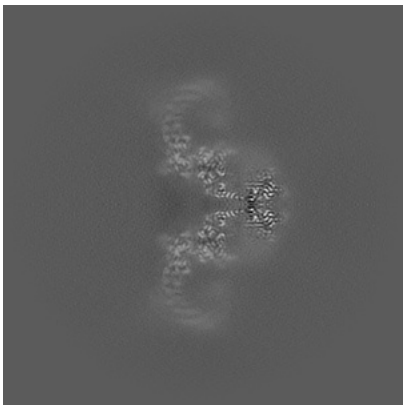
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

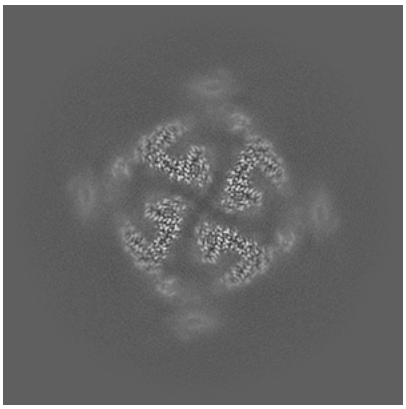
6.2.1 Primary map



X Index: 230

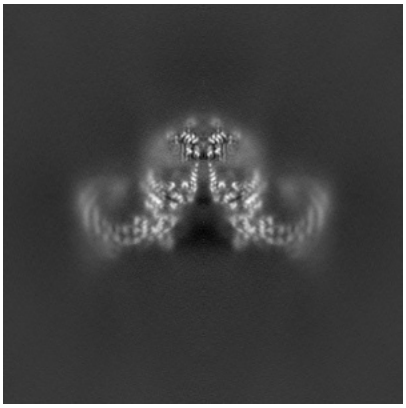


Y Index: 230

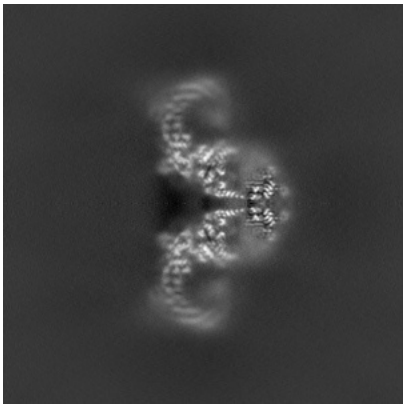


Z Index: 230

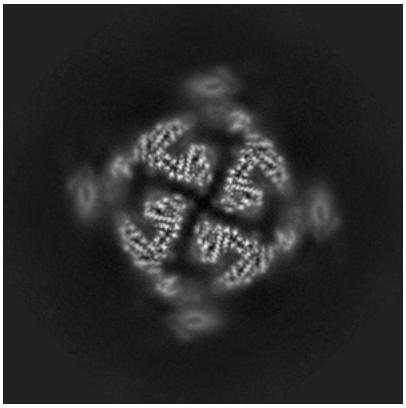
6.2.2 Raw map



X Index: 230



Y Index: 230

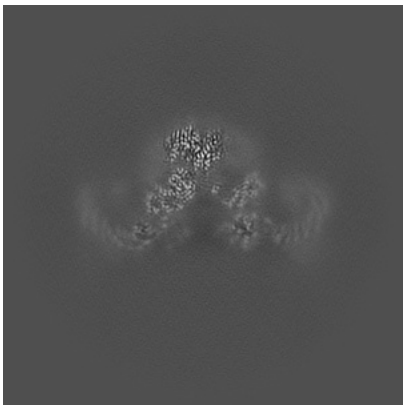


Z Index: 230

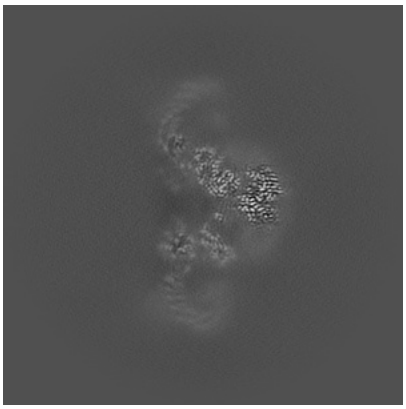
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

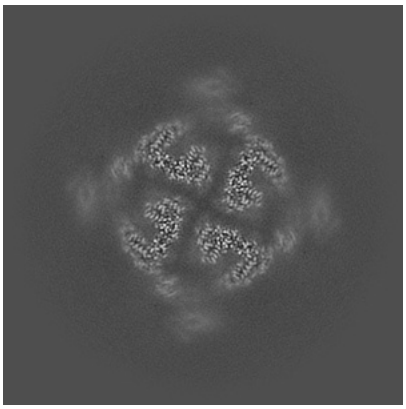
6.3.1 Primary map



X Index: 236

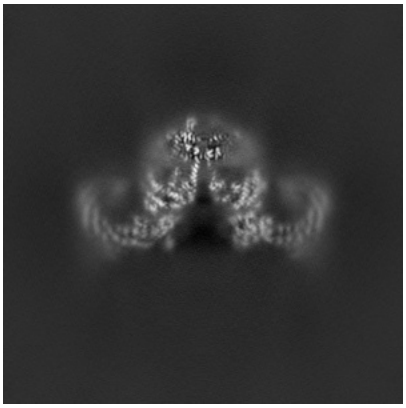


Y Index: 236

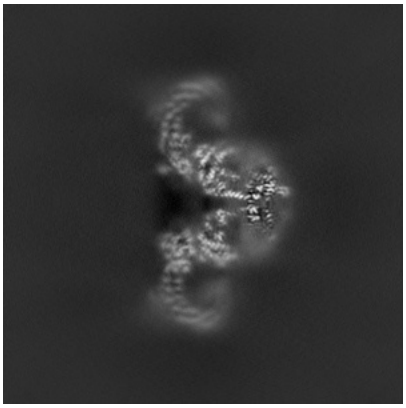


Z Index: 229

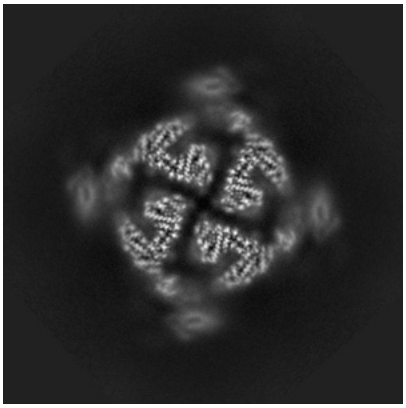
6.3.2 Raw map



X Index: 232



Y Index: 232

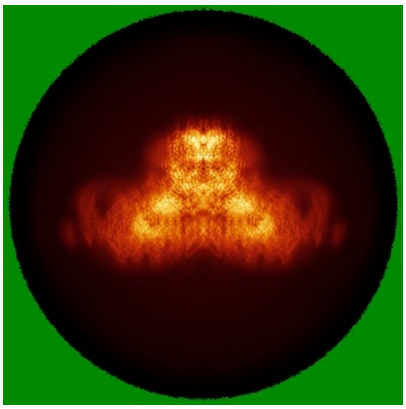


Z Index: 230

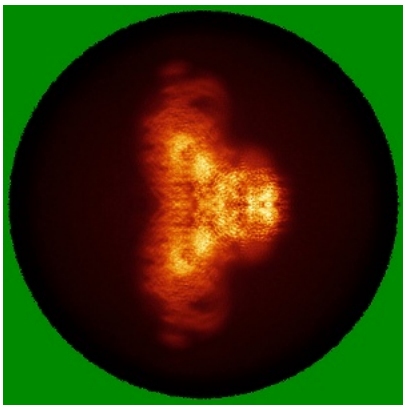
The images above show the largest variance slices of the map in three orthogonal directions.

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

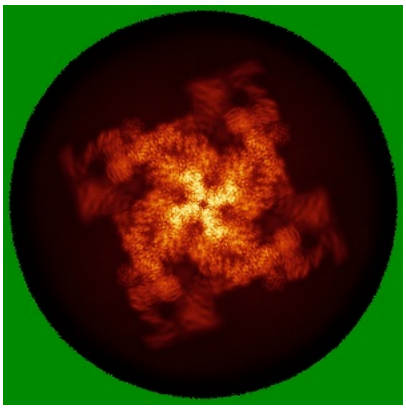
6.4.1 Primary map



X



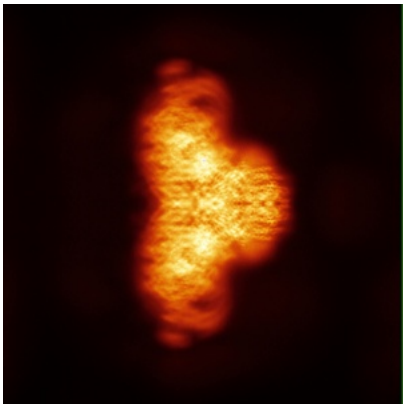
Y



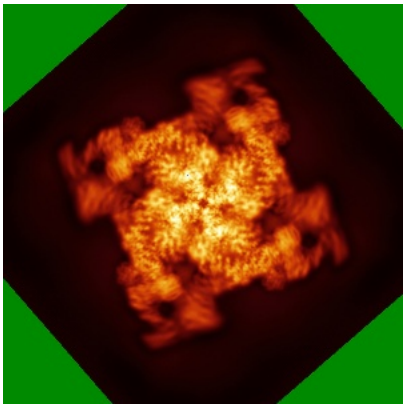
Z

6.4.2 Raw map

X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

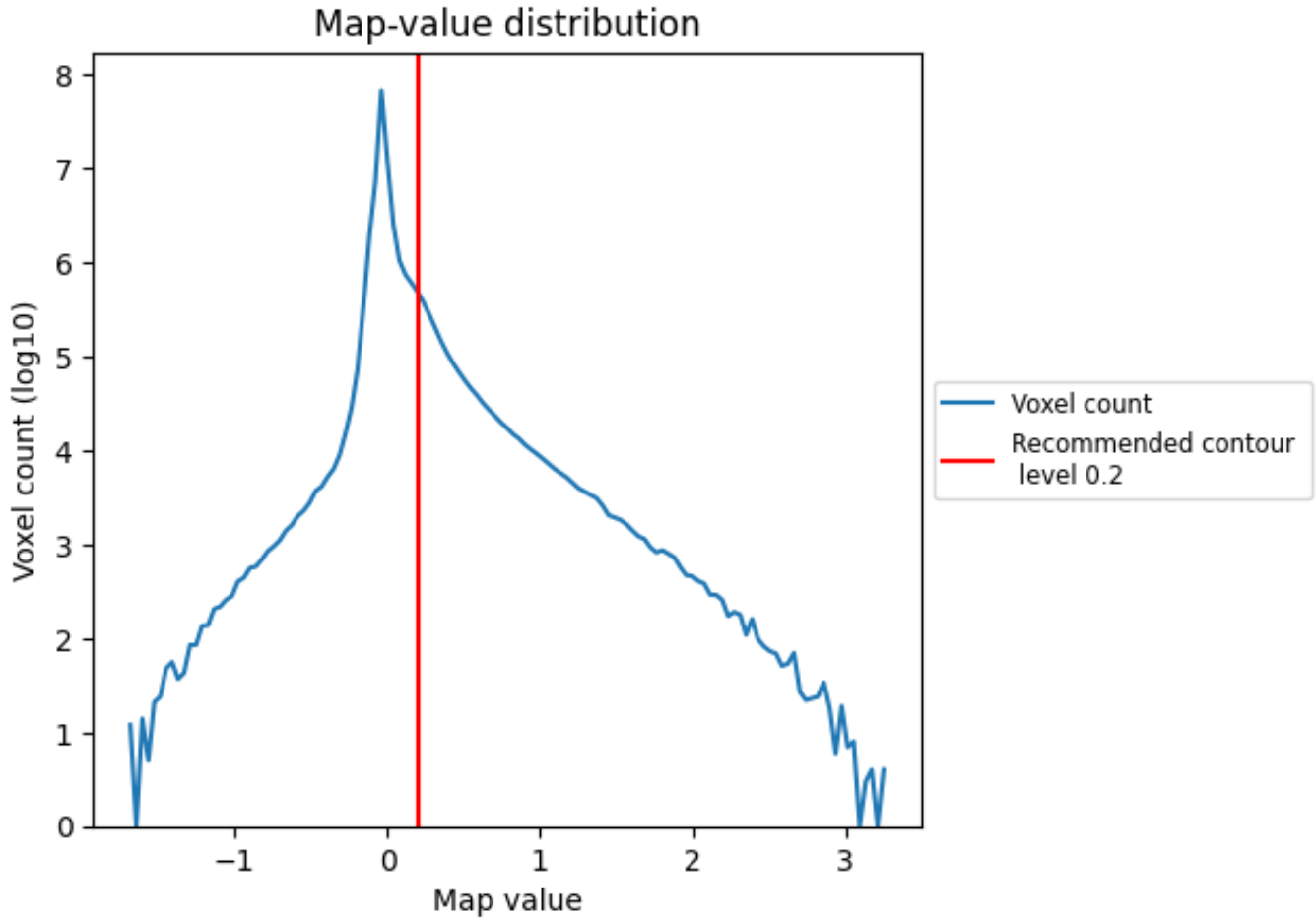
6.6 Mask visualisation (i)

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

7 Map analysis

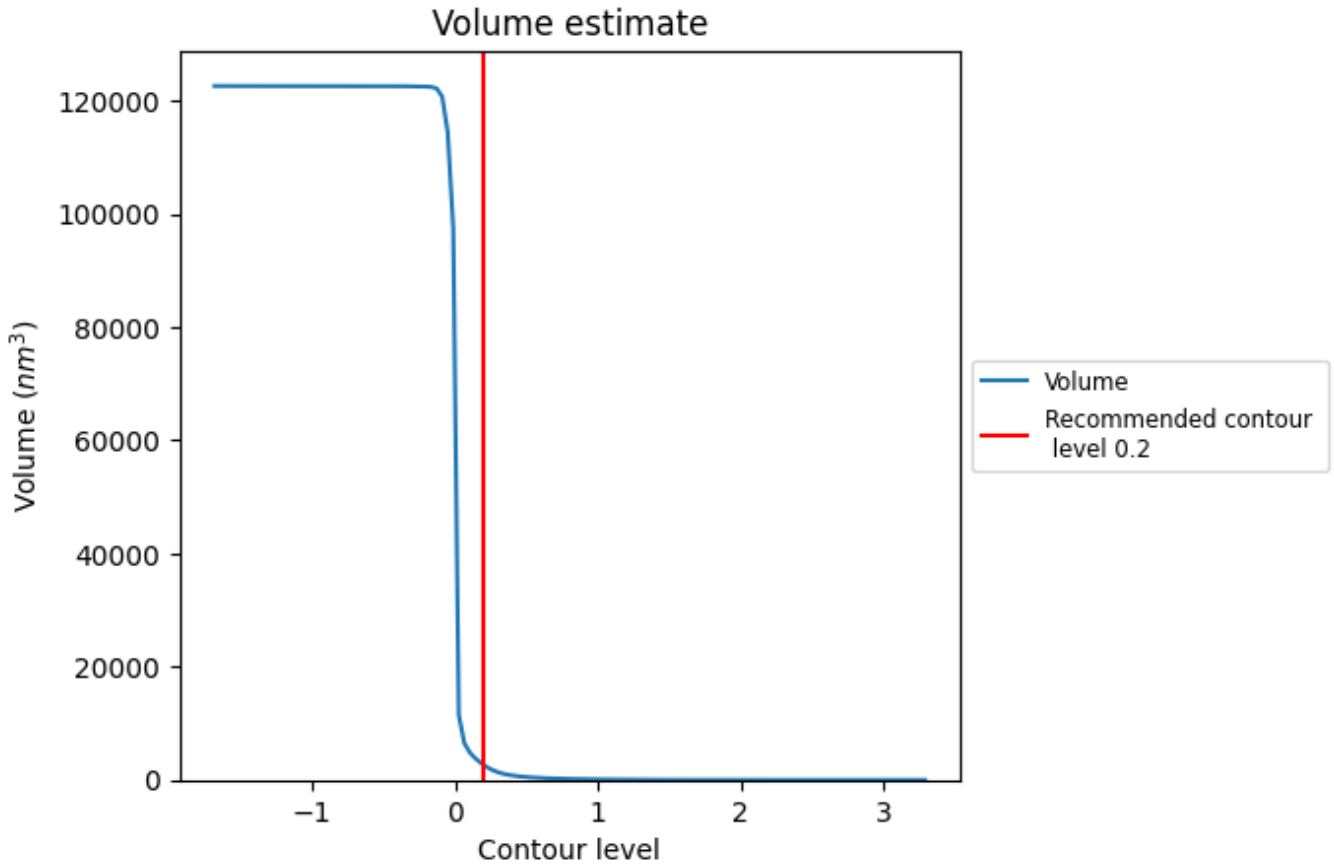
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

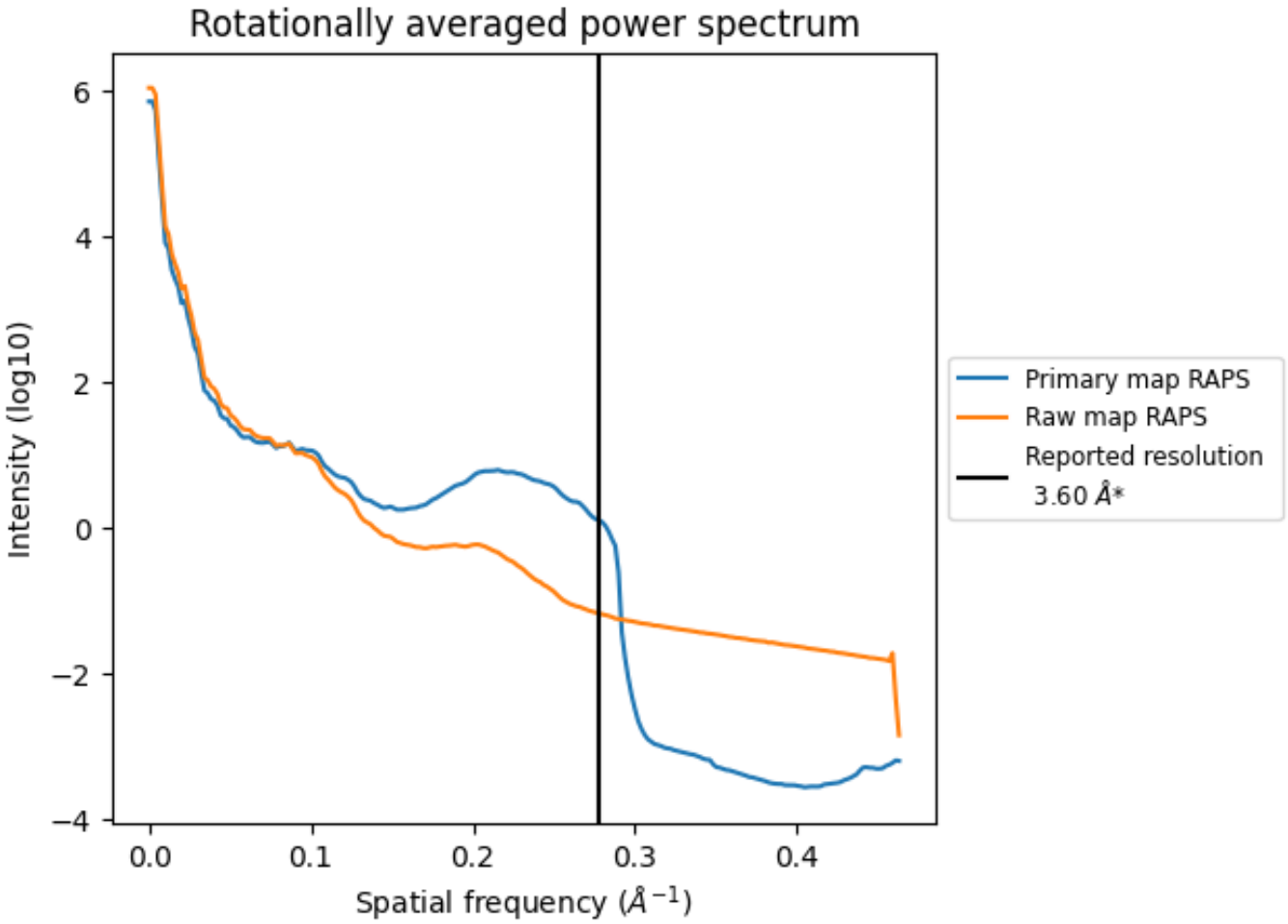
7.2 Volume estimate



The volume at the recommended contour level is 2673 nm^3; this corresponds to an approximate mass of 2415 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)

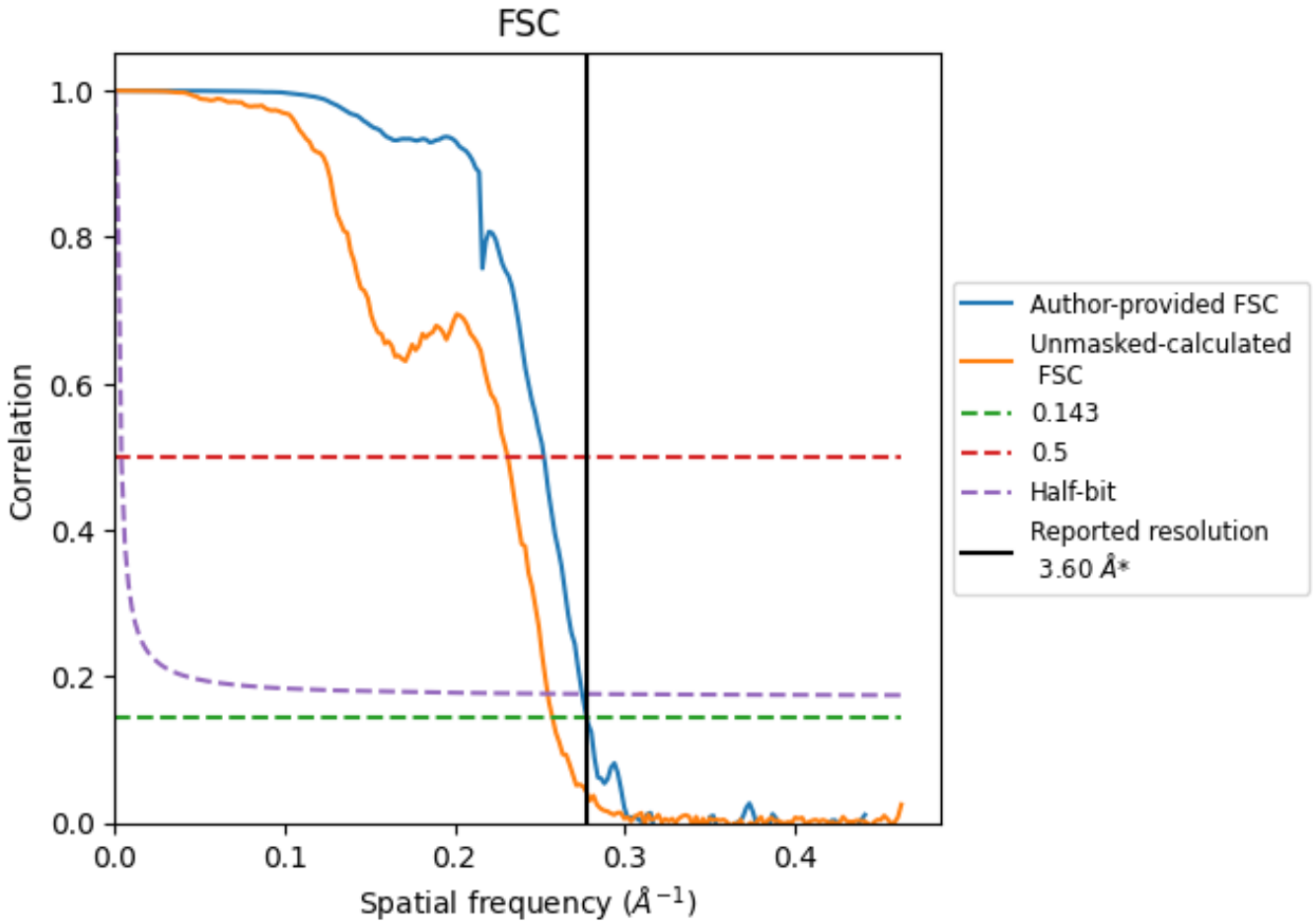


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

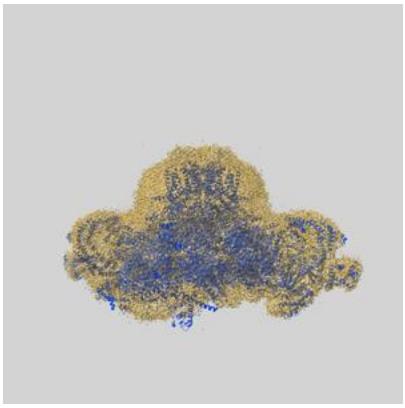
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	3.96	3.64
Unmasked-calculated*	3.88	4.32	3.92

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

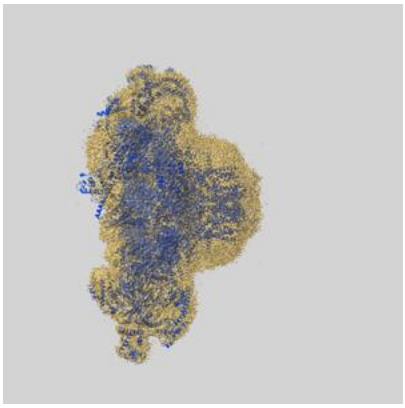
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27712 and PDB model 8DTZ. Per-residue inclusion information can be found in section 3 on page 5.

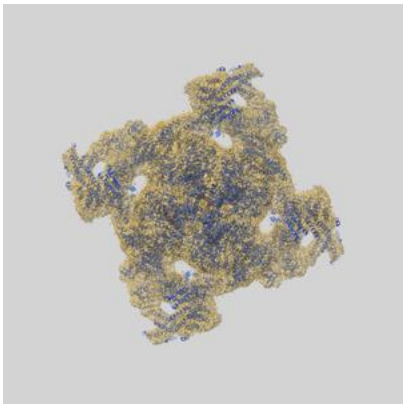
9.1 Map-model overlay



X



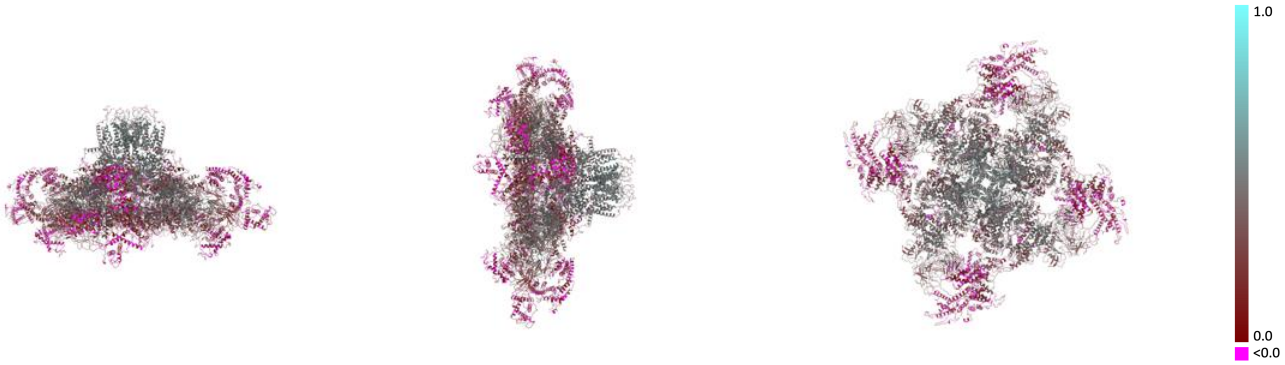
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

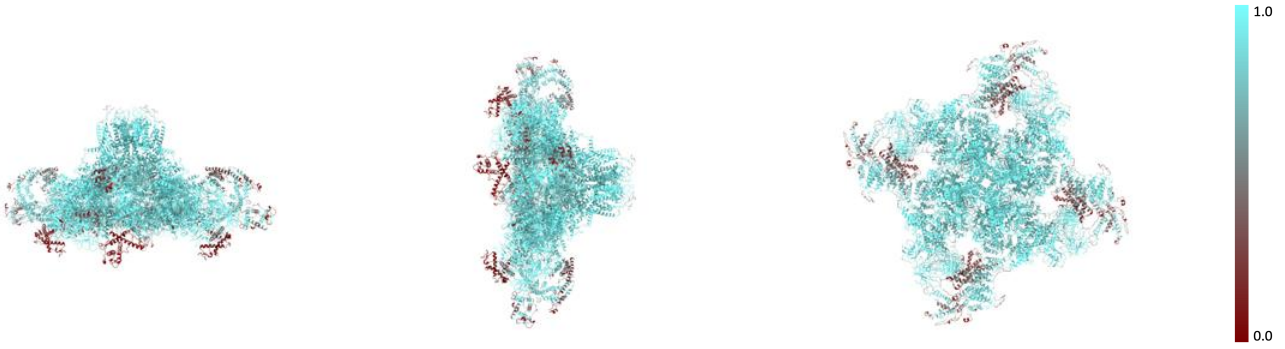
9.2 Q-score mapped to coordinate model (i)



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.

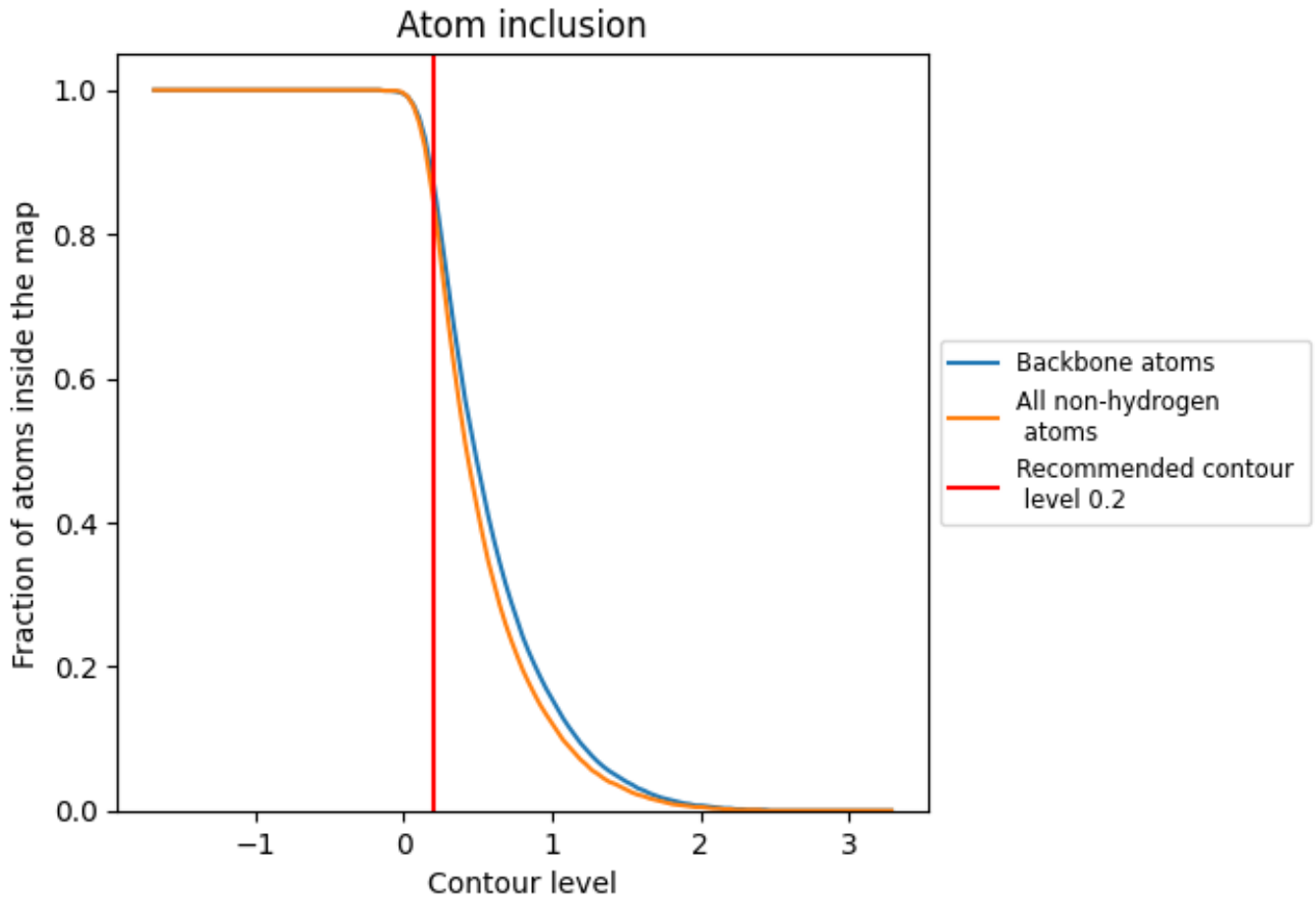
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.3020
A	0.8450	0.3010
B	0.8450	0.3000
C	0.8460	0.3000
D	0.8450	0.3010
E	0.9380	0.3560
F	0.9370	0.3550
G	0.9340	0.3570
H	0.9370	0.3580