Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 02:33 PM EDT

PDB ID	:	5TB4
EMDB ID	:	EMD-8395
Title	:	Structure of rabbit RyR1 (EGTA-only dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-11
Resolution	:	4.50 Å(reported)

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:

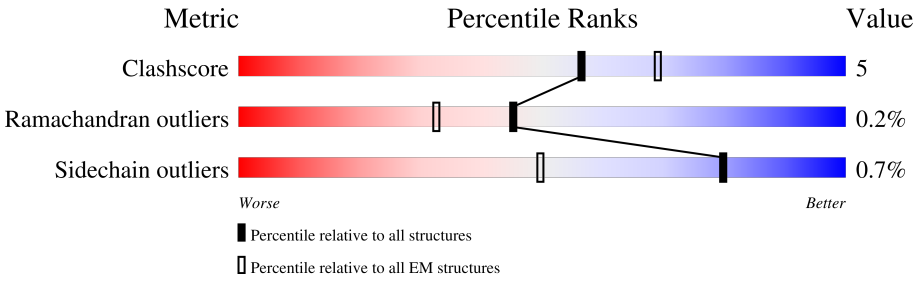
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	108	27% 84% 15%
1	F	108	28% 81% 19%
1	H	108	26% 85% 14%
1	J	108	28% 83% 16%
2	B	4416	39% 84% 10% 5%
2	E	4416	39% 84% 10% 5%
2	G	4416	39% 84% 10% 5%
2	I	4416	39% 84% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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

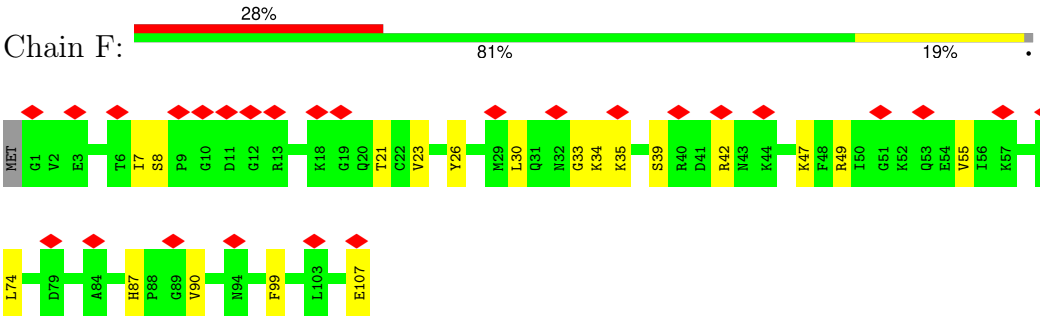
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

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.

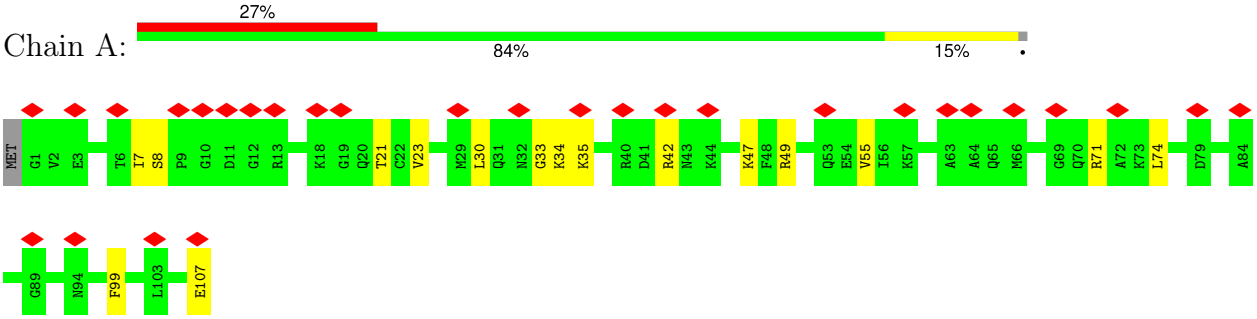
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



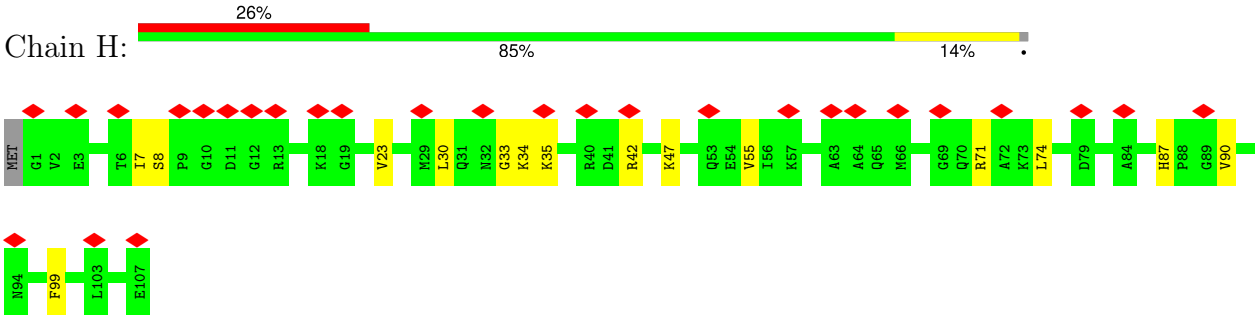
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



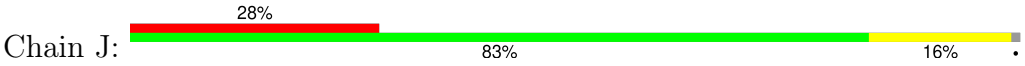
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

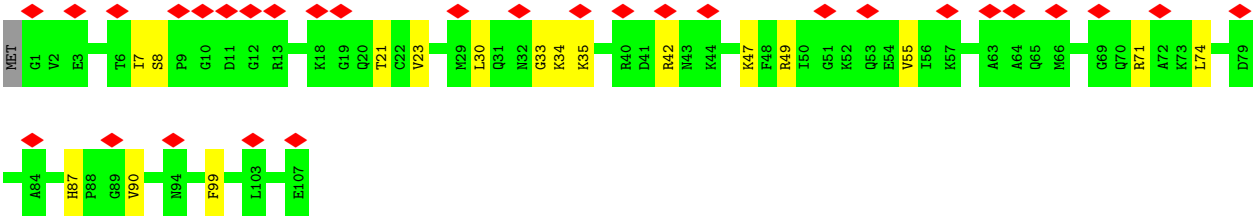
Chain H:



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

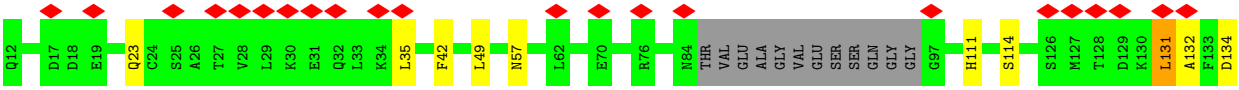
Chain J:

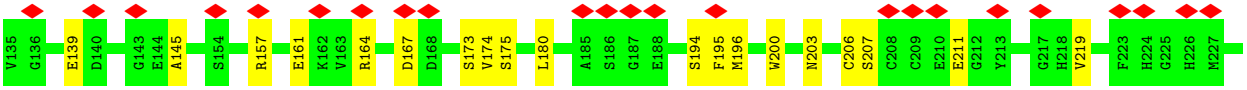


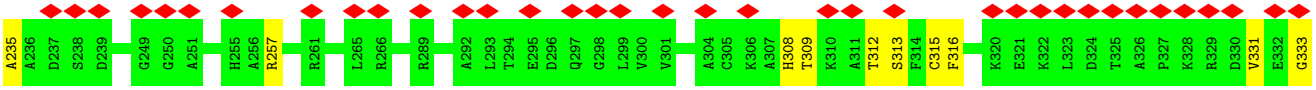


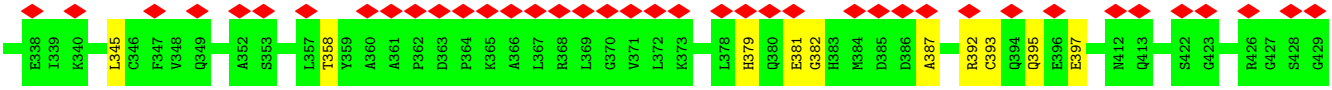
• Molecule 2: Ryanodine receptor 1

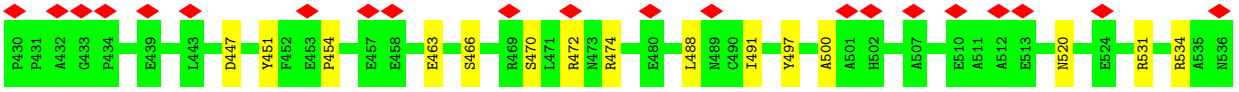
Chain B:

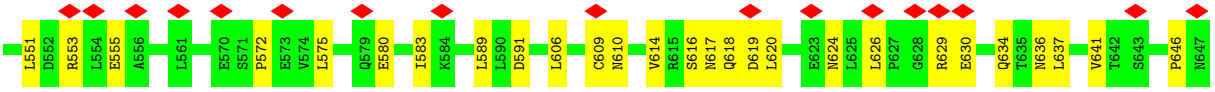


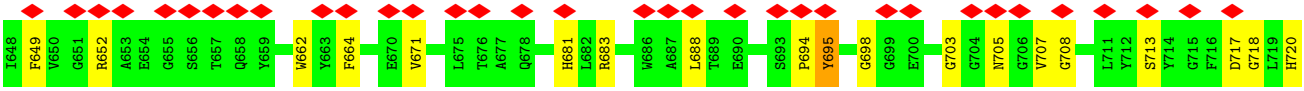


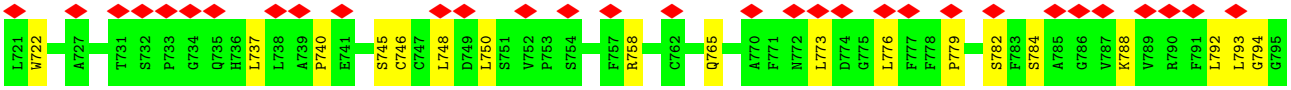


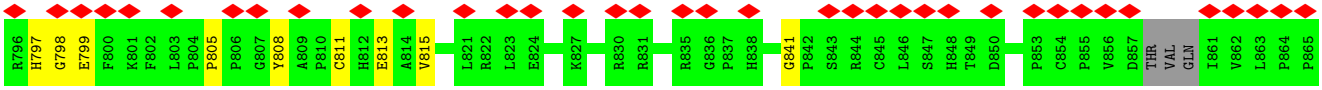


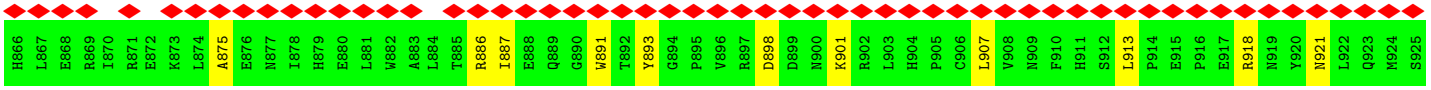


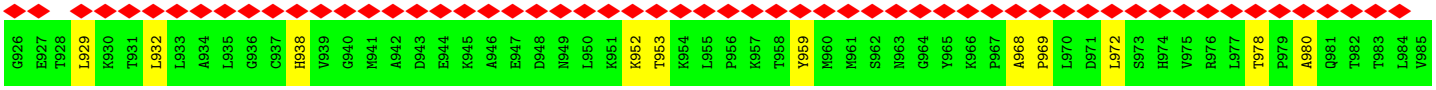


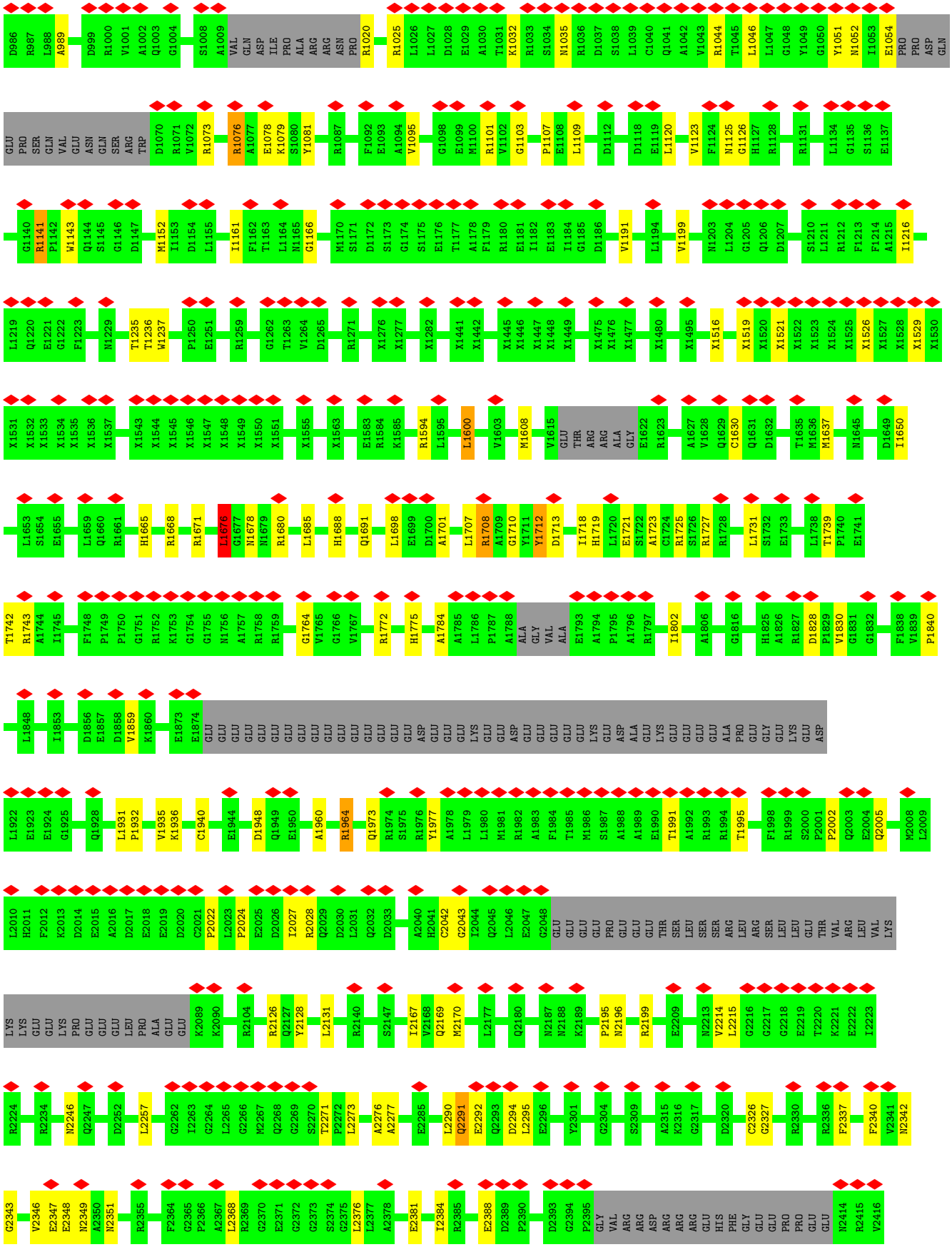


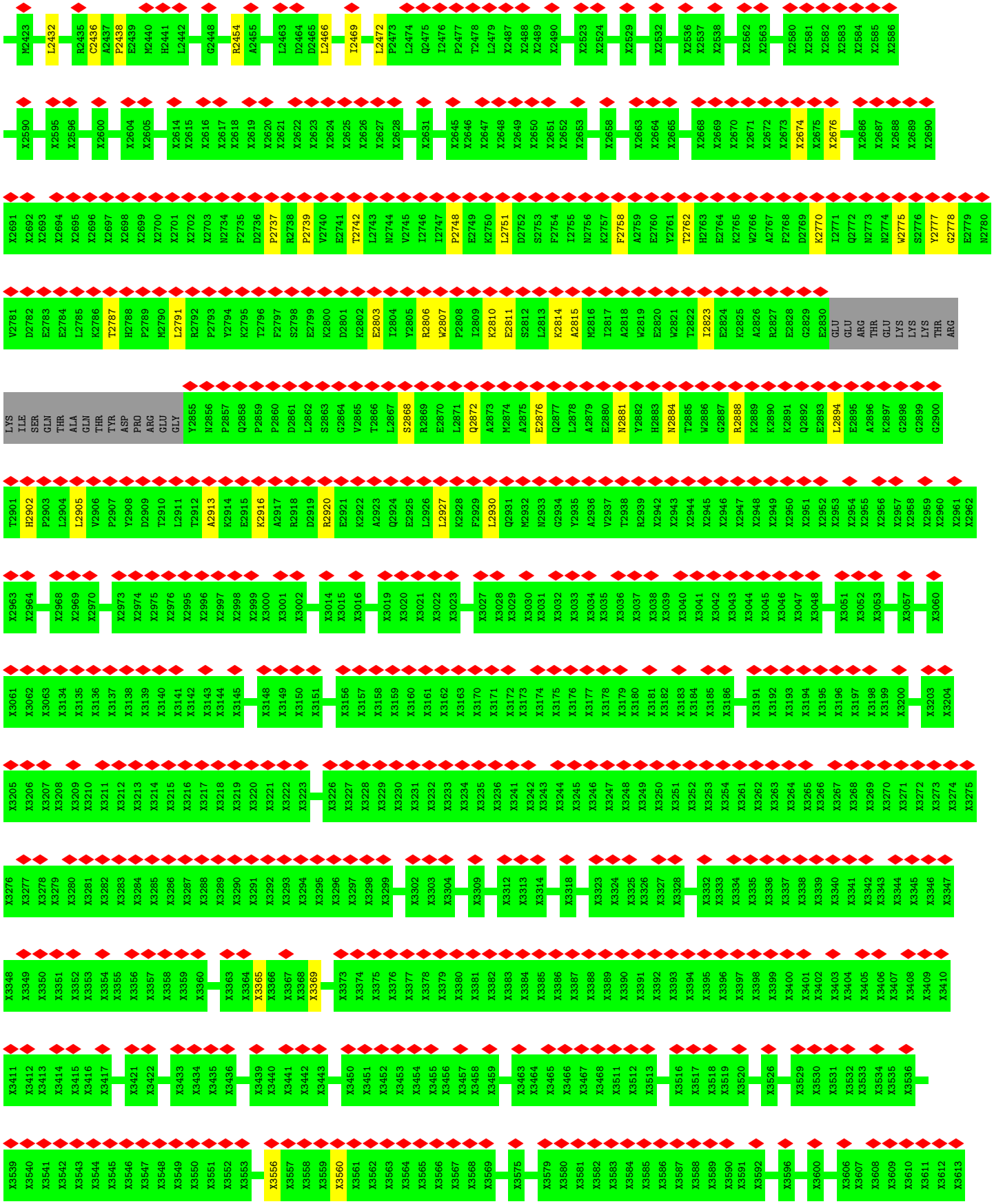








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X2590 X2595 X2596 X2600 X2604 X2605 X2614 X2615 X2616 X2617 X2618 X2619 X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2627 X2628 X2631 X2645 X2646 X2647 X2648 X2649 X2650 X2651 X2652 X2653 X2658 X2663 X2664 X2665 X2668 X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2686 X2687 X2688 X2689 X2690
X2691 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 Y2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780
V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG
LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900
T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2955 X2956 X2957 X2958 X2959 X2960 X2961 X2962
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X3205 X3206 X3207 X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223 X3226 X3227 X3228 X3229 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275
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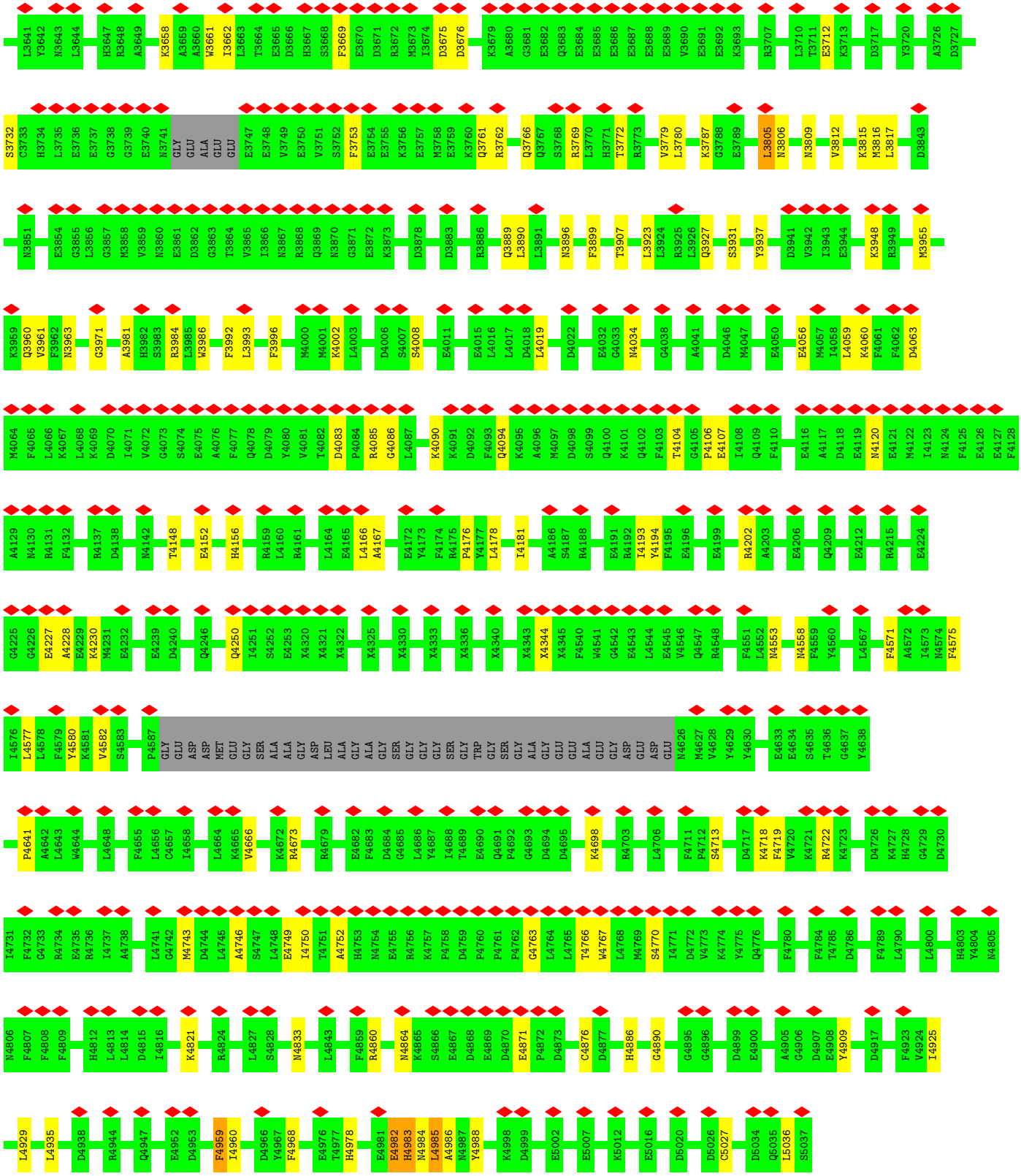
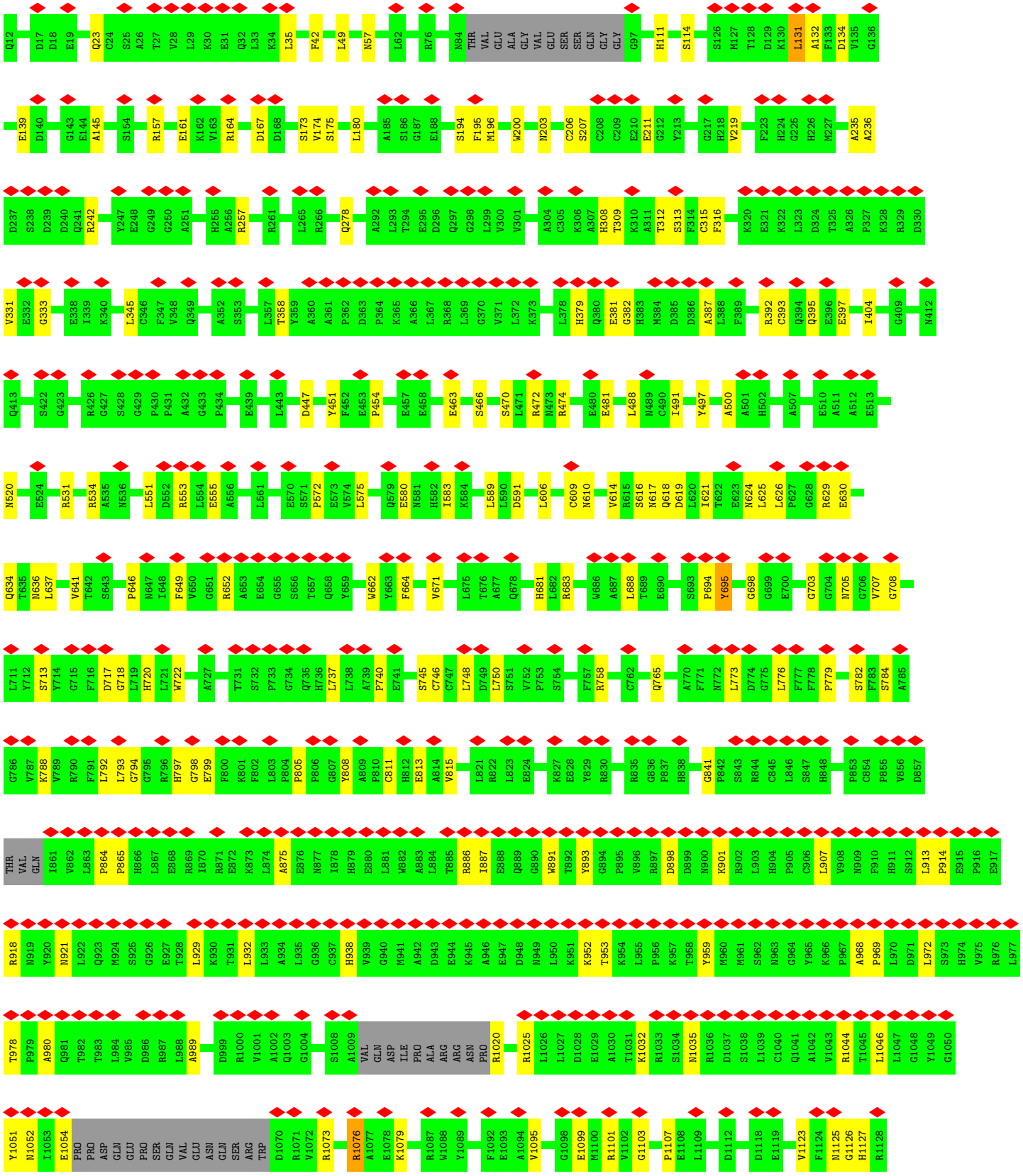
X3411 X3412 X3413 X3414 X3415 X3416 X3417 X3421 X3422 X3433 X3434 X3435 X3436 X3439 X3440 X3441 X3442 X3443 X3450 X3451 X3452 X3453 X3454 X3455 X3456 X3457 X3458 X3459 X3463 X3464 X3465 X3466 X3467 X3468 X3511 X3512 X3513 X3516 X3517 X3518 X3519 X3520 X3526 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3536
X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3575 X3579 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3592 X3596 X3600 X3606 X3607 X3608 X3609 X3610 X3611 X3612 X3613



- Molecule 2: Ryanodine receptor 1

Chain E: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E139 D140 G143 E144 A145 S154 R157 E161 K162 V163 R164 D167 D168 S173 V174 S175 L180 A185 S186 G187 E188 S194 F195 M196 W200 N203 C206 S207 C208 C209 E210 E211 G212 Y213 G217 H218 V219 F223 H224 G225 H226 M227 A235 A236
D237 S238 D239 D240 Q241 R242 Y247 E248 G249 G250 A251 H255 A256 R257 R261 L265 R266 Q278 A292 L293 T294 E295 D296 Q297 G298 L299 V300 V301 A304 C305 K306 A307 H308 T309 K310 A311 T312 S313 F314 C315 F316 K320 E321 K322 L323 D324 T325 A326 P327 K328 R329 D330
V331 E332 G333 E338 I339 K340 L345 C346 F347 V348 Q349 A352 S353 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 K373 L378 H379 Q380 E381 G382 H383 M384 D385 D386 A387 L388 F389 R392 C393 Q394 Q395 E396 E397 I404 G409 N412
Q413 S422 G423 R426 G427 S428 G429 P430 P431 A432 G433 P434 E439 L443 D447 Y451 F452 E453 P454 E457 E458 E463 S466 S470 L471 R472 N473 R474 E480 E481 L488 N489 C490 I491 Y497 A500 A501 H502 A507 E510 A511 A512 E513
N520 E524 R531 R534 A535 N536 L551 D552 R553 L554 E555 A556 L561 E570 S571 P572 E573 V574 L575 Q579 E580 N581 H582 I583 K584 L589 L590 D591 L606 C609 N610 V614 R615 S616 N617 Q618 D619 L620 I621 T622 E623 N624 L625 L626 P627 G628 R629 E630
Q634 T635 N636 L637 V641 T642 S643 P646 N647 I648 F649 V650 G651 R652 A653 E654 G655 S656 T657 Q658 Y659 W662 Y663 F664 V671 L675 T676 A677 Q678 H681 L682 R683 W686 A687 L688 T689 E690 S693 P694 Y695 G698 G699 E700 G703 G704 N705 G706 V707 G708
L711 Y712 S713 Y714 G715 F716 D717 G718 L719 H720 L721 W722 A727 T731 S732 P733 G734 Q735 H736 L737 L738 A739 P740 E741 S745 C746 C747 L748 D749 L750 S751 V752 P753 S754 F757 R758 C762 Q765 A770 F771 N772 L773 D774 G775 L776 F777 F778 P779 S782 F783 S784 A785
G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 H797 G798 E799 F800 K801 F802 L803 P804 P805 P806 G807 Y808 A809 P810 C811 H812 E813 A814 V815 L821 R822 L823 E824 K827 E828 Y829 R830 R835 G836 P837 H838 G841 P842 S843 R844 C845 L846 S847 H848 P853 C854 P855 V856 D857
THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917
R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977
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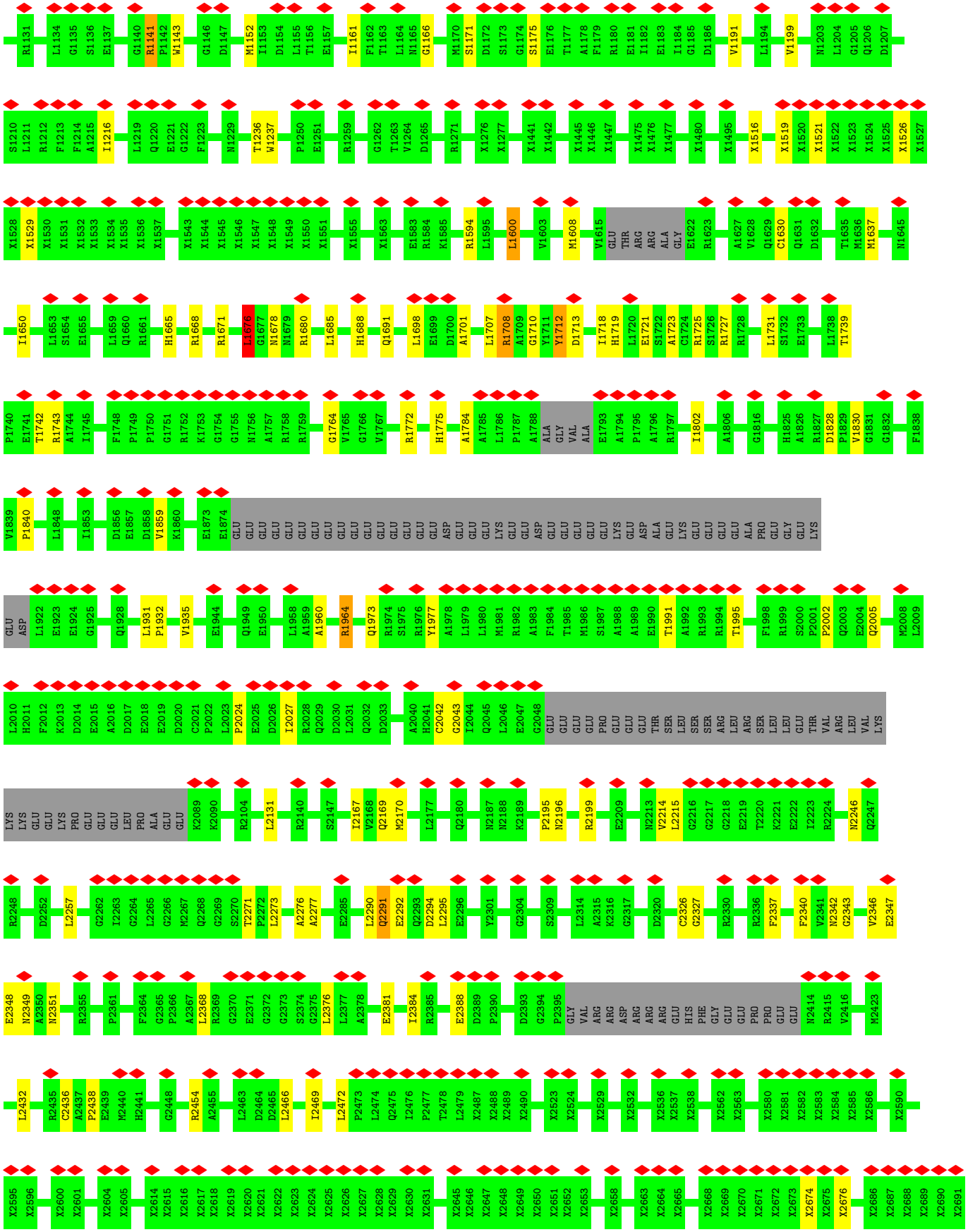

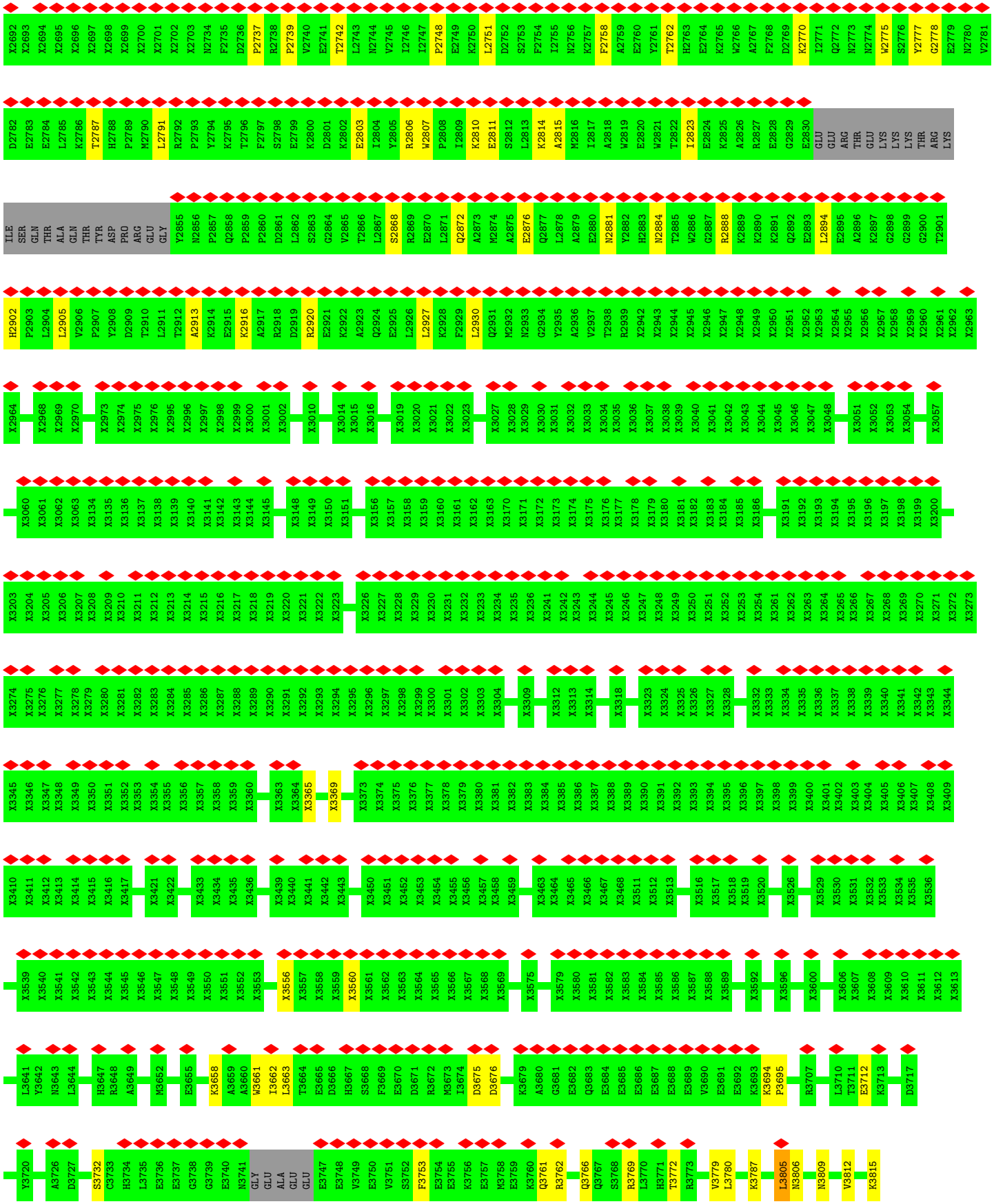
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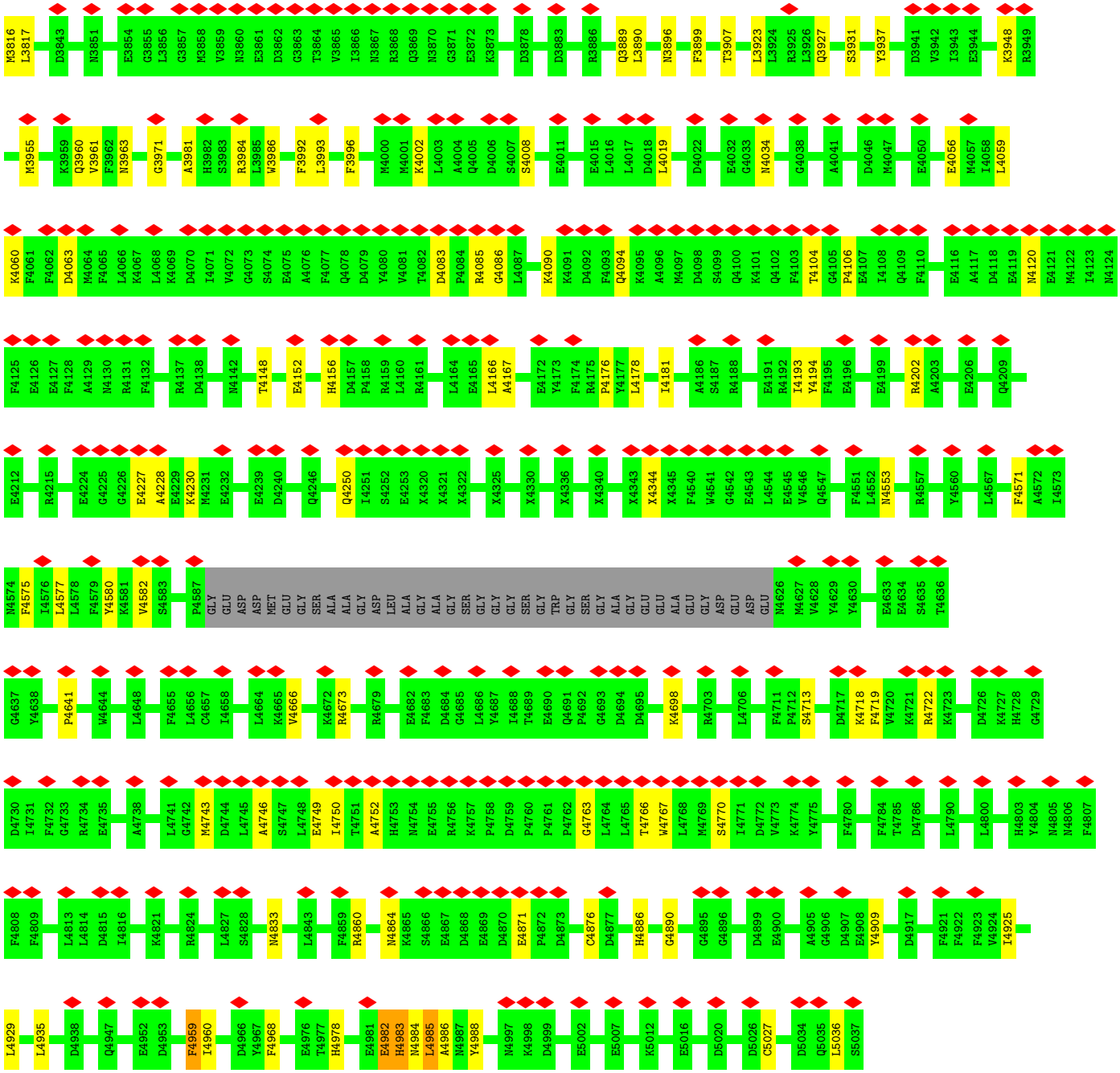
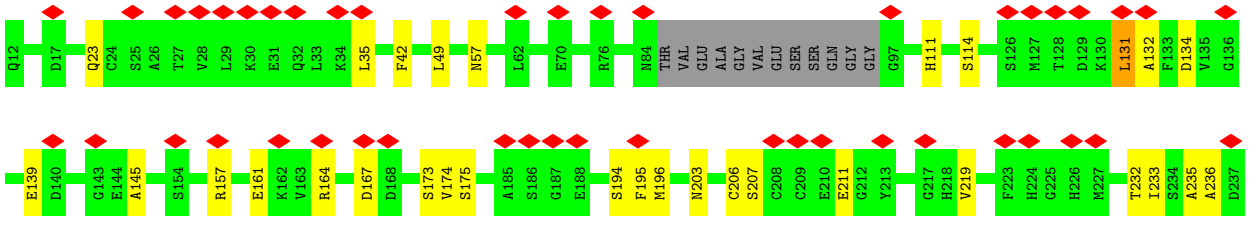
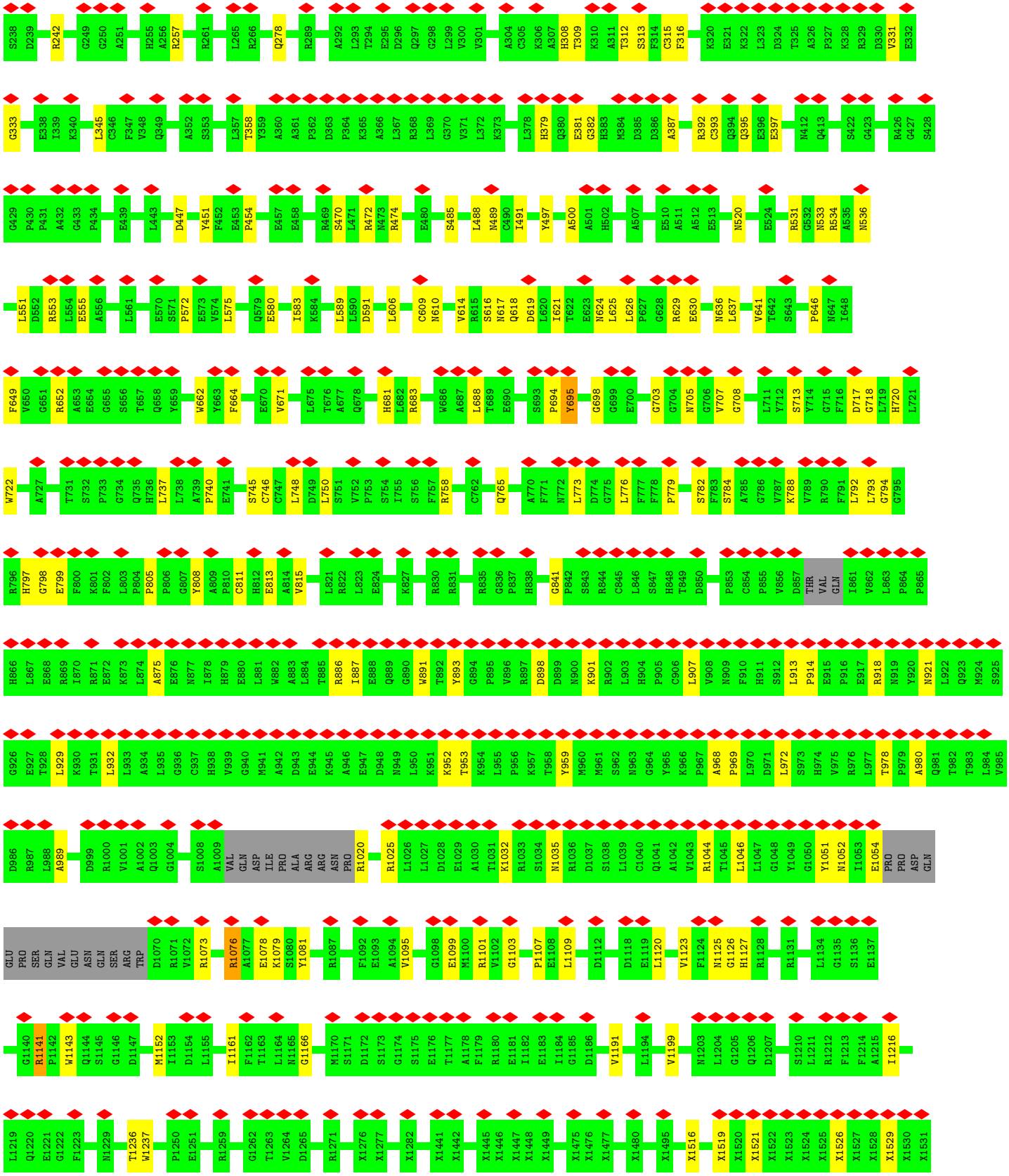


• Molecule 2: Ryanodine receptor 1

Chain I:

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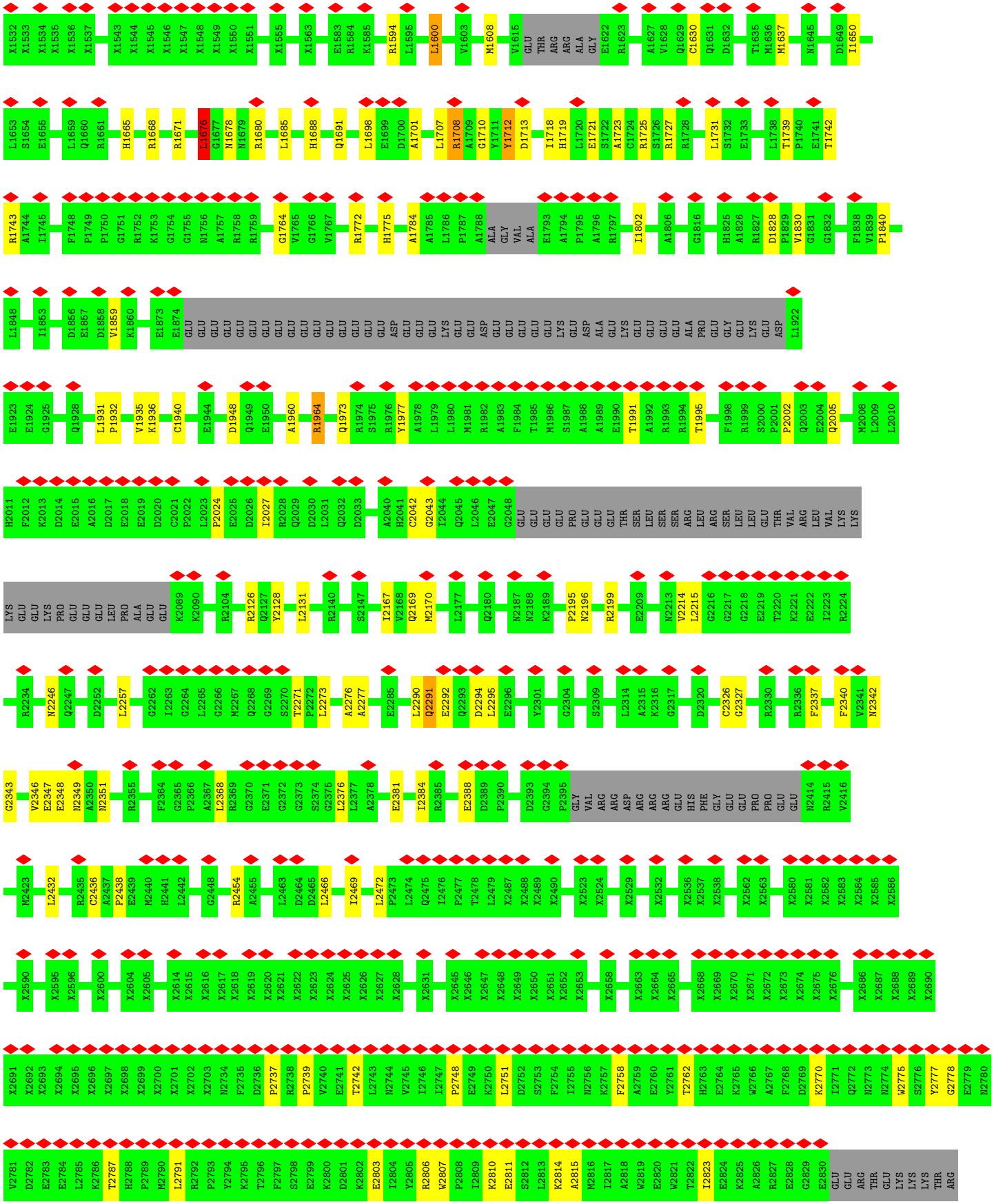

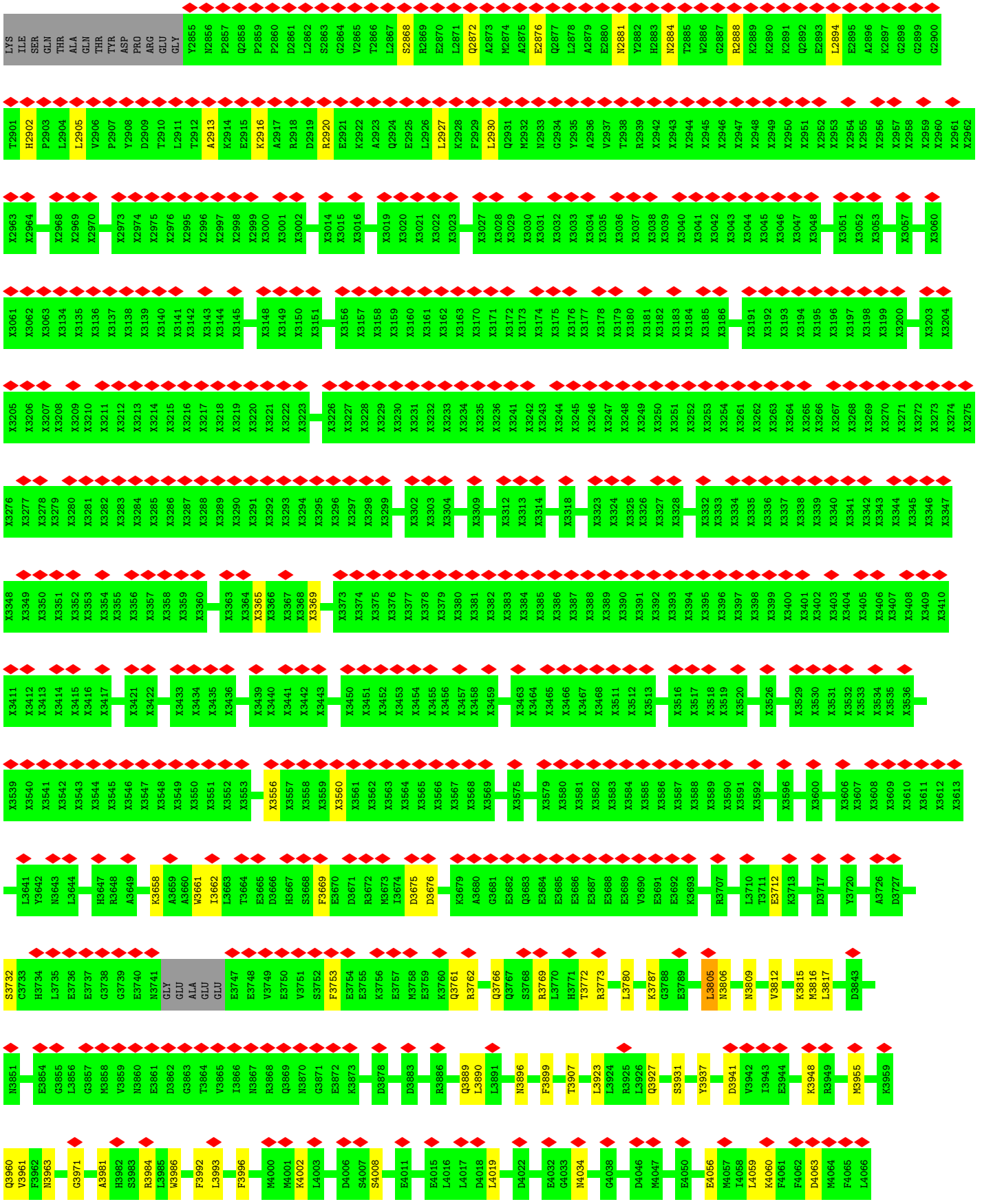
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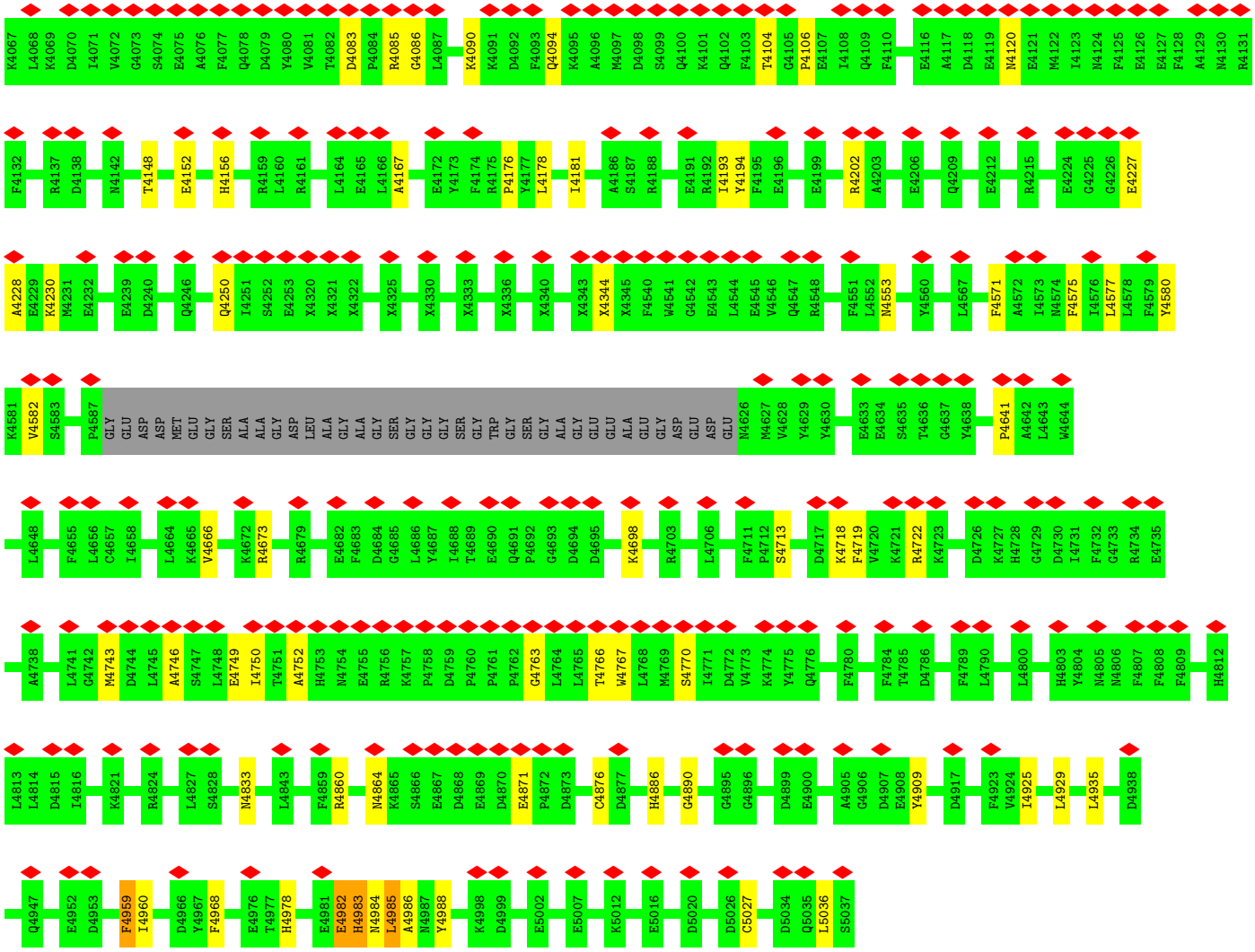
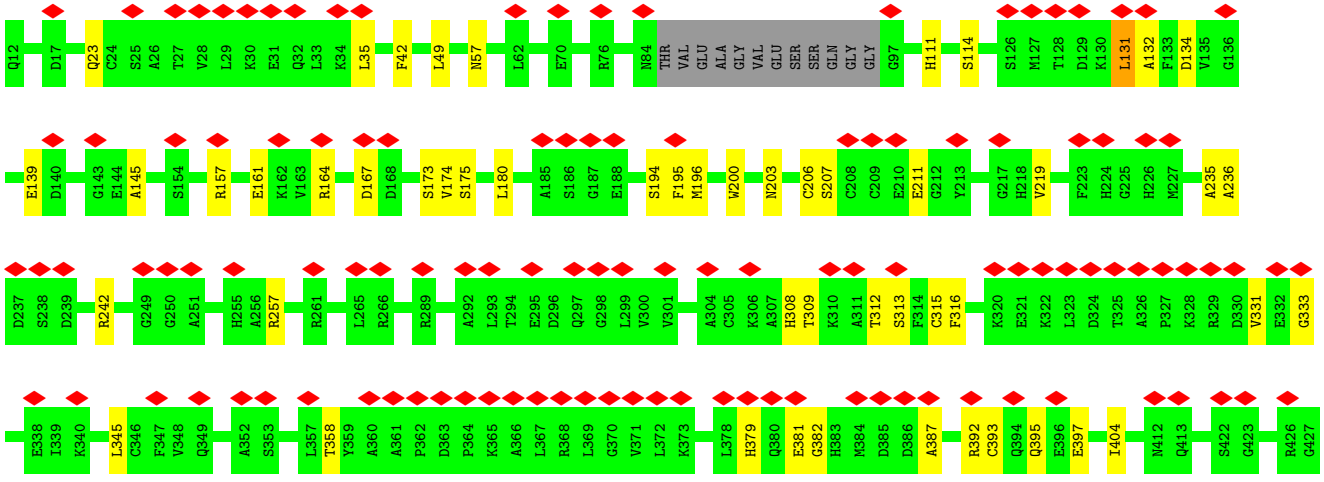
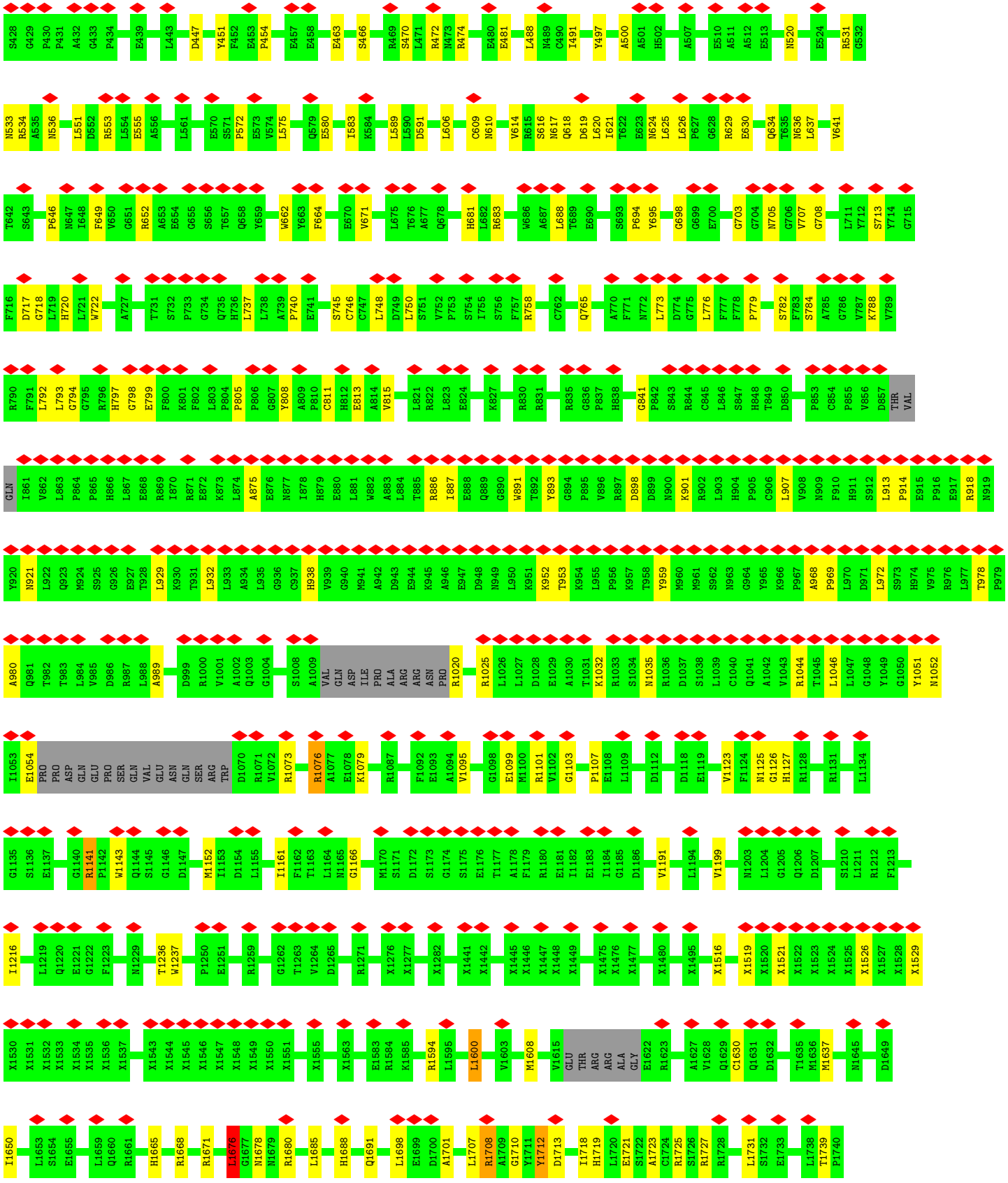


• Molecule 2: Ryanodine receptor 1

Chain G:

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A980 Q981 T982 T983 L984 V985 D986 R987 L988 A989 D999 R1000 V1001 A1002 Q1003 G1004 S1008 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 R1025 L1026 L1027 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052
I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 R1076 A1077 E1078 K1079 R1087 F1092 E1093 A1094 V1095 G1098 E1099 M1100 R1101 V1102 G1103 P1107 E1108 L1109 D1112 D1118 E1119 V1123 F1124 N1125 G1126 H1127 R1128 R1131 L1134
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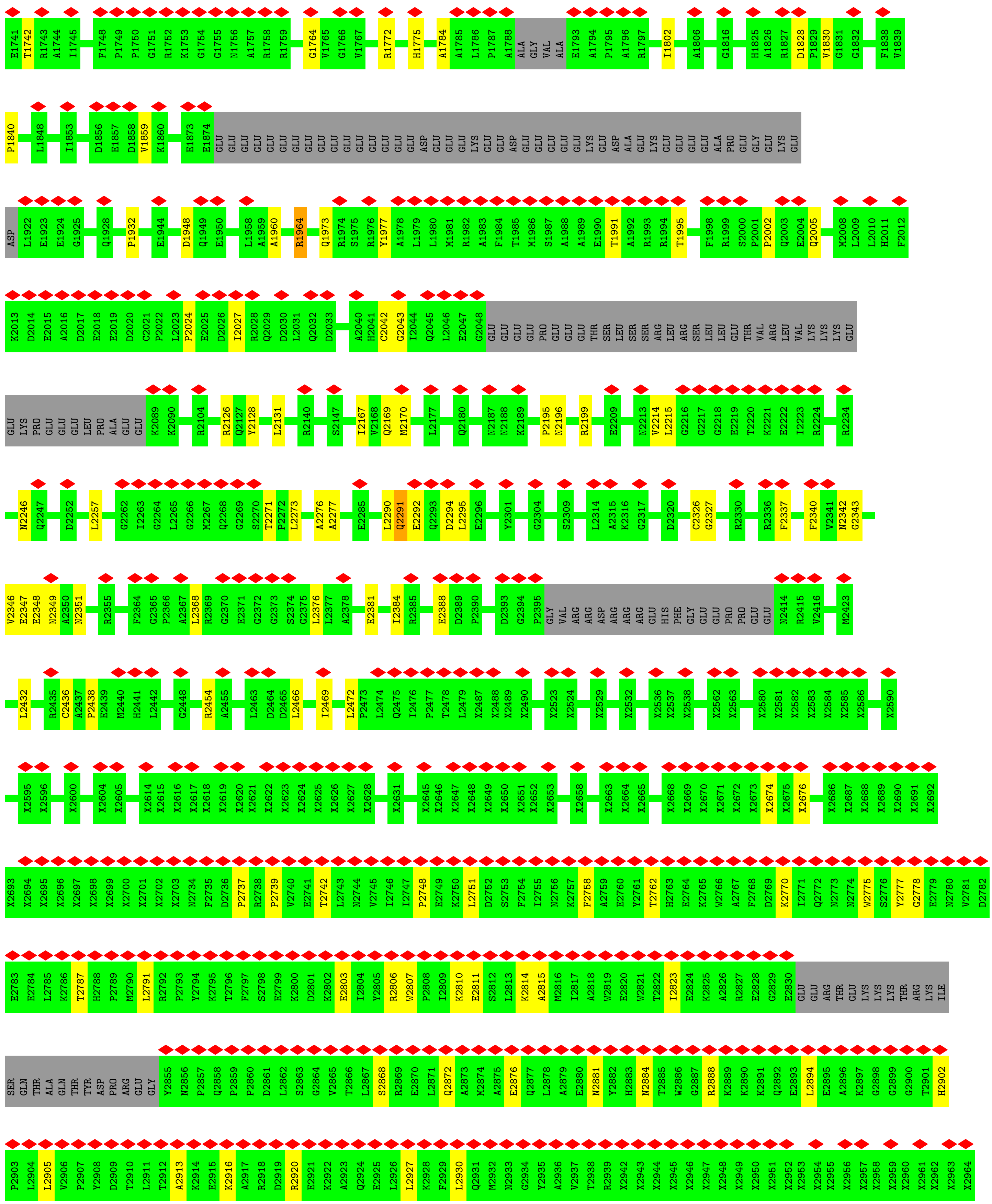
I1650 L1653 S1654 E1655 L1659 Q1660 R1661 H1665 R1668 R1671 L1676 G1677 N1678 M1679 R1680 L1685 H1688 Q1691 L1698 E1699 D1700 A1701 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 S1722 A1723 C1724 R1725 S1726 R1727 R1728 L1731 S1732 E1733 L1738 T1739 P1740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P1840 L1848 I1853 D1856 E1857 D1858 V1859 K1860 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU
ASP L1922 E1923 E1924 G1925 Q1928 P1932 E1944 D1948 Q1949 E1950 L1958 A1959 A1960 R1964 Q1973 R1974 S1975 R1976 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 M2008 L2009 L2010 H2011 F2012
K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 P2022 L2023 P2024 E2025 D2026 I2027 R2028 Q2029 D2030 L2031 Q2032 D2033 A2040 H2041 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU
GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 K2090 R2104 R2126 Q2127 Y2128 L2131 R2140 S2147 I2167 V2168 Q2169 M2170 L2177 Q2180 N2187 N2188 K2189 P2195 N2196 R2199 E2209 N2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 R2234
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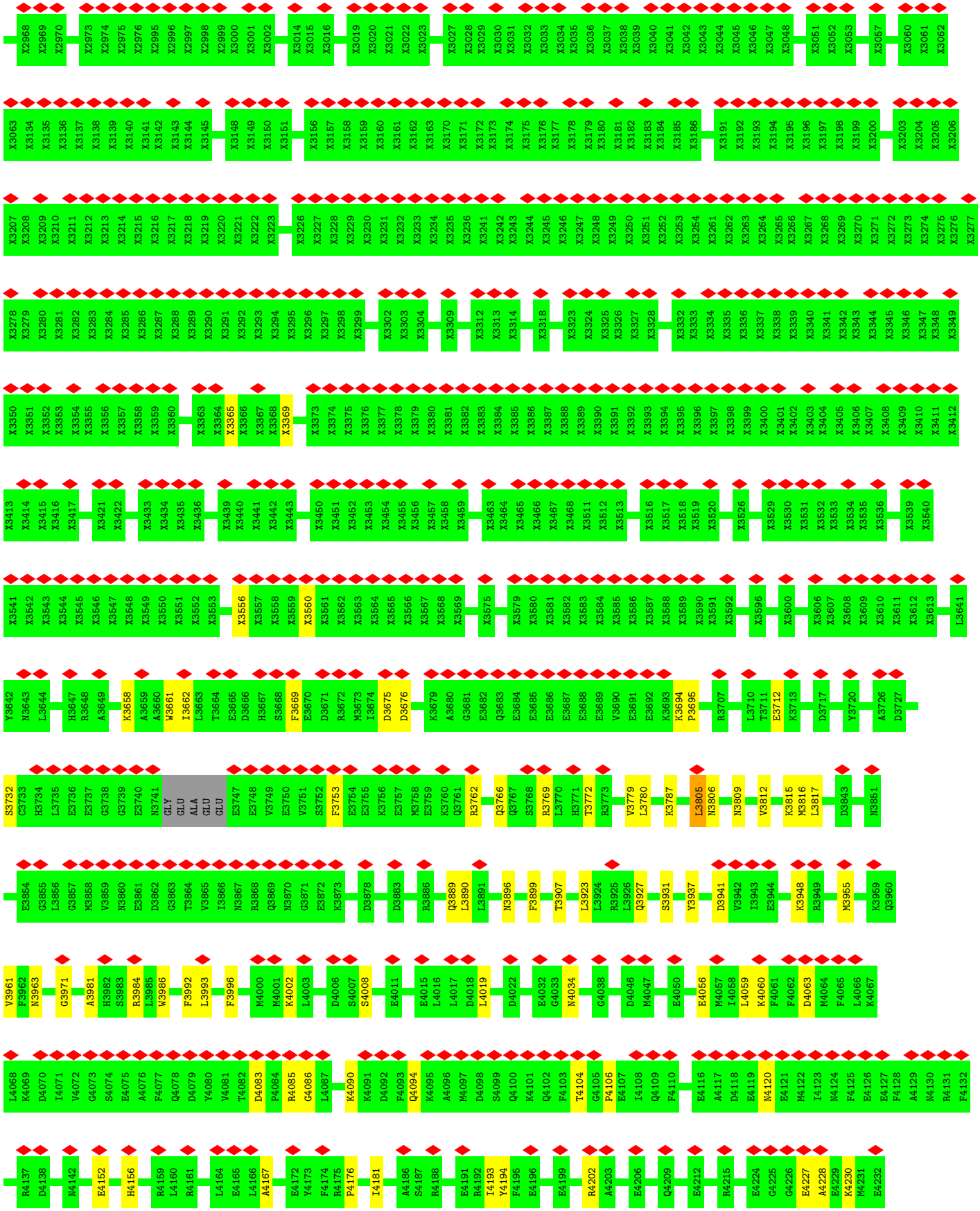
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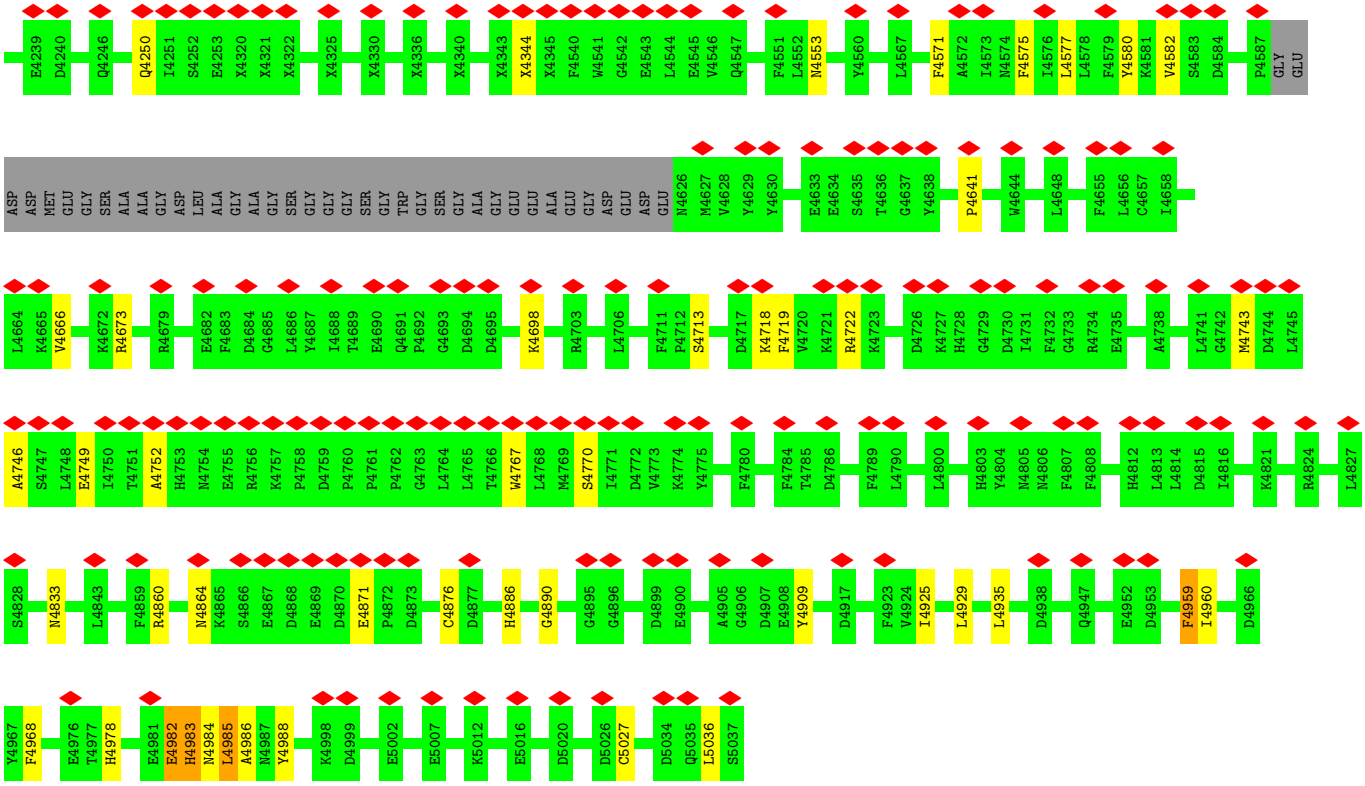
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Y4967 F4968 E4976 T4977 H4978 E4981 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 K4998 D4999 E5002 E5007 K5012 E5016 D5020 D5026 C5027 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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	0.31	0/834	0.51	0/1123
1	F	0.31	0/834	0.51	0/1123
1	H	0.31	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.55	6/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.55	24/142628 (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	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	695	TYR	C-N	5.28	1.44	1.34
2	I	695	TYR	C-N	5.28	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	695	TYR	C-N	5.28	1.44	1.34
2	E	695	TYR	C-N	5.26	1.44	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	E	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	G	131	LEU	CA-CB-CG	8.22	134.20	115.30
2	I	131	LEU	CA-CB-CG	8.21	134.18	115.30
2	I	1600	LEU	CA-CB-CG	6.73	130.78	115.30
2	B	1600	LEU	CA-CB-CG	6.71	130.75	115.30
2	E	1600	LEU	CA-CB-CG	6.71	130.75	115.30
2	G	1600	LEU	CA-CB-CG	6.70	130.71	115.30
2	G	1676	LEU	CA-CB-CG	6.39	130.01	115.30
2	B	1676	LEU	CA-CB-CG	6.39	130.00	115.30
2	I	1676	LEU	CA-CB-CG	6.39	130.00	115.30
2	E	1676	LEU	CA-CB-CG	6.38	129.98	115.30
2	I	2290	LEU	CA-CB-CG	5.65	128.30	115.30
2	B	2290	LEU	CA-CB-CG	5.65	128.30	115.30
2	E	2290	LEU	CA-CB-CG	5.65	128.30	115.30
2	G	2290	LEU	CA-CB-CG	5.62	128.23	115.30
2	B	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	E	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	I	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	G	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	B	4985	LEU	CA-CB-CG	5.37	127.66	115.30
2	E	4985	LEU	CA-CB-CG	5.37	127.66	115.30
2	I	4985	LEU	CA-CB-CG	5.37	127.66	115.30
2	G	4985	LEU	CA-CB-CG	5.37	127.66	115.30

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	624	ASN	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	624	ASN	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	624	ASN	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	624	ASN	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	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	818	0	824	11	0
1	F	818	0	824	12	0
1	H	818	0	824	9	0
1	J	818	0	824	11	0
2	B	29499	0	24757	259	0
2	E	29499	0	24757	259	0
2	G	29499	0	24757	251	0
2	I	29499	0	24757	256	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121272	0	102324	1040	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 5.

All (1040) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.51	0.76
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.51	0.76
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.51	0.75
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.51	0.74
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.57	0.70
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.57	0.69
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.57	0.69
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.57	0.68
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.76	0.67
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.76	0.66
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.31	0.66
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.31	0.66
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.31	0.65
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.76	0.65
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.31	0.65
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.76	0.65
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.80	0.63
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.82	0.62
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.82	0.62
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.82	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.82	0.62
1:J:35:LYS:HD3	2:I:636:ASN:HD21	1.65	0.62
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.73	0.62
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.73	0.62
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.73	0.61
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.82	0.61
1:F:35:LYS:HD3	2:E:636:ASN:HD21	1.65	0.61
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.82	0.61
1:H:35:LYS:HD3	2:G:636:ASN:HD21	1.65	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.82	0.61
2:I:379:HIS:HD2	2:I:382:GLY:H	1.49	0.61
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.82	0.61
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.82	0.61
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.82	0.61
1:A:35:LYS:HD3	2:B:636:ASN:HD21	1.65	0.61
1:J:34:LYS:HD3	2:I:629:ARG:HD2	1.83	0.60
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.73	0.60
1:A:34:LYS:HD3	2:B:629:ARG:HD2	1.82	0.60
2:B:379:HIS:HD2	2:B:382:GLY:H	1.49	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:E:2347:GLU:O	2:E:2351:ASN:N	2.32	0.60
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:HIS:HD2	2:E:382:GLY:H	1.49	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.84	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.67	0.60
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.82	0.60
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.82	0.59
2:B:2347:GLU:O	2:B:2351:ASN:N	2.32	0.59
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.84	0.59
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.84	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.83	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.59
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.68	0.59
2:I:331:VAL:HG12	2:I:333:GLY:H	1.67	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.68	0.59
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.68	0.59
2:E:626:LEU:HD23	2:E:630:GLU:H	1.68	0.59
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.36	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.68	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.58
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.84	0.58
2:E:331:VAL:HG12	2:E:333:GLY:H	1.67	0.58
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.84	0.58
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.84	0.58
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.84	0.58
2:G:2347:GLU:O	2:G:2351:ASN:N	2.32	0.58
2:I:626:LEU:HD23	2:I:630:GLU:H	1.68	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.67	0.58
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.84	0.58
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.86	0.58
2:G:379:HIS:HD2	2:G:382:GLY:H	1.49	0.58
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.36	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.58
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.86	0.58
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.85	0.58
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.36	0.57
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.86	0.57
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.39	0.57
2:G:626:LEU:HD23	2:G:630:GLU:H	1.68	0.57
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.40	0.57
2:B:626:LEU:HD23	2:B:630:GLU:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.57
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.86	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.78	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.78	0.57
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.40	0.57
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.86	0.57
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.38	0.57
2:B:652:ARG:HD3	2:B:773:LEU:HD13	1.87	0.57
2:B:4983:HIS:N	2:B:4983:HIS:CD2	2.73	0.57
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.86	0.57
2:I:315:CYS:SG	2:I:316:PHE:N	2.78	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.57
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.57
2:G:315:CYS:SG	2:G:316:PHE:N	2.78	0.57
2:G:4983:HIS:N	2:G:4983:HIS:CD2	2.73	0.57
2:I:652:ARG:HD3	2:I:773:LEU:HD13	1.87	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.38	0.57
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.57
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.87	0.56
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.87	0.56
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.87	0.56
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.38	0.56
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.36	0.56
2:E:652:ARG:HD3	2:E:773:LEU:HD13	1.87	0.56
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.39	0.56
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.38	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.86	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.86	0.56
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.87	0.56
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.56
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.88	0.56
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.56
2:E:1076:ARG:HB3	2:E:1191:VAL:HG23	1.89	0.55
2:E:4983:HIS:N	2:E:4983:HIS:CD2	2.73	0.55
2:I:1671:ARG:HH21	2:I:1713:ASP:HB3	1.71	0.55
2:G:652:ARG:HD3	2:G:773:LEU:HD13	1.87	0.55
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.88	0.55
2:E:3993:LEU:HA	2:E:3996:PHE:HB2	1.88	0.55
2:I:2347:GLU:O	2:I:2351:ASN:N	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.87	0.55
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.40	0.55
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.87	0.55
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.55
2:G:1076:ARG:HB3	2:G:1191:VAL:HG23	1.89	0.55
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.89	0.55
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.89	0.55
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.89	0.55
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.89	0.55
2:I:1076:ARG:HB3	2:I:1191:VAL:HG23	1.88	0.55
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.89	0.55
2:I:3993:LEU:HA	2:I:3996:PHE:HB2	1.89	0.55
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.55
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.75	0.55
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.88	0.55
2:G:3993:LEU:HA	2:G:3996:PHE:HB2	1.89	0.55
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.40	0.55
2:B:1076:ARG:HB3	2:B:1191:VAL:HG23	1.88	0.55
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.75	0.55
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.40	0.55
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.40	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.89	0.55
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.55
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.40	0.55
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.55
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.88	0.55
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.40	0.55
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.89	0.54
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.40	0.54
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.89	0.54
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.72	0.54
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.88	0.54
2:E:1671:ARG:HH21	2:E:1713:ASP:HB3	1.71	0.54
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.88	0.54
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.75	0.54
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.88	0.54
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.40	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.40	0.54
2:G:1671:ARG:HH21	2:G:1713:ASP:HB3	1.71	0.54
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3993:LEU:HA	2:B:3996:PHE:HB2	1.88	0.54
2:E:161:GLU:OE2	2:G:3984:ARG:NH2	2.41	0.54
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.40	0.54
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.88	0.54
2:B:1671:ARG:HH21	2:B:1713:ASP:HB3	1.71	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.41	0.54
2:E:3732:SER:O	2:E:3766:GLN:NE2	2.41	0.54
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.41	0.54
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.72	0.54
2:G:4960:ILE:HG21	2:G:4988:TYR:HE2	1.73	0.54
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.89	0.54
2:G:3732:SER:O	2:G:3766:GLN:NE2	2.41	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.80	0.53
2:I:3732:SER:O	2:I:3766:GLN:NE2	2.41	0.53
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.41	0.53
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.40	0.53
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.40	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.91	0.53
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.72	0.53
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.72	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.91	0.53
2:B:1052:ASN:ND2	2:B:1054:GLU:OE2	2.42	0.53
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.90	0.53
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.41	0.53
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.91	0.53
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.91	0.53
2:B:3732:SER:O	2:B:3766:GLN:NE2	2.41	0.53
2:B:4056:GLU:O	2:B:4060:LYS:N	2.36	0.53
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.53
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.42	0.53
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.89	0.53
2:B:161:GLU:OE2	2:E:3984:ARG:NH2	2.42	0.53
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.53
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.90	0.53
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.91	0.53
2:I:4960:ILE:HG21	2:I:4988:TYR:HE2	1.73	0.53
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.74	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.91	0.53
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.42	0.53
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.91	0.52
2:E:4960:ILE:HG21	2:E:4988:TYR:HE2	1.73	0.52
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.42	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.52
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:E:1052:ASN:ND2	2:E:1054:GLU:OE2	2.42	0.52
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.91	0.52
2:I:1052:ASN:ND2	2:I:1054:GLU:OE2	2.42	0.52
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.90	0.52
2:G:1052:ASN:ND2	2:G:1054:GLU:OE2	2.42	0.52
2:B:173:SER:OG	2:B:174:VAL:N	2.43	0.52
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.52
2:I:4056:GLU:O	2:I:4060:LYS:N	2.36	0.52
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.42	0.52
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.74	0.52
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.42	0.52
2:G:4090:LYS:O	2:G:4094:GLN:N	2.42	0.52
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.90	0.52
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.92	0.52
2:B:4960:ILE:HG21	2:B:4988:TYR:HE2	1.73	0.52
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:I:173:SER:OG	2:I:174:VAL:N	2.43	0.52
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.43	0.52
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.80	0.52
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.92	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:G:4056:GLU:O	2:G:4060:LYS:N	2.36	0.52
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.41	0.51
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.43	0.51
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.51
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.74	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.80	0.51
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.92	0.51
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.41	0.51
2:E:173:SER:OG	2:E:174:VAL:N	2.43	0.51
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.90	0.51
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.43	0.51
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.92	0.51
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3948:LYS:NZ	2:B:4008:SER:O	2.44	0.51
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.43	0.51
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.92	0.51
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.93	0.51
2:B:3984:ARG:NH2	2:I:161:GLU:OE2	2.43	0.51
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.43	0.51
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.92	0.51
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.93	0.51
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.92	0.51
2:B:2195:PRO:HB3	2:B:2246:ASN:HD21	1.76	0.51
2:E:2195:PRO:HB3	2:E:2246:ASN:HD21	1.76	0.51
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.93	0.51
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.93	0.51
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.44	0.51
2:G:173:SER:OG	2:G:174:VAL:N	2.43	0.51
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.50
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.43	0.50
2:I:3984:ARG:NH2	2:G:161:GLU:OE2	2.43	0.50
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.92	0.50
2:E:3948:LYS:NZ	2:E:4008:SER:O	2.44	0.50
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.94	0.50
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.92	0.50
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.94	0.50
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.41	0.50
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.50
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.50
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.42	0.50
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.93	0.50
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.94	0.50
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.94	0.50
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.77	0.50
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.77	0.50
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.94	0.50
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.94	0.50
2:E:4059:LEU:O	2:E:4063:ASP:N	2.45	0.50
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.50
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.94	0.50
2:I:2195:PRO:HB3	2:I:2246:ASN:HD21	1.76	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.50
2:E:4056:GLU:O	2:E:4060:LYS:N	2.36	0.49
2:I:913:LEU:O	2:I:918:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.93	0.49
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.49
2:B:913:LEU:O	2:B:918:ARG:NH2	2.45	0.49
2:E:609:CYS:SG	2:E:610:ASN:N	2.85	0.49
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.94	0.49
2:I:3948:LYS:NZ	2:I:4008:SER:O	2.44	0.49
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.49
2:G:609:CYS:SG	2:G:610:ASN:N	2.85	0.49
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.76	0.49
2:G:2195:PRO:HB3	2:G:2246:ASN:HD21	1.76	0.49
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.94	0.49
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.43	0.49
2:I:4059:LEU:O	2:I:4063:ASP:N	2.45	0.49
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.94	0.49
2:B:451:TYR:O	2:B:474:ARG:NH1	2.43	0.49
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.95	0.49
2:B:3753:PHE:HE2	2:B:4718:LYS:HB2	1.77	0.49
2:B:4059:LEU:O	2:B:4063:ASP:N	2.45	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.49
2:E:1991:THR:O	2:E:1995:THR:OG1	2.30	0.49
2:E:4090:LYS:O	2:E:4094:GLN:N	2.42	0.49
2:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.77	0.49
2:G:1991:THR:O	2:G:1995:THR:OG1	2.30	0.49
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.94	0.49
2:E:913:LEU:O	2:E:918:ARG:NH2	2.45	0.49
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.77	0.49
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.49
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.49
2:I:609:CYS:SG	2:I:610:ASN:N	2.85	0.49
2:I:3992:PHE:O	2:I:3996:PHE:N	2.43	0.49
2:G:913:LEU:O	2:G:918:ARG:NH2	2.45	0.49
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.94	0.49
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.93	0.49
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.49
2:E:4978:HIS:HE1	2:E:5027:CYS:SG	2.36	0.49
2:I:132:ALA:HA	2:I:194:SER:HB2	1.95	0.49
2:G:132:ALA:HA	2:G:194:SER:HB2	1.95	0.49
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.93	0.49
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.94	0.49
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.76	0.49
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2868:SER:O	2:E:2872:GLN:N	2.39	0.49
2:I:683:ARG:NH1	2:I:707:VAL:O	2.44	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.49
2:I:4090:LYS:O	2:I:4094:GLN:N	2.42	0.49
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.49
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.49
2:I:3753:PHE:HE2	2:I:4718:LYS:HB2	1.77	0.49
2:G:4059:LEU:O	2:G:4063:ASP:N	2.45	0.49
2:G:4978:HIS:HE1	2:G:5027:CYS:SG	2.36	0.49
2:B:1991:THR:O	2:B:1995:THR:OG1	2.30	0.49
2:B:4978:HIS:HE1	2:B:5027:CYS:SG	2.36	0.49
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.94	0.49
2:E:3753:PHE:HE2	2:E:4718:LYS:HB2	1.77	0.49
2:I:1991:THR:O	2:I:1995:THR:OG1	2.30	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.95	0.49
2:G:3948:LYS:NZ	2:G:4008:SER:O	2.44	0.49
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.94	0.48
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.94	0.48
2:I:4978:HIS:HE1	2:I:5027:CYS:SG	2.36	0.48
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.44	0.48
2:G:683:ARG:NH1	2:G:707:VAL:O	2.44	0.48
2:B:609:CYS:SG	2:B:610:ASN:N	2.85	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.48
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:G:3753:PHE:HE2	2:G:4718:LYS:HB2	1.78	0.48
2:E:132:ALA:HA	2:E:194:SER:HB2	1.95	0.48
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.94	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.95	0.48
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.94	0.48
2:B:132:ALA:HA	2:B:194:SER:HB2	1.95	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.79	0.48
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.47	0.48
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.79	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.48
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.29	0.48
2:E:4571:PHE:O	2:E:4575:PHE:N	2.46	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.46	0.48
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4571:PHE:O	2:B:4575:PHE:N	2.46	0.48
2:B:683:ARG:NH1	2:B:707:VAL:O	2.44	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.42	0.48
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.47	0.48
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.79	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:I:395:GLN:HG3	2:I:397:GLU:H	1.79	0.48
2:I:1973:GLN:HE22	2:I:2005:GLN:HE22	1.62	0.48
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.42	0.48
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.41	0.48
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.79	0.48
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.79	0.48
2:B:929:LEU:HD23	2:B:932:LEU:HD12	1.96	0.48
2:B:4090:LYS:O	2:B:4094:GLN:N	2.42	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.47	0.48
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.44	0.48
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.47	0.48
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.96	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.39	0.48
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.79	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.79	0.47
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.44	0.47
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.96	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.47	0.47
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.47	0.47
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.47
2:B:1973:GLN:HE22	2:B:2005:GLN:HE22	1.62	0.47
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.32	0.47
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.47	0.47
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.32	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:1973:GLN:HE22	2:G:2005:GLN:HE22	1.62	0.47
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.79	0.47
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.97	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.46	0.47
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.96	0.47
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.96	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.79	0.47
2:I:929:LEU:HD23	2:I:932:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.47	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.47
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.97	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.47
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.79	0.47
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.96	0.47
2:B:2810:LYS:HB3	2:B:2814:LYS:HE3	1.97	0.47
2:E:1723:ALA:HB1	2:E:1775:HIS:HD2	1.80	0.47
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.79	0.47
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.47
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.97	0.47
2:B:219:VAL:O	2:B:392:ARG:NH1	2.48	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.32	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.79	0.47
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.47	0.47
2:G:219:VAL:O	2:G:392:ARG:NH1	2.48	0.47
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.47
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.32	0.47
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.97	0.47
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.29	0.47
2:E:1973:GLN:HE22	2:E:2005:GLN:HE22	1.62	0.47
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.42	0.47
2:I:219:VAL:O	2:I:392:ARG:NH1	2.48	0.47
2:I:345:LEU:HD22	2:I:387:ALA:HB1	1.97	0.47
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.47
2:E:345:LEU:HD22	2:E:387:ALA:HB1	1.97	0.47
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.88	0.47
2:E:2810:LYS:HB3	2:E:2814:LYS:HE3	1.97	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.88	0.47
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.79	0.47
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.97	0.47
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.73	0.47
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.79	0.47
2:B:345:LEU:HD22	2:B:387:ALA:HB1	1.97	0.46
2:B:1701:ALA:HB1	2:B:1830:VAL:HG22	1.97	0.46
2:B:1723:ALA:HB1	2:B:1775:HIS:HD2	1.80	0.46
2:B:3806:ASN:HA	2:B:3890:LEU:HD13	1.98	0.46
2:I:1701:ALA:HB1	2:I:1830:VAL:HG22	1.97	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.80	0.46
2:G:164:ARG:N	2:G:167:ASP:OD2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:345:LEU:HD22	2:G:387:ALA:HB1	1.97	0.46
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.46
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.49	0.46
2:B:792:LEU:HD22	2:B:799:GLU:H	1.80	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.39	0.46
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.98	0.46
2:E:929:LEU:HD23	2:E:932:LEU:HD12	1.96	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.46
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.79	0.46
2:G:792:LEU:HD22	2:G:799:GLU:H	1.80	0.46
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.96	0.46
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.98	0.46
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.39	0.46
2:E:1701:ALA:HB1	2:E:1830:VAL:HG22	1.97	0.46
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.97	0.46
2:E:219:VAL:O	2:E:392:ARG:NH1	2.48	0.46
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.79	0.46
2:E:463:GLU:O	2:E:466:SER:OG	2.30	0.46
2:E:2913:ALA:HA	2:E:2916:LYS:HB2	1.98	0.46
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.97	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.47	0.46
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.73	0.46
2:G:2913:ALA:HA	2:G:2916:LYS:HB2	1.98	0.46
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.97	0.46
2:I:4982:GLU:HB3	2:I:4983:HIS:CD2	2.51	0.46
2:G:2810:LYS:HB3	2:G:2814:LYS:HE3	1.97	0.46
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	1.98	0.46
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.49	0.46
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.88	0.46
2:B:2913:ALA:HA	2:B:2916:LYS:HB2	1.98	0.46
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.98	0.46
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.28	0.46
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.98	0.46
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	1.97	0.46
2:G:1723:ALA:HB1	2:G:1775:HIS:HD2	1.80	0.46
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	3.04	0.46
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.98	0.46
2:B:1516:UNK:N	2:B:1529:UNK:O	2.49	0.46
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.79	0.46
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.46
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.98	0.46
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.51	0.46
2:I:3927:GLN:O	2:I:3931:SER:N	2.47	0.46
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.98	0.46
2:G:929:LEU:HD23	2:G:932:LEU:HD12	1.96	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.51	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.80	0.46
2:E:683:ARG:NH1	2:E:707:VAL:O	2.44	0.46
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.49	0.46
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.46
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.46
2:G:1516:UNK:N	2:G:1529:UNK:O	2.49	0.46
2:G:1701:ALA:HB1	2:G:1830:VAL:HG22	1.97	0.46
2:G:2758:PHE:O	2:G:2762:THR:N	2.47	0.46
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	3.04	0.46
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.46
2:G:978:THR:HB	2:G:980:ALA:H	1.80	0.46
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.88	0.46
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.79	0.46
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.96	0.46
2:B:195:PHE:HB3	2:B:196:MET:HG2	1.98	0.46
2:B:2381:GLU:HA	2:B:2384:ILE:HD12	1.98	0.46
2:B:3992:PHE:O	2:B:3996:PHE:N	2.43	0.46
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.46
2:E:4344:UNK:N	2:I:4909:TYR:OH	2.49	0.46
2:I:1516:UNK:N	2:I:1529:UNK:O	2.49	0.46
2:I:2913:ALA:HA	2:I:2916:LYS:HB2	1.98	0.46
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.81	0.45
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.81	0.45
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.45
2:I:2810:LYS:HB3	2:I:2814:LYS:HE3	1.97	0.45
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.43	0.45
2:E:1516:UNK:N	2:E:1529:UNK:O	2.49	0.45
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.49	0.45
2:I:3806:ASN:HA	2:I:3890:LEU:HD13	1.98	0.45
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	3.04	0.45
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.99	0.45
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.80	0.45
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.45
2:B:4982:GLU:HB3	2:B:4983:HIS:CD2	2.51	0.45
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.80	0.45
2:E:4982:GLU:HB3	2:E:4983:HIS:CD2	2.51	0.45
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.52	0.45
2:G:2346:VAL:HG13	2:G:2349:ASN:H	1.82	0.45
2:G:2381:GLU:HA	2:G:2384:ILE:HD12	1.99	0.45
2:E:195:PHE:HB3	2:E:196:MET:HG2	1.98	0.45
2:E:2381:GLU:HA	2:E:2384:ILE:HD12	1.98	0.45
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.49	0.45
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.49	0.45
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	1.99	0.45
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.97	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.51	0.45
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.49	0.45
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.99	0.45
2:E:2758:PHE:O	2:E:2762:THR:N	2.47	0.45
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.49	0.45
2:I:2346:VAL:HG13	2:I:2349:ASN:H	1.82	0.45
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.49	0.45
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.28	0.45
2:G:3806:ASN:HA	2:G:3890:LEU:HD13	1.98	0.45
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.45
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.49	0.45
2:E:662:TRP:H	2:E:748:LEU:HB3	1.82	0.45
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.51	0.45
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	3.04	0.45
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.45
2:I:1723:ALA:HB1	2:I:1775:HIS:HD2	1.80	0.45
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.98	0.45
2:G:662:TRP:H	2:G:748:LEU:HB3	1.82	0.45
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.49	0.45
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	1.98	0.45
2:B:2346:VAL:HG13	2:B:2349:ASN:H	1.82	0.45
2:E:792:LEU:HD22	2:E:799:GLU:H	1.80	0.45
2:E:2214:VAL:HG23	2:E:2215:LEU:HD12	1.99	0.45
2:E:2346:VAL:HG13	2:E:2349:ASN:H	1.82	0.45
2:I:792:LEU:HD22	2:I:799:GLU:H	1.80	0.45
2:I:2381:GLU:HA	2:I:2384:ILE:HD12	1.98	0.45
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.99	0.45
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.50	0.45
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.52	0.45
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	1.98	0.45
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	1.99	0.45
2:E:3806:ASN:HA	2:E:3890:LEU:HD13	1.98	0.45
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.50	0.45
2:I:2214:VAL:HG23	2:I:2215:LEU:HD12	1.99	0.45
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.52	0.45
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	1.99	0.45
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.50	0.45
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.99	0.45
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.49	0.45
2:G:4982:GLU:HB3	2:G:4983:HIS:CD2	2.51	0.45
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	1.99	0.45
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.97	0.45
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.50	0.45
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	1.99	0.45
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.50	0.44
2:I:195:PHE:HB3	2:I:196:MET:HG2	1.98	0.44
2:I:718:GLY:HA3	2:I:737:LEU:HA	2.00	0.44
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	1.99	0.44
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.99	0.44
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.77	0.44
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.35	0.44
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.50	0.44
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	1.99	0.44
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.99	0.44
2:E:875:ALA:HB1	2:E:921:ASN:HB3	1.99	0.44
2:E:3927:GLN:O	2:E:3931:SER:N	2.47	0.44
2:I:1973:GLN:O	2:I:1977:TYR:N	2.49	0.44
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.44
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	2.00	0.44
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.81	0.44
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.82	0.44
2:B:718:GLY:HA3	2:B:737:LEU:HA	2.00	0.44
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	2.00	0.44
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.99	0.44
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.35	0.44
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.81	0.44
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.98	0.44
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:VAL:HA	2:E:1784:ALA:HA	2.00	0.44
2:B:164:ARG:N	2:B:167:ASP:OD2	2.47	0.44
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.50	0.44
2:E:4959:PHE:O	2:E:4959:PHE:CG	2.71	0.44
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.83	0.44
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.99	0.44
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.52	0.44
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.80	0.44
2:B:4344:UNK:N	2:G:4909:TYR:OH	2.50	0.44
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.44
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.50	0.44
2:G:4959:PHE:O	2:G:4959:PHE:CG	2.71	0.44
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	2.00	0.44
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.00	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CG	2.71	0.44
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.82	0.44
2:G:3941:ASP:OD1	2:G:3941:ASP:N	2.50	0.44
2:G:4886:HIS:O	2:G:4890:GLY:N	2.50	0.44
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.53	0.44
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	2.00	0.44
2:I:875:ALA:HB1	2:I:921:ASN:HB3	1.99	0.44
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	1.99	0.44
2:I:2902:HIS:HB3	2:I:2905:LEU:HG	2.00	0.44
2:B:875:ALA:HB1	2:B:921:ASN:HB3	1.99	0.44
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.51	0.44
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	1.99	0.44
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.98	0.44
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.43	0.44
2:G:875:ALA:HB1	2:G:921:ASN:HB3	1.99	0.44
2:G:1973:GLN:O	2:G:1977:TYR:N	2.49	0.44
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.50	0.44
2:B:134:ASP:OD1	2:B:134:ASP:N	2.50	0.44
2:B:662:TRP:H	2:B:748:LEU:HB3	1.82	0.44
2:B:811:CYS:HB3	2:B:815:VAL:HG11	2.00	0.44
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.50	0.44
2:I:451:TYR:O	2:I:474:ARG:NH1	2.43	0.44
2:I:2868:SER:O	2:I:2872:GLN:N	2.39	0.44
2:G:2902:HIS:HB3	2:G:2905:LEU:HG	2.00	0.44
2:B:4909:TYR:OH	2:G:4344:UNK:N	2.51	0.43
2:B:4959:PHE:O	2:B:4959:PHE:CG	2.71	0.43
2:E:2902:HIS:HB3	2:E:2905:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.51	0.43
2:G:111:HIS:HD2	2:G:114:SER:H	1.65	0.43
2:G:4181:ILE:HG23	2:G:4193:ILE:HB	2.00	0.43
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.83	0.43
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.99	0.43
2:E:811:CYS:HB3	2:E:815:VAL:HG11	2.00	0.43
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.51	0.43
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.00	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.84	0.43
2:E:4713:SER:HA	2:E:4718:LYS:HE2	2.00	0.43
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.39	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.82	0.43
2:G:195:PHE:HB3	2:G:196:MET:HG2	1.98	0.43
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.00	0.43
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.29	0.43
2:G:3365:UNK:O	2:G:3369:UNK:N	2.52	0.43
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.00	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.00	0.43
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.53	0.43
2:E:1973:GLN:O	2:E:1977:TYR:N	2.49	0.43
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.77	0.43
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.29	0.43
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.50	0.43
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.00	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	1.99	0.43
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.01	0.43
2:E:1152:MET:HB2	2:E:1161:ILE:HB	2.00	0.43
2:E:3992:PHE:O	2:E:3996:PHE:N	2.43	0.43
2:I:662:TRP:H	2:I:748:LEU:HB3	1.82	0.43
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.53	0.43
2:G:718:GLY:HA3	2:G:737:LEU:HA	2.00	0.43
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.50	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.53	0.43
2:B:938:HIS:N	2:B:1054:GLU:O	2.52	0.43
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.52	0.43
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.43
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.00	0.43
2:G:134:ASP:OD1	2:G:134:ASP:N	2.50	0.43
2:G:811:CYS:HB3	2:G:815:VAL:HG11	2.00	0.43
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.82	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.84	0.43
2:E:111:HIS:HD2	2:E:114:SER:H	1.66	0.43
2:E:718:GLY:HA3	2:E:737:LEU:HA	2.00	0.43
2:I:4181:ILE:HG23	2:I:4193:ILE:HB	2.00	0.43
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.52	0.43
2:B:794:GLY:H	2:B:798:GLY:HA3	1.84	0.43
2:E:134:ASP:N	2:E:134:ASP:OD1	2.50	0.43
2:E:3761:GLN:NE2	2:E:4750:ILE:O	2.50	0.43
2:I:811:CYS:HB3	2:I:815:VAL:HG11	2.00	0.43
2:G:180:LEU:O	2:G:200:TRP:NE1	2.43	0.43
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.51	0.43
2:G:4713:SER:HA	2:G:4718:LYS:HE2	2.00	0.43
2:B:1973:GLN:O	2:B:1977:TYR:N	2.49	0.43
2:E:794:GLY:H	2:E:798:GLY:HA3	1.84	0.43
2:E:4984:ASN:C	2:E:4986:ALA:H	2.22	0.43
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.00	0.43
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.52	0.43
2:I:4984:ASN:C	2:I:4986:ALA:H	2.22	0.43
2:B:111:HIS:HD2	2:B:114:SER:H	1.65	0.43
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.43
2:B:1152:MET:HB2	2:B:1161:ILE:HB	2.00	0.43
2:B:4713:SER:HA	2:B:4718:LYS:HE2	2.00	0.43
2:E:938:HIS:N	2:E:1054:GLU:O	2.52	0.43
2:E:4181:ILE:HG23	2:E:4193:ILE:HB	2.00	0.43
2:I:111:HIS:HD2	2:I:114:SER:H	1.65	0.43
2:I:134:ASP:OD1	2:I:134:ASP:N	2.50	0.43
2:I:4713:SER:HA	2:I:4718:LYS:HE2	2.00	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.43
2:G:3927:GLN:O	2:G:3931:SER:N	2.47	0.43
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.84	0.43
2:G:4984:ASN:C	2:G:4986:ALA:H	2.22	0.43
2:B:1936:LYS:O	2:B:1940:CYS:N	2.48	0.43
2:B:2170:MET:HG3	2:B:2214:VAL:HG12	2.01	0.43
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.28	0.43
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.43
2:E:4909:TYR:OH	2:I:4344:UNK:N	2.52	0.43
2:G:1101:ARG:HG2	2:G:1125:ASN:HA	2.01	0.43
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.72	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.42
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.83	0.42
2:I:1152:MET:HB2	2:I:1161:ILE:HB	2.00	0.42
2:I:4181:ILE:HG13	2:I:4988:TYR:CE1	2.54	0.42
2:G:1152:MET:HB2	2:G:1161:ILE:HB	2.00	0.42
2:G:2438:PRO:HG2	2:G:2454:ARG:HB2	2.01	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.50	0.42
2:B:4181:ILE:HG13	2:B:4988:TYR:CE1	2.54	0.42
2:E:1739:THR:H	2:E:1742:THR:HB	1.85	0.42
2:E:4886:HIS:O	2:E:4890:GLY:N	2.50	0.42
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.01	0.42
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.46	0.42
2:I:2170:MET:HG3	2:I:2214:VAL:HG12	2.01	0.42
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.84	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.46	0.42
2:G:1948:ASP:OD1	2:G:2126:ARG:NH2	2.49	0.42
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.93	0.42
2:B:1739:THR:H	2:B:1742:THR:HB	1.85	0.42
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	2.02	0.42
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	2.02	0.42
2:E:893:TYR:HD1	2:E:907:LEU:HB2	1.85	0.42
2:E:2170:MET:HG3	2:E:2214:VAL:HG12	2.01	0.42
2:E:4181:ILE:HG13	2:E:4988:TYR:CE1	2.54	0.42
2:E:4250:GLN:O	2:E:4553:ASN:ND2	2.53	0.42
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.72	0.42
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	2.02	0.42
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	2.02	0.42
2:I:4959:PHE:CD1	2:I:4959:PHE:O	2.72	0.42
2:G:649:PHE:HB3	2:G:776:LEU:HD13	2.00	0.42
2:G:2170:MET:HG3	2:G:2214:VAL:HG12	2.01	0.42
2:B:893:TYR:HD1	2:B:907:LEU:HB2	1.85	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.42
2:E:145:ALA:HA	2:E:175:SER:HB3	2.01	0.42
2:E:180:LEU:O	2:E:200:TRP:NE1	2.43	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.42
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.85	0.42
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.42
2:I:145:ALA:HA	2:I:175:SER:HB3	2.01	0.42
2:I:652:ARG:HD2	2:I:750:LEU:HB3	2.02	0.42
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.42	0.42
2:I:758:ARG:HH22	2:I:805:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.42
2:I:1739:THR:H	2:I:1742:THR:HB	1.85	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.50	0.42
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.84	0.42
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.42
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.85	0.42
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.42
1:J:30:LEU:HB3	1:J:33:GLY:HA3	2.01	0.42
2:B:4959:PHE:CD1	2:B:4959:PHE:O	2.72	0.42
2:B:4984:ASN:C	2:B:4986:ALA:H	2.22	0.42
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.93	0.42
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.42
2:E:2438:PRO:HG2	2:E:2454:ARG:HB2	2.01	0.42
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.02	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.42
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.00	0.42
2:I:708:GLY:HA3	2:I:722:TRP:HB3	2.01	0.42
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.02	0.42
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.53	0.42
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.02	0.42
2:G:794:GLY:H	2:G:798:GLY:HA3	1.84	0.42
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	1.99	0.42
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.53	0.42
2:G:1739:THR:H	2:G:1742:THR:HB	1.85	0.42
1:F:30:LEU:HB3	1:F:33:GLY:HA3	2.01	0.42
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.01	0.42
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.52	0.42
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.39	0.42
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	2.02	0.42
2:I:794:GLY:H	2:I:798:GLY:HA3	1.84	0.42
2:I:2432:LEU:O	2:I:2436:CYS:N	2.52	0.42
2:G:793:LEU:HD12	2:G:797:HIS:H	1.85	0.42
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	2.02	0.42
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.41	0.42
2:B:1101:ARG:HG2	2:B:1125:ASN:HA	2.01	0.42
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.02	0.42
2:B:3927:GLN:O	2:B:3931:SER:N	2.47	0.42
2:B:4181:ILE:HG23	2:B:4193:ILE:HB	2.00	0.42
2:E:621:ILE:O	2:E:625:LEU:N	2.49	0.42
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.01	0.42
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.85	0.42
2:I:2438:PRO:HG2	2:I:2454:ARG:HB2	2.01	0.42
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.42
2:G:621:ILE:O	2:G:625:LEU:N	2.49	0.42
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.00	0.42
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	2.02	0.42
1:A:30:LEU:HB3	1:A:33:GLY:HA3	2.01	0.42
2:B:652:ARG:HD2	2:B:750:LEU:HB3	2.02	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.02	0.42
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.02	0.42
2:B:2432:LEU:O	2:B:2436:CYS:N	2.52	0.42
2:E:758:ARG:HH22	2:E:805:PRO:HD3	1.85	0.42
2:E:793:LEU:HD12	2:E:797:HIS:H	1.85	0.42
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.00	0.42
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.46	0.42
2:E:2432:LEU:O	2:E:2436:CYS:N	2.52	0.42
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.02	0.42
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.42
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.02	0.42
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.35	0.42
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.01	0.42
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.02	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.02	0.42
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.42	0.42
2:G:3992:PHE:O	2:G:3996:PHE:N	2.43	0.42
2:B:145:ALA:HA	2:B:175:SER:HB3	2.01	0.42
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.02	0.42
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.53	0.42
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.38	0.42
2:I:4250:GLN:O	2:I:4553:ASN:ND2	2.53	0.42
2:G:451:TYR:O	2:G:474:ARG:NH1	2.43	0.42
2:G:914:PRO:O	2:G:918:ARG:N	2.52	0.42
2:B:758:ARG:HH22	2:B:805:PRO:HD3	1.84	0.42
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.73	0.42
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	2.02	0.42
2:I:614:VAL:HA	2:I:2169:GLN:HB3	2.02	0.42
2:G:893:TYR:HD1	2:G:907:LEU:HB2	1.85	0.42
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.93	0.42
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.02	0.42
2:G:2128:TYR:HB3	2:G:3669:PHE:HB3	2.02	0.42
2:G:4250:GLN:O	2:G:4553:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.03	0.41
2:B:4250:GLN:O	2:B:4553:ASN:ND2	2.53	0.41
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.85	0.41
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.85	0.41
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	2.02	0.41
2:G:758:ARG:HH22	2:G:805:PRO:HD3	1.84	0.41
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.85	0.41
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.86	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.02	0.41
2:B:2384:ILE:O	2:B:2388:GLU:N	2.53	0.41
2:I:621:ILE:O	2:I:625:LEU:N	2.49	0.41
2:I:2384:ILE:O	2:I:2388:GLU:N	2.53	0.41
2:G:652:ARG:HD2	2:G:750:LEU:HB3	2.02	0.41
1:F:21:THR:HA	1:F:49:ARG:HA	2.03	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.41
2:B:3556:UNK:O	2:B:3560:UNK:N	2.54	0.41
2:E:1101:ARG:HG2	2:E:1125:ASN:HA	2.01	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.02	0.41
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.03	0.41
2:G:157:ARG:HH21	2:G:164:ARG:HD2	1.86	0.41
2:G:708:GLY:HA3	2:G:722:TRP:HB3	2.01	0.41
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.02	0.41
2:G:2384:ILE:O	2:G:2388:GLU:N	2.53	0.41
2:G:4181:ILE:HG13	2:G:4988:TYR:CE1	2.54	0.41
2:G:4719:PHE:HD1	2:G:4722:ARG:HD3	1.85	0.41
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.00	0.41
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.35	0.41
2:B:708:GLY:HA3	2:B:722:TRP:HB3	2.01	0.41
2:B:793:LEU:HD12	2:B:797:HIS:H	1.85	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.38	0.41
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.02	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.03	0.41
2:E:2384:ILE:O	2:E:2388:GLU:N	2.53	0.41
2:I:3556:UNK:O	2:I:3560:UNK:N	2.54	0.41
2:I:3941:ASP:OD1	2:I:3941:ASP:N	2.50	0.41
2:G:145:ALA:HA	2:G:175:SER:HB3	2.01	0.41
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.35	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.02	0.41
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	2.02	0.41
1:H:30:LEU:HB3	1:H:33:GLY:HA3	2.01	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2777:TYR:HD1	2:B:2791:LEU:HB2	1.86	0.41
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.54	0.41
2:B:4886:HIS:O	2:B:4890:GLY:N	2.50	0.41
2:E:614:VAL:HA	2:E:2169:GLN:HB3	2.02	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.02	0.41
2:E:708:GLY:HA3	2:E:722:TRP:HB3	2.01	0.41
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.02	0.41
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.02	0.41
2:I:1948:ASP:OD1	2:I:2126:ARG:NH2	2.49	0.41
1:F:21:THR:N	1:F:107:GLU:OE1	2.43	0.41
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.41
2:B:2438:PRO:HG2	2:B:2454:ARG:HB2	2.01	0.41
2:B:4156:HIS:CE1	2:B:5036:LEU:HD11	2.56	0.41
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.41
2:E:3556:UNK:O	2:E:3560:UNK:N	2.54	0.41
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	2.02	0.41
2:I:157:ARG:HH21	2:I:164:ARG:HD2	1.86	0.41
2:I:793:LEU:HD12	2:I:797:HIS:H	1.85	0.41
2:I:893:TYR:HD1	2:I:907:LEU:HB2	1.85	0.41
2:I:1101:ARG:HG2	2:I:1125:ASN:HA	2.01	0.41
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.93	0.41
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.85	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.41
2:G:614:VAL:HA	2:G:2169:GLN:HB3	2.02	0.41
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	2.02	0.41
2:B:1931:LEU:HD13	2:B:1935:VAL:HG11	2.03	0.41
2:B:3761:GLN:NE2	2:B:4750:ILE:O	2.50	0.41
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.85	0.41
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	2.02	0.41
2:I:3761:GLN:NE2	2:I:4750:ILE:O	2.50	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.03	0.41
1:A:21:THR:N	1:A:107:GLU:OE1	2.43	0.41
1:J:21:THR:HA	1:J:49:ARG:HA	2.03	0.41
2:B:2128:TYR:HB3	2:B:3669:PHE:HB3	2.02	0.41
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.36	0.41
2:E:652:ARG:HD2	2:E:750:LEU:HB3	2.02	0.41
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.54	0.41
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.03	0.41
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.41
2:I:4156:HIS:CE1	2:I:5036:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:938:HIS:N	2:G:1054:GLU:O	2.52	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.38	0.41
1:F:26:TYR:N	1:F:39:SER:OG	2.48	0.41
1:A:21:THR:HA	1:A:49:ARG:HA	2.03	0.41
2:B:157:ARG:HH21	2:B:164:ARG:HD2	1.86	0.41
2:B:180:LEU:O	2:B:200:TRP:NE1	2.43	0.41
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.03	0.41
2:B:4056:GLU:HG2	2:B:4166:LEU:HD23	2.03	0.41
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.53	0.41
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.41	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.38	0.41
2:E:4719:PHE:HD1	2:E:4722:ARG:HD3	1.85	0.41
2:I:278:GLN:N	2:I:315:CYS:SG	2.91	0.41
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.02	0.41
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.73	0.41
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.02	0.41
2:I:2777:TYR:HD1	2:I:2791:LEU:HB2	1.86	0.41
2:G:236:ALA:HA	2:G:242:ARG:HD2	2.03	0.41
2:G:953:THR:HB	2:G:969:PRO:HD2	2.03	0.41
2:G:2777:TYR:HD1	2:G:2791:LEU:HB2	1.86	0.41
2:G:3556:UNK:O	2:G:3560:UNK:N	2.54	0.41
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.85	0.41
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.86	0.41
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.54	0.41
2:B:4148:THR:HG21	2:B:4178:LEU:HD21	2.03	0.41
2:B:4719:PHE:HD1	2:B:4722:ARG:HD3	1.85	0.41
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.85	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.93	0.41
2:E:1931:LEU:HD13	2:E:1935:VAL:HG11	2.03	0.41
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.02	0.41
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.03	0.41
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	2.02	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.41
2:I:2128:TYR:HB3	2:I:3669:PHE:HB3	2.02	0.41
2:I:4719:PHE:HD1	2:I:4722:ARG:HD3	1.85	0.41
2:G:2432:LEU:O	2:G:2436:CYS:N	2.52	0.41
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.02	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.55	0.40
2:E:206:CYS:SG	2:E:207:SER:N	2.94	0.40
2:E:278:GLN:N	2:E:315:CYS:SG	2.91	0.40
2:E:953:THR:HB	2:E:969:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.96	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.94	0.40
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.03	0.40
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.85	0.40
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.02	0.40
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.96	0.40
1:J:7:ILE:HD13	1:J:71:ARG:HG2	2.04	0.40
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.03	0.40
2:B:953:THR:HB	2:B:969:PRO:HD2	2.03	0.40
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	2.02	0.40
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	2.02	0.40
2:B:1948:ASP:OD1	2:B:2126:ARG:NH2	2.49	0.40
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.35	0.40
2:E:1171:SER:OG	2:E:1175:SER:N	2.44	0.40
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.02	0.40
2:E:4148:THR:HG21	2:E:4178:LEU:HD21	2.03	0.40
2:I:232:THR:OG1	2:I:233:ILE:N	2.55	0.40
2:I:1931:LEU:HD13	2:I:1935:VAL:HG11	2.03	0.40
2:I:1936:LYS:O	2:I:1940:CYS:N	2.48	0.40
2:I:4886:HIS:O	2:I:4890:GLY:N	2.50	0.40
2:G:404:ILE:HD13	2:G:481:GLU:HG3	2.03	0.40
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.85	0.40
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.40
2:G:4156:HIS:CE1	2:G:5036:LEU:HD11	2.56	0.40
1:A:7:ILE:HD13	1:A:71:ARG:HG2	2.04	0.40
2:B:463:GLU:O	2:B:466:SER:OG	2.30	0.40
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.85	0.40
2:B:1078:GLU:HB2	2:B:1235:THR:HG22	2.04	0.40
2:E:404:ILE:HD13	2:E:481:GLU:HG3	2.03	0.40
2:E:3663:LEU:H	2:E:3663:LEU:HG	1.77	0.40
2:E:4056:GLU:HG2	2:E:4166:LEU:HD23	2.03	0.40
2:I:485:SER:O	2:I:489:ASN:N	2.44	0.40
2:I:914:PRO:O	2:I:918:ARG:N	2.52	0.40
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.54	0.40
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.03	0.40
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.03	0.40
2:B:206:CYS:SG	2:B:207:SER:N	2.94	0.40
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.86	0.40
2:E:914:PRO:O	2:E:918:ARG:N	2.52	0.40
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	2.02	0.40
2:E:2777:TYR:HD1	2:E:2791:LEU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.85	0.40
2:I:236:ALA:HA	2:I:242:ARG:HD2	2.03	0.40
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.86	0.40
2:I:4148:THR:HG21	2:I:4178:LEU:HD21	2.03	0.40
2:G:206:CYS:SG	2:G:207:SER:N	2.94	0.40
2:G:463:GLU:O	2:G:466:SER:OG	2.30	0.40
2:G:2674:UNK:O	2:G:2676:UNK:N	2.55	0.40
2:B:4060:LYS:NZ	2:B:4107:GLU:OE2	2.41	0.40
2:B:4821:LYS:HE2	2:B:4821:LYS:HB3	1.94	0.40
2:E:157:ARG:HH21	2:E:164:ARG:HD2	1.86	0.40
2:E:236:ALA:HA	2:E:242:ARG:HD2	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.37	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.55	0.40
2:I:953:THR:HB	2:I:969:PRO:HD2	2.03	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	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	H	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	44	78
2	E	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	44	78
2	G	3235/4416 (73%)	2891 (89%)	337 (10%)	7 (0%)	44	78
2	I	3235/4416 (73%)	2893 (89%)	335 (10%)	7 (0%)	44	78
All	All	13360/18096 (74%)	11956 (90%)	1376 (10%)	28 (0%)	45	78

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	I	1708	ARG
2	I	1932	PRO
2	G	1708	ARG
2	G	1932	PRO
2	B	4641	PRO
2	B	4982	GLU
2	B	4985	LEU
2	E	4641	PRO
2	E	4982	GLU
2	E	4985	LEU
2	I	4641	PRO
2	I	4982	GLU
2	I	4985	LEU
2	G	4641	PRO
2	G	4982	GLU
2	G	4985	LEU
2	B	1840	PRO
2	B	2292	GLU
2	E	1840	PRO
2	E	2292	GLU
2	I	1840	PRO
2	I	2292	GLU
2	G	1840	PRO
2	G	2292	GLU

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	88/89 (99%)	88 (100%)	0	100 100
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3022 (82%)	2476 (99%)	17 (1%)	81 87
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	81 87
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	81 87
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	81 87
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	80 87

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3762	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4959	PHE
2	B	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3762	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN

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Mol	Chain	Res	Type
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4959	PHE
2	E	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3762	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4959	PHE
2	I	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3762	ARG
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4959	PHE
2	G	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	520	ASN
2	B	765	GLN
2	B	1158	ASN
2	B	1678	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1952	GLN
2	B	2005	GLN
2	B	2127	GLN
2	B	3767	GLN
2	B	3809	ASN
2	B	3896	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4054	ASN
2	B	4120	ASN
2	B	4553	ASN
2	B	4978	HIS
2	B	4987	ASN
2	E	57	ASN
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	520	ASN
2	E	765	GLN
2	E	1158	ASN
2	E	1678	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1952	GLN
2	E	2005	GLN
2	E	2127	GLN

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Mol	Chain	Res	Type
2	E	3767	GLN
2	E	3809	ASN
2	E	3896	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4054	ASN
2	E	4120	ASN
2	E	4553	ASN
2	E	4978	HIS
2	E	4987	ASN
2	I	57	ASN
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	479	GLN
2	I	520	ASN
2	I	765	GLN
2	I	1158	ASN
2	I	1678	ASN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1952	GLN
2	I	2005	GLN
2	I	2127	GLN
2	I	3767	GLN
2	I	3809	ASN
2	I	3896	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4054	ASN
2	I	4120	ASN
2	I	4553	ASN
2	I	4978	HIS
2	I	4987	ASN
2	G	57	ASN
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	520	ASN

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Mol	Chain	Res	Type
2	G	765	GLN
2	G	1158	ASN
2	G	1678	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1952	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	3767	GLN
2	G	3809	ASN
2	G	3896	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4054	ASN
2	G	4120	ASN
2	G	4553	ASN
2	G	4978	HIS
2	G	4987	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.04
1	E	4345:UNK	C	4540:PHE	N	74.04
1	I	4345:UNK	C	4540:PHE	N	74.04
1	G	4345:UNK	C	4540:PHE	N	74.04
1	B	3613:UNK	C	3639:THR	N	46.14
1	E	3613:UNK	C	3639:THR	N	46.14
1	I	3613:UNK	C	3639:THR	N	46.14
1	G	3613:UNK	C	3639:THR	N	46.14
1	B	4253:GLU	C	4320:UNK	N	27.75
1	E	4253:GLU	C	4320:UNK	N	27.75
1	I	4253:GLU	C	4320:UNK	N	27.75
1	G	4253:GLU	C	4320:UNK	N	27.75
1	B	3163:UNK	C	3170:UNK	N	15.37
1	E	3163:UNK	C	3170:UNK	N	15.37
1	I	3163:UNK	C	3170:UNK	N	15.37
1	G	3163:UNK	C	3170:UNK	N	15.37
1	B	3468:UNK	C	3511:UNK	N	14.99
1	E	3468:UNK	C	3511:UNK	N	14.99
1	I	3468:UNK	C	3511:UNK	N	14.99
1	G	3468:UNK	C	3511:UNK	N	14.99
1	B	3063:UNK	C	3134:UNK	N	14.98

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3063:UNK	C	3134:UNK	N	14.98
1	I	3063:UNK	C	3134:UNK	N	14.98
1	G	3063:UNK	C	3134:UNK	N	14.98
1	B	2703:UNK	C	2734:ASN	N	14.84
1	E	2703:UNK	C	2734:ASN	N	14.84
1	I	2703:UNK	C	2734:ASN	N	14.84
1	G	2703:UNK	C	2734:ASN	N	14.84
1	B	3236:UNK	C	3241:UNK	N	13.23
1	E	3236:UNK	C	3241:UNK	N	13.23
1	I	3236:UNK	C	3241:UNK	N	13.23
1	G	3236:UNK	C	3241:UNK	N	13.23
1	B	2976:UNK	C	2995:UNK	N	12.15
1	E	2976:UNK	C	2995:UNK	N	12.15
1	I	2976:UNK	C	2995:UNK	N	12.15
1	G	2976:UNK	C	2995:UNK	N	12.15
1	B	1564:UNK	C	1573:MET	N	11.93
1	E	1564:UNK	C	1573:MET	N	11.93
1	I	1564:UNK	C	1573:MET	N	11.93
1	G	1564:UNK	C	1573:MET	N	11.93
1	B	3254:UNK	C	3261:UNK	N	7.98
1	E	3254:UNK	C	3261:UNK	N	7.98
1	I	3254:UNK	C	3261:UNK	N	7.98
1	G	3254:UNK	C	3261:UNK	N	7.98
1	B	1297:UNK	C	1430:UNK	N	5.84
1	E	1297:UNK	C	1430:UNK	N	5.84
1	I	1297:UNK	C	1430:UNK	N	5.84
1	G	1297:UNK	C	1430:UNK	N	5.84
1	B	2479:LEU	C	2487:UNK	N	3.80
1	E	2479:LEU	C	2487:UNK	N	3.80
1	I	2479:LEU	C	2487:UNK	N	3.80
1	G	2479:LEU	C	2487:UNK	N	3.80
1	B	2939:ARG	C	2942:UNK	N	3.24
1	E	2939:ARG	C	2942:UNK	N	3.24
1	I	2939:ARG	C	2942:UNK	N	3.24
1	G	2939:ARG	C	2942:UNK	N	3.24

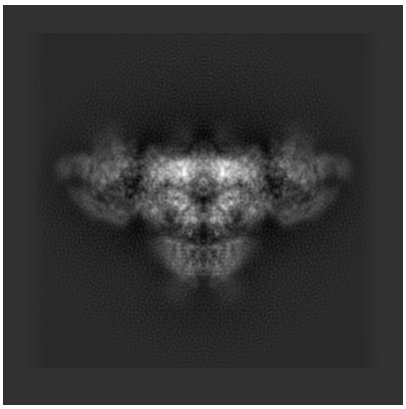
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8395. These allow visual inspection of the internal detail of the map and identification of artifacts.

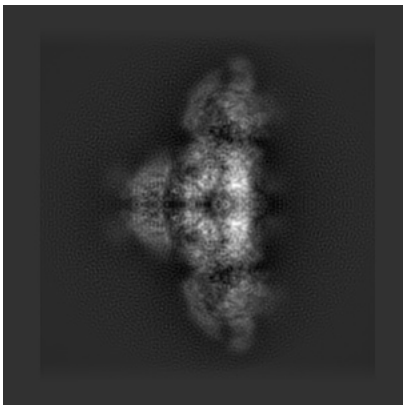
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

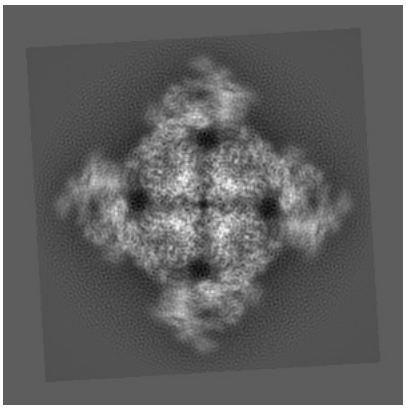
6.1.1 Primary map



X

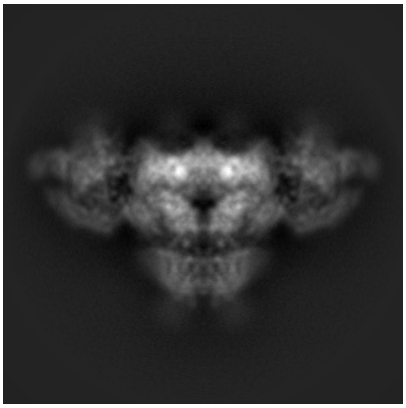


Y

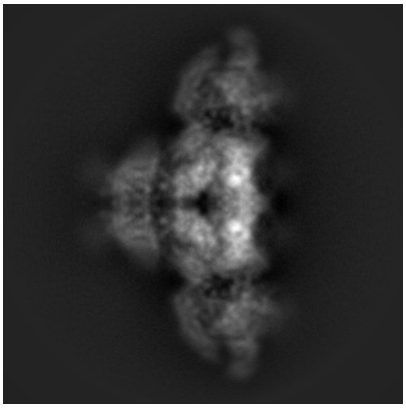


Z

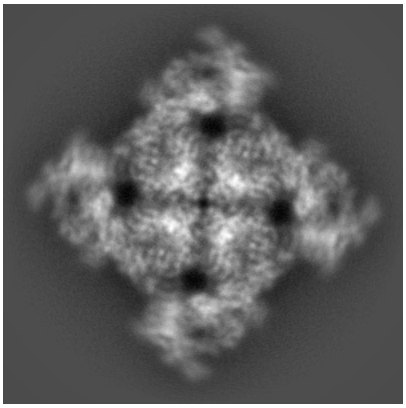
6.1.2 Raw map



X



Y



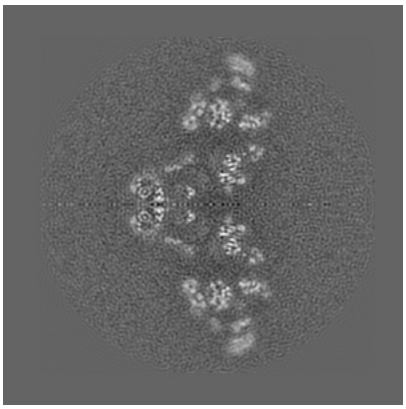
Z

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

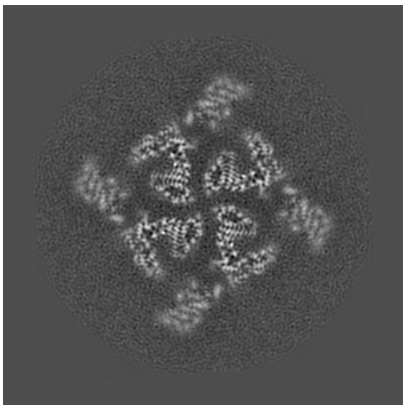
6.2 Central slices (i)

6.2.1 Primary map

X Index: 200

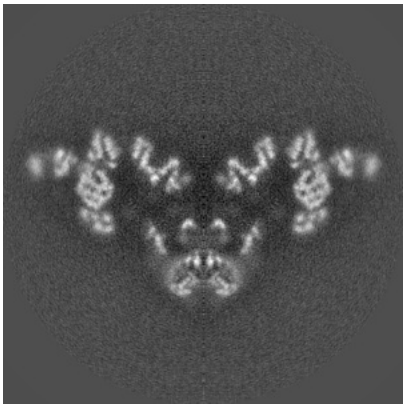


Y Index: 200

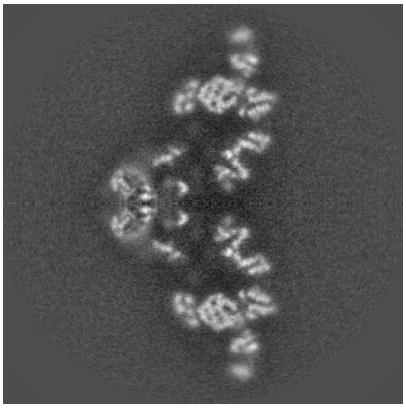


Z Index: 200

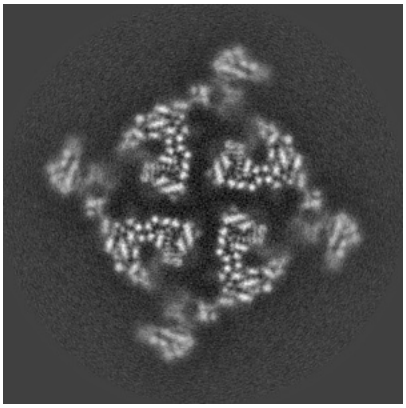
6.2.2 Raw map



X Index: 168



Y Index: 168

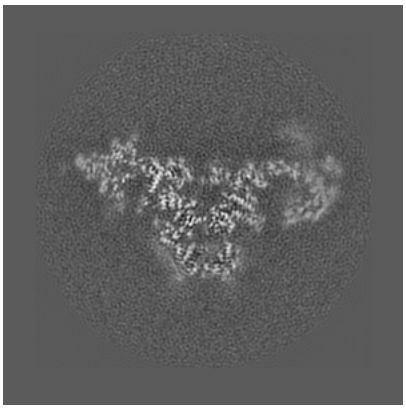


Z Index: 168

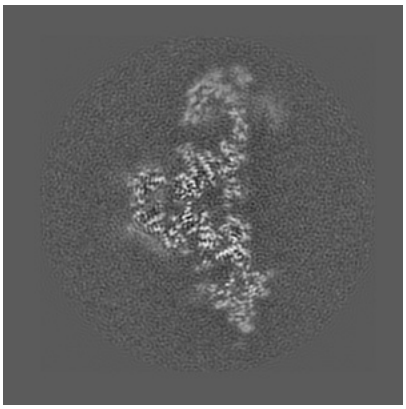
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

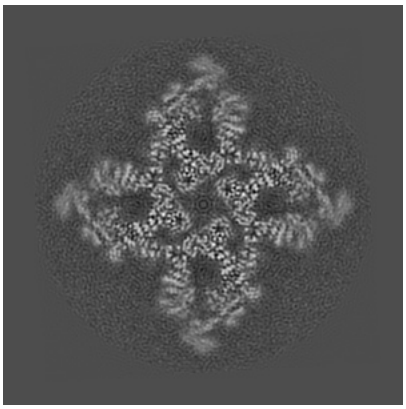
6.3.1 Primary map



X Index: 217

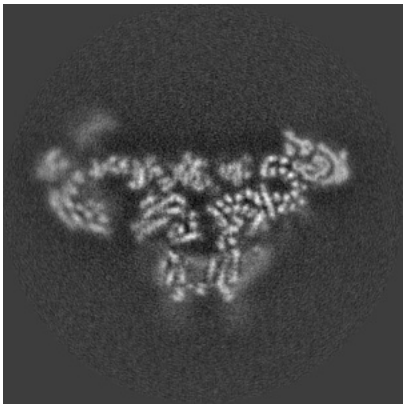


Y Index: 183

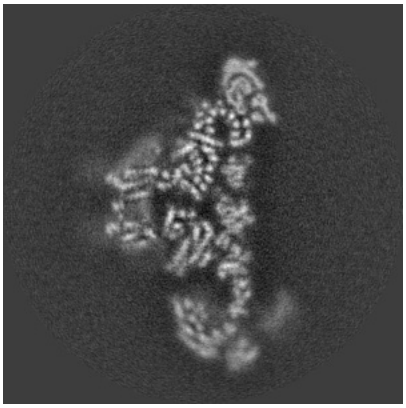


Z Index: 232

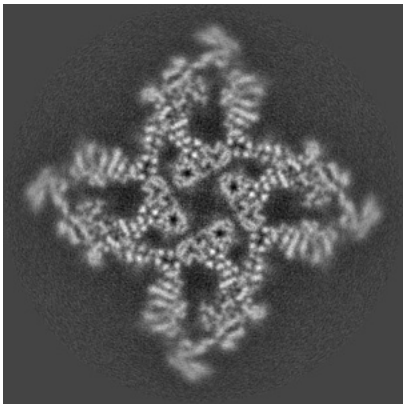
6.3.2 Raw map



X Index: 147



Y Index: 189

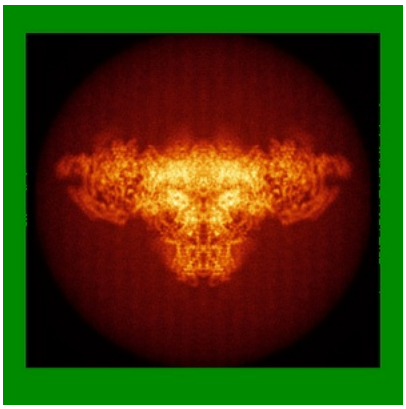


Z Index: 195

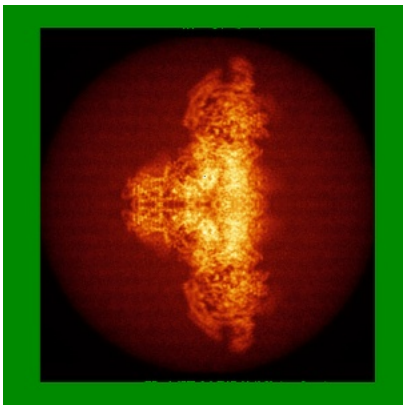
The images above show the largest variance slices of the map in three orthogonal directions.

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

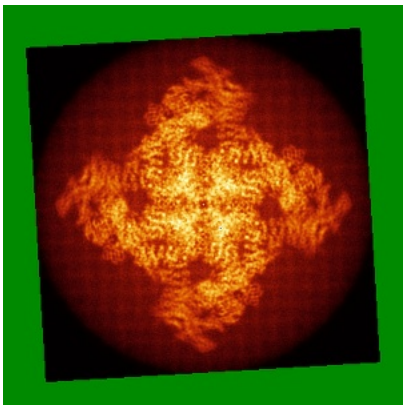
6.4.1 Primary map



X

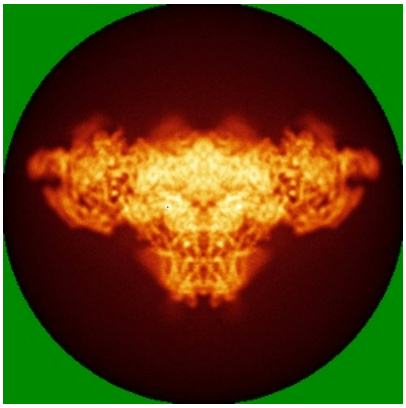


Y

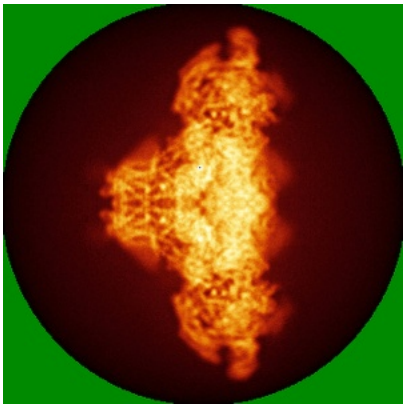


Z

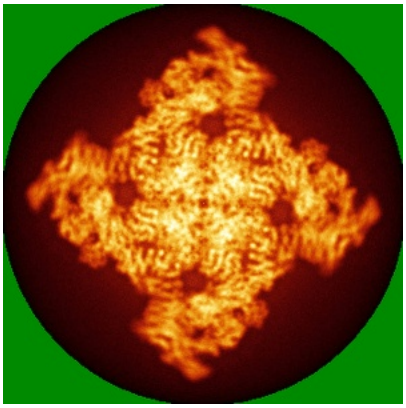
6.4.2 Raw map



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 0.025. 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.

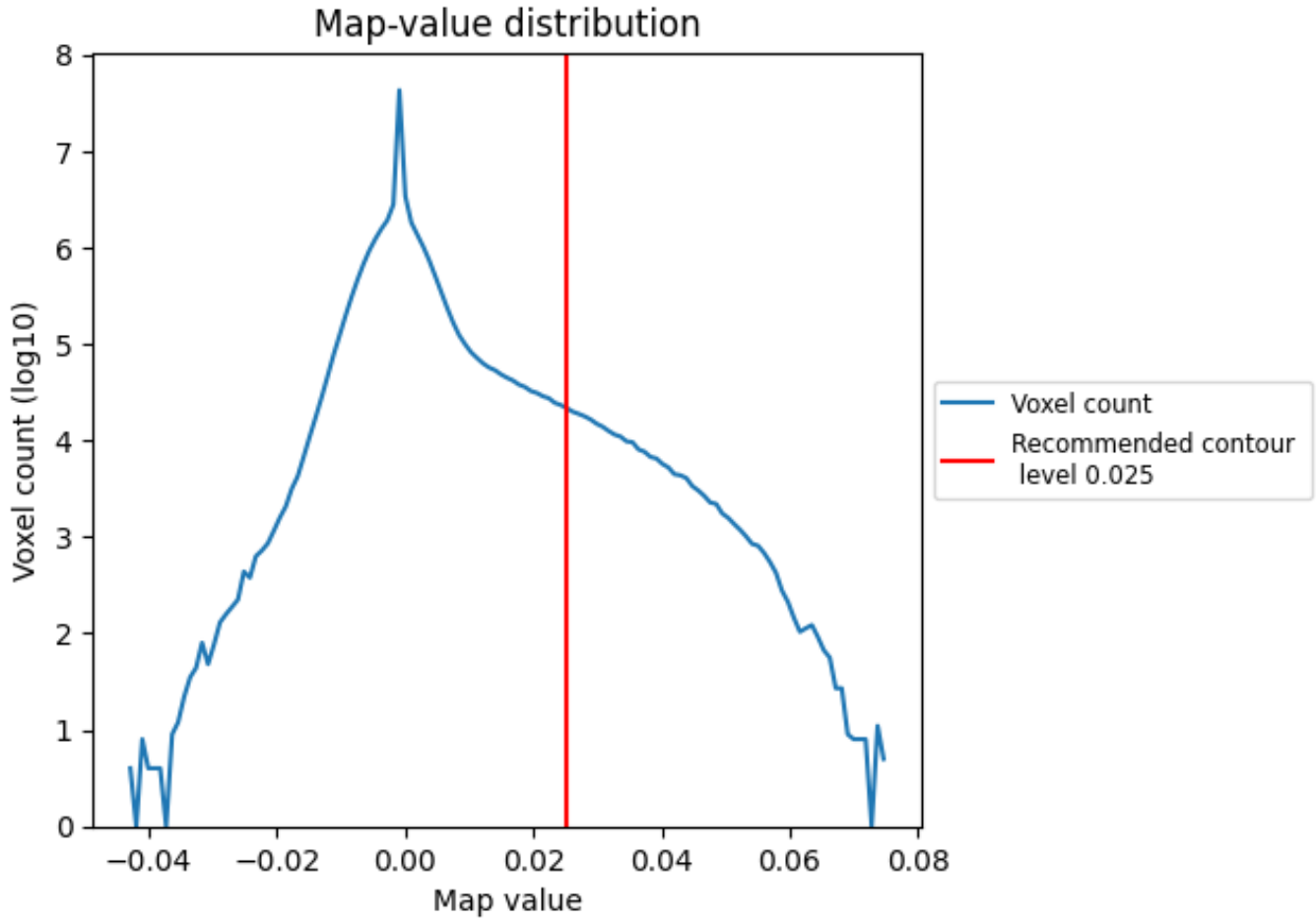
6.6 Mask visualisation (i)

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

7 Map analysis

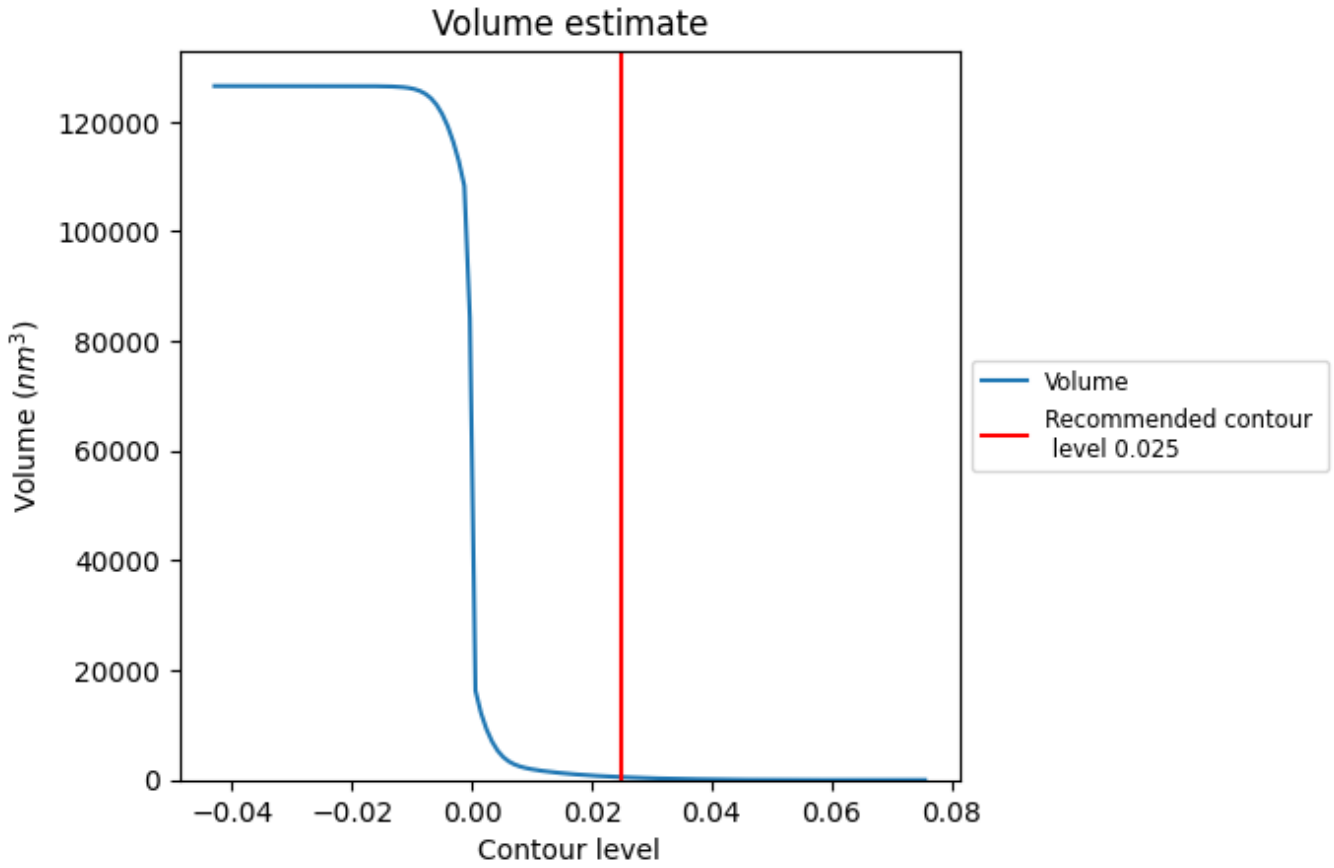
This section contains the results of statistical analysis of the map.

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.

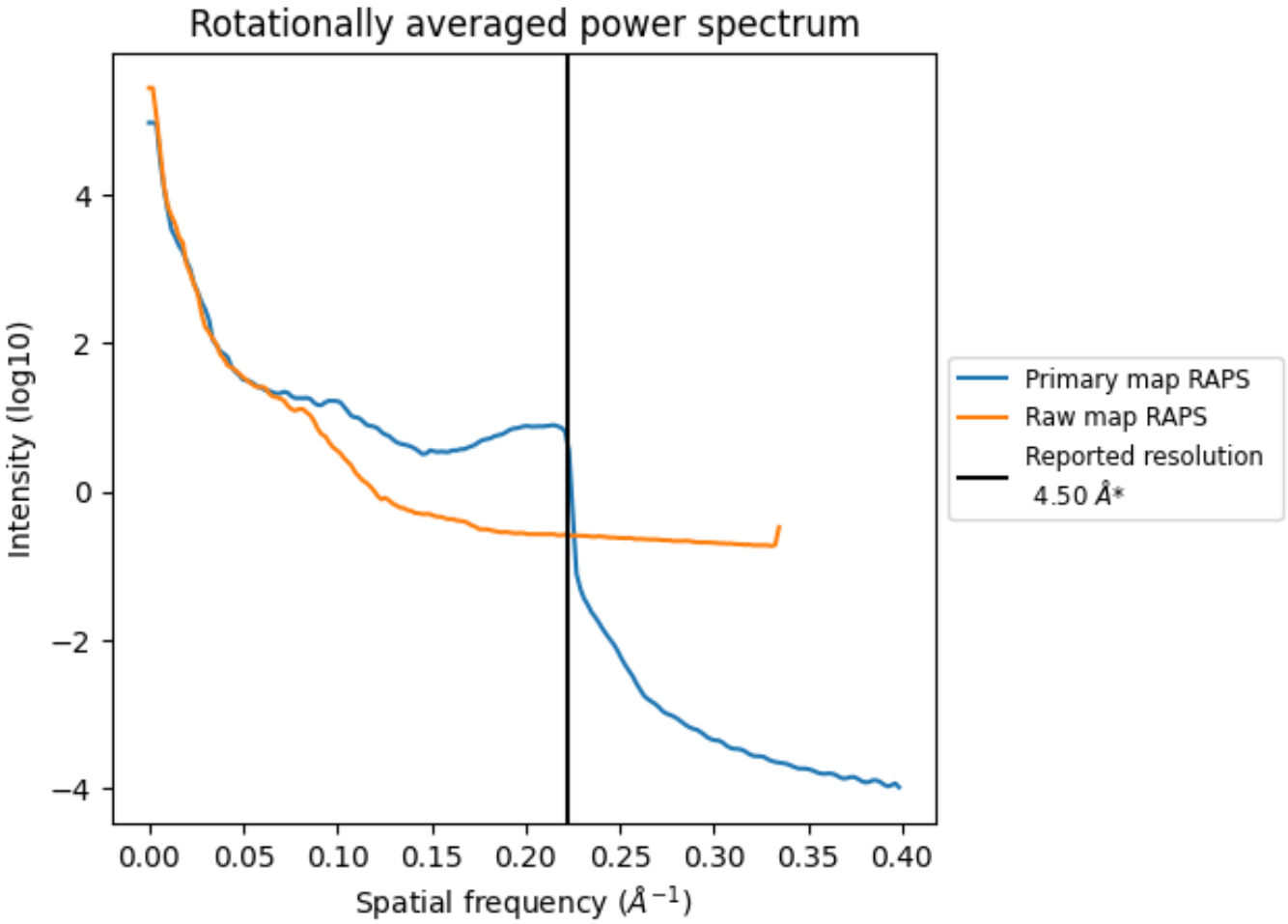
7.2 Volume estimate



The volume at the recommended contour level is 516 nm^3; this corresponds to an approximate mass of 466 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)

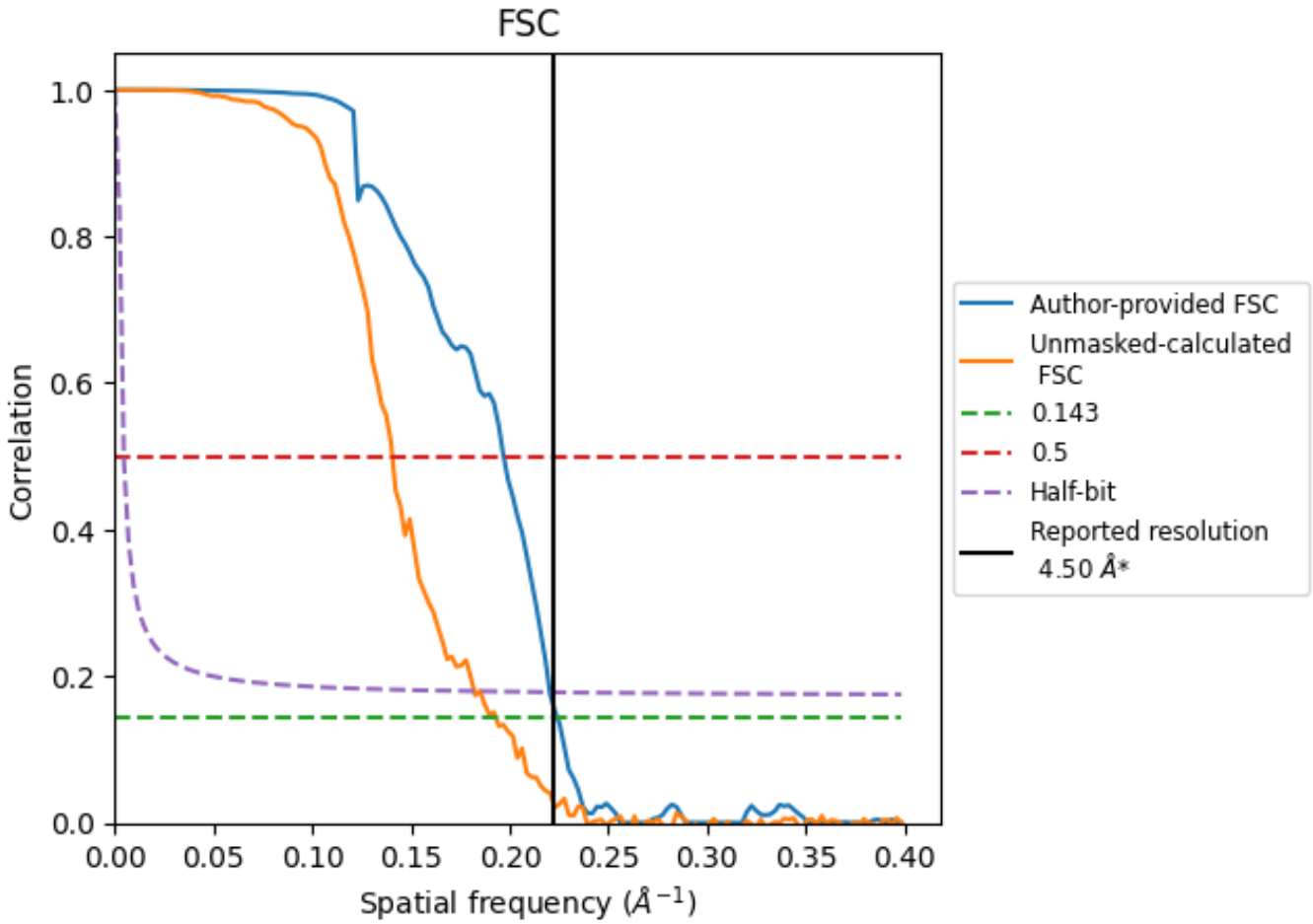


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

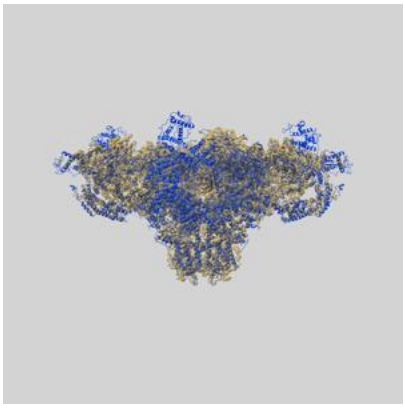
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.46	5.08	4.54
Unmasked-calculated*	5.18	7.11	5.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.18 differs from the reported value 4.5 by more than 10 %

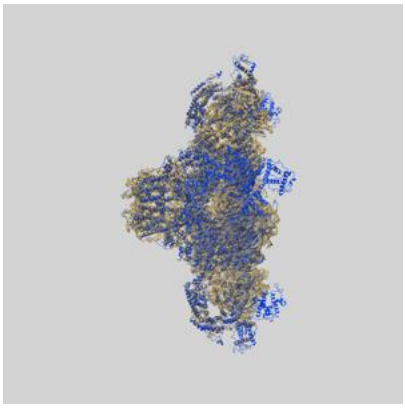
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8395 and PDB model 5TB4. Per-residue inclusion information can be found in section 3 on page 4.

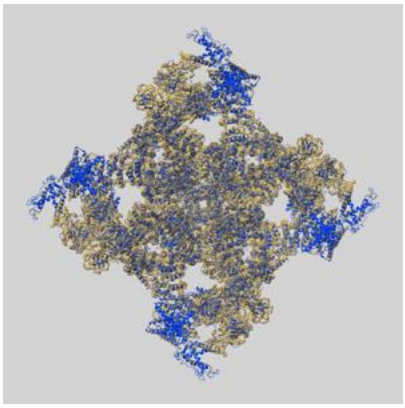
9.1 Map-model overlay



X



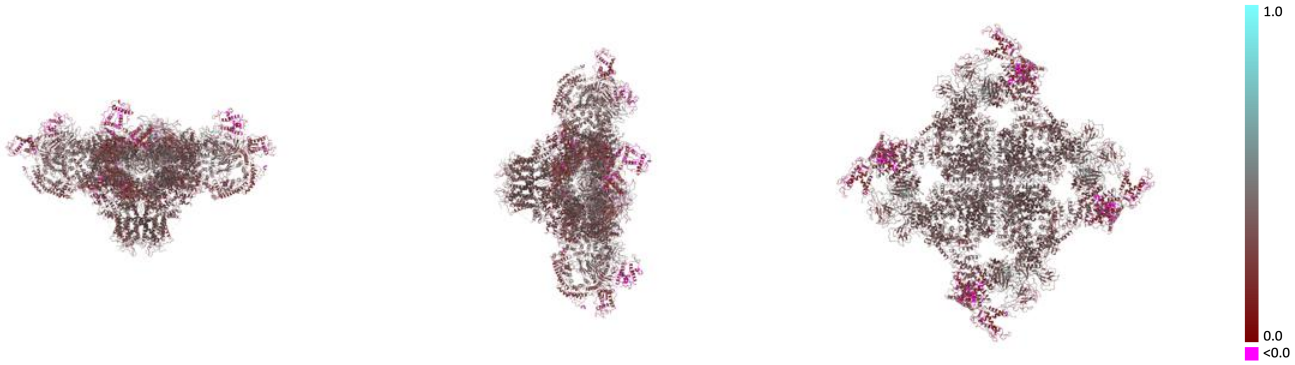
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

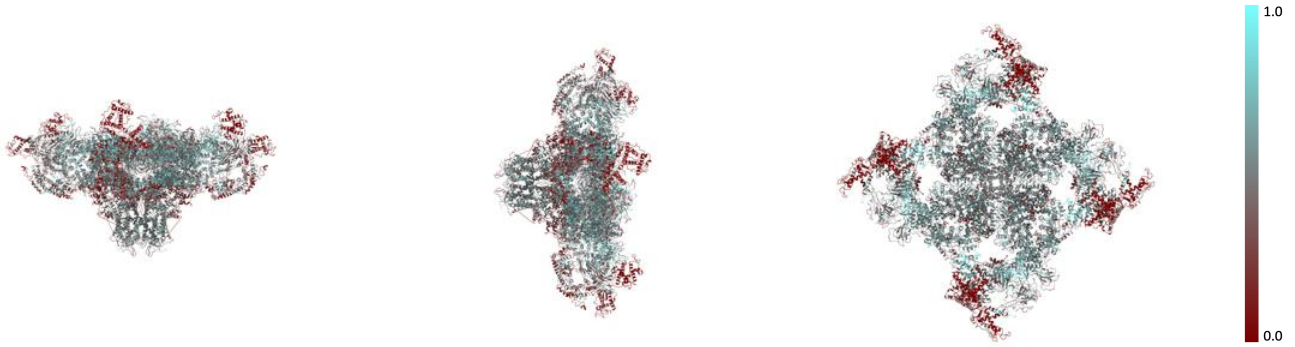
9.2 Q-score mapped to coordinate model (i)



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.

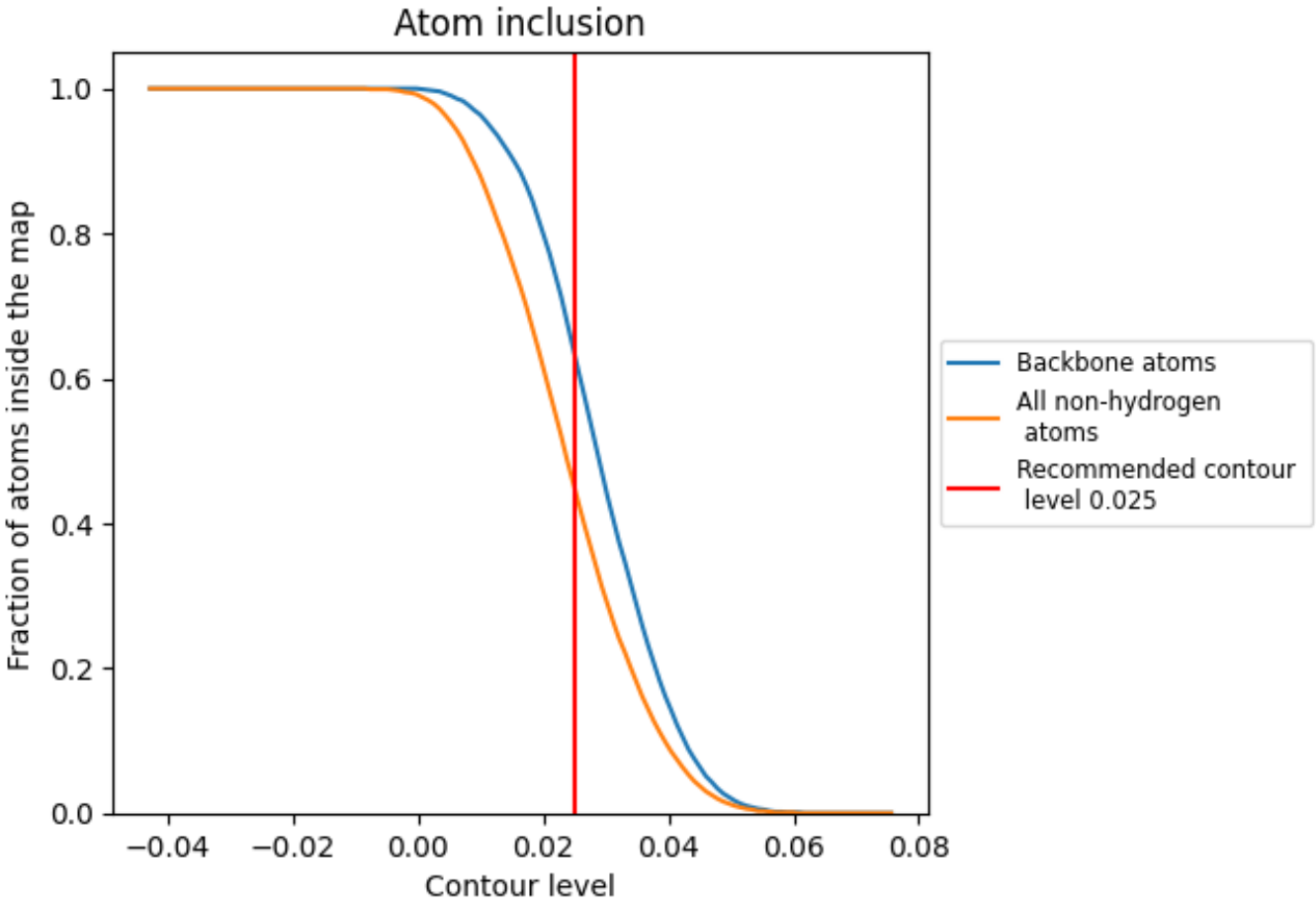
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 45% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4480	0.3170
A	0.4810	0.3380
B	0.4470	0.3160
E	0.4470	0.3160
F	0.4740	0.3420
G	0.4470	0.3160
H	0.4790	0.3410
I	0.4470	0.3160
J	0.4800	0.3400