Full wwPDB EM Validation Report ⓘ

Dec 4, 2024 – 01:19 PM EST

PDB ID	:	9CGP
EMDB ID	:	EMD-45584
Title	:	RyR1 disease mutant Y523S with FKBP12.6, nanodisc and inhibitor dantrolene in the absence of calcium with refined P1 domain
Authors	:	Iyer, K.A.; Samso, M.
Deposited on	:	2024-06-30
Resolution	:	3.34 Å(reported)
Based on initial model	:	7T64

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:

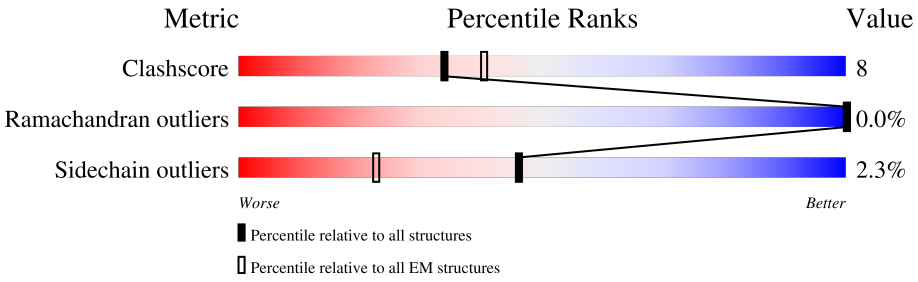
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.34 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	5037	8% 68% 16% 15%
1	B	5037	8% 69% 15% 15%
1	C	5037	8% 68% 16% 15%
1	D	5037	8% 68% 16% 15%
2	E	107	69% 31%
2	F	107	74% 26%
2	G	107	72% 27%
2	H	107	70% 29%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 132860 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	B	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	C	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	D	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	TYR	engineered mutation	UNP P11716
B	523	SER	TYR	engineered mutation	UNP P11716
C	523	SER	TYR	engineered mutation	UNP P11716
D	523	SER	TYR	engineered mutation	UNP P11716

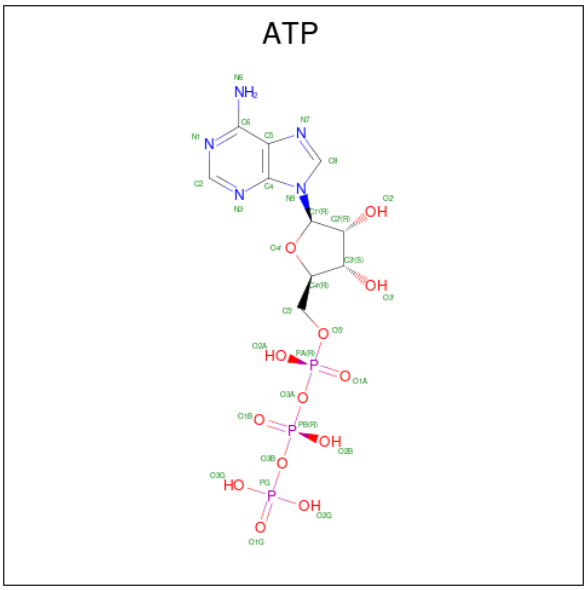
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	F	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	G	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	H	107	Total 786	C 498	N 137	O 148	S 3	0	0

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

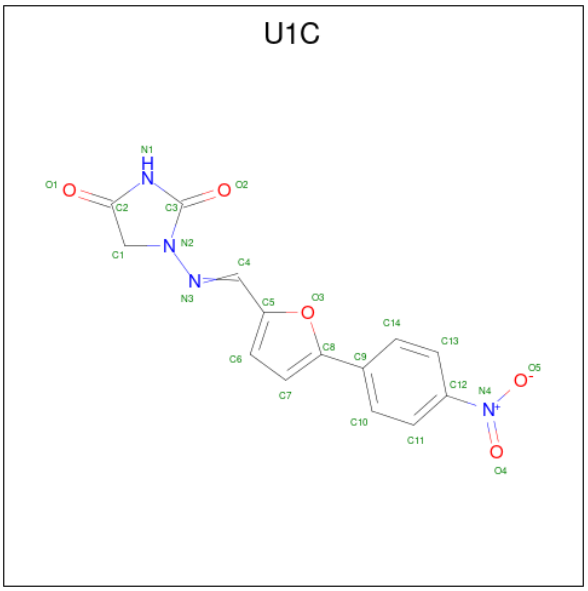
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

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



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

- Molecule 5 is Dantrolene (three-letter code: U1C) (formula: $C_{14}H_{10}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



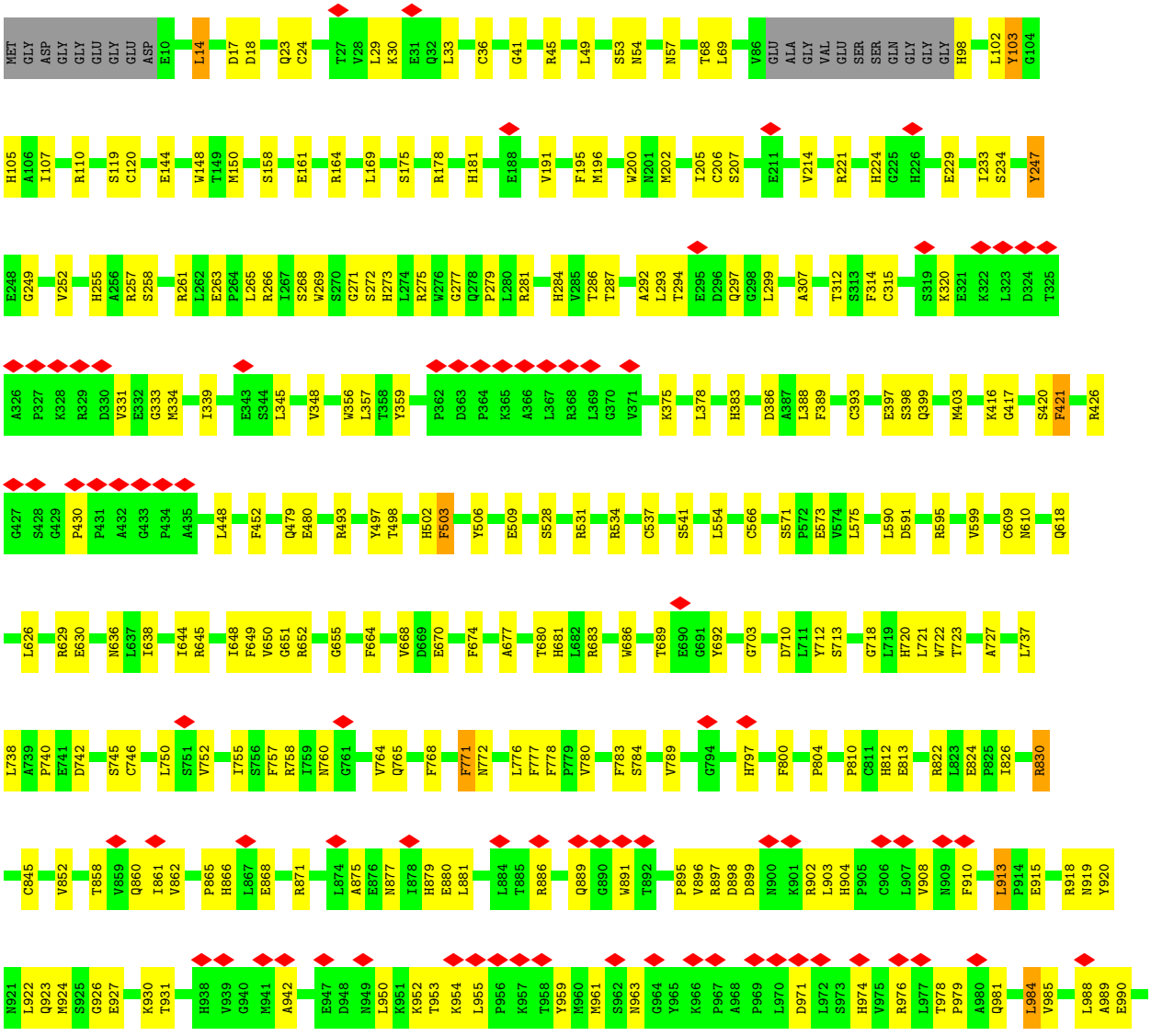
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			23	14	4	5	
5	B	1	Total	C	N	O	0
			23	14	4	5	
5	C	1	Total	C	N	O	0
			23	14	4	5	
5	D	1	Total	C	N	O	0
			23	14	4	5	

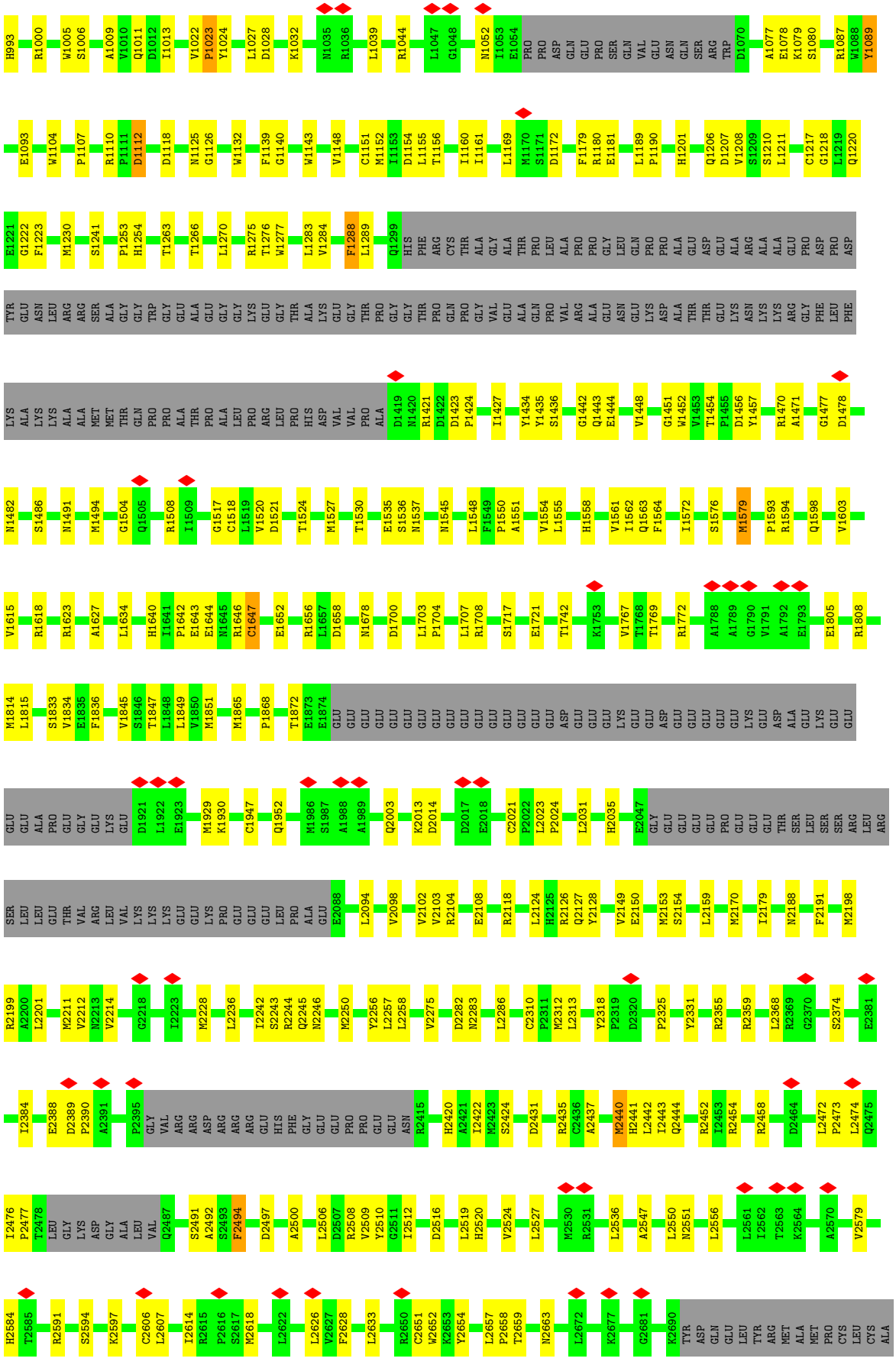
3 Residue-property plots (i)

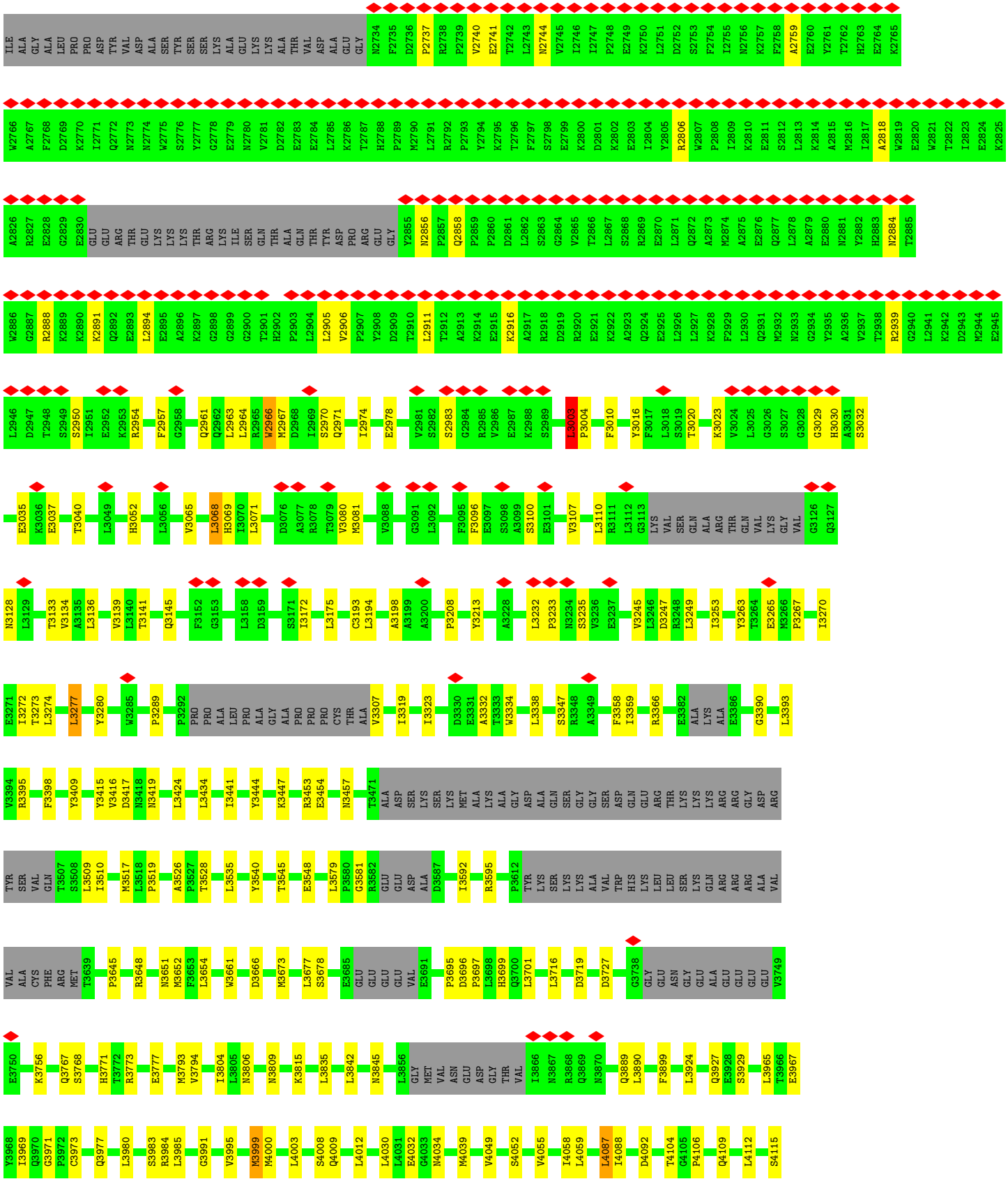
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

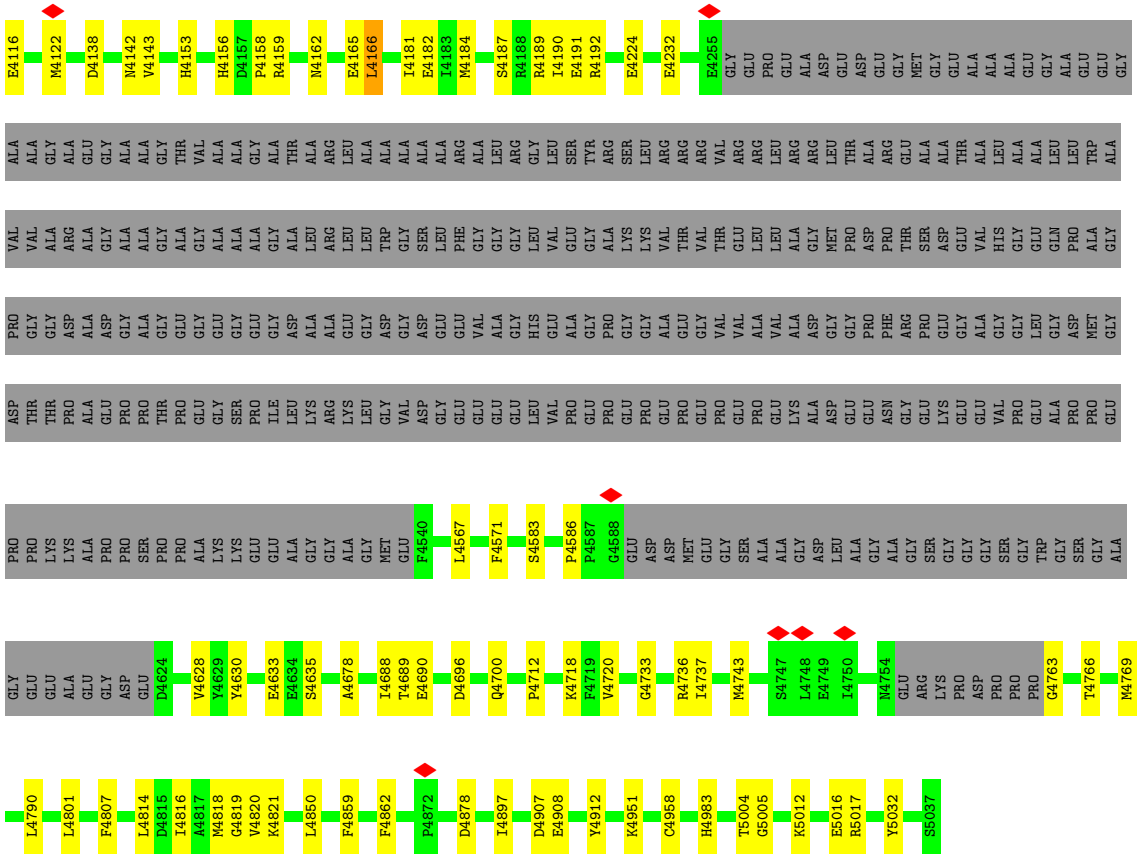
- Molecule 1: Ryanodine receptor 1

Chain A:



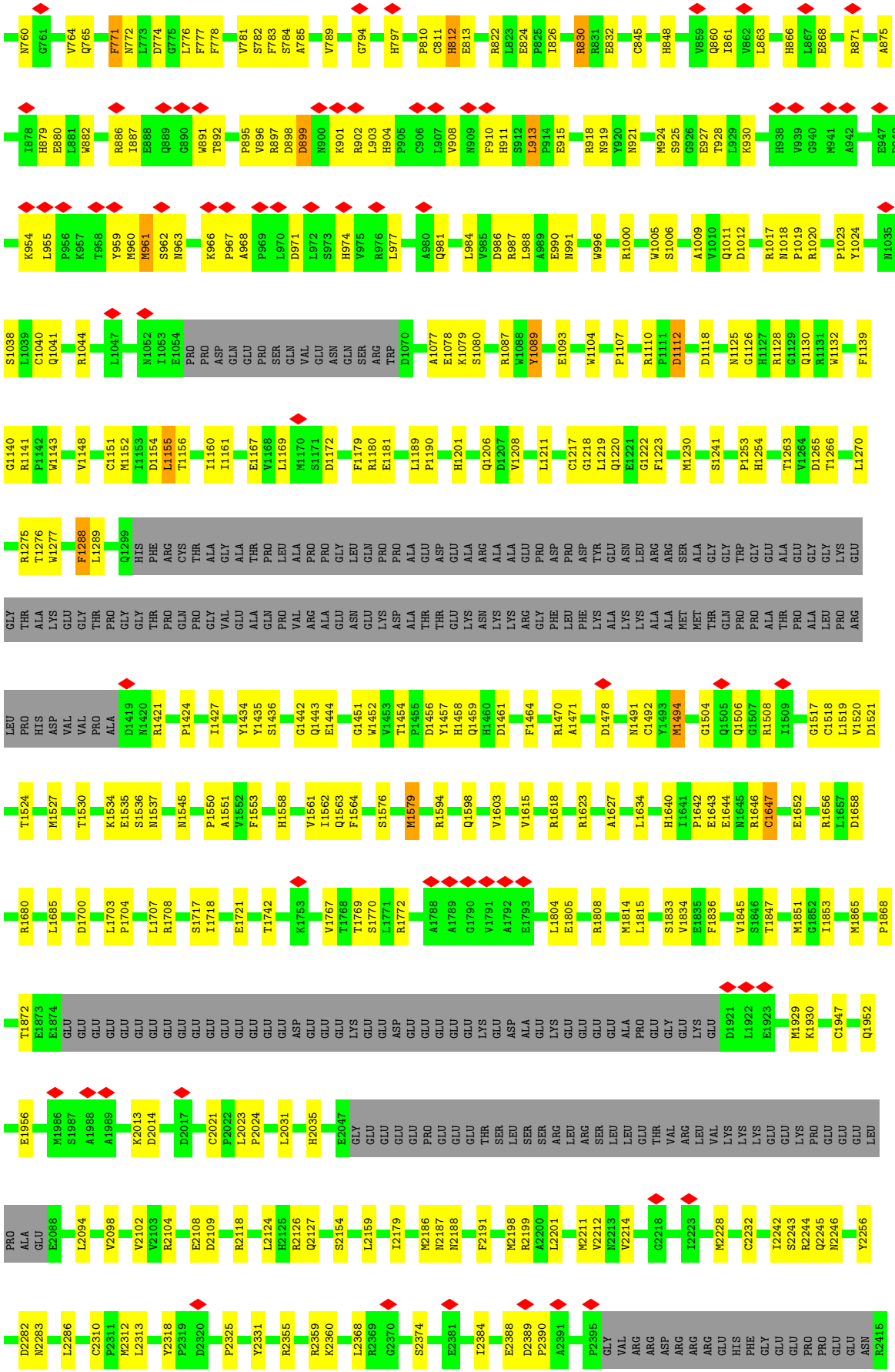


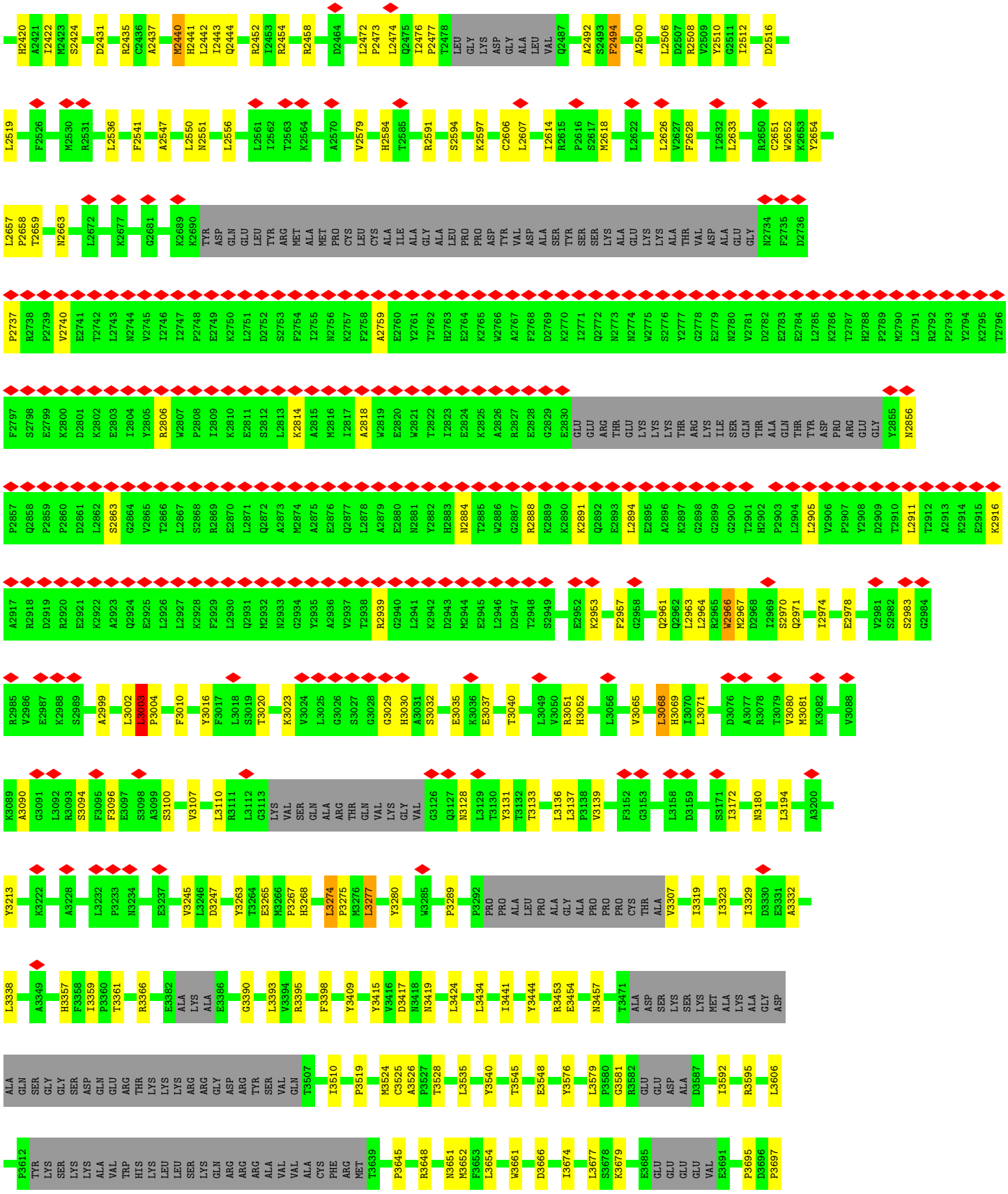

ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY
N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765
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 G2940 L2941 K2942 D2943 M2944 E2945
L2946 D2947 T2948 S2949 S2950 I2951 E2952 K2953 R2954 F2957 G2958 Q2961 Q2962 L2963 L2964 R2965 W2966 M2967 D2968 I2969 S2970 Q2971 I2974 E2978 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 L3003 P3004 F3010 Y3016 F3017 L3018 S3019 T3020 K3023 V3024 L3025 G3026 S3027 G3028 G3029 H3030 A3031 S3032
E3035 K3036 E3037 T3040 L3049 H3052 L3056 V3065 L3068 H3069 I3070 L3071 D3076 A3077 R3078 T3079 V3080 M3081 V3088 G3091 L3092 F3095 F3096 E3097 S3098 A3099 S3100 E3101 V3107 L3110 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL G3126 Q3127
N3128 L3129 T3133 V3134 A3135 L3136 V3139 L3140 T3141 Q3145 F3152 G3153 L3158 D3159 S3171 I3172 L3175 G3193 L3194 A3198 A3199 A3200 P3208 Y3213 A3228 L3232 P3233 N3234 S3235 V3236 E3237 V3245 L3246 D3247 R3248 L3249 I3253 Y3263 T3264 E3265 M3266 P3267 I3270
E3271 I3272 T3273 L3274 L3277 Y3280 W3285 P3289 P3292 PRO PRO ALA LEU PRO ALA GLY ALA PRO PRO PRO CYS THR ALA V3307 I3319 I3323 D3330 E3331 A3332 T3333 W3334 L3338 S3347 R3348 A3349 F3358 I3359 R3366 E3382 ALA LYS ALA E3386 G3390 L3393
V3394 R3395 F3398 Y3409 Y3415 V3416 D3417 N3418 N3419 L3424 L3434 I3441 Y3444 K3447 R3453 E3454 N3457 T3471 ALA ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG ARG GLY ASP ARG
TYR SER VAL GLN T3507 S3508 L3509 I3510 M3517 L3518 P3519 A3526 P3527 T3528 L3535 Y3540 T3545 E3548 L3579 P3580 G3581 R3582 GLU GLU ASP ALA D3587 I3592 R3595 P3612 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG GLY ALA VAL
VAL ALA CYS PHE ARG MET T3639 P3645 R3648 N3651 M3652 F3653 L3654 W3661 D3666 M3673 L3677 S3678 E3685 GLU GLU GLU GLU VAL E3691 P3695 D3696 P3697 L3698 H3699 Q3700 L3701 L3716 D3719 D3727 G3738 GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU V3749
E3750 K3756 Q3767 S3768 H3771 T3772 R3773 E3777 M3793 V3794 I3804 L3805 N3806 N3809 K3815 L3835 L3842 N3845 L3856 GLY MET VAL ASN GLU ASP GLY THR VAL I3866 N3867 R3868 Q3869 N3870 Q3889 L3890 F3899 L3924 Q3927 E3928 S3929 L3965 T3966 E3967
Y3968 I3969 Q3970 G3971 P3972 C3973 Q3977 L3980 S3983 R3984 L3985 G3991 V3995 M3999 M4000 L4003 S4008 Q4009 L4012 L4030 L4031 E4032 G4033 N4034 M4039 V4049 S4052 V4055 I4058 L4059 L4087 I4088 D4092 T4104 G4105 P4106 Q4109 L4112 S4115



• Molecule 1: Ryanodine receptor 1

Chain B:




H2420 A2421 I2422 M2423 S2424 D2431 R2435 C2436 A2437 M2440 H2441 L2442 I2443 Q2444 R2452 I2453 R2454 R2458 D2464 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 LEU GLY LYS ASP GLY ALA LEU VAL Q2487 A2492 S2493 F2494 A2500 L2506 D2507 R2508 V2509 Y2510 G2511 I2512 D2516
L2519 F2526 M2530 R2531 L2536 F2541 A2547 L2550 N2551 L2556 L2561 I2562 T2563 K2564 A2570 V2579 H2584 T2585 R2591 S2594 K2597 C2606 L2607 I2614 R2615 P2616 S2617 M2618 L2622 L2626 V2627 F2628 I2632 L2633 R2650 C2651 W2652 K2653 Y2654
L2657 P2658 T2659 N2663 L2672 K2677 G2681 K2689 K2690 TYR ASP GLN GLU LEU TYR ARG MET ALA MET PRO CYS LEU CYS ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736
P2737 R2738 P2739 V2740 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
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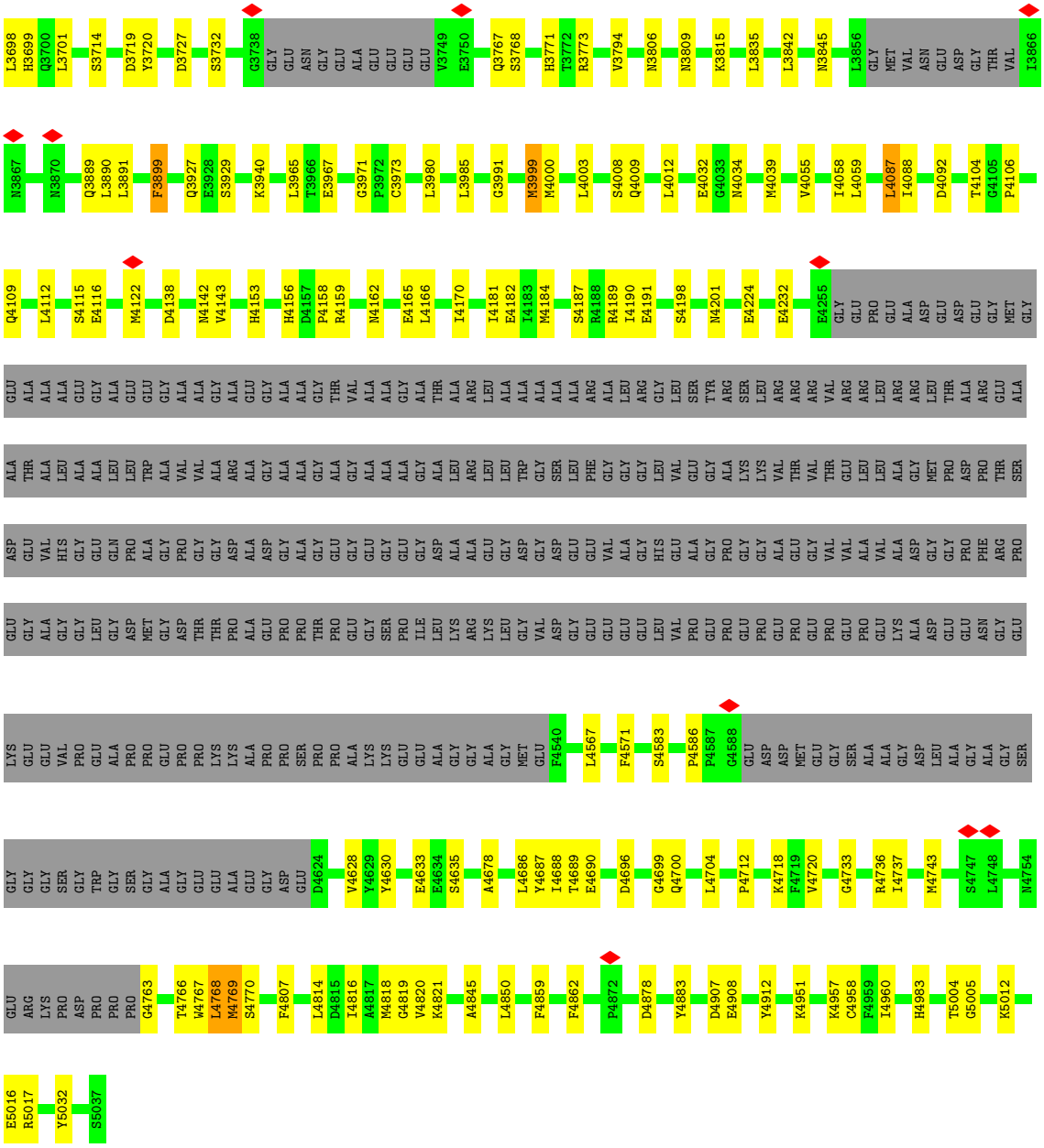
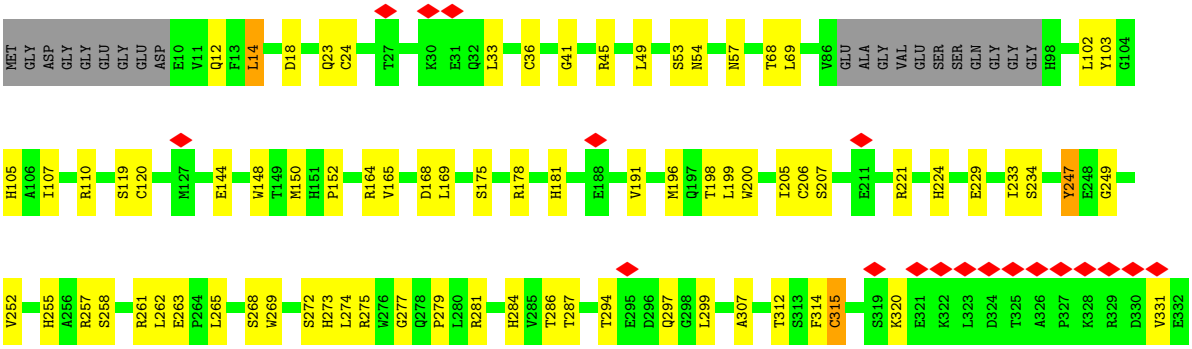
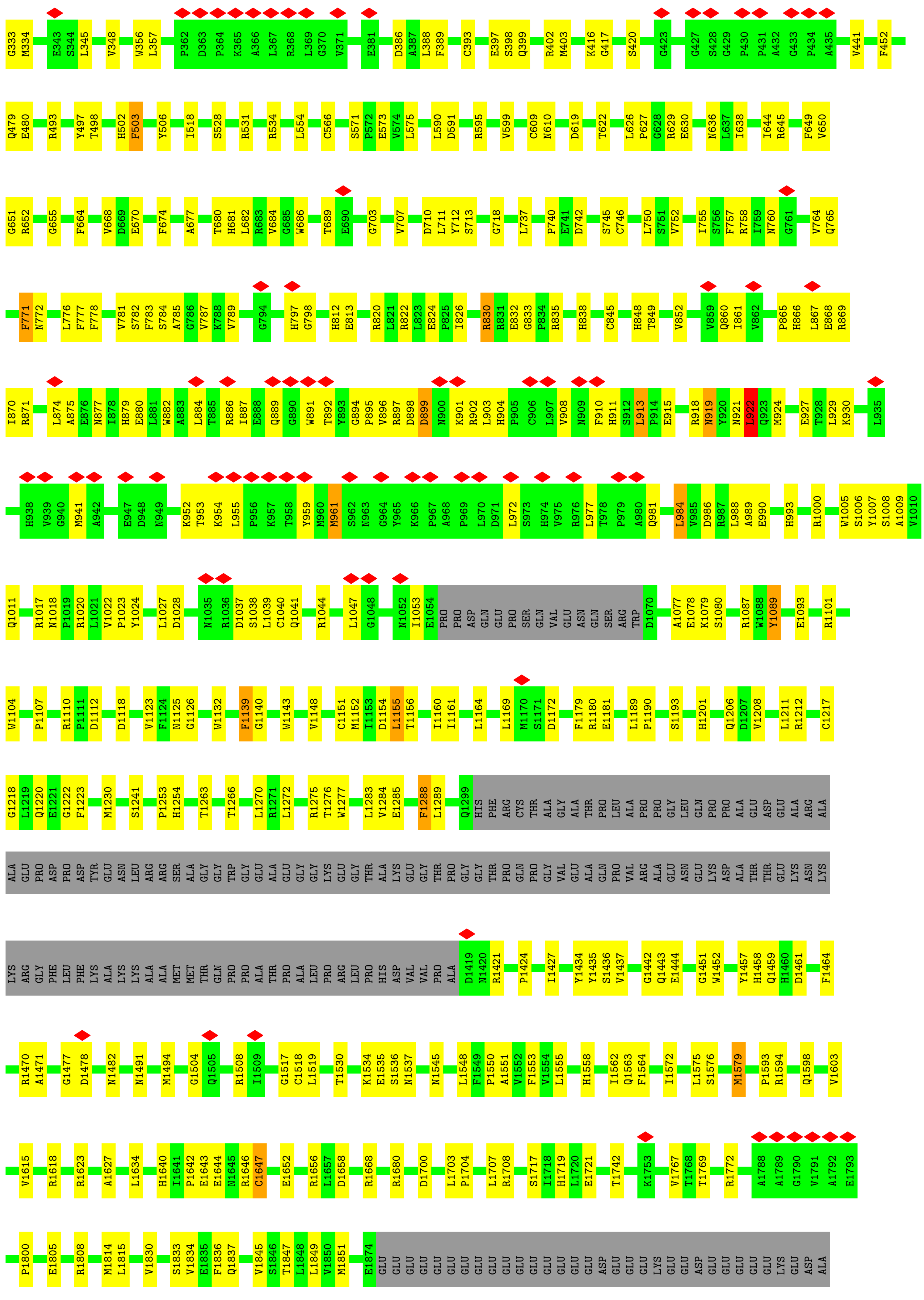
R2985 V2986 E2987 K2988 S2989 A2999 L3002 L3003 P3004 F3010 Y3016 F3017 L3018 S3019 T3020 K3023 V3024 L3025 G3026 S3027 G3028 G3029 H3030 A3031 S3032 E3035 K3036 E3037 T3040 L3049 V3050 R3051 H3052 L3056 V3065 L3068 H3069 I3070 L3071 D3076 A3077 R3078 T3079 V3080 M3081 K3082 V3088
K3089 A3090 G3091 L3092 R3093 S3094 F3095 F3096 E3097 S3098 A3099 S3100 V3107 L3110 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL G3126 Q3127 N3128 L3129 T3130 Y3131 T3132 T3133 L3136 L3137 P3138 V3139 F3152 G3153 L3158 D3159 S3171 I3172 N3180 L3194 A3200
Y3213 K3222 A3228 L3232 P3233 N3234 E3237 V3245 L3246 D3247 Y3263 T3264 E3265 M3266 P3267 H3268 L3274 P3275 M3276 L3277 Y3280 W3285 P3289 P3292 PRO PRO PRO ALA LEU PRO ALA GLY ALA PRO PRO PRO CYS THR ALA V3307 I3319 I3323 I3329 D3330 E3331 A3332
L3338 A3349 H3357 F3358 I3359 P3360 T3361 R3366 E3382 ALA LYS ALA E3386 G3390 L3393 V3394 R3395 F3398 Y3409 Y3415 V3416 D3417 N3418 N3419 L3424 L3434 I3441 Y3444 R3453 E3454 N3457 T3471 ALA ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP
ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG ARG TYR SER VAL GLN T3507 I3510 P3519 M3524 C3525 A3526 P3527 T3528 L3535 Y3540 T3545 E3548 Y3576 L3579 P3580 G3581 R3582 GLU GLU ASP ALA D3587 I3592 R3595 L3606
P3612 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3645 R3648 N3651 M3652 F3653 L3654 W3661 D3666 I3674 L3677 S3678 K3679 E3685 GLU GLU GLU GLU VAL E3691 P3695 D3696 P3697



• Molecule 1: Ryanodine receptor 1

Chain C:

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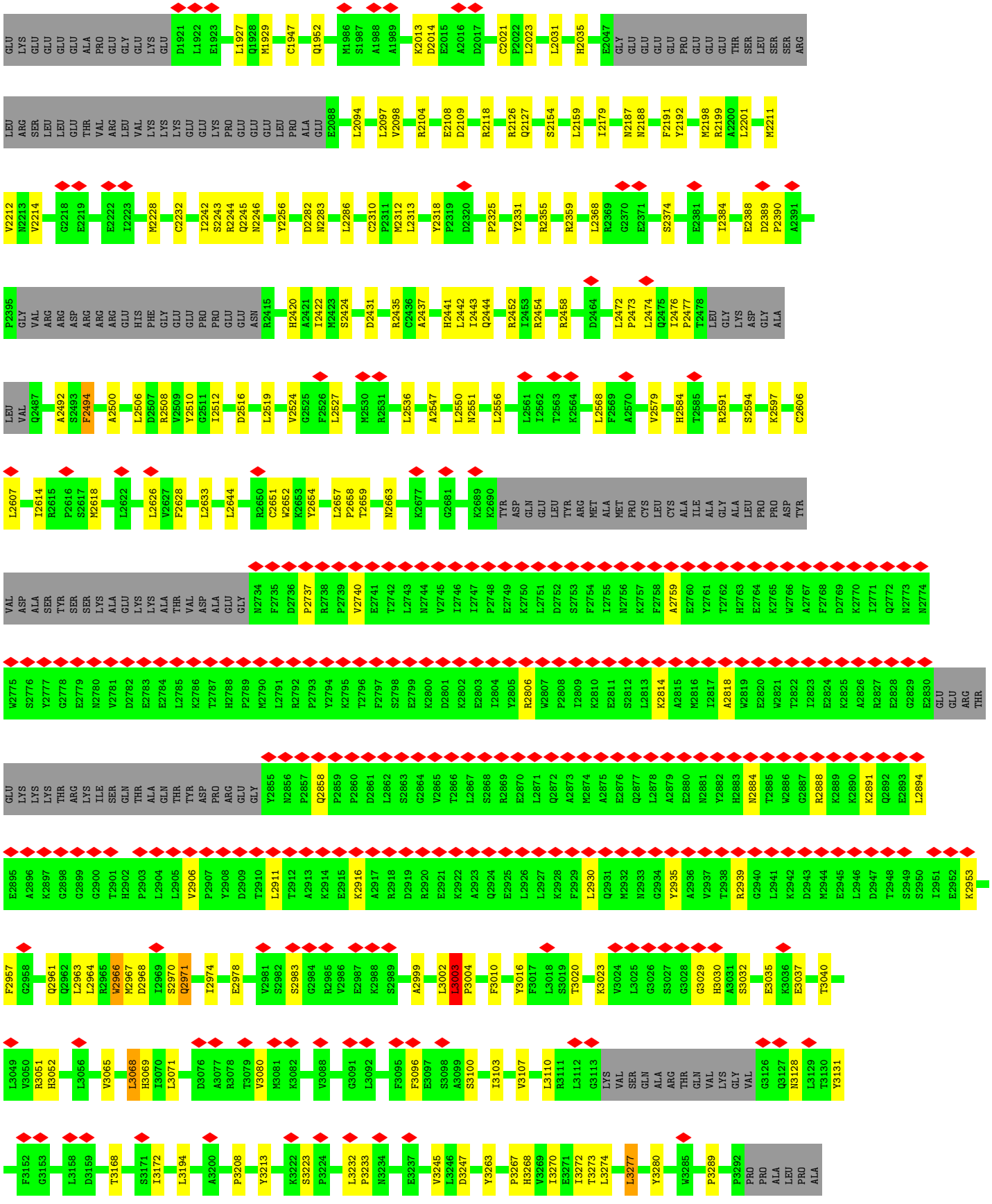
Q479 E480 R493 Y497 T498 H502 F503 Y506 I518 S528 R531 R534 L554 C566 S571 P572 E573 V574 L575 L590 D591 R595 V599 C609 N610 D619 T622 L626 P627 G628 R629 E630 N636 L637 I638 I644 R645 F649 V650
G651 R652 G655 F664 V668 D669 E670 F674 A677 T680 H681 L682 R683 V684 G685 W686 T689 E690 G703 V707 D710 L711 Y712 S713 G718 L737 P740 E741 D742 S745 C746 L750 S751 V752 I755 S756 F757 R758 I759 N760 G761 V764 Q765
F771 N772 L776 F777 F778 V781 S782 F783 S784 A785 G786 V787 K788 V789 G794 H797 G798 H812 E813 R820 L821 R822 L823 E824 P825 I826 R830 R831 E832 G833 P834 R835 H838 C845 H848 T849 V852 V859 Q860 I861 V862 P865 H866 L867 E868 R869
I870 R871 L874 A875 E876 N877 T878 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 R918 N919 Y920 N921 L922 Q923 M924 E927 T928 L929 K930 L935
H938 V939 G940 M941 A942 E947 D948 N949 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 T978 P979 A980 Q981 L984 V985 D986 R987 L988 A989 E990 H993 R1000 W1005 S1006 Y1007 S1008 A1009 V1010
Q1011 R1017 N1018 P1019 R1020 L1021 V1022 P1023 Y1024 L1027 D1028 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 R1044 L1047 G1048 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 A1077 E1078 K1079 S1080 R1087 W1088 Y1089 E1093 R1101
W1104 P1107 R1110 P1111 D1112 D1118 V1123 F1124 N1125 G1126 W1132 F1139 G1140 W1143 V1148 C1151 M1152 I1153 D1154 L1155 T1156 I1160 I1161 L1164 L1169 M1170 S1171 D1172 F1179 R1180 E1181 L1189 P1190 S1193 H1201 Q1206 D1207 V1208 L1211 R1212 C1217
G1218 L1219 Q1220 E1221 G1222 F1223 M1230 S1241 P1253 H1254 T1263 T1266 L1270 R1271 L1272 R1275 T1276 W1277 L1283 V1284 E1285 F1288 L1289 Q1299 HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA
ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS
LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 P1424 I1427 Y1434 Y1435 S1436 V1437 G1442 Q1443 E1444 G1451 W1452 Y1457 H1458 Q1459 H1460 D1461 F1464
R1470 A1471 G1477 D1478 N1482 N1491 M1494 G1504 Q1505 R1508 I1509 G1517 C1518 L1519 T1530 K1534 E1535 S1536 N1537 N1545 L1548 F1549 P1550 A1551 V1552 F1553 V1554 L1555 H1558 I1562 Q1563 F1564 I1572 L1575 S1576 M1579 P1593 R1594 Q1598 V1603
V1615 R1618 R1623 A1627 L1634 H1640 I1641 P1642 E1643 E1644 N1645 R1646 C1647 E1652 R1656 L1657 D1658 R1668 R1680 D1700 L1703 P1704 L1707 R1708 S1717 I1718 H1719 L1720 E1721 T1742 K1753 V1767 T1768 T1769 R1772 A1788 A1789 G1790 V1791 A1792 E1793
P1800 E1805 R1808 M1814 L1815 V1830 S1833 V1834 E1835 F1836 Q1837 V1845 S1846 T1847 L1848 L1849 V1850 M1851 E1874 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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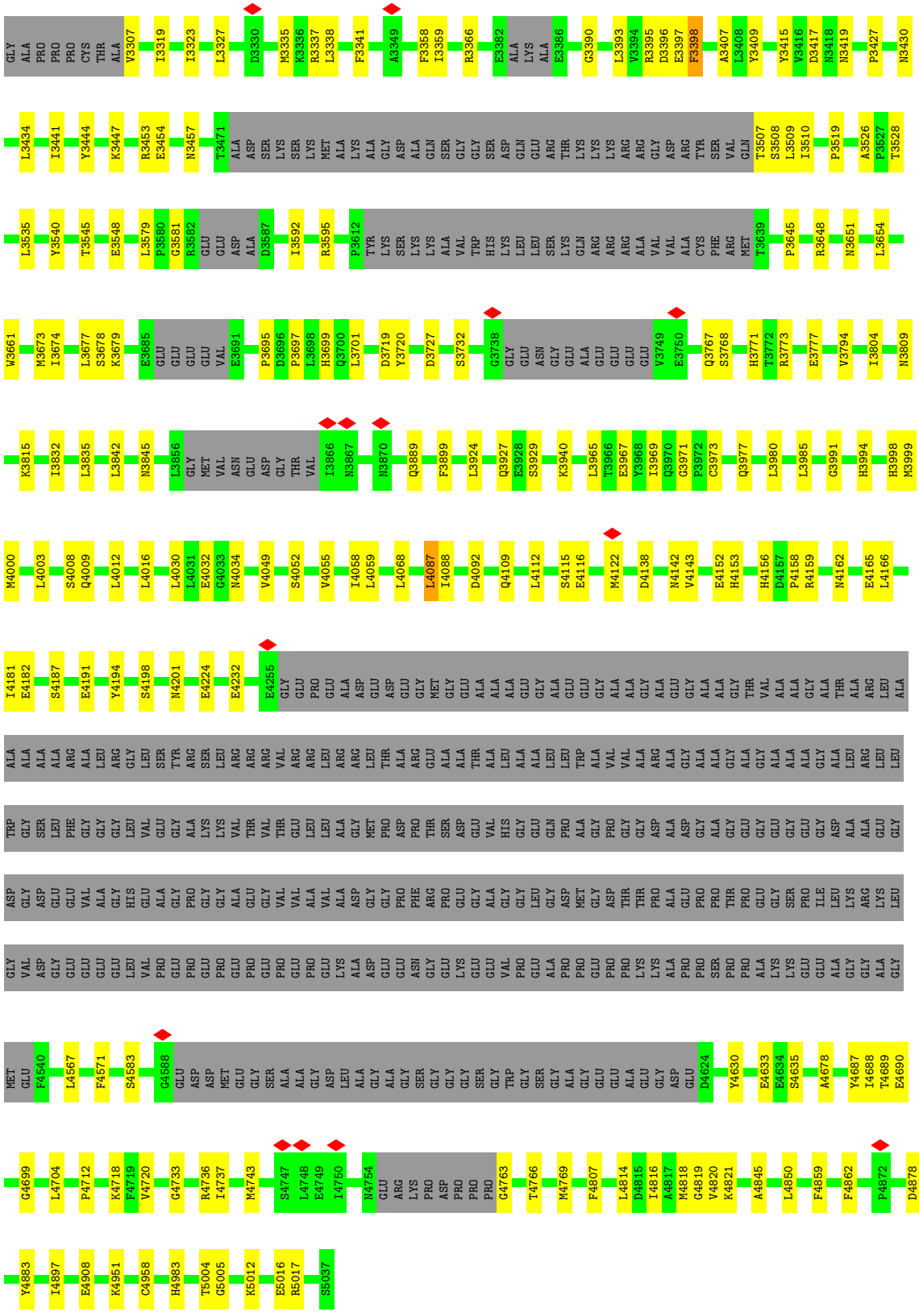
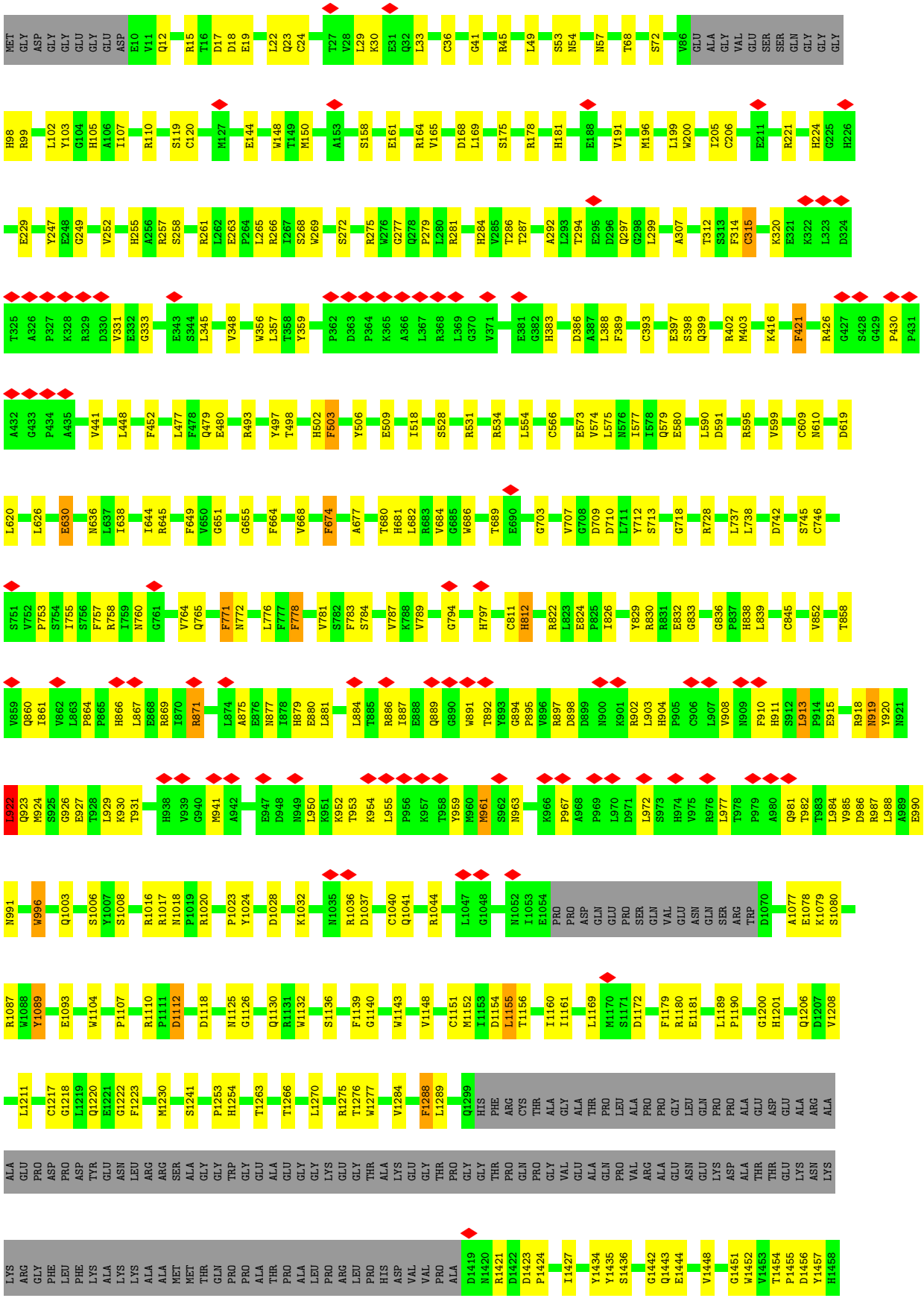
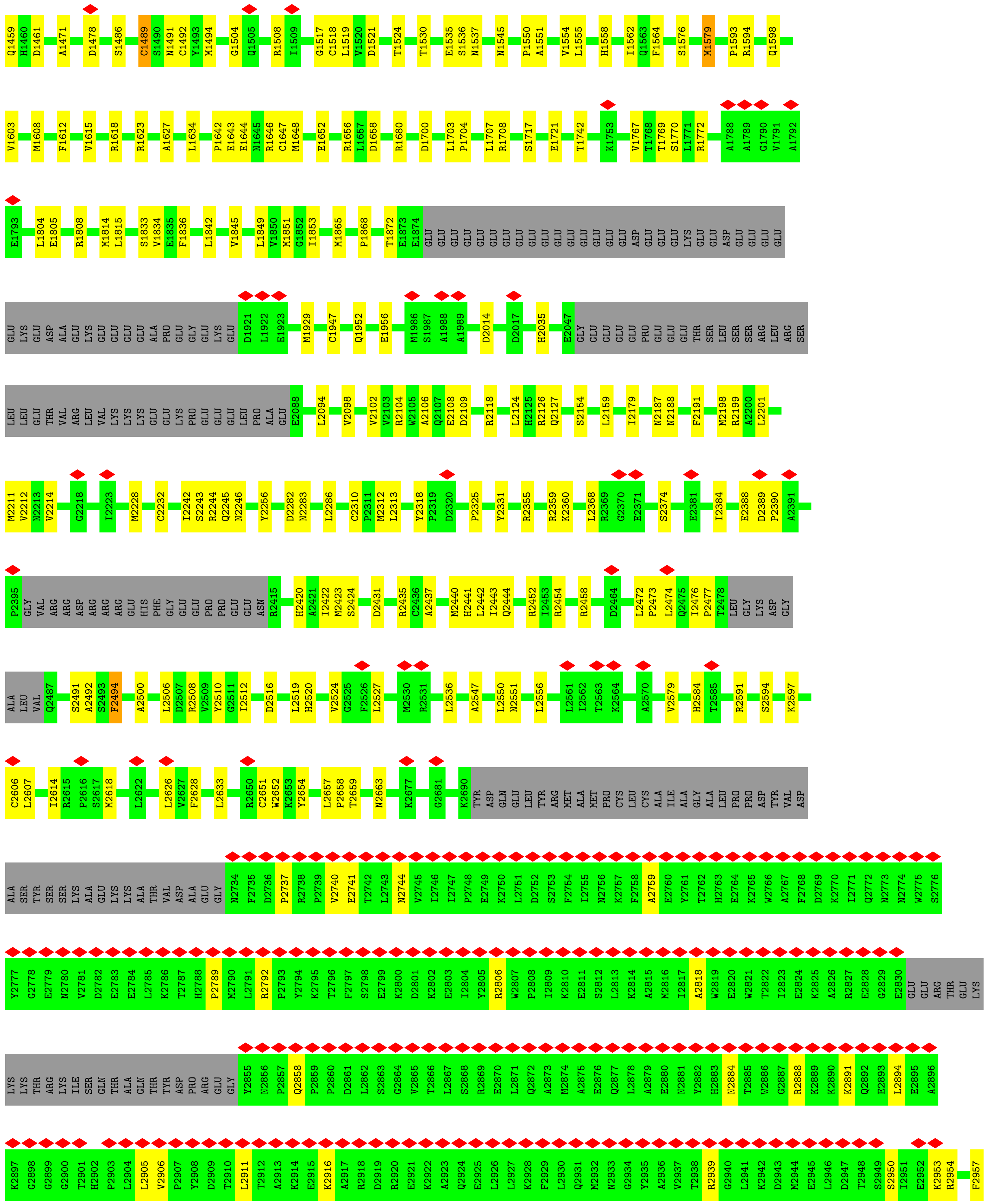
LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 L2094 L2097 V2098 R2104 E2108 D2109 R2118 R2126 Q2127 S2154 L2159 I2179 N2187 N2188 F2191 Y2192 M2198 R2199 A2200 L2201 M2211
V2212 N2213 V2214 G2218 E2219 E2222 I2223 M2228 C2232 I2242 S2243 R2244 Q2245 N2246 Y2256 D2282 N2283 L2286 C2310 P2311 M2312 L2313 Y2318 P2319 D2320 P2325 Y2331 R2355 R2359 L2368 R2369 G2370 E2371 S2374 E2381 I2384 E2388 D2389 P2390 A2391
P2395 GLY VAL ARG ARG ASP ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU ASN R2415 H2420 A2421 I2422 M2423 S2424 D2431 R2435 C2436 A2437 H2441 L2442 I2443 Q2444 R2452 I2453 R2454 R2458 D2464 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 LEU GLY LYS ASP GLY ALA
LEU VAL Q2487 A2492 S2493 F2494 A2500 L2506 D2507 R2508 V2509 Y2510 G2511 I2512 D2516 L2519 V2524 G2525 F2526 L2527 M2530 R2531 L2536 A2547 L2550 N2551 L2556 L2561 I2562 T2563 K2564 L2568 F2569 A2570 V2579 H2584 T2585 R2591 S2594 K2597 C2606
L2607 I2614 R2615 P2616 S2617 M2618 L2622 L2626 V2627 F2628 L2633 L2644 R2650 C2651 W2652 K2653 Y2654 L2657 P2658 T2659 N2663 K2677 G2681 K2689 K2690 TYR ASP GLN GLU LEU TYR ARG MET ALA MET PRO CYS LEU CYS ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR
VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 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 P2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 G2940 L2941 K2942 D2943 M2944 E2945 L2946 D2947 T2948 S2949 S2950 I2951 E2952 K2953
F2957 G2958 Q2961 Q2962 L2963 L2964 R2965 W2966 M2967 D2968 I2969 S2970 Q2971 I2974 E2978 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 A2999 L3002 L3003 P3004 F3010 Y3016 F3017 L3018 S3019 T3020 K3023 V3024 L3025 G3026 S3027 G3028 G3029 H3030 A3031 S3032 E3035 K3036 E3037 T3040
L3049 V3050 R3051 H3052 L3056 V3065 L3068 H3069 I3070 L3071 D3076 A3077 R3078 T3079 V3080 M3081 K3082 V3088 G3091 L3092 F3095 F3096 E3097 S3098 A3099 S3100 I3103 Y3107 L3110 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL G3126 G3127 N3128 L3129 T3130 Y3131
F3152 G3153 L3158 D3159 T3168 S3171 I3172 L3194 A3200 P3208 Y3213 K3222 S3223 P3224 L3232 P3233 N3234 E3237 V3245 L3246 D3247 Y3263 P3267 H3268 V3269 I3270 E3271 I3272 T3273 L3274 L3277 Y3280 W3285 P3289 P3292 PRO PRO ALA LEU PRO ALA



• Molecule 1: Ryanodine receptor 1

Chain D:

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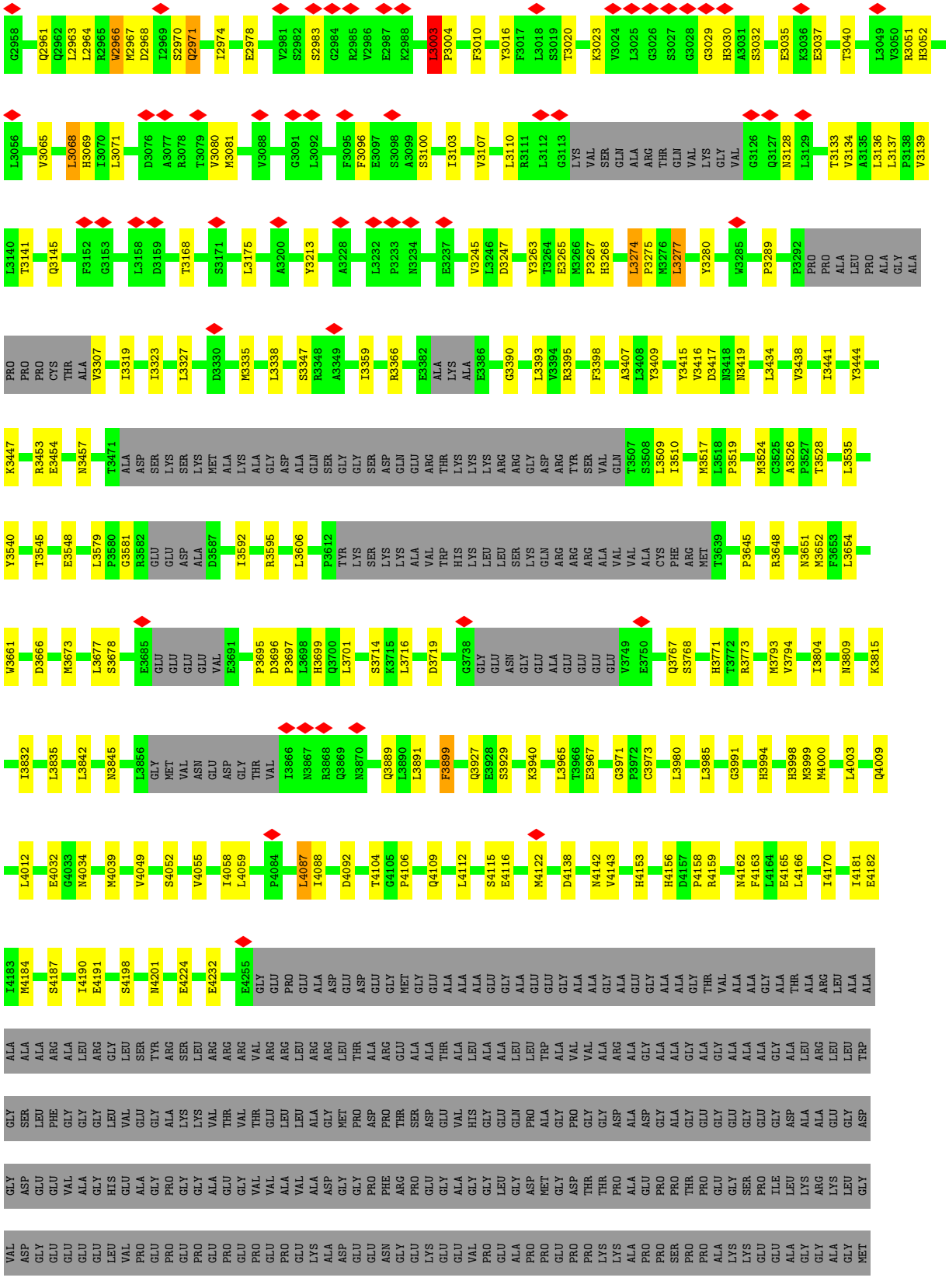
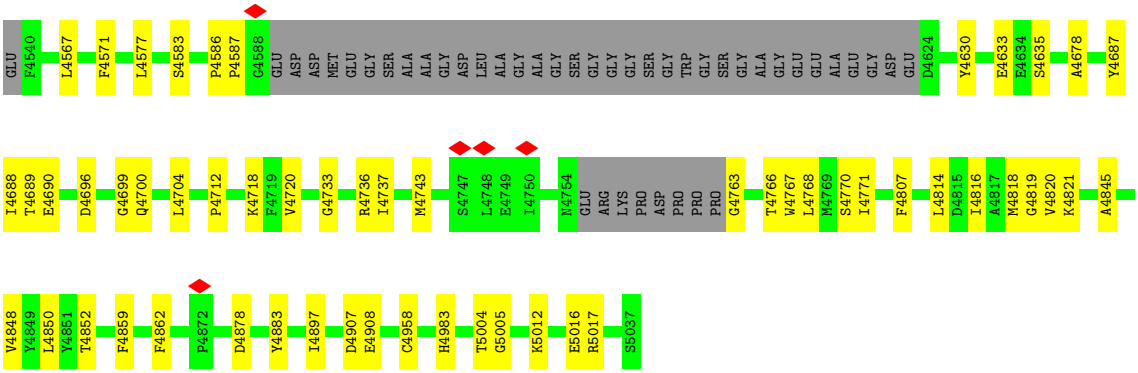
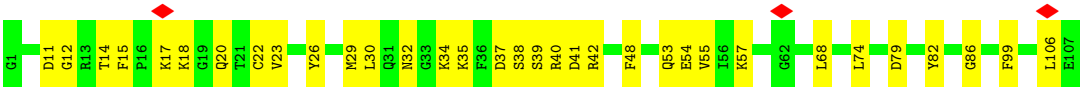
V1603 M1608 F1612 V1615 R1618 R1623 A1627 L1634 P1642 E1643 E1644 N1645 R1646 C1647 M1648 E1652 R1656 L1657 D1658 R1680 D1700 L1703 P1704 L1707 R1708 S1717 E1721 T1742 K1753 V1767 T1768 T1769 S1770 L1771 R1772 A1788 A1789 G1790 V1791 A1792
E1793 L1804 E1805 R1808 M1814 L1815 S1833 V1834 E1835 F1836 L1842 V1845 L1849 V1850 M1851 G1852 I1853 M1865 P1868 T1872 E1873 E1874 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 D1921 L1922 E1923 M1929 C1947 Q1952 E1956 M1986 S1987 A1988 A1989 D2014 D2017 H2035 E2047 GLY 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 E2088 L2094 V2098 V2102 V2103 R2104 W2105 A2106 Q2107 E2108 D2109 R2118 L2124 H2125 R2126 Q2127 S2154 L2159 I2179 N2187 N2188 F2191 M2198 R2199 A2200 L2201
M2211 V2212 N2213 V2214 G2218 I2223 M2228 C2232 I2242 S2243 R2244 Q2245 N2246 Y2256 D2282 N2283 L2286 C2310 P2311 M2312 L2313 Y2318 P2319 D2320 P2325 Y2331 R2355 R2359 K2360 L2368 R2369 G2370 E2371 S2374 E2381 I2384 E2388 D2389 P2390 A2391
P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU ASN R2415 H2420 A2421 I2422 M2423 S2424 D2431 R2435 C2436 A2437 M2440 H2441 L2442 I2443 Q2444 R2452 I2453 R2454 R2458 D2464 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 LEU GLY LYS ASP GLY
ALA LEU VAL Q2487 S2491 A2492 S2493 F2494 A2500 L2506 D2507 R2508 V2509 Y2510 G2511 I2512 D2516 L2519 H2520 V2524 G2525 F2526 L2527 M2530 R2531 L2536 A2547 L2550 N2551 L2556 L2561 I2562 T2563 K2564 A2570 V2579 H2584 T2585 R2591 S2594 K2597
C2606 L2607 I2614 R2615 P2616 S2617 M2618 L2622 L2626 V2627 F2628 L2633 R2650 C2651 W2652 K2653 Y2654 L2657 P2658 T2659 N2663 K2677 G2681 K2690 TYR ASP GLN GLU LEU TYR ARG MET ALA MET PRO CYS LEU CYS ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP
ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 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 S2859 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 G2940 L2941 K2942 D2943 M2944 E2945 L2946 D2947 T2948 S2949 S2950 I2951 E2952 K2953 R2954 F2957





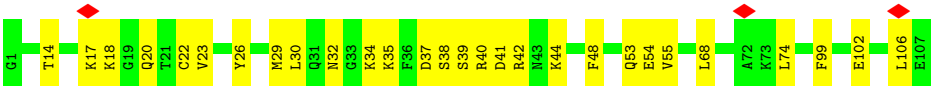
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



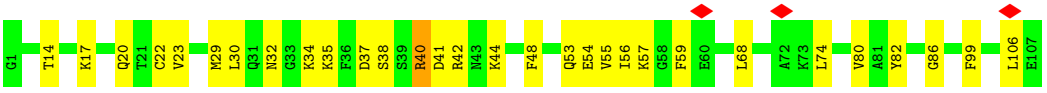
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



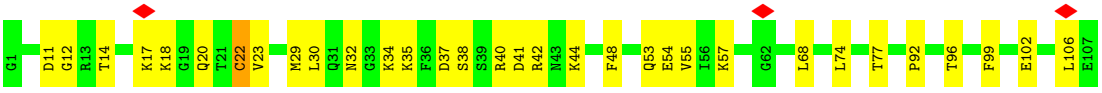
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249034	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.277	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, U1C, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/33082	0.48	3/45015 (0.0%)
1	B	0.24	0/33082	0.47	2/45015 (0.0%)
1	C	0.24	0/33082	0.48	4/45015 (0.0%)
1	D	0.25	0/33082	0.48	5/45015 (0.0%)
2	E	0.26	0/802	0.52	0/1086
2	F	0.27	0/802	0.54	0/1086
2	G	0.27	0/802	0.55	0/1086
2	H	0.26	0/802	0.52	0/1086
All	All	0.25	0/135536	0.48	14/184404 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3003	LEU	CA-CB-CG	7.13	131.69	115.30
1	C	3003	LEU	CA-CB-CG	7.11	131.64	115.30
1	D	3003	LEU	CA-CB-CG	7.03	131.48	115.30
1	A	3003	LEU	CA-CB-CG	7.00	131.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	922	LEU	CA-CB-CG	6.73	130.77	115.30
1	D	922	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	984	LEU	CA-CB-CG	5.78	128.60	115.30
1	B	3274	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	2644	LEU	CA-CB-CG	5.41	127.75	115.30
1	C	14	LEU	CA-CB-CG	5.40	127.73	115.30
1	D	3274	LEU	CA-CB-CG	5.33	127.55	115.30
1	D	988	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	14	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	832	GLU	CB-CA-C	5.06	120.52	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	626	LEU	Peptide
1	B	626	LEU	Peptide
1	C	626	LEU	Peptide
1	D	626	LEU	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	32374	0	30869	505	0
1	B	32374	0	30869	488	0
1	C	32374	0	30869	498	0
1	D	32374	0	30869	514	0
2	E	786	0	766	22	0
2	F	786	0	766	20	0
2	G	786	0	766	21	0
2	H	786	0	766	26	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
All	All	132860	0	126588	2070	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 8.

All (2070) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:830:ARG:HD3	1:D:1612:PHE:CE2	1.70	1.26
1:D:1454:THR:CG2	1:D:1456:ASP:OD1	2.09	0.99
1:D:830:ARG:CD	1:D:1612:PHE:CE2	2.45	0.99
1:D:1454:THR:HG23	1:D:1456:ASP:OD1	1.63	0.97
1:B:4763:GLY:N	1:B:4766:THR:HG1	1.62	0.95
1:D:833:GLY:HA3	1:D:838:HIS:HD2	1.32	0.92
1:D:830:ARG:NH1	1:D:1612:PHE:CD2	2.39	0.91
1:C:4763:GLY:N	1:C:4766:THR:HG1	1.75	0.85
1:C:707:VAL:HG23	1:C:713:SER:OG	1.78	0.83
1:D:4763:GLY:N	1:D:4766:THR:HG1	1.76	0.83
1:D:3003:LEU:HD12	1:D:3004:PRO:HD3	1.60	0.83
1:D:897:ARG:HG2	1:D:898:ASP:H	1.44	0.82
1:C:911:HIS:ND1	1:C:911:HIS:O	2.12	0.82
1:B:3003:LEU:HD12	1:B:3004:PRO:HD3	1.61	0.81
1:B:609:CYS:SG	1:B:610:ASN:N	2.53	0.81
1:B:1451:GLY:HA3	1:B:1494:MET:HB3	1.62	0.81
1:C:69:LEU:HD11	1:C:107:ILE:HD11	1.63	0.81
1:C:3003:LEU:HD12	1:C:3004:PRO:HD3	1.60	0.81
1:A:3003:LEU:HD12	1:A:3004:PRO:HD3	1.61	0.81
1:C:609:CYS:SG	1:C:610:ASN:N	2.53	0.81
1:B:707:VAL:HG23	1:B:713:SER:OG	1.81	0.80
1:D:609:CYS:SG	1:D:610:ASN:N	2.53	0.80
1:D:1454:THR:HG21	1:D:1456:ASP:OD1	1.81	0.79
1:D:830:ARG:NH1	1:D:1612:PHE:HD2	1.82	0.78
1:A:609:CYS:SG	1:A:610:ASN:N	2.53	0.78
1:C:1437:VAL:HG13	1:C:1562:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.67	0.76
1:D:3277:LEU:HA	1:D:3280:TYR:HB3	1.66	0.76
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.67	0.76
1:D:833:GLY:HA3	1:D:838:HIS:CD2	2.20	0.76
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.66	0.76
1:B:3277:LEU:HA	1:B:3280:TYR:HB3	1.68	0.75
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.67	0.75
1:C:3277:LEU:HA	1:C:3280:TYR:HB3	1.68	0.75
1:A:4763:GLY:N	1:A:4766:THR:HG1	1.83	0.74
1:D:686:TRP:HE1	1:D:746:CYS:HG	1.36	0.74
1:A:3277:LEU:HA	1:A:3280:TYR:HB3	1.69	0.73
1:B:205:ILE:HG22	1:B:206:CYS:H	1.54	0.72
1:C:3651:ASN:HA	1:C:3654:LEU:HD12	1.71	0.72
1:B:1018:ASN:HD21	1:B:1020:ARG:HG2	1.53	0.72
1:D:1130:GLN:NE2	1:D:1136:SER:OG	2.23	0.72
1:D:3651:ASN:HA	1:D:3654:LEU:HD12	1.72	0.72
1:B:897:ARG:HG2	1:B:898:ASP:H	1.55	0.71
1:C:897:ARG:HG2	1:C:898:ASP:H	1.56	0.71
1:A:897:ARG:HG2	1:A:898:ASP:H	1.56	0.71
1:A:3651:ASN:HA	1:A:3654:LEU:HD12	1.71	0.71
1:D:102:LEU:HB3	1:D:105:HIS:CD2	2.25	0.71
1:D:205:ILE:HG22	1:D:206:CYS:H	1.54	0.71
1:A:638:ILE:HG21	1:A:703:GLY:HA3	1.73	0.70
1:A:942:ALA:HB2	1:A:1052:ASN:HB3	1.73	0.70
1:A:2651:CYS:SG	1:A:2652:TRP:N	2.65	0.70
1:B:686:TRP:HE1	1:B:746:CYS:HG	1.38	0.70
1:D:794:GLY:O	1:D:812:HIS:ND1	2.25	0.69
1:D:2651:CYS:SG	1:D:2652:TRP:N	2.65	0.69
1:B:2651:CYS:SG	1:B:2652:TRP:N	2.65	0.69
1:B:3651:ASN:HA	1:B:3654:LEU:HD12	1.72	0.69
1:A:4850:LEU:HD11	1:B:4814:LEU:HB2	1.74	0.69
1:B:2626:LEU:HG	1:B:2628:PHE:H	1.58	0.69
1:D:830:ARG:CD	1:D:1612:PHE:HE2	2.04	0.69
1:A:4814:LEU:HB2	1:D:4850:LEU:HD11	1.75	0.69
1:B:681:HIS:HB3	1:B:784:SER:HB3	1.73	0.69
1:A:2524:VAL:HA	1:A:2527:LEU:HD23	1.74	0.69
1:C:2651:CYS:SG	1:C:2652:TRP:N	2.64	0.69
1:B:1128:ARG:HB2	1:B:1130:GLN:HE21	1.58	0.69
1:A:2626:LEU:HG	1:A:2628:PHE:H	1.58	0.68
1:B:4850:LEU:HD11	1:C:4814:LEU:HB2	1.74	0.68
1:C:2626:LEU:HG	1:C:2628:PHE:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:ILE:HG21	1:D:703:GLY:HA3	1.75	0.68
1:D:4820:VAL:HG23	1:D:4821:LYS:H	1.59	0.68
1:C:4850:LEU:HD11	1:D:4814:LEU:HB2	1.75	0.68
1:B:638:ILE:HG21	1:B:703:GLY:HA3	1.76	0.68
1:A:4820:VAL:HG23	1:A:4821:LYS:H	1.59	0.68
1:C:629:ARG:O	1:C:630:GLU:HG3	1.93	0.68
1:C:861:ILE:HB	1:C:930:LYS:HZ2	1.58	0.68
1:B:4820:VAL:HG23	1:B:4821:LYS:H	1.59	0.68
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.76	0.68
1:D:830:ARG:HD3	1:D:1612:PHE:CZ	2.26	0.67
1:D:961:MET:HE2	1:D:963:ASN:H	1.58	0.67
1:B:2441:HIS:HA	1:B:2444:GLN:HB3	1.76	0.67
1:C:14:LEU:HD11	1:C:69:LEU:HD13	1.75	0.67
1:D:2626:LEU:HG	1:D:2628:PHE:H	1.58	0.67
1:B:629:ARG:O	1:B:630:GLU:HG3	1.95	0.67
1:A:102:LEU:HB3	1:A:105:HIS:CD2	2.30	0.67
1:C:4820:VAL:HG23	1:C:4821:LYS:H	1.61	0.66
1:D:2579:VAL:HG22	1:D:2594:SER:HB2	1.78	0.66
1:A:590:LEU:HB2	1:A:599:VAL:HG11	1.78	0.66
1:C:638:ILE:HG21	1:C:703:GLY:HA3	1.77	0.66
1:D:23:GLN:NE2	1:D:36:CYS:SG	2.69	0.66
1:C:977:LEU:HB3	1:C:981:GLN:HB2	1.78	0.66
1:C:2579:VAL:HG22	1:C:2594:SER:HB2	1.77	0.66
1:D:102:LEU:HB3	1:D:105:HIS:HD2	1.61	0.66
1:D:3716:LEU:HD13	1:D:3793:MET:HG2	1.78	0.66
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.76	0.65
1:B:2214:VAL:HG21	1:B:2228:MET:HE1	1.77	0.65
1:C:12:GLN:HE22	1:C:14:LEU:HD22	1.61	0.65
1:C:3697:PRO:O	1:C:3701:LEU:N	2.24	0.65
1:A:3716:LEU:HD13	1:A:3793:MET:HG2	1.78	0.65
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.76	0.65
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.77	0.65
1:B:772:ASN:HD22	1:B:1471:ALA:H	1.42	0.65
2:F:37:ASP:OD1	2:F:42:ARG:NH2	2.30	0.65
1:C:23:GLN:NE2	1:C:36:CYS:SG	2.69	0.65
1:D:590:LEU:HB2	1:D:599:VAL:HG11	1.79	0.65
1:D:2442:LEU:HG	1:D:2443:ILE:HG12	1.79	0.65
1:A:868:GLU:O	1:A:871:ARG:HG3	1.95	0.65
1:C:590:LEU:HB2	1:C:599:VAL:HG11	1.78	0.65
1:A:2579:VAL:HG22	1:A:2594:SER:HB2	1.77	0.65
1:A:3697:PRO:O	1:A:3701:LEU:N	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2579:VAL:HG22	1:B:2594:SER:HB2	1.78	0.64
1:A:3080:VAL:HG13	1:A:3081:MET:HE3	1.79	0.64
1:A:879:HIS:NE2	1:A:908:VAL:O	2.29	0.64
1:D:861:ILE:O	1:D:930:LYS:NZ	2.31	0.64
1:D:664:PHE:HB3	1:D:746:CYS:HB3	1.78	0.64
1:D:1804:LEU:HD12	1:D:1853:ILE:HG21	1.79	0.64
1:C:3052:HIS:NE2	1:C:3128:ASN:O	2.30	0.63
1:A:629:ARG:O	1:A:630:GLU:HG3	1.98	0.63
1:C:1459:GLN:HE22	1:C:1461:ASP:HB2	1.63	0.63
1:D:681:HIS:HB3	1:D:784:SER:HB3	1.80	0.63
1:D:1459:GLN:HE22	1:D:1461:ASP:HB2	1.63	0.63
1:A:23:GLN:NE2	1:A:36:CYS:SG	2.72	0.63
1:B:3319:ILE:HD11	1:B:3338:LEU:HD11	1.79	0.63
1:D:977:LEU:HB3	1:D:981:GLN:HB2	1.80	0.63
1:C:2214:VAL:HG21	1:C:2228:MET:HE1	1.80	0.63
1:A:348:VAL:HG13	1:A:357:LEU:HD23	1.80	0.63
1:B:348:VAL:HG13	1:B:357:LEU:HD23	1.81	0.63
1:B:3080:VAL:HG13	1:B:3081:MET:HE3	1.80	0.63
2:G:23:VAL:HG21	2:G:106:LEU:HB2	1.80	0.63
2:E:37:ASP:OD1	2:E:42:ARG:NH2	2.32	0.63
1:A:2961:GLN:HA	1:A:2964:LEU:HB3	1.81	0.63
1:A:664:PHE:HB3	1:A:746:CYS:HB3	1.81	0.63
1:A:1457:TYR:HA	1:A:1491:ASN:HD22	1.63	0.63
1:C:879:HIS:NE2	1:C:908:VAL:O	2.31	0.63
1:A:722:TRP:CD1	1:A:727:ALA:HA	2.34	0.62
1:B:794:GLY:O	1:B:812:HIS:ND1	2.27	0.62
1:D:3697:PRO:O	1:D:3701:LEU:N	2.26	0.62
2:H:37:ASP:OD1	2:H:42:ARG:NH2	2.32	0.62
1:A:2441:HIS:HA	1:A:2444:GLN:HB3	1.81	0.62
1:B:1804:LEU:HD12	1:B:1853:ILE:HG21	1.80	0.62
1:C:2961:GLN:HA	1:C:2964:LEU:HB3	1.81	0.62
1:C:4166:LEU:HD23	1:C:4166:LEU:H	1.64	0.62
1:B:4088:ILE:HB	1:B:4092:ASP:HB2	1.81	0.62
2:F:23:VAL:HG21	2:F:106:LEU:HB2	1.80	0.62
2:H:23:VAL:HG21	2:H:106:LEU:HB2	1.79	0.62
1:A:1576:SER:HA	1:A:1579:MET:HB2	1.82	0.62
1:B:590:LEU:HB2	1:B:599:VAL:HG11	1.80	0.62
1:C:3592:ILE:HA	1:C:3595:ARG:HE	1.64	0.62
1:D:879:HIS:NE2	1:D:908:VAL:O	2.28	0.62
2:G:37:ASP:OD1	2:G:42:ARG:NH2	2.32	0.62
1:A:1289:LEU:HB2	1:A:1550:PRO:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4003:LEU:HG	1:B:4009:GLN:HG3	1.82	0.62
1:D:3592:ILE:HA	1:D:3595:ARG:HE	1.64	0.62
1:B:961:MET:HE2	1:B:963:ASN:H	1.64	0.62
1:D:2214:VAL:HG21	1:D:2228:MET:HE1	1.82	0.62
1:D:4088:ILE:HB	1:D:4092:ASP:HB2	1.82	0.62
1:A:2214:VAL:HG21	1:A:2228:MET:HE1	1.81	0.62
2:E:74:LEU:HB2	2:E:99:PHE:HB2	1.82	0.62
1:A:1742:THR:HG22	1:A:1769:THR:HG21	1.82	0.61
1:A:205:ILE:HG22	1:A:206:CYS:H	1.65	0.61
1:A:988:LEU:HG	1:A:1039:LEU:HD12	1.81	0.61
1:B:1289:LEU:HB2	1:B:1550:PRO:HD2	1.81	0.61
1:B:3697:PRO:O	1:B:3701:LEU:N	2.30	0.61
1:C:1457:TYR:HA	1:C:1491:ASN:HD22	1.65	0.61
1:A:681:HIS:HB3	1:A:784:SER:HB3	1.82	0.61
1:C:3016:TYR:HA	1:C:3029:GLY:HA2	1.82	0.61
1:A:737:LEU:HD23	1:A:738:LEU:H	1.65	0.61
1:D:348:VAL:HG13	1:D:357:LEU:HD23	1.81	0.61
1:D:677:ALA:HB1	2:H:40:ARG:HB3	1.82	0.61
1:D:1457:TYR:HA	1:D:1491:ASN:HD22	1.65	0.61
1:A:4088:ILE:HB	1:A:4092:ASP:HB2	1.83	0.61
1:D:1576:SER:HA	1:D:1579:MET:HB2	1.81	0.61
2:G:74:LEU:HB2	2:G:99:PHE:HB2	1.83	0.61
1:A:2472:LEU:HD12	1:A:2473:PRO:HD2	1.83	0.61
1:A:4003:LEU:HG	1:A:4009:GLN:HG3	1.83	0.61
1:C:4003:LEU:HG	1:C:4009:GLN:HG3	1.82	0.61
1:A:895:PRO:HG2	1:A:896:VAL:HG23	1.83	0.61
1:B:645:ARG:HB3	1:B:826:ILE:HD11	1.83	0.61
1:D:299:LEU:HD11	1:D:314:PHE:HZ	1.66	0.61
1:B:765:GLN:NE2	1:B:1478:ASP:OD1	2.34	0.61
1:D:1742:THR:HG22	1:D:1769:THR:HG21	1.83	0.61
1:B:1576:SER:HA	1:B:1579:MET:HB2	1.82	0.60
1:C:645:ARG:HB3	1:C:826:ILE:HD11	1.83	0.60
1:B:1742:THR:HG22	1:B:1769:THR:HG21	1.83	0.60
1:C:1742:THR:HG22	1:C:1769:THR:HG21	1.83	0.60
1:D:737:LEU:HD23	1:D:738:LEU:H	1.65	0.60
1:D:4712:PRO:O	1:D:4718:LYS:NZ	2.34	0.60
2:F:74:LEU:HB2	2:F:99:PHE:HB2	1.83	0.60
1:B:892:THR:OG1	1:B:902:ARG:O	2.18	0.60
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.34	0.60
1:B:2472:LEU:HD12	1:B:2473:PRO:HD2	1.84	0.60
1:C:1545:ASN:OD1	2:G:32:ASN:ND2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:765:GLN:NE2	1:D:1478:ASP:OD1	2.34	0.60
1:B:3016:TYR:HA	1:B:3029:GLY:HA2	1.84	0.60
1:C:1451:GLY:HA3	1:C:1494:MET:HB3	1.82	0.60
1:D:797:HIS:HB3	1:D:1623:ARG:HH21	1.66	0.60
1:A:2967:MET:HA	1:A:2970:SER:HB3	1.84	0.60
1:A:3592:ILE:HA	1:A:3595:ARG:HE	1.65	0.60
1:C:2591:ARG:O	1:C:2594:SER:OG	2.18	0.60
1:D:2659:THR:O	1:D:2663:ASN:ND2	2.35	0.60
1:D:3016:TYR:HA	1:D:3029:GLY:HA2	1.82	0.60
1:A:2474:LEU:HA	1:A:2494:PHE:HD2	1.67	0.60
1:B:879:HIS:NE2	1:B:908:VAL:O	2.31	0.60
1:C:986:ASP:N	1:C:986:ASP:OD1	2.33	0.60
1:C:4088:ILE:HB	1:C:4092:ASP:HB2	1.83	0.60
1:C:4158:PRO:O	1:C:4162:ASN:ND2	2.35	0.60
1:B:299:LEU:HD11	1:B:314:PHE:HZ	1.67	0.60
1:B:3052:HIS:NE2	1:B:3128:ASN:O	2.34	0.60
1:C:205:ILE:HG22	1:C:206:CYS:H	1.66	0.60
1:C:348:VAL:HG13	1:C:357:LEU:HD23	1.83	0.60
1:C:765:GLN:NE2	1:C:1478:ASP:OD1	2.35	0.60
1:D:421:PHE:HB3	1:D:426:ARG:HH21	1.67	0.60
2:H:74:LEU:HB2	2:H:99:PHE:HB2	1.84	0.60
1:B:659:TYR:HE1	1:B:1006:SER:HB3	1.66	0.60
1:C:1289:LEU:HB2	1:C:1550:PRO:HD2	1.83	0.60
1:D:2911:LEU:HB2	1:D:2916:LYS:HD3	1.84	0.60
1:B:1012:ASP:HB3	1:B:1017:ARG:HG3	1.84	0.60
1:D:3080:VAL:HG13	1:D:3081:MET:HE3	1.82	0.60
1:A:645:ARG:HB3	1:A:826:ILE:HD11	1.84	0.59
1:C:2472:LEU:HD12	1:C:2473:PRO:HD2	1.83	0.59
1:D:1289:LEU:HB2	1:D:1550:PRO:HD2	1.83	0.59
1:D:2472:LEU:HD12	1:D:2473:PRO:HD2	1.84	0.59
2:G:53:GLN:HG2	2:G:54:GLU:H	1.66	0.59
1:A:961:MET:HE2	1:A:963:ASN:H	1.67	0.59
1:A:3016:TYR:HA	1:A:3029:GLY:HA2	1.83	0.59
1:C:3040:THR:HG21	1:C:3080:VAL:HG21	1.85	0.59
1:D:649:PHE:HB3	1:D:776:LEU:HD22	1.84	0.59
1:A:765:GLN:NE2	1:A:1478:ASP:OD1	2.34	0.59
1:A:4712:PRO:O	1:A:4718:LYS:NZ	2.34	0.59
1:B:630:GLU:HA	1:B:1642:PRO:HB2	1.84	0.59
1:B:668:VAL:HG22	1:B:789:VAL:HG12	1.85	0.59
1:D:645:ARG:HD3	1:D:826:ILE:HG12	1.83	0.59
1:D:686:TRP:NE1	1:D:746:CYS:SG	2.72	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:TYR:CE1	1:B:1006:SER:HB3	2.37	0.59
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	1.83	0.59
1:B:2961:GLN:HA	1:B:2964:LEU:HB3	1.82	0.59
1:C:1104:TRP:NE1	1:C:1151:CYS:SG	2.75	0.59
1:A:4158:PRO:O	1:A:4162:ASN:ND2	2.35	0.59
1:B:150:MET:HB3	1:B:169:LEU:HD13	1.84	0.59
1:B:649:PHE:HB3	1:B:776:LEU:HD22	1.85	0.59
1:B:1457:TYR:HA	1:B:1491:ASN:HD22	1.66	0.59
1:B:2967:MET:HA	1:B:2970:SER:HB3	1.84	0.59
1:D:265:LEU:HD23	1:D:279:PRO:HB2	1.85	0.59
1:D:1104:TRP:NE1	1:D:1151:CYS:SG	2.76	0.59
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	1.85	0.59
1:C:107:ILE:N	1:C:148:TRP:O	2.34	0.59
1:D:707:VAL:HG23	1:D:713:SER:HB2	1.85	0.59
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.36	0.59
1:A:797:HIS:HB3	1:A:1623:ARG:HH21	1.66	0.59
1:A:813:GLU:OE1	1:A:813:GLU:N	2.36	0.59
1:A:2659:THR:O	1:A:2663:ASN:ND2	2.36	0.59
1:B:4712:PRO:O	1:B:4718:LYS:NZ	2.34	0.59
1:C:4712:PRO:O	1:C:4718:LYS:NZ	2.33	0.59
1:D:709:ASP:OD1	1:D:713:SER:OG	2.20	0.59
1:D:772:ASN:HD22	1:D:1471:ALA:H	1.49	0.59
1:A:2452:ARG:NH1	1:D:175:SER:O	2.36	0.59
1:A:2911:LEU:HB2	1:A:2916:LYS:HD3	1.84	0.59
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.35	0.59
1:D:168:ASP:HB3	1:D:199:LEU:HB3	1.84	0.59
1:D:331:VAL:HG22	1:D:333:GLY:H	1.68	0.59
2:E:11:ASP:OD1	2:E:12:GLY:N	2.36	0.59
1:A:421:PHE:HB3	1:A:426:ARG:HH21	1.68	0.58
1:A:3409:TYR:HE2	1:A:3510:ILE:HG23	1.68	0.58
1:B:4158:PRO:O	1:B:4162:ASN:ND2	2.36	0.58
1:C:265:LEU:HD23	1:C:279:PRO:HB2	1.85	0.58
1:C:331:VAL:HG22	1:C:333:GLY:H	1.68	0.58
1:A:331:VAL:HG22	1:A:333:GLY:H	1.67	0.58
1:B:797:HIS:HB3	1:B:1623:ARG:HH21	1.66	0.58
1:B:895:PRO:HG2	1:B:896:VAL:HG23	1.84	0.58
1:D:986:ASP:OD1	1:D:986:ASP:N	2.36	0.58
1:A:1545:ASN:OD1	2:E:32:ASN:ND2	2.34	0.58
1:B:3096:PHE:O	1:B:3100:SER:N	2.36	0.58
1:D:574:VAL:HA	1:D:577:ILE:HD12	1.85	0.58
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:GLU:N	1:C:813:GLU:OE1	2.36	0.58
1:D:1118:ASP:OD1	1:D:1118:ASP:N	2.36	0.58
2:E:23:VAL:HG21	2:E:106:LEU:HB2	1.85	0.58
1:A:1451:GLY:HA3	1:A:1494:MET:HB3	1.84	0.58
1:D:3052:HIS:NE2	1:D:3128:ASN:O	2.36	0.58
1:B:2659:THR:O	1:B:2663:ASN:ND2	2.36	0.58
1:C:1576:SER:HA	1:C:1579:MET:HB2	1.83	0.58
1:C:3409:TYR:HE2	1:C:3510:ILE:HG23	1.67	0.58
1:D:4733:GLY:HA3	1:D:4736:ARG:HG3	1.85	0.58
2:E:53:GLN:HG2	2:E:54:GLU:H	1.67	0.58
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.84	0.58
1:C:686:TRP:HE1	1:C:746:CYS:HG	1.48	0.58
1:D:1545:ASN:OD1	2:H:32:ASN:ND2	2.35	0.58
2:H:17:LYS:NZ	2:H:18:LYS:O	2.36	0.58
1:B:4733:GLY:HA3	1:B:4736:ARG:HG3	1.86	0.58
1:C:668:VAL:HG22	1:C:789:VAL:HG12	1.85	0.58
1:C:2911:LEU:HB2	1:C:2916:LYS:HD3	1.84	0.58
2:G:17:LYS:H	2:G:20:GLN:HE22	1.50	0.58
2:H:11:ASP:OD1	2:H:12:GLY:N	2.37	0.58
1:A:1000:ARG:HG3	1:A:1005:TRP:HB2	1.86	0.58
1:C:393:CYS:SG	1:C:398:SER:OG	2.62	0.58
1:D:19:GLU:HB2	1:D:205:ILE:HB	1.86	0.58
1:D:150:MET:HB3	1:D:169:LEU:HD13	1.86	0.58
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.85	0.58
1:A:534:ARG:NH2	1:A:573:GLU:OE2	2.37	0.57
1:A:4733:GLY:HA3	1:A:4736:ARG:HG3	1.86	0.57
1:C:534:ARG:NH2	1:C:573:GLU:OE2	2.37	0.57
1:C:649:PHE:HB3	1:C:776:LEU:HD22	1.85	0.57
1:C:4733:GLY:HA3	1:C:4736:ARG:HG3	1.85	0.57
1:D:534:ARG:NH2	1:D:573:GLU:OE2	2.36	0.57
1:A:668:VAL:HG22	1:A:789:VAL:HG12	1.86	0.57
1:B:175:SER:O	1:C:2452:ARG:NH1	2.37	0.57
1:C:636:ASN:HD21	2:G:35:LYS:HE3	1.69	0.57
1:C:2659:THR:O	1:C:2663:ASN:ND2	2.37	0.57
1:D:668:VAL:HG22	1:D:789:VAL:HG12	1.86	0.57
1:D:927:GLU:O	1:D:931:THR:HG23	2.04	0.57
2:E:14:THR:HG21	2:E:68:LEU:HD12	1.86	0.57
2:F:53:GLN:HG2	2:F:54:GLU:H	1.68	0.57
1:A:175:SER:O	1:B:2452:ARG:NH1	2.38	0.57
1:B:331:VAL:HG22	1:B:333:GLY:H	1.68	0.57
1:B:1104:TRP:NE1	1:B:1151:CYS:SG	2.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1452:TRP:HE1	1:C:1518:CYS:HB3	1.70	0.57
1:A:1104:TRP:NE1	1:A:1151:CYS:SG	2.77	0.57
1:A:3980:LEU:HD23	1:A:3985:LEU:HD22	1.85	0.57
1:B:737:LEU:HD23	1:B:738:LEU:H	1.69	0.57
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.36	0.57
1:C:2967:MET:HA	1:C:2970:SER:HB3	1.86	0.57
1:C:3415:TYR:O	1:C:3419:ASN:ND2	2.37	0.57
1:D:2968:ASP:O	1:D:2971:GLN:NE2	2.29	0.57
1:B:3409:TYR:HE2	1:B:3510:ILE:HG23	1.70	0.57
1:C:3096:PHE:O	1:C:3100:SER:N	2.36	0.57
1:D:2961:GLN:HA	1:D:2964:LEU:HB3	1.87	0.57
1:B:651:GLY:HA3	1:B:776:LEU:HA	1.85	0.57
1:A:221:ARG:NH1	1:A:258:SER:OG	2.38	0.57
1:B:574:VAL:HA	1:B:577:ILE:HD12	1.85	0.57
1:B:2911:LEU:HB2	1:B:2916:LYS:HD3	1.86	0.57
1:C:221:ARG:NH1	1:C:258:SER:OG	2.37	0.57
1:C:865:PRO:HA	1:C:868:GLU:HB3	1.86	0.57
1:C:1164:LEU:HD23	1:C:1169:LEU:HB3	1.86	0.57
1:D:1241:SER:HA	1:D:1603:VAL:HG12	1.86	0.57
1:D:2524:VAL:HA	1:D:2527:LEU:HD23	1.85	0.57
1:D:4158:PRO:O	1:D:4162:ASN:ND2	2.37	0.57
1:A:651:GLY:HA3	1:A:776:LEU:HA	1.86	0.57
1:A:3666:ASP:OD1	1:A:3666:ASP:N	2.38	0.57
1:C:4567:LEU:HB2	1:C:4816:ILE:HG21	1.87	0.57
1:D:895:PRO:HD2	1:D:903:LEU:HD13	1.85	0.57
1:A:299:LEU:HD11	1:A:314:PHE:HZ	1.68	0.57
1:B:1140:GLY:HA3	1:B:1169:LEU:HD12	1.87	0.57
1:D:3409:TYR:HE2	1:D:3510:ILE:HG23	1.70	0.57
1:A:393:CYS:SG	1:A:398:SER:OG	2.62	0.57
1:B:636:ASN:HD21	2:F:35:LYS:HE3	1.69	0.57
1:B:737:LEU:HD23	1:B:738:LEU:N	2.20	0.57
1:B:4696:ASP:O	1:B:4700:GLN:NE2	2.38	0.57
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	1.87	0.57
1:D:2967:MET:HA	1:D:2970:SER:HB3	1.87	0.57
1:D:3366:ARG:HA	1:D:3441:ILE:HD11	1.86	0.57
1:A:3052:HIS:NE2	1:A:3128:ASN:O	2.37	0.56
1:B:393:CYS:SG	1:B:398:SER:OG	2.63	0.56
1:B:753:PRO:HB2	1:B:771:PHE:CD2	2.40	0.56
1:D:860:GLN:OE1	1:D:860:GLN:N	2.38	0.56
1:A:636:ASN:HD21	2:E:35:LYS:HE3	1.70	0.56
1:A:2737:PRO:HG3	1:A:2888:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LEU:HD23	1:B:279:PRO:HB2	1.87	0.56
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.37	0.56
1:C:14:LEU:HD12	1:C:18:ASP:HB3	1.86	0.56
1:D:3415:TYR:O	1:D:3419:ASN:ND2	2.38	0.56
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.38	0.56
1:A:644:ILE:HD11	1:A:1615:VAL:HG21	1.87	0.56
1:A:1140:GLY:HA3	1:A:1169:LEU:HD12	1.86	0.56
1:B:677:ALA:HB1	2:F:40:ARG:HB3	1.87	0.56
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.85	0.56
1:C:3270:ILE:HA	1:C:3274:LEU:HD21	1.86	0.56
1:D:1089:TYR:HB2	1:D:1152:MET:HG2	1.87	0.56
1:D:1140:GLY:HA3	1:D:1169:LEU:HD12	1.87	0.56
2:H:53:GLN:HG2	2:H:54:GLU:H	1.69	0.56
1:A:3415:TYR:O	1:A:3419:ASN:ND2	2.38	0.56
1:C:3335:MET:HB3	1:C:3407:ALA:HB2	1.87	0.56
1:D:636:ASN:HD21	2:H:35:LYS:HE3	1.70	0.56
1:D:910:PHE:HA	1:D:913:LEU:HD11	1.87	0.56
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.39	0.56
1:B:1241:SER:HA	1:B:1603:VAL:HG12	1.86	0.56
1:B:3980:LEU:HD23	1:B:3985:LEU:HD22	1.87	0.56
1:D:689:THR:HB	1:D:778:PHE:CZ	2.40	0.56
1:D:1424:PRO:HA	1:D:1427:ILE:HG22	1.87	0.56
1:D:2118:ARG:NH2	1:D:3719:ASP:OD1	2.37	0.56
1:B:977:LEU:HB3	1:B:981:GLN:HB2	1.88	0.56
1:B:4678:ALA:HB1	1:B:4720:VAL:HG21	1.87	0.56
1:C:860:GLN:N	1:C:860:GLN:OE1	2.38	0.56
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.87	0.56
1:A:4678:ALA:HB1	1:A:4720:VAL:HG21	1.87	0.56
1:B:860:GLN:OE1	1:B:860:GLN:N	2.39	0.56
1:C:664:PHE:HB3	1:C:746:CYS:HB3	1.88	0.56
1:D:221:ARG:NH1	1:D:258:SER:OG	2.38	0.56
1:A:150:MET:HB3	1:A:169:LEU:HD13	1.87	0.56
1:A:452:PHE:O	1:A:528:SER:OG	2.24	0.56
1:A:4567:LEU:HB2	1:A:4816:ILE:HG21	1.88	0.56
1:B:910:PHE:HA	1:B:913:LEU:HD11	1.86	0.56
1:C:651:GLY:HA3	1:C:776:LEU:HA	1.88	0.56
1:C:2884:ASN:OD1	1:C:2888:ARG:NH1	2.39	0.56
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.38	0.56
1:C:4769:MET:N	1:C:4769:MET:SD	2.79	0.56
1:D:1452:TRP:HE1	1:D:1518:CYS:HB3	1.71	0.56
1:D:2512:ILE:HG22	1:D:2516:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3980:LEU:HD23	1:D:3985:LEU:HD22	1.87	0.56
1:A:2591:ARG:O	1:A:2594:SER:OG	2.19	0.56
1:C:882:TRP:HZ3	1:C:921:ASN:HD21	1.53	0.56
1:C:895:PRO:HD2	1:C:903:LEU:HD13	1.86	0.56
1:C:3366:ARG:HA	1:C:3441:ILE:HD11	1.87	0.56
1:D:393:CYS:SG	1:D:398:SER:OG	2.63	0.56
1:D:2737:PRO:HG3	1:D:2888:ARG:HD2	1.88	0.56
1:D:4567:LEU:HB2	1:D:4816:ILE:HG21	1.88	0.56
1:A:1112:ASP:OD1	1:A:1112:ASP:N	2.36	0.56
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.36	0.56
1:A:2118:ARG:NH2	1:A:3719:ASP:OD1	2.37	0.56
1:A:2740:VAL:HG21	1:A:2818:ALA:HB1	1.88	0.56
1:B:221:ARG:NH1	1:B:258:SER:OG	2.38	0.56
1:B:2891:LYS:HA	1:B:2894:LEU:HD12	1.88	0.56
1:B:4232:GLU:OE2	1:B:5017:ARG:NH2	2.39	0.56
1:C:830:ARG:NH2	1:C:832:GLU:OE2	2.36	0.56
1:C:3980:LEU:HD23	1:C:3985:LEU:HD22	1.87	0.56
1:A:2884:ASN:OD1	1:A:2888:ARG:NH1	2.39	0.55
1:B:4567:LEU:HB2	1:B:4816:ILE:HG21	1.88	0.55
1:C:2740:VAL:HG21	1:C:2818:ALA:HB1	1.88	0.55
1:D:864:PRO:HD2	1:D:867:LEU:HD12	1.87	0.55
1:D:1003:GLN:O	1:D:1016:ARG:NH2	2.39	0.55
1:D:3319:ILE:HD11	1:D:3338:LEU:HD11	1.87	0.55
1:D:5012:LYS:NZ	1:D:5016:GLU:OE2	2.39	0.55
1:A:107:ILE:N	1:A:148:TRP:O	2.38	0.55
1:B:2512:ILE:HG22	1:B:2516:ASP:HB3	1.87	0.55
1:C:5012:LYS:NZ	1:C:5016:GLU:OE2	2.40	0.55
1:D:12:GLN:HG3	1:D:165:VAL:HA	1.88	0.55
1:D:4696:ASP:O	1:D:4700:GLN:NE2	2.40	0.55
1:A:229:GLU:HA	1:A:249:GLY:HA3	1.89	0.55
1:A:1241:SER:HA	1:A:1603:VAL:HG12	1.87	0.55
1:B:102:LEU:HB3	1:B:105:HIS:CD2	2.41	0.55
1:B:2740:VAL:HG21	1:B:2818:ALA:HB1	1.88	0.55
1:B:4087:LEU:HD22	1:B:4122:MET:HA	1.88	0.55
1:C:175:SER:O	1:D:2452:ARG:NH1	2.38	0.55
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.38	0.55
1:B:861:ILE:HB	1:B:930:LYS:HZ2	1.71	0.55
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.36	0.55
1:C:2737:PRO:HG3	1:C:2888:ARG:HD2	1.88	0.55
1:D:3666:ASP:OD1	1:D:3666:ASP:N	2.38	0.55
1:A:772:ASN:HD22	1:A:1471:ALA:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2737:PRO:HG3	1:B:2888:ARG:HD2	1.87	0.55
1:C:150:MET:HB3	1:C:169:LEU:HD13	1.88	0.55
1:C:299:LEU:HD11	1:C:314:PHE:HZ	1.71	0.55
1:C:452:PHE:O	1:C:528:SER:OG	2.24	0.55
1:C:755:ILE:HG13	1:C:771:PHE:CZ	2.42	0.55
1:A:677:ALA:HB1	2:E:40:ARG:HB3	1.88	0.55
1:A:4696:ASP:O	1:A:4700:GLN:NE2	2.40	0.55
1:B:1089:TYR:HB2	1:B:1152:MET:HG2	1.88	0.55
1:C:797:HIS:HB3	1:C:1623:ARG:HH21	1.70	0.55
1:C:2118:ARG:NH2	1:C:3719:ASP:OD1	2.38	0.55
1:C:4032:GLU:OE2	1:C:5004:THR:OG1	2.25	0.55
1:A:14:LEU:HD11	1:A:69:LEU:HD13	1.88	0.55
1:A:3270:ILE:HA	1:A:3274:LEU:HD21	1.88	0.55
1:B:2884:ASN:OD1	1:B:2888:ARG:NH1	2.39	0.55
1:B:5012:LYS:NZ	1:B:5016:GLU:OE2	2.39	0.55
1:C:689:THR:HB	1:C:778:PHE:CZ	2.42	0.55
1:C:2420:HIS:N	1:C:2492:ALA:O	2.40	0.55
1:D:107:ILE:N	1:D:148:TRP:O	2.38	0.55
1:D:4224:GLU:OE2	1:D:4224:GLU:N	2.40	0.55
1:A:399:GLN:O	1:A:403:MET:HG3	2.06	0.55
1:A:3366:ARG:HA	1:A:3441:ILE:HD11	1.88	0.55
1:A:5012:LYS:NZ	1:A:5016:GLU:OE2	2.39	0.55
1:B:2244:ARG:NH1	1:B:2283:ASN:OD1	2.40	0.55
1:B:3415:TYR:O	1:B:3419:ASN:ND2	2.40	0.55
1:C:4678:ALA:HB1	1:C:4720:VAL:HG21	1.89	0.55
1:D:2244:ARG:NH1	1:D:2283:ASN:OD1	2.40	0.55
1:D:2884:ASN:OD1	1:D:2888:ARG:NH1	2.39	0.55
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.39	0.55
1:A:3417:ASP:OD1	1:A:3417:ASP:N	2.40	0.55
1:B:103:TYR:HE2	1:B:152:PRO:HA	1.71	0.55
1:D:1530:THR:HG22	1:D:1535:GLU:HA	1.89	0.55
1:D:3335:MET:HB3	1:D:3407:ALA:HB2	1.89	0.55
1:D:3678:SER:OG	1:D:3773:ARG:NH2	2.39	0.55
1:A:2512:ILE:HG22	1:A:2516:ASP:HB3	1.87	0.55
1:B:2654:TYR:HA	1:B:2657:LEU:HD23	1.89	0.55
1:B:4166:LEU:HD23	1:B:4166:LEU:H	1.70	0.55
1:C:1504:GLY:O	1:C:1508:ARG:NH1	2.40	0.55
1:C:2098:VAL:HG11	1:C:2127:GLN:HG3	1.88	0.55
1:C:4224:GLU:N	1:C:4224:GLU:OE1	2.40	0.55
1:D:3245:VAL:HG12	1:D:3247:ASP:H	1.72	0.55
1:A:649:PHE:HB3	1:A:776:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3319:ILE:HD11	1:A:3338:LEU:HD11	1.89	0.54
1:A:4818:MET:SD	1:A:4819:GLY:N	2.81	0.54
1:B:229:GLU:HA	1:B:249:GLY:HA3	1.89	0.54
1:B:284:HIS:ND1	1:B:287:THR:OG1	2.33	0.54
1:B:1018:ASN:ND2	1:B:1020:ARG:HG2	2.22	0.54
1:C:1028:ASP:OD1	1:C:1028:ASP:N	2.40	0.54
1:C:1140:GLY:HA3	1:C:1169:LEU:HD12	1.89	0.54
1:C:1530:THR:HG22	1:C:1535:GLU:HA	1.89	0.54
1:D:2654:TYR:HA	1:D:2657:LEU:HD23	1.89	0.54
1:A:4032:GLU:OE2	1:A:5004:THR:OG1	2.24	0.54
1:B:534:ARG:NH2	1:B:573:GLU:OE2	2.35	0.54
1:B:2098:VAL:HG11	1:B:2127:GLN:HG3	1.89	0.54
1:B:4224:GLU:N	1:B:4224:GLU:OE2	2.40	0.54
1:D:580:GLU:HG3	1:D:620:LEU:HD21	1.89	0.54
1:D:867:LEU:HD22	1:D:929:LEU:HD11	1.88	0.54
1:A:910:PHE:HA	1:A:913:LEU:HD11	1.90	0.54
1:B:753:PRO:HB2	1:B:771:PHE:HD2	1.72	0.54
1:C:49:LEU:HD11	1:C:191:VAL:HG23	1.90	0.54
1:D:871:ARG:NH1	1:D:922:LEU:O	2.40	0.54
1:A:2891:LYS:HA	1:A:2894:LEU:HD12	1.90	0.54
1:A:3678:SER:OG	1:A:3773:ARG:NH2	2.41	0.54
1:B:4818:MET:SD	1:B:4819:GLY:N	2.81	0.54
1:C:3678:SER:OG	1:C:3773:ARG:NH2	2.41	0.54
1:C:4232:GLU:OE2	1:C:5017:ARG:NH2	2.40	0.54
1:A:144:GLU:O	1:A:175:SER:OG	2.25	0.54
1:D:2740:VAL:HG21	1:D:2818:ALA:HB1	1.89	0.54
1:D:4688:ILE:HD12	1:D:4737:ILE:HD12	1.90	0.54
1:A:54:ASN:HD22	1:A:57:ASN:HD21	1.54	0.54
1:A:1704:PRO:HG2	1:A:1707:LEU:HB2	1.90	0.54
1:A:3096:PHE:O	1:A:3100:SER:N	2.35	0.54
1:A:4688:ILE:HD12	1:A:4737:ILE:HD12	1.90	0.54
1:B:1152:MET:HB2	1:B:1161:ILE:O	2.08	0.54
1:B:1459:GLN:NE2	1:B:1470:ARG:HE	2.05	0.54
1:A:1658:ASP:N	1:A:1658:ASP:OD1	2.40	0.54
1:B:619:ASP:OD2	1:B:1680:ARG:NH2	2.37	0.54
1:D:4818:MET:SD	1:D:4819:GLY:N	2.81	0.54
1:B:1160:ILE:HB	1:B:1179:PHE:HD2	1.73	0.54
1:B:4768:LEU:HD12	1:B:4769:MET:SD	2.48	0.54
1:C:1089:TYR:HB2	1:C:1152:MET:HG2	1.89	0.54
1:C:3323:ILE:HD11	1:C:3338:LEU:HD22	1.90	0.54
1:D:2891:LYS:HA	1:D:2894:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.38	0.54
1:A:1089:TYR:HB2	1:A:1152:MET:HG2	1.89	0.54
1:A:3673:MET:O	1:A:3677:LEU:HB2	2.08	0.54
1:A:4224:GLU:N	1:A:4224:GLU:OE2	2.40	0.54
1:C:4087:LEU:HD22	1:C:4122:MET:HA	1.88	0.54
1:D:651:GLY:HA3	1:D:776:LEU:HA	1.88	0.54
1:A:1530:THR:HG22	1:A:1535:GLU:HA	1.90	0.54
1:A:2244:ARG:NH1	1:A:2283:ASN:OD1	2.40	0.54
1:B:659:TYR:OH	1:B:1017:ARG:HD3	2.07	0.54
1:B:1040:CYS:O	1:B:1044:ARG:HG2	2.07	0.54
1:B:2118:ARG:NH2	1:B:3719:ASP:OD1	2.37	0.54
1:C:2244:ARG:NH1	1:C:2283:ASN:OD1	2.40	0.54
1:C:2953:LYS:HA	1:C:2957:PHE:HB3	1.90	0.54
1:D:1704:PRO:HG2	1:D:1707:LEU:HB2	1.90	0.54
1:D:4032:GLU:OE2	1:D:5004:THR:OG1	2.25	0.54
1:A:1504:GLY:O	1:A:1508:ARG:NH1	2.41	0.53
1:A:2654:TYR:HA	1:A:2657:LEU:HD23	1.90	0.53
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.40	0.53
1:D:54:ASN:HD22	1:D:57:ASN:HD21	1.55	0.53
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.89	0.53
1:D:1443:GLN:NE2	1:D:1444:GLU:O	2.41	0.53
1:D:2420:HIS:N	1:D:2492:ALA:O	2.41	0.53
1:A:205:ILE:HG22	1:A:206:CYS:N	2.24	0.53
1:A:4162:ASN:HA	1:A:4165:GLU:HG2	1.89	0.53
1:B:644:ILE:HD11	1:B:1615:VAL:HG21	1.90	0.53
1:C:3319:ILE:HD11	1:C:3338:LEU:HD11	1.90	0.53
1:A:871:ARG:HH12	1:A:926:GLY:HA3	1.72	0.53
1:A:4769:MET:N	1:A:4769:MET:SD	2.81	0.53
1:B:813:GLU:HG3	1:B:1009:ALA:H	1.74	0.53
1:B:2420:HIS:CE1	1:B:2424:SER:HB3	2.43	0.53
1:B:2953:LYS:HA	1:B:2957:PHE:HB3	1.90	0.53
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.42	0.53
1:C:1241:SER:HA	1:C:1603:VAL:HG12	1.91	0.53
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.90	0.53
1:A:745:SER:HB3	1:A:758:ARG:HB2	1.91	0.53
1:B:1180:ARG:O	1:B:1181:GLU:HG2	2.09	0.53
1:B:4032:GLU:OE2	1:B:5004:THR:OG1	2.25	0.53
1:C:554:LEU:HD23	1:C:1593:PRO:HD3	1.90	0.53
1:C:681:HIS:HB3	1:C:784:SER:HB3	1.89	0.53
1:C:972:LEU:HD22	1:C:1044:ARG:HB3	1.90	0.53
1:C:2441:HIS:HA	1:C:2444:GLN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:GLU:HA	1:D:249:GLY:HA3	1.89	0.53
1:D:3133:THR:HA	1:D:3137:LEU:HD12	1.89	0.53
1:D:4003:LEU:HG	1:D:4009:GLN:HG3	1.90	0.53
1:B:1530:THR:HG22	1:B:1535:GLU:HA	1.91	0.53
1:C:54:ASN:HD22	1:C:57:ASN:HD21	1.56	0.53
1:C:4688:ILE:HD12	1:C:4737:ILE:HD12	1.91	0.53
1:D:24:CYS:HB2	1:D:200:TRP:HA	1.91	0.53
1:D:4055:VAL:HA	1:D:4058:ILE:HD12	1.90	0.53
2:H:17:LYS:H	2:H:20:GLN:HE22	1.56	0.53
1:B:3417:ASP:N	1:B:3417:ASP:OD1	2.42	0.53
1:C:1424:PRO:HA	1:C:1427:ILE:HG22	1.90	0.53
1:C:3417:ASP:N	1:C:3417:ASP:OD1	2.39	0.53
2:H:17:LYS:HG3	2:H:18:LYS:H	1.73	0.53
1:B:1772:ARG:NH2	1:B:1952:GLN:OE1	2.42	0.53
1:B:3366:ARG:HA	1:B:3441:ILE:HD11	1.90	0.53
1:B:4688:ILE:HD12	1:B:4737:ILE:HD12	1.91	0.53
1:C:3037:GLU:O	1:C:3040:THR:OG1	2.26	0.53
1:C:3673:MET:O	1:C:3677:LEU:HB2	2.08	0.53
1:D:3438:VAL:HG11	1:D:3517:MET:CE	2.39	0.53
1:B:984:LEU:O	1:B:988:LEU:HG	2.09	0.53
1:C:745:SER:HB3	1:C:758:ARG:HB2	1.90	0.53
1:C:1180:ARG:O	1:C:1181:GLU:HG2	2.09	0.53
1:C:2654:TYR:HA	1:C:2657:LEU:HD23	1.91	0.53
1:A:1424:PRO:HA	1:A:1427:ILE:HG22	1.90	0.53
1:A:5004:THR:OG1	1:A:5005:GLY:N	2.42	0.53
1:B:1461:ASP:HB3	1:B:1464:PHE:HB2	1.91	0.53
1:B:3245:VAL:HG12	1:B:3247:ASP:H	1.71	0.53
1:B:3794:VAL:HG21	1:B:3835:LEU:HD11	1.91	0.53
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.41	0.53
1:A:4087:LEU:HD22	1:A:4122:MET:HA	1.91	0.53
1:B:1079:LYS:HA	1:B:1189:LEU:HD11	1.91	0.53
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.42	0.53
1:B:4820:VAL:HG23	1:B:4821:LYS:N	2.24	0.53
1:C:1704:PRO:HG2	1:C:1707:LEU:HB2	1.91	0.53
1:D:2420:HIS:CE1	1:D:2424:SER:HB3	2.44	0.53
1:A:692:TYR:CD1	1:A:713:SER:OG	2.59	0.52
1:A:871:ARG:HH21	1:A:922:LEU:HD23	1.74	0.52
1:C:205:ILE:HG22	1:C:206:CYS:N	2.24	0.52
1:C:1160:ILE:HB	1:C:1179:PHE:HD2	1.74	0.52
1:C:1436:SER:HA	1:C:1517:GLY:HA2	1.90	0.52
1:D:1180:ARG:O	1:D:1181:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ARG:NH2	1:A:922:LEU:O	2.43	0.52
1:C:3545:THR:HG23	1:C:3548:GLU:H	1.73	0.52
1:C:4818:MET:SD	1:C:4819:GLY:N	2.82	0.52
1:C:5004:THR:OG1	1:C:5005:GLY:N	2.43	0.52
1:D:1079:LYS:HA	1:D:1189:LEU:HD11	1.91	0.52
1:D:1160:ILE:HB	1:D:1179:PHE:HD2	1.74	0.52
1:D:3673:MET:O	1:D:3677:LEU:HB2	2.09	0.52
1:A:265:LEU:HD11	1:A:281:ARG:HD3	1.91	0.52
1:B:1704:PRO:HG2	1:B:1707:LEU:HB2	1.91	0.52
1:D:119:SER:OG	1:D:120:CYS:N	2.43	0.52
1:D:981:GLN:O	1:D:985:VAL:HG23	2.10	0.52
1:A:3545:THR:HG23	1:A:3548:GLU:H	1.74	0.52
1:B:452:PHE:O	1:B:528:SER:OG	2.22	0.52
1:B:1504:GLY:O	1:B:1508:ARG:NH1	2.40	0.52
1:C:229:GLU:HA	1:C:249:GLY:HA3	1.90	0.52
1:C:913:LEU:HB2	1:C:918:ARG:HG2	1.92	0.52
1:C:2891:LYS:HA	1:C:2894:LEU:HD12	1.90	0.52
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.41	0.52
1:A:981:GLN:O	1:A:985:VAL:HG23	2.10	0.52
1:C:24:CYS:HB2	1:C:200:TRP:HA	1.91	0.52
1:D:3545:THR:HG23	1:D:3548:GLU:H	1.73	0.52
1:A:49:LEU:HD11	1:A:191:VAL:HG23	1.91	0.52
1:B:882:TRP:HZ3	1:B:921:ASN:HD21	1.58	0.52
1:B:1443:GLN:NE2	1:B:1444:GLU:O	2.41	0.52
1:C:119:SER:OG	1:C:120:CYS:N	2.43	0.52
1:D:41:GLY:O	1:D:45:ARG:NH1	2.43	0.52
1:D:4087:LEU:HD22	1:D:4122:MET:HA	1.91	0.52
1:A:1079:LYS:HA	1:A:1189:LEU:HD11	1.92	0.52
1:A:3453:ARG:O	1:A:3457:ASN:ND2	2.43	0.52
1:B:498:THR:H	1:B:503:PHE:HE2	1.57	0.52
1:B:4055:VAL:HA	1:B:4058:ILE:HD12	1.92	0.52
1:C:910:PHE:HA	1:C:913:LEU:HD11	1.92	0.52
1:D:3579:LEU:HG	1:D:3581:GLY:H	1.75	0.52
1:B:772:ASN:ND2	1:B:1471:ALA:H	2.08	0.52
1:C:1079:LYS:HA	1:C:1189:LEU:HD11	1.92	0.52
1:C:1435:TYR:HB3	1:C:1575:LEU:HG	1.92	0.52
1:C:4633:GLU:HG2	1:C:4635:SER:H	1.75	0.52
1:D:554:LEU:HD23	1:D:1593:PRO:HD3	1.91	0.52
1:D:1152:MET:HB2	1:D:1161:ILE:O	2.09	0.52
1:D:3453:ARG:O	1:D:3457:ASN:ND2	2.43	0.52
1:A:1443:GLN:NE2	1:A:1444:GLU:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2243:SER:OG	1:A:2245:GLN:OE1	2.28	0.52
1:A:2856:ASN:OD1	1:A:2856:ASN:N	2.43	0.52
1:B:49:LEU:HD11	1:B:191:VAL:HG23	1.92	0.52
1:B:2420:HIS:N	1:B:2492:ALA:O	2.42	0.52
1:D:674:PHE:N	1:D:680:THR:OG1	2.43	0.52
1:D:982:THR:HA	1:D:985:VAL:HG23	1.92	0.52
1:D:1772:ARG:NH2	1:D:1952:GLN:OE1	2.43	0.52
1:D:4696:ASP:OD1	1:D:4696:ASP:N	2.37	0.52
1:A:1110:ARG:NH2	1:A:1112:ASP:OD2	2.43	0.52
1:A:1180:ARG:O	1:A:1181:GLU:HG2	2.10	0.52
1:A:3037:GLU:O	1:A:3040:THR:OG1	2.26	0.52
1:B:830:ARG:NH2	1:B:832:GLU:OE2	2.38	0.52
1:B:1208:VAL:HA	1:B:1211:LEU:HD12	1.91	0.52
1:B:3545:THR:HG23	1:B:3548:GLU:H	1.74	0.52
1:C:1152:MET:HB2	1:C:1161:ILE:O	2.09	0.52
1:C:1277:TRP:CD1	1:C:1277:TRP:O	2.63	0.52
1:D:644:ILE:HD11	1:D:1615:VAL:HG21	1.92	0.52
1:D:1110:ARG:NH2	1:D:1112:ASP:OD2	2.43	0.52
1:D:1172:ASP:OD1	1:D:1172:ASP:N	2.43	0.52
1:D:5004:THR:OG1	1:D:5005:GLY:N	2.42	0.52
1:A:416:LYS:HD3	1:A:416:LYS:C	2.30	0.51
1:A:4633:GLU:HG2	1:A:4635:SER:H	1.75	0.51
1:C:984:LEU:O	1:C:988:LEU:HG	2.09	0.51
1:C:4055:VAL:HA	1:C:4058:ILE:HD12	1.92	0.51
1:D:3417:ASP:OD1	1:D:3417:ASP:N	2.40	0.51
1:A:976:ARG:HA	1:A:1044:ARG:HH12	1.74	0.51
1:A:2420:HIS:CE1	1:A:2424:SER:HB3	2.45	0.51
1:B:961:MET:CE	1:B:963:ASN:H	2.23	0.51
1:D:284:HIS:ND1	1:D:287:THR:OG1	2.34	0.51
1:D:1208:VAL:HA	1:D:1211:LEU:HD12	1.93	0.51
1:D:1504:GLY:O	1:D:1508:ARG:NH1	2.40	0.51
1:A:3110:LEU:HD12	1:A:3175:LEU:HD11	1.92	0.51
1:C:871:ARG:NH2	1:C:922:LEU:HB2	2.24	0.51
1:C:1562:ILE:HD12	1:C:1563:GLN:H	1.74	0.51
1:C:2420:HIS:CE1	1:C:2424:SER:HB3	2.46	0.51
1:D:3096:PHE:O	1:D:3100:SER:N	2.36	0.51
1:A:119:SER:OG	1:A:120:CYS:N	2.42	0.51
1:A:674:PHE:N	1:A:680:THR:OG1	2.42	0.51
1:A:1152:MET:HB2	1:A:1161:ILE:O	2.10	0.51
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.21	0.51
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.93	0.51
1:B:2154:SER:HB3	1:B:2188:ASN:HD21	1.75	0.51
1:B:3453:ARG:O	1:B:3457:ASN:ND2	2.43	0.51
1:C:1270:LEU:O	1:C:1564:PHE:N	2.36	0.51
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.78	0.51
1:D:1112:ASP:OD1	1:D:1112:ASP:N	2.36	0.51
1:D:4633:GLU:HG2	1:D:4635:SER:H	1.75	0.51
1:A:3065:VAL:O	1:A:3069:HIS:ND1	2.43	0.51
1:B:19:GLU:HB2	1:B:205:ILE:HB	1.91	0.51
1:B:1172:ASP:OD1	1:B:1172:ASP:N	2.44	0.51
1:B:4187:SER:OG	1:B:4191:GLU:OE2	2.27	0.51
1:B:4766:THR:HA	1:B:4769:MET:HE1	1.92	0.51
1:C:989:ALA:HA	1:C:1039:LEU:HG	1.92	0.51
1:D:745:SER:HB3	1:D:758:ARG:HB2	1.91	0.51
1:A:860:GLN:OE1	1:A:860:GLN:N	2.44	0.51
1:A:886:ARG:NH2	1:A:889:GLN:OE1	2.44	0.51
1:A:1078:GLU:OE1	1:A:1080:SER:OG	2.29	0.51
1:B:119:SER:OG	1:B:120:CYS:N	2.43	0.51
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.20	0.51
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.40	0.51
1:C:299:LEU:HD22	1:C:357:LEU:HD11	1.92	0.51
1:C:645:ARG:HD3	1:C:826:ILE:HG13	1.91	0.51
1:C:674:PHE:N	1:C:680:THR:OG1	2.36	0.51
1:C:686:TRP:NE1	1:C:746:CYS:SG	2.76	0.51
1:C:772:ASN:HD22	1:C:1471:ALA:H	1.59	0.51
1:C:2512:ILE:HG22	1:C:2516:ASP:HB3	1.91	0.51
1:C:3263:TYR:O	1:C:3267:PRO:HD2	2.11	0.51
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.43	0.51
1:D:452:PHE:O	1:D:528:SER:OG	2.24	0.51
1:D:1078:GLU:OE1	1:D:1080:SER:OG	2.29	0.51
1:D:4162:ASN:HA	1:D:4165:GLU:HG2	1.92	0.51
2:E:17:LYS:HG3	2:E:18:LYS:H	1.74	0.51
2:E:17:LYS:H	2:E:20:GLN:HE22	1.57	0.51
1:B:24:CYS:HB2	1:B:200:TRP:HA	1.92	0.51
1:B:181:HIS:CG	1:B:196:MET:HB2	2.46	0.51
1:B:1078:GLU:OE1	1:B:1080:SER:OG	2.29	0.51
1:B:2243:SER:OG	1:B:2245:GLN:OE1	2.29	0.51
1:B:5004:THR:OG1	1:B:5005:GLY:N	2.42	0.51
1:C:3453:ARG:O	1:C:3457:ASN:ND2	2.42	0.51
1:D:961:MET:CE	1:D:963:ASN:H	2.24	0.51
1:D:2243:SER:OG	1:D:2245:GLN:OE1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:ARG:HD3	1:A:826:ILE:HG13	1.93	0.51
1:A:895:PRO:HD2	1:A:903:LEU:HD23	1.93	0.51
1:A:2420:HIS:N	1:A:2492:ALA:O	2.43	0.51
1:B:1545:ASN:ND2	2:F:32:ASN:HD22	2.09	0.51
1:B:4633:GLU:HG2	1:B:4635:SER:H	1.76	0.51
1:C:320:LYS:HB3	1:C:356:TRP:NE1	2.26	0.51
1:C:1658:ASP:N	1:C:1658:ASP:OD1	2.41	0.51
1:A:554:LEU:HD23	1:A:1593:PRO:HD3	1.92	0.51
1:A:3969:ILE:HD13	1:A:4030:LEU:HD13	1.92	0.51
1:B:960:MET:SD	1:B:966:LYS:NZ	2.83	0.51
1:B:1110:ARG:NH2	1:B:1112:ASP:OD2	2.43	0.51
1:B:3666:ASP:OD1	1:B:3666:ASP:N	2.37	0.51
1:C:1139:PHE:CE1	1:C:1169:LEU:HD11	2.45	0.51
1:C:3337:ARG:HG2	1:C:3341:PHE:HE2	1.75	0.51
1:C:3965:LEU:HD22	1:C:3980:LEU:HD21	1.93	0.51
1:D:181:HIS:CG	1:D:196:MET:HB2	2.46	0.51
1:A:498:THR:H	1:A:503:PHE:HE2	1.57	0.51
1:A:2191:PHE:HA	1:A:2198:MET:HE3	1.92	0.51
1:A:4055:VAL:HA	1:A:4058:ILE:HD12	1.92	0.51
1:B:689:THR:HB	1:B:778:PHE:CZ	2.45	0.51
1:C:3395:ARG:HG2	1:C:3453:ARG:HH22	1.75	0.51
1:C:3579:LEU:HG	1:C:3581:GLY:H	1.76	0.51
2:G:48:PHE:CE1	2:G:55:VAL:HG21	2.46	0.51
1:A:3579:LEU:HG	1:A:3581:GLY:H	1.76	0.50
1:A:3965:LEU:HD22	1:A:3980:LEU:HD21	1.92	0.50
1:B:41:GLY:O	1:B:45:ARG:NH1	2.44	0.50
1:B:813:GLU:OE1	1:B:813:GLU:N	2.43	0.50
1:C:1284:VAL:HG22	1:C:1555:LEU:HD13	1.94	0.50
1:C:4187:SER:OG	1:C:4191:GLU:OE2	2.28	0.50
1:D:3037:GLU:O	1:D:3040:THR:OG1	2.25	0.50
1:A:668:VAL:HB	1:A:742:ASP:OD1	2.12	0.50
1:A:1717:SER:HA	1:A:1721:GLU:HB2	1.92	0.50
1:B:107:ILE:N	1:B:148:TRP:O	2.40	0.50
1:B:986:ASP:OD1	1:B:986:ASP:N	2.42	0.50
1:B:3674:ILE:HG13	1:B:3732:SER:HB2	1.92	0.50
1:C:990:GLU:HG2	1:C:1024:TYR:CE2	2.46	0.50
1:C:1717:SER:HA	1:C:1721:GLU:HB2	1.93	0.50
1:A:681:HIS:O	1:A:783:PHE:HA	2.10	0.50
1:A:989:ALA:HA	1:A:1039:LEU:HG	1.93	0.50
1:B:1452:TRP:HE1	1:B:1518:CYS:HB3	1.76	0.50
1:D:4187:SER:OG	1:D:4191:GLU:OE2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:HB3	1:A:356:TRP:NE1	2.27	0.50
1:A:1160:ILE:HB	1:A:1179:PHE:HD2	1.75	0.50
1:A:2104:ARG:NH1	1:A:2108:GLU:OE2	2.43	0.50
1:A:2474:LEU:HA	1:A:2494:PHE:CD2	2.46	0.50
1:B:645:ARG:HD3	1:B:826:ILE:HG13	1.93	0.50
1:C:1263:THR:N	1:C:1266:THR:O	2.38	0.50
1:C:4958:CYS:SG	1:C:4983:HIS:HD2	2.34	0.50
1:D:1263:THR:N	1:D:1266:THR:O	2.38	0.50
1:A:3645:PRO:HG2	1:A:3648:ARG:HH11	1.77	0.50
1:B:1289:LEU:HD12	1:B:1550:PRO:HG2	1.94	0.50
1:B:3927:GLN:HE21	1:B:3991:GLY:HA3	1.76	0.50
1:C:1288:PHE:HE1	1:C:1598:GLN:HB2	1.77	0.50
1:C:3927:GLN:HE21	1:C:3991:GLY:HA3	1.77	0.50
1:C:4008:SER:OG	1:C:4009:GLN:OE1	2.26	0.50
1:D:718:GLY:HA3	1:D:737:LEU:HA	1.93	0.50
1:D:1717:SER:HA	1:D:1721:GLU:HB2	1.93	0.50
1:D:3065:VAL:O	1:D:3069:HIS:ND1	2.45	0.50
1:A:41:GLY:O	1:A:45:ARG:NH1	2.44	0.50
1:A:284:HIS:ND1	1:A:287:THR:OG1	2.34	0.50
1:A:4003:LEU:HD21	1:A:4012:LEU:HB3	1.93	0.50
1:C:1078:GLU:OE1	1:C:1080:SER:OG	2.29	0.50
1:C:1110:ARG:NH2	1:C:1112:ASP:OD2	2.43	0.50
1:C:4820:VAL:HG23	1:C:4821:LYS:N	2.24	0.50
1:D:4820:VAL:HG23	1:D:4821:LYS:N	2.24	0.50
2:E:48:PHE:CE1	2:E:55:VAL:HG21	2.47	0.50
1:A:1289:LEU:HD12	1:A:1550:PRO:HG2	1.94	0.50
1:A:2440:MET:SD	1:A:2442:LEU:N	2.84	0.50
1:A:3263:TYR:O	1:A:3267:PRO:HD2	2.12	0.50
1:B:307:ALA:HB1	1:B:312:THR:HG21	1.94	0.50
1:B:1263:THR:HG22	1:B:1266:THR:HB	1.94	0.50
1:B:1717:SER:HA	1:B:1721:GLU:HB2	1.93	0.50
1:C:884:LEU:HG	1:C:959:TYR:HE2	1.77	0.50
1:C:2243:SER:OG	1:C:2245:GLN:OE1	2.29	0.50
1:D:299:LEU:HD22	1:D:357:LEU:HD11	1.94	0.50
1:D:498:THR:H	1:D:503:PHE:HE2	1.59	0.50
1:D:4908:GLU:O	1:D:4908:GLU:HG2	2.12	0.50
2:H:30:LEU:HD21	2:H:92:PRO:HD2	1.93	0.50
1:A:3927:GLN:HE21	1:A:3991:GLY:HA3	1.77	0.50
1:B:144:GLU:O	1:B:175:SER:OG	2.26	0.50
1:B:4003:LEU:HD21	1:B:4012:LEU:HB3	1.93	0.50
1:C:1172:ASP:OD1	1:C:1172:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2963:LEU:HA	1:C:2966:TRP:HB2	1.93	0.50
1:D:320:LYS:HB3	1:D:356:TRP:NE1	2.27	0.50
1:D:2154:SER:HB3	1:D:2188:ASN:HD21	1.76	0.50
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.45	0.50
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.30	0.50
1:A:1155:LEU:H	1:A:1155:LEU:HD12	1.77	0.50
1:B:72:SER:O	1:B:105:HIS:ND1	2.45	0.50
1:B:2104:ARG:NH1	1:B:2108:GLU:OE2	2.44	0.50
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.38	0.50
1:C:1208:VAL:HA	1:C:1211:LEU:HD12	1.94	0.50
1:C:1644:GLU:OE1	1:C:1646:ARG:NE	2.43	0.50
1:C:3969:ILE:HD13	1:C:4030:LEU:HD13	1.92	0.50
1:D:3965:LEU:HD22	1:D:3980:LEU:HD21	1.94	0.50
2:F:14:THR:OG1	2:F:68:LEU:N	2.45	0.50
1:A:502:HIS:CE1	1:A:1263:THR:HA	2.47	0.49
1:A:4820:VAL:HG23	1:A:4821:LYS:N	2.25	0.49
1:B:895:PRO:HD2	1:B:903:LEU:HD23	1.94	0.49
1:C:3645:PRO:HG2	1:C:3648:ARG:HH11	1.77	0.49
1:D:2104:ARG:NH1	1:D:2108:GLU:OE2	2.43	0.49
1:B:1288:PHE:HE1	1:B:1598:GLN:HB2	1.77	0.49
1:B:1424:PRO:HA	1:B:1427:ILE:HG22	1.94	0.49
1:B:3677:LEU:HD22	1:B:3697:PRO:HG3	1.95	0.49
1:C:1289:LEU:HD12	1:C:1550:PRO:HG2	1.94	0.49
1:C:2187:ASN:OD1	1:C:2187:ASN:N	2.44	0.49
1:C:3390:GLY:HA2	1:C:3393:LEU:HD12	1.95	0.49
1:D:2591:ARG:O	1:D:2594:SER:OG	2.30	0.49
1:A:1703:LEU:HD23	1:A:1704:PRO:HD2	1.93	0.49
1:B:4696:ASP:OD1	1:B:4696:ASP:N	2.39	0.49
1:C:181:HIS:CG	1:C:196:MET:HB2	2.47	0.49
1:C:2104:ARG:NH1	1:C:2108:GLU:OE2	2.45	0.49
1:D:822:ARG:NH2	1:D:824:GLU:OE1	2.46	0.49
1:D:3927:GLN:HE21	1:D:3991:GLY:HA3	1.77	0.49
1:A:4908:GLU:O	1:A:4908:GLU:HG2	2.12	0.49
1:B:1277:TRP:O	1:B:1277:TRP:CD1	2.65	0.49
1:C:1155:LEU:H	1:C:1155:LEU:HD12	1.77	0.49
1:D:3695:PRO:HD2	1:D:3699:HIS:HB2	1.94	0.49
1:A:4878:ASP:OD1	1:A:4878:ASP:N	2.44	0.49
1:B:649:PHE:HE2	1:B:845:CYS:HB2	1.76	0.49
1:B:1703:LEU:HD23	1:B:1704:PRO:HD2	1.94	0.49
1:B:2474:LEU:HA	1:B:2494:PHE:HD2	1.76	0.49
1:C:252:VAL:HB	1:C:257:ARG:HH12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2556:LEU:HD21	1:C:2597:LYS:HA	1.95	0.49
1:D:224:HIS:HE2	1:D:386:ASP:HA	1.78	0.49
1:A:1087:ARG:NE	1:A:1222:GLY:O	2.46	0.49
1:A:1208:VAL:HA	1:A:1211:LEU:HD12	1.94	0.49
1:A:3136:LEU:HA	1:A:3139:VAL:HG22	1.94	0.49
1:A:3535:LEU:HD23	1:A:3535:LEU:H	1.77	0.49
1:A:3677:LEU:HG	1:A:3697:PRO:HG2	1.94	0.49
1:B:4878:ASP:OD1	1:B:4878:ASP:N	2.44	0.49
1:C:668:VAL:HB	1:C:742:ASP:OD1	2.13	0.49
1:D:4958:CYS:SG	1:D:4983:HIS:HD2	2.35	0.49
1:A:877:ASN:O	1:A:880:GLU:HG3	2.12	0.49
1:A:1270:LEU:O	1:A:1564:PHE:N	2.41	0.49
1:A:2431:ASP:OD1	1:A:2435:ARG:NE	2.46	0.49
1:B:320:LYS:HB3	1:B:356:TRP:NE1	2.27	0.49
1:B:684:VAL:HG12	1:B:781:VAL:HG12	1.95	0.49
1:B:990:GLU:HG2	1:B:1024:TYR:CZ	2.47	0.49
1:B:1112:ASP:OD1	1:B:1112:ASP:N	2.36	0.49
1:B:3535:LEU:HD23	1:B:3535:LEU:H	1.77	0.49
1:A:2098:VAL:HG11	1:A:2127:GLN:HG3	1.95	0.49
1:B:3698:LEU:HD12	1:B:3773:ARG:HG3	1.95	0.49
1:B:3965:LEU:HD22	1:B:3980:LEU:HD21	1.94	0.49
1:B:4000:MET:HE1	1:B:4058:ILE:HG12	1.95	0.49
1:C:41:GLY:O	1:C:45:ARG:NH1	2.46	0.49
1:A:307:ALA:HB1	1:A:312:THR:HG21	1.94	0.49
1:A:3395:ARG:HG2	1:A:3453:ARG:HH22	1.78	0.49
1:B:810:PRO:HD2	1:B:813:GLU:OE1	2.13	0.49
1:C:144:GLU:O	1:C:175:SER:OG	2.26	0.49
1:C:2657:LEU:N	1:C:2658:PRO:HD2	2.28	0.49
1:D:3395:ARG:HG2	1:D:3453:ARG:HH22	1.78	0.49
1:A:822:ARG:NH2	1:A:824:GLU:OE1	2.45	0.49
1:B:2325:PRO:HB3	1:B:2422:ILE:HA	1.94	0.49
1:B:3695:PRO:HD2	1:B:3699:HIS:HB2	1.95	0.49
1:C:644:ILE:HD11	1:C:1615:VAL:HG21	1.95	0.49
1:C:2474:LEU:HA	1:C:2494:PHE:HD2	1.78	0.49
1:D:668:VAL:HB	1:D:742:ASP:OD1	2.13	0.49
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.31	0.49
1:D:1459:GLN:NE2	1:D:1461:ASP:HB2	2.27	0.49
1:D:2950:SER:HB3	1:D:2954:ARG:HH21	1.78	0.49
1:D:4115:SER:OG	1:D:4116:GLU:N	2.46	0.49
1:A:649:PHE:HE2	1:A:845:CYS:HB2	1.78	0.48
1:B:252:VAL:HB	1:B:257:ARG:HH12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:ARG:NH2	1:B:824:GLU:OE1	2.46	0.48
1:B:971:ASP:O	1:B:974:HIS:NE2	2.46	0.48
1:B:2431:ASP:O	1:B:2435:ARG:HG2	2.13	0.48
1:B:2657:LEU:N	1:B:2658:PRO:HD2	2.28	0.48
1:C:1047:LEU:HD12	1:C:1053:ILE:HD12	1.95	0.48
1:C:3427:PRO:HG2	1:C:3579:LEU:HD12	1.95	0.48
1:D:1703:LEU:HD23	1:D:1704:PRO:HD2	1.93	0.48
1:D:2282:ASP:OD1	1:D:2282:ASP:N	2.46	0.48
1:D:2440:MET:HG3	1:D:2441:HIS:H	1.78	0.48
1:D:3390:GLY:HA2	1:D:3393:LEU:HD12	1.95	0.48
2:F:14:THR:HG21	2:F:68:LEU:HB2	1.95	0.48
1:A:689:THR:HB	1:A:778:PHE:CZ	2.48	0.48
1:A:993:HIS:ND1	1:A:1023:PRO:O	2.45	0.48
1:B:284:HIS:HD1	1:B:287:THR:HG1	1.56	0.48
1:B:1930:LYS:HE3	1:B:1930:LYS:HB3	1.69	0.48
1:B:3409:TYR:CE2	1:B:3510:ILE:HG23	2.48	0.48
1:C:1459:GLN:NE2	1:C:1461:ASP:HB2	2.27	0.48
1:D:144:GLU:O	1:D:175:SER:OG	2.24	0.48
1:D:307:ALA:HB1	1:D:312:THR:HG21	1.94	0.48
1:D:2191:PHE:HA	1:D:2198:MET:HE3	1.95	0.48
1:D:2953:LYS:HA	1:D:2957:PHE:HB3	1.94	0.48
1:A:813:GLU:HG3	1:A:1009:ALA:H	1.77	0.48
1:A:2282:ASP:OD1	1:A:2282:ASP:N	2.46	0.48
1:B:668:VAL:HB	1:B:742:ASP:OD1	2.14	0.48
1:B:977:LEU:HG	1:B:1044:ARG:HH11	1.77	0.48
1:B:3133:THR:HA	1:B:3137:LEU:HD12	1.94	0.48
1:C:294:THR:HG23	1:C:297:GLN:H	1.78	0.48
1:C:1112:ASP:OD1	1:C:1112:ASP:N	2.37	0.48
1:C:2154:SER:HB3	1:C:2188:ASN:HD21	1.78	0.48
1:D:689:THR:OG1	1:D:689:THR:O	2.30	0.48
1:D:1087:ARG:NE	1:D:1222:GLY:O	2.45	0.48
1:D:3263:TYR:O	1:D:3267:PRO:HD2	2.13	0.48
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.31	0.48
1:B:2191:PHE:HA	1:B:2198:MET:HE3	1.95	0.48
1:B:3645:PRO:HG2	1:B:3648:ARG:HH11	1.77	0.48
1:D:753:PRO:HB2	1:D:771:PHE:CD2	2.49	0.48
1:D:1277:TRP:O	1:D:1277:TRP:CD1	2.66	0.48
1:A:978:THR:HG22	1:A:979:PRO:HD2	1.95	0.48
1:A:2657:LEU:N	1:A:2658:PRO:HD2	2.28	0.48
1:B:653:ALA:HB2	1:B:848:HIS:HD2	1.79	0.48
1:B:4115:SER:OG	1:B:4116:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:875:ALA:HB1	1:C:910:PHE:CZ	2.48	0.48
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.31	0.48
1:C:2814:LYS:HD3	1:C:2814:LYS:HA	1.66	0.48
1:C:3245:VAL:HG12	1:C:3247:ASP:H	1.77	0.48
1:D:252:VAL:HB	1:D:257:ARG:HH12	1.78	0.48
1:D:920:TYR:HD1	1:D:923:GLN:HE21	1.62	0.48
1:D:3068:LEU:HA	1:D:3071:LEU:HB2	1.95	0.48
1:D:3794:VAL:HG21	1:D:3835:LEU:HD11	1.96	0.48
2:E:53:GLN:HG2	2:E:54:GLU:N	2.29	0.48
2:H:38:SER:OG	2:H:41:ASP:OD2	2.30	0.48
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.96	0.48
1:B:3068:LEU:HA	1:B:3071:LEU:HB2	1.96	0.48
1:C:677:ALA:HB1	2:G:40:ARG:HB3	1.96	0.48
1:C:2384:ILE:O	1:C:2388:GLU:HG2	2.14	0.48
1:C:4908:GLU:HG2	1:C:4908:GLU:O	2.14	0.48
1:D:2384:ILE:O	1:D:2388:GLU:HG2	2.13	0.48
2:E:30:LEU:N	2:E:34:LYS:O	2.46	0.48
1:A:718:GLY:HA3	1:A:737:LEU:HA	1.95	0.48
1:A:750:LEU:C	1:A:752:VAL:H	2.16	0.48
1:A:1772:ARG:NH2	1:A:1952:GLN:OE1	2.46	0.48
1:A:2506:LEU:HD12	1:A:2510:TYR:HB2	1.96	0.48
1:A:3794:VAL:HG21	1:A:3835:LEU:HD11	1.96	0.48
1:A:4166:LEU:HD23	1:A:4166:LEU:H	1.78	0.48
1:B:1087:ARG:NE	1:B:1222:GLY:O	2.46	0.48
1:C:102:LEU:HB3	1:C:105:HIS:CD2	2.49	0.48
1:D:49:LEU:HD11	1:D:191:VAL:HG23	1.95	0.48
1:D:416:LYS:HD3	1:D:416:LYS:C	2.34	0.48
1:D:1284:VAL:HG22	1:D:1555:LEU:HD13	1.95	0.48
1:D:1868:PRO:O	1:D:1872:THR:OG1	2.24	0.48
1:D:3535:LEU:HD23	1:D:3535:LEU:H	1.79	0.48
2:F:17:LYS:H	2:F:20:GLN:HE22	1.60	0.48
1:A:1435:TYR:HE1	1:A:1452:TRP:CZ2	2.32	0.48
1:A:4000:MET:HE2	1:A:4058:ILE:HG12	1.95	0.48
1:B:1093:GLU:HG2	1:B:1148:VAL:HG12	1.96	0.48
1:B:1833:SER:OG	1:B:1834:VAL:N	2.47	0.48
1:B:3065:VAL:O	1:B:3069:HIS:ND1	2.47	0.48
1:B:4767:TRP:O	1:B:4770:SER:OG	2.26	0.48
1:C:1220:GLN:NE2	1:D:3519:PRO:O	2.45	0.48
1:D:919:ASN:O	1:D:923:GLN:HG2	2.13	0.48
1:D:2355:ARG:HB3	1:D:2359:ARG:HH21	1.79	0.48
1:D:3645:PRO:HG2	1:D:3648:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:ILE:HB	1:A:930:LYS:HZ1	1.79	0.48
1:A:1217:CYS:SG	1:A:1218:GLY:N	2.86	0.48
1:A:1700:ASP:HB3	1:A:1703:LEU:HD12	1.96	0.48
1:A:1833:SER:OG	1:A:1834:VAL:N	2.47	0.48
1:A:3032:SER:N	1:A:3035:GLU:OE1	2.45	0.48
1:A:3319:ILE:HG13	1:A:3338:LEU:HD21	1.95	0.48
1:A:4059:LEU:HD21	1:A:4143:VAL:HG11	1.95	0.48
1:B:54:ASN:HD22	1:B:57:ASN:HD21	1.60	0.48
1:B:868:GLU:HA	1:B:871:ARG:HG3	1.95	0.48
1:B:4059:LEU:HD21	1:B:4143:VAL:HG11	1.96	0.48
1:B:4958:CYS:SG	1:B:4983:HIS:HD2	2.37	0.48
1:C:822:ARG:NH2	1:C:824:GLU:OE1	2.46	0.48
1:C:4003:LEU:HD21	1:C:4012:LEU:HB3	1.95	0.48
1:C:4115:SER:OG	1:C:4116:GLU:N	2.46	0.48
1:C:4878:ASP:OD1	1:C:4878:ASP:N	2.44	0.48
1:D:1018:ASN:OD1	1:D:1020:ARG:NE	2.46	0.48
1:D:1087:ARG:HB3	1:D:1223:PHE:CD1	2.49	0.48
1:D:1486:SER:O	1:D:1486:SER:OG	2.30	0.48
1:D:2098:VAL:HG11	1:D:2127:GLN:HG3	1.96	0.48
1:D:2506:LEU:HD12	1:D:2510:TYR:HB2	1.95	0.48
1:D:2657:LEU:N	1:D:2658:PRO:HD2	2.28	0.48
1:A:252:VAL:HB	1:A:257:ARG:HH12	1.78	0.48
1:A:571:SER:O	1:A:571:SER:OG	2.32	0.48
1:B:1520:VAL:HG12	1:B:1527:MET:HG2	1.96	0.48
1:B:2282:ASP:N	1:B:2282:ASP:OD1	2.46	0.48
1:B:2506:LEU:HD12	1:B:2510:TYR:HB2	1.95	0.48
1:B:4908:GLU:HG2	1:B:4908:GLU:O	2.12	0.48
1:C:1443:GLN:NE2	1:C:1444:GLU:O	2.44	0.48
1:C:1833:SER:OG	1:C:1834:VAL:N	2.47	0.48
1:C:3051:ARG:HG3	1:C:3052:HIS:H	1.79	0.48
1:D:1833:SER:OG	1:D:1834:VAL:N	2.47	0.48
1:A:3198:ALA:HB1	1:A:3280:TYR:HB2	1.95	0.47
1:A:4115:SER:OG	1:A:4116:GLU:N	2.46	0.47
1:A:4696:ASP:OD1	1:A:4696:ASP:N	2.38	0.47
1:B:277:GLY:HA2	1:B:315:CYS:SG	2.54	0.47
1:C:399:GLN:O	1:C:403:MET:HG3	2.14	0.47
1:C:2974:ILE:O	1:C:2978:GLU:N	2.43	0.47
1:C:3359:ILE:HD11	1:C:3434:LEU:HB2	1.96	0.47
1:D:892:THR:OG1	1:D:902:ARG:O	2.25	0.47
1:D:1289:LEU:HD12	1:D:1550:PRO:HG2	1.95	0.47
1:D:4059:LEU:HD21	1:D:4143:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:THR:HG21	2:G:68:LEU:HB2	1.95	0.47
1:B:224:HIS:HE2	1:B:386:ASP:HA	1.79	0.47
1:B:3395:ARG:HG2	1:B:3453:ARG:HH22	1.79	0.47
1:C:681:HIS:O	1:C:783:PHE:HA	2.14	0.47
1:C:861:ILE:O	1:C:930:LYS:NZ	2.44	0.47
1:C:1452:TRP:HE3	1:C:1548:LEU:HB3	1.79	0.47
1:C:2431:ASP:O	1:C:2435:ARG:HG2	2.14	0.47
1:D:689:THR:HB	1:D:778:PHE:HZ	1.79	0.47
1:D:1288:PHE:HE1	1:D:1598:GLN:HB2	1.79	0.47
1:A:299:LEU:HD22	1:A:357:LEU:HD11	1.95	0.47
1:A:359:TYR:HB2	1:A:383:HIS:HE1	1.78	0.47
1:A:2355:ARG:HB3	1:A:2359:ARG:HH21	1.79	0.47
1:A:3409:TYR:CE2	1:A:3510:ILE:HG23	2.48	0.47
1:B:416:LYS:C	1:B:416:LYS:HD3	2.34	0.47
1:B:3592:ILE:HA	1:B:3595:ARG:HE	1.79	0.47
1:C:571:SER:O	1:C:571:SER:OG	2.32	0.47
1:C:848:HIS:CE1	1:C:849:THR:HG23	2.49	0.47
1:C:1040:CYS:O	1:C:1044:ARG:HG2	2.13	0.47
1:C:1125:ASN:HB2	1:C:1132:TRP:HD1	1.79	0.47
1:D:3032:SER:N	1:D:3035:GLU:OE1	2.46	0.47
1:A:1644:GLU:OE1	1:A:1646:ARG:NE	2.43	0.47
1:A:2013:LYS:HE3	1:A:2031:LEU:HD23	1.95	0.47
1:B:1457:TYR:CZ	1:B:1459:GLN:HB2	2.48	0.47
1:B:2814:LYS:HD3	1:B:2814:LYS:HA	1.66	0.47
1:C:497:TYR:HA	1:C:503:PHE:CE2	2.50	0.47
1:C:877:ASN:O	1:C:880:GLU:HG3	2.14	0.47
1:C:1087:ARG:HB3	1:C:1223:PHE:CD1	2.49	0.47
1:C:2242:ILE:HG23	1:C:2246:ASN:HD22	1.80	0.47
1:C:2506:LEU:HD12	1:C:2510:TYR:HB2	1.95	0.47
1:C:3768:SER:HA	1:C:3771:HIS:ND1	2.30	0.47
2:F:53:GLN:HG2	2:F:54:GLU:N	2.29	0.47
2:H:53:GLN:HG2	2:H:54:GLU:N	2.28	0.47
1:A:2556:LEU:HD21	1:A:2597:LYS:HA	1.96	0.47
1:A:2963:LEU:HA	1:A:2966:TRP:HB2	1.96	0.47
1:B:595:ARG:NH2	1:B:1643:GLU:OE1	2.46	0.47
1:B:898:ASP:O	1:B:901:LYS:N	2.43	0.47
2:G:53:GLN:HG2	2:G:54:GLU:N	2.29	0.47
1:A:24:CYS:HB2	1:A:200:TRP:HA	1.96	0.47
1:A:1087:ARG:HB3	1:A:1223:PHE:CD1	2.49	0.47
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.96	0.47
1:B:1155:LEU:HD12	1:B:1155:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2094:LEU:O	1:B:2098:VAL:HG12	2.14	0.47
1:B:2983:SER:O	1:B:2983:SER:OG	2.30	0.47
1:C:630:GLU:HA	1:C:1642:PRO:HB2	1.96	0.47
1:C:3068:LEU:HA	1:C:3071:LEU:HB2	1.97	0.47
1:D:772:ASN:ND2	1:D:1471:ALA:H	2.10	0.47
1:D:1700:ASP:HB3	1:D:1703:LEU:HD12	1.96	0.47
1:D:2242:ILE:HG23	1:D:2246:ASN:HD22	1.80	0.47
1:A:224:HIS:HE2	1:A:386:ASP:HA	1.79	0.47
1:A:1011:GLN:NE2	1:A:1013:ILE:HG12	2.29	0.47
1:A:1277:TRP:CD1	1:A:1277:TRP:O	2.67	0.47
1:A:2257:LEU:HD21	1:A:2275:VAL:HG13	1.96	0.47
1:A:2310:CYS:HB3	1:A:2313:LEU:HD23	1.97	0.47
1:B:913:LEU:HB2	1:B:918:ARG:HG2	1.96	0.47
1:B:1217:CYS:SG	1:B:1218:GLY:N	2.87	0.47
1:B:2013:LYS:HE3	1:B:2031:LEU:HD23	1.96	0.47
1:B:2384:ILE:O	1:B:2388:GLU:HG2	2.13	0.47
1:B:2389:ASP:N	1:B:2390:PRO:HD3	2.30	0.47
1:B:3003:LEU:HD12	1:B:3004:PRO:CD	2.40	0.47
1:B:3037:GLU:O	1:B:3040:THR:OG1	2.27	0.47
1:B:3136:LEU:HA	1:B:3139:VAL:HG22	1.97	0.47
1:B:3263:TYR:O	1:B:3267:PRO:HD2	2.13	0.47
1:C:205:ILE:CG2	1:C:206:CYS:H	2.27	0.47
1:C:1000:ARG:HB3	1:C:1005:TRP:HB2	1.95	0.47
1:C:3842:LEU:O	1:C:3929:SER:OG	2.28	0.47
1:D:277:GLY:HA2	1:D:315:CYS:SG	2.55	0.47
1:D:877:ASN:O	1:D:880:GLU:HG3	2.15	0.47
1:D:1708:ARG:NH1	1:D:1836:PHE:O	2.47	0.47
1:D:2389:ASP:N	1:D:2390:PRO:HD3	2.30	0.47
1:D:4000:MET:HE2	1:D:4058:ILE:HG12	1.97	0.47
2:H:22:CYS:O	2:H:48:PHE:N	2.48	0.47
1:A:1452:TRP:HE1	1:A:1518:CYS:HB3	1.79	0.47
1:A:3842:LEU:O	1:A:3929:SER:OG	2.28	0.47
1:B:2310:CYS:HB3	1:B:2313:LEU:HD23	1.97	0.47
1:B:3768:SER:HA	1:B:3771:HIS:ND1	2.29	0.47
1:C:1018:ASN:OD1	1:C:1020:ARG:NH1	2.48	0.47
1:D:2431:ASP:O	1:D:2435:ARG:HG2	2.15	0.47
1:D:3768:SER:HA	1:D:3771:HIS:ND1	2.29	0.47
1:D:4159:ARG:HA	1:D:4162:ASN:HD21	1.80	0.47
1:A:772:ASN:ND2	1:A:1471:ALA:H	2.13	0.47
1:A:2431:ASP:O	1:A:2435:ARG:HG2	2.15	0.47
1:A:2500:ALA:HB1	1:A:2550:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3359:ILE:HD11	1:A:3434:LEU:HB2	1.97	0.47
1:A:4034:ASN:HD21	1:A:4153:HIS:CE1	2.33	0.47
1:B:399:GLN:O	1:B:403:MET:HG3	2.15	0.47
1:B:2440:MET:SD	1:B:2442:LEU:N	2.88	0.47
1:B:2963:LEU:HA	1:B:2966:TRP:HB2	1.97	0.47
1:C:895:PRO:HG2	1:C:896:VAL:HG23	1.96	0.47
1:C:1703:LEU:HD23	1:C:1704:PRO:HD2	1.95	0.47
1:D:2102:VAL:HG11	1:D:2124:LEU:HB2	1.97	0.47
2:E:38:SER:OG	2:E:41:ASP:OD2	2.32	0.47
1:B:1700:ASP:HB3	1:B:1703:LEU:HD12	1.97	0.47
1:C:813:GLU:HG3	1:C:1009:ALA:H	1.80	0.47
1:C:2389:ASP:N	1:C:2390:PRO:HD3	2.29	0.47
1:D:1125:ASN:HB2	1:D:1132:TRP:HD1	1.79	0.47
1:D:2310:CYS:HB3	1:D:2313:LEU:HD23	1.97	0.47
2:F:30:LEU:N	2:F:34:LYS:O	2.48	0.47
2:H:57:LYS:HB3	2:H:57:LYS:HE2	1.75	0.47
1:A:2094:LEU:O	1:A:2098:VAL:HG12	2.15	0.46
1:A:4958:CYS:SG	1:A:4983:HIS:HD2	2.37	0.46
1:B:1087:ARG:HB3	1:B:1223:PHE:CD1	2.50	0.46
1:B:3390:GLY:HA2	1:B:3393:LEU:HD12	1.96	0.46
1:C:224:HIS:HE2	1:C:386:ASP:HA	1.80	0.46
1:C:307:ALA:HB1	1:C:312:THR:HG21	1.96	0.46
1:C:498:THR:H	1:C:503:PHE:HE2	1.62	0.46
1:C:1708:ARG:NH1	1:C:1836:PHE:O	2.48	0.46
1:C:2968:ASP:O	1:C:2971:GLN:NE2	2.32	0.46
1:C:4059:LEU:HD21	1:C:4143:VAL:HG11	1.96	0.46
1:A:630:GLU:HA	1:A:1642:PRO:HB2	1.98	0.46
1:A:915:GLU:HA	1:A:918:ARG:HB2	1.97	0.46
1:B:664:PHE:HB3	1:B:746:CYS:HB3	1.96	0.46
1:B:1270:LEU:O	1:B:1564:PHE:N	2.42	0.46
1:C:1277:TRP:O	1:C:1277:TRP:HD1	1.98	0.46
1:D:2441:HIS:HA	1:D:2444:GLN:HB3	1.96	0.46
1:D:3051:ARG:HD2	1:D:3051:ARG:HA	1.74	0.46
1:D:3409:TYR:CE2	1:D:3510:ILE:HG23	2.48	0.46
1:A:861:ILE:HB	1:A:930:LYS:NZ	2.30	0.46
1:A:1930:LYS:HE3	1:A:1930:LYS:HB3	1.70	0.46
1:A:3133:THR:HG23	1:A:3134:VAL:HG13	1.96	0.46
1:A:3141:THR:O	1:A:3145:GLN:HG2	2.14	0.46
1:C:750:LEU:C	1:C:752:VAL:H	2.18	0.46
1:C:3032:SER:N	1:C:3035:GLU:OE1	2.46	0.46
1:C:3409:TYR:CE2	1:C:3510:ILE:HG23	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:595:ARG:NH2	1:D:1643:GLU:OE1	2.48	0.46
1:D:884:LEU:HG	1:D:959:TYR:HE2	1.81	0.46
1:D:4034:ASN:HD21	1:D:4153:HIS:CE1	2.34	0.46
1:D:4878:ASP:OD1	1:D:4878:ASP:N	2.44	0.46
1:A:755:ILE:HG13	1:A:771:PHE:CZ	2.50	0.46
1:B:977:LEU:HG	1:B:1044:ARG:NH1	2.30	0.46
1:B:3107:VAL:HA	1:B:3110:LEU:HB2	1.97	0.46
1:B:3999:MET:HE1	1:B:4003:LEU:HD22	1.97	0.46
1:C:2094:LEU:O	1:C:2098:VAL:HG12	2.14	0.46
1:D:18:ASP:OD1	1:D:19:GLU:N	2.49	0.46
1:D:502:HIS:CE1	1:D:1263:THR:HA	2.50	0.46
1:D:2614:ILE:O	1:D:2618:MET:N	2.49	0.46
1:A:1288:PHE:HE1	1:A:1598:GLN:HB2	1.79	0.46
1:A:1452:TRP:HE3	1:A:1548:LEU:HB3	1.81	0.46
1:A:2983:SER:O	1:A:2983:SER:OG	2.29	0.46
1:B:292:ALA:O	1:B:299:LEU:HD12	2.16	0.46
1:B:299:LEU:HD22	1:B:357:LEU:HD11	1.96	0.46
1:C:861:ILE:HB	1:C:930:LYS:NZ	2.29	0.46
1:C:924:MET:HA	1:C:927:GLU:OE2	2.15	0.46
1:C:977:LEU:HG	1:C:1044:ARG:HH21	1.81	0.46
1:C:1087:ARG:NE	1:C:1222:GLY:O	2.47	0.46
1:D:1077:ALA:HB3	1:D:1190:PRO:HD2	1.98	0.46
2:G:22:CYS:SG	2:G:48:PHE:HB3	2.55	0.46
2:H:30:LEU:N	2:H:34:LYS:O	2.47	0.46
1:A:181:HIS:CG	1:A:196:MET:HB2	2.50	0.46
1:A:205:ILE:CG2	1:A:206:CYS:H	2.27	0.46
1:A:1470:ARG:HD3	1:A:1470:ARG:HA	1.70	0.46
1:C:3065:VAL:O	1:C:3069:HIS:ND1	2.48	0.46
1:D:441:VAL:HG13	1:D:518:ILE:HD11	1.97	0.46
1:D:913:LEU:HB2	1:D:918:ARG:HG2	1.98	0.46
1:A:2389:ASP:N	1:A:2390:PRO:HD3	2.31	0.46
1:A:3696:ASP:CG	1:A:3697:PRO:HD3	2.35	0.46
1:B:284:HIS:CE1	1:B:286:THR:HB	2.50	0.46
1:C:591:ASP:OD1	1:C:1594:ARG:NH1	2.48	0.46
1:C:1470:ARG:HD3	1:C:1470:ARG:HA	1.71	0.46
1:C:2282:ASP:OD1	1:C:2282:ASP:N	2.47	0.46
1:D:830:ARG:NE	1:D:1612:PHE:HE2	2.13	0.46
1:D:886:ARG:NH2	1:D:889:GLN:OE1	2.44	0.46
1:D:2906:VAL:HG11	1:D:2911:LEU:HA	1.97	0.46
2:H:44:LYS:HD2	2:H:44:LYS:HA	1.80	0.46
1:A:3768:SER:HA	1:A:3771:HIS:ND1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4159:ARG:HA	1:A:4162:ASN:HD21	1.81	0.46
1:B:830:ARG:HH12	1:B:832:GLU:HG3	1.81	0.46
1:B:2242:ILE:HG23	1:B:2246:ASN:HD22	1.80	0.46
1:C:772:ASN:ND2	1:C:1471:ALA:H	2.13	0.46
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.96	0.46
1:C:1452:TRP:CE3	1:C:1548:LEU:HB3	2.51	0.46
1:C:1772:ARG:NH2	1:C:1952:GLN:OE1	2.48	0.46
1:C:2310:CYS:HB3	1:C:2313:LEU:HD23	1.98	0.46
1:C:3845:ASN:N	1:C:3845:ASN:OD1	2.49	0.46
1:C:4109:GLN:HA	1:C:4112:LEU:HD12	1.97	0.46
1:D:1155:LEU:H	1:D:1155:LEU:HD12	1.80	0.46
1:D:1217:CYS:SG	1:D:1218:GLY:N	2.88	0.46
1:D:2094:LEU:O	1:D:2098:VAL:HG12	2.16	0.46
1:D:2431:ASP:OD1	1:D:2435:ARG:NE	2.46	0.46
1:A:2150:GLU:HA	1:A:2153:MET:HB2	1.98	0.46
1:A:3068:LEU:HA	1:A:3071:LEU:HB2	1.98	0.46
1:A:3390:GLY:HA2	1:A:3393:LEU:HD12	1.98	0.46
1:B:2556:LEU:HD21	1:B:2597:LYS:HA	1.97	0.46
1:B:3845:ASN:N	1:B:3845:ASN:OD1	2.49	0.46
1:B:4034:ASN:HD21	1:B:4153:HIS:CE1	2.34	0.46
1:C:284:HIS:ND1	1:C:287:THR:OG1	2.33	0.46
1:C:416:LYS:C	1:C:416:LYS:HD3	2.37	0.46
1:C:718:GLY:HA3	1:C:737:LEU:HA	1.96	0.46
1:D:924:MET:HA	1:D:927:GLU:OE2	2.15	0.46
1:D:1093:GLU:HG2	1:D:1148:VAL:HG12	1.98	0.46
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.97	0.46
1:D:1454:THR:OG1	1:D:1455:PRO:HD2	2.15	0.46
1:D:2556:LEU:HD21	1:D:2597:LYS:HA	1.97	0.46
1:D:3438:VAL:HG11	1:D:3517:MET:HE1	1.98	0.46
2:H:14:THR:HG21	2:H:68:LEU:HB2	1.98	0.46
1:A:359:TYR:HB2	1:A:383:HIS:CE1	2.51	0.46
1:A:595:ARG:NH2	1:A:1643:GLU:OE1	2.49	0.46
1:A:954:LYS:HA	1:A:954:LYS:HD2	1.79	0.46
1:A:2950:SER:HB3	1:A:2954:ARG:HH21	1.80	0.46
1:B:630:GLU:HA	1:B:1642:PRO:CB	2.45	0.46
1:B:861:ILE:O	1:B:930:LYS:NZ	2.48	0.46
1:B:3329:ILE:HG12	1:B:3332:ALA:HB2	1.97	0.46
1:C:168:ASP:HB3	1:C:199:LEU:HB3	1.97	0.46
1:C:284:HIS:CE1	1:C:286:THR:HB	2.51	0.46
1:C:886:ARG:NH2	1:C:889:GLN:OE1	2.47	0.46
1:D:630:GLU:HA	1:D:1642:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1767:VAL:HG12	1:D:1767:VAL:O	2.16	0.46
1:D:3133:THR:HG23	1:D:3134:VAL:HG13	1.98	0.46
1:A:871:ARG:NH2	1:A:922:LEU:HD23	2.31	0.45
1:A:1220:GLN:NE2	1:B:3519:PRO:O	2.47	0.45
1:A:2154:SER:HB3	1:A:2188:ASN:HD21	1.81	0.45
1:A:2242:ILE:HG23	1:A:2246:ASN:HD22	1.81	0.45
1:A:2491:SER:O	1:A:2491:SER:OG	2.31	0.45
1:B:755:ILE:HG13	1:B:771:PHE:CZ	2.51	0.45
1:B:1534:LYS:HA	1:B:1534:LYS:HD2	1.82	0.45
1:B:1708:ARG:NH1	1:B:1836:PHE:O	2.48	0.45
1:B:2591:ARG:O	1:B:2594:SER:OG	2.30	0.45
1:B:3032:SER:N	1:B:3035:GLU:OE1	2.45	0.45
1:B:4162:ASN:HA	1:B:4165:GLU:HG2	1.98	0.45
1:B:4586:PRO:HB3	1:B:4628:VAL:HG21	1.98	0.45
1:C:24:CYS:SG	1:C:198:THR:OG1	2.74	0.45
1:C:502:HIS:CE1	1:C:1263:THR:HA	2.51	0.45
1:C:3526:ALA:HB2	1:C:3595:ARG:HH12	1.81	0.45
2:F:22:CYS:SG	2:F:48:PHE:HB3	2.55	0.45
1:A:1022:VAL:HG23	1:A:1027:LEU:HG	1.98	0.45
1:A:3323:ILE:HD11	1:A:3338:LEU:HD22	1.99	0.45
1:B:263:GLU:HB3	1:B:281:ARG:HB2	1.99	0.45
1:B:1077:ALA:HB3	1:B:1190:PRO:HD2	1.98	0.45
1:B:1868:PRO:O	1:B:1872:THR:OG1	2.25	0.45
1:C:531:ARG:HA	1:C:566:CYS:SG	2.56	0.45
1:C:2474:LEU:HA	1:C:2494:PHE:CD2	2.52	0.45
1:C:3971:GLY:O	1:C:3973:CYS:N	2.49	0.45
1:D:1008:SER:HB3	1:D:1017:ARG:HB3	1.98	0.45
1:A:102:LEU:HD12	1:A:161:GLU:O	2.16	0.45
1:A:1077:ALA:HB3	1:A:1190:PRO:HD2	1.98	0.45
1:A:1708:ARG:NH1	1:A:1836:PHE:O	2.48	0.45
1:A:1868:PRO:O	1:A:1872:THR:OG1	2.25	0.45
1:A:2384:ILE:O	1:A:2388:GLU:HG2	2.17	0.45
1:A:3999:MET:HE3	1:A:4003:LEU:HB2	1.97	0.45
1:B:899:ASP:HB2	1:B:902:ARG:CZ	2.46	0.45
1:B:4181:ILE:HG22	1:B:4182:GLU:H	1.81	0.45
1:C:2500:ALA:HB1	1:C:2550:LEU:HD22	1.97	0.45
1:D:68:THR:HG23	1:D:110:ARG:HB2	1.99	0.45
1:D:399:GLN:O	1:D:403:MET:HG3	2.15	0.45
1:D:1270:LEU:O	1:D:1564:PHE:N	2.37	0.45
1:A:531:ARG:HA	1:A:566:CYS:SG	2.56	0.45
1:A:591:ASP:OD1	1:A:1594:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2906:VAL:HG11	1:A:2911:LEU:HA	1.99	0.45
1:A:3208:PRO:HD2	1:A:3245:VAL:HG22	1.98	0.45
1:A:3245:VAL:HG12	1:A:3247:ASP:H	1.81	0.45
1:A:3804:ILE:HD12	1:A:3804:ILE:HA	1.87	0.45
1:B:1767:VAL:O	1:B:1767:VAL:HG12	2.17	0.45
1:C:1077:ALA:HB3	1:C:1190:PRO:HD2	1.99	0.45
1:C:1275:ARG:HG3	1:C:1276:THR:HG23	1.97	0.45
1:D:684:VAL:HG12	1:D:781:VAL:HG12	1.99	0.45
1:D:755:ILE:HG13	1:D:771:PHE:CZ	2.52	0.45
2:H:48:PHE:CE1	2:H:55:VAL:HG21	2.51	0.45
1:A:269:TRP:CD1	1:A:272:SER:HB2	2.52	0.45
1:A:284:HIS:CE1	1:A:286:THR:HB	2.52	0.45
1:A:1521:ASP:OD1	1:A:1524:THR:OG1	2.31	0.45
1:B:168:ASP:HB3	1:B:199:LEU:HB3	1.99	0.45
1:B:2614:ILE:O	1:B:2618:MET:N	2.49	0.45
1:C:269:TRP:NE1	1:C:333:GLY:O	2.50	0.45
1:C:441:VAL:HG13	1:C:518:ILE:HD11	1.97	0.45
1:C:1435:TYR:HE1	1:C:1452:TRP:CZ2	2.34	0.45
1:C:3107:VAL:HA	1:C:3110:LEU:HB2	1.97	0.45
1:D:2474:LEU:HA	1:D:2494:PHE:HD2	1.82	0.45
2:E:22:CYS:SG	2:E:48:PHE:HB3	2.57	0.45
1:A:430:PRO:HB2	1:A:509:GLU:HB2	1.99	0.45
1:A:899:ASP:HB2	1:A:902:ARG:CZ	2.47	0.45
1:A:1520:VAL:HG12	1:A:1527:MET:HG2	1.97	0.45
1:B:2974:ILE:O	1:B:2978:GLU:N	2.46	0.45
1:B:3068:LEU:H	1:B:3068:LEU:HD12	1.82	0.45
1:C:1562:ILE:HD12	1:C:1563:GLN:N	2.32	0.45
1:C:2191:PHE:HA	1:C:2198:MET:HE3	1.98	0.45
1:C:2983:SER:O	1:C:2983:SER:OG	2.29	0.45
1:C:3003:LEU:HD12	1:C:3004:PRO:CD	2.40	0.45
1:D:4181:ILE:HG22	1:D:4182:GLU:H	1.82	0.45
1:A:2442:LEU:HG	1:A:2443:ILE:HG12	1.98	0.45
1:A:3526:ALA:HB2	1:A:3595:ARG:HH12	1.82	0.45
1:B:875:ALA:HB1	1:B:910:PHE:CZ	2.51	0.45
1:B:959:TYR:HB3	1:B:967:PRO:HD2	1.98	0.45
1:B:1263:THR:N	1:B:1266:THR:O	2.47	0.45
1:C:263:GLU:HB3	1:C:281:ARG:HB2	1.98	0.45
1:C:977:LEU:CG	1:C:1044:ARG:HH21	2.30	0.45
1:D:871:ARG:HH22	1:D:922:LEU:HD13	1.80	0.45
1:D:894:GLY:HA3	1:D:903:LEU:HD22	1.98	0.45
1:D:986:ASP:HB3	1:D:1036:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1008:SER:HB2	1:D:1017:ARG:NH2	2.32	0.45
1:D:3319:ILE:HG13	1:D:3338:LEU:HD21	1.97	0.45
1:D:3524:MET:H	1:D:3524:MET:HG2	1.57	0.45
2:F:38:SER:OG	2:F:41:ASP:OD2	2.31	0.45
2:G:80:VAL:HG23	2:G:80:VAL:O	2.16	0.45
1:A:3995:VAL:O	1:A:3999:MET:HB2	2.17	0.45
1:A:4181:ILE:HG22	1:A:4182:GLU:H	1.81	0.45
1:B:269:TRP:NE1	1:B:333:GLY:O	2.49	0.45
1:C:479:GLN:O	1:C:479:GLN:NE2	2.50	0.45
1:C:961:MET:HE3	1:C:961:MET:H	1.82	0.45
1:C:1434:TYR:HA	1:C:1519:LEU:HD23	1.98	0.45
1:C:2442:LEU:HG	1:C:2443:ILE:HG12	1.99	0.45
1:C:3794:VAL:HG21	1:C:3835:LEU:HD11	1.99	0.45
1:C:4181:ILE:HG22	1:C:4182:GLU:H	1.82	0.45
1:D:430:PRO:HB2	1:D:509:GLU:HB2	1.98	0.45
1:D:531:ARG:HA	1:D:566:CYS:SG	2.56	0.45
2:F:48:PHE:CE1	2:F:55:VAL:HG21	2.51	0.45
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.84	0.45
1:A:681:HIS:NE2	1:A:683:ARG:HD2	2.32	0.45
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.97	0.45
1:A:3347:SER:O	1:A:3347:SER:OG	2.29	0.45
1:B:760:ASN:N	1:B:760:ASN:OD1	2.49	0.45
1:B:915:GLU:HA	1:B:918:ARG:HB2	1.98	0.45
1:B:924:MET:HA	1:B:927:GLU:OE2	2.16	0.45
1:B:1000:ARG:HB3	1:B:1005:TRP:HB2	1.98	0.45
1:C:417:GLY:O	1:C:420:SER:OG	2.35	0.45
1:C:2013:LYS:HE3	1:C:2031:LEU:HD23	1.97	0.45
1:D:1770:SER:OG	1:D:1956:GLU:OE2	2.28	0.45
1:D:4848:VAL:O	1:D:4852:THR:OG1	2.32	0.45
1:A:103:TYR:HB2	1:A:161:GLU:O	2.17	0.45
1:A:292:ALA:O	1:A:299:LEU:HD12	2.17	0.45
1:A:1172:ASP:OD1	1:A:1172:ASP:N	2.44	0.45
1:A:1767:VAL:O	1:A:1767:VAL:HG12	2.17	0.45
1:B:2474:LEU:HA	1:B:2494:PHE:CD2	2.50	0.45
1:C:1093:GLU:HG2	1:C:1148:VAL:HG12	1.99	0.45
1:C:1217:CYS:SG	1:C:1218:GLY:N	2.90	0.45
1:C:1767:VAL:O	1:C:1767:VAL:HG12	2.17	0.45
1:D:266:ARG:NH2	1:D:331:VAL:O	2.37	0.45
1:D:1037:ASP:O	1:D:1041:GLN:HG2	2.16	0.45
1:D:1769:THR:O	1:D:1769:THR:OG1	2.34	0.45
1:D:3398:PHE:HB3	1:D:3454:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3434:LEU:O	1:D:3438:VAL:HG12	2.17	0.45
2:E:17:LYS:NZ	2:E:18:LYS:O	2.46	0.45
1:A:417:GLY:O	1:A:420:SER:OG	2.35	0.44
1:A:721:LEU:HD21	1:A:768:PHE:CZ	2.53	0.44
1:A:3845:ASN:OD1	1:A:3845:ASN:N	2.49	0.44
1:B:925:SER:O	1:B:928:THR:OG1	2.32	0.44
1:B:2187:ASN:OD1	1:B:2187:ASN:N	2.43	0.44
1:B:2759:ALA:HB2	1:B:2806:ARG:HH22	1.83	0.44
1:B:3526:ALA:O	1:B:3528:THR:N	2.50	0.44
1:C:24:CYS:HB3	1:C:200:TRP:CE3	2.53	0.44
1:C:710:ASP:O	1:C:712:TYR:N	2.50	0.44
1:D:15:ARG:O	1:D:98:HIS:ND1	2.39	0.44
1:D:269:TRP:CD1	1:D:272:SER:HB2	2.53	0.44
1:D:649:PHE:HE2	1:D:845:CYS:HB2	1.82	0.44
1:D:2187:ASN:OD1	1:D:2187:ASN:N	2.44	0.44
2:G:57:LYS:HB3	2:G:57:LYS:HE2	1.78	0.44
1:A:3971:GLY:O	1:A:3973:CYS:N	2.50	0.44
1:B:1685:LEU:HD23	1:B:1718:ILE:HD11	1.99	0.44
1:C:277:GLY:HA2	1:C:315:CYS:SG	2.57	0.44
1:C:3398:PHE:HB3	1:C:3454:GLU:HG2	1.98	0.44
1:D:292:ALA:O	1:D:299:LEU:HD12	2.17	0.44
1:D:757:PHE:HB2	1:D:764:VAL:HG11	1.99	0.44
1:D:2325:PRO:HB3	1:D:2422:ILE:HA	2.00	0.44
1:D:3526:ALA:O	1:D:3528:THR:N	2.50	0.44
1:D:4109:GLN:HA	1:D:4112:LEU:HD12	2.00	0.44
1:A:830:ARG:HE	1:A:830:ARG:HB3	1.58	0.44
1:A:886:ARG:HB3	1:A:891:TRP:CD1	2.53	0.44
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.83	0.44
1:A:1452:TRP:CE3	1:A:1548:LEU:HB3	2.52	0.44
1:A:4189:ARG:NE	1:A:5032:TYR:OH	2.29	0.44
1:B:269:TRP:CD1	1:B:272:SER:HB2	2.52	0.44
1:B:531:ARG:HA	1:B:566:CYS:SG	2.56	0.44
1:B:2355:ARG:HB3	1:B:2359:ARG:HH21	1.82	0.44
1:B:2500:ALA:HB1	1:B:2550:LEU:HD22	1.99	0.44
1:C:3110:LEU:HD23	1:C:3110:LEU:HA	1.85	0.44
1:C:3695:PRO:HD2	1:C:3699:HIS:HB2	1.98	0.44
1:D:24:CYS:HB3	1:D:200:TRP:CE3	2.53	0.44
1:D:2474:LEU:HA	1:D:2494:PHE:CD2	2.52	0.44
1:D:2491:SER:O	1:D:2491:SER:OG	2.32	0.44
1:A:2003:GLN:HA	1:A:3652:MET:HE1	1.98	0.44
1:B:3842:LEU:O	1:B:3929:SER:OG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2614:ILE:O	1:C:2618:MET:N	2.50	0.44
1:C:2858:GLN:H	1:C:2858:GLN:HG3	1.67	0.44
1:C:4034:ASN:HD21	1:C:4153:HIS:CE1	2.35	0.44
1:B:710:ASP:O	1:B:712:TYR:N	2.50	0.44
1:B:1128:ARG:HD3	1:B:1130:GLN:NE2	2.33	0.44
1:B:4159:ARG:HA	1:B:4162:ASN:HD21	1.82	0.44
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.29	0.44
1:C:757:PHE:HB2	1:C:764:VAL:HG11	1.99	0.44
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.99	0.44
1:C:2325:PRO:HB3	1:C:2422:ILE:HA	2.00	0.44
1:C:3172:ILE:HG21	1:C:3194:LEU:HD21	1.99	0.44
1:D:477:LEU:HD12	1:D:477:LEU:HA	1.90	0.44
1:D:497:TYR:HA	1:D:503:PHE:CE2	2.52	0.44
1:D:1206:GLN:NE2	1:D:1230:MET:O	2.51	0.44
1:D:2500:ALA:HB1	1:D:2550:LEU:HD22	2.00	0.44
1:D:2974:ILE:O	1:D:2978:GLU:N	2.44	0.44
1:D:4003:LEU:HD21	1:D:4012:LEU:HB3	1.98	0.44
1:A:263:GLU:HB3	1:A:281:ARG:HB2	1.99	0.44
1:A:479:GLN:O	1:A:479:GLN:NE2	2.51	0.44
1:A:497:TYR:HA	1:A:503:PHE:CE2	2.53	0.44
1:A:686:TRP:NE1	1:A:746:CYS:SG	2.77	0.44
1:A:760:ASN:N	1:A:760:ASN:OD1	2.49	0.44
1:A:1000:ARG:HD2	1:A:1005:TRP:CG	2.52	0.44
1:A:2536:LEU:HA	1:A:2584:HIS:CE1	2.53	0.44
1:B:24:CYS:HB3	1:B:200:TRP:CE3	2.53	0.44
1:B:3579:LEU:HG	1:B:3581:GLY:H	1.82	0.44
1:C:1700:ASP:HB3	1:C:1703:LEU:HD12	1.99	0.44
1:C:4000:MET:HE2	1:C:4058:ILE:HG12	1.99	0.44
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.30	0.44
1:D:760:ASN:N	1:D:760:ASN:OD1	2.49	0.44
1:D:1454:THR:HG22	1:D:1491:ASN:HA	1.99	0.44
2:G:30:LEU:N	2:G:34:LYS:O	2.48	0.44
2:H:77:THR:HA	2:H:96:THR:HG22	2.00	0.44
1:A:1125:ASN:HB2	1:A:1132:TRP:HD1	1.83	0.44
1:A:1263:THR:N	1:A:1266:THR:O	2.41	0.44
1:A:3999:MET:HB3	1:A:3999:MET:HE2	1.78	0.44
1:A:4583:SER:HB3	1:A:4630:TYR:HE2	1.83	0.44
1:B:68:THR:HG23	1:B:110:ARG:HB2	2.00	0.44
1:B:3274:LEU:HG	1:B:3275:PRO:HD3	1.99	0.44
1:B:4109:GLN:HA	1:B:4112:LEU:HD12	2.00	0.44
1:B:4769:MET:SD	1:B:4769:MET:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:TRP:CD1	1:C:272:SER:HB2	2.52	0.44
1:C:3535:LEU:HD23	1:C:3535:LEU:H	1.83	0.44
1:D:102:LEU:HD12	1:D:161:GLU:O	2.17	0.44
1:D:830:ARG:NE	1:D:1612:PHE:CE2	2.83	0.44
1:D:954:LYS:HA	1:D:954:LYS:HD2	1.80	0.44
1:D:1644:GLU:OE1	1:D:1646:ARG:NE	2.42	0.44
1:D:3971:GLY:O	1:D:3973:CYS:N	2.50	0.44
2:G:38:SER:OG	2:G:41:ASP:OD2	2.35	0.44
1:A:158:SER:N	1:A:161:GLU:OE1	2.49	0.44
1:A:2614:ILE:O	1:A:2618:MET:N	2.51	0.44
1:A:4008:SER:OG	1:A:4009:GLN:OE1	2.24	0.44
1:C:68:THR:HG23	1:C:110:ARG:HB2	1.99	0.44
1:D:1040:CYS:O	1:D:1044:ARG:HG2	2.18	0.44
1:D:3526:ALA:HB2	1:D:3595:ARG:HH12	1.82	0.44
1:D:3845:ASN:OD1	1:D:3845:ASN:N	2.49	0.44
2:G:14:THR:OG1	2:G:68:LEU:N	2.51	0.44
1:A:1435:TYR:CZ	1:A:1550:PRO:HB3	2.53	0.44
1:A:4586:PRO:HB3	1:A:4628:VAL:HG21	1.98	0.44
1:B:30:LYS:HA	1:B:30:LYS:HD3	1.84	0.44
1:B:2368:LEU:HA	1:B:2374:SER:HB2	2.00	0.44
1:C:3289:PRO:HG2	1:C:3307:VAL:HG22	1.99	0.44
1:D:619:ASP:OD2	1:D:1680:ARG:NH2	2.50	0.44
1:D:2983:SER:O	1:D:2983:SER:OG	2.29	0.44
1:D:3359:ILE:HD11	1:D:3434:LEU:HB2	2.00	0.44
2:F:17:LYS:HD3	2:F:17:LYS:N	2.33	0.44
1:A:68:THR:HG23	1:A:110:ARG:HB2	2.00	0.43
1:A:277:GLY:HA2	1:A:315:CYS:SG	2.57	0.43
1:A:279:PRO:HA	1:A:314:PHE:O	2.18	0.43
1:A:757:PHE:HB2	1:A:764:VAL:HG11	1.99	0.43
1:A:1486:SER:O	1:A:1486:SER:OG	2.29	0.43
1:A:2258:LEU:HD12	1:A:2258:LEU:HA	1.87	0.43
1:B:2431:ASP:OD1	1:B:2435:ARG:NE	2.47	0.43
1:C:798:GLY:HA2	1:C:1623:ARG:HD3	1.99	0.43
1:C:1125:ASN:OD1	1:C:1126:GLY:N	2.51	0.43
1:C:2159:LEU:HD22	1:C:2201:LEU:HD21	2.00	0.43
1:D:269:TRP:NE1	1:D:333:GLY:O	2.51	0.43
1:D:448:LEU:HD23	1:D:448:LEU:HA	1.84	0.43
1:D:1805:GLU:OE2	1:D:1808:ARG:NH2	2.51	0.43
1:D:3940:LYS:HE2	1:D:3940:LYS:HB2	1.83	0.43
1:A:375:LYS:HB2	1:A:375:LYS:HE3	1.81	0.43
1:A:652:ARG:HG2	1:A:750:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3249:LEU:O	1:A:3253:ILE:HG12	2.18	0.43
1:A:3526:ALA:O	1:A:3528:THR:N	2.51	0.43
1:B:1018:ASN:HA	1:B:1019:PRO:HD3	1.78	0.43
1:B:3289:PRO:HG2	1:B:3307:VAL:HG22	2.00	0.43
1:C:651:GLY:H	1:C:776:LEU:HD23	1.83	0.43
1:C:1283:LEU:HD12	1:C:1283:LEU:HA	1.84	0.43
1:C:1652:GLU:OE1	1:C:1656:ARG:NH2	2.51	0.43
1:C:3327:LEU:HD12	1:C:3327:LEU:HA	1.82	0.43
1:D:263:GLU:HB3	1:D:281:ARG:HB2	1.99	0.43
1:D:1139:PHE:CE1	1:D:1169:LEU:HD11	2.53	0.43
2:H:22:CYS:SG	2:H:23:VAL:N	2.91	0.43
1:A:865:PRO:HA	1:A:868:GLU:HB2	2.00	0.43
1:A:1079:LYS:HG3	1:A:1107:PRO:HB3	2.00	0.43
1:A:1634:LEU:HD12	1:A:1634:LEU:HA	1.79	0.43
1:A:1805:GLU:OE2	1:A:1808:ARG:NH2	2.52	0.43
1:A:3424:LEU:HD23	1:A:3424:LEU:HA	1.86	0.43
1:A:3695:PRO:HD2	1:A:3699:HIS:HB2	1.99	0.43
1:A:4763:GLY:N	1:A:4766:THR:OG1	2.49	0.43
1:B:268:SER:OG	1:B:269:TRP:N	2.51	0.43
1:B:689:THR:HB	1:B:778:PHE:HZ	1.83	0.43
1:C:760:ASN:OD1	1:C:760:ASN:N	2.50	0.43
1:C:1442:GLY:HA3	1:C:1558:HIS:CD2	2.53	0.43
1:C:1461:ASP:HB3	1:C:1464:PHE:HB2	2.01	0.43
1:C:2536:LEU:HA	1:C:2584:HIS:CE1	2.53	0.43
1:C:2606:CYS:SG	1:C:2607:LEU:N	2.91	0.43
1:C:3051:ARG:HA	1:C:3051:ARG:HD2	1.73	0.43
1:D:919:ASN:O	1:D:922:LEU:HD12	2.18	0.43
1:D:1815:LEU:HD12	1:D:1815:LEU:HA	1.90	0.43
1:D:2368:LEU:HA	1:D:2374:SER:HB2	2.01	0.43
1:D:4583:SER:HB3	1:D:4630:TYR:HE2	1.83	0.43
1:A:2325:PRO:HB3	1:A:2422:ILE:HA	2.00	0.43
1:A:2476:ILE:HD12	1:A:2477:PRO:HD2	2.01	0.43
1:A:3232:LEU:HD12	1:A:3233:PRO:HD2	1.99	0.43
1:A:4187:SER:OG	1:A:4191:GLU:OE2	2.28	0.43
1:B:417:GLY:O	1:B:420:SER:OG	2.35	0.43
1:B:686:TRP:NE1	1:B:746:CYS:SG	2.75	0.43
1:B:757:PHE:HB2	1:B:764:VAL:HG11	1.99	0.43
1:B:960:MET:HG3	1:B:966:LYS:HG3	2.01	0.43
1:B:986:ASP:HB3	1:B:1036:ARG:HE	1.82	0.43
1:B:1000:ARG:HD2	1:B:1005:TRP:CG	2.53	0.43
1:B:1125:ASN:OD1	1:B:1126:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1436:SER:HA	1:B:1517:GLY:HA2	1.99	0.43
1:B:1457:TYR:O	1:B:1458:HIS:ND1	2.51	0.43
1:C:830:ARG:HH12	1:C:832:GLU:HG3	1.83	0.43
1:C:3677:LEU:HG	1:C:3697:PRO:HG2	2.00	0.43
1:C:3999:MET:HE2	1:C:4016:LEU:HD13	1.99	0.43
1:C:4162:ASN:HA	1:C:4165:GLU:HG2	2.00	0.43
1:D:681:HIS:O	1:D:783:PHE:HA	2.19	0.43
1:D:1842:LEU:HD23	1:D:1842:LEU:HA	1.89	0.43
1:D:2556:LEU:HD11	1:D:2597:LYS:HA	2.01	0.43
1:D:3842:LEU:O	1:D:3929:SER:OG	2.30	0.43
1:D:4845:ALA:O	1:D:4883:TYR:OH	2.34	0.43
1:A:1206:GLN:NE2	1:A:1230:MET:O	2.52	0.43
1:B:591:ASP:OD1	1:B:1594:ARG:NH1	2.51	0.43
1:B:718:GLY:HA3	1:B:737:LEU:HA	2.00	0.43
1:B:1141:ARG:NH2	1:B:1167:GLU:OE2	2.51	0.43
1:B:1805:GLU:OE2	1:B:1808:ARG:NH2	2.52	0.43
1:B:2159:LEU:HD22	1:B:2201:LEU:HD21	2.00	0.43
1:B:4189:ARG:NE	1:B:5032:TYR:OH	2.29	0.43
1:B:4583:SER:HB3	1:B:4630:TYR:HE2	1.83	0.43
1:B:4951:LYS:HE2	1:B:4951:LYS:HB2	1.88	0.43
1:C:103:TYR:HE1	1:C:152:PRO:HA	1.83	0.43
1:C:1125:ASN:HB2	1:C:1132:TRP:CD1	2.53	0.43
1:C:2759:ALA:HB2	1:C:2806:ARG:HH22	1.84	0.43
1:C:3103:ILE:HD11	1:C:3168:THR:HG22	2.00	0.43
1:C:4583:SER:HB3	1:C:4630:TYR:HE2	1.83	0.43
1:D:575:LEU:HD22	1:D:609:CYS:HB2	2.00	0.43
1:A:268:SER:OG	1:A:269:TRP:N	2.52	0.43
1:A:294:THR:HG23	1:A:297:GLN:H	1.83	0.43
1:A:1125:ASN:OD1	1:A:1126:GLY:N	2.51	0.43
1:A:2520:HIS:O	1:A:2524:VAL:HG23	2.19	0.43
1:B:224:HIS:HB2	1:B:388:LEU:HG	2.01	0.43
1:B:561:LEU:HD11	1:B:589:LEU:HD21	2.00	0.43
1:B:886:ARG:HB3	1:B:891:TRP:CD1	2.53	0.43
1:B:2313:LEU:HB3	1:B:2318:TYR:HD2	1.84	0.43
1:B:3524:MET:H	1:B:3524:MET:HG2	1.65	0.43
1:B:3971:GLY:O	1:B:3973:CYS:N	2.50	0.43
1:C:1805:GLU:OE2	1:C:1808:ARG:NH2	2.51	0.43
1:C:1947:CYS:HB3	1:C:2126:ARG:HH21	1.84	0.43
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.32	0.43
1:D:591:ASP:OD1	1:D:1594:ARG:NH1	2.52	0.43
1:D:977:LEU:H	1:D:1044:ARG:NH2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1442:GLY:HA3	1:D:1558:HIS:CD2	2.54	0.43
2:G:56:ILE:HG22	2:G:59:PHE:H	1.83	0.43
2:H:68:LEU:HD23	2:H:68:LEU:HA	1.80	0.43
1:A:871:ARG:HH12	1:A:926:GLY:CA	2.32	0.43
1:A:2212:VAL:HG22	1:A:2256:TYR:CZ	2.54	0.43
1:B:479:GLN:O	1:B:479:GLN:NE2	2.50	0.43
1:B:955:LEU:HD13	1:B:959:TYR:CG	2.53	0.43
1:B:1442:GLY:HA3	1:B:1558:HIS:CD2	2.54	0.43
1:B:2476:ILE:HD12	1:B:2477:PRO:HD2	2.01	0.43
1:C:649:PHE:HE2	1:C:845:CYS:HB2	1.83	0.43
1:C:2228:MET:HE3	1:C:2228:MET:HB3	1.91	0.43
1:D:294:THR:HG23	1:D:297:GLN:H	1.84	0.43
1:D:858:THR:OG1	1:D:930:LYS:HG3	2.18	0.43
1:D:881:LEU:HD12	1:D:881:LEU:HA	1.84	0.43
1:D:1006:SER:O	1:D:1017:ARG:NH1	2.51	0.43
1:D:3347:SER:O	1:D:3347:SER:OG	2.29	0.43
2:H:17:LYS:O	2:H:18:LYS:HG2	2.19	0.43
1:A:269:TRP:NE1	1:A:333:GLY:O	2.52	0.43
1:B:359:TYR:HB2	1:B:383:HIS:CE1	2.54	0.43
1:B:2556:LEU:HD11	1:B:2597:LYS:HA	2.01	0.43
1:B:3357:HIS:O	1:B:3361:THR:HG23	2.18	0.43
1:C:3232:LEU:HD12	1:C:3233:PRO:HD2	1.99	0.43
1:D:915:GLU:HA	1:D:918:ARG:HB2	2.00	0.43
1:D:1849:LEU:HD23	1:D:1849:LEU:HA	1.86	0.43
1:D:2159:LEU:HD22	1:D:2201:LEU:HD21	2.01	0.43
1:D:3447:LYS:HA	1:D:3447:LYS:HD2	1.75	0.43
1:D:4907:ASP:O	1:D:4908:GLU:HB3	2.19	0.43
1:A:858:THR:OG1	1:A:930:LYS:HG3	2.19	0.43
1:A:913:LEU:HB2	1:A:918:ARG:HG2	1.99	0.43
1:A:1277:TRP:O	1:A:1277:TRP:HD1	2.02	0.43
1:A:2310:CYS:O	1:A:2312:MET:N	2.52	0.43
1:A:2556:LEU:HD11	1:A:2597:LYS:HA	2.01	0.43
1:A:3235:SER:O	1:A:3235:SER:OG	2.35	0.43
1:B:2199:ARG:HG3	1:B:2246:ASN:OD1	2.19	0.43
1:B:2536:LEU:HA	1:B:2584:HIS:CE1	2.53	0.43
1:B:2856:ASN:OD1	1:B:2856:ASN:N	2.52	0.43
1:B:3398:PHE:HB3	1:B:3454:GLU:HG2	2.00	0.43
1:C:684:VAL:HG12	1:C:781:VAL:HG12	2.00	0.43
1:C:977:LEU:HB3	1:C:981:GLN:CB	2.48	0.43
1:C:1022:VAL:HG23	1:C:1027:LEU:HG	2.01	0.43
1:C:1288:PHE:HA	1:C:1551:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2021:CYS:SG	1:C:2023:LEU:HB3	2.59	0.43
1:D:268:SER:OG	1:D:269:TRP:N	2.52	0.43
1:D:402:ARG:HA	1:D:402:ARG:HD2	1.85	0.43
1:D:1634:LEU:HD12	1:D:1634:LEU:HA	1.79	0.43
1:D:1652:GLU:OE1	1:D:1656:ARG:NH2	2.52	0.43
1:D:3141:THR:O	1:D:3145:GLN:HG2	2.19	0.43
1:A:30:LYS:HA	1:A:30:LYS:HD3	1.83	0.43
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.26	0.43
1:A:990:GLU:HG2	1:A:1024:TYR:CE2	2.53	0.43
1:A:3509:LEU:HD12	1:A:3509:LEU:HA	1.84	0.43
1:A:4109:GLN:HA	1:A:4112:LEU:HD12	2.00	0.43
1:A:4689:THR:OG1	1:A:4690:GLU:N	2.52	0.43
1:B:1770:SER:OG	1:B:1956:GLU:OE2	2.28	0.43
1:B:2283:ASN:HB3	1:B:2286:LEU:H	1.84	0.43
1:B:3172:ILE:HG21	1:B:3194:LEU:HD21	2.01	0.43
1:B:3263:TYR:O	1:B:3265:GLU:N	2.52	0.43
1:C:919:ASN:O	1:C:922:LEU:HD12	2.18	0.43
1:C:1272:LEU:HD11	1:C:1285:GLU:OE1	2.18	0.43
1:C:2556:LEU:HD11	1:C:2597:LYS:HA	2.01	0.43
1:C:2916:LYS:HA	1:C:2916:LYS:HD2	1.80	0.43
1:D:359:TYR:HB2	1:D:383:HIS:CE1	2.54	0.43
1:D:1028:ASP:O	1:D:1032:LYS:HG3	2.19	0.43
1:D:3274:LEU:HG	1:D:3275:PRO:HD3	2.01	0.43
1:D:3994:HIS:O	1:D:3998:HIS:ND1	2.50	0.43
1:A:971:ASP:O	1:A:974:HIS:NE2	2.51	0.42
1:A:981:GLN:HA	1:A:984:LEU:HD23	2.01	0.42
1:A:3519:PRO:O	1:D:1220:GLN:NE2	2.50	0.42
1:B:294:THR:HG23	1:B:297:GLN:H	1.84	0.42
1:B:2310:CYS:O	1:B:2312:MET:N	2.52	0.42
1:B:3359:ILE:HD11	1:B:3434:LEU:HB2	2.01	0.42
1:C:670:GLU:HA	1:C:740:PRO:HB3	2.01	0.42
1:C:2310:CYS:O	1:C:2312:MET:N	2.52	0.42
1:C:2355:ARG:HB3	1:C:2359:ARG:HH21	1.84	0.42
1:C:2454:ARG:HG2	1:C:2458:ARG:HH12	1.84	0.42
1:C:2476:ILE:HD12	1:C:2477:PRO:HD2	2.00	0.42
1:C:3447:LYS:HD2	1:C:3447:LYS:HA	1.74	0.42
1:C:3771:HIS:HD2	1:C:3815:LYS:HD2	1.84	0.42
1:D:29:LEU:HD12	1:D:30:LYS:N	2.34	0.42
1:D:479:GLN:O	1:D:479:GLN:NE2	2.50	0.42
1:D:1436:SER:HA	1:D:1517:GLY:HA2	2.01	0.42
1:D:2283:ASN:HB3	1:D:2286:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2606:CYS:SG	1:D:2607:LEU:N	2.92	0.42
1:D:3677:LEU:HG	1:D:3697:PRO:HG2	2.01	0.42
1:A:14:LEU:HD12	1:A:18:ASP:HB3	2.01	0.42
1:A:266:ARG:NH2	1:A:331:VAL:O	2.35	0.42
1:A:881:LEU:HD12	1:A:881:LEU:HA	1.78	0.42
1:A:1283:LEU:HD12	1:A:1283:LEU:HA	1.84	0.42
1:A:1442:GLY:HA3	1:A:1558:HIS:CD2	2.54	0.42
1:A:2035:HIS:CE1	1:A:3661:TRP:HB3	2.54	0.42
1:A:2149:VAL:O	1:A:2153:MET:N	2.49	0.42
1:A:2967:MET:H	1:A:2967:MET:HG2	1.60	0.42
1:A:3398:PHE:HB3	1:A:3454:GLU:HG2	2.00	0.42
1:B:497:TYR:HA	1:B:503:PHE:CE2	2.54	0.42
1:B:1079:LYS:HG3	1:B:1107:PRO:HB3	2.01	0.42
1:B:1459:GLN:HA	1:B:1459:GLN:OE1	2.19	0.42
1:B:4198:SER:HB3	1:B:4201:ASN:ND2	2.34	0.42
1:C:345:LEU:HD22	1:C:389:PHE:HB3	2.01	0.42
1:C:595:ARG:NH2	1:C:1643:GLU:OE1	2.50	0.42
1:C:655:GLY:HA3	1:C:852:VAL:HG12	2.01	0.42
1:C:1206:GLN:NE2	1:C:1230:MET:O	2.51	0.42
1:C:2283:ASN:HB3	1:C:2286:LEU:H	1.84	0.42
1:C:2431:ASP:OD1	1:C:2435:ARG:NE	2.49	0.42
1:C:2999:ALA:HA	1:C:3002:LEU:HG	2.00	0.42
1:C:4198:SER:HB3	1:C:4201:ASN:ND2	2.34	0.42
1:C:4897:ILE:HD12	1:C:4897:ILE:HA	1.89	0.42
1:D:2199:ARG:HG3	1:D:2246:ASN:OD1	2.19	0.42
1:D:4049:VAL:O	1:D:4052:SER:OG	2.35	0.42
1:D:4198:SER:HB3	1:D:4201:ASN:ND2	2.35	0.42
1:A:902:ARG:O	1:A:903:LEU:HD12	2.19	0.42
1:A:993:HIS:NE2	1:A:1027:LEU:HD11	2.34	0.42
1:A:2454:ARG:HG2	1:A:2458:ARG:HH12	1.85	0.42
1:A:3289:PRO:HG2	1:A:3307:VAL:HG22	2.00	0.42
1:A:3332:ALA:HB1	1:A:3334:TRP:CD1	2.54	0.42
1:B:12:GLN:HE21	1:B:14:LEU:HD11	1.84	0.42
1:B:1037:ASP:O	1:B:1041:GLN:HG2	2.18	0.42
1:B:1125:ASN:HB2	1:B:1132:TRP:HD1	1.84	0.42
1:B:2964:LEU:HA	1:B:2967:MET:HE2	2.02	0.42
1:C:273:HIS:HE1	1:C:334:MET:HG3	1.84	0.42
1:C:882:TRP:HZ3	1:C:921:ASN:ND2	2.17	0.42
1:C:899:ASP:HB2	1:C:902:ARG:CZ	2.49	0.42
1:C:1634:LEU:HD12	1:C:1634:LEU:HA	1.79	0.42
1:C:4689:THR:OG1	1:C:4690:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1434:TYR:HA	1:D:1519:LEU:HD23	2.01	0.42
1:D:2476:ILE:HD12	1:D:2477:PRO:HD2	2.00	0.42
1:D:3804:ILE:HD12	1:D:3804:ILE:HA	1.87	0.42
1:D:4184:MET:HB2	1:D:4190:ILE:HD13	2.02	0.42
1:A:345:LEU:HD22	1:A:389:PHE:HB3	2.00	0.42
1:A:710:ASP:O	1:A:712:TYR:N	2.52	0.42
1:A:1253:PRO:HB2	1:A:1254:HIS:CE1	2.54	0.42
1:A:3756:LYS:HE2	1:A:3756:LYS:HB3	1.86	0.42
1:B:725:HIS:O	1:B:725:HIS:ND1	2.52	0.42
1:C:887:ILE:HG13	1:C:891:TRP:O	2.20	0.42
1:C:1640:HIS:HA	1:C:1647:CYS:HA	2.01	0.42
1:C:2547:ALA:O	1:C:2551:ASN:ND2	2.52	0.42
1:C:3208:PRO:HD2	1:C:3245:VAL:HG22	2.02	0.42
1:D:871:ARG:HH11	1:D:926:GLY:HA3	1.83	0.42
1:D:1125:ASN:OD1	1:D:1126:GLY:N	2.52	0.42
1:D:1253:PRO:HB2	1:D:1254:HIS:CE1	2.54	0.42
1:D:1451:GLY:HA3	1:D:1494:MET:HG2	2.02	0.42
2:E:29:MET:HA	2:E:35:LYS:HA	2.01	0.42
1:A:670:GLU:HA	1:A:740:PRO:HB3	2.00	0.42
1:A:886:ARG:HB3	1:A:891:TRP:HD1	1.85	0.42
1:A:2103:VAL:HG13	1:A:3696:ASP:OD2	2.19	0.42
1:A:3806:ASN:HA	1:A:3890:LEU:HD21	2.01	0.42
1:A:4184:MET:HB2	1:A:4190:ILE:HD13	2.02	0.42
1:B:273:HIS:HE1	1:B:334:MET:HG3	1.84	0.42
1:B:345:LEU:HD22	1:B:389:PHE:HB3	2.01	0.42
1:B:954:LYS:HD2	1:B:954:LYS:HA	1.83	0.42
1:B:1263:THR:HG23	1:B:1265:ASP:H	1.85	0.42
1:B:1618:ARG:HG2	1:B:1627:ALA:HB3	2.01	0.42
1:B:1652:GLU:OE1	1:B:1656:ARG:NH2	2.53	0.42
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.85	0.42
1:C:2199:ARG:HG3	1:C:2246:ASN:OD1	2.19	0.42
1:C:4951:LYS:HE2	1:C:4951:LYS:HB2	1.88	0.42
1:D:710:ASP:O	1:D:712:TYR:N	2.52	0.42
1:D:887:ILE:HG13	1:D:891:TRP:O	2.19	0.42
1:D:977:LEU:HD12	1:D:1044:ARG:HH21	1.83	0.42
1:D:2858:GLN:H	1:D:2858:GLN:HG3	1.67	0.42
1:D:3263:TYR:O	1:D:3265:GLU:N	2.53	0.42
1:A:924:MET:HA	1:A:927:GLU:OE2	2.18	0.42
1:A:2313:LEU:HB3	1:A:2318:TYR:HD2	1.84	0.42
1:A:3107:VAL:HA	1:A:3110:LEU:HB2	2.02	0.42
1:B:266:ARG:NH2	1:B:331:VAL:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2035:HIS:CE1	1:B:3661:TRP:HB3	2.55	0.42
1:B:2442:LEU:HG	1:B:2443:ILE:HG12	2.01	0.42
1:C:1719:HIS:CE1	1:C:1800:PRO:HB2	2.55	0.42
1:C:2035:HIS:CE1	1:C:3661:TRP:HB3	2.55	0.42
1:C:3526:ALA:O	1:C:3528:THR:N	2.52	0.42
1:D:950:LEU:HD23	1:D:950:LEU:HA	1.84	0.42
1:D:3289:PRO:HG2	1:D:3307:VAL:HG22	2.00	0.42
1:D:3438:VAL:HG11	1:D:3517:MET:HE3	2.01	0.42
1:D:3771:HIS:HD2	1:D:3815:LYS:HD2	1.84	0.42
2:G:29:MET:HA	2:G:35:LYS:HA	2.02	0.42
1:A:255:HIS:ND1	1:A:480:GLU:OE2	2.52	0.42
1:A:575:LEU:HD22	1:A:609:CYS:HB2	2.02	0.42
1:A:1436:SER:HA	1:A:1517:GLY:HA2	2.01	0.42
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.00	0.42
1:A:2974:ILE:O	1:A:2978:GLU:N	2.44	0.42
1:A:3771:HIS:HD2	1:A:3815:LYS:HD2	1.84	0.42
1:A:4907:ASP:O	1:A:4908:GLU:HB3	2.19	0.42
1:B:1288:PHE:CE1	1:B:1598:GLN:HB2	2.54	0.42
1:B:2021:CYS:SG	1:B:2023:LEU:HB3	2.60	0.42
1:B:2606:CYS:SG	1:B:2607:LEU:N	2.92	0.42
1:C:233:ILE:HG22	1:C:234:SER:N	2.35	0.42
1:C:268:SER:OG	1:C:269:TRP:N	2.51	0.42
1:C:575:LEU:HD22	1:C:609:CYS:HB2	2.02	0.42
1:C:952:LYS:HG2	1:C:953:THR:H	1.84	0.42
1:C:993:HIS:NE2	1:C:1027:LEU:HD11	2.35	0.42
1:C:1079:LYS:HG3	1:C:1107:PRO:HB3	2.00	0.42
1:C:1101:ARG:HB3	1:C:1123:VAL:HG21	2.00	0.42
1:C:1618:ARG:HG2	1:C:1627:ALA:HB3	2.01	0.42
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.84	0.42
1:C:3396:ASP:OD1	1:C:3397:GLU:N	2.53	0.42
1:C:4159:ARG:HA	1:C:4162:ASN:HD21	1.84	0.42
1:D:981:GLN:O	1:D:984:LEU:HG	2.19	0.42
1:D:990:GLU:HG2	1:D:1024:TYR:CZ	2.55	0.42
1:D:2212:VAL:HG22	1:D:2256:TYR:CZ	2.55	0.42
1:D:3068:LEU:H	1:D:3068:LEU:HD12	1.84	0.42
1:D:3136:LEU:HA	1:D:3139:VAL:HG22	2.01	0.42
1:D:4586:PRO:HA	1:D:4587:PRO:HD3	1.91	0.42
1:A:875:ALA:HB1	1:A:910:PHE:CZ	2.55	0.42
1:A:1275:ARG:HG3	1:A:1276:THR:HG23	2.01	0.42
1:A:2159:LEU:HD22	1:A:2201:LEU:HD21	2.02	0.42
1:A:2236:LEU:HD22	1:A:2250:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2759:ALA:HB2	1:A:2806:ARG:HH22	1.84	0.42
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.85	0.42
1:A:3447:LYS:HA	1:A:3447:LYS:HD2	1.75	0.42
1:B:575:LEU:HD22	1:B:609:CYS:HB2	2.01	0.42
1:B:1470:ARG:HA	1:B:1470:ARG:HD3	1.70	0.42
1:B:4845:ALA:O	1:B:4883:TYR:OH	2.36	0.42
1:C:33:LEU:HG	1:C:53:SER:OG	2.20	0.42
1:C:2212:VAL:HG22	1:C:2256:TYR:CZ	2.55	0.42
1:C:3272:ILE:HG13	1:C:3273:THR:HG22	2.02	0.42
1:C:3509:LEU:HD12	1:C:3509:LEU:HA	1.84	0.42
1:D:829:TYR:HE2	1:D:1608:MET:HG2	1.85	0.42
1:D:875:ALA:HB1	1:D:910:PHE:CZ	2.55	0.42
1:D:1275:ARG:HG3	1:D:1276:THR:HG23	2.01	0.42
1:D:2035:HIS:CE1	1:D:3661:TRP:HB3	2.55	0.42
1:D:2360:LYS:HE3	1:D:2360:LYS:HB2	1.95	0.42
1:D:3696:ASP:CG	1:D:3697:PRO:HD3	2.39	0.42
2:E:57:LYS:HB3	2:E:57:LYS:HE2	1.76	0.42
2:H:29:MET:HA	2:H:35:LYS:HA	2.02	0.42
1:A:17:ASP:HB2	1:A:98:HIS:HE1	1.84	0.42
1:A:723:THR:HG21	1:A:768:PHE:HE2	1.85	0.42
1:A:1618:ARG:HG2	1:A:1627:ALA:HB3	2.01	0.42
1:A:2199:ARG:HG3	1:A:2246:ASN:OD1	2.20	0.42
1:A:2283:ASN:HB3	1:A:2286:LEU:H	1.84	0.42
1:B:233:ILE:HG22	1:B:234:SER:N	2.35	0.42
1:B:681:HIS:O	1:B:783:PHE:HA	2.20	0.42
1:B:3323:ILE:HD11	1:B:3338:LEU:HD22	2.01	0.42
1:B:4008:SER:OG	1:B:4009:GLN:OE1	2.27	0.42
1:C:892:THR:OG1	1:C:902:ARG:O	2.28	0.42
1:C:1000:ARG:HD2	1:C:1000:ARG:HA	1.81	0.42
1:C:1849:LEU:HD23	1:C:1849:LEU:HA	1.87	0.42
1:C:2313:LEU:HB3	1:C:2318:TYR:HD2	1.84	0.42
1:C:3674:ILE:HG13	1:C:3732:SER:HB2	2.02	0.42
1:C:4049:VAL:O	1:C:4052:SER:OG	2.32	0.42
1:D:299:LEU:HD12	1:D:299:LEU:HA	1.81	0.42
1:D:1947:CYS:HB3	1:D:2126:ARG:HH21	1.84	0.42
1:D:2741:GLU:HB3	1:D:2744:ASN:HB2	2.01	0.42
1:D:2963:LEU:HA	1:D:2966:TRP:HB2	2.01	0.42
1:D:3323:ILE:HD11	1:D:3338:LEU:HD22	2.01	0.42
1:D:3714:SER:O	1:D:3714:SER:OG	2.37	0.42
1:A:33:LEU:HG	1:A:53:SER:OG	2.20	0.42
1:A:233:ILE:HG22	1:A:234:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:PHE:HA	1:A:1551:ALA:HA	2.02	0.42
1:A:1947:CYS:HB3	1:A:2126:ARG:HH21	1.85	0.42
1:A:2021:CYS:SG	1:A:2023:LEU:HB3	2.60	0.42
1:A:3777:GLU:H	1:A:3777:GLU:HG2	1.64	0.42
1:B:913:LEU:H	1:B:913:LEU:HD12	1.85	0.42
1:B:1275:ARG:HG3	1:B:1276:THR:HG23	2.01	0.42
1:B:2454:ARG:HG2	1:B:2458:ARG:HH12	1.84	0.42
1:B:3771:HIS:HD2	1:B:3815:LYS:HD2	1.84	0.42
1:C:107:ILE:HG22	1:C:148:TRP:HB2	2.01	0.42
1:C:224:HIS:HB2	1:C:388:LEU:HG	2.02	0.42
1:C:915:GLU:HA	1:C:918:ARG:HB2	2.01	0.42
1:C:2930:LEU:HB2	1:C:2935:TYR:HB3	2.02	0.42
1:C:3940:LYS:HB2	1:C:3940:LYS:HE2	1.83	0.42
1:D:22:LEU:HB3	1:D:200:TRP:CE3	2.55	0.42
1:D:33:LEU:HG	1:D:53:SER:OG	2.20	0.42
1:D:1008:SER:HB2	1:D:1017:ARG:CZ	2.50	0.42
1:D:1079:LYS:HG3	1:D:1107:PRO:HB3	2.01	0.42
1:D:1536:SER:OG	1:D:1537:ASN:N	2.53	0.42
1:D:2310:CYS:O	1:D:2312:MET:N	2.52	0.42
1:D:4767:TRP:O	1:D:4770:SER:OG	2.35	0.42
1:A:920:TYR:HD1	1:A:923:GLN:HE21	1.68	0.41
1:A:2858:GLN:H	1:A:2858:GLN:HG3	1.67	0.41
1:A:3172:ILE:HG21	1:A:3194:LEU:HD21	2.01	0.41
1:B:880:GLU:HG3	1:B:968:ALA:H	1.84	0.41
1:B:1220:GLN:HG3	1:C:3519:PRO:HB3	2.02	0.41
1:B:1644:GLU:OE1	1:B:1646:ARG:NE	2.42	0.41
1:B:4170:ILE:HD13	1:B:4170:ILE:HA	1.94	0.41
1:C:867:LEU:O	1:C:870:ILE:HG22	2.19	0.41
1:C:1435:TYR:CZ	1:C:1550:PRO:HB3	2.55	0.41
1:C:2179:ILE:HD11	1:C:2228:MET:HG2	2.02	0.41
1:C:3677:LEU:HG	1:C:3697:PRO:CG	2.50	0.41
1:C:4845:ALA:O	1:C:4883:TYR:OH	2.35	0.41
1:D:72:SER:H	1:D:99:ARG:HH12	1.68	0.41
1:D:2905:LEU:HD23	1:D:2905:LEU:H	1.83	0.41
2:E:48:PHE:HE1	2:E:55:VAL:HG21	1.84	0.41
1:A:24:CYS:HB3	1:A:200:TRP:CE3	2.54	0.41
1:A:655:GLY:HA3	1:A:852:VAL:HG12	2.01	0.41
1:A:952:LYS:HG2	1:A:953:THR:H	1.85	0.41
1:A:1028:ASP:O	1:A:1032:LYS:HG3	2.20	0.41
1:A:1640:HIS:HA	1:A:1647:CYS:HA	2.02	0.41
1:A:1652:GLU:OE1	1:A:1656:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1849:LEU:HD23	1:A:1849:LEU:HA	1.87	0.41
1:A:2179:ILE:HD11	1:A:2228:MET:HG2	2.02	0.41
1:A:3983:SER:OG	1:A:3984:ARG:N	2.54	0.41
1:B:1253:PRO:HB2	1:B:1254:HIS:CE1	2.54	0.41
1:B:3051:ARG:HD2	1:B:3051:ARG:HA	1.62	0.41
1:B:3806:ASN:HA	1:B:3890:LEU:HD21	2.01	0.41
1:B:4907:ASP:O	1:B:4908:GLU:HB3	2.19	0.41
1:B:4957:LYS:HB3	1:B:4957:LYS:HE2	1.88	0.41
1:C:833:GLY:HA3	1:C:838:HIS:ND1	2.35	0.41
1:C:1037:ASP:O	1:C:1041:GLN:HG2	2.20	0.41
1:C:1927:LEU:HD22	1:C:2097:LEU:HD11	2.02	0.41
1:C:3994:HIS:O	1:C:3998:HIS:ND1	2.49	0.41
1:D:833:GLY:N	1:D:836:GLY:O	2.52	0.41
1:D:955:LEU:HD13	1:D:959:TYR:CG	2.55	0.41
1:D:987:ARG:O	1:D:991:ASN:ND2	2.43	0.41
1:D:2520:HIS:O	1:D:2524:VAL:HG23	2.20	0.41
1:D:3103:ILE:HD11	1:D:3168:THR:HG22	2.02	0.41
1:D:3416:VAL:HG21	1:D:3517:MET:SD	2.60	0.41
2:G:44:LYS:HA	2:G:44:LYS:HD2	1.81	0.41
1:A:955:LEU:HD13	1:A:959:TYR:CG	2.54	0.41
1:A:1139:PHE:CE1	1:A:1169:LEU:HD11	2.55	0.41
1:A:2236:LEU:HD23	1:A:2236:LEU:HA	1.90	0.41
1:A:4951:LYS:HE2	1:A:4951:LYS:HB2	1.88	0.41
1:B:255:HIS:ND1	1:B:480:GLU:OE2	2.54	0.41
1:B:774:ASP:O	1:B:848:HIS:ND1	2.52	0.41
1:B:1634:LEU:HD12	1:B:1634:LEU:HA	1.79	0.41
1:C:619:ASP:OD2	1:C:1680:ARG:NH2	2.48	0.41
1:C:682:LEU:HD12	1:C:787:VAL:HG12	2.00	0.41
1:C:2906:VAL:HG11	1:C:2911:LEU:HA	2.03	0.41
1:C:3777:GLU:H	1:C:3777:GLU:HG2	1.64	0.41
1:D:393:CYS:HB2	1:D:397:GLU:HG3	2.03	0.41
1:D:881:LEU:HD23	1:D:1041:GLN:HG3	2.02	0.41
1:D:913:LEU:H	1:D:913:LEU:HD12	1.84	0.41
1:D:1521:ASP:OD1	1:D:1524:THR:OG1	2.32	0.41
1:A:778:PHE:HB2	1:A:780:VAL:HG13	2.01	0.41
1:B:1521:ASP:OD1	1:B:1524:THR:OG1	2.33	0.41
1:B:2541:PHE:HD1	1:B:2541:PHE:HA	1.81	0.41
1:B:3940:LYS:HB2	1:B:3940:LYS:HE2	1.83	0.41
1:C:12:GLN:HB2	1:C:165:VAL:HG13	2.03	0.41
1:C:255:HIS:ND1	1:C:480:GLU:OE2	2.54	0.41
1:C:711:LEU:HD12	1:C:1470:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2524:VAL:HA	1:C:2527:LEU:HD23	2.02	0.41
1:D:284:HIS:CE1	1:D:286:THR:HB	2.55	0.41
1:D:884:LEU:O	1:D:887:ILE:HG22	2.21	0.41
1:D:1288:PHE:HA	1:D:1551:ALA:HA	2.03	0.41
1:D:3110:LEU:HD12	1:D:3175:LEU:HD11	2.02	0.41
1:D:3592:ILE:HA	1:D:3595:ARG:NE	2.34	0.41
1:D:4689:THR:OG1	1:D:4690:GLU:N	2.53	0.41
1:A:537:CYS:O	1:A:541:SER:OG	2.39	0.41
1:A:1284:VAL:HG22	1:A:1555:LEU:HD13	2.02	0.41
1:A:1434:TYR:HB2	1:A:1572:ILE:HG21	2.02	0.41
1:A:2458:ARG:NH2	1:A:2509:VAL:O	2.54	0.41
1:A:3416:VAL:HG21	1:A:3517:MET:SD	2.60	0.41
1:B:393:CYS:HB2	1:B:397:GLU:HG3	2.03	0.41
1:B:830:ARG:HE	1:B:830:ARG:HB3	1.67	0.41
1:B:987:ARG:O	1:B:991:ASN:ND2	2.46	0.41
1:B:1139:PHE:CE1	1:B:1169:LEU:HD11	2.55	0.41
1:B:1206:GLN:NE2	1:B:1230:MET:O	2.52	0.41
1:C:689:THR:HB	1:C:778:PHE:HZ	1.84	0.41
1:C:874:LEU:HD13	1:C:929:LEU:HD21	2.02	0.41
1:D:224:HIS:HB2	1:D:388:LEU:HG	2.02	0.41
1:D:996:TRP:C	1:D:996:TRP:CD1	2.93	0.41
1:D:3040:THR:HG21	1:D:3080:VAL:HG21	2.01	0.41
1:D:3509:LEU:HD12	1:D:3509:LEU:HA	1.85	0.41
1:D:3832:ILE:HD13	1:D:3832:ILE:HA	1.97	0.41
1:A:14:LEU:HD22	1:A:202:MET:HE2	2.01	0.41
1:A:4897:ILE:HD12	1:A:4897:ILE:HA	1.91	0.41
1:B:72:SER:H	1:B:99:ARG:HH12	1.69	0.41
1:B:902:ARG:O	1:B:903:LEU:HD12	2.20	0.41
1:B:2547:ALA:O	1:B:2551:ASN:ND2	2.54	0.41
1:B:3714:SER:O	1:B:3714:SER:OG	2.36	0.41
1:B:3891:LEU:HD22	1:B:3899:PHE:CE2	2.56	0.41
1:B:4689:THR:OG1	1:B:4690:GLU:N	2.53	0.41
1:C:402:ARG:HA	1:C:402:ARG:HD2	1.85	0.41
1:C:913:LEU:H	1:C:913:LEU:HD12	1.85	0.41
1:C:3068:LEU:HD12	1:C:3068:LEU:H	1.85	0.41
1:C:3430:ASN:OD1	1:C:3430:ASN:N	2.54	0.41
1:D:345:LEU:HD22	1:D:389:PHE:HB3	2.01	0.41
1:D:1851:MET:HB2	1:D:1853:ILE:HG13	2.03	0.41
1:D:2454:ARG:HG2	1:D:2458:ARG:HH12	1.85	0.41
1:D:3107:VAL:HA	1:D:3110:LEU:HB2	2.03	0.41
1:D:3327:LEU:HA	1:D:3327:LEU:HD12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3359:ILE:HD13	1:D:3359:ILE:HA	1.93	0.41
1:A:206:CYS:N	1:A:271:GLY:HA3	2.36	0.41
1:A:247:TYR:OH	1:A:388:LEU:HD11	2.20	0.41
1:A:650:VAL:HG12	1:A:777:PHE:HB2	2.02	0.41
1:A:800:PHE:HD2	1:A:804:PRO:HG3	1.86	0.41
1:A:2741:GLU:HB3	1:A:2744:ASN:HB2	2.02	0.41
1:B:1288:PHE:HA	1:B:1551:ALA:HA	2.03	0.41
1:B:2179:ILE:HD11	1:B:2228:MET:HG2	2.02	0.41
1:B:2999:ALA:HA	1:B:3002:LEU:HG	2.03	0.41
1:B:4686:LEU:HD23	1:B:4687:TYR:CE1	2.55	0.41
1:C:630:GLU:HA	1:C:1642:PRO:CB	2.51	0.41
1:C:955:LEU:HD13	1:C:959:TYR:CG	2.55	0.41
1:D:839:LEU:O	1:D:1200:GLY:N	2.46	0.41
1:D:2536:LEU:HA	1:D:2584:HIS:CE1	2.55	0.41
1:D:2547:ALA:O	1:D:2551:ASN:ND2	2.54	0.41
1:D:3606:LEU:HD12	1:D:3606:LEU:HA	1.93	0.41
1:A:293:LEU:HD22	1:A:378:LEU:HD13	2.02	0.41
1:A:927:GLU:O	1:A:931:THR:HG23	2.21	0.41
1:A:1207:ASP:O	1:A:1210:SER:N	2.52	0.41
1:A:2102:VAL:HG11	1:A:2124:LEU:HB2	2.03	0.41
1:A:2606:CYS:SG	1:A:2607:LEU:N	2.91	0.41
1:A:4182:GLU:OE2	1:A:4192:ARG:NH1	2.54	0.41
1:B:12:GLN:HB2	1:B:165:VAL:HG13	2.03	0.41
1:B:29:LEU:HD12	1:B:30:LYS:N	2.36	0.41
1:B:205:ILE:HG22	1:B:206:CYS:N	2.30	0.41
1:B:4859:PHE:HB3	1:B:4862:PHE:HD2	1.86	0.41
1:C:622:THR:O	1:C:627:PRO:HD3	2.21	0.41
1:C:1253:PRO:HB2	1:C:1254:HIS:CE1	2.55	0.41
1:C:1536:SER:OG	1:C:1537:ASN:N	2.53	0.41
1:D:959:TYR:HB3	1:D:967:PRO:HD2	2.03	0.41
1:D:1618:ARG:HG2	1:D:1627:ALA:HB3	2.02	0.41
1:D:2313:LEU:HB3	1:D:2318:TYR:HD2	1.84	0.41
1:D:2759:ALA:HB2	1:D:2806:ARG:HH22	1.85	0.41
1:D:3891:LEU:HG	1:D:3899:PHE:CE2	2.55	0.41
1:D:4859:PHE:HB3	1:D:4862:PHE:HD2	1.86	0.41
2:G:82:TYR:HB3	2:G:86:GLY:HA2	2.03	0.41
1:A:29:LEU:HD12	1:A:30:LYS:N	2.35	0.41
1:A:320:LYS:HB3	1:A:356:TRP:CD1	2.56	0.41
1:A:2023:LEU:HG	1:A:2024:PRO:HD2	2.02	0.41
1:A:3263:TYR:O	1:A:3265:GLU:N	2.54	0.41
1:A:3272:ILE:HG13	1:A:3273:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4790:LEU:HD23	1:A:4790:LEU:HA	1.92	0.41
1:A:4801:LEU:HD12	1:A:4801:LEU:HA	1.94	0.41
1:B:707:VAL:HG12	1:B:782:SER:HB3	2.02	0.41
1:B:1434:TYR:HA	1:B:1519:LEU:HD23	2.01	0.41
1:B:1536:SER:OG	1:B:1537:ASN:N	2.53	0.41
1:B:2228:MET:HE3	1:B:2228:MET:HB3	1.98	0.41
1:B:3606:LEU:HD12	1:B:3606:LEU:HA	1.93	0.41
1:B:4184:MET:HB2	1:B:4190:ILE:HD13	2.02	0.41
1:B:4763:GLY:N	1:B:4766:THR:OG1	2.40	0.41
1:C:393:CYS:HB2	1:C:397:GLU:HG3	2.03	0.41
1:C:772:ASN:ND2	1:C:1470:ARG:HA	2.35	0.41
1:C:784:SER:OG	1:C:785:ALA:N	2.53	0.41
1:C:1041:GLN:O	1:C:1044:ARG:HB2	2.21	0.41
1:C:1668:ARG:HE	1:C:1668:ARG:HB2	1.58	0.41
1:C:1847:THR:O	1:C:1851:MET:HG3	2.21	0.41
1:C:2368:LEU:HA	1:C:2374:SER:HB2	2.02	0.41
1:C:3592:ILE:HA	1:C:3595:ARG:NE	2.34	0.41
1:D:866:HIS:HA	1:D:869:ARG:HD3	2.03	0.41
1:D:952:LYS:HG2	1:D:953:THR:H	1.85	0.41
1:D:2106:ALA:HB3	1:D:3696:ASP:OD1	2.21	0.41
1:D:2179:ILE:HD11	1:D:2228:MET:HG2	2.02	0.41
1:D:2789:PRO:O	1:D:2792:ARG:NH1	2.53	0.41
1:D:4897:ILE:HD12	1:D:4897:ILE:HA	1.92	0.41
2:E:26:TYR:CE1	2:E:39:SER:HB3	2.55	0.41
2:F:29:MET:HA	2:F:35:LYS:HA	2.02	0.41
1:A:206:CYS:SG	1:A:207:SER:N	2.94	0.41
1:A:1536:SER:OG	1:A:1537:ASN:N	2.53	0.41
1:A:4049:VAL:O	1:A:4052:SER:OG	2.34	0.41
1:B:375:LYS:HE3	1:B:375:LYS:HB2	1.81	0.41
1:B:674:PHE:N	1:B:680:THR:OG1	2.54	0.41
1:B:886:ARG:HB3	1:B:891:TRP:HD1	1.86	0.41
1:C:206:CYS:SG	1:C:207:SER:N	2.93	0.41
1:C:247:TYR:OH	1:C:388:LEU:HD11	2.20	0.41
1:C:860:GLN:HG2	1:C:860:GLN:O	2.21	0.41
1:C:1101:ARG:HB2	1:C:1193:SER:HB3	2.03	0.41
1:D:49:LEU:HD21	1:D:191:VAL:HG23	2.03	0.41
1:D:255:HIS:ND1	1:D:480:GLU:OE2	2.53	0.41
1:D:655:GLY:HA3	1:D:852:VAL:HG12	2.03	0.41
1:D:1277:TRP:O	1:D:1277:TRP:HD1	2.04	0.41
1:D:4577:LEU:HD23	1:D:4577:LEU:HA	1.95	0.41
1:A:273:HIS:HE1	1:A:334:MET:HG3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1477:GLY:HA2	1:A:1482:ASN:O	2.21	0.40
1:A:1847:THR:O	1:A:1851:MET:HG3	2.21	0.40
1:A:2098:VAL:CG1	1:A:2127:GLN:HG3	2.51	0.40
1:B:299:LEU:HD12	1:B:299:LEU:HA	1.81	0.40
1:B:650:VAL:HG12	1:B:777:PHE:HB2	2.03	0.40
1:B:1815:LEU:HD12	1:B:1815:LEU:HA	1.89	0.40
1:B:3424:LEU:HA	1:B:3424:LEU:HD23	1.87	0.40
1:C:835:ARG:HH12	1:C:1212:ARG:HG3	1.87	0.40
1:C:952:LYS:HE2	1:C:952:LYS:HB3	1.97	0.40
1:C:1457:TYR:O	1:C:1458:HIS:ND1	2.54	0.40
1:C:1830:VAL:HB	1:C:1837:GLN:HG3	2.04	0.40
1:C:3832:ILE:HD13	1:C:3832:ILE:HA	1.97	0.40
1:C:4859:PHE:HB3	1:C:4862:PHE:HD2	1.86	0.40
1:D:17:ASP:HB2	1:D:98:HIS:HE1	1.86	0.40
1:D:320:LYS:HB3	1:D:356:TRP:CD1	2.56	0.40
1:A:4859:PHE:HB3	1:A:4862:PHE:HD2	1.85	0.40
1:B:996:TRP:CD1	1:B:996:TRP:C	2.94	0.40
1:B:1640:HIS:HA	1:B:1647:CYS:HA	2.04	0.40
1:B:2905:LEU:H	1:B:2905:LEU:HD23	1.86	0.40
1:C:262:LEU:HD13	1:C:274:LEU:HD22	2.04	0.40
1:C:901:LYS:HE3	1:C:903:LEU:HD12	2.03	0.40
1:C:954:LYS:HA	1:C:954:LYS:HD2	1.85	0.40
1:C:1434:TYR:HB2	1:C:1572:ILE:HG21	2.02	0.40
1:C:3507:THR:HB	1:C:3508:SER:H	1.74	0.40
1:D:869:ARG:NH2	1:D:941:MET:HE1	2.36	0.40
1:D:3103:ILE:H	1:D:3103:ILE:HG12	1.76	0.40
1:D:4170:ILE:HD13	1:D:4170:ILE:HA	1.94	0.40
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.34	0.40
2:E:82:TYR:HB3	2:E:86:GLY:HA2	2.04	0.40
1:A:810:PRO:HD2	1:A:813:GLU:OE1	2.21	0.40
1:B:670:GLU:HA	1:B:740:PRO:HB3	2.02	0.40
1:B:2360:LYS:HE3	1:B:2360:LYS:HB2	1.93	0.40
1:C:650:VAL:HG12	1:C:777:PHE:HB2	2.04	0.40
1:C:1519:LEU:HD23	1:C:1519:LEU:HA	1.95	0.40
1:C:1534:LYS:HD2	1:C:1534:LYS:HA	1.82	0.40
1:D:830:ARG:CZ	1:D:1612:PHE:CE2	3.04	0.40
1:D:918:ARG:O	1:D:922:LEU:HG	2.22	0.40
1:A:214:VAL:HG11	1:A:339:ILE:HG13	2.04	0.40
1:A:2359:ARG:HE	1:A:2359:ARG:HB2	1.77	0.40
1:A:2497:ASP:HA	1:A:2547:ALA:HB2	2.03	0.40
1:A:2547:ALA:O	1:A:2551:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2905:LEU:H	1:A:2905:LEU:HD23	1.87	0.40
1:B:784:SER:OG	1:B:785:ALA:N	2.54	0.40
1:B:863:LEU:H	1:B:863:LEU:HD23	1.87	0.40
1:B:887:ILE:HG13	1:B:891:TRP:O	2.21	0.40
1:B:961:MET:HE2	1:B:962:SER:N	2.37	0.40
1:B:2102:VAL:HG11	1:B:2124:LEU:HB2	2.03	0.40
1:B:3090:ALA:O	1:B:3094:SER:N	2.46	0.40
1:B:3180:ASN:OD1	1:B:3180:ASN:N	2.54	0.40
1:B:4958:CYS:C	1:B:4960:ILE:H	2.25	0.40
1:C:869:ARG:NH2	1:C:941:MET:HE1	2.37	0.40
1:C:1008:SER:HB2	1:C:1017:ARG:CZ	2.51	0.40
1:D:682:LEU:HD12	1:D:787:VAL:HG12	2.04	0.40
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.87	0.40
1:D:4771:ILE:HD13	1:D:4771:ILE:HA	1.90	0.40
2:F:44:LYS:HA	2:F:44:LYS:HD2	1.79	0.40
1:A:393:CYS:HB2	1:A:397:GLU:HG3	2.04	0.40
1:A:648:ILE:HG12	1:A:648:ILE:O	2.21	0.40
1:A:1093:GLU:HG2	1:A:1148:VAL:HG12	2.02	0.40
1:A:2368:LEU:HA	1:A:2374:SER:HB2	2.04	0.40
1:B:33:LEU:HG	1:B:53:SER:OG	2.20	0.40
1:B:1847:THR:O	1:B:1851:MET:HG3	2.22	0.40
1:B:1947:CYS:HB3	1:B:2126:ARG:HH21	1.86	0.40
1:B:2023:LEU:HG	1:B:2024:PRO:HD2	2.03	0.40
1:B:2212:VAL:HG22	1:B:2256:TYR:CZ	2.56	0.40
1:B:2440:MET:SD	1:B:2442:LEU:HB3	2.61	0.40
1:C:707:VAL:HG12	1:C:782:SER:HB3	2.03	0.40
1:C:1180:ARG:NE	1:C:1180:ARG:HA	2.36	0.40
1:C:1477:GLY:HA2	1:C:1482:ASN:O	2.22	0.40
1:C:3804:ILE:HD12	1:C:3804:ILE:HA	1.87	0.40
1:D:158:SER:N	1:D:161:GLU:OE1	2.54	0.40
1:D:359:TYR:HB2	1:D:383:HIS:HE1	1.86	0.40
1:D:972:LEU:HD22	1:D:1044:ARG:HB3	2.03	0.40
1:D:1562:ILE:HD13	1:D:1562:ILE:HA	1.94	0.40
1:D:4055:VAL:HG11	1:D:4163:PHE:HZ	1.87	0.40
2:F:26:TYR:CE1	2:F:39:SER:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4214/5037 (84%)	3883 (92%)	329 (8%)	2 (0%)	100	100
1	B	4214/5037 (84%)	3873 (92%)	340 (8%)	1 (0%)	100	100
1	C	4214/5037 (84%)	3878 (92%)	334 (8%)	2 (0%)	100	100
1	D	4214/5037 (84%)	3886 (92%)	327 (8%)	1 (0%)	100	100
2	E	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
2	F	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	G	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	H	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
All	All	17276/20576 (84%)	15878 (92%)	1392 (8%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	862	VAL
1	C	899	ASP
1	A	1023	PRO
1	C	1023	PRO
1	D	1023	PRO
1	B	1023	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3334/4276 (78%)	3266 (98%)	68 (2%)	50 72
1	B	3334/4276 (78%)	3244 (97%)	90 (3%)	40 65
1	C	3334/4276 (78%)	3260 (98%)	74 (2%)	47 70
1	D	3334/4276 (78%)	3259 (98%)	75 (2%)	47 70
2	E	80/88 (91%)	78 (98%)	2 (2%)	42 67
2	F	80/88 (91%)	79 (99%)	1 (1%)	65 79
2	G	80/88 (91%)	79 (99%)	1 (1%)	65 79
2	H	80/88 (91%)	79 (99%)	1 (1%)	65 79
All	All	13656/17456 (78%)	13344 (98%)	312 (2%)	46 69

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TYR
1	A	164	ARG
1	A	178	ARG
1	A	195	PHE
1	A	247	TYR
1	A	261	ARG
1	A	275	ARG
1	A	421	PHE
1	A	493	ARG
1	A	503	PHE
1	A	506	TYR
1	A	720	HIS
1	A	771	PHE
1	A	812	HIS
1	A	830	ARG
1	A	866	HIS
1	A	904	HIS
1	A	913	LEU
1	A	919	ASN
1	A	1006	SER
1	A	1089	TYR
1	A	1112	ASP
1	A	1143	TRP
1	A	1288	PHE
1	A	1421	ARG
1	A	1423	ASP
1	A	1563	GLN

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Mol	Chain	Res	Type
1	A	1579	MET
1	A	1647	CYS
1	A	1814	MET
1	A	1865	MET
1	A	1929	MET
1	A	2014	ASP
1	A	2128	TYR
1	A	2170	MET
1	A	2211	MET
1	A	2331	TYR
1	A	2440	MET
1	A	2494	PHE
1	A	2519	LEU
1	A	2633	LEU
1	A	2939	ARG
1	A	2957	PHE
1	A	2966	TRP
1	A	2971	GLN
1	A	3003	LEU
1	A	3010	PHE
1	A	3030	HIS
1	A	3068	LEU
1	A	3193	CYS
1	A	3213	TYR
1	A	3277	LEU
1	A	3358	PHE
1	A	3444	TYR
1	A	3540	TYR
1	A	3727	ASP
1	A	3899	PHE
1	A	3924	LEU
1	A	3977	GLN
1	A	3999	MET
1	A	4039	MET
1	A	4087	LEU
1	A	4156	HIS
1	A	4166	LEU
1	A	4571	PHE
1	A	4743	MET
1	A	4807	PHE
1	A	4912	TYR
1	B	103	TYR

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Mol	Chain	Res	Type
1	B	131	LEU
1	B	164	ARG
1	B	178	ARG
1	B	195	PHE
1	B	247	TYR
1	B	261	ARG
1	B	275	ARG
1	B	421	PHE
1	B	493	ARG
1	B	503	PHE
1	B	506	TYR
1	B	579	GLN
1	B	659	TYR
1	B	674	PHE
1	B	714	TYR
1	B	721	LEU
1	B	771	PHE
1	B	811	CYS
1	B	812	HIS
1	B	830	ARG
1	B	866	HIS
1	B	899	ASP
1	B	904	HIS
1	B	911	HIS
1	B	913	LEU
1	B	919	ASN
1	B	961	MET
1	B	1011	GLN
1	B	1038	SER
1	B	1089	TYR
1	B	1112	ASP
1	B	1143	TRP
1	B	1155	LEU
1	B	1219	LEU
1	B	1288	PHE
1	B	1421	ARG
1	B	1435	TYR
1	B	1492	CYS
1	B	1494	MET
1	B	1506	GLN
1	B	1553	PHE
1	B	1563	GLN

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Mol	Chain	Res	Type
1	B	1579	MET
1	B	1647	CYS
1	B	1814	MET
1	B	1865	MET
1	B	1929	MET
1	B	2014	ASP
1	B	2109	ASP
1	B	2186	MET
1	B	2211	MET
1	B	2232	CYS
1	B	2331	TYR
1	B	2440	MET
1	B	2494	PHE
1	B	2519	LEU
1	B	2633	LEU
1	B	2863	SER
1	B	2939	ARG
1	B	2966	TRP
1	B	2971	GLN
1	B	3003	LEU
1	B	3010	PHE
1	B	3030	HIS
1	B	3068	LEU
1	B	3131	TYR
1	B	3213	TYR
1	B	3268	HIS
1	B	3277	LEU
1	B	3444	TYR
1	B	3525	CYS
1	B	3540	TYR
1	B	3576	TYR
1	B	3652	MET
1	B	3679	LYS
1	B	3720	TYR
1	B	3727	ASP
1	B	3899	PHE
1	B	3999	MET
1	B	4039	MET
1	B	4087	LEU
1	B	4156	HIS
1	B	4571	PHE
1	B	4704	LEU

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Mol	Chain	Res	Type
1	B	4743	MET
1	B	4768	LEU
1	B	4769	MET
1	B	4807	PHE
1	B	4912	TYR
1	C	164	ARG
1	C	178	ARG
1	C	247	TYR
1	C	261	ARG
1	C	275	ARG
1	C	315	CYS
1	C	493	ARG
1	C	503	PHE
1	C	506	TYR
1	C	652	ARG
1	C	771	PHE
1	C	812	HIS
1	C	820	ARG
1	C	830	ARG
1	C	866	HIS
1	C	904	HIS
1	C	913	LEU
1	C	919	ASN
1	C	922	LEU
1	C	961	MET
1	C	984	LEU
1	C	1006	SER
1	C	1011	GLN
1	C	1038	SER
1	C	1089	TYR
1	C	1139	PHE
1	C	1143	TRP
1	C	1155	LEU
1	C	1288	PHE
1	C	1421	ARG
1	C	1553	PHE
1	C	1579	MET
1	C	1647	CYS
1	C	1814	MET
1	C	1929	MET
1	C	2014	ASP
1	C	2109	ASP

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Mol	Chain	Res	Type
1	C	2192	TYR
1	C	2211	MET
1	C	2232	CYS
1	C	2331	TYR
1	C	2494	PHE
1	C	2519	LEU
1	C	2568	LEU
1	C	2633	LEU
1	C	2939	ARG
1	C	2966	TRP
1	C	2971	GLN
1	C	3003	LEU
1	C	3010	PHE
1	C	3030	HIS
1	C	3068	LEU
1	C	3131	TYR
1	C	3213	TYR
1	C	3223	SER
1	C	3268	HIS
1	C	3277	LEU
1	C	3358	PHE
1	C	3398	PHE
1	C	3444	TYR
1	C	3540	TYR
1	C	3679	LYS
1	C	3720	TYR
1	C	3727	ASP
1	C	3899	PHE
1	C	3924	LEU
1	C	3977	GLN
1	C	4068	LEU
1	C	4087	LEU
1	C	4156	HIS
1	C	4571	PHE
1	C	4704	LEU
1	C	4743	MET
1	C	4807	PHE
1	D	103	TYR
1	D	164	ARG
1	D	178	ARG
1	D	247	TYR
1	D	261	ARG

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Mol	Chain	Res	Type
1	D	275	ARG
1	D	315	CYS
1	D	421	PHE
1	D	493	ARG
1	D	503	PHE
1	D	506	TYR
1	D	579	GLN
1	D	630	GLU
1	D	674	PHE
1	D	771	PHE
1	D	778	PHE
1	D	811	CYS
1	D	812	HIS
1	D	871	ARG
1	D	904	HIS
1	D	911	HIS
1	D	913	LEU
1	D	919	ASN
1	D	922	LEU
1	D	961	MET
1	D	996	TRP
1	D	1089	TYR
1	D	1112	ASP
1	D	1143	TRP
1	D	1155	LEU
1	D	1288	PHE
1	D	1421	ARG
1	D	1423	ASP
1	D	1435	TYR
1	D	1489	CYS
1	D	1492	CYS
1	D	1579	MET
1	D	1647	CYS
1	D	1648	MET
1	D	1814	MET
1	D	1865	MET
1	D	1929	MET
1	D	2014	ASP
1	D	2109	ASP
1	D	2211	MET
1	D	2232	CYS
1	D	2331	TYR

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Mol	Chain	Res	Type
1	D	2423	MET
1	D	2494	PHE
1	D	2519	LEU
1	D	2633	LEU
1	D	2939	ARG
1	D	2966	TRP
1	D	2971	GLN
1	D	3003	LEU
1	D	3010	PHE
1	D	3030	HIS
1	D	3068	LEU
1	D	3213	TYR
1	D	3268	HIS
1	D	3277	LEU
1	D	3444	TYR
1	D	3540	TYR
1	D	3652	MET
1	D	3899	PHE
1	D	3999	MET
1	D	4039	MET
1	D	4087	LEU
1	D	4156	HIS
1	D	4166	LEU
1	D	4571	PHE
1	D	4704	LEU
1	D	4743	MET
1	D	4768	LEU
1	D	4807	PHE
2	E	15	PHE
2	E	79	ASP
2	F	18	LYS
2	G	40	ARG
2	H	22	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	181	HIS
1	A	772	ASN
1	A	1011	GLN
1	A	1130	GLN

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Mol	Chain	Res	Type
1	A	1563	GLN
1	A	1696	HIS
1	A	2005	GLN
1	A	2112	GLN
1	A	2176	ASN
1	A	2188	ASN
1	A	2246	ASN
1	A	2247	GLN
1	A	2663	ASN
1	A	3013	HIS
1	A	3837	GLN
1	A	4162	ASN
1	A	4650	HIS
1	A	4700	GLN
1	B	772	ASN
1	B	1130	GLN
1	B	1545	ASN
1	B	1563	GLN
1	B	2005	GLN
1	B	2112	GLN
1	B	2188	ASN
1	B	2246	ASN
1	B	2247	GLN
1	B	2663	ASN
1	B	3013	HIS
1	B	3837	GLN
1	B	3882	GLN
1	B	4162	ASN
1	B	4650	HIS
1	B	4700	GLN
1	B	4983	HIS
1	C	12	GLN
1	C	23	GLN
1	C	181	HIS
1	C	772	ASN
1	C	1130	GLN
1	C	2005	GLN
1	C	2112	GLN
1	C	2176	ASN
1	C	2188	ASN
1	C	2246	ASN
1	C	2247	GLN

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Mol	Chain	Res	Type
1	C	2663	ASN
1	C	3013	HIS
1	C	3837	GLN
1	C	4162	ASN
1	C	4650	HIS
1	D	23	GLN
1	D	772	ASN
1	D	838	HIS
1	D	1011	GLN
1	D	1130	GLN
1	D	2005	GLN
1	D	2112	GLN
1	D	2176	ASN
1	D	2188	ASN
1	D	2246	ASN
1	D	2247	GLN
1	D	2663	ASN
1	D	3013	HIS
1	D	3837	GLN
1	D	4162	ASN
1	D	4650	HIS
1	D	4700	GLN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	U1C	C	5103	-	23,25,25	6.21	12 (52%)	26,35,35	3.18	9 (34%)
4	ATP	C	5102	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
5	U1C	A	5103	-	23,25,25	6.21	12 (52%)	26,35,35	3.20	9 (34%)
4	ATP	D	5102	-	28,33,33	0.65	0	34,52,52	0.58	1 (2%)
5	U1C	B	5103	-	23,25,25	6.19	12 (52%)	26,35,35	3.20	9 (34%)
5	U1C	D	5103	-	23,25,25	6.20	12 (52%)	26,35,35	3.19	9 (34%)
4	ATP	A	5102	-	28,33,33	0.65	0	34,52,52	0.58	1 (2%)
4	ATP	B	5102	-	28,33,33	0.66	0	34,52,52	0.58	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	U1C	C	5103	-	-	1/7/25/25	0/3/3/3
4	ATP	C	5102	-	-	9/18/38/38	0/3/3/3
5	U1C	A	5103	-	-	1/7/25/25	0/3/3/3
4	ATP	D	5102	-	-	9/18/38/38	0/3/3/3
5	U1C	B	5103	-	-	1/7/25/25	0/3/3/3
5	U1C	D	5103	-	-	1/7/25/25	0/3/3/3
4	ATP	A	5102	-	-	9/18/38/38	0/3/3/3
4	ATP	B	5102	-	-	9/18/38/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5103	U1C	C1-N2	-18.77	1.32	1.45
5	A	5103	U1C	C1-N2	-18.76	1.32	1.45
5	D	5103	U1C	C1-N2	-18.64	1.32	1.45
5	B	5103	U1C	C1-N2	-18.59	1.32	1.45
5	B	5103	U1C	C1-C2	-10.54	1.39	1.51
5	D	5103	U1C	C1-C2	-10.54	1.39	1.51
5	C	5103	U1C	C1-C2	-10.51	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5103	U1C	C1-C2	-10.49	1.39	1.51
5	B	5103	U1C	O4-N4	10.46	1.40	1.22
5	A	5103	U1C	O4-N4	10.42	1.40	1.22
5	C	5103	U1C	O4-N4	10.41	1.40	1.22
5	D	5103	U1C	O4-N4	10.41	1.40	1.22
5	A	5103	U1C	O2-C3	9.84	1.40	1.23
5	B	5103	U1C	O2-C3	9.81	1.40	1.23
5	C	5103	U1C	O2-C3	9.81	1.40	1.23
5	D	5103	U1C	O2-C3	9.80	1.40	1.23
5	A	5103	U1C	O1-C2	8.68	1.40	1.23
5	B	5103	U1C	O1-C2	8.67	1.40	1.23
5	D	5103	U1C	O1-C2	8.67	1.40	1.23
5	C	5103	U1C	O1-C2	8.61	1.40	1.23
5	B	5103	U1C	C4-N3	6.66	1.45	1.27
5	C	5103	U1C	C4-N3	6.66	1.45	1.27
5	D	5103	U1C	C4-N3	6.66	1.45	1.27
5	A	5103	U1C	C4-N3	6.66	1.45	1.27
5	D	5103	U1C	C3-N2	-5.27	1.32	1.37
5	B	5103	U1C	C3-N2	-5.24	1.32	1.37
5	C	5103	U1C	C3-N2	-5.23	1.32	1.37
5	A	5103	U1C	C3-N2	-5.22	1.32	1.37
5	B	5103	U1C	C5-C4	4.23	1.53	1.45
5	A	5103	U1C	C5-C4	4.22	1.53	1.45
5	A	5103	U1C	C9-C8	4.19	1.53	1.46
5	D	5103	U1C	C5-C4	4.19	1.53	1.45
5	C	5103	U1C	C9-C8	4.17	1.53	1.46
5	B	5103	U1C	C9-C8	4.15	1.53	1.46
5	C	5103	U1C	C5-C4	4.15	1.53	1.45
5	D	5103	U1C	C9-C8	4.13	1.53	1.46
5	D	5103	U1C	N2-N3	3.86	1.41	1.37
5	C	5103	U1C	N2-N3	3.81	1.41	1.37
5	A	5103	U1C	N2-N3	3.79	1.41	1.37
5	B	5103	U1C	N2-N3	3.77	1.41	1.37
5	A	5103	U1C	C3-N1	-3.29	1.32	1.38
5	C	5103	U1C	C3-N1	-3.25	1.32	1.38
5	B	5103	U1C	C3-N1	-3.22	1.32	1.38
5	D	5103	U1C	C3-N1	-3.22	1.32	1.38
5	A	5103	U1C	C2-N1	-2.94	1.32	1.37
5	B	5103	U1C	C2-N1	-2.90	1.32	1.37
5	D	5103	U1C	C2-N1	-2.90	1.32	1.37
5	C	5103	U1C	C2-N1	-2.85	1.32	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	5103	U1C	C2-C1-N2	8.41	106.93	101.45
5	B	5103	U1C	C2-C1-N2	8.40	106.92	101.45
5	A	5103	U1C	C2-C1-N2	8.38	106.91	101.45
5	D	5103	U1C	C2-C1-N2	8.37	106.90	101.45
5	B	5103	U1C	C1-N2-C3	-7.36	108.27	112.31
5	A	5103	U1C	C1-N2-C3	-7.32	108.29	112.31
5	D	5103	U1C	C1-N2-C3	-7.29	108.31	112.31
5	A	5103	U1C	C3-N2-N3	7.24	125.89	119.83
5	C	5103	U1C	C1-N2-C3	-7.24	108.33	112.31
5	B	5103	U1C	C3-N2-N3	7.17	125.83	119.83
5	D	5103	U1C	C3-N2-N3	7.15	125.80	119.83
5	C	5103	U1C	C3-N2-N3	7.13	125.79	119.83
5	B	5103	U1C	C2-N1-C3	-4.84	108.22	112.47
5	D	5103	U1C	C2-N1-C3	-4.84	108.22	112.47
5	C	5103	U1C	C2-N1-C3	-4.81	108.25	112.47
5	A	5103	U1C	C2-N1-C3	-4.75	108.30	112.47
5	A	5103	U1C	C5-C4-N3	-4.32	110.43	118.74
5	C	5103	U1C	C5-C4-N3	-4.27	110.52	118.74
5	D	5103	U1C	C5-C4-N3	-4.27	110.52	118.74
5	B	5103	U1C	C5-C4-N3	-4.27	110.52	118.74
5	B	5103	U1C	N1-C3-N2	3.65	109.63	106.12
5	D	5103	U1C	N1-C3-N2	3.63	109.61	106.12
5	A	5103	U1C	N1-C3-N2	3.62	109.59	106.12
5	C	5103	U1C	N1-C3-N2	3.61	109.58	106.12
5	C	5103	U1C	C7-C8-C9	-3.43	125.57	128.77
5	D	5103	U1C	C7-C8-C9	-3.42	125.57	128.77
5	B	5103	U1C	C7-C8-C9	-3.42	125.58	128.77
5	A	5103	U1C	C7-C8-C9	-3.40	125.59	128.77
5	A	5103	U1C	O2-C3-N2	-2.69	125.13	127.67
5	B	5103	U1C	O2-C3-N2	-2.64	125.18	127.67
5	C	5103	U1C	O2-C3-N2	-2.60	125.22	127.67
5	D	5103	U1C	O2-C3-N2	-2.60	125.22	127.67
5	A	5103	U1C	C1-N2-N3	-2.54	125.82	127.64
5	C	5103	U1C	C1-N2-N3	-2.46	125.88	127.64
5	D	5103	U1C	C1-N2-N3	-2.45	125.89	127.64
5	B	5103	U1C	C1-N2-N3	-2.43	125.90	127.64
4	C	5102	ATP	C5-C6-N6	2.34	123.88	120.31
4	A	5102	ATP	C5-C6-N6	2.32	123.85	120.31
4	B	5102	ATP	C5-C6-N6	2.29	123.81	120.31
4	D	5102	ATP	C5-C6-N6	2.29	123.80	120.31

There are no chirality outliers.

All (40) torsion outliers are listed below:

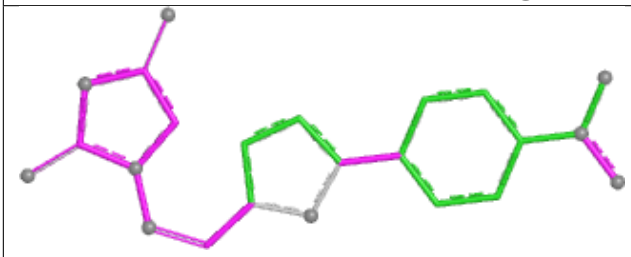
Mol	Chain	Res	Type	Atoms
4	A	5102	ATP	C5'-O5'-PA-O1A
4	A	5102	ATP	C5'-O5'-PA-O2A
4	A	5102	ATP	C5'-O5'-PA-O3A
4	A	5102	ATP	O4'-C4'-C5'-O5'
4	B	5102	ATP	C5'-O5'-PA-O1A
4	B	5102	ATP	C5'-O5'-PA-O2A
4	B	5102	ATP	C5'-O5'-PA-O3A
4	B	5102	ATP	O4'-C4'-C5'-O5'
4	C	5102	ATP	C5'-O5'-PA-O1A
4	C	5102	ATP	C5'-O5'-PA-O2A
4	C	5102	ATP	C5'-O5'-PA-O3A
4	C	5102	ATP	O4'-C4'-C5'-O5'
4	D	5102	ATP	C5'-O5'-PA-O1A
4	D	5102	ATP	C5'-O5'-PA-O2A
4	D	5102	ATP	C5'-O5'-PA-O3A
4	D	5102	ATP	O4'-C4'-C5'-O5'
5	A	5103	U1C	C5-C4-N3-N2
5	B	5103	U1C	C5-C4-N3-N2
5	C	5103	U1C	C5-C4-N3-N2
5	D	5103	U1C	C5-C4-N3-N2
4	A	5102	ATP	C3'-C4'-C5'-O5'
4	B	5102	ATP	C3'-C4'-C5'-O5'
4	C	5102	ATP	C3'-C4'-C5'-O5'
4	D	5102	ATP	C3'-C4'-C5'-O5'
4	A	5102	ATP	PB-O3A-PA-O2A
4	B	5102	ATP	PB-O3A-PA-O2A
4	C	5102	ATP	PB-O3A-PA-O2A
4	D	5102	ATP	PB-O3A-PA-O2A
4	A	5102	ATP	C4'-C5'-O5'-PA
4	B	5102	ATP	C4'-C5'-O5'-PA
4	C	5102	ATP	C4'-C5'-O5'-PA
4	D	5102	ATP	C4'-C5'-O5'-PA
4	A	5102	ATP	PG-O3B-PB-O2B
4	B	5102	ATP	PG-O3B-PB-O2B
4	C	5102	ATP	PG-O3B-PB-O2B
4	D	5102	ATP	PG-O3B-PB-O2B
4	A	5102	ATP	PB-O3A-PA-O1A
4	B	5102	ATP	PB-O3A-PA-O1A
4	C	5102	ATP	PB-O3A-PA-O1A
4	D	5102	ATP	PB-O3A-PA-O1A

There are no ring outliers.

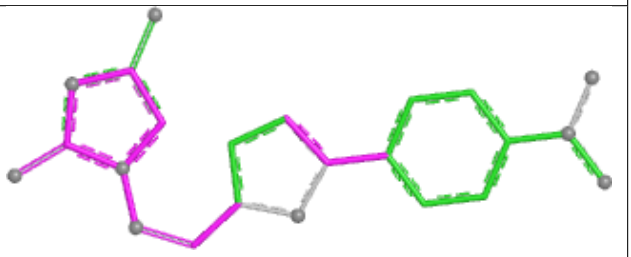
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

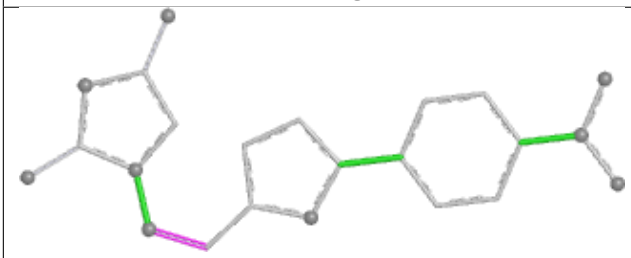
Ligand U1C C 5103



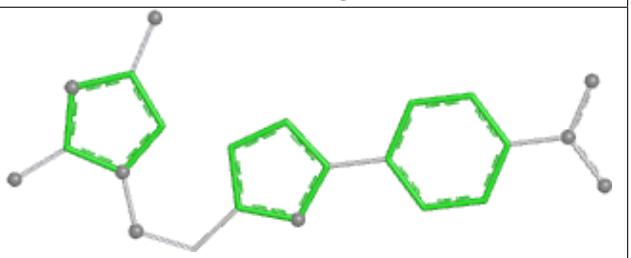
Bond lengths



Bond angles

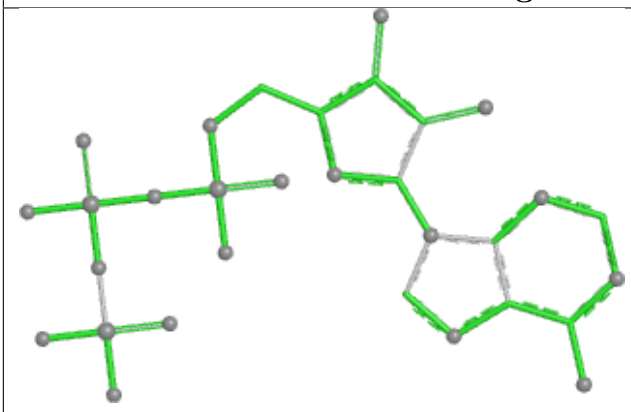


Torsions

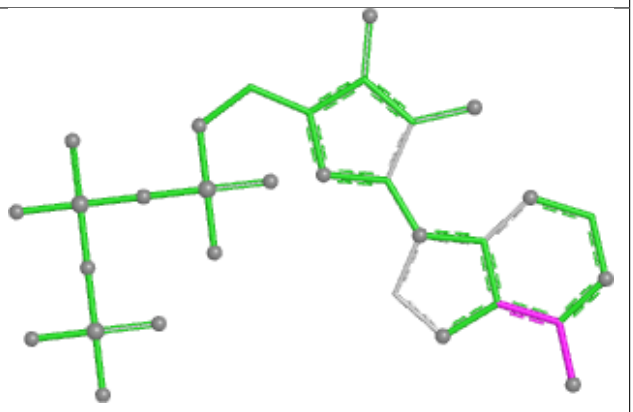


Rings

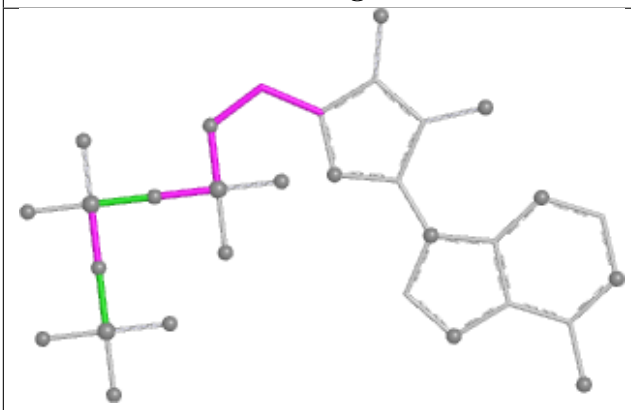
Ligand ATP C 5102



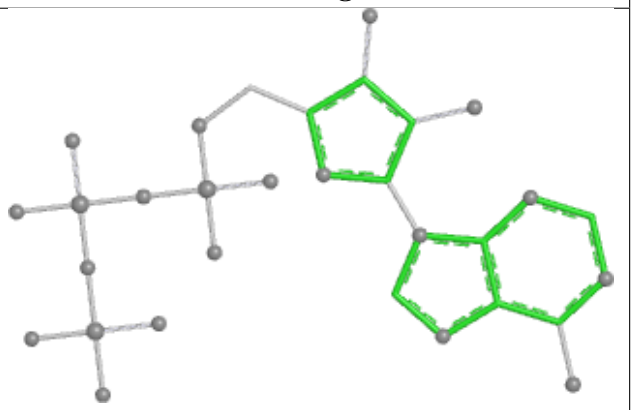
Bond lengths



Bond angles

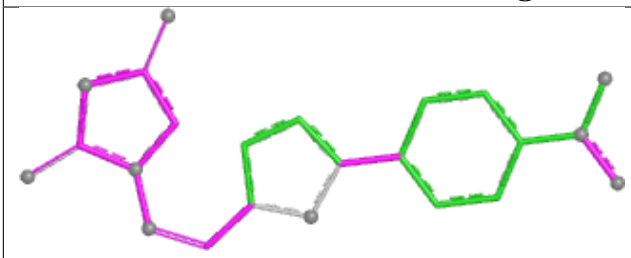


Torsions

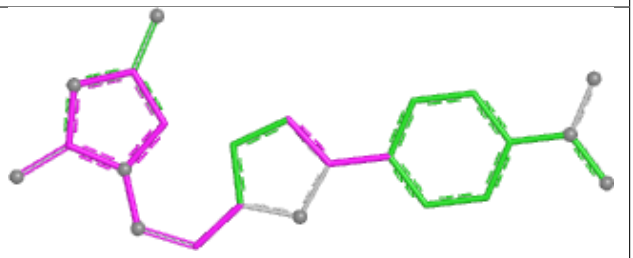


Rings

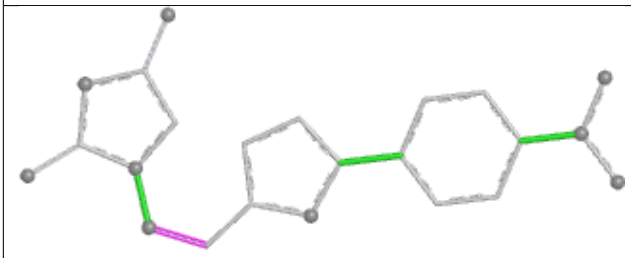
Ligand U1C A 5103



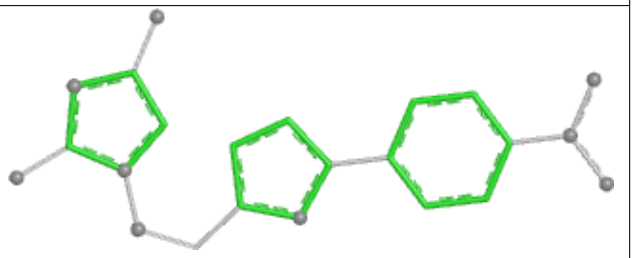
Bond lengths



Bond angles

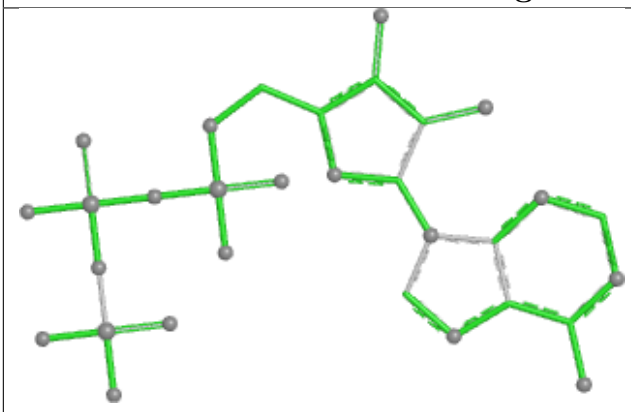


Torsions

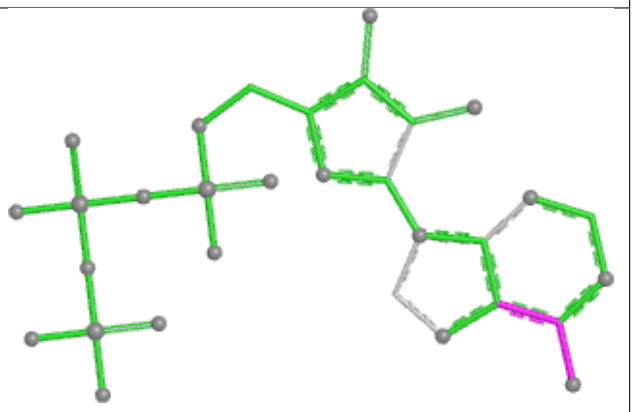


Rings

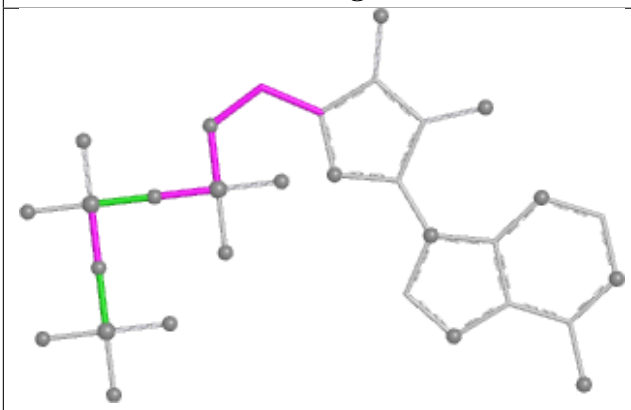
Ligand ATP D 5102



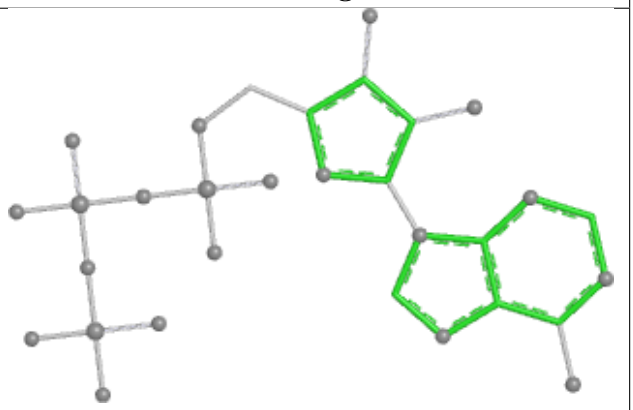
Bond lengths



Bond angles

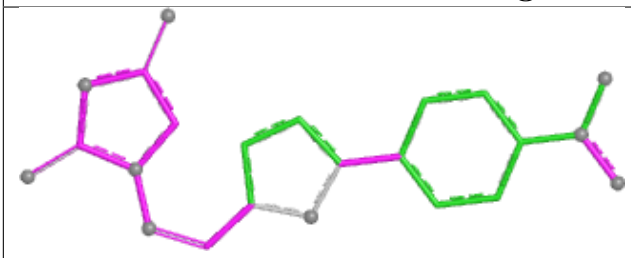


Torsions

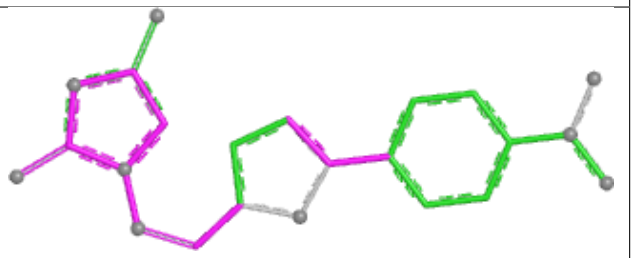


Rings

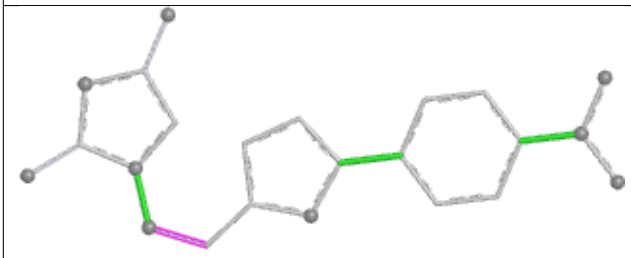
Ligand U1C B 5103



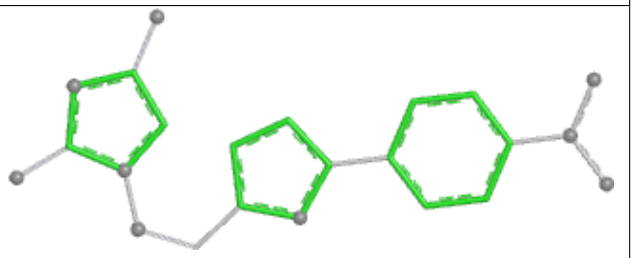
Bond lengths



Bond angles

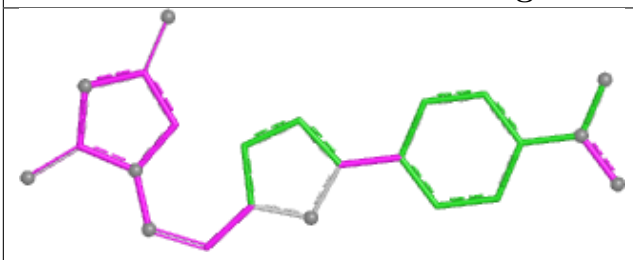


Torsions

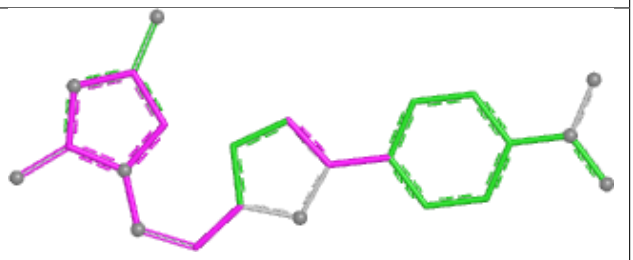


Rings

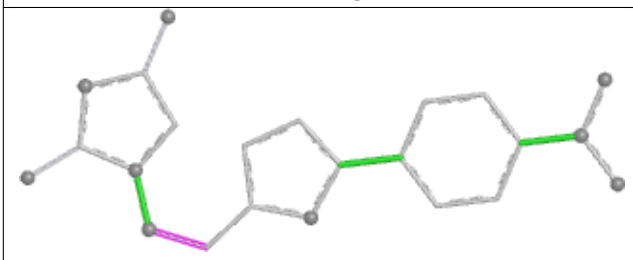
Ligand U1C D 5103



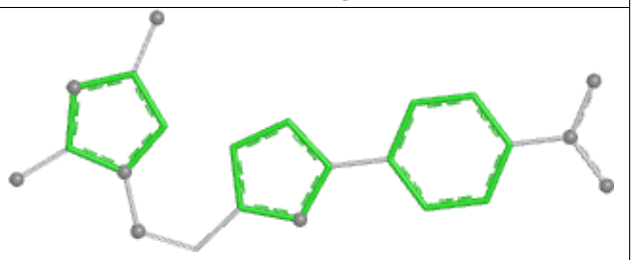
Bond lengths



Bond angles

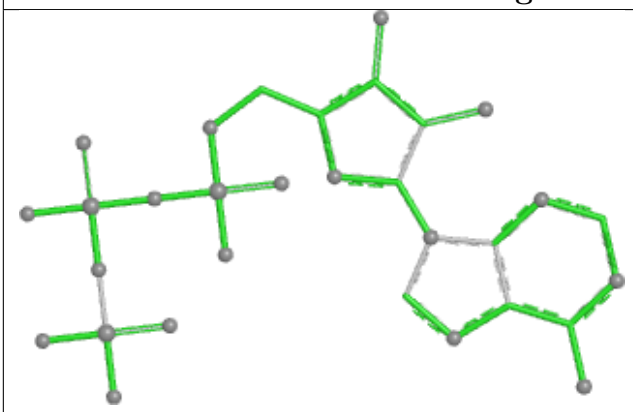


Torsions

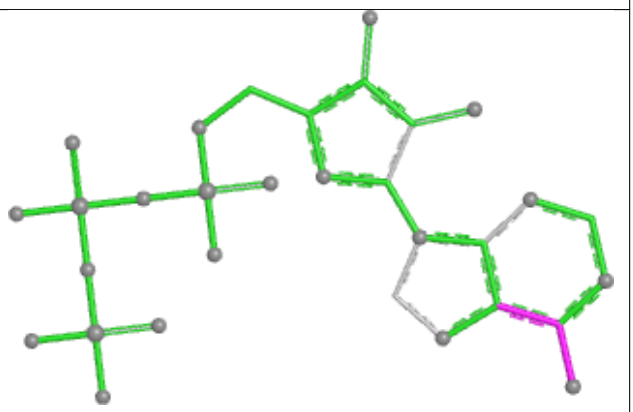


Rings

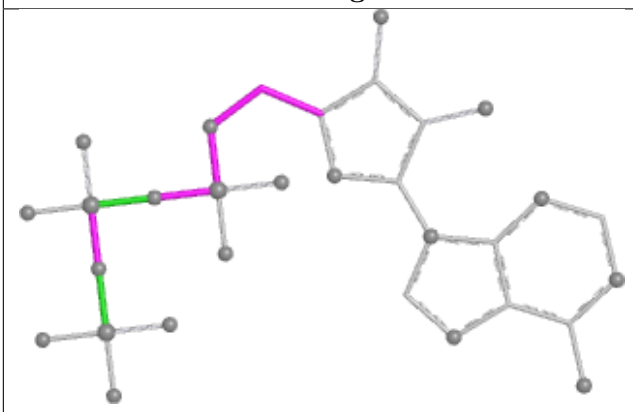
Ligand ATP A 5102



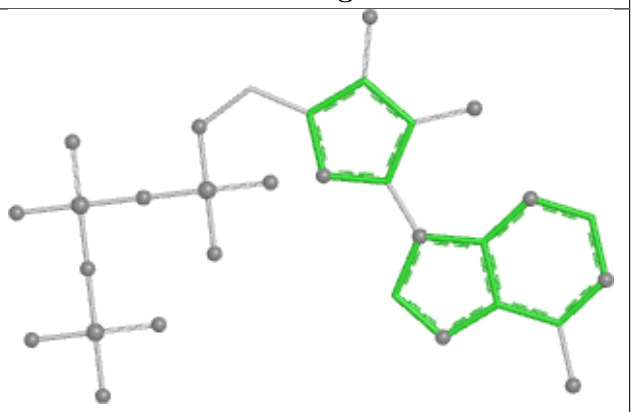
Bond lengths



Bond angles

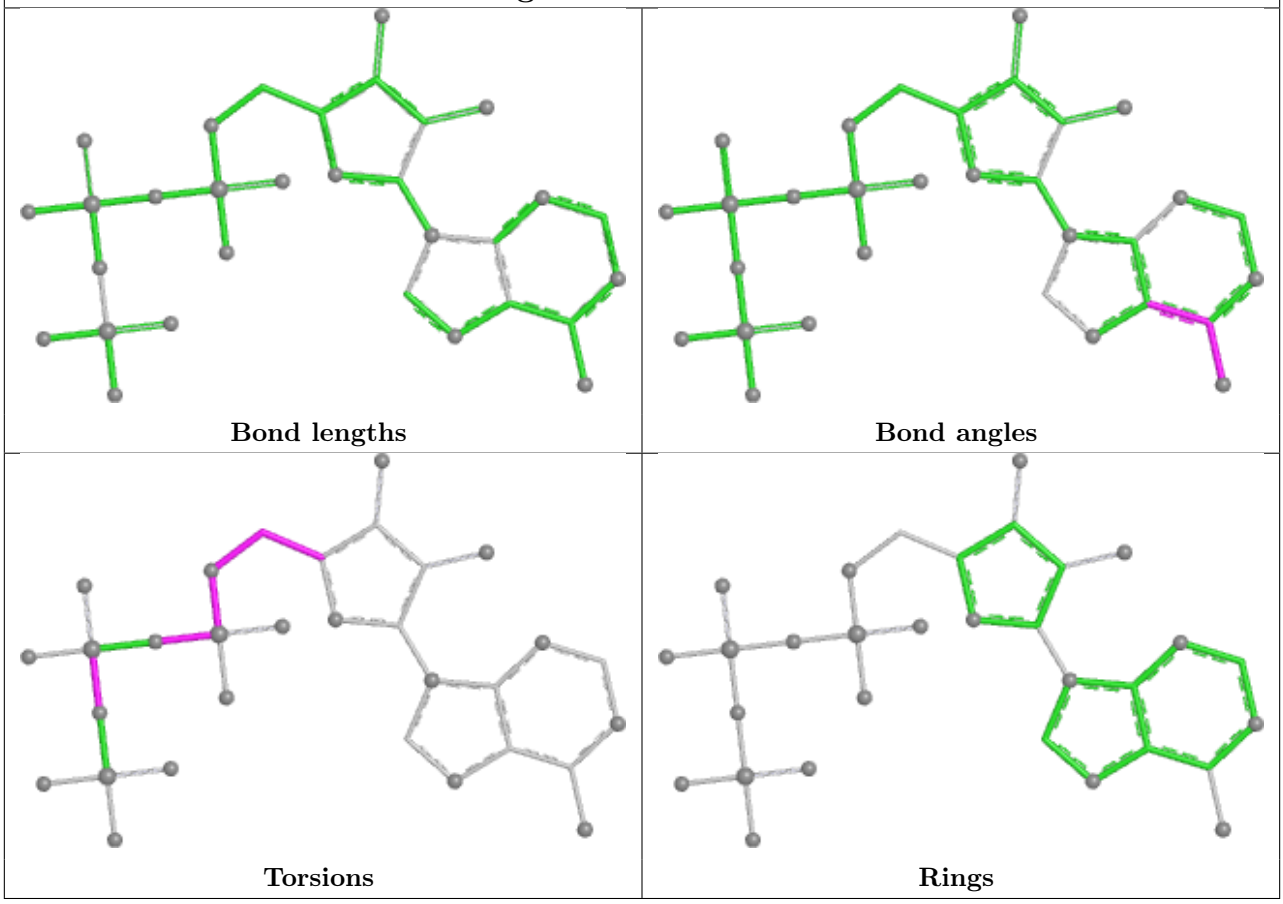


Torsions



Rings

Ligand ATP B 5102



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

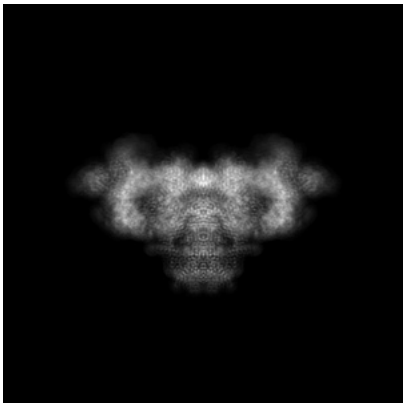
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45584. These allow visual inspection of the internal detail of the map and identification of artifacts.

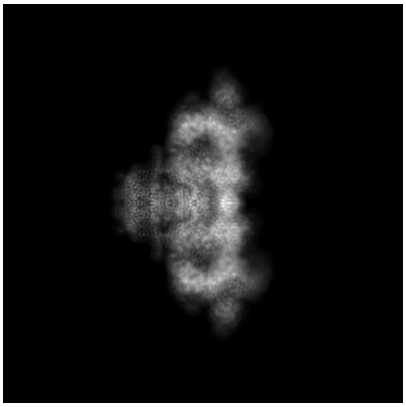
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

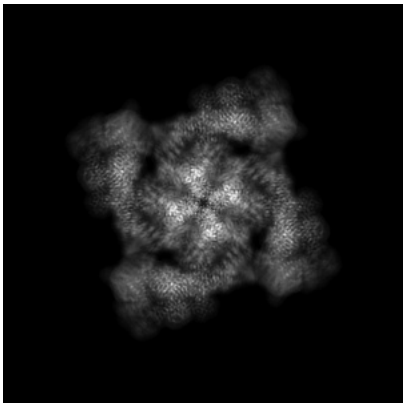
6.1.1 Primary map



X



Y

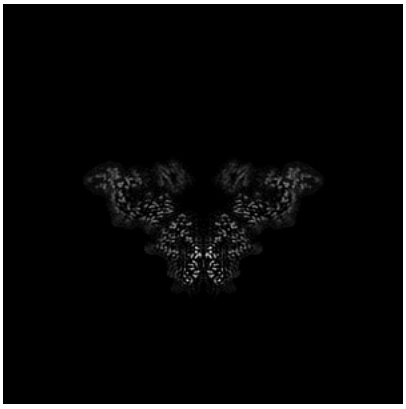


Z

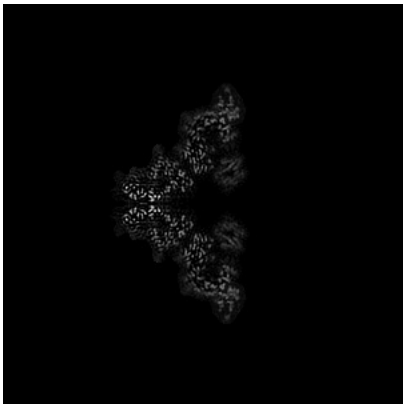
The images above show the map projected in three orthogonal directions.

6.2 Central slices

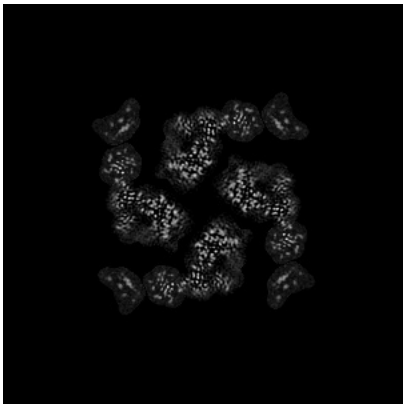
6.2.1 Primary map



X Index: 232



Y Index: 232

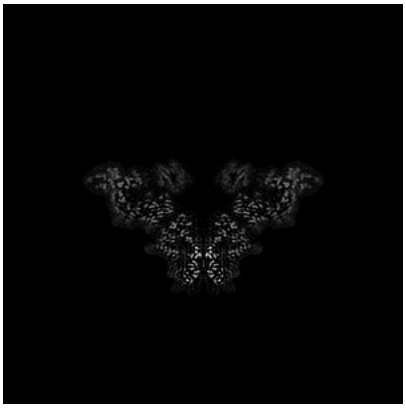


Z Index: 232

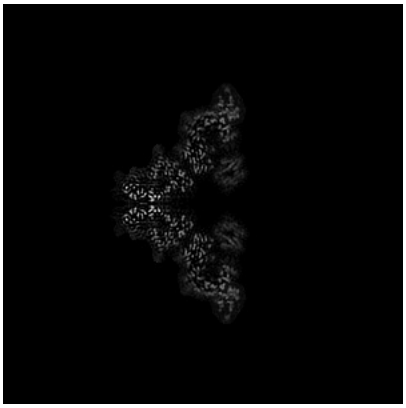
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

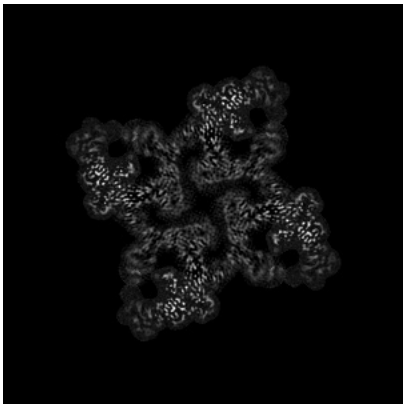
6.3.1 Primary map



X Index: 232



Y Index: 232

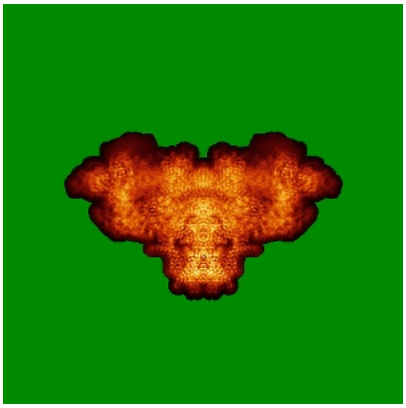


Z Index: 261

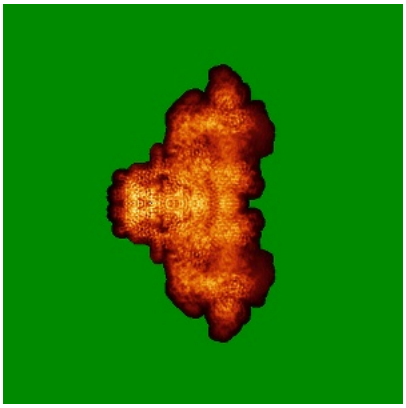
The images above show the largest variance slices of the map in three orthogonal directions.

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

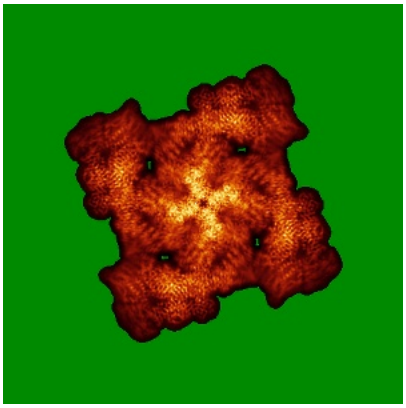
6.4.1 Primary map



X



Y

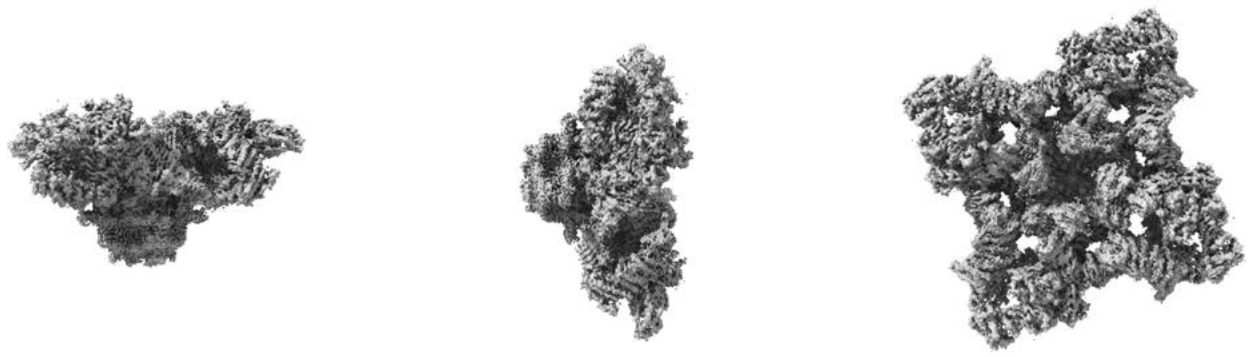


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

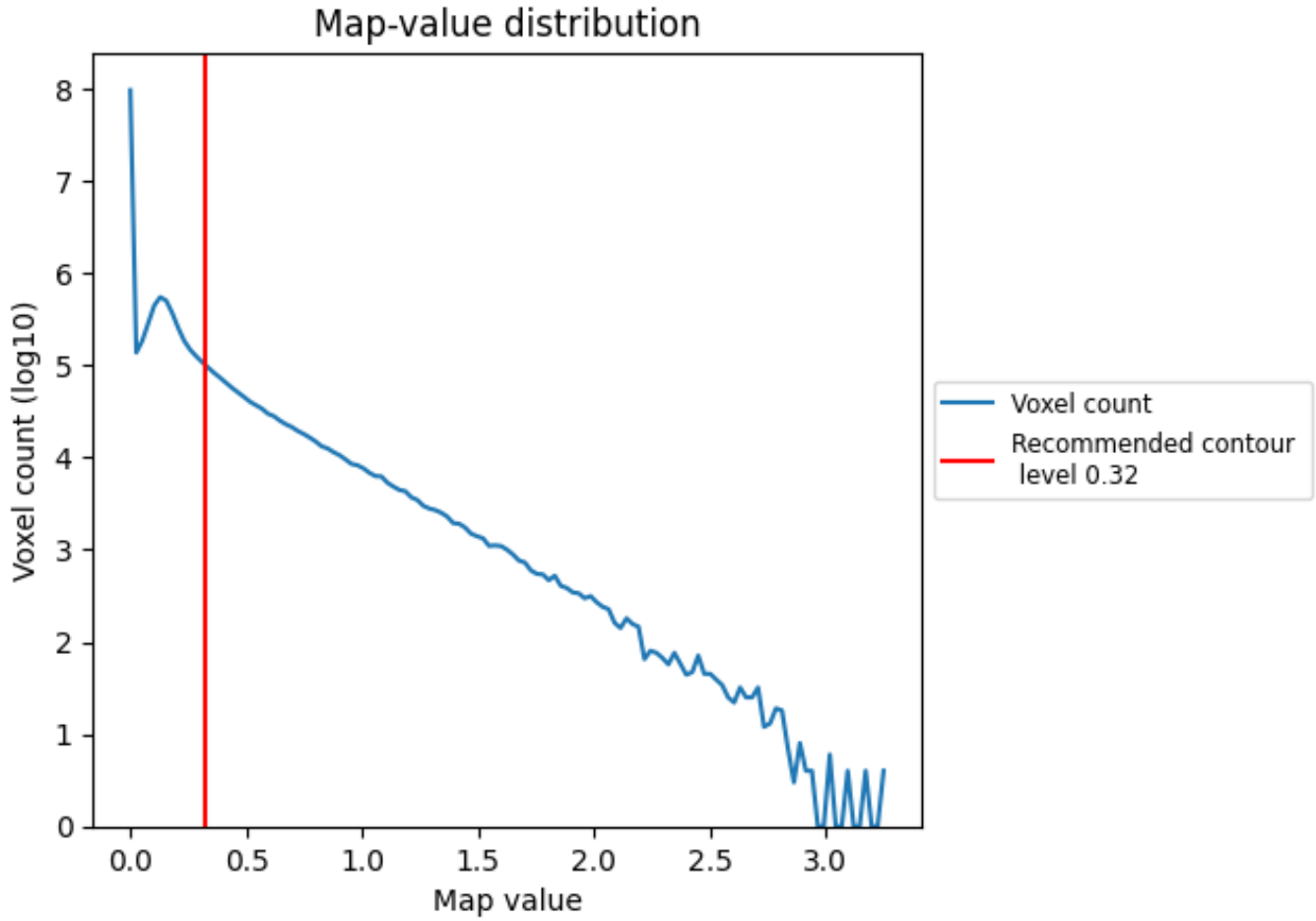
6.6 Mask visualisation (i)

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

7 Map analysis

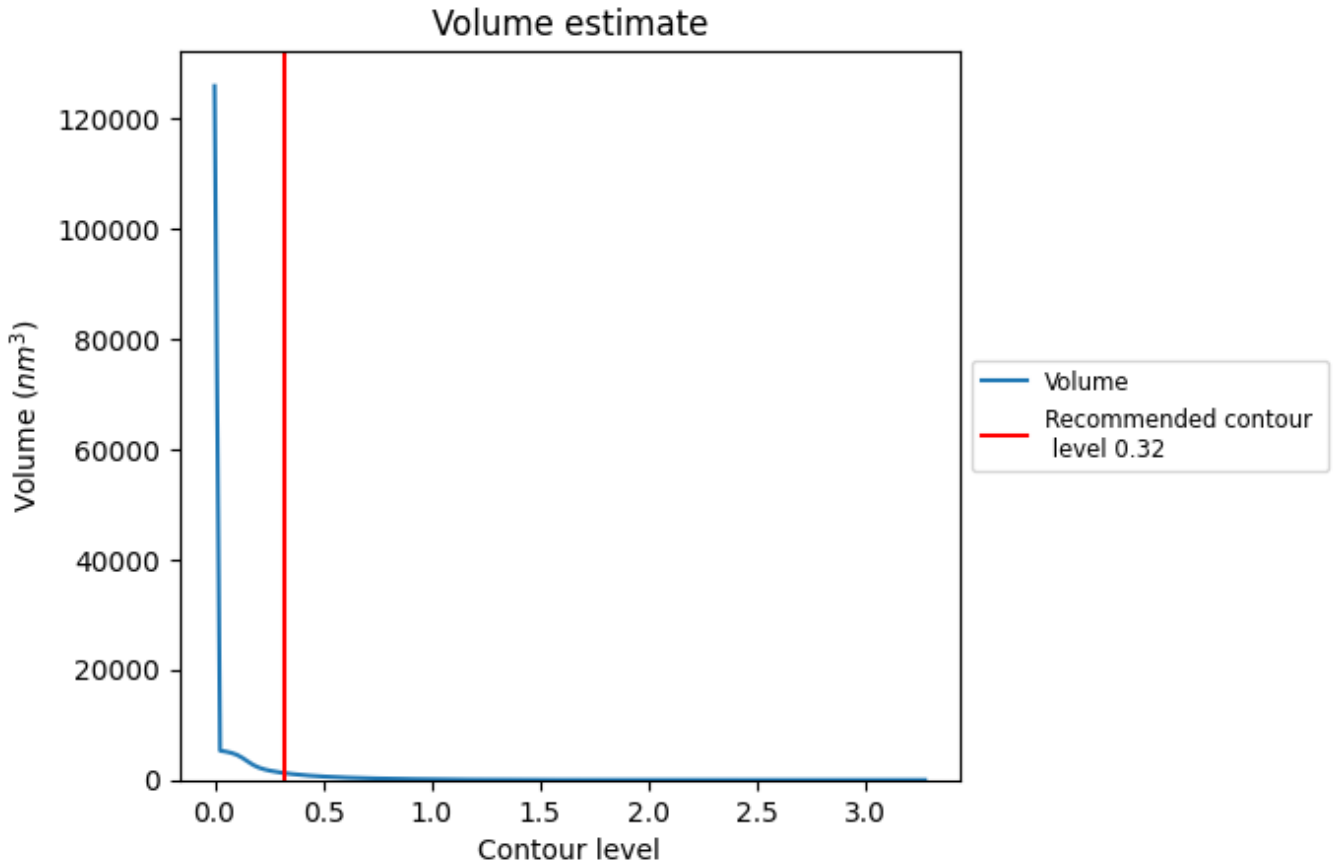
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

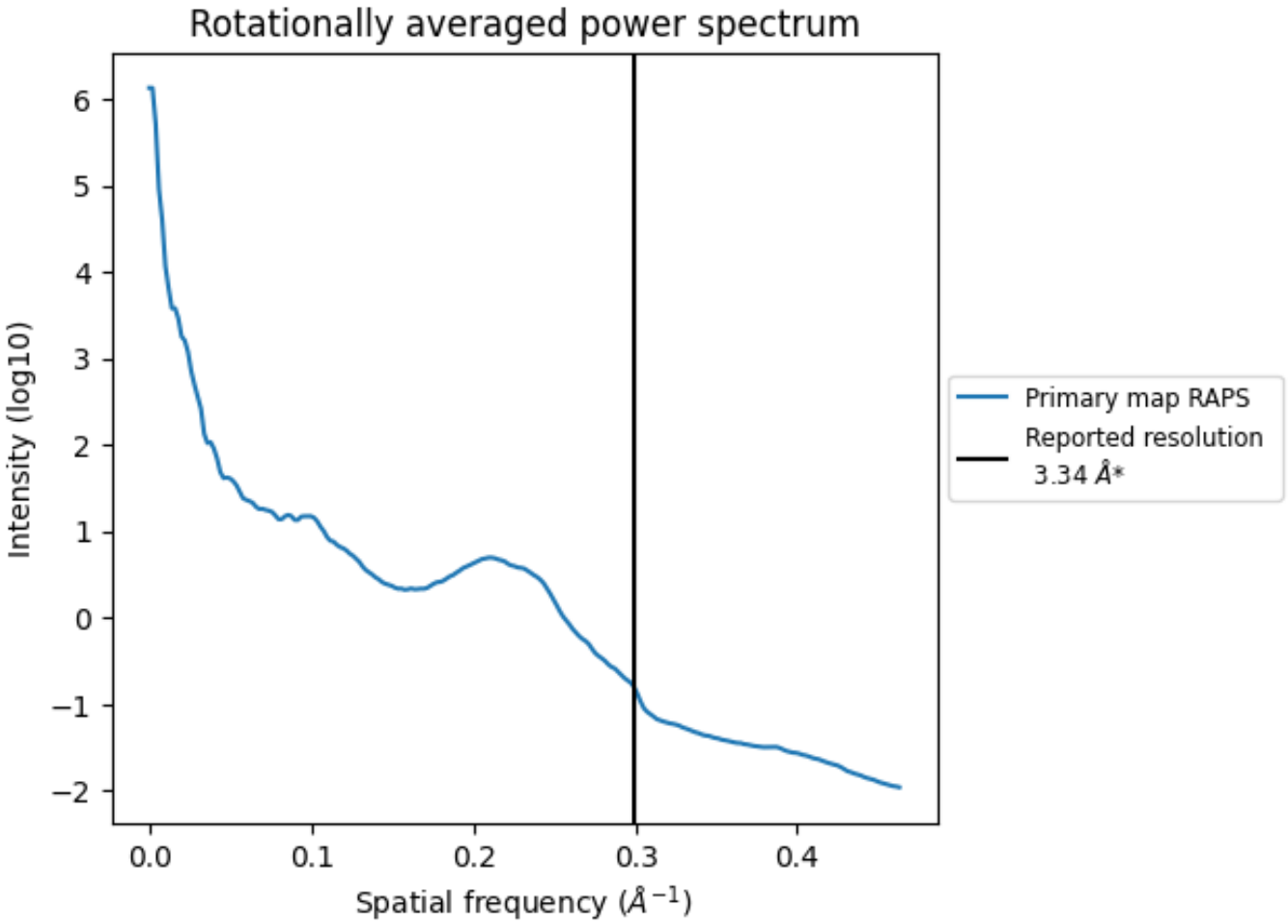
7.2 Volume estimate



The volume at the recommended contour level is 1262 nm^3; this corresponds to an approximate mass of 1140 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 0.299 Å^{-1}

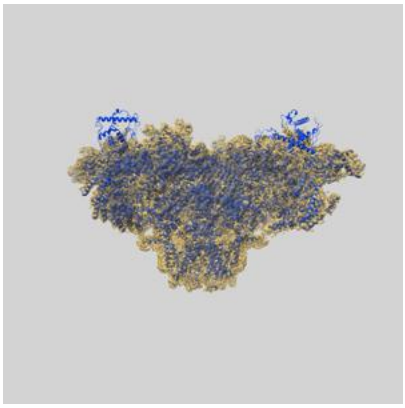
8 Fourier-Shell correlation

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

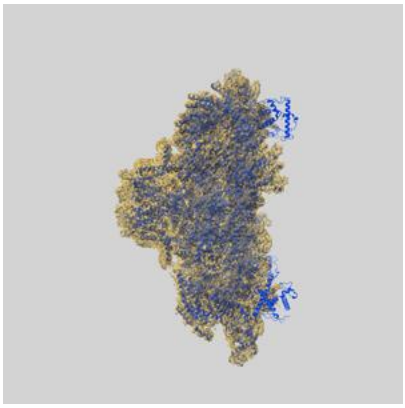
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45584 and PDB model 9CGP. Per-residue inclusion information can be found in section 3 on page 6.

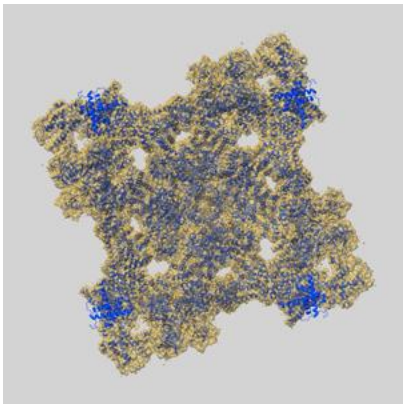
9.1 Map-model overlay



X



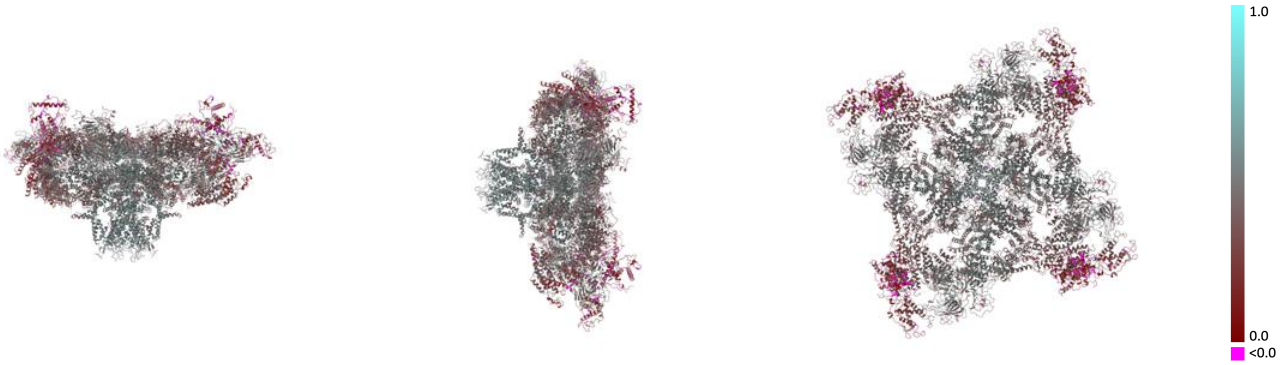
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.32 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.

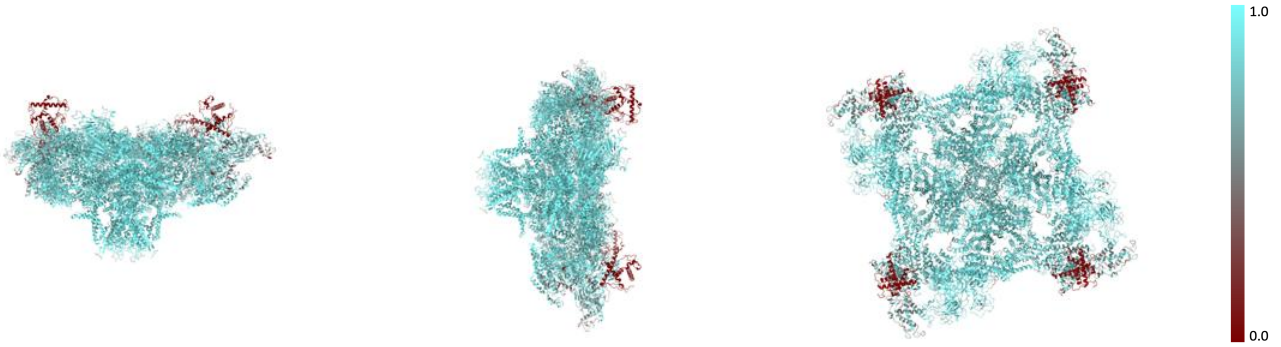
9.2 Q-score mapped to coordinate model (i)



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.

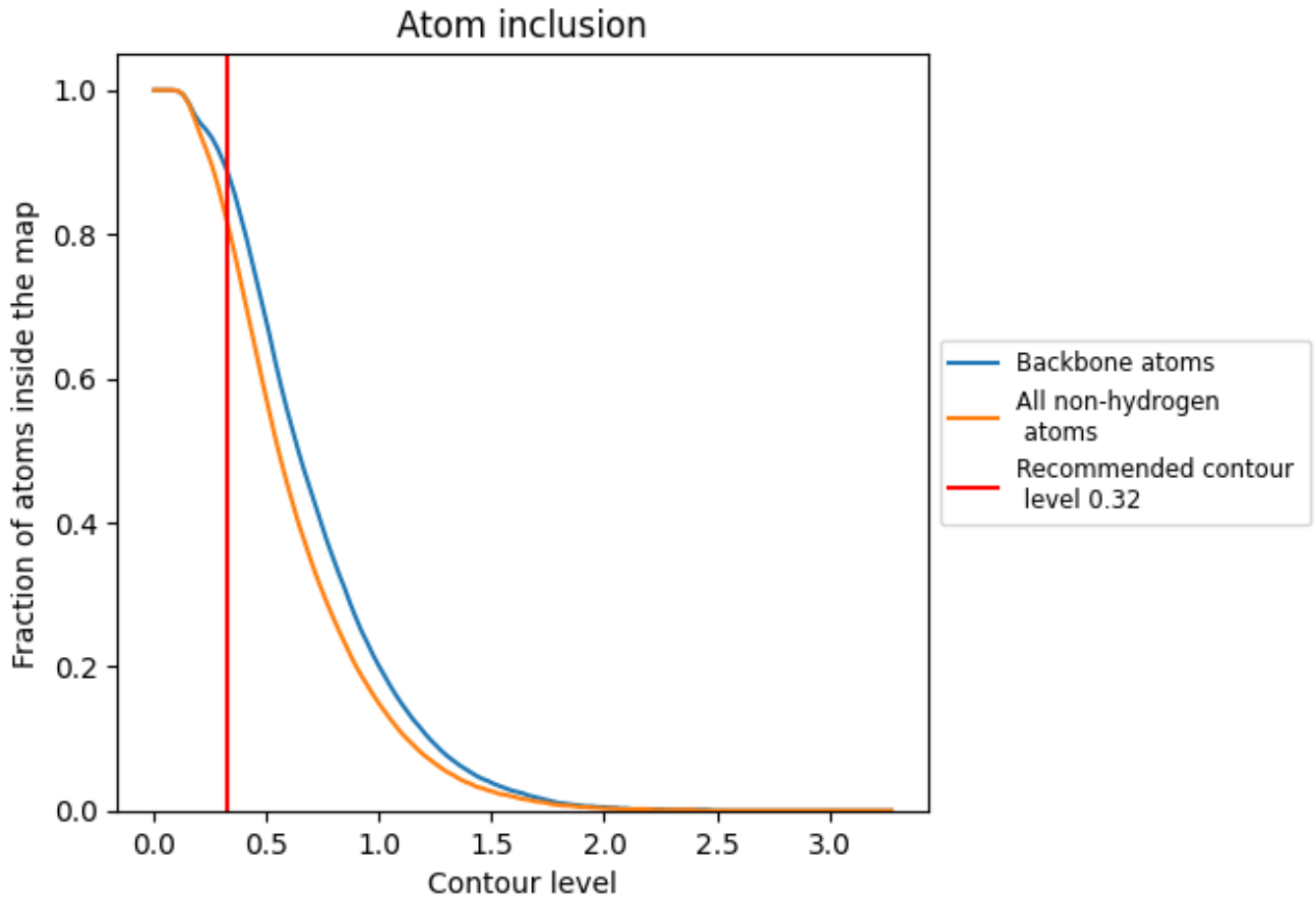
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.32).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.4080
A	0.8210	0.4070
B	0.8220	0.4080
C	0.8210	0.4070
D	0.8230	0.4080
E	0.8530	0.4190
F	0.8480	0.4210
G	0.8490	0.4200
H	0.8490	0.4230