



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:19 PM UTC

PDB ID : 8UQ4 / pdb\_00008uq4  
EMDB ID : EMD-42460  
Title : Structure of human RyR2-S2808D in the subprimed state in the presence of H<sub>2</sub>O<sub>2</sub>/NOC-12/GSH  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2023-10-23  
Resolution : 3.64 Å(reported)  
Based on initial model : 7UA5

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

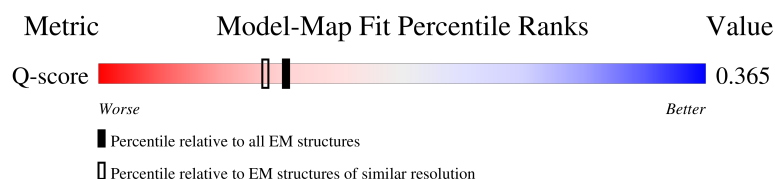
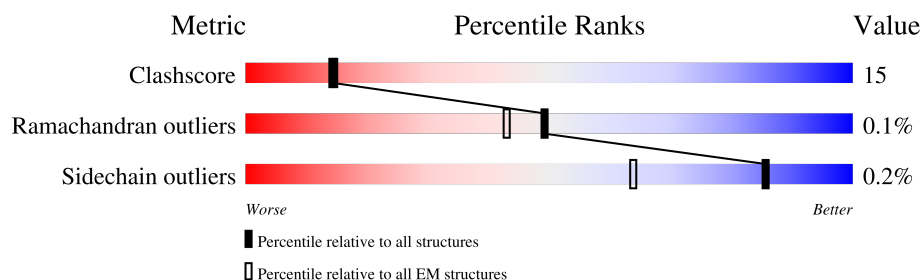
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

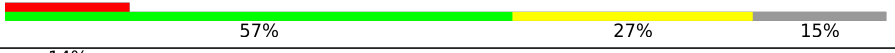
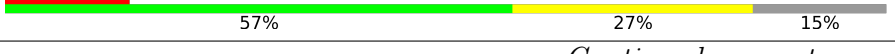
The reported resolution of this entry is 3.64 Å.

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.



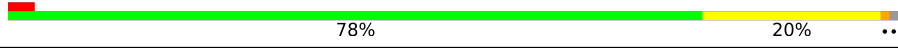
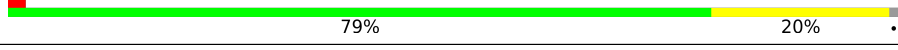
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11633 ( 3.14 - 4.14 )                                    |

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  $\geq 3$ , 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  $\leq 5\%$ . 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     | 4967   |  |
| 1   | B     | 4967   |  |
| 1   | C     | 4967   |  |
| 1   | D     | 4967   |  |

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| Mol | Chain | Length | Quality of chain                                                                            |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 2   | E     | 108    |  80%19%.  |
| 2   | F     | 108    |  79%20%.  |
| 2   | G     | 108    |  78%20%.. |
| 2   | H     | 108    |  79%20%.  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 138608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 1   | A     | 4224     | Total | C     | N    | O    | S   | 2       | 0     |
|     |       |          | 33771 | 21516 | 5745 | 6280 | 230 |         |       |
| 1   | B     | 4224     | Total | C     | N    | O    | S   | 2       | 0     |
|     |       |          | 33771 | 21516 | 5745 | 6280 | 230 |         |       |
| 1   | C     | 4224     | Total | C     | N    | O    | S   | 2       | 0     |
|     |       |          | 33771 | 21516 | 5745 | 6280 | 230 |         |       |
| 1   | D     | 4224     | Total | C     | N    | O    | S   | 2       | 0     |
|     |       |          | 33771 | 21516 | 5745 | 6280 | 230 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 2808    | ASP      | SER    | engineered mutation | UNP Q92736 |
| B     | 2808    | ASP      | SER    | engineered mutation | UNP Q92736 |
| C     | 2808    | ASP      | SER    | engineered mutation | UNP Q92736 |
| D     | 2808    | ASP      | SER    | engineered mutation | UNP Q92736 |

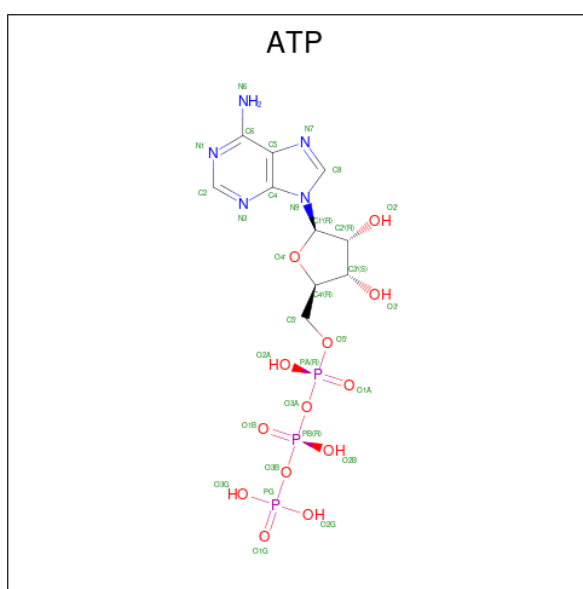
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

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

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: 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 | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

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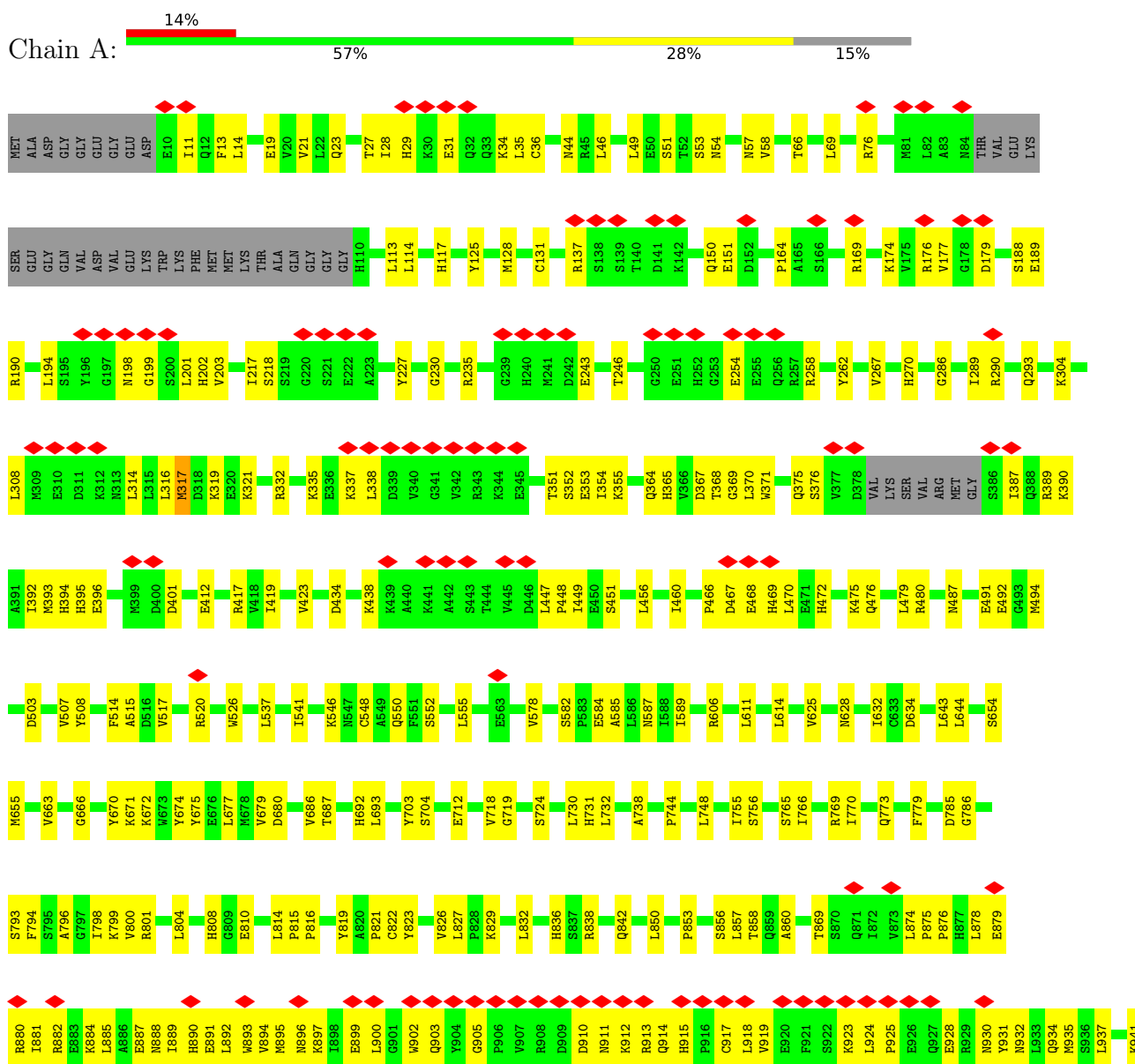
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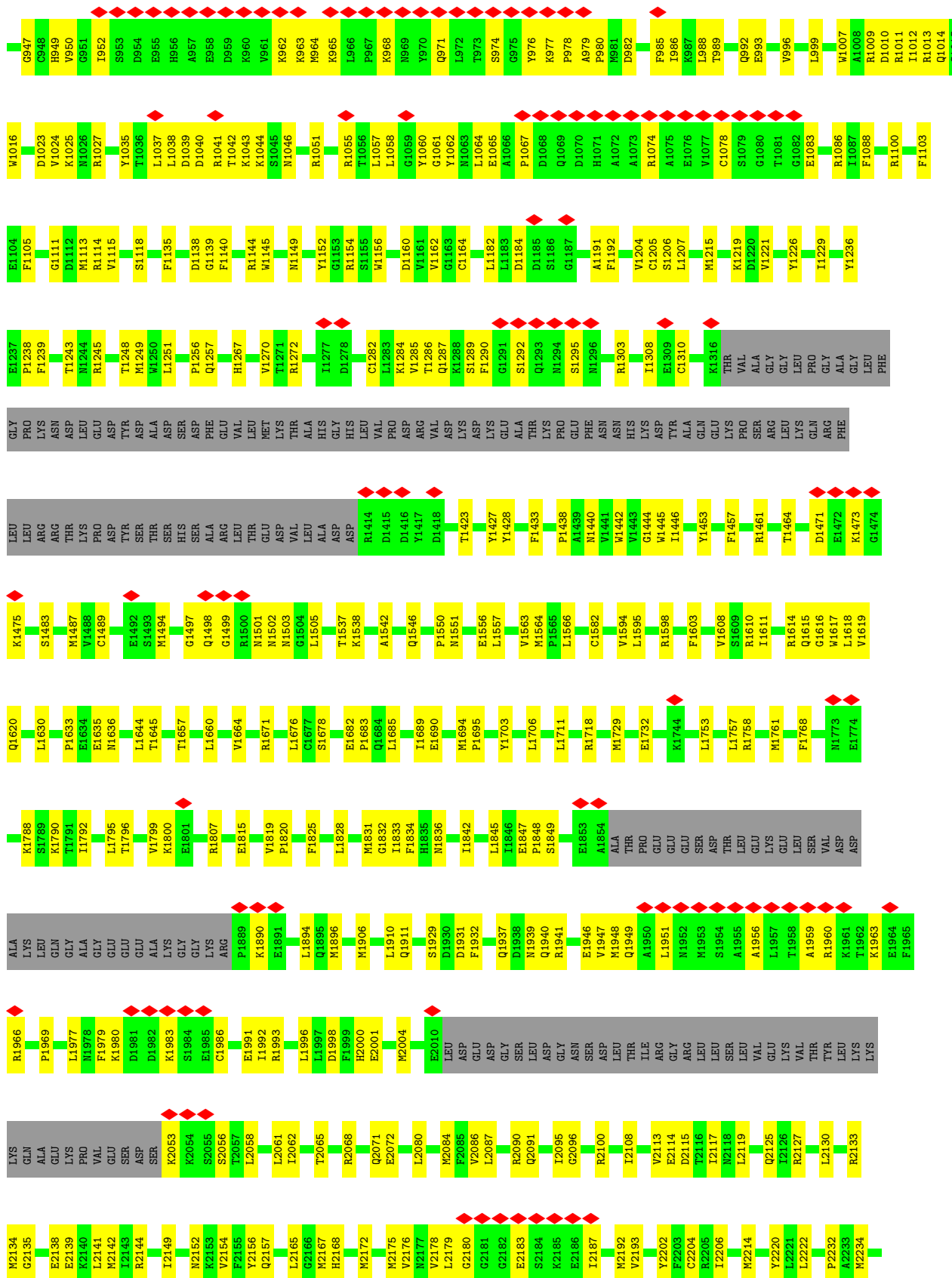
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 4   | D     | 1        | 31    | 10 | 5 | 13 | 3 | 0       |

### 3 Residue-property plots

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

#### • Molecule 1: Ryanodine receptor 2





|       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| K3144 | Q3077 | E3002 | I2930 | F2869 | G2820 | Y2743 | Y2680 | L2525 | Q2441 | P2364 | D2241 |
| S3145 | G3078 | M3003 | A2936 | L2870 | THR   | G2744 | K2681 | P2526 | N2442 | ASN   | V2242 |
| S3146 | Q3079 | L3007 | Y2939 | L2871 | SER   | E2745 | S2682 | T2529 | A2243 | SER   | A2244 |
| Y3147 | F3080 | F3008 | Y2939 | P2873 | GLN   | I2746 | S2683 | R2530 | T2444 | SER   |       |
| V3148 | T3081 | G3009 | F2943 | Y2874 | VAL   | Y2747 | N2684 | L2534 | A2446 | LYS   | V2247 |
| E3149 | K3010 | F3009 | D2944 | Y2875 | VAL   | S2748 | V2685 | F2535 | K2447 | SER   | N2248 |
| R3150 | T3011 | K3010 | G2945 | T2876 | ASP   | D2749 | V2686 | L2623 | V2461 | THR   | D2249 |
| Q3151 | L3014 | D2946 | G2946 | L2877 | ALA   | S2750 | S2687 | A2536 | L2452 | LEU   | N2250 |
| R3152 | V3015 | G2947 | G2947 | T2878 | ALA   | S2751 | N2688 | G2537 | E2453 | ASP   |       |
| L3159 | R3016 | S2947 | S2947 | T2879 | HIS   | K2752 | N2689 | H2540 | N2456 | THR   | L2253 |
| F3162 | H3017 | R2948 | R2948 | A2880 | G2821 | V2753 | E2690 | H2541 | F2460 | GLU   | R2258 |
| A3163 | R3018 | K2880 | K2880 | E2881 | Q2822 | Q2754 | K2691 | A2542 | C2461 | GLU   | E2259 |
| G3164 | T3019 | K2881 | K2881 | E2882 | P2823 | P2755 | Q2692 | E2543 | P2462 | E2377 | F2260 |
| A3165 | S3020 | K2882 | K2882 | K2883 | R2824 | L2756 | S2693 | S2543 | P2462 | D2379 | K2264 |
| F3166 | F3022 | A2883 | A2883 | A2884 | A2825 | M2757 | S2694 | L2544 | K2465 | D2380 | V2265 |
| F3167 | G3023 | D2885 | D2885 | D2886 | L2826 | K2758 | N2695 | L2545 |       | H2383 | V2266 |
| V3168 | N3024 | E2887 | E2887 | E2888 | D2827 | P2759 | D2696 | L2548 | M2468 |       | A2270 |
| A3169 | A3026 | K2888 | K2888 | K2889 | H2828 | Y2760 | S2697 | L2549 | V2469 |       | G2273 |
| F3170 | T3027 | K2890 | K2890 | Q2889 | S2829 | L2762 | G2699 | Y2553 | F2471 |       |       |
| L3171 | S3028 | D2891 | D2891 | D2892 | N2830 | L2763 | N2700 | L2554 |       | M2389 | Q2278 |
| T3172 | V3030 | L2893 | L2893 | L2894 | V2831 | S2764 | F2701 | L2555 | R2474 | T2390 |       |
| H3173 | H3034 | L2895 | L2895 | L2896 | T2832 | E2765 | N2702 | S2556 | Y2475 | F2391 | V2281 |
| H3174 | L3035 | F2895 | F2895 | F2896 | L2833 | K2766 | P2703 | K2557 | Y2476 | L2396 |       |
| L3175 | L3036 | K2897 | K2897 | K2898 | S2834 | E2767 | Q2704 | Q2565 | D2482 | Q2401 | N2290 |
| D3176 | G3037 | L2899 | L2899 | L2899 | R2835 | K2768 | P2705 | R2566 | F2483 | N2291 | N2291 |
| F3177 | Q3038 | Q2897 | Q2897 | Q2898 | D2836 | E2769 | P2706 | L2485 | L2484 | P2292 | P2292 |
| H3178 | T3039 | L2898 | L2898 | L2899 | L2837 | L2770 | D2707 | L2488 | L2485 | G2295 | G2295 |
| N3179 | L3040 | N2899 | N2899 | N2899 | L2838 | Y2771 | D2707 | L2488 | L2485 | E2296 | E2296 |
| L3180 | D3041 | G2900 | G2900 | G2900 | A2839 | Q2773 | T2708 | L2488 | L2485 | R2297 | R2297 |
| Y3181 | A3042 | Y2901 | Y2901 | Y2901 | M2840 | L2779 | S2709 | L2488 | L2485 | M2406 | M2406 |
| Y3184 | R3043 | F2975 | F2975 | F2975 | E2842 | K2655 | K2655 | G2491 | G2491 | H2407 | H2407 |
| N3185 | T3044 | K2976 | K2976 | K2976 | M2843 | K2656 | K2656 | F2492 | F2492 | L2408 | L2408 |
| T3186 | V3045 | H2978 | H2978 | H2978 | N2844 | Y2657 | S2583 | D2495 | D2495 | K2413 | K2413 |
| K3187 | K3046 | R2979 | R2979 | R2979 | E2845 | E2658 | N2584 | A2500 | A2500 | G2414 | G2414 |
| S3188 | K3047 | L2980 | L2980 | L2980 | E2846 | Q2659 | N2585 | S2501 | S2501 | E2415 | E2415 |
| E3191 | T3048 | Y2981 | Y2981 | Y2981 | N2847 | L2661 | E2660 | L2502 | L2502 | A2416 | A2416 |
| R3192 | G3049 | F2982 | F2982 | F2982 | Y2848 | F2662 | H2587 | D2503 | D2503 | L2417 | L2417 |
| A3193 | L3050 | L2983 | L2983 | L2983 | H2849 | L2664 | L2589 | T2504 | T2504 | R2418 | R2418 |
| A3194 | Y3053 | S2984 | S2984 | S2984 | N2850 | A2665 | R2590 | L2507 | L2507 | L2419 | L2419 |
| L3195 | R3058 | A2985 | A2985 | A2985 | V2852 | L2666 | R2591 | S2508 | S2508 | R2424 | R2424 |
| S3196 | A3059 | K2986 | K2986 | K2986 | A2853 | P2667 | V2593 | T2510 | T2510 | S2425 | S2425 |
| F3197 | F3060 | S2987 | S2987 | S2987 | K2854 | C2668 | N2511 | D2511 | D2511 | L2426 | L2426 |
| P3198 | K3064 | R2988 | R2988 | R2988 | K2855 | L2792 | K2723 | M2512 | M2512 | I2427 | I2427 |
| N3200 | A3065 | L2989 | L2989 | L2989 | K2856 | G2795 | Y2724 | L2513 | L2513 | R2420 | R2420 |
| V3201 | S3066 | C2990 | C2990 | C2990 | H2857 | S2797 | E2726 | R2514 | R2514 | D2431 | D2431 |
| D3202 | L3068 | S2992 | S2992 | S2992 | E2859 | M2798 | H2727 | L2518 | L2518 | G2434 | G2434 |
| T3203 | E3069 | G2993 | G2993 | G2993 | L2860 | Y2801 | H2729 | N2605 | N2605 | V2435 | V2435 |
| V3204 | K3072 | A2996 | A2996 | A2996 | E2861 | N2802 | D2730 | P2606 | P2606 | I2436 | I2436 |
| L3208 | K3076 | K2999 | K2999 | K2999 | K2863 | ARG   | K2731 | L2610 | L2610 | S2437 | S2437 |
| F3209 |       | E3000 | E3000 | E3000 | C2864 | THR   | D2675 | N2612 | N2612 | L2438 | L2438 |
| S3210 |       | F2925 | F2925 | F2925 | G2865 | ARG   | P2677 | H2613 | H2613 |       |       |
| L3211 |       | L2926 | L2926 | L2926 | G2866 | ILE   | P2678 | Y2614 | Y2614 |       |       |
| E3212 |       | L2929 | L2929 | L2929 | H2868 | ASP   | N2739 |       |       |       |       |

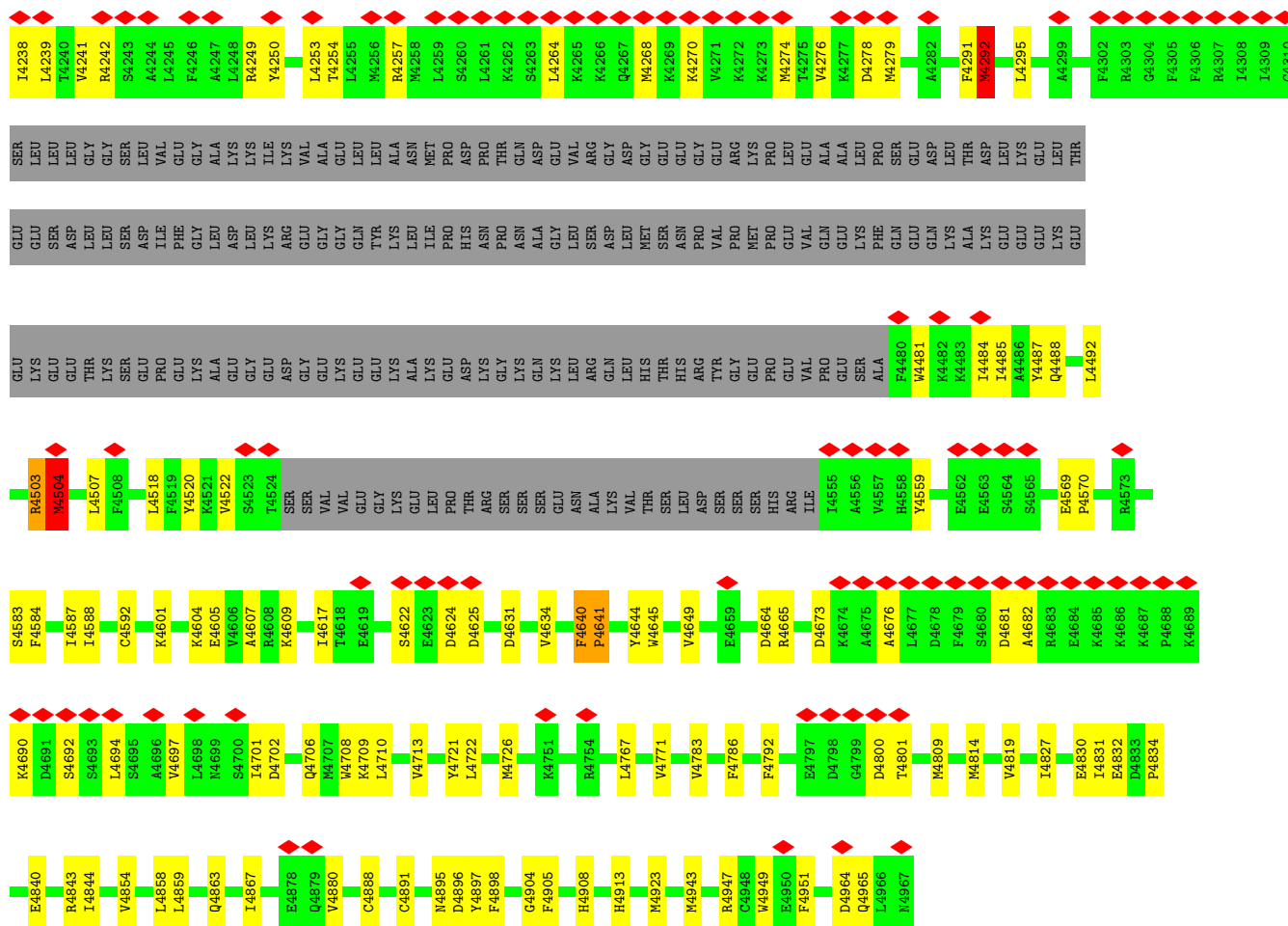




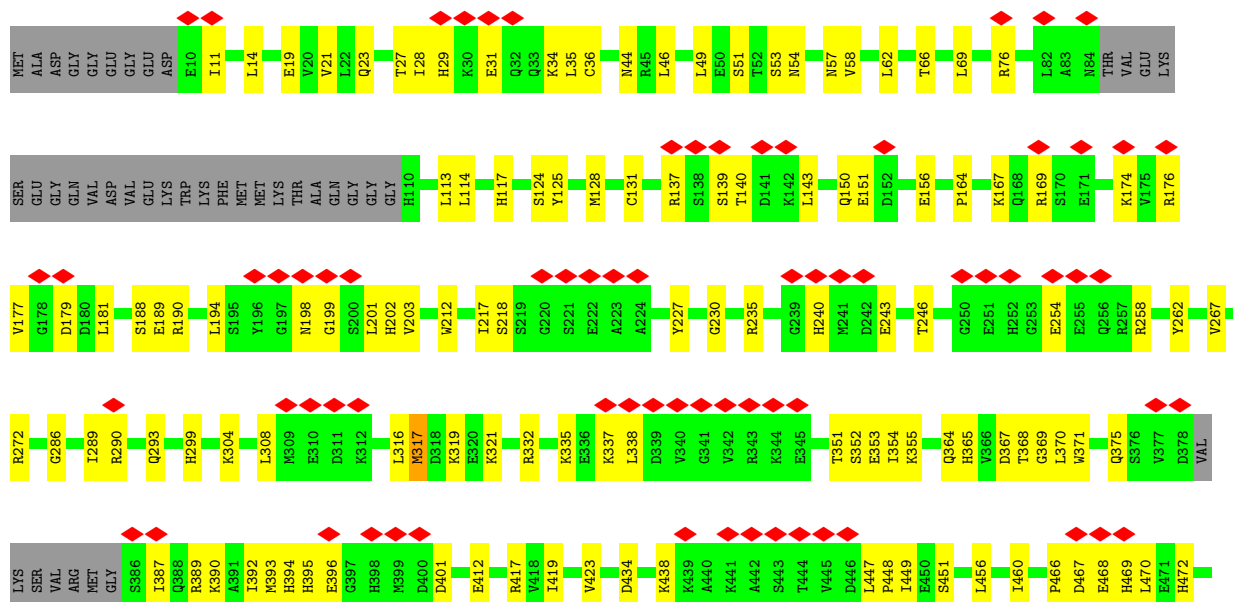


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| E3000 | K3001 | E3002 | M3003 | L3007 | F3008 | G3009 | K3010 | L3011 | L3014 | V3015 | R3016 | H3017 | K3018 | L3019 | S3020 | E3022 | F3022 | G3023 | N3024 | D3025 | A3026 | L2926 | L2929 | I2930 | A2936 | Y2939 | G2945 | G2946 | S2947 | R2948 | G2949 | K2950 | G2951 | E2952 | H2953 | F2954 | E2957 | L2960 | K2961 | F2962 | K2965 | V2966 | L2967 | L2968 | P2969 | L2970 | I2971 | D2972 | Q2973 | L2974 | F2975 | K2976 | N2977 | H2978 | R2979 | L2980 | Y2981 | F2982 | L2983 | S2984 | A2985 | A2986 | S2987 | R2988 | P2989 | L2990 | A3064 | A3065 | L3068 | E3069 | M3072 |
| G2866 | N2867 | H2868 | P2869 | L2870 | L2871 | N2872 | P2873 | T2874 | D2875 | L2877 | L2878 | A2879 | K2880 | E2881 | K2882 | A2883 | K2884 | D2885 | R2886 | E2887 | K2888 | A2889 | K2890 | D2891 | L2892 | L2893 | K2894 | F2895 | L2896 | Q2897 | L2898 | N2899 | G2900 | Y2901 | A2902 | V2903 | S2904 | R2905 | G2906 | F2907 | K2908 | D2909 | L2910 | E2911 | L2912 | D2913 | T2914 | P2915 | S2916 | L2917 | E2918 | K2919 | R2920 | F2921 | A2922 | Y2923 | S2924 | F2925 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| ARG   | ILE   | ASP   | GLN   | THR   | SER   | GLN   | VAL   | SER   | VAL   | ASP   | ALA   | ALA   | HIS   | G2820 | Y2821 | S2822 | P2823 | R2824 | A2825 | I2826 | D2827 | M2828 | S2829 | M2830 | V2831 | T2832 | L2833 | S2834 | R2835 | D2836 | L2837 | H2838 | A2839 | M2840 | A2841 | E2842 | M2843 | M2844 | A2845 | E2846 | M2847 | Y2848 | H2849 | M2850 | I2851 | W2852 | A2853 | K2854 | K2855 | K2856 | K2857 | M2858 | E2859 | L2860 | E2861 | S2862 | K2863 | G2864 | G2865 |       |       |       |       |       |       |       |       |       |       |       |       |
| I2742 | Y2743 | G2744 | E2745 | T2746 | Y2747 | S2748 | D2749 | S2750 | S2751 | K2752 | Q2753 | Q2754 | P2755 | L2756 | M2757 | K2758 | P2759 | Y2760 | K2761 | L2762 | L2763 | S2764 | E2765 | K2766 | E2767 | K2768 | E2769 | I2770 | Y2771 | R2772 | W2773 | S2778 | L2779 | K2780 | M2781 | M2782 | L2783 | A2784 | G2785 | W2787 | R2788 | I2789 | E2790 | A2791 | L2792 | R2793 | E2794 | D2795 | S2797 | L2798 | A2799 | N2802 | ARG   | THR   | ARG   |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| H2613 | Y2614 | E2615 | R2616 | K2619 | Y2620 | Y2621 | L2623 | P2624 | G2625 | G2626 | W2627 | F2630 | S2634 | E2635 | E2636 | E2637 | L2638 | H2639 | L2640 | S2641 | R2642 | K2643 | L2644 | F2645 | W2646 | G2647 | I2648 | F2649 | D2650 | A2651 | L2652 | K2655 | K2656 | Y2657 | E2658 | Q2659 | E2660 | L2661 | F2662 | K2663 | L2664 | A2665 | L2666 | P2667 | C2668 | L2669 | S2670 | A2671 | V2672 | A2673 | G2674 | A2675 | L2676 | P2677 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| P2678 | D2679 | M2680 | E2682 | S2683 | N2684 | Y2685 | V2686 | S2687 | M2688 | M2689 | E2690 | K2691 | Q2692 | S2693 | S2694 | H2695 | D2696 | S2697 | E2698 | G2699 | N2700 | F2701 | N2702 | P2703 | Q2704 | P2705 | V2706 | L2707 | T2708 | S2709 | N2710 | L2711 | T2712 | L2713 | P2714 | E2715 | K2716 | L2717 | E2718 | Y2719 | F2720 | L2721 | N2722 | K2723 | Y2724 | A2725 | E2726 | H2727 | S2728 | H2729 | D2730 | K2731 | W2732 | L2737 | A2738 | H2739 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| I2742 | Y2743 | G2744 | E2745 | T2746 | Y2747 | S2748 | D2749 | S2750 | S2751 | K2752 | Q2753 | Q2754 | P2755 | L2756 | M2757 | K2758 | P2759 | Y2760 | K2761 | L2762 | L2763 | S2764 | E2765 | K2766 | E2767 | K2768 | E2769 | I2770 | Y2771 | R2772 | W2773 | S2778 | L2779 | K2780 | M2781 | M2782 | L2783 | A2784 | G2785 | W2787 | R2788 | I2789 | E2790 | A2791 | L2792 | R2793 | E2794 | D2795 | S2797 | L2798 | A2799 | N2802 | ARG   | THR   | ARG   |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G2866 | N2867 | H2868 | P2869 | L2870 | L2871 | N2872 | P2873 | T2874 | D2875 | L2877 | L2878 | A2879 | K2880 | E2881 | K2882 | A2883 | K2884 | D2885 | R2886 | E2887 | K2888 | A2889 | K2890 | D2891 | L2892 | L2893 | K2894 | F2895 | L2896 | Q2897 | L2898 | N2899 | G2900 | Y2901 | A2902 | V2903 | S2904 | R2905 | G2906 | F2907 | K2908 | D2909 | L2910 | E2911 | L2912 | D2913 | T2914 | P2915 | S2916 | L2917 | E2918 | K2919 | R2920 | F2921 | A2922 | Y2923 | S2924 | F2925 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| L2926 | L2929 | I2930 | A2936 | Y2939 | G2945 | G2946 | S2947 | R2948 | G2949 | K2950 | G2951 | E2952 | H2953 | F2954 | E2957 | L2960 | K2961 | F2962 | K2965 | V2966 | L2967 | L2968 | P2969 | L2970 | I2971 | D2972 | Q2973 | L2974 | F2975 | K2976 | N2977 | H2978 | R2979 | L2980 | Y2981 | F2982 | L2983 | S2984 | A2985 | A2986 | S2987 | R2988 | P2989 | L2990 | C2991 | S2992 | G2993 | A2996 | N2998 | K2999 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |





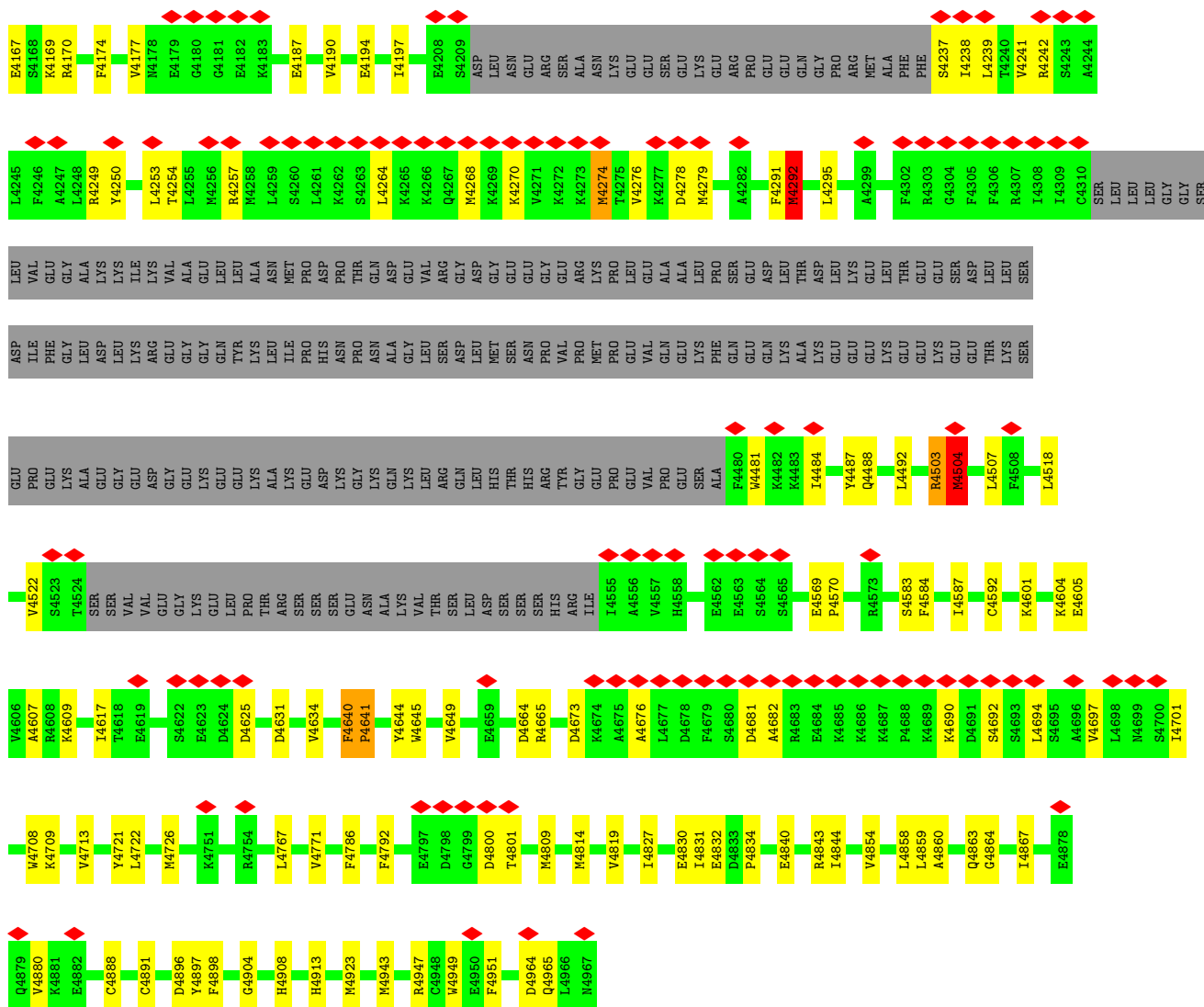
• Molecule 1: Ryanodine receptor 2



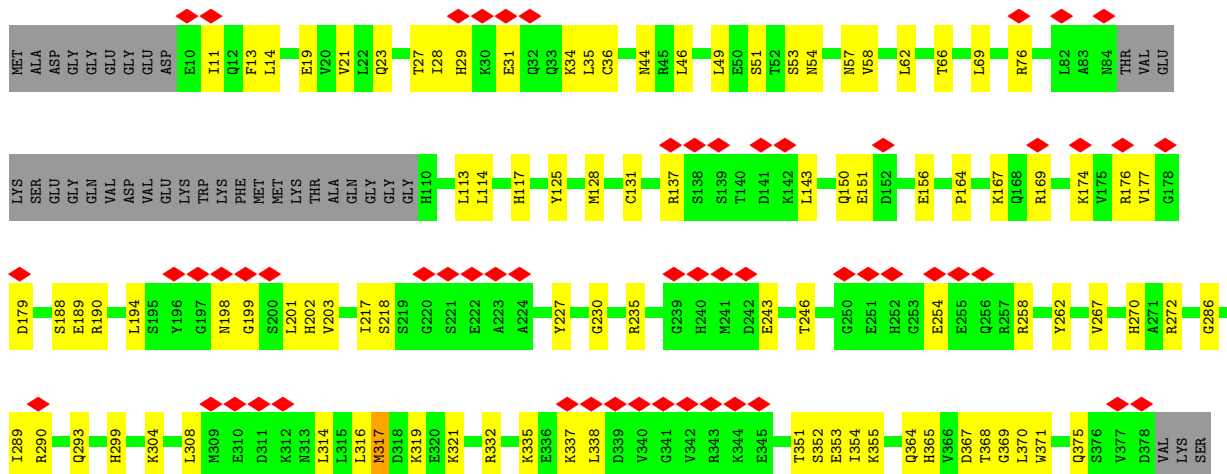


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| L2926 | L2929 | L2930 | A2936 | Y2939 | G2945 | G2946 | G2947 | R2948 | G2949 | K2950 | G2951 | E2952 | H2953 | F2954 | E2957 | L2960 | K2961 | F2962 | K2965 | V2966 | V2967 | L2968 | P2969 | L2970 | L2971 | D2972 | Q2973 | Y2974 | K2975 | F2976 | N2977 | H2978 | R2979 | L2980 | Y2981 | L2982 | S2984 | A2985 | A2986 | S2987 | R2988 | P2989 | L2990 | C2991 | S2992 | G2993 | A2996 | N2997 | K2998 | K2999 |       |       |       |       |       |       |       |       |       |
| G2866 | N2867 | H2868 | P2869 | L2870 | L2871 | V2872 | P2873 | R2874 | D2875 | L2876 | G2877 | T2878 | A2879 | K2880 | E2881 | K2882 | A2883 | K2884 | D2885 | R2886 | E2887 | K2888 | A2889 | Q2890 | D2891 | L2892 | L2893 | K2894 | F2895 | L2896 | L2897 | D2898 | N2899 | G2900 | Y2901 | A2902 | V2903 | S2904 | R2905 | F2907 | K2908 | D2909 | L2910 | E2911 | L2912 | D2913 | T2914 | P2915 | S2916 | L2917 | K2918 | K2919 | R2920 | F2921 | A2922 | S2923 | F2924 | F2925 |       |
| Y2743 | G2744 | E2745 | L2746 | V2747 | L2748 | D2749 | S2750 | S2751 | K2752 | G2753 | G2754 | P2755 | L2756 | K2757 | K2758 | P2759 | V2760 | K2761 | L2762 | L2763 | S2764 | E2765 | K2766 | E2767 | K2768 | E2769 | L2770 | L2771 | K2772 | K2773 | S2778 | K2779 | K2780 | L2781 | K2782 | L2783 | A2784 | W2785 | G2786 | W2787 | R2788 | L2789 | E2790 | R2791 | T2792 | K2793 | E2794 | G2795 | K2796 | S2797 | W2798 | A2799 | L2800 | Y2801 | N2802 | ARG   | THR   | ARG   |       |
| ARG   | ILE   | ASP   | GLN   | THR   | SER   | GLN   | VAL   | SER   | VAL   | ASP   | ALA   | ALA   | HIS   | G2820 | Y2821 | S2822 | P2823 | R2824 | A2825 | L2826 | D2827 | M2828 | S2829 | N2830 | V2831 | L2832 | L2833 | L2834 | S2835 | D2836 | L2837 | H2838 | A2839 | M2840 | A2841 | E2842 | M2843 | M2844 | A2845 | E2846 | M2847 | Y2848 | H2849 | N2850 | L2851 | V2852 | K2853 | K2854 | K2855 | K2856 | K2857 | M2858 | E2859 | L2860 | E2861 | S2862 | K2863 | G2864 | G2865 |
| D2679 | T2680 | M2681 | E2682 | S2683 | N2684 | V2685 | V2686 | S2687 | M2688 | E2689 | E2690 | K2691 | Q2692 | S2693 | S2694 | M2695 | D2696 | S2697 | E2698 | G2699 | N2700 | F2701 | N2702 | P2703 | Q2704 | P2705 | V2706 | D2707 | T2708 | S2709 | N2710 | L2711 | T2712 | L2713 | P2714 | E2715 | K2716 | K2663 | L2664 | A2665 | L2666 | P2667 | C2668 | L2669 | S2670 | A2671 | V2672 | A2673 | G2674 | A2675 | L2676 | P2677 | P2678 |       |       |       |       |       |       |
| Y2614 | E2615 | R2616 | K2619 | V2620 | Y2621 | C2622 | L2623 | A2624 | G2625 | G2626 | W2627 | F2630 | S2634 | E2635 | E2636 | E2637 | L2638 | H2639 | L2640 | S2641 | R2642 | L2643 | L2644 | F2645 | G2646 | L2647 | L2648 | F2649 | D2650 | A2651 | L2652 | K2655 | K2656 | Y2657 | E2658 | S2659 | Q2660 | L2661 | F2662 | K2663 | L2664 | A2665 | L2666 | P2667 | C2668 | L2669 | S2670 | A2671 | V2672 | A2673 | G2674 | A2675 | L2676 | P2677 | P2678 |       |       |       |       |
| L2525 | P2526 | R2530 | L2534 | F2535 | A2536 | G2537 | H2540 | H2541 | A2542 | S2543 | L2544 | L2545 | L2548 | L2549 | Y2553 | R2554 | L2555 | K2556 | Q2557 | Q2558 | D2557 | S2558 | F2559 | E2570 | L2580 | P2581 | L2582 | S2583 | M2584 | M2585 | Q2586 | H2587 | L2588 | L2589 | R2590 | R2591 | L2592 | V2593 | F2594 | H2602 | A2603 | K2604 | M2605 | W2612 | L2610 | T2611 | N2612 | H2613 |       |       |       |       |       |       |       |       |       |       |       |
| G2437 | L2438 | Q2441 | P2442 | T2443 | T2444 | L2445 | K2447 | V2451 | V2452 | E2453 | M2456 | F2460 | C2461 | P2462 | K2465 | V2468 | V2469 | L2470 | F2471 | R2474 | V2475 | Y2476 | D2482 | F2483 | L2484 | L2485 | L2486 | L2487 | E2488 | E2489 | V2490 | G2491 | F2492 | D2495 | A2500 | S2501 | L2502 | D2503 | T2504 | L2507 | S2508 | T2510 | D2511 | W2512 | C2521 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| D2360 | S2363 | P2364 | ASN   | SER   | GLY   | SER   | SER   | LYS   | THR   | LEU   | ASP   | THR   | GLU   | E2377 | D2378 | D2379 | D2380 | H2383 | N2386 | M2389 | T2390 | F2391 | I2396 | R2401 | C2402 | A2403 | M2406 | H2407 | L2408 | I2409 | K2413 | G2414 | E2415 | A2416 | R2417 | L2418 | I2419 | R2420 | L2423 | R2424 | S2425 | L2426 | L2427 | D2431 | G2434 | V2435 | L2436 |       |       |       |       |       |       |       |       |       |       |       |       |
| D2241 | V2242 | A2243 | A2244 | V2247 | M2248 | D2249 | N2250 | L2253 | R2258 | E2259 | P2260 | K2264 | V2265 | V2266 | A2270 | G2273 | Q2278 | V2281 | D2287 | V2290 | N2291 | P2292 | G2295 | E2296 | R2297 | F2301 | R2303 | F2304 | F2307 | R2322 | R2326 | R2327 | G2332 | R2336 | G2337 | E2338 | I2353 | R2359 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G2135 | E2138 | E2139 | K2140 | L2141 | M2142 | J2143 | L2144 | I2149 | M2150 | N2151 | N2152 | J2153 | V2154 | V2155 | V2156 | Q2157 | L2165 | M2167 | H2168 | M2172 | M2175 | V2176 | V2178 | L2179 | G2180 | G2181 | G2182 | E2183 | S2184 | K2185 | E2186 | I2187 | M2192 | V2193 | Y2202 | F2203 | C2204 | R2205 | T2206 | M2214 | Q2215 | L2216 | R2217 | L2221 | L2222 | L2130 | R2133 | M2134 |       |       |       |       |       |       |       |       |       |       |       |
| P1969 | L1977 | N1978 | F1979 | K1980 | D1981 | D1982 | K1983 | S1984 | E1985 | C1986 | E1991 | I1992 | R1993 | L1996 | L1997 | D1998 | F1999 | H2000 | E2001 | M2004 | E2010 | LEU   | ASP   | GLU   | ASP   | GLY   | SER   | LEU   | ASP   | GLY   | ASN   | SER   | ASP   | LEU   | THR   | ILE   | ARG   | GLY   | ARG   | LEU   | LEU   | SER   | VAL   | GLU   | LYS   | VAL   | THR   | TVR   | LEU   | LYS   | LYS   |       |       |       |       |       |       |       |       |

|       |       |       |       |       |       |     |     |     |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-----|-----|-----|-------|-------|-------|-------|-------|
| K4056 | Q3955 | S3825 | E3678 | SER   | PRO   | GLN | VAL | ALA | I3280 | M3215 | L3140 | K3076 | E3000 |
| H4057 | M3956 | G3826 | K3679 | LYS   | ALA   | THR | PHE | GLU | L3281 | E3216 | L3140 | Q3077 | K3001 |
| T4063 | K3957 | G3827 | L3687 | ALA   | ILE   | SER | ILE | ALA | K3282 | E3217 | K3144 | Q3078 | E3002 |
| F4064 | L3958 | E3827 | Y3688 | TRP   | TRP   | ILE | TRP | ARG | I3283 | E3218 | S3145 | Q3079 | M3003 |
| L4066 | L3968 | K3828 | M3689 | VAL   | GLN   | VAL | SER | ASP | I3284 | V3219 | I3146 | F3080 | L3007 |
| L4067 | M3972 | D3832 | A3690 | HIS   | MET   | ALA | LYS | MET | N3286 | E3220 | Y3147 | F3008 | G3009 |
| E4071 | D3973 | F3835 | Y3691 | LYS   | ALA   | ALA | SER | SER | K3287 |       | V3148 | HIS   | K3010 |
| T4072 | K3975 | L3846 | M3695 | LEU   | LEU   | LEU | HIS | GLU | L3288 |       | E3149 | ARG   | L3011 |
| D4073 | K3976 | A3696 | A3696 | LEU   | LEU   | LEU | ASN | ALA | I3227 |       | Q3151 | ASN   | L3014 |
| E4074 | D3977 | N3851 | C3699 | LYS   | ASP   | PRO | LYS | LEU | T3229 |       | R3152 | GLN   | V3015 |
| V3979 | M3978 | S3852 | H3700 | GLN   | PRO   | ILE | ARG | LEU | F3232 |       | F3162 | PRO   | R3016 |
| V3980 | K3979 | D3853 | D3701 | ARG   | ASN   | GLY | GLN | LEU | G3293 |       | A3163 | G3089 | H3017 |
| M3981 | K3981 | F3854 | E3702 | THR   | THR   | LEU | ASN | GLU | A3294 |       | G3164 | V3090 | R3018 |
| M3985 | M3985 | Q3855 | GLU   | ASP   | ASP   | ILE | PHE | THR | M3295 |       | A3165 | T3091 | I3019 |
| L3986 | L3986 | L3858 | ASP   | THR   | THR   | CYS | VAL | THR | K3297 |       | F3167 | Q3092 | S3020 |
| M3999 | M3999 | Q3882 | ASP   | SER   | SER   | ALA | VAL | ALA | R3298 |       | V3168 | Y3096 | F3022 |
| V4000 | V4000 | E3883 | GLY   | ASP   | PRO   | GLY | GLN | ARG | F3303 |       | A3169 | T3097 | G3023 |
| M4001 | M4001 | S3884 | GLU   | GLU   | PRO   | ASP | ASN | ALA | K3304 |       | F3170 | T3098 | R3024 |
| M4002 | M4002 | W3890 | GLU   | LYS   | LYS   | GLN | ASN | LEU | G3305 |       | A3171 | V3099 | D3025 |
| L4003 | L4003 | Y3891 | THR   | THR   | THR   | GLU | ASN | LEU | I3306 |       | L3171 | A3100 | A3026 |
| V4004 | V4004 | E3710 | V3711 | VAL   | VAL   | ILE | MET | ALA | I3307 |       | F3172 | L3102 | T3029 |
| E4005 | E4005 | K3712 | K3712 | GLU   | GLU   | ALA | PHE | TYR | N3308 |       | T3173 | P3103 | V3030 |
| S4006 | S4006 | Q3722 | Q3722 | ARG   | VAL   | LEU | LEU | PRO | K3309 |       | M3104 | M3104 | H3034 |
| E4011 | E4011 | K3723 | K3723 | LEU   | VAL   | LEU | ILE | LEU | V3310 |       | D3176 | L3105 | L3035 |
| L4014 | L4014 | Q3727 | Q3727 | ASP   | ASP   | LYS | THR | LEU | K3311 |       | K3177 | S3106 | L3036 |
| L4021 | L4021 | K3728 | K3728 | ILE   | ILE   | ASN | ASP | ILE | E3251 |       | R3178 | S3107 | G3037 |
| K4022 | K4022 | A3913 | A3913 | ALA   | ALA   | ARG | THR | ARG | Q3312 |       | K3179 | F3108 | Q3038 |
| L4023 | L4023 | K3914 | K3914 | ASN   | VAL   | PHE | LYS | PHE | K3313 |       | I3180 | F3109 | T3039 |
| L4026 | L4026 | H3615 | H3615 | VAL   | VAL   | SER | SER | VAL | G3253 |       | Y3181 | E3110 | L3040 |
| L4115 | L4115 | Q3915 | Q3915 | LEU   | LEU   | LYS | LYS | ASP | P3254 |       | Y3184 | H3111 | D3041 |
| T4117 | T4117 | V3916 | V3916 | PHE   | PHE   | LYS | MET | TYR | N3256 |       | N3185 | Q3114 | A3042 |
| F4118 | F4118 | L3920 | L3920 | HIS   | HIS   | THR | SER | ASN | F3319 |       | T3186 | F3117 | R3043 |
| L4119 | L4119 | G3926 | G3926 | LEU   | LEU   | GLU | LYS | ALA | L3320 |       | K3187 | G3118 | V3045 |
| E4120 | E4120 | P3927 | P3927 | GLU   | GLU   | ASP | VAL | TRP | L3321 |       | S3188 | G3119 | K3046 |
| A4122 | A4122 | C3928 | C3928 | LYS   | LYS   | VAL | SER | VAL | L3322 |       |       | D3120 | T3048 |
| E4123 | E4123 | T3929 | T3929 | ARG   | ARG   | ASP | ASP | LYS | M3323 |       |       | L3121 | G3049 |
| Y4128 | Y4128 | Q3932 | Q3932 | E3650 | E3650 | ILE | GLN | PRO | K3325 |       | E3191 | L3123 | L3050 |
| R4135 | R4135 | Q3933 | Q3933 | P3651 | P3651 | ILE | GLU | GLU | L3326 |       | R3192 | E3124 | V3053 |
| E4137 | E4137 | S3934 | S3934 | P3652 | P3652 | ARG | LYS | PRO | K3327 |       | A3193 | D3125 | R3058 |
| R4147 | R4147 | L3935 | L3935 | E3653 | E3653 | THR | LYS | GLU | K3328 |       | A3194 | V3126 | F3060 |
| Y4148 | Y4148 | L3940 | L3940 | E3654 | E3654 | ASN | MET | ALA | K3329 |       | S3196 | Q3127 | K3064 |
| V4149 | V4149 | V3944 | V3944 | D3655 | D3655 | ILE | LYS | GLU | A3330 |       | S3196 | Q3127 | A3064 |
| S4155 | S4155 | V3945 | V3945 | E3656 | E3656 | HIS | ARG | GLU | L3331 |       | L3197 | V3128 | A3065 |
| Q4159 | Q4159 | F3946 | F3946 | E3657 | E3657 | LEU | LYS | LEU | T3332 |       | P3198 | S3129 | L3068 |
|       |       | L3948 | L3948 | T3658 | T3658 | GLY | ASP | PHE | K3333 |       | T3199 | C3130 | E3069 |
|       |       | H3949 | H3949 | K3659 | K3659 | LYS | ARG | MET | V3334 |       | R3200 | Y3131 |       |
|       |       | V3950 | V3950 | R3660 | R3660 | VAL | TYR | VAL | E3202 |       | V3201 | R3132 |       |
|       |       | F3951 | F3951 | V3661 | V3661 | GLN | SER | ALA | D3203 |       | V3204 | L3133 |       |
|       |       |       |       | Q3666 | Q3666 | ASP | MET | GLU | E3337 |       | T3278 | S3136 |       |
|       |       |       |       | T3674 | T3674 | LEU |     |     | ASP   |       | L3208 | HIS   |       |
|       |       |       |       |       |       | LYS |     |     | HIS   |       | P3209 | L3137 |       |
|       |       |       |       |       |       |     |     |     | LEU   |       | S3210 | L3211 |       |
|       |       |       |       |       |       |     |     |     | LYS   |       | E3212 | Y3138 |       |
|       |       |       |       |       |       |     |     |     |       |       | K3213 | A3139 |       |
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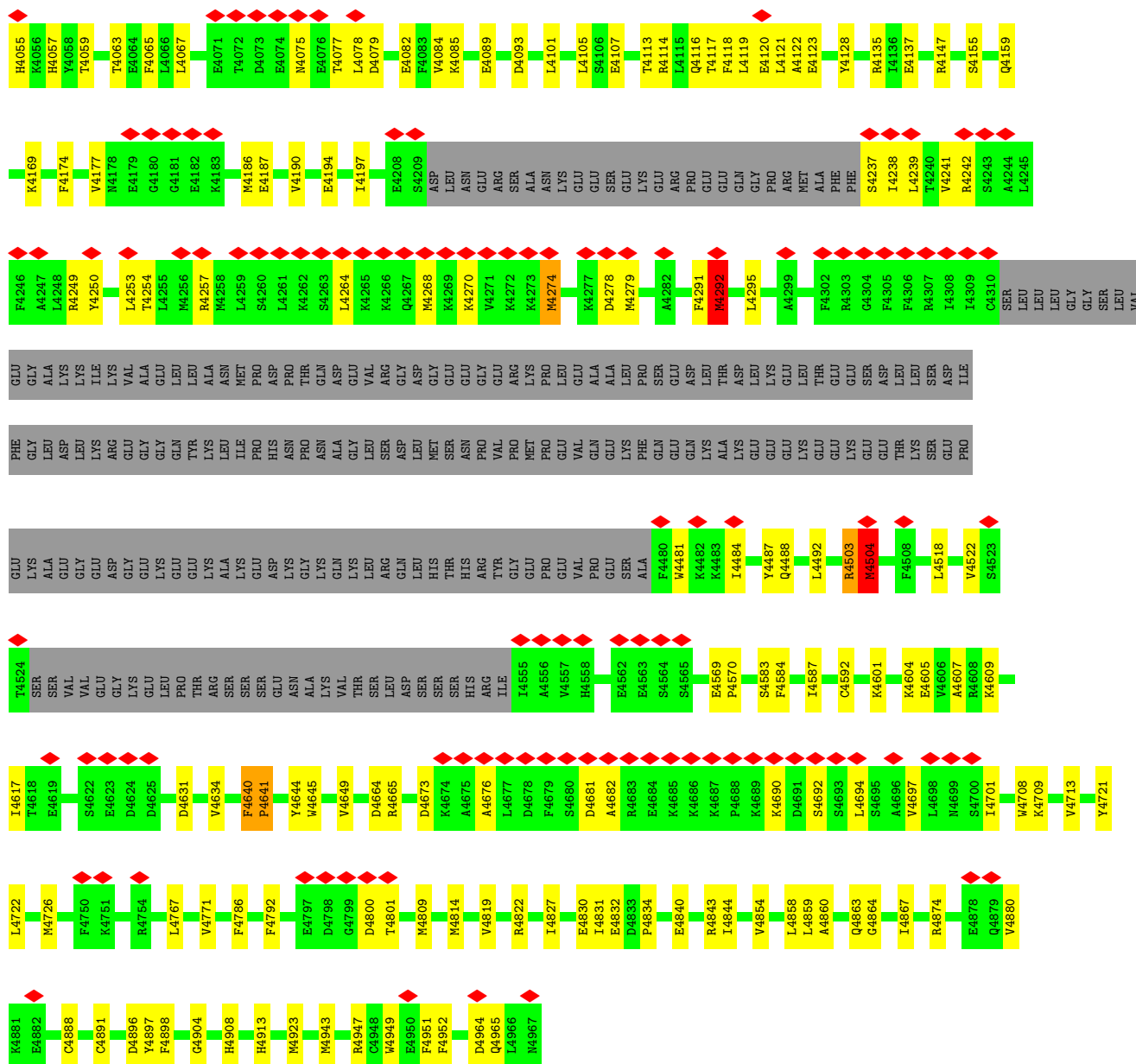
• Molecule 1: Ryanodine receptor 2



|       |       |     |     |       |       |       |      |      |      |      |
|-------|-------|-----|-----|-------|-------|-------|------|------|------|------|
| M1761 | R1614 | G1N | GLY | R1100 | I1012 | L937  | H877 | F779 | L479 | VAL  |
| F1768 | Q1615 | ARG | LEU | F1103 | R1013 | K941  | L878 | D785 | R480 | ARG  |
| N1773 | G1616 | PHE | GLY | E1104 | Q1014 | L946  | E879 | G786 | M487 | GLY  |
| E1774 | W1617 | LEU | GLY | F1105 | W1016 | G947  | I881 | S793 | E491 | S386 |
| K1788 | L1618 | LEU | PRO | M1113 | D1023 | G948  | R882 | F794 | E492 | I387 |
| S1789 | V1619 | ARG | ASN | E1237 | V1024 | H949  | E883 | S795 | G493 | Q388 |
| K1790 | Q1620 | THR | ASP | F1239 | V1025 | H950  | K884 | A796 | M494 | R389 |
| T1791 | L1630 | PRO | GLY | G951  | N1026 | G951  | K885 | G797 | M655 | K390 |
| I1792 | P1633 | ASP | ASP | S1118 | R1027 | I952  | A886 | I798 | D503 | A391 |
| L1795 | P1633 | TYR | TYR | D1126 | Y1035 | S953  | E887 | K799 | I392 | I392 |
| V1799 | E1634 | ASP | ASP | Q1126 | T1036 | D954  | N888 | V800 | M393 | M393 |
| K1800 | S1493 | THR | ALA | F1135 | L1037 | E955  | E891 | V507 | M394 | H394 |
| E1801 | G1497 | SER | SER | D1138 | L1038 | H956  | H890 | Y508 | H395 | H395 |
| R1807 | Q1498 | ASP | ASP | G1139 | D1039 | A957  | E891 | F514 | E396 | E396 |
| E1815 | G1499 | ALA | PHE | R1144 | R1040 | E958  | H893 | Y674 | M399 | M399 |
| V1819 | R1500 | ARG | GLY | W1145 | R1041 | D959  | E894 | Y675 | D400 | D400 |
| P1820 | N1501 | LEU | LEU | W1145 | T1042 | K960  | M896 | L677 | D401 | D401 |
| F1825 | N1503 | GLY | MET | N1149 | K1043 | V961  | K897 | M678 | E412 | E412 |
| L1829 | G1504 | VAL | THR | T1271 | S1045 | K962  | I898 | D680 | R417 | R417 |
| P1833 | L1505 | ALA | ALA | Y1152 | L1050 | K963  | E899 | V686 | V418 | V418 |
| Q1834 | D1512 | ASP | HIS | G1153 | R1051 | N964  | E901 | T687 | I419 | I419 |
| E1835 | G1516 | LEU | GLY | R1154 | L1057 | K965  | W902 | H692 | V423 | V423 |
| H1836 | T1537 | PRO | LEU | S1155 | T1056 | L966  | Q903 | L693 | D434 | D434 |
| P1848 | K1538 | ARG | ASP | W1156 | L1057 | P967  | Y904 | S704 | K438 | K438 |
| S1849 | K1538 | ARG | ASP | D1160 | L1058 | K968  | G905 | Q550 | K439 | K439 |
| E1853 | A1542 | VAL | VAL | V1161 | G1059 | N969  | G905 | E712 | A440 | A440 |
| A1854 | A1542 | ASP | ASP | V1162 | G1060 | Y970  | Q907 | S552 | K441 | K441 |
| ALA   | A1542 | ASP | ASP | C1164 | Y1061 | Q971  | L972 | V718 | A442 | A442 |
| THR   | A1542 | ASP | ASP | L1177 | Y1062 | L973  | R908 | G719 | S443 | S443 |
| PRO   | A1542 | ASP | ASP | L1182 | N1063 | S974  | D909 | S724 | T444 | T444 |
| GLY   | A1542 | ASP | ASP | L1183 | L1064 | G975  | D910 | E563 | V445 | V445 |
| GLY   | A1542 | ASP | ASP | D1184 | E1065 | Y976  | N911 | V578 | D446 | D446 |
| ASP   | A1542 | ASP | ASP | D1185 | A1066 | K977  | K912 | S822 | L447 | L447 |
| ASN   | A1542 | ASP | ASP | S1186 | D1067 | P978  | R913 | P583 | P448 | P448 |
| ASN   | A1542 | ASP | ASP | G1187 | Q1069 | A979  | H915 | A585 | I449 | I449 |
| HIS   | A1542 | ASP | ASP | A1191 | D1070 | P980  | P916 | L748 | E450 | E450 |
| ASP   | A1542 | ASP | ASP | K1193 | H1071 | N981  | C917 | N587 | S451 | S451 |
| TYR   | A1542 | ASP | ASP | V1204 | H1072 | D982  | L918 | I588 | L456 | L456 |
| ALA   | A1542 | ASP | ASP | C1205 | A1073 | F985  | E920 | I755 | I460 | I460 |
| GLY   | A1542 | ASP | ASP | S1206 | R1074 | I986  | F921 | S765 | P466 | P466 |
| PRO   | A1542 | ASP | ASP | L1207 | A1076 | K987  | S870 | I766 | D467 | D467 |
| VAL   | A1542 | ASP | ASP | M1215 | V1077 | T989  | Q871 | L614 | E468 | E468 |
| THR   | A1542 | ASP | ASP | K1219 | S1079 | Q992  | V873 | I770 | H469 | H469 |
| GLY   | A1542 | ASP | ASP | V1221 | G1080 | E993  | L874 | Q773 | L470 | L470 |
| GLY   | A1542 | ASP | ASP | ALA   | T1081 | V996  | P875 | N628 | E471 | E471 |
| GLY   | A1542 | ASP | ASP | ALA   | E1082 | L999  | P876 |      | H472 | H472 |
| GLY   | A1542 | ASP | ASP | ALA   | E1083 | W1007 |      |      | K475 | K475 |
| GLY   | A1542 | ASP | ASP | ALA   | F1088 | A1008 |      |      | Q476 | Q476 |
| GLY   | A1542 | ASP | ASP | ALA   |       | R1009 |      |      |      |      |
| GLY   | A1542 | ASP | ASP | ALA   |       | D1010 |      |      |      |      |
| GLY   | A1542 | ASP | ASP | ALA   |       | R1011 |      |      |      |      |
| GLY   | A1542 | ASP | ASP | ALA   |       | M935  |      |      |      |      |
| GLY   | A1542 | ASP | ASP | ALA   |       | S936  |      |      |      |      |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2865 | G2866 | M2867 | H2868 | L2869 | L2870 | L2871 | L2872 | L2873 | L2874 | L2875 | L2876 | L2877 | L2878 | L2879 | L2880 | E2881 | K2882 | L2883 | L2884 | L2885 | L2886 | E2887 | K2888 | A2889 | Q2890 | L2891 | L2892 | L2893 | L2894 | F2895 | L2896 | L2897 | L2898 | L2899 | L2900 | L2901 | A2902 | L2903 | S2904 | L2905 | L2906 | L2907 | L2908 | L2909 | L2910 | E2911 | L2912 | L2913 | L2914 | L2915 | L2916 | L2917 | L2918 | L2919 | L2920 | L2921 | L2922 | L2923 | S2924 |
| ARG   | ARG   | ILE   | ASP   | GLN   | THR   | THR   | GLN   | GLN   | VAL   | VAL   | ASP   | ALA   | HIS   | G2820 | Y2821 | S2822 | P2823 | R2824 | A2825 | L2826 | D2827 | M2828 | S2829 | N2830 | N2831 | T2832 | L2833 | S2834 | R2835 | R2836 | L2837 | H2838 | A2839 | M2840 | A2841 | E2842 | M2843 | M2844 | A2845 | E2846 | N2847 | Y2848 | H2849 | H2850 | T2851 | L2852 | A2853 | K2854 | K2855 | K2856 | K2857 | E2858 | L2859 | L2860 | E2861 | S2862 | K2863 | G2864 |       |
| I2742 | Y2743 | G2744 | E2745 | L2746 | Y2747 | S2748 | D2749 | S2750 | S2751 | K2752 | V2753 | Q2754 | P2755 | L2756 | M2757 | K2758 | P2759 | Y2760 | K2761 | L2762 | L2763 | S2764 | E2765 | K2766 | E2767 | K2768 | E2769 | L2770 | Y2771 | R2772 | W2773 | S2778 | L2779 | K2780 | L2781 | M2782 | L2783 | A2784 | G2785 | W2786 | W2787 | R2788 | L2789 | E2790 | L2791 | L2792 | K2793 | E2794 | D2795 | G2796 | S2797 | M2798 | A2799 | L2800 | Y2801 | W2802 | ARG   | THR   |       |
| P2678 | D2679 | Y2680 | E2681 | E2682 | S2683 | M2684 | Y2685 | L2686 | S2687 | M2688 | M2689 | E2690 | K2691 | Q2692 | S2693 | S2694 | M2695 | D2696 | S2697 | E2698 | G2699 | N2700 | F2701 | M2702 | T2703 | Q2704 | P2705 | T2706 | D2707 | L2708 | S2709 | M2710 | L2711 | T2712 | L2713 | P2714 | E2715 | K2716 | L2717 | E2718 | Y2719 | F2720 | L2721 | K2722 | K2723 | Y2724 | A2725 | E2726 | H2727 | S2728 | H2729 | D2730 | K2731 | W2732 | L2737 | A2738 | M2739 |       |       |
| Y2614 | E2615 | R2616 | K2619 | Y2620 | Y2621 | C2622 | L2623 | P2624 | G2625 | G2626 | W2627 | F2630 | S2634 | E2635 | E2636 | E2637 | H2638 | H2639 | S2641 | R2642 | K2643 | L2644 | F2645 | L2646 | G2647 | L2648 | F2649 | D2650 | A2651 | L2652 | Q2653 | K2654 | K2655 | R2656 | Y2657 | E2658 | Q2659 | L2660 | F2662 | K2663 | L2664 | A2665 | L2666 | P2667 | C2668 | L2669 | S2670 | A2671 | V2672 | G2674 | A2675 | L2676 | F2677 |       |       |       |       |       |       |
| L2525 | P2526 | T2529 | R2530 | L2534 | F2535 | A2536 | G2537 | H2540 | H2541 | A2542 | S2543 | L2544 | T2545 | L2548 | L2549 | Y2553 | L2554 | L2555 | S2556 | K2557 | Q2565 | R2566 | L2568 | F2569 | E2570 | L2580 | R2581 | P2582 | S2583 | M2584 | Q2585 | Q2586 | H2587 | L2588 | L2589 | R2590 | R2591 | L2592 | V2593 | F2594 | H2602 | A2603 | K2604 | M2605 | M2612 | P2606 | L2610 | T2611 | N2612 | H2613 |       |       |       |       |       |       |       |       |       |
| S2437 | L2438 | Q2441 | M2442 | P2443 | T2444 | L2445 | A2446 | K2447 | V2451 | V2452 | E2453 | M2456 | F2460 | C2461 | P2462 | K2465 | M2468 | Y2469 | L2470 | F2471 | R2474 | V2475 | Y2476 | D2482 | F2483 | L2484 | L2485 | H2486 | L2487 | L2488 | E2489 | V2490 | G2491 | F2492 | D2495 | A2500 | S2501 | L2502 | D2503 | T2504 | L2507 | S2508 | A2509 | T2510 | M2511 | M2512 | C2521 |       |       |       |       |       |       |       |       |       |       |       |       |
| D2360 | S2363 | P2364 | ASN   | GLY   | GLY   | SER   | SER   | THR   | LEU   | ASP   | THR   | GLU   | GLU   | E2377 | E2378 | D2379 | D2380 | H2383 | N2386 | M2389 | T2390 | F2391 | L2396 | R2401 | C2402 | A2403 | M2406 | H2407 | L2408 | L2409 | K2413 | G2414 | E2415 | A2416 | L2417 | R2418 | L2419 | R2420 | L2423 | R2424 | S2425 | L2426 | I2427 | D2431 | G2434 | V2435 | I2436 |       |       |       |       |       |       |       |       |       |       |       |       |
| A2233 | M2234 | D2241 | A2243 | A2244 | V2247 | M2248 | D2249 | N2250 | L2253 | R2258 | E2259 | P2260 | K2264 | V2265 | V2266 | A2270 | G2273 | G2278 | V2281 | V2290 | M2291 | P2292 | G2295 | E2296 | R2297 | F2301 | L2302 | R2303 | F2304 | F2307 | R2322 | R2326 | R2327 | G2332 | R2336 | G2337 | E2338 | L2353 | R2359 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| R2133 | M2134 | G2135 | E2138 | E2139 | K2140 | L2141 | M2142 | D2143 | R2144 | T2149 | M2150 | N2151 | N2152 | K2153 | V2154 | F2155 | Y2156 | Q2157 | L2165 | G2166 | N2167 | H2168 | M2172 | M2175 | V2176 | R2177 | V2178 | L2179 | G2180 | G2181 | G2182 | E2183 | S2184 | K2185 | E2186 | I2187 | M2192 | V2193 | Y2202 | F2203 | C2204 | R2205 | L2206 | M2214 | Y2220 | L2221 | L2222 | P2232 |       |       |       |       |       |       |       |       |       |       |       |
| LYS   | LYS   | GLN   | ALA   | GLU   | LYS   | PRO   | VAL   | GLU   | SER   | SER   | K2053 | K2054 | S2055 | S2056 | T2057 | L2058 | L2061 | L2062 | T2065 | R2068 | Q2071 | E2072 | L2080 | M2084 | P2085 | V2086 | L2087 | R2090 | Q2091 | T2095 | G2096 | R2100 | I2108 | V2113 | E2114 | D2115 | T2116 | L2117 | M2118 | L2119 | Q2125 | T2126 | R2127 | S2128 | L2129 | L2130 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| SER   | VAL   | ASP   | ALA   | LYS   | LEU   | GLN   | ALA   | GLY   | LYS   | ARG   | P1889 | K1890 | E1891 | L1894 | Q1895 | M1896 | M1906 | L1910 | Q1911 | D1931 | F1932 | Q1937 | H1938 | N1939 | Q1940 | R1941 | E1946 | V1947 | M1948 | Q1949 | A1950 | L1951 | M1952 | M1953 | S1954 | A1955 | A1956 | L1957 | T1958 | A1959 | R1960 | K1961 | T1962 | K1963 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Q3955 | Q3956 | M3957 | L3958 | L3968 | K3972 | L3973 | L3974 | Q3975 | K3976 | B3977 | K3978 | L3979 | K3980 | K3981 | K3985 | L3986 | K3989 | V4000 | L4001 | L4002 | L4003 | V4004 | E4005 | S4006 | E4011 | L4014 | Q3900 | Q3901 | V3912 | A3913 | K3914 | Q3915 | V3916 | L3920 | G3926 | P3927 | C3928 | T3929 | Q3932 | Q3933 | S3934 | L3935 | L3940 | V3944 | V3945 | G3946 | F3947 | M4052 | E4053 | S4054 |       |       |       |       |       |       |       |
| T3821 | E3822 | E3823 | G3824 | S3825 | G3826 | E3827 | K3828 | D3832 | F3835 | L3846 | M3851 | S3852 | D3853 | F3854 | Q3855 | Q3882 | E3883 | S3884 | W3890 | Y3891 | D3896 | E3900 | Q3901 | V3912 | A3913 | K3914 | Q3915 | V3916 | L3920 | G3926 | P3927 | C3928 | T3929 | Q3932 | Q3933 | S3934 | L3935 | L3940 | V3944 | V3945 | G3946 | F3947 | M3819 | V3820 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| E3678 | K3679 | L3687 | M3688 | M3689 | A3690 | Y3691 | M3695 | A3696 | C3699 | H3700 | F3701 | E3702 | GLU   | ASP   | ASP   | ASP   | GLY   | GLU   | E3710 | V3711 | K3712 | F3714 | K3717 | Q3722 | K3723 | Q3728 | A3729 | L3731 | H3732 | P3753 | I3765 | V3773 | K3776 | M3777 | L3803 | D3804 | L3805 | E3815 | G3816 | L3817 | G3818 | M3819 | V3820 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| ARG   | SER   | LYS   | ALA   | VAL   | TRP   | HIS   | LEU   | LEU   | SER   | LYS   | GLN   | LYS   | LEU   | LEU   | ASP   | ASP   | ASP   | GLY   | GLU   | E3710 | V3711 | K3712 | F3714 | K3717 | Q3722 | K3723 | Q3728 | A3729 | L3731 | H3732 | P3753 | I3765 | V3773 | K3776 | M3777 | L3803 | D3804 | L3805 | E3815 | G3816 | L3817 | G3818 | M3819 | V3820 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| ASP   | PRO   | ALA   | ILE   | TRP   | GLN   | MET   | ALA   | ALA   | LYS   | TRP   | LYS   | ASP   | LEU   | LEU   | PRO   | ASP   | THR   | ASP   | THR   | ASP   | GLY   | GLU   | ARG   | VAL   | LEU   | LEU   | VAL   | LEU   | LEU   | LEU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   |       |       |       |       |       |       |       |       |       |       |
| GLU   | VAL   | PHE   | ILE   | TYR   | TRP   | SER   | LYS   | GLU   | ASN   | PHE   | LYS   | ARG   | GLU   | LEU   | ARG   | ILE   | GLN   | ASN   | ILE   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   | VAL   |       |       |       |       |       |       |       |       |       |
| LYS   | ALA   | GLU   | ALA   | TRP   | GLY   | ASP   | MET   | SER   | ALA   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   | GLU   |       |       |       |       |       |       |       |       |       |       |
| K3279 | I3280 | K3281 | K3282 | I3283 | I3284 | Y3285 | K3286 | K3287 | K3288 | G3289 | I3290 | D3291 | E3292 | G3293 | A3294 | K3295 | K3296 | K3297 | K3298 | F3302 | S3303 | Q3304 | P3305 | T3306 | T3307 | T3308 | K3309 | V3310 | K3311 | Q3312 | Q3313 | L3314 | L3315 | K3316 | T3317 | H3318 | F3319 | L3320 | P3321 | L3322 | K3323 | E3324 | L3326 | K3327 | K3328 | A3329 | A3330 | A3331 | T3332 | V3333 | V3334 | S3335 | K3336 | E3337 | ASP   | HIS   | LEU   |
| L3214 | M3215 | E3216 | E3217 | I3218 | V3219 | E3220 | I3226 | K3227 | L3228 | T3229 | Q3230 | M3231 | P3232 | K3233 | V3234 | M3235 | E3236 | V3237 | I3238 | L3239 | P3240 | K3241 | S3242 | C3243 | S3244 | Y3245 | K3246 | W3249 | K3250 | E3251 | H3252 | G3253 | P3254 | E3255 | N3256 | K3257 | P3258 | E3259 | K3260 | A3261 | E3262 | M3263 | C3264 | C3265 | T3266 | A3267 | L3268 | N3269 | S3270 | E3271 | H3272 | M3273 | K3274 | L3275 | L3276 | L3277 | G3278 |
| L3140 | K3141 | S3145 | S3146 | I3147 | Y3147 | E3148 | E3149 | R3150 | Q3151 | F3162 | A3163 | G3164 | A3165 | F3166 | P3167 | V3168 | A3169 | F3170 | L3171 | E3172 | T3173 | H3174 | L3175 | D3176 | K3177 | H3178 | N3179 | I3180 | Y3181 | Y3184 | N3185 | T3186 | K3187 | S3188 | E3191 | R3192 | A3193 | A3194 | L3195 | S3196 | L3197 | P3198 | T3199 | N3200 | V3201 | E3202 | D3203 | L3204 | T3205 | T3206 | P3207 | S3208 | S3209 | L3210 | L3211 | E3212 | K3213 |
| K3076 | Q3077 | G3078 | Q3079 | F3080 | F3081 | HIS   | THR   | ARG   | ASN   | GLN   | PRO   | K3088 | G3089 | V3090 | T3091 | Q3092 | Y3096 | T3097 | T3098 | V3099 | A3100 | L3101 | L3102 | P3103 | M3104 | L3105 | S3106 | L3107 | L3108 | F3109 | E3110 | H3111 | Q3114 | F3117 | G3118 | E3119 | D3120 | L3121 | I3122 | L3123 | E3124 | D3125 | V3126 | Q3127 | V3128 | S3129 | C3130 | Y3131 | R3132 | T3133 | L3134 | T3135 | S3136 | L3137 | Y3138 | A3139 |       |
| E3000 | K3001 | E3002 | M3003 | L3007 | F3008 | C3009 | K3010 | L3011 | L3014 | V3015 | R3016 | H3017 | R3018 | L3019 | S3020 | L3021 | F3022 | G3023 | D3025 | A3026 | I3029 | V3030 | H3034 | I3035 | V2966 | G3037 | Q3038 | T3039 | L3040 | D3041 | A3042 | R3043 | V3045 | M3046 | K3047 | T3048 | G3049 | L3050 | V3053 | R3058 | A3059 | F3060 | A3064 | A3065 | L3068 | E3069 | M3072 | A2996 | K2999 |       |       |       |       |       |       |       |       |
| F2925 | L2926 | L2929 | I2930 | A2936 | Y2939 | G2945 | G2946 | S2947 | R2948 | G2949 | K2950 | G2951 | E2952 | H2953 | F2954 | E2957 | I2960 | K2961 | F2962 | K2965 | V2966 | V2967 | L2968 | P2969 | L2970 | I2971 | D2972 | Q2973 | Y2974 | F2975 | K2976 | V2977 | H2978 | R2979 | L2980 | V2981 | F2982 | L2983 | S2984 | A2985 | A2986 | S2987 | R2988 | P2989 | L2990 | C2991 | S2992 | G2993 | A2996 | K2999 |       |       |       |       |       |       |       |



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

Chain E: 80% 19%

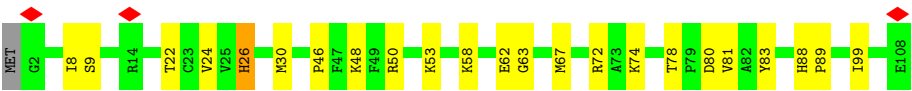
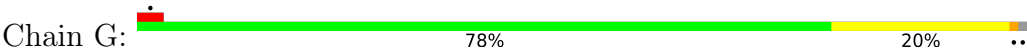


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

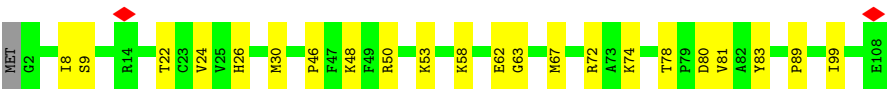
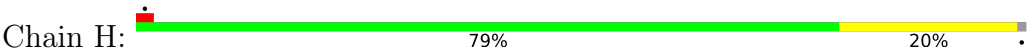
Chain F: 79% 20%



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



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



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C4                               | Depositor |
| Number of particles used             | 19753                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 58                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.474                                   | Depositor |
| Minimum map value                    | -0.018                                  | Depositor |
| Average map value                    | 0.010                                   | Depositor |
| Map value standard deviation         | 0.024                                   | Depositor |
| Recommended contour level            | 0.12                                    | Depositor |
| Map size (Å)                         | 424.96, 424.96, 424.96                  | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.83, 0.83, 0.83                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.17         | 0/34511     | 0.44        | 5/46614 (0.0%)   |
| 1   | B     | 0.17         | 0/34511     | 0.44        | 5/46614 (0.0%)   |
| 1   | C     | 0.17         | 0/34511     | 0.44        | 5/46614 (0.0%)   |
| 1   | D     | 0.17         | 0/34511     | 0.44        | 5/46614 (0.0%)   |
| 2   | E     | 0.16         | 0/834       | 0.38        | 0/1123           |
| 2   | F     | 0.16         | 0/834       | 0.38        | 0/1123           |
| 2   | G     | 0.16         | 0/834       | 0.38        | 0/1123           |
| 2   | H     | 0.16         | 0/834       | 0.38        | 0/1123           |
| All | All   | 0.17         | 0/141380    | 0.44        | 20/190948 (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                   | 3                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 3                   |
| 1   | D     | 0                   | 3                   |
| All | All   | 0                   | 12                  |

There are no bond length outliers.

All (20) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1   | B     | 4292 | MET  | CB-CG-SD | 7.48 | 135.13      | 112.70   |
| 1   | C     | 4292 | MET  | CB-CG-SD | 7.47 | 135.12      | 112.70   |
| 1   | D     | 4292 | MET  | CB-CG-SD | 7.47 | 135.10      | 112.70   |
| 1   | A     | 4292 | MET  | CB-CG-SD | 7.45 | 135.05      | 112.70   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | D     | 2512 | MET  | CB-CG-SD | 5.48  | 129.15      | 112.70   |
| 1   | B     | 2512 | MET  | CB-CG-SD | 5.48  | 129.15      | 112.70   |
| 1   | C     | 2512 | MET  | CB-CG-SD | 5.48  | 129.13      | 112.70   |
| 1   | A     | 2512 | MET  | CB-CG-SD | 5.47  | 129.12      | 112.70   |
| 1   | D     | 1836 | ASN  | CB-CA-C  | -5.31 | 110.01      | 117.23   |
| 1   | B     | 1836 | ASN  | CB-CA-C  | -5.30 | 110.02      | 117.23   |
| 1   | C     | 1836 | ASN  | CB-CA-C  | -5.30 | 110.02      | 117.23   |
| 1   | A     | 1836 | ASN  | CB-CA-C  | -5.30 | 110.03      | 117.23   |
| 1   | C     | 4503 | ARG  | CA-C-N   | -5.16 | 113.03      | 122.38   |
| 1   | C     | 4503 | ARG  | C-N-CA   | -5.16 | 113.03      | 122.38   |
| 1   | D     | 4503 | ARG  | CA-C-N   | -5.16 | 113.03      | 122.38   |
| 1   | D     | 4503 | ARG  | C-N-CA   | -5.16 | 113.03      | 122.38   |
| 1   | A     | 4503 | ARG  | CA-C-N   | -5.15 | 113.05      | 122.38   |
| 1   | A     | 4503 | ARG  | C-N-CA   | -5.15 | 113.05      | 122.38   |
| 1   | B     | 4503 | ARG  | CA-C-N   | -5.13 | 113.09      | 122.38   |
| 1   | B     | 4503 | ARG  | C-N-CA   | -5.13 | 113.09      | 122.38   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 2988 | ARG  | Peptide |
| 1   | A     | 4504 | MET  | Peptide |
| 1   | A     | 4640 | PHE  | Peptide |
| 1   | B     | 2988 | ARG  | Peptide |
| 1   | B     | 4504 | MET  | Peptide |
| 1   | B     | 4640 | PHE  | Peptide |
| 1   | C     | 2988 | ARG  | Peptide |
| 1   | C     | 4504 | MET  | Peptide |
| 1   | C     | 4640 | PHE  | Peptide |
| 1   | D     | 2988 | ARG  | Peptide |
| 1   | D     | 4504 | MET  | Peptide |
| 1   | D     | 4640 | PHE  | Peptide |

## 5.2 Too-close contacts ⓘ

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     | 33771  | 0        | 33455    | 1064    | 0            |
| 1   | B     | 33771  | 0        | 33455    | 1059    | 0            |
| 1   | C     | 33771  | 0        | 33455    | 1046    | 0            |
| 1   | D     | 33771  | 0        | 33455    | 1046    | 0            |
| 2   | E     | 818    | 0        | 821      | 19      | 0            |
| 2   | F     | 818    | 0        | 821      | 19      | 0            |
| 2   | G     | 818    | 0        | 821      | 20      | 0            |
| 2   | H     | 818    | 0        | 821      | 21      | 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     | 62     | 0        | 24       | 4       | 0            |
| 4   | B     | 62     | 0        | 24       | 4       | 0            |
| 4   | C     | 62     | 0        | 24       | 4       | 0            |
| 4   | D     | 62     | 0        | 24       | 4       | 0            |
| All | All   | 138608 | 0        | 137200   | 4220    | 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 15.

All (4220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1611:ILE:HD11 | 1:B:1618:LEU:HB2  | 1.49                     | 0.93              |
| 1:D:1611:ILE:HD11 | 1:D:1618:LEU:HB2  | 1.49                     | 0.92              |
| 1:A:1611:ILE:HD11 | 1:A:1618:LEU:HB2  | 1.49                     | 0.91              |
| 1:C:1611:ILE:HD11 | 1:C:1618:LEU:HB2  | 1.49                     | 0.90              |
| 1:B:2905:ARG:HE   | 1:B:2906:GLY:H    | 1.22                     | 0.88              |
| 1:A:2905:ARG:HE   | 1:A:2906:GLY:H    | 1.22                     | 0.88              |
| 1:C:2905:ARG:HE   | 1:C:2906:GLY:H    | 1.22                     | 0.88              |
| 1:D:2905:ARG:HE   | 1:D:2906:GLY:H    | 1.22                     | 0.87              |
| 2:E:50:ARG:HE     | 2:E:53:LYS:HG3    | 1.38                     | 0.87              |
| 2:H:50:ARG:HE     | 2:H:53:LYS:HG3    | 1.38                     | 0.87              |
| 2:G:50:ARG:HE     | 2:G:53:LYS:HG3    | 1.38                     | 0.87              |
| 1:D:317:MET:SD    | 1:D:321:LYS:NZ    | 2.49                     | 0.86              |
| 2:F:50:ARG:HE     | 2:F:53:LYS:HG3    | 1.38                     | 0.85              |
| 1:C:317:MET:SD    | 1:C:321:LYS:NZ    | 2.49                     | 0.85              |
| 1:A:317:MET:SD    | 1:A:321:LYS:NZ    | 2.49                     | 0.85              |
| 1:C:4834:PRO:HB3  | 1:C:4843:ARG:HD3  | 1.59                     | 0.85              |
| 1:B:317:MET:SD    | 1:B:321:LYS:NZ    | 2.49                     | 0.85              |
| 1:D:2585:MET:HE3  | 1:D:2616:ARG:HH22 | 1.41                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4834:PRO:HB3  | 1:A:4843:ARG:HD3  | 1.58                     | 0.85              |
| 1:B:2585:MET:HE3  | 1:B:2616:ARG:HH22 | 1.41                     | 0.84              |
| 1:B:4834:PRO:HB3  | 1:B:4843:ARG:HD3  | 1.58                     | 0.84              |
| 1:A:2585:MET:HE3  | 1:A:2616:ARG:HH22 | 1.41                     | 0.83              |
| 1:D:4834:PRO:HB3  | 1:D:4843:ARG:HD3  | 1.58                     | 0.83              |
| 1:C:290:ARG:NH1   | 1:C:351:THR:O     | 2.12                     | 0.83              |
| 1:B:290:ARG:NH1   | 1:B:351:THR:O     | 2.12                     | 0.83              |
| 1:C:3065:ALA:HB1  | 1:C:3132:ARG:HH12 | 1.43                     | 0.83              |
| 1:A:1689:ILE:HA   | 1:A:1703:TYR:HE1  | 1.43                     | 0.83              |
| 1:D:3065:ALA:HB1  | 1:D:3132:ARG:HH12 | 1.44                     | 0.83              |
| 1:C:2585:MET:HE3  | 1:C:2616:ARG:HH22 | 1.41                     | 0.83              |
| 1:A:290:ARG:NH1   | 1:A:351:THR:O     | 2.12                     | 0.82              |
| 1:D:1689:ILE:HA   | 1:D:1703:TYR:HE1  | 1.43                     | 0.82              |
| 1:C:1689:ILE:HA   | 1:C:1703:TYR:HE1  | 1.43                     | 0.82              |
| 1:B:1689:ILE:HA   | 1:B:1703:TYR:HE1  | 1.43                     | 0.81              |
| 1:D:290:ARG:NH1   | 1:D:351:THR:O     | 2.12                     | 0.81              |
| 1:A:3065:ALA:HB1  | 1:A:3132:ARG:HH12 | 1.44                     | 0.81              |
| 1:B:3065:ALA:HB1  | 1:B:3132:ARG:HH12 | 1.43                     | 0.80              |
| 1:C:2826:ILE:HD12 | 1:D:1501:ASN:HB2  | 1.65                     | 0.79              |
| 1:C:2139:GLU:HG3  | 1:C:2192:MET:HB2  | 1.63                     | 0.79              |
| 1:D:2139:GLU:HG3  | 1:D:2192:MET:HB2  | 1.63                     | 0.79              |
| 1:A:2139:GLU:HG3  | 1:A:2192:MET:HB2  | 1.63                     | 0.78              |
| 1:C:2682:GLU:HB3  | 1:C:2919:LYS:HB3  | 1.65                     | 0.78              |
| 1:D:3945:VAL:HG23 | 1:D:4006:SER:HB3  | 1.65                     | 0.78              |
| 1:B:2139:GLU:HG3  | 1:B:2192:MET:HB2  | 1.63                     | 0.78              |
| 1:A:3945:VAL:HG23 | 1:A:4006:SER:HB3  | 1.65                     | 0.78              |
| 1:C:3945:VAL:HG23 | 1:C:4006:SER:HB3  | 1.65                     | 0.78              |
| 1:C:466:PRO:HG2   | 1:C:479:LEU:HD12  | 1.66                     | 0.78              |
| 1:B:949:HIS:HB3   | 1:B:1065:GLU:HB2  | 1.66                     | 0.77              |
| 1:B:2826:ILE:HD12 | 1:C:1501:ASN:HB2  | 1.66                     | 0.77              |
| 1:D:949:HIS:HB3   | 1:D:1065:GLU:HB2  | 1.66                     | 0.77              |
| 1:A:905:GLY:HA3   | 1:A:914:GLN:HB3   | 1.67                     | 0.77              |
| 1:B:2682:GLU:HB3  | 1:B:2919:LYS:HB3  | 1.66                     | 0.77              |
| 1:D:905:GLY:HA3   | 1:D:914:GLN:HB3   | 1.67                     | 0.77              |
| 1:B:3945:VAL:HG23 | 1:B:4006:SER:HB3  | 1.65                     | 0.77              |
| 1:C:949:HIS:HB3   | 1:C:1065:GLU:HB2  | 1.66                     | 0.77              |
| 1:A:4584:PHE:HA   | 1:A:4726:MET:HE1  | 1.67                     | 0.77              |
| 1:D:4584:PHE:HA   | 1:D:4726:MET:HE1  | 1.67                     | 0.77              |
| 1:A:2830:ASN:ND2  | 1:B:1551:ASN:O    | 2.17                     | 0.76              |
| 1:D:2682:GLU:HB3  | 1:D:2919:LYS:HB3  | 1.66                     | 0.76              |
| 1:A:949:HIS:HB3   | 1:A:1065:GLU:HB2  | 1.66                     | 0.76              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:2657:TYR:HA   | 1:D:2662:PHE:HE2 | 1.51                     | 0.76              |
| 1:B:905:GLY:HA3   | 1:B:914:GLN:HB3  | 1.67                     | 0.76              |
| 1:C:905:GLY:HA3   | 1:C:914:GLN:HB3  | 1.67                     | 0.76              |
| 1:C:2657:TYR:HA   | 1:C:2662:PHE:HE2 | 1.51                     | 0.76              |
| 1:A:466:PRO:HG2   | 1:A:479:LEU:HD12 | 1.66                     | 0.76              |
| 1:C:2545:ILE:HD11 | 1:C:2584:MET:HG2 | 1.68                     | 0.76              |
| 1:D:466:PRO:HG2   | 1:D:479:LEU:HD12 | 1.66                     | 0.75              |
| 1:A:2657:TYR:HA   | 1:A:2662:PHE:HE2 | 1.51                     | 0.75              |
| 1:A:2682:GLU:HB3  | 1:A:2919:LYS:HB3 | 1.66                     | 0.75              |
| 1:B:4584:PHE:HA   | 1:B:4726:MET:HE1 | 1.67                     | 0.75              |
| 1:A:2465:LYS:NZ   | 1:A:2495:ASP:OD2 | 2.20                     | 0.75              |
| 1:B:466:PRO:HG2   | 1:B:479:LEU:HD12 | 1.66                     | 0.75              |
| 1:C:988:LEU:HB2   | 1:C:1055:ARG:HE  | 1.52                     | 0.75              |
| 1:D:988:LEU:HB2   | 1:D:1055:ARG:HE  | 1.52                     | 0.75              |
| 1:B:2545:ILE:HD11 | 1:B:2584:MET:HG2 | 1.68                     | 0.74              |
| 1:B:2670:SER:HB2  | 1:B:2973:GLN:HG2 | 1.69                     | 0.74              |
| 1:C:4584:PHE:HA   | 1:C:4726:MET:HE1 | 1.67                     | 0.74              |
| 1:D:2545:ILE:HD11 | 1:D:2584:MET:HG2 | 1.68                     | 0.74              |
| 1:A:2545:ILE:HD11 | 1:A:2584:MET:HG2 | 1.68                     | 0.74              |
| 1:C:2670:SER:HB2  | 1:C:2973:GLN:HG2 | 1.69                     | 0.74              |
| 1:D:584:GLU:HA    | 1:D:587:ASN:HD22 | 1.53                     | 0.74              |
| 1:B:584:GLU:HA    | 1:B:587:ASN:HD22 | 1.52                     | 0.74              |
| 1:B:988:LEU:HB2   | 1:B:1055:ARG:HE  | 1.52                     | 0.74              |
| 1:C:584:GLU:HA    | 1:C:587:ASN:HD22 | 1.52                     | 0.74              |
| 1:B:930:ASN:O     | 1:B:934:GLN:NE2  | 2.21                     | 0.74              |
| 1:A:930:ASN:O     | 1:A:934:GLN:NE2  | 2.21                     | 0.74              |
| 1:A:584:GLU:HA    | 1:A:587:ASN:HD22 | 1.52                     | 0.73              |
| 1:D:930:ASN:O     | 1:D:934:GLN:NE2  | 2.21                     | 0.73              |
| 1:A:2670:SER:HB2  | 1:A:2973:GLN:HG2 | 1.69                     | 0.73              |
| 1:B:11:ILE:HD12   | 1:B:176:ARG:HG2  | 1.70                     | 0.73              |
| 1:A:988:LEU:HB2   | 1:A:1055:ARG:HE  | 1.52                     | 0.73              |
| 1:B:2657:TYR:HA   | 1:B:2662:PHE:HE2 | 1.51                     | 0.73              |
| 1:C:3674:THR:O    | 1:C:3679:LYS:NZ  | 2.22                     | 0.73              |
| 1:B:3890:TRP:HB3  | 1:C:76:ARG:HD2   | 1.69                     | 0.73              |
| 1:D:2670:SER:HB2  | 1:D:2973:GLN:HG2 | 1.69                     | 0.73              |
| 1:B:2745:GLU:HA   | 1:B:2755:PRO:HB3 | 1.71                     | 0.73              |
| 1:A:2791:ARG:NH1  | 1:A:2901:TYR:OH  | 2.22                     | 0.73              |
| 1:B:2791:ARG:NH1  | 1:B:2901:TYR:OH  | 2.22                     | 0.73              |
| 1:B:4690:LYS:HG3  | 1:B:4692:SER:H   | 1.54                     | 0.73              |
| 1:C:11:ILE:HD12   | 1:C:176:ARG:HG2  | 1.70                     | 0.73              |
| 1:C:2745:GLU:HA   | 1:C:2755:PRO:HB3 | 1.71                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2975:PHE:O    | 1:A:2979:ARG:HB3  | 1.89                     | 0.73              |
| 1:C:2465:LYS:NZ   | 1:C:2495:ASP:OD2  | 2.20                     | 0.73              |
| 1:D:2745:GLU:HA   | 1:D:2755:PRO:HB3  | 1.71                     | 0.73              |
| 1:A:2745:GLU:HA   | 1:A:2755:PRO:HB3  | 1.71                     | 0.72              |
| 1:B:2689:MET:HE2  | 1:B:2785:TRP:HB3  | 1.71                     | 0.72              |
| 1:C:930:ASN:O     | 1:C:934:GLN:NE2   | 2.21                     | 0.72              |
| 1:D:2465:LYS:NZ   | 1:D:2495:ASP:OD2  | 2.20                     | 0.72              |
| 1:B:2975:PHE:O    | 1:B:2979:ARG:HB3  | 1.89                     | 0.72              |
| 1:C:2241:ASP:OD1  | 1:C:2297:ARG:NH2  | 2.22                     | 0.72              |
| 1:A:11:ILE:HD12   | 1:A:176:ARG:HG2   | 1.70                     | 0.72              |
| 1:B:552:SER:HA    | 1:B:555:LEU:HD23  | 1.72                     | 0.72              |
| 1:D:2241:ASP:OD1  | 1:D:2297:ARG:NH2  | 2.22                     | 0.72              |
| 1:A:2689:MET:HE2  | 1:A:2785:TRP:HB3  | 1.71                     | 0.72              |
| 1:C:2590:ARG:NH2  | 1:C:2875:ASP:OD2  | 2.23                     | 0.72              |
| 1:D:2791:ARG:NH1  | 1:D:2901:TYR:OH   | 2.22                     | 0.72              |
| 1:B:2465:LYS:NZ   | 1:B:2495:ASP:OD2  | 2.20                     | 0.72              |
| 1:C:879:GLU:OE1   | 1:C:880:ARG:NH2   | 2.23                     | 0.72              |
| 1:C:2791:ARG:NH1  | 1:C:2901:TYR:OH   | 2.22                     | 0.72              |
| 1:D:2975:PHE:O    | 1:D:2979:ARG:HB3  | 1.89                     | 0.72              |
| 1:A:3674:THR:O    | 1:A:3679:LYS:NZ   | 2.22                     | 0.72              |
| 1:B:2590:ARG:NH2  | 1:B:2875:ASP:OD2  | 2.23                     | 0.72              |
| 1:C:552:SER:HA    | 1:C:555:LEU:HD23  | 1.72                     | 0.72              |
| 1:C:3890:TRP:HB3  | 1:D:76:ARG:HD2    | 1.71                     | 0.72              |
| 1:D:552:SER:HA    | 1:D:555:LEU:HD23  | 1.72                     | 0.72              |
| 1:A:1501:ASN:HB2  | 1:D:2826:ILE:HD12 | 1.72                     | 0.72              |
| 1:B:879:GLU:OE1   | 1:B:880:ARG:NH2   | 2.23                     | 0.72              |
| 1:C:4690:LYS:HG3  | 1:C:4692:SER:H    | 1.54                     | 0.72              |
| 1:D:353:GLU:HG3   | 1:D:354:ILE:HD12  | 1.71                     | 0.72              |
| 1:A:2590:ARG:NH2  | 1:A:2875:ASP:OD2  | 2.23                     | 0.72              |
| 1:A:4690:LYS:HG3  | 1:A:4692:SER:H    | 1.54                     | 0.72              |
| 1:D:2581:ARG:HD2  | 1:D:2582:PRO:HD2  | 1.72                     | 0.72              |
| 1:D:3674:THR:O    | 1:D:3679:LYS:NZ   | 2.22                     | 0.72              |
| 1:A:552:SER:HA    | 1:A:555:LEU:HD23  | 1.72                     | 0.72              |
| 1:A:3016:ARG:HH22 | 1:A:3101:LEU:HD22 | 1.55                     | 0.72              |
| 1:D:11:ILE:HD12   | 1:D:176:ARG:HG2   | 1.70                     | 0.72              |
| 1:A:881:ILE:O     | 1:A:884:LYS:NZ    | 2.22                     | 0.71              |
| 1:B:3674:THR:O    | 1:B:3679:LYS:NZ   | 2.22                     | 0.71              |
| 1:D:4690:LYS:HG3  | 1:D:4692:SER:H    | 1.54                     | 0.71              |
| 1:A:2581:ARG:HD2  | 1:A:2582:PRO:HD2  | 1.72                     | 0.71              |
| 1:D:876:PRO:HA    | 1:D:880:ARG:HB2   | 1.72                     | 0.71              |
| 1:A:2326:ARG:NH2  | 1:B:189:GLU:O     | 2.24                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:353:GLU:HG3   | 1:B:354:ILE:HD12  | 1.71                     | 0.71              |
| 1:B:876:PRO:HA    | 1:B:880:ARG:HB2   | 1.73                     | 0.71              |
| 1:B:881:ILE:O     | 1:B:884:LYS:NZ    | 2.22                     | 0.71              |
| 1:B:2178:VAL:HG21 | 1:B:2192:MET:HE1  | 1.73                     | 0.71              |
| 1:A:2241:ASP:OD1  | 1:A:2297:ARG:NH2  | 2.22                     | 0.71              |
| 1:B:2241:ASP:OD1  | 1:B:2297:ARG:NH2  | 2.22                     | 0.71              |
| 1:B:3016:ARG:HH22 | 1:B:3101:LEU:HD22 | 1.55                     | 0.71              |
| 1:C:2975:PHE:O    | 1:C:2979:ARG:HB3  | 1.89                     | 0.71              |
| 1:D:881:ILE:O     | 1:D:884:LYS:NZ    | 2.22                     | 0.71              |
| 1:A:879:GLU:OE1   | 1:A:880:ARG:NH2   | 2.23                     | 0.71              |
| 1:A:4819:VAL:HG12 | 1:A:4830:GLU:HG3  | 1.73                     | 0.71              |
| 1:B:887:GLU:HA    | 1:B:890:HIS:HD1   | 1.55                     | 0.71              |
| 1:C:353:GLU:HG3   | 1:C:354:ILE:HD12  | 1.71                     | 0.71              |
| 1:D:2590:ARG:NH2  | 1:D:2875:ASP:OD2  | 2.23                     | 0.71              |
| 1:C:876:PRO:HA    | 1:C:880:ARG:HB2   | 1.72                     | 0.71              |
| 1:C:881:ILE:O     | 1:C:884:LYS:NZ    | 2.22                     | 0.71              |
| 1:C:2178:VAL:HG21 | 1:C:2192:MET:HE1  | 1.73                     | 0.71              |
| 1:C:2581:ARG:HD2  | 1:C:2582:PRO:HD2  | 1.72                     | 0.71              |
| 1:A:876:PRO:HA    | 1:A:880:ARG:HB2   | 1.72                     | 0.71              |
| 1:B:4819:VAL:HG12 | 1:B:4830:GLU:HG3  | 1.73                     | 0.71              |
| 1:D:879:GLU:OE1   | 1:D:880:ARG:NH2   | 2.23                     | 0.71              |
| 1:A:235:ARG:NH2   | 1:A:412:GLU:OE2   | 2.24                     | 0.71              |
| 1:D:2178:VAL:HG21 | 1:D:2192:MET:HE1  | 1.73                     | 0.71              |
| 1:D:3016:ARG:HH22 | 1:D:3101:LEU:HD22 | 1.55                     | 0.71              |
| 2:G:89:PRO:HB2    | 1:C:1671:ARG:HH21 | 1.56                     | 0.70              |
| 1:C:235:ARG:NH2   | 1:C:412:GLU:OE2   | 2.24                     | 0.70              |
| 1:C:887:GLU:HA    | 1:C:890:HIS:HD1   | 1.55                     | 0.70              |
| 1:D:887:GLU:HA    | 1:D:890:HIS:HD1   | 1.55                     | 0.70              |
| 1:D:2689:MET:HE2  | 1:D:2785:TRP:HB3  | 1.71                     | 0.70              |
| 1:A:353:GLU:HG3   | 1:A:354:ILE:HD12  | 1.71                     | 0.70              |
| 1:A:2266:VAL:HG12 | 1:A:2327:ARG:HD2  | 1.73                     | 0.70              |
| 2:F:89:PRO:HB2    | 1:B:1671:ARG:HH21 | 1.56                     | 0.70              |
| 1:B:3043:ARG:HE   | 1:B:3117:PHE:HA   | 1.56                     | 0.70              |
| 1:A:3043:ARG:HE   | 1:A:3117:PHE:HA   | 1.56                     | 0.70              |
| 1:C:4819:VAL:HG12 | 1:C:4830:GLU:HG3  | 1.73                     | 0.70              |
| 1:A:887:GLU:HA    | 1:A:890:HIS:HD1   | 1.55                     | 0.70              |
| 1:A:2178:VAL:HG21 | 1:A:2192:MET:HE1  | 1.73                     | 0.70              |
| 1:B:2581:ARG:HD2  | 1:B:2582:PRO:HD2  | 1.72                     | 0.70              |
| 1:C:2689:MET:HE2  | 1:C:2785:TRP:HB3  | 1.71                     | 0.70              |
| 1:C:3214:LEU:HD21 | 1:C:3242:LEU:HD21 | 1.74                     | 0.70              |
| 1:A:337:LYS:NZ    | 1:A:369:GLY:O     | 2.25                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:842:GLN:HB2   | 1:B:1603:PHE:HB2  | 1.74                     | 0.70              |
| 1:C:2266:VAL:HG12 | 1:C:2327:ARG:HD2  | 1.73                     | 0.70              |
| 1:D:235:ARG:NH2   | 1:D:412:GLU:OE2   | 2.24                     | 0.70              |
| 1:D:337:LYS:NZ    | 1:D:369:GLY:O     | 2.25                     | 0.70              |
| 1:C:903:GLN:HB2   | 1:C:913:ARG:HG3   | 1.74                     | 0.69              |
| 1:D:3043:ARG:HE   | 1:D:3117:PHE:HA   | 1.56                     | 0.69              |
| 1:D:4819:VAL:HG12 | 1:D:4830:GLU:HG3  | 1.73                     | 0.69              |
| 1:C:799:LYS:NZ    | 1:C:1620:GLN:OE1  | 2.26                     | 0.69              |
| 1:C:3016:ARG:HH22 | 1:C:3101:LEU:HD22 | 1.55                     | 0.69              |
| 1:C:4279:MET:HE2  | 1:D:4484:ILE:HG22 | 1.73                     | 0.69              |
| 1:B:235:ARG:NH2   | 1:B:412:GLU:OE2   | 2.24                     | 0.69              |
| 1:D:3607:PRO:HG2  | 1:D:3610:ASN:HB2  | 1.74                     | 0.69              |
| 1:A:842:GLN:HB2   | 1:A:1603:PHE:HB2  | 1.74                     | 0.69              |
| 1:A:2886:ARG:O    | 1:A:2890:GLN:NE2  | 2.25                     | 0.69              |
| 1:B:1498:GLN:NE2  | 1:B:1499:GLY:O    | 2.26                     | 0.69              |
| 1:C:1498:GLN:NE2  | 1:C:1499:GLY:O    | 2.26                     | 0.69              |
| 1:D:2072:GLU:O    | 1:D:3660:ARG:NH1  | 2.26                     | 0.69              |
| 1:D:2886:ARG:O    | 1:D:2890:GLN:NE2  | 2.25                     | 0.69              |
| 1:B:3109:PHE:HD1  | 1:B:3162:PHE:HA   | 1.57                     | 0.69              |
| 1:C:337:LYS:NZ    | 1:C:369:GLY:O     | 2.25                     | 0.69              |
| 1:C:3109:PHE:HD1  | 1:C:3162:PHE:HA   | 1.57                     | 0.69              |
| 1:D:2266:VAL:HG12 | 1:D:2327:ARG:HD2  | 1.73                     | 0.69              |
| 1:B:3607:PRO:HG2  | 1:B:3610:ASN:HB2  | 1.74                     | 0.69              |
| 1:D:387:ILE:HD12  | 1:D:389:ARG:HG3   | 1.74                     | 0.69              |
| 1:D:3109:PHE:HD1  | 1:D:3162:PHE:HA   | 1.57                     | 0.69              |
| 1:A:903:GLN:HB2   | 1:A:913:ARG:HG3   | 1.74                     | 0.69              |
| 1:B:2326:ARG:NH2  | 1:C:189:GLU:O     | 2.24                     | 0.69              |
| 1:C:2764:SER:OG   | 1:C:2767:GLU:OE1  | 2.10                     | 0.69              |
| 1:A:387:ILE:HD12  | 1:A:389:ARG:HG3   | 1.74                     | 0.69              |
| 1:B:337:LYS:NZ    | 1:B:369:GLY:O     | 2.25                     | 0.69              |
| 1:B:903:GLN:HB2   | 1:B:913:ARG:HG3   | 1.74                     | 0.69              |
| 1:B:2764:SER:OG   | 1:B:2767:GLU:OE1  | 2.10                     | 0.69              |
| 1:C:2886:ARG:O    | 1:C:2890:GLN:NE2  | 2.25                     | 0.69              |
| 1:D:890:HIS:HA    | 1:D:893:TRP:HE3   | 1.58                     | 0.69              |
| 1:D:3214:LEU:HD21 | 1:D:3242:LEU:HD21 | 1.74                     | 0.69              |
| 1:B:799:LYS:NZ    | 1:B:1620:GLN:OE1  | 2.26                     | 0.69              |
| 1:B:2266:VAL:HG12 | 1:B:2327:ARG:HD2  | 1.73                     | 0.69              |
| 1:B:2886:ARG:O    | 1:B:2890:GLN:NE2  | 2.25                     | 0.69              |
| 1:D:799:LYS:NZ    | 1:D:1620:GLN:OE1  | 2.26                     | 0.69              |
| 1:D:842:GLN:HB2   | 1:D:1603:PHE:HB2  | 1.74                     | 0.69              |
| 1:D:1498:GLN:NE2  | 1:D:1499:GLY:O    | 2.26                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:890:HIS:HA    | 1:A:893:TRP:HE3   | 1.58                     | 0.69              |
| 1:A:2764:SER:OG   | 1:A:2767:GLU:OE1  | 2.10                     | 0.69              |
| 1:A:3214:LEU:HD21 | 1:A:3242:LEU:HD21 | 1.74                     | 0.69              |
| 1:D:2764:SER:OG   | 1:D:2767:GLU:OE1  | 2.10                     | 0.69              |
| 1:D:3696:ALA:O    | 1:D:3700:HIS:ND1  | 2.26                     | 0.69              |
| 1:A:799:LYS:NZ    | 1:A:1620:GLN:OE1  | 2.26                     | 0.68              |
| 1:A:1498:GLN:NE2  | 1:A:1499:GLY:O    | 2.26                     | 0.68              |
| 1:A:2072:GLU:O    | 1:A:3660:ARG:NH1  | 2.25                     | 0.68              |
| 1:B:2072:GLU:O    | 1:B:3660:ARG:NH1  | 2.26                     | 0.68              |
| 1:D:2456:MET:HE2  | 1:D:2462:PRO:HD3  | 1.75                     | 0.68              |
| 1:C:2326:ARG:NH2  | 1:D:189:GLU:O     | 2.26                     | 0.68              |
| 1:B:3214:LEU:HD21 | 1:B:3242:LEU:HD21 | 1.74                     | 0.68              |
| 1:C:2072:GLU:O    | 1:C:3660:ARG:NH1  | 2.25                     | 0.68              |
| 1:C:3043:ARG:HE   | 1:C:3117:PHE:HA   | 1.56                     | 0.68              |
| 1:D:903:GLN:HB2   | 1:D:913:ARG:HG3   | 1.74                     | 0.68              |
| 1:B:387:ILE:HD12  | 1:B:389:ARG:HG3   | 1.74                     | 0.68              |
| 1:A:3109:PHE:HD1  | 1:A:3162:PHE:HA   | 1.57                     | 0.68              |
| 1:C:842:GLN:HB2   | 1:C:1603:PHE:HB2  | 1.74                     | 0.68              |
| 1:C:2456:MET:HE2  | 1:C:2462:PRO:HD3  | 1.75                     | 0.68              |
| 1:C:3607:PRO:HG2  | 1:C:3610:ASN:HB2  | 1.74                     | 0.68              |
| 1:D:4187:GLU:OE2  | 1:D:4947:ARG:NH2  | 2.27                     | 0.68              |
| 1:B:4279:MET:HE2  | 1:C:4484:ILE:HG22 | 1.74                     | 0.68              |
| 1:B:890:HIS:HA    | 1:B:893:TRP:HE3   | 1.58                     | 0.68              |
| 1:C:885:LEU:HD12  | 1:C:888:ASN:HB3   | 1.76                     | 0.68              |
| 1:C:890:HIS:HA    | 1:C:893:TRP:HE3   | 1.58                     | 0.68              |
| 1:A:1473:LYS:HE3  | 1:A:1475:LYS:HB2  | 1.76                     | 0.68              |
| 1:A:3607:PRO:HG2  | 1:A:3610:ASN:HB2  | 1.74                     | 0.68              |
| 1:B:1473:LYS:HE3  | 1:B:1475:LYS:HB2  | 1.76                     | 0.68              |
| 1:C:1685:LEU:O    | 1:C:1689:ILE:HG12 | 1.93                     | 0.68              |
| 1:B:1685:LEU:O    | 1:B:1689:ILE:HG12 | 1.93                     | 0.68              |
| 1:B:885:LEU:HD12  | 1:B:888:ASN:HB3   | 1.76                     | 0.67              |
| 1:B:3696:ALA:O    | 1:B:3700:HIS:ND1  | 2.26                     | 0.67              |
| 1:B:989:THR:OG1   | 1:B:992:GLN:OE1   | 2.12                     | 0.67              |
| 1:C:989:THR:OG1   | 1:C:992:GLN:OE1   | 2.12                     | 0.67              |
| 1:A:885:LEU:HD12  | 1:A:888:ASN:HB3   | 1.76                     | 0.67              |
| 1:B:4187:GLU:OE2  | 1:B:4947:ARG:NH2  | 2.27                     | 0.67              |
| 1:C:2445:ILE:HG22 | 1:C:2451:VAL:HG22 | 1.77                     | 0.67              |
| 1:C:4888:CYS:HB3  | 1:C:4891:CYS:SG   | 2.35                     | 0.67              |
| 1:B:2445:ILE:HG22 | 1:B:2451:VAL:HG22 | 1.77                     | 0.67              |
| 1:C:3700:HIS:HB3  | 1:C:3702:GLU:HG2  | 1.77                     | 0.67              |
| 1:D:885:LEU:HD12  | 1:D:888:ASN:HB3   | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1685:LEU:O    | 1:A:1689:ILE:HG12 | 1.93                     | 0.67              |
| 1:C:387:ILE:HD12  | 1:C:389:ARG:HG3   | 1.74                     | 0.67              |
| 1:C:4187:GLU:OE2  | 1:C:4947:ARG:NH2  | 2.27                     | 0.67              |
| 1:D:1685:LEU:O    | 1:D:1689:ILE:HG12 | 1.93                     | 0.67              |
| 1:B:4664:ASP:OD1  | 1:B:4665:ARG:N    | 2.28                     | 0.67              |
| 1:A:164:PRO:HB3   | 1:A:169:ARG:HB2   | 1.77                     | 0.67              |
| 1:A:2554:ARG:HH12 | 1:A:2699:GLY:HA2  | 1.60                     | 0.67              |
| 1:B:2456:MET:HE2  | 1:B:2462:PRO:HD3  | 1.75                     | 0.67              |
| 1:A:989:THR:OG1   | 1:A:992:GLN:OE1   | 2.12                     | 0.67              |
| 1:A:1310:CYS:HB2  | 1:A:1537:THR:H    | 1.59                     | 0.67              |
| 1:B:1310:CYS:HB2  | 1:B:1537:THR:H    | 1.59                     | 0.67              |
| 1:D:188:SER:HB2   | 1:D:190:ARG:HH11  | 1.60                     | 0.67              |
| 1:D:4888:CYS:HB3  | 1:D:4891:CYS:SG   | 2.34                     | 0.67              |
| 1:C:164:PRO:HB3   | 1:C:169:ARG:HB2   | 1.77                     | 0.67              |
| 1:D:2831:VAL:O    | 1:D:2894:LYS:NZ   | 2.28                     | 0.67              |
| 1:B:1703:TYR:HD2  | 1:B:1820:PRO:HB2  | 1.60                     | 0.66              |
| 1:D:2427:ILE:O    | 1:D:2476:TYR:OH   | 2.14                     | 0.66              |
| 1:D:2666:LEU:HD11 | 1:D:2969:PRO:HB2  | 1.77                     | 0.66              |
| 1:A:2831:VAL:O    | 1:A:2894:LYS:NZ   | 2.28                     | 0.66              |
| 1:B:4888:CYS:HB3  | 1:B:4891:CYS:SG   | 2.34                     | 0.66              |
| 1:D:3108:LEU:HA   | 1:D:3111:HIS:CE1  | 2.31                     | 0.66              |
| 1:A:3696:ALA:O    | 1:A:3700:HIS:ND1  | 2.26                     | 0.66              |
| 1:D:164:PRO:HB3   | 1:D:169:ARG:HB2   | 1.77                     | 0.66              |
| 1:A:3890:TRP:HB3  | 1:B:76:ARG:HD2    | 1.78                     | 0.66              |
| 1:C:3261:ALA:O    | 1:C:3262:GLU:HG3  | 1.95                     | 0.66              |
| 1:D:989:THR:OG1   | 1:D:992:GLN:OE1   | 2.12                     | 0.66              |
| 1:D:3261:ALA:O    | 1:D:3262:GLU:HG3  | 1.95                     | 0.66              |
| 1:A:2427:ILE:O    | 1:A:2476:TYR:OH   | 2.13                     | 0.66              |
| 1:A:3261:ALA:O    | 1:A:3262:GLU:HG3  | 1.95                     | 0.66              |
| 1:B:188:SER:HB2   | 1:B:190:ARG:HH11  | 1.60                     | 0.66              |
| 1:C:188:SER:HB2   | 1:C:190:ARG:HH11  | 1.60                     | 0.66              |
| 1:C:1473:LYS:HE3  | 1:C:1475:LYS:HB2  | 1.76                     | 0.66              |
| 1:C:3108:LEU:HA   | 1:C:3111:HIS:CE1  | 2.31                     | 0.66              |
| 1:A:2456:MET:HE2  | 1:A:2462:PRO:HD3  | 1.75                     | 0.66              |
| 1:A:4187:GLU:OE2  | 1:A:4947:ARG:NH2  | 2.27                     | 0.66              |
| 1:C:3696:ALA:O    | 1:C:3700:HIS:ND1  | 2.26                     | 0.66              |
| 1:D:1473:LYS:HE3  | 1:D:1475:LYS:HB2  | 1.76                     | 0.66              |
| 1:D:2445:ILE:HG22 | 1:D:2451:VAL:HG22 | 1.77                     | 0.66              |
| 1:D:2554:ARG:HH12 | 1:D:2699:GLY:HA2  | 1.60                     | 0.66              |
| 1:A:4888:CYS:HB3  | 1:A:4891:CYS:SG   | 2.35                     | 0.66              |
| 1:C:2666:LEU:HD11 | 1:C:2969:PRO:HB2  | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4664:ASP:OD1  | 1:C:4665:ARG:N    | 2.28                     | 0.66              |
| 1:A:3108:LEU:HA   | 1:A:3111:HIS:CE1  | 2.31                     | 0.66              |
| 1:B:2877:LEU:HB3  | 1:B:2881:GLU:OE2  | 1.96                     | 0.66              |
| 1:D:1310:CYS:HB2  | 1:D:1537:THR:H    | 1.59                     | 0.66              |
| 1:D:3109:PHE:HE1  | 1:D:3162:PHE:HD1  | 1.43                     | 0.66              |
| 1:D:4664:ASP:OD1  | 1:D:4665:ARG:N    | 2.28                     | 0.66              |
| 1:A:1986:CYS:O    | 1:A:1993:ARG:NH2  | 2.29                     | 0.66              |
| 1:B:2849:HIS:CE1  | 1:B:2877:LEU:HD11 | 2.31                     | 0.66              |
| 1:B:3261:ALA:O    | 1:B:3262:GLU:HG3  | 1.95                     | 0.66              |
| 1:B:3700:HIS:HB3  | 1:B:3702:GLU:HG2  | 1.77                     | 0.66              |
| 1:C:2507:LEU:O    | 1:C:2510:THR:OG1  | 2.14                     | 0.66              |
| 1:C:2831:VAL:O    | 1:C:2894:LYS:NZ   | 2.28                     | 0.66              |
| 1:D:1986:CYS:O    | 1:D:1993:ARG:NH2  | 2.29                     | 0.66              |
| 1:A:189:GLU:O     | 1:D:2326:ARG:NH2  | 2.29                     | 0.66              |
| 1:A:2436:ILE:HG22 | 1:A:2491:GLY:HA3  | 1.78                     | 0.66              |
| 1:A:2826:ILE:HD12 | 1:B:1501:ASN:HB2  | 1.77                     | 0.66              |
| 1:B:3231:MET:HE3  | 1:B:3233:HIS:HB2  | 1.77                     | 0.66              |
| 1:C:1310:CYS:HB2  | 1:C:1537:THR:H    | 1.59                     | 0.66              |
| 1:D:1011:ARG:HG3  | 1:D:1016:TRP:HB2  | 1.78                     | 0.66              |
| 1:A:2621:TYR:OH   | 1:A:2637:GLU:OE2  | 2.14                     | 0.65              |
| 1:B:164:PRO:HB3   | 1:B:169:ARG:HB2   | 1.77                     | 0.65              |
| 1:C:332:ARG:NH2   | 1:C:338:LEU:O     | 2.30                     | 0.65              |
| 1:C:2427:ILE:O    | 1:C:2476:TYR:OH   | 2.14                     | 0.65              |
| 1:A:188:SER:HB2   | 1:A:190:ARG:HH11  | 1.60                     | 0.65              |
| 1:A:2445:ILE:HG22 | 1:A:2451:VAL:HG22 | 1.77                     | 0.65              |
| 1:B:332:ARG:NH2   | 1:B:338:LEU:O     | 2.30                     | 0.65              |
| 1:B:2554:ARG:HH12 | 1:B:2699:GLY:HA2  | 1.60                     | 0.65              |
| 1:B:2831:VAL:O    | 1:B:2894:LYS:NZ   | 2.28                     | 0.65              |
| 1:C:3231:MET:HE3  | 1:C:3233:HIS:HB2  | 1.77                     | 0.65              |
| 1:A:3231:MET:HE3  | 1:A:3233:HIS:HB2  | 1.77                     | 0.65              |
| 1:A:3700:HIS:HB3  | 1:A:3702:GLU:HG2  | 1.77                     | 0.65              |
| 1:B:3108:LEU:HA   | 1:B:3111:HIS:CE1  | 2.31                     | 0.65              |
| 1:C:2877:LEU:HB3  | 1:C:2881:GLU:OE2  | 1.96                     | 0.65              |
| 1:D:1980:LYS:O    | 1:D:1983:LYS:NZ   | 2.30                     | 0.65              |
| 1:A:4664:ASP:OD1  | 1:A:4665:ARG:N    | 2.28                     | 0.65              |
| 1:B:1980:LYS:O    | 1:B:1983:LYS:NZ   | 2.30                     | 0.65              |
| 1:C:3294:ALA:HA   | 1:C:3297:LYS:HE2  | 1.79                     | 0.65              |
| 1:B:2436:ILE:HG22 | 1:B:2491:GLY:HA3  | 1.78                     | 0.65              |
| 1:B:3803:LEU:HB2  | 1:B:3884:SER:HB2  | 1.79                     | 0.65              |
| 1:C:1703:TYR:HD2  | 1:C:1820:PRO:HB2  | 1.60                     | 0.65              |
| 1:D:2877:LEU:HB3  | 1:D:2881:GLU:OE2  | 1.96                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3231:MET:HE3  | 1:D:3233:HIS:HB2  | 1.77                     | 0.65              |
| 1:A:3803:LEU:HB2  | 1:A:3884:SER:HB2  | 1.79                     | 0.65              |
| 1:B:2621:TYR:OH   | 1:B:2637:GLU:OE2  | 2.14                     | 0.65              |
| 1:B:3109:PHE:HE1  | 1:B:3162:PHE:HD1  | 1.43                     | 0.65              |
| 1:D:332:ARG:NH2   | 1:D:338:LEU:O     | 2.30                     | 0.65              |
| 1:D:2849:HIS:CE1  | 1:D:2877:LEU:HD11 | 2.31                     | 0.65              |
| 1:D:3294:ALA:HA   | 1:D:3297:LYS:HE2  | 1.79                     | 0.65              |
| 1:A:1011:ARG:HG3  | 1:A:1016:TRP:HB2  | 1.78                     | 0.65              |
| 1:A:2634:SER:O    | 1:A:2635:GLU:HG3  | 1.97                     | 0.65              |
| 1:A:2877:LEU:HB3  | 1:A:2881:GLU:OE2  | 1.96                     | 0.65              |
| 1:B:2427:ILE:O    | 1:B:2476:TYR:OH   | 2.14                     | 0.65              |
| 1:C:2621:TYR:OH   | 1:C:2637:GLU:OE2  | 2.14                     | 0.65              |
| 1:A:1703:TYR:HD2  | 1:A:1820:PRO:HB2  | 1.60                     | 0.65              |
| 1:A:3016:ARG:O    | 1:A:3018:ARG:NH1  | 2.30                     | 0.65              |
| 1:A:3294:ALA:HA   | 1:A:3297:LYS:HE2  | 1.79                     | 0.65              |
| 1:B:1986:CYS:O    | 1:B:1993:ARG:NH2  | 2.29                     | 0.65              |
| 1:C:1011:ARG:HG3  | 1:C:1016:TRP:HB2  | 1.78                     | 0.65              |
| 1:C:1980:LYS:O    | 1:C:1983:LYS:NZ   | 2.30                     | 0.65              |
| 1:C:3260:ARG:HA   | 1:C:3263:MET:HE2  | 1.79                     | 0.65              |
| 1:D:3016:ARG:O    | 1:D:3018:ARG:NH1  | 2.30                     | 0.65              |
| 1:A:1980:LYS:O    | 1:A:1983:LYS:NZ   | 2.30                     | 0.65              |
| 1:A:2666:LEU:HD11 | 1:A:2969:PRO:HB2  | 1.77                     | 0.65              |
| 1:B:1011:ARG:HG3  | 1:B:1016:TRP:HB2  | 1.78                     | 0.65              |
| 1:C:2436:ILE:HG22 | 1:C:2491:GLY:HA3  | 1.78                     | 0.65              |
| 1:C:2554:ARG:HH12 | 1:C:2699:GLY:HA2  | 1.60                     | 0.65              |
| 1:D:1703:TYR:HD2  | 1:D:1820:PRO:HB2  | 1.60                     | 0.65              |
| 1:A:332:ARG:NH2   | 1:A:338:LEU:O     | 2.30                     | 0.65              |
| 1:B:2634:SER:O    | 1:B:2635:GLU:HG3  | 1.97                     | 0.65              |
| 1:C:2504:THR:O    | 1:C:2508:SER:N    | 2.30                     | 0.65              |
| 1:C:3293:GLY:H    | 1:C:3296:MET:HE1  | 1.62                     | 0.65              |
| 1:D:3260:ARG:HA   | 1:D:3263:MET:HE2  | 1.79                     | 0.65              |
| 1:A:2849:HIS:CE1  | 1:A:2877:LEU:HD11 | 2.31                     | 0.64              |
| 1:A:3109:PHE:HE1  | 1:A:3162:PHE:HD1  | 1.43                     | 0.64              |
| 1:A:3293:GLY:H    | 1:A:3296:MET:HE1  | 1.62                     | 0.64              |
| 1:B:3260:ARG:HA   | 1:B:3263:MET:HE2  | 1.79                     | 0.64              |
| 1:C:1986:CYS:O    | 1:C:1993:ARG:NH2  | 2.29                     | 0.64              |
| 1:D:2725:ALA:O    | 1:D:2771:TYR:OH   | 2.15                     | 0.64              |
| 1:A:1703:TYR:CD2  | 1:A:1820:PRO:HB2  | 2.33                     | 0.64              |
| 1:B:2666:LEU:HD11 | 1:B:2969:PRO:HB2  | 1.77                     | 0.64              |
| 1:B:3293:GLY:H    | 1:B:3296:MET:HE1  | 1.62                     | 0.64              |
| 1:C:2725:ALA:O    | 1:C:2771:TYR:OH   | 2.15                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3260:ARG:HA   | 1:A:3263:MET:HE2  | 1.79                     | 0.64              |
| 1:B:1800:LYS:HA   | 1:B:1890:LYS:HZ1  | 1.63                     | 0.64              |
| 1:B:2556:SER:O    | 1:B:2602:HIS:NE2  | 2.26                     | 0.64              |
| 1:B:3016:ARG:O    | 1:B:3018:ARG:NH1  | 2.30                     | 0.64              |
| 1:C:3016:ARG:O    | 1:C:3018:ARG:NH1  | 2.30                     | 0.64              |
| 1:D:2507:LEU:O    | 1:D:2510:THR:OG1  | 2.14                     | 0.64              |
| 1:D:3700:HIS:HB3  | 1:D:3702:GLU:HG2  | 1.77                     | 0.64              |
| 1:A:243:GLU:HG3   | 1:A:262:TYR:HB3   | 1.80                     | 0.64              |
| 1:C:2968:LEU:HB3  | 1:C:2969:PRO:HD3  | 1.80                     | 0.64              |
| 1:C:4601:LYS:O    | 1:C:4604:LYS:HG2  | 1.98                     | 0.64              |
| 1:D:1703:TYR:CD2  | 1:D:1820:PRO:HB2  | 2.33                     | 0.64              |
| 1:D:3803:LEU:HB2  | 1:D:3884:SER:HB2  | 1.79                     | 0.64              |
| 1:B:878:LEU:HD21  | 1:B:950:VAL:HG21  | 1.79                     | 0.64              |
| 1:B:3294:ALA:HA   | 1:B:3297:LYS:HE2  | 1.79                     | 0.64              |
| 1:D:878:LEU:HD21  | 1:D:950:VAL:HG21  | 1.79                     | 0.64              |
| 1:A:2273:GLY:O    | 1:A:2336:ARG:NH2  | 2.30                     | 0.64              |
| 1:C:1703:TYR:CD2  | 1:C:1820:PRO:HB2  | 2.33                     | 0.64              |
| 1:D:2504:THR:O    | 1:D:2508:SER:N    | 2.30                     | 0.64              |
| 1:D:3293:GLY:H    | 1:D:3296:MET:HE1  | 1.62                     | 0.64              |
| 1:B:2847:ASN:OD1  | 1:B:2848:TYR:N    | 2.31                     | 0.64              |
| 1:C:2849:HIS:CE1  | 1:C:2877:LEU:HD11 | 2.31                     | 0.64              |
| 1:D:2436:ILE:HG22 | 1:D:2491:GLY:HA3  | 1.78                     | 0.64              |
| 1:A:290:ARG:HB2   | 1:A:293:GLN:HB2   | 1.80                     | 0.64              |
| 1:B:4601:LYS:O    | 1:B:4604:LYS:HG2  | 1.98                     | 0.64              |
| 1:D:2847:ASN:OD1  | 1:D:2848:TYR:N    | 2.31                     | 0.64              |
| 1:B:2168:HIS:HB2  | 1:B:2214:MET:HE1  | 1.81                     | 0.64              |
| 1:A:2847:ASN:OD1  | 1:A:2848:TYR:N    | 2.31                     | 0.63              |
| 1:C:3109:PHE:HE1  | 1:C:3162:PHE:HD1  | 1.43                     | 0.63              |
| 1:A:2507:LEU:O    | 1:A:2510:THR:OG1  | 2.14                     | 0.63              |
| 1:A:2968:LEU:HB3  | 1:A:2969:PRO:HD3  | 1.79                     | 0.63              |
| 1:A:4484:ILE:HG22 | 1:D:4279:MET:HE2  | 1.81                     | 0.63              |
| 1:C:3803:LEU:HB2  | 1:C:3884:SER:HB2  | 1.79                     | 0.63              |
| 1:A:515:ALA:O     | 1:A:520:ARG:NH2   | 2.31                     | 0.63              |
| 1:A:878:LEU:HD21  | 1:A:950:VAL:HG21  | 1.79                     | 0.63              |
| 1:A:4943:MET:HE2  | 1:A:4951:PHE:HD1  | 1.64                     | 0.63              |
| 1:B:2658:GLU:OE1  | 1:B:2661:LEU:N    | 2.30                     | 0.63              |
| 1:C:290:ARG:HB2   | 1:C:293:GLN:HB2   | 1.80                     | 0.63              |
| 1:D:4943:MET:HE2  | 1:D:4951:PHE:HD1  | 1.64                     | 0.63              |
| 1:A:730:LEU:HD11  | 2:E:8:ILE:HA      | 1.80                     | 0.63              |
| 1:A:891:GLU:HA    | 1:A:894:VAL:HG22  | 1.81                     | 0.63              |
| 1:A:2168:HIS:HB2  | 1:A:2214:MET:HE1  | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:89:PRO:HB2    | 1:D:1671:ARG:HH21 | 1.62                     | 0.63              |
| 1:B:243:GLU:HG3   | 1:B:262:TYR:HB3   | 1.79                     | 0.63              |
| 1:B:1703:TYR:CD2  | 1:B:1820:PRO:HB2  | 2.33                     | 0.63              |
| 1:C:1800:LYS:HA   | 1:C:1890:LYS:HZ1  | 1.63                     | 0.63              |
| 1:D:2621:TYR:OH   | 1:D:2637:GLU:OE2  | 2.14                     | 0.63              |
| 1:A:76:ARG:HD2    | 1:D:3890:TRP:HB3  | 1.81                     | 0.63              |
| 1:B:879:GLU:HA    | 1:B:882:ARG:HB3   | 1.80                     | 0.63              |
| 1:C:243:GLU:HG3   | 1:C:262:TYR:HB3   | 1.79                     | 0.63              |
| 1:C:891:GLU:HA    | 1:C:894:VAL:HG22  | 1.81                     | 0.63              |
| 1:C:2634:SER:O    | 1:C:2635:GLU:HG3  | 1.97                     | 0.63              |
| 1:C:2847:ASN:OD1  | 1:C:2848:TYR:N    | 2.31                     | 0.63              |
| 1:D:891:GLU:HA    | 1:D:894:VAL:HG22  | 1.81                     | 0.63              |
| 1:B:2717:LEU:HD11 | 1:B:2789:ILE:HD11 | 1.80                     | 0.63              |
| 1:D:515:ALA:O     | 1:D:520:ARG:NH2   | 2.32                     | 0.63              |
| 1:A:718:VAL:HG23  | 1:A:793:SER:HB3   | 1.81                     | 0.63              |
| 1:A:1800:LYS:HA   | 1:A:1890:LYS:HZ3  | 1.64                     | 0.63              |
| 1:B:891:GLU:HA    | 1:B:894:VAL:HG22  | 1.81                     | 0.63              |
| 1:B:4943:MET:HE2  | 1:B:4951:PHE:HD1  | 1.64                     | 0.63              |
| 1:C:2168:HIS:HB2  | 1:C:2214:MET:HE1  | 1.81                     | 0.63              |
| 1:C:2713:ILE:HD12 | 1:C:2718:GLU:HB3  | 1.81                     | 0.63              |
| 1:C:2717:LEU:HD11 | 1:C:2789:ILE:HD11 | 1.80                     | 0.63              |
| 1:D:243:GLU:HG3   | 1:D:262:TYR:HB3   | 1.79                     | 0.63              |
| 1:D:555:LEU:HD21  | 1:D:578:VAL:HG11  | 1.81                     | 0.63              |
| 1:D:2968:LEU:HB3  | 1:D:2969:PRO:HD3  | 1.80                     | 0.63              |
| 1:A:555:LEU:HD21  | 1:A:578:VAL:HG11  | 1.81                     | 0.63              |
| 1:A:2713:ILE:HD12 | 1:A:2718:GLU:HB3  | 1.81                     | 0.63              |
| 1:A:4601:LYS:O    | 1:A:4604:LYS:HG2  | 1.98                     | 0.63              |
| 1:C:878:LEU:HD21  | 1:C:950:VAL:HG21  | 1.79                     | 0.63              |
| 1:C:2488:LEU:HA   | 1:C:2492:PHE:HB2  | 1.81                     | 0.63              |
| 1:D:893:TRP:HA    | 1:D:896:ASN:ND2   | 2.14                     | 0.63              |
| 1:B:2488:LEU:HA   | 1:B:2492:PHE:HB2  | 1.81                     | 0.63              |
| 1:D:2634:SER:O    | 1:D:2635:GLU:HG3  | 1.97                     | 0.63              |
| 1:D:3108:LEU:HD12 | 1:D:3111:HIS:HE1  | 1.64                     | 0.63              |
| 1:A:2725:ALA:O    | 1:A:2771:TYR:OH   | 2.15                     | 0.62              |
| 1:C:4943:MET:HE2  | 1:C:4951:PHE:HD1  | 1.64                     | 0.62              |
| 1:D:290:ARG:HB2   | 1:D:293:GLN:HB2   | 1.80                     | 0.62              |
| 1:D:2053:LYS:NZ   | 1:D:2056:SER:OG   | 2.33                     | 0.62              |
| 1:D:3260:ARG:HD3  | 1:D:3264:CYS:HB2  | 1.81                     | 0.62              |
| 1:A:2504:THR:O    | 1:A:2508:SER:N    | 2.30                     | 0.62              |
| 2:G:89:PRO:HB2    | 1:C:1671:ARG:NH2  | 2.14                     | 0.62              |
| 1:B:2273:GLY:O    | 1:B:2336:ARG:NH2  | 2.30                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2968:LEU:HB3  | 1:B:2969:PRO:HD3  | 1.79                     | 0.62              |
| 1:D:1800:LYS:HA   | 1:D:1890:LYS:HZ3  | 1.64                     | 0.62              |
| 1:D:2713:ILE:HD12 | 1:D:2718:GLU:HB3  | 1.81                     | 0.62              |
| 1:D:2789:ILE:HB   | 1:D:2901:TYR:HB3  | 1.81                     | 0.62              |
| 1:A:2053:LYS:NZ   | 1:A:2056:SER:OG   | 2.32                     | 0.62              |
| 1:A:3108:LEU:HD12 | 1:A:3111:HIS:HE1  | 1.64                     | 0.62              |
| 1:B:3108:LEU:HD12 | 1:B:3111:HIS:HE1  | 1.64                     | 0.62              |
| 1:C:893:TRP:HA    | 1:C:896:ASN:ND2   | 2.14                     | 0.62              |
| 1:D:2168:HIS:HB2  | 1:D:2214:MET:HE1  | 1.81                     | 0.62              |
| 1:D:4601:LYS:O    | 1:D:4604:LYS:HG2  | 1.98                     | 0.62              |
| 1:B:515:ALA:O     | 1:B:520:ARG:NH2   | 2.32                     | 0.62              |
| 1:B:1969:PRO:HB3  | 1:B:3611:LEU:HD11 | 1.80                     | 0.62              |
| 1:B:2713:ILE:HD12 | 1:B:2718:GLU:HB3  | 1.81                     | 0.62              |
| 1:C:2053:LYS:NZ   | 1:C:2056:SER:OG   | 2.32                     | 0.62              |
| 1:B:801:ARG:NH1   | 1:B:1615:GLN:O    | 2.33                     | 0.62              |
| 1:C:2142:MET:HE3  | 1:C:2192:MET:HG2  | 1.82                     | 0.62              |
| 1:D:879:GLU:HA    | 1:D:882:ARG:HB3   | 1.80                     | 0.62              |
| 1:D:2142:MET:HE3  | 1:D:2192:MET:HG2  | 1.82                     | 0.62              |
| 1:A:893:TRP:HA    | 1:A:896:ASN:ND2   | 2.14                     | 0.62              |
| 1:A:2658:GLU:OE1  | 1:A:2661:LEU:N    | 2.30                     | 0.62              |
| 1:B:290:ARG:HB2   | 1:B:293:GLN:HB2   | 1.80                     | 0.62              |
| 1:B:555:LEU:HD21  | 1:B:578:VAL:HG11  | 1.81                     | 0.62              |
| 1:B:2053:LYS:NZ   | 1:B:2056:SER:OG   | 2.32                     | 0.62              |
| 1:C:194:LEU:HD11  | 1:C:201:LEU:HB3   | 1.82                     | 0.62              |
| 1:C:879:GLU:HA    | 1:C:882:ARG:HB3   | 1.80                     | 0.62              |
| 1:A:1042:THR:O    | 1:A:1046:ASN:ND2  | 2.33                     | 0.62              |
| 1:A:4504:MET:N    | 1:A:4504:MET:SD   | 2.73                     | 0.62              |
| 1:B:1042:THR:O    | 1:B:1046:ASN:ND2  | 2.33                     | 0.62              |
| 1:C:1611:ILE:HB   | 1:C:1615:GLN:HB2  | 1.82                     | 0.62              |
| 1:C:3260:ARG:HD3  | 1:C:3264:CYS:HB2  | 1.81                     | 0.62              |
| 1:D:194:LEU:HD11  | 1:D:201:LEU:HB3   | 1.82                     | 0.62              |
| 1:A:1630:LEU:HD22 | 1:A:1644:LEU:HD11 | 1.82                     | 0.62              |
| 1:A:2488:LEU:HA   | 1:A:2492:PHE:HB2  | 1.81                     | 0.62              |
| 1:A:2717:LEU:HD11 | 1:A:2789:ILE:HD11 | 1.80                     | 0.62              |
| 1:A:2789:ILE:HB   | 1:A:2901:TYR:HB3  | 1.82                     | 0.62              |
| 1:B:4504:MET:N    | 1:B:4504:MET:SD   | 2.73                     | 0.62              |
| 1:C:2789:ILE:HB   | 1:C:2901:TYR:HB3  | 1.82                     | 0.62              |
| 1:C:3016:ARG:HH21 | 1:C:3096:TYR:HE2  | 1.46                     | 0.62              |
| 1:D:1611:ILE:HB   | 1:D:1615:GLN:HB2  | 1.82                     | 0.62              |
| 1:D:1630:LEU:HD22 | 1:D:1644:LEU:HD11 | 1.82                     | 0.62              |
| 1:D:4504:MET:N    | 1:D:4504:MET:SD   | 2.73                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:893:TRP:HA    | 1:B:896:ASN:ND2   | 2.14                     | 0.62              |
| 1:B:915:HIS:HB3   | 1:B:918:LEU:HB2   | 1.82                     | 0.62              |
| 1:B:1630:LEU:HD22 | 1:B:1644:LEU:HD11 | 1.82                     | 0.62              |
| 1:C:555:LEU:HD21  | 1:C:578:VAL:HG11  | 1.81                     | 0.62              |
| 1:C:1630:LEU:HD22 | 1:C:1644:LEU:HD11 | 1.82                     | 0.62              |
| 1:C:1969:PRO:HB3  | 1:C:3611:LEU:HD11 | 1.81                     | 0.62              |
| 1:D:718:VAL:HG23  | 1:D:793:SER:HB3   | 1.81                     | 0.62              |
| 1:A:915:HIS:HB3   | 1:A:918:LEU:HB2   | 1.82                     | 0.62              |
| 1:B:3016:ARG:HH21 | 1:B:3096:TYR:HE2  | 1.46                     | 0.62              |
| 1:D:801:ARG:NH1   | 1:D:1615:GLN:O    | 2.33                     | 0.62              |
| 1:D:2541:HIS:HB3  | 1:D:2544:LEU:HG   | 1.82                     | 0.62              |
| 1:A:879:GLU:HA    | 1:A:882:ARG:HB3   | 1.80                     | 0.61              |
| 1:A:1969:PRO:HB3  | 1:A:3611:LEU:HD11 | 1.81                     | 0.61              |
| 1:A:4052:MET:SD   | 1:A:4063:THR:HG23 | 2.40                     | 0.61              |
| 1:A:4063:THR:O    | 1:A:4067:LEU:HD12 | 2.00                     | 0.61              |
| 1:C:718:VAL:HG23  | 1:C:793:SER:HB3   | 1.81                     | 0.61              |
| 1:C:1042:THR:O    | 1:C:1046:ASN:ND2  | 2.33                     | 0.61              |
| 1:C:3108:LEU:HD12 | 1:C:3111:HIS:HE1  | 1.64                     | 0.61              |
| 1:C:3311:LYS:HG3  | 1:C:3313:GLN:H    | 1.65                     | 0.61              |
| 1:C:4832:GLU:O    | 1:C:4843:ARG:NH2  | 2.33                     | 0.61              |
| 1:A:2377:GLU:OE2  | 1:A:2383:HIS:NE2  | 2.34                     | 0.61              |
| 1:C:4063:THR:O    | 1:C:4067:LEU:HD12 | 2.00                     | 0.61              |
| 1:C:4504:MET:SD   | 1:C:4504:MET:N    | 2.73                     | 0.61              |
| 1:D:4063:THR:O    | 1:D:4067:LEU:HD12 | 2.00                     | 0.61              |
| 1:A:3016:ARG:HH21 | 1:A:3096:TYR:HE2  | 1.46                     | 0.61              |
| 1:B:2142:MET:HE3  | 1:B:2192:MET:HG2  | 1.82                     | 0.61              |
| 1:B:4052:MET:SD   | 1:B:4063:THR:HG23 | 2.40                     | 0.61              |
| 1:C:2273:GLY:O    | 1:C:2336:ARG:NH2  | 2.30                     | 0.61              |
| 1:D:915:HIS:HB3   | 1:D:918:LEU:HB2   | 1.82                     | 0.61              |
| 1:A:801:ARG:NH1   | 1:A:1615:GLN:O    | 2.33                     | 0.61              |
| 1:B:2789:ILE:HB   | 1:B:2901:TYR:HB3  | 1.82                     | 0.61              |
| 1:C:515:ALA:O     | 1:C:520:ARG:NH2   | 2.31                     | 0.61              |
| 1:D:1042:THR:O    | 1:D:1046:ASN:ND2  | 2.33                     | 0.61              |
| 1:D:4832:GLU:O    | 1:D:4843:ARG:NH2  | 2.33                     | 0.61              |
| 1:A:3236:GLU:HG3  | 1:A:3237:VAL:HG13 | 1.83                     | 0.61              |
| 1:B:194:LEU:HD11  | 1:B:201:LEU:HB3   | 1.82                     | 0.61              |
| 1:C:2594:PHE:HZ   | 1:C:2697:SER:HA   | 1.66                     | 0.61              |
| 1:C:3689:MET:HE3  | 1:C:3753:PRO:HB2  | 1.83                     | 0.61              |
| 1:C:4052:MET:SD   | 1:C:4063:THR:HG23 | 2.40                     | 0.61              |
| 1:D:3016:ARG:HH21 | 1:D:3096:TYR:HE2  | 1.46                     | 0.61              |
| 1:A:1611:ILE:HB   | 1:A:1615:GLN:HB2  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2142:MET:HE3  | 1:A:2192:MET:HG2  | 1.82                     | 0.61              |
| 1:A:2594:PHE:HZ   | 1:A:2697:SER:HA   | 1.66                     | 0.61              |
| 1:A:2657:TYR:HA   | 1:A:2662:PHE:CE2  | 2.36                     | 0.61              |
| 1:B:4063:THR:O    | 1:B:4067:LEU:HD12 | 2.00                     | 0.61              |
| 1:C:2377:GLU:OE2  | 1:C:2383:HIS:NE2  | 2.33                     | 0.61              |
| 1:D:2488:LEU:HA   | 1:D:2492:PHE:HB2  | 1.81                     | 0.61              |
| 1:D:3228:TYR:HB2  | 1:D:3295:TRP:CZ2  | 2.36                     | 0.61              |
| 1:A:2926:LEU:HD23 | 1:A:3003:MET:HG3  | 1.83                     | 0.61              |
| 1:A:3260:ARG:HD3  | 1:A:3264:CYS:HB2  | 1.81                     | 0.61              |
| 1:A:3689:MET:HE3  | 1:A:3753:PRO:HB2  | 1.83                     | 0.61              |
| 1:A:4011:GLU:HB3  | 1:A:4121:LEU:HD23 | 1.83                     | 0.61              |
| 1:B:2507:LEU:O    | 1:B:2510:THR:OG1  | 2.14                     | 0.61              |
| 1:C:992:GLN:O     | 1:C:996:VAL:HG23  | 2.01                     | 0.61              |
| 1:C:2541:HIS:HB3  | 1:C:2544:LEU:HG   | 1.82                     | 0.61              |
| 1:D:2377:GLU:OE2  | 1:D:2383:HIS:NE2  | 2.34                     | 0.61              |
| 1:D:2556:SER:O    | 1:D:2602:HIS:NE2  | 2.26                     | 0.61              |
| 1:D:2717:LEU:HD11 | 1:D:2789:ILE:HD11 | 1.80                     | 0.61              |
| 1:A:2502:LEU:HD23 | 1:A:2507:LEU:HD13 | 1.82                     | 0.61              |
| 1:B:718:VAL:HG23  | 1:B:793:SER:HB3   | 1.81                     | 0.61              |
| 1:B:1267:HIS:HB3  | 1:B:1287:GLN:HE21 | 1.66                     | 0.61              |
| 1:B:2502:LEU:HD23 | 1:B:2507:LEU:HD13 | 1.83                     | 0.61              |
| 1:B:2716:LYS:HG3  | 1:B:2717:LEU:HD22 | 1.82                     | 0.61              |
| 1:B:2926:LEU:HD23 | 1:B:3003:MET:HG3  | 1.83                     | 0.61              |
| 1:B:4859:LEU:O    | 1:B:4863:GLN:NE2  | 2.34                     | 0.61              |
| 1:C:1941:ARG:HE   | 1:C:3609:TYR:HB2  | 1.66                     | 0.61              |
| 1:C:3072:MET:HB2  | 1:C:3140:LEU:HD21 | 1.83                     | 0.61              |
| 1:C:3228:TYR:HB2  | 1:C:3295:TRP:CZ2  | 2.36                     | 0.61              |
| 1:D:992:GLN:O     | 1:D:996:VAL:HG23  | 2.01                     | 0.61              |
| 1:A:69:LEU:HD13   | 1:A:113:LEU:HD11  | 1.82                     | 0.61              |
| 1:A:992:GLN:O     | 1:A:996:VAL:HG23  | 2.01                     | 0.61              |
| 1:A:1267:HIS:HB3  | 1:A:1287:GLN:HE21 | 1.66                     | 0.61              |
| 1:A:2541:HIS:HB3  | 1:A:2544:LEU:HG   | 1.82                     | 0.61              |
| 1:A:4832:GLU:O    | 1:A:4843:ARG:NH2  | 2.33                     | 0.61              |
| 1:B:69:LEU:HD13   | 1:B:113:LEU:HD11  | 1.82                     | 0.61              |
| 1:B:3260:ARG:HD3  | 1:B:3264:CYS:HB2  | 1.81                     | 0.61              |
| 1:B:3689:MET:HE3  | 1:B:3753:PRO:HB2  | 1.83                     | 0.61              |
| 1:B:4011:GLU:HB3  | 1:B:4121:LEU:HD23 | 1.83                     | 0.61              |
| 1:C:915:HIS:HB3   | 1:C:918:LEU:HB2   | 1.82                     | 0.61              |
| 1:C:1043:LYS:HA   | 1:C:1046:ASN:HD21 | 1.66                     | 0.61              |
| 1:D:3072:MET:HB2  | 1:D:3140:LEU:HD21 | 1.83                     | 0.61              |
| 1:D:3236:GLU:HG3  | 1:D:3237:VAL:HG13 | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4859:LEU:O    | 1:A:4863:GLN:NE2  | 2.34                     | 0.61              |
| 1:C:950:VAL:HG22  | 1:C:1064:LEU:HD22 | 1.83                     | 0.61              |
| 1:D:1969:PRO:HB3  | 1:D:3611:LEU:HD11 | 1.81                     | 0.61              |
| 1:D:2716:LYS:HG3  | 1:D:2717:LEU:HD22 | 1.82                     | 0.61              |
| 1:D:4052:MET:SD   | 1:D:4063:THR:HG23 | 2.40                     | 0.61              |
| 1:A:4187:GLU:OE1  | 1:A:4949:TRP:NE1  | 2.24                     | 0.60              |
| 1:B:950:VAL:HG22  | 1:B:1064:LEU:HD22 | 1.83                     | 0.60              |
| 1:B:992:GLN:O     | 1:B:996:VAL:HG23  | 2.01                     | 0.60              |
| 1:B:1611:ILE:HB   | 1:B:1615:GLN:HB2  | 1.82                     | 0.60              |
| 1:B:2504:THR:O    | 1:B:2508:SER:N    | 2.30                     | 0.60              |
| 1:C:69:LEU:HD13   | 1:C:113:LEU:HD11  | 1.82                     | 0.60              |
| 1:C:2716:LYS:HG3  | 1:C:2717:LEU:HD22 | 1.82                     | 0.60              |
| 1:D:2273:GLY:O    | 1:D:2336:ARG:NH2  | 2.30                     | 0.60              |
| 1:D:2545:ILE:HD12 | 1:D:2580:LEU:HD11 | 1.83                     | 0.60              |
| 1:D:2657:TYR:HA   | 1:D:2662:PHE:CE2  | 2.35                     | 0.60              |
| 1:D:2926:LEU:HD23 | 1:D:3003:MET:HG3  | 1.83                     | 0.60              |
| 1:A:2716:LYS:HG3  | 1:A:2717:LEU:HD22 | 1.82                     | 0.60              |
| 1:A:3030:VAL:O    | 1:A:3034:HIS:HD2  | 1.84                     | 0.60              |
| 1:A:3228:TYR:HB2  | 1:A:3295:TRP:CZ2  | 2.36                     | 0.60              |
| 1:B:4075:ASN:OD1  | 1:B:4077:THR:OG1  | 2.18                     | 0.60              |
| 1:B:4832:GLU:O    | 1:B:4843:ARG:NH2  | 2.33                     | 0.60              |
| 1:D:2658:GLU:OE1  | 1:D:2661:LEU:N    | 2.30                     | 0.60              |
| 1:D:3689:MET:HE3  | 1:D:3753:PRO:HB2  | 1.83                     | 0.60              |
| 1:A:194:LEU:HD11  | 1:A:201:LEU:HB3   | 1.82                     | 0.60              |
| 1:A:2360:ASP:OD2  | 1:A:2383:HIS:ND1  | 2.30                     | 0.60              |
| 2:G:50:ARG:NE     | 2:G:53:LYS:HG3    | 2.15                     | 0.60              |
| 1:B:2657:TYR:HA   | 1:B:2662:PHE:CE2  | 2.36                     | 0.60              |
| 1:D:69:LEU:HD13   | 1:D:113:LEU:HD11  | 1.82                     | 0.60              |
| 1:D:3030:VAL:O    | 1:D:3034:HIS:HD2  | 1.84                     | 0.60              |
| 1:D:3311:LYS:HG3  | 1:D:3313:GLN:H    | 1.65                     | 0.60              |
| 1:A:2413:LYS:HD2  | 1:A:2416:ALA:H    | 1.66                     | 0.60              |
| 1:A:3311:LYS:HG3  | 1:A:3313:GLN:H    | 1.65                     | 0.60              |
| 1:C:1792:ILE:HG12 | 1:C:1842:ILE:HD13 | 1.84                     | 0.60              |
| 1:C:2556:SER:O    | 1:C:2602:HIS:NE2  | 2.26                     | 0.60              |
| 1:C:3236:GLU:HG3  | 1:C:3237:VAL:HG13 | 1.83                     | 0.60              |
| 1:D:905:GLY:N     | 1:D:915:HIS:H     | 2.00                     | 0.60              |
| 1:D:4859:LEU:O    | 1:D:4863:GLN:NE2  | 2.34                     | 0.60              |
| 1:B:1941:ARG:HE   | 1:B:3609:TYR:HB2  | 1.66                     | 0.60              |
| 1:B:2570:GLU:HG2  | 1:B:2605:MET:HG3  | 1.83                     | 0.60              |
| 1:B:2725:ALA:O    | 1:B:2771:TYR:OH   | 2.15                     | 0.60              |
| 1:B:3072:MET:HB2  | 1:B:3140:LEU:HD21 | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2570:GLU:HG2  | 1:C:2605:MET:HG3  | 1.83                     | 0.60              |
| 1:D:1043:LYS:HA   | 1:D:1046:ASN:HD21 | 1.66                     | 0.60              |
| 1:D:1267:HIS:HB3  | 1:D:1287:GLN:HE21 | 1.66                     | 0.60              |
| 1:A:1941:ARG:HE   | 1:A:3609:TYR:HB2  | 1.66                     | 0.60              |
| 1:A:3069:GLU:HA   | 1:A:3072:MET:HG3  | 1.84                     | 0.60              |
| 1:A:3072:MET:HB2  | 1:A:3140:LEU:HD21 | 1.83                     | 0.60              |
| 1:A:4270:LYS:NZ   | 1:A:4278:ASP:OD1  | 2.35                     | 0.60              |
| 1:B:905:GLY:N     | 1:B:915:HIS:H     | 2.00                     | 0.60              |
| 1:B:2377:GLU:OE2  | 1:B:2383:HIS:NE2  | 2.34                     | 0.60              |
| 1:B:3108:LEU:HD12 | 1:B:3111:HIS:CE1  | 2.37                     | 0.60              |
| 1:B:3111:HIS:HA   | 1:B:3114:GLN:HG3  | 1.84                     | 0.60              |
| 1:B:3311:LYS:HG3  | 1:B:3313:GLN:H    | 1.65                     | 0.60              |
| 1:B:4187:GLU:OE1  | 1:B:4949:TRP:NE1  | 2.24                     | 0.60              |
| 1:C:3108:LEU:HD12 | 1:C:3111:HIS:CE1  | 2.37                     | 0.60              |
| 1:D:2436:ILE:HA   | 1:D:2465:LYS:HE3  | 1.84                     | 0.60              |
| 1:A:950:VAL:HG22  | 1:A:1064:LEU:HD22 | 1.83                     | 0.60              |
| 1:A:1303:ARG:NH2  | 1:A:1635:GLU:OE1  | 2.35                     | 0.60              |
| 1:A:1792:ILE:HG12 | 1:A:1842:ILE:HD13 | 1.84                     | 0.60              |
| 1:A:2691:LYS:HE3  | 1:A:2850:ASN:ND2  | 2.17                     | 0.60              |
| 1:B:3030:VAL:O    | 1:B:3034:HIS:HD2  | 1.84                     | 0.60              |
| 1:C:4859:LEU:O    | 1:C:4863:GLN:NE2  | 2.34                     | 0.60              |
| 1:D:4014:LEU:HD13 | 1:D:4122:ALA:HB2  | 1.84                     | 0.60              |
| 1:A:905:GLY:N     | 1:A:915:HIS:H     | 2.00                     | 0.60              |
| 1:A:2556:SER:O    | 1:A:2602:HIS:NE2  | 2.26                     | 0.60              |
| 2:G:83:TYR:OH     | 1:C:1768:PHE:O    | 2.18                     | 0.60              |
| 2:H:83:TYR:OH     | 1:D:1768:PHE:O    | 2.14                     | 0.60              |
| 1:B:1043:LYS:HA   | 1:B:1046:ASN:HD21 | 1.66                     | 0.60              |
| 1:B:2541:HIS:HB3  | 1:B:2544:LEU:HG   | 1.82                     | 0.60              |
| 1:B:2691:LYS:HE3  | 1:B:2850:ASN:ND2  | 2.17                     | 0.60              |
| 1:B:3228:TYR:HB2  | 1:B:3295:TRP:CZ2  | 2.36                     | 0.60              |
| 1:C:3111:HIS:HA   | 1:C:3114:GLN:HG3  | 1.84                     | 0.60              |
| 1:D:2594:PHE:HZ   | 1:D:2697:SER:HA   | 1.66                     | 0.60              |
| 1:D:3069:GLU:HA   | 1:D:3072:MET:HG3  | 1.84                     | 0.60              |
| 1:A:1768:PHE:O    | 2:E:83:TYR:OH     | 2.15                     | 0.60              |
| 1:B:3279:ASN:O    | 1:B:3283:ILE:HG13 | 2.02                     | 0.60              |
| 1:B:4270:LYS:NZ   | 1:B:4278:ASP:OD1  | 2.35                     | 0.60              |
| 1:C:3279:ASN:O    | 1:C:3283:ILE:HG13 | 2.02                     | 0.60              |
| 1:C:4011:GLU:HB3  | 1:C:4121:LEU:HD23 | 1.83                     | 0.60              |
| 1:C:4014:LEU:HD13 | 1:C:4122:ALA:HB2  | 1.84                     | 0.60              |
| 1:D:950:VAL:HG22  | 1:D:1064:LEU:HD22 | 1.83                     | 0.60              |
| 1:D:4270:LYS:NZ   | 1:D:4278:ASP:OD1  | 2.35                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1043:LYS:HA   | 1:A:1046:ASN:HD21 | 1.66                     | 0.60              |
| 1:A:3111:HIS:HA   | 1:A:3114:GLN:HG3  | 1.84                     | 0.60              |
| 1:B:3254:PRO:HD2  | 1:B:3268:LEU:H    | 1.67                     | 0.60              |
| 1:C:2830:ASN:ND2  | 1:D:1551:ASN:O    | 2.33                     | 0.60              |
| 1:C:2979:ARG:HB2  | 1:C:3039:THR:HG22 | 1.84                     | 0.60              |
| 1:C:4270:LYS:NZ   | 1:C:4278:ASP:OD1  | 2.35                     | 0.60              |
| 1:D:2502:LEU:HD23 | 1:D:2507:LEU:HD13 | 1.82                     | 0.60              |
| 1:D:2691:LYS:HE3  | 1:D:2850:ASN:ND2  | 2.17                     | 0.60              |
| 1:D:3108:LEU:HD12 | 1:D:3111:HIS:CE1  | 2.37                     | 0.60              |
| 1:D:4011:GLU:HB3  | 1:D:4121:LEU:HD23 | 1.83                     | 0.60              |
| 1:A:3108:LEU:HD12 | 1:A:3111:HIS:CE1  | 2.37                     | 0.59              |
| 1:A:3171:LEU:HB3  | 1:A:3211:LEU:HB2  | 1.84                     | 0.59              |
| 1:B:2744:GLY:HA3  | 1:B:2753:VAL:HB   | 1.84                     | 0.59              |
| 1:D:4584:PHE:CA   | 1:D:4726:MET:HE1  | 2.32                     | 0.59              |
| 1:A:2521:CYS:HA   | 1:A:2525:LEU:HD12 | 1.84                     | 0.59              |
| 1:C:801:ARG:NH1   | 1:C:1615:GLN:O    | 2.33                     | 0.59              |
| 1:C:1795:LEU:HD23 | 1:C:1842:ILE:HD11 | 1.84                     | 0.59              |
| 1:D:885:LEU:O     | 1:D:889:ILE:HG13  | 2.02                     | 0.59              |
| 1:D:1792:ILE:HG12 | 1:D:1842:ILE:HD13 | 1.84                     | 0.59              |
| 1:B:885:LEU:O     | 1:B:889:ILE:HG13  | 2.02                     | 0.59              |
| 1:B:1303:ARG:NH2  | 1:B:1635:GLU:OE1  | 2.35                     | 0.59              |
| 1:B:1792:ILE:HG12 | 1:B:1842:ILE:HD13 | 1.84                     | 0.59              |
| 1:C:3254:PRO:HD2  | 1:C:3268:LEU:H    | 1.67                     | 0.59              |
| 1:D:1303:ARG:NH2  | 1:D:1635:GLU:OE1  | 2.35                     | 0.59              |
| 1:D:4075:ASN:OD1  | 1:D:4077:THR:OG1  | 2.18                     | 0.59              |
| 1:A:885:LEU:O     | 1:A:889:ILE:HG13  | 2.02                     | 0.59              |
| 1:B:2413:LYS:HD2  | 1:B:2416:ALA:H    | 1.66                     | 0.59              |
| 1:B:2594:PHE:HZ   | 1:B:2697:SER:HA   | 1.65                     | 0.59              |
| 1:B:2979:ARG:HB2  | 1:B:3039:THR:HG22 | 1.84                     | 0.59              |
| 1:C:905:GLY:N     | 1:C:915:HIS:H     | 2.00                     | 0.59              |
| 1:C:1303:ARG:NH2  | 1:C:1635:GLU:OE1  | 2.35                     | 0.59              |
| 1:C:4584:PHE:CA   | 1:C:4726:MET:HE1  | 2.32                     | 0.59              |
| 1:D:644:LEU:HD13  | 1:D:1630:LEU:HD21 | 1.84                     | 0.59              |
| 1:D:1941:ARG:HE   | 1:D:3609:TYR:HB2  | 1.66                     | 0.59              |
| 1:B:3236:GLU:HG3  | 1:B:3237:VAL:HG13 | 1.83                     | 0.59              |
| 1:C:693:LEU:HD22  | 1:C:798:ILE:HD12  | 1.85                     | 0.59              |
| 1:C:1256:PRO:HG2  | 1:C:1453:TYR:HB2  | 1.84                     | 0.59              |
| 1:C:1267:HIS:HB3  | 1:C:1287:GLN:HE21 | 1.66                     | 0.59              |
| 1:C:2436:ILE:HA   | 1:C:2465:LYS:HE3  | 1.84                     | 0.59              |
| 2:H:50:ARG:NE     | 2:H:53:LYS:HG3    | 2.15                     | 0.59              |
| 1:B:1256:PRO:HG2  | 1:B:1453:TYR:HB2  | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1795:LEU:HD23 | 1:B:1842:ILE:HD11 | 1.85                     | 0.59              |
| 1:B:2521:CYS:HA   | 1:B:2525:LEU:HD12 | 1.84                     | 0.59              |
| 1:B:2984:SER:O    | 1:B:2996:ALA:N    | 2.35                     | 0.59              |
| 1:B:4584:PHE:CA   | 1:B:4726:MET:HE1  | 2.32                     | 0.59              |
| 1:C:3030:VAL:O    | 1:C:3034:HIS:HD2  | 1.84                     | 0.59              |
| 1:C:3171:LEU:HB3  | 1:C:3211:LEU:HB2  | 1.85                     | 0.59              |
| 1:D:1795:LEU:HD23 | 1:D:1842:ILE:HD11 | 1.85                     | 0.59              |
| 1:D:2979:ARG:HB2  | 1:D:3039:THR:HG22 | 1.84                     | 0.59              |
| 1:D:3171:LEU:HB3  | 1:D:3211:LEU:HB2  | 1.85                     | 0.59              |
| 1:D:3254:PRO:HD2  | 1:D:3268:LEU:H    | 1.67                     | 0.59              |
| 1:A:2979:ARG:HB2  | 1:A:3039:THR:HG22 | 1.84                     | 0.59              |
| 1:B:2545:ILE:HD12 | 1:B:2580:LEU:HD11 | 1.83                     | 0.59              |
| 1:C:2502:LEU:HD23 | 1:C:2507:LEU:HD13 | 1.83                     | 0.59              |
| 1:C:2691:LYS:HE3  | 1:C:2850:ASN:ND2  | 2.17                     | 0.59              |
| 1:D:625:VAL:HG12  | 1:D:2133:ARG:HD3  | 1.85                     | 0.59              |
| 1:D:2413:LYS:HD2  | 1:D:2416:ALA:H    | 1.66                     | 0.59              |
| 1:D:2570:GLU:HG2  | 1:D:2605:MET:HG3  | 1.83                     | 0.59              |
| 1:A:2545:ILE:HD12 | 1:A:2580:LEU:HD11 | 1.83                     | 0.59              |
| 1:A:3254:PRO:HD2  | 1:A:3268:LEU:H    | 1.67                     | 0.59              |
| 1:C:2926:LEU:HD23 | 1:C:3003:MET:HG3  | 1.83                     | 0.59              |
| 1:D:1256:PRO:HG2  | 1:D:1453:TYR:HB2  | 1.84                     | 0.59              |
| 1:A:625:VAL:HG12  | 1:A:2133:ARG:HD3  | 1.85                     | 0.59              |
| 1:A:2744:GLY:HA3  | 1:A:2753:VAL:HB   | 1.84                     | 0.59              |
| 2:F:89:PRO:HB2    | 1:B:1671:ARG:NH2  | 2.17                     | 0.59              |
| 1:C:4027:THR:HA   | 1:C:4032:PHE:HD1  | 1.68                     | 0.59              |
| 1:D:2521:CYS:HA   | 1:D:2525:LEU:HD12 | 1.84                     | 0.59              |
| 1:D:2744:GLY:HA3  | 1:D:2753:VAL:HB   | 1.84                     | 0.59              |
| 1:D:4027:THR:HA   | 1:D:4032:PHE:HD1  | 1.68                     | 0.59              |
| 1:A:693:LEU:HD22  | 1:A:798:ILE:HD12  | 1.85                     | 0.59              |
| 1:A:2570:GLU:HG2  | 1:A:2605:MET:HG3  | 1.83                     | 0.59              |
| 1:A:3279:ASN:O    | 1:A:3283:ILE:HG13 | 2.02                     | 0.59              |
| 1:A:4027:THR:HA   | 1:A:4032:PHE:HD1  | 1.68                     | 0.59              |
| 1:B:4014:LEU:HD13 | 1:B:4122:ALA:HB2  | 1.84                     | 0.59              |
| 1:B:4027:THR:HA   | 1:B:4032:PHE:HD1  | 1.68                     | 0.59              |
| 1:C:644:LEU:HD13  | 1:C:1630:LEU:HD21 | 1.84                     | 0.59              |
| 1:C:885:LEU:O     | 1:C:889:ILE:HG13  | 2.02                     | 0.59              |
| 1:C:2413:LYS:HD2  | 1:C:2416:ALA:H    | 1.66                     | 0.59              |
| 1:C:2545:ILE:HD12 | 1:C:2580:LEU:HD11 | 1.83                     | 0.59              |
| 1:D:3111:HIS:HA   | 1:D:3114:GLN:HG3  | 1.84                     | 0.59              |
| 1:D:3279:ASN:O    | 1:D:3283:ILE:HG13 | 2.02                     | 0.59              |
| 1:D:4187:GLU:OE1  | 1:D:4949:TRP:NE1  | 2.24                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:974:SER:HB3   | 1:A:976:TYR:HD2   | 1.68                     | 0.58              |
| 1:A:1795:LEU:HD23 | 1:A:1842:ILE:HD11 | 1.85                     | 0.58              |
| 1:C:625:VAL:HG12  | 1:C:2133:ARG:HD3  | 1.85                     | 0.58              |
| 1:C:1906:MET:HA   | 1:C:1906:MET:HE3  | 1.85                     | 0.58              |
| 1:A:3240:PRO:HB3  | 1:A:3302:PHE:HD2  | 1.68                     | 0.58              |
| 1:A:4014:LEU:HD13 | 1:A:4122:ALA:HB2  | 1.84                     | 0.58              |
| 1:A:4584:PHE:CA   | 1:A:4726:MET:HE1  | 2.32                     | 0.58              |
| 1:B:974:SER:HB3   | 1:B:976:TYR:HD2   | 1.68                     | 0.58              |
| 1:B:3069:GLU:HA   | 1:B:3072:MET:HG3  | 1.84                     | 0.58              |
| 1:B:3171:LEU:HB3  | 1:B:3211:LEU:HB2  | 1.85                     | 0.58              |
| 1:B:3240:PRO:HB3  | 1:B:3302:PHE:HD2  | 1.68                     | 0.58              |
| 1:B:4481:TRP:HZ2  | 1:B:4694:LEU:HB2  | 1.68                     | 0.58              |
| 1:C:2521:CYS:HA   | 1:C:2525:LEU:HD12 | 1.84                     | 0.58              |
| 1:C:2657:TYR:HA   | 1:C:2662:PHE:CE2  | 2.35                     | 0.58              |
| 1:C:2744:GLY:HA3  | 1:C:2753:VAL:HB   | 1.84                     | 0.58              |
| 1:C:3234:VAL:HA   | 1:C:3238:ILE:HG12 | 1.85                     | 0.58              |
| 1:C:3281:LEU:HB3  | 1:C:3322:LEU:HG   | 1.85                     | 0.58              |
| 1:D:686:VAL:HG11  | 1:D:796:ALA:HB3   | 1.85                     | 0.58              |
| 1:D:892:LEU:HA    | 1:D:895:MET:HE2   | 1.85                     | 0.58              |
| 1:A:1256:PRO:HG2  | 1:A:1453:TYR:HB2  | 1.85                     | 0.58              |
| 1:A:1906:MET:HA   | 1:A:1906:MET:HE3  | 1.85                     | 0.58              |
| 1:A:2436:ILE:HA   | 1:A:2465:LYS:HE3  | 1.84                     | 0.58              |
| 1:B:1007:TRP:NE1  | 4:B:5003:ATP:O3G  | 2.36                     | 0.58              |
| 1:C:66:THR:HG1    | 1:C:124:SER:HG    | 1.51                     | 0.58              |
| 1:C:2722:ASN:O    | 1:C:2723:LYS:HG2  | 2.04                     | 0.58              |
| 1:C:2984:SER:O    | 1:C:2996:ALA:N    | 2.35                     | 0.58              |
| 1:A:686:VAL:HG11  | 1:A:796:ALA:HB3   | 1.85                     | 0.58              |
| 1:A:2138:GLU:HA   | 1:A:2141:LEU:HD12 | 1.86                     | 0.58              |
| 1:A:4481:TRP:HZ2  | 1:A:4694:LEU:HB2  | 1.68                     | 0.58              |
| 1:B:686:VAL:HG11  | 1:B:796:ALA:HB3   | 1.85                     | 0.58              |
| 1:B:693:LEU:HD22  | 1:B:798:ILE:HD12  | 1.85                     | 0.58              |
| 1:B:2436:ILE:HA   | 1:B:2465:LYS:HE3  | 1.84                     | 0.58              |
| 1:B:3234:VAL:HA   | 1:B:3238:ILE:HG12 | 1.85                     | 0.58              |
| 1:C:2658:GLU:OE1  | 1:C:2661:LEU:N    | 2.30                     | 0.58              |
| 1:C:4045:LYS:HG2  | 1:C:4078:LEU:HD23 | 1.85                     | 0.58              |
| 1:D:2722:ASN:O    | 1:D:2723:LYS:HG2  | 2.04                     | 0.58              |
| 1:A:2722:ASN:O    | 1:A:2723:LYS:HG2  | 2.04                     | 0.58              |
| 1:B:892:LEU:HA    | 1:B:895:MET:HE2   | 1.86                     | 0.58              |
| 1:C:892:LEU:HA    | 1:C:895:MET:HE2   | 1.85                     | 0.58              |
| 1:D:3281:LEU:HB3  | 1:D:3322:LEU:HG   | 1.85                     | 0.58              |
| 1:A:892:LEU:HA    | 1:A:895:MET:HE2   | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2843:MET:HA   | 1:A:2846:GLU:HG3  | 1.86                     | 0.58              |
| 1:C:2138:GLU:HA   | 1:C:2141:LEU:HD12 | 1.86                     | 0.58              |
| 1:C:2553:TYR:CE1  | 1:C:2557:LYS:HE2  | 2.39                     | 0.58              |
| 1:C:2639:HIS:O    | 1:C:2643:LYS:HG3  | 2.04                     | 0.58              |
| 1:D:4481:TRP:HZ2  | 1:D:4694:LEU:HB2  | 1.68                     | 0.58              |
| 1:A:2445:ILE:HA   | 1:A:2451:VAL:HA   | 1.86                     | 0.58              |
| 1:A:2984:SER:O    | 1:A:2996:ALA:N    | 2.35                     | 0.58              |
| 1:A:3234:VAL:HA   | 1:A:3238:ILE:HG12 | 1.85                     | 0.58              |
| 1:B:2138:GLU:HA   | 1:B:2141:LEU:HD12 | 1.86                     | 0.58              |
| 1:C:3069:GLU:HA   | 1:C:3072:MET:HG3  | 1.84                     | 0.58              |
| 1:C:3732:HIS:O    | 1:C:3776:LYS:NZ   | 2.37                     | 0.58              |
| 1:D:686:VAL:HG13  | 1:D:687:THR:HG23  | 1.86                     | 0.58              |
| 1:D:2627:TRP:HB2  | 1:D:2630:PHE:HB2  | 1.86                     | 0.58              |
| 1:D:3234:VAL:HA   | 1:D:3238:ILE:HG12 | 1.85                     | 0.58              |
| 1:A:644:LEU:HD13  | 1:A:1630:LEU:HD21 | 1.84                     | 0.58              |
| 1:C:3269:ASN:OD1  | 1:C:3270:SER:N    | 2.37                     | 0.58              |
| 1:D:1016:TRP:CE2  | 1:D:1027:ARG:HG3  | 2.39                     | 0.58              |
| 1:D:2445:ILE:HA   | 1:D:2451:VAL:HA   | 1.86                     | 0.58              |
| 1:D:3269:ASN:OD1  | 1:D:3270:SER:N    | 2.37                     | 0.58              |
| 1:D:4045:LYS:HG2  | 1:D:4078:LEU:HD23 | 1.85                     | 0.58              |
| 1:B:2553:TYR:CE1  | 1:B:2557:LYS:HE2  | 2.39                     | 0.58              |
| 1:B:3219:VAL:HG22 | 1:B:3279:ASN:HD21 | 1.69                     | 0.58              |
| 1:B:3269:ASN:OD1  | 1:B:3270:SER:N    | 2.37                     | 0.58              |
| 1:C:3283:ILE:HA   | 1:C:3286:ASN:HD21 | 1.69                     | 0.58              |
| 1:D:1946:GLU:HA   | 1:D:1949:GLN:HG3  | 1.86                     | 0.58              |
| 1:D:2138:GLU:HA   | 1:D:2141:LEU:HD12 | 1.86                     | 0.58              |
| 1:D:2843:MET:HA   | 1:D:2846:GLU:HG3  | 1.86                     | 0.58              |
| 1:A:1946:GLU:HA   | 1:A:1949:GLN:HG3  | 1.86                     | 0.58              |
| 1:A:2553:TYR:CE1  | 1:A:2557:LYS:HE2  | 2.39                     | 0.58              |
| 1:A:3219:VAL:HG22 | 1:A:3279:ASN:HD21 | 1.69                     | 0.58              |
| 1:A:3281:LEU:HB3  | 1:A:3322:LEU:HG   | 1.85                     | 0.58              |
| 1:B:1016:TRP:CE2  | 1:B:1027:ARG:HG3  | 2.39                     | 0.58              |
| 1:B:4045:LYS:HG2  | 1:B:4078:LEU:HD23 | 1.85                     | 0.58              |
| 1:C:587:ASN:OD1   | 1:C:2133:ARG:NH2  | 2.37                     | 0.58              |
| 1:C:4187:GLU:OE1  | 1:C:4949:TRP:NE1  | 2.24                     | 0.58              |
| 1:C:4481:TRP:HZ2  | 1:C:4694:LEU:HB2  | 1.68                     | 0.58              |
| 1:D:2553:TYR:CE1  | 1:D:2557:LYS:HE2  | 2.39                     | 0.58              |
| 1:D:2639:HIS:O    | 1:D:2643:LYS:HG3  | 2.04                     | 0.58              |
| 1:D:4641:PRO:HB3  | 1:D:4644:TYR:HB3  | 1.86                     | 0.58              |
| 1:A:2686:VAL:HG13 | 1:A:2688:MET:HE3  | 1.86                     | 0.57              |
| 1:A:3219:VAL:HG22 | 1:A:3279:ASN:ND2  | 2.20                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:625:VAL:HG12  | 1:B:2133:ARG:HD3  | 1.85                     | 0.57              |
| 1:C:1016:TRP:CE2  | 1:C:1027:ARG:HG3  | 2.39                     | 0.57              |
| 1:D:974:SER:HB3   | 1:D:976:TYR:HD2   | 1.68                     | 0.57              |
| 1:D:2686:VAL:HG13 | 1:D:2688:MET:HE3  | 1.86                     | 0.57              |
| 1:A:1016:TRP:CE2  | 1:A:1027:ARG:HG3  | 2.39                     | 0.57              |
| 1:A:1671:ARG:HH21 | 2:E:89:PRO:HB2    | 1.69                     | 0.57              |
| 2:E:50:ARG:NE     | 2:E:53:LYS:HG3    | 2.15                     | 0.57              |
| 1:B:644:LEU:HD13  | 1:B:1630:LEU:HD21 | 1.85                     | 0.57              |
| 1:B:2843:MET:HA   | 1:B:2846:GLU:HG3  | 1.86                     | 0.57              |
| 1:B:3219:VAL:HG22 | 1:B:3279:ASN:ND2  | 2.20                     | 0.57              |
| 1:B:3281:LEU:HB3  | 1:B:3322:LEU:HG   | 1.85                     | 0.57              |
| 1:C:2583:SER:HA   | 1:C:2586:GLN:HE22 | 1.69                     | 0.57              |
| 1:C:2627:TRP:HB2  | 1:C:2630:PHE:HB2  | 1.86                     | 0.57              |
| 1:C:3240:PRO:HB3  | 1:C:3302:PHE:HD2  | 1.68                     | 0.57              |
| 1:D:1471:ASP:OD1  | 1:D:1475:LYS:N    | 2.37                     | 0.57              |
| 1:D:3283:ILE:HA   | 1:D:3286:ASN:HD21 | 1.69                     | 0.57              |
| 1:C:887:GLU:HA    | 1:C:890:HIS:ND1   | 2.19                     | 0.57              |
| 1:C:974:SER:HB3   | 1:C:976:TYR:HD2   | 1.68                     | 0.57              |
| 1:C:3219:VAL:HG22 | 1:C:3279:ASN:ND2  | 2.19                     | 0.57              |
| 1:D:1906:MET:HA   | 1:D:1906:MET:HE3  | 1.85                     | 0.57              |
| 1:A:587:ASN:OD1   | 1:A:2133:ARG:NH2  | 2.37                     | 0.57              |
| 1:A:3269:ASN:OD1  | 1:A:3270:SER:N    | 2.37                     | 0.57              |
| 1:B:1946:GLU:HA   | 1:B:1949:GLN:HG3  | 1.86                     | 0.57              |
| 1:B:2565:GLN:O    | 1:B:2569:ILE:HD12 | 2.05                     | 0.57              |
| 1:C:686:VAL:HG13  | 1:C:687:THR:HG23  | 1.86                     | 0.57              |
| 1:D:3219:VAL:HG22 | 1:D:3279:ASN:ND2  | 2.19                     | 0.57              |
| 1:A:2639:HIS:O    | 1:A:2643:LYS:HG3  | 2.04                     | 0.57              |
| 1:B:1144:ARG:HG3  | 1:B:1152:TYR:HB3  | 1.86                     | 0.57              |
| 1:D:587:ASN:OD1   | 1:D:2133:ARG:NH2  | 2.37                     | 0.57              |
| 1:D:693:LEU:HD22  | 1:D:798:ILE:HD12  | 1.85                     | 0.57              |
| 1:D:2583:SER:HA   | 1:D:2586:GLN:HE22 | 1.69                     | 0.57              |
| 1:D:3240:PRO:HB3  | 1:D:3302:PHE:HD2  | 1.68                     | 0.57              |
| 1:A:1007:TRP:NE1  | 4:A:5003:ATP:O3G  | 2.36                     | 0.57              |
| 1:A:2565:GLN:O    | 1:A:2569:ILE:HD12 | 2.05                     | 0.57              |
| 1:A:2999:LYS:HA   | 1:A:3002:GLU:OE1  | 2.05                     | 0.57              |
| 1:A:4864:GLY:HA2  | 1:D:4867:ILE:HG12 | 1.87                     | 0.57              |
| 1:B:1471:ASP:OD1  | 1:B:1475:LYS:N    | 2.37                     | 0.57              |
| 1:B:2722:ASN:O    | 1:B:2723:LYS:HG2  | 2.03                     | 0.57              |
| 1:C:1946:GLU:HA   | 1:C:1949:GLN:HG3  | 1.86                     | 0.57              |
| 1:C:3219:VAL:HG22 | 1:C:3279:ASN:HD21 | 1.69                     | 0.57              |
| 1:C:4641:PRO:HB3  | 1:C:4644:TYR:HB3  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:887:GLU:HA    | 1:D:890:HIS:ND1   | 2.19                     | 0.57              |
| 1:A:1471:ASP:OD1  | 1:A:1475:LYS:N    | 2.37                     | 0.57              |
| 1:A:2583:SER:HA   | 1:A:2586:GLN:HE22 | 1.69                     | 0.57              |
| 1:A:4120:GLU:HA   | 1:A:4123:GLU:OE2  | 2.05                     | 0.57              |
| 1:A:4641:PRO:HB3  | 1:A:4644:TYR:HB3  | 1.86                     | 0.57              |
| 2:H:89:PRO:HB2    | 1:D:1671:ARG:NH2  | 2.20                     | 0.57              |
| 1:B:887:GLU:HA    | 1:B:890:HIS:ND1   | 2.19                     | 0.57              |
| 1:C:1007:TRP:NE1  | 4:C:5003:ATP:O3G  | 2.36                     | 0.57              |
| 1:D:1910:LEU:HD22 | 1:D:2062:ILE:HD11 | 1.87                     | 0.57              |
| 1:D:2726:GLU:HG3  | 1:D:2760:TYR:HB3  | 1.87                     | 0.57              |
| 2:E:58:LYS:HE2    | 2:E:81:VAL:HG12   | 1.87                     | 0.57              |
| 1:C:1910:LEU:HD22 | 1:C:2062:ILE:HD11 | 1.87                     | 0.57              |
| 1:D:2360:ASP:OD2  | 1:D:2383:HIS:ND1  | 2.30                     | 0.57              |
| 1:D:2999:LYS:HA   | 1:D:3002:GLU:OE1  | 2.05                     | 0.57              |
| 1:A:686:VAL:HG13  | 1:A:687:THR:HG23  | 1.86                     | 0.57              |
| 1:A:1910:LEU:HD22 | 1:A:2062:ILE:HD11 | 1.87                     | 0.57              |
| 1:A:2726:GLU:HG3  | 1:A:2760:TYR:HB3  | 1.87                     | 0.57              |
| 1:A:2768:LYS:HB3  | 1:A:2772:ARG:HD3  | 1.87                     | 0.57              |
| 1:A:4518:LEU:HD23 | 1:B:4809:MET:HE3  | 1.87                     | 0.57              |
| 1:B:2639:HIS:O    | 1:B:2643:LYS:HG3  | 2.04                     | 0.57              |
| 1:B:2999:LYS:HA   | 1:B:3002:GLU:OE1  | 2.05                     | 0.57              |
| 1:C:686:VAL:HG11  | 1:C:796:ALA:HB3   | 1.85                     | 0.57              |
| 1:D:3240:PRO:HB3  | 1:D:3302:PHE:CD2  | 2.40                     | 0.57              |
| 1:A:1144:ARG:NH1  | 1:A:1191:ALA:O    | 2.33                     | 0.57              |
| 1:A:2627:TRP:HB2  | 1:A:2630:PHE:HB2  | 1.86                     | 0.57              |
| 1:A:3065:ALA:O    | 1:A:3068:LEU:HG   | 2.05                     | 0.57              |
| 1:B:587:ASN:OD1   | 1:B:2133:ARG:NH2  | 2.37                     | 0.57              |
| 1:B:2445:ILE:HA   | 1:B:2451:VAL:HA   | 1.86                     | 0.57              |
| 1:B:3283:ILE:HA   | 1:B:3286:ASN:HD21 | 1.68                     | 0.57              |
| 1:B:3732:HIS:O    | 1:B:3776:LYS:NZ   | 2.37                     | 0.57              |
| 1:C:2172:MET:O    | 1:C:2176:VAL:HG23 | 2.05                     | 0.57              |
| 1:C:2445:ILE:HA   | 1:C:2451:VAL:HA   | 1.86                     | 0.57              |
| 1:D:34:LYS:N      | 1:D:53:SER:OG     | 2.38                     | 0.57              |
| 1:D:3102:LEU:HD23 | 1:D:3105:LEU:HD21 | 1.87                     | 0.57              |
| 1:D:4120:GLU:HA   | 1:D:4123:GLU:OE2  | 2.05                     | 0.57              |
| 1:D:4800:ASP:OD1  | 1:D:4801:THR:N    | 2.38                     | 0.57              |
| 1:A:3290:ILE:HG13 | 1:A:3291:ASP:H    | 1.70                     | 0.56              |
| 2:H:8:ILE:HA      | 1:D:730:LEU:HD11  | 1.87                     | 0.56              |
| 2:H:58:LYS:HE2    | 2:H:81:VAL:HG12   | 1.87                     | 0.56              |
| 1:B:1906:MET:HA   | 1:B:1906:MET:HE3  | 1.85                     | 0.56              |
| 1:C:2843:MET:HA   | 1:C:2846:GLU:HG3  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3134:LEU:HB2  | 1:C:3162:PHE:CE2  | 2.40                     | 0.56              |
| 1:A:4045:LYS:HG2  | 1:A:4078:LEU:HD23 | 1.85                     | 0.56              |
| 1:B:3065:ALA:O    | 1:B:3068:LEU:HG   | 2.05                     | 0.56              |
| 1:B:3240:PRO:HB3  | 1:B:3302:PHE:CD2  | 2.40                     | 0.56              |
| 1:C:1144:ARG:HG3  | 1:C:1152:TYR:HB3  | 1.86                     | 0.56              |
| 1:C:2999:LYS:HA   | 1:C:3002:GLU:OE1  | 2.05                     | 0.56              |
| 1:C:3026:ALA:O    | 1:C:3030:VAL:HG23 | 2.05                     | 0.56              |
| 1:D:1144:ARG:NH1  | 1:D:1191:ALA:O    | 2.33                     | 0.56              |
| 1:D:2565:GLN:O    | 1:D:2569:ILE:HD12 | 2.05                     | 0.56              |
| 1:A:2204:CYS:SG   | 1:A:2214:MET:HG3  | 2.46                     | 0.56              |
| 1:A:3102:LEU:HD23 | 1:A:3105:LEU:HD21 | 1.87                     | 0.56              |
| 1:A:3732:HIS:O    | 1:A:3776:LYS:NZ   | 2.37                     | 0.56              |
| 1:B:254:GLU:CD    | 1:B:258:ARG:HE    | 2.14                     | 0.56              |
| 1:B:375:GLN:N     | 1:B:390:LYS:O     | 2.34                     | 0.56              |
| 1:B:686:VAL:HG13  | 1:B:687:THR:HG23  | 1.86                     | 0.56              |
| 1:B:977:LYS:HB2   | 1:B:980:PRO:HG3   | 1.87                     | 0.56              |
| 1:B:1910:LEU:HD22 | 1:B:2062:ILE:HD11 | 1.87                     | 0.56              |
| 1:B:2488:LEU:HD21 | 1:B:2548:LEU:HD22 | 1.88                     | 0.56              |
| 1:B:2583:SER:HA   | 1:B:2586:GLN:HE22 | 1.69                     | 0.56              |
| 1:B:2686:VAL:HG13 | 1:B:2688:MET:HE3  | 1.86                     | 0.56              |
| 1:B:2768:LYS:HB3  | 1:B:2772:ARG:HD3  | 1.87                     | 0.56              |
| 1:C:34:LYS:N      | 1:C:53:SER:OG     | 2.38                     | 0.56              |
| 1:C:879:GLU:HG3   | 1:C:937:LEU:HG    | 1.87                     | 0.56              |
| 1:C:2619:LYS:HZ1  | 1:C:2627:TRP:CD1  | 2.22                     | 0.56              |
| 1:D:335:LYS:NZ    | 1:D:401:ASP:OD2   | 2.31                     | 0.56              |
| 1:D:2445:ILE:HG13 | 1:D:2865:GLY:HA2  | 1.88                     | 0.56              |
| 1:D:2984:SER:O    | 1:D:2996:ALA:N    | 2.35                     | 0.56              |
| 1:A:1144:ARG:HG3  | 1:A:1152:TYR:HB3  | 1.86                     | 0.56              |
| 1:A:2125:GLN:OE1  | 1:A:2144:ARG:NH1  | 2.39                     | 0.56              |
| 1:A:3026:ALA:O    | 1:A:3030:VAL:HG23 | 2.05                     | 0.56              |
| 1:A:3134:LEU:HB2  | 1:A:3162:PHE:CE2  | 2.40                     | 0.56              |
| 1:A:4075:ASN:OD1  | 1:A:4077:THR:OG1  | 2.18                     | 0.56              |
| 1:B:2176:VAL:HG22 | 1:B:2220:TYR:CZ   | 2.41                     | 0.56              |
| 1:B:3134:LEU:HB2  | 1:B:3162:PHE:CE2  | 2.40                     | 0.56              |
| 1:B:3290:ILE:HG13 | 1:B:3291:ASP:H    | 1.70                     | 0.56              |
| 1:B:4673:ASP:HB3  | 1:B:4676:ALA:HB3  | 1.87                     | 0.56              |
| 1:C:2565:GLN:O    | 1:C:2569:ILE:HD12 | 2.05                     | 0.56              |
| 1:C:3240:PRO:HB3  | 1:C:3302:PHE:CD2  | 2.40                     | 0.56              |
| 1:D:1007:TRP:NE1  | 4:D:5003:ATP:O3G  | 2.36                     | 0.56              |
| 1:D:2488:LEU:HD21 | 1:D:2548:LEU:HD22 | 1.88                     | 0.56              |
| 1:D:3219:VAL:HG22 | 1:D:3279:ASN:HD21 | 1.69                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1226:TYR:HD1  | 1:A:1229:ILE:HD11 | 1.71                     | 0.56              |
| 1:A:2765:GLU:OE2  | 1:A:2772:ARG:NH2  | 2.38                     | 0.56              |
| 1:A:3283:ILE:HA   | 1:A:3286:ASN:HD21 | 1.69                     | 0.56              |
| 1:A:4800:ASP:OD1  | 1:A:4801:THR:N    | 2.38                     | 0.56              |
| 1:B:34:LYS:N      | 1:B:53:SER:OG     | 2.38                     | 0.56              |
| 1:B:2627:TRP:HB2  | 1:B:2630:PHE:HB2  | 1.86                     | 0.56              |
| 1:B:3026:ALA:O    | 1:B:3030:VAL:HG23 | 2.06                     | 0.56              |
| 1:C:1226:TYR:HD1  | 1:C:1229:ILE:HD11 | 1.71                     | 0.56              |
| 1:C:1471:ASP:OD1  | 1:C:1475:LYS:N    | 2.37                     | 0.56              |
| 1:D:2172:MET:O    | 1:D:2176:VAL:HG23 | 2.05                     | 0.56              |
| 1:A:2172:MET:O    | 1:A:2176:VAL:HG23 | 2.05                     | 0.56              |
| 1:A:2619:LYS:HZ1  | 1:A:2627:TRP:CD1  | 2.24                     | 0.56              |
| 1:A:4673:ASP:HB3  | 1:A:4676:ALA:HB3  | 1.87                     | 0.56              |
| 1:A:4709:LYS:O    | 1:A:4713:VAL:HG23 | 2.06                     | 0.56              |
| 1:B:2172:MET:O    | 1:B:2176:VAL:HG23 | 2.05                     | 0.56              |
| 1:B:3252:HIS:C    | 1:B:3260:ARG:HH22 | 2.13                     | 0.56              |
| 1:B:4641:PRO:HB3  | 1:B:4644:TYR:HB3  | 1.86                     | 0.56              |
| 1:C:2659:GLN:O    | 1:C:2663:LYS:HG2  | 2.06                     | 0.56              |
| 1:C:2687:SER:C    | 1:C:2688:MET:HE2  | 2.31                     | 0.56              |
| 1:C:2726:GLU:HG3  | 1:C:2760:TYR:HB3  | 1.87                     | 0.56              |
| 1:D:2619:LYS:HZ1  | 1:D:2627:TRP:CD1  | 2.24                     | 0.56              |
| 1:D:3134:LEU:HB2  | 1:D:3162:PHE:CE2  | 2.40                     | 0.56              |
| 1:A:254:GLU:CD    | 1:A:258:ARG:HE    | 2.14                     | 0.56              |
| 1:A:2445:ILE:HG13 | 1:A:2865:GLY:HA2  | 1.88                     | 0.56              |
| 1:A:3252:HIS:C    | 1:A:3260:ARG:HH22 | 2.13                     | 0.56              |
| 1:B:2204:CYS:SG   | 1:B:2214:MET:HG3  | 2.46                     | 0.56              |
| 1:B:4709:LYS:O    | 1:B:4713:VAL:HG23 | 2.06                     | 0.56              |
| 1:D:977:LYS:HB2   | 1:D:980:PRO:HG3   | 1.87                     | 0.56              |
| 1:D:2176:VAL:HG22 | 1:D:2220:TYR:CZ   | 2.41                     | 0.56              |
| 1:D:3252:HIS:C    | 1:D:3260:ARG:HH22 | 2.13                     | 0.56              |
| 1:A:879:GLU:HG3   | 1:A:937:LEU:HG    | 1.87                     | 0.56              |
| 1:A:887:GLU:HA    | 1:A:890:HIS:ND1   | 2.19                     | 0.56              |
| 1:B:2659:GLN:O    | 1:B:2663:LYS:HG2  | 2.06                     | 0.56              |
| 1:B:4800:ASP:OD1  | 1:B:4801:THR:N    | 2.38                     | 0.56              |
| 1:C:2176:VAL:HG22 | 1:C:2220:TYR:CZ   | 2.41                     | 0.56              |
| 1:D:2765:GLU:OE2  | 1:D:2772:ARG:NH2  | 2.38                     | 0.56              |
| 1:D:2857:LYS:O    | 1:D:2860:LEU:HG   | 2.06                     | 0.56              |
| 1:D:3290:ILE:HG13 | 1:D:3291:ASP:H    | 1.70                     | 0.56              |
| 1:A:3240:PRO:HB3  | 1:A:3302:PHE:CD2  | 2.40                     | 0.56              |
| 1:B:3257:ASN:HD21 | 1:B:3260:ARG:HH21 | 1.54                     | 0.56              |
| 1:B:4120:GLU:HA   | 1:B:4123:GLU:OE2  | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2204:CYS:SG   | 1:C:2214:MET:HG3  | 2.46                     | 0.56              |
| 1:C:2686:VAL:HG13 | 1:C:2688:MET:HE3  | 1.86                     | 0.56              |
| 1:C:3102:LEU:HD23 | 1:C:3105:LEU:HD21 | 1.87                     | 0.56              |
| 1:C:3290:ILE:HG13 | 1:C:3291:ASP:H    | 1.70                     | 0.56              |
| 1:D:2443:PRO:HB3  | 1:D:2453:GLU:HA   | 1.87                     | 0.56              |
| 1:D:2687:SER:C    | 1:D:2688:MET:HE2  | 2.31                     | 0.56              |
| 1:A:34:LYS:N      | 1:A:53:SER:OG     | 2.38                     | 0.56              |
| 1:A:2443:PRO:HB3  | 1:A:2453:GLU:HA   | 1.88                     | 0.56              |
| 1:B:2644:LEU:O    | 1:B:2648:ILE:HG13 | 2.06                     | 0.56              |
| 1:B:2830:ASN:ND2  | 1:C:1551:ASN:O    | 2.31                     | 0.56              |
| 1:C:3065:ALA:O    | 1:C:3068:LEU:HG   | 2.05                     | 0.56              |
| 1:D:1144:ARG:HG3  | 1:D:1152:TYR:HB3  | 1.86                     | 0.56              |
| 1:D:1226:TYR:HD1  | 1:D:1229:ILE:HD11 | 1.71                     | 0.56              |
| 1:D:2125:GLN:OE1  | 1:D:2144:ARG:NH1  | 2.39                     | 0.56              |
| 1:A:1757:LEU:HD22 | 1:A:2117:ILE:HD11 | 1.88                     | 0.55              |
| 1:A:2687:SER:C    | 1:A:2688:MET:HE2  | 2.31                     | 0.55              |
| 2:F:50:ARG:NE     | 2:F:53:LYS:HG3    | 2.15                     | 0.55              |
| 2:G:58:LYS:HE2    | 2:G:81:VAL:HG12   | 1.87                     | 0.55              |
| 1:B:3102:LEU:HD23 | 1:B:3105:LEU:HD21 | 1.87                     | 0.55              |
| 1:B:3211:LEU:HD23 | 1:B:3215:MET:HE1  | 1.89                     | 0.55              |
| 1:C:755:ILE:HG13  | 1:C:770:ILE:HD13  | 1.89                     | 0.55              |
| 1:C:977:LYS:HB2   | 1:C:980:PRO:HG3   | 1.87                     | 0.55              |
| 1:C:2488:LEU:HD21 | 1:C:2548:LEU:HD22 | 1.87                     | 0.55              |
| 1:C:4673:ASP:HB3  | 1:C:4676:ALA:HB3  | 1.87                     | 0.55              |
| 1:D:879:GLU:HG3   | 1:D:937:LEU:HG    | 1.87                     | 0.55              |
| 1:A:2659:GLN:O    | 1:A:2663:LYS:HG2  | 2.06                     | 0.55              |
| 1:A:2857:LYS:O    | 1:A:2860:LEU:HG   | 2.06                     | 0.55              |
| 1:B:2125:GLN:OE1  | 1:B:2144:ARG:NH1  | 2.39                     | 0.55              |
| 1:B:2726:GLU:HG3  | 1:B:2760:TYR:HB3  | 1.87                     | 0.55              |
| 1:B:2765:GLU:OE2  | 1:B:2772:ARG:NH2  | 2.38                     | 0.55              |
| 1:B:3285:TYR:CD1  | 1:B:3325:LYS:HG2  | 2.41                     | 0.55              |
| 1:B:4031:THR:O    | 1:B:4034:GLU:HG3  | 2.07                     | 0.55              |
| 1:C:3252:HIS:C    | 1:C:3260:ARG:HH22 | 2.13                     | 0.55              |
| 1:C:4709:LYS:O    | 1:C:4713:VAL:HG23 | 2.06                     | 0.55              |
| 1:C:4800:ASP:OD1  | 1:C:4801:THR:N    | 2.38                     | 0.55              |
| 1:D:375:GLN:N     | 1:D:390:LYS:O     | 2.34                     | 0.55              |
| 1:D:666:GLY:HA2   | 1:D:1012:ILE:HG21 | 1.87                     | 0.55              |
| 1:D:755:ILE:HG13  | 1:D:770:ILE:HD13  | 1.88                     | 0.55              |
| 1:D:2204:CYS:SG   | 1:D:2214:MET:HG3  | 2.46                     | 0.55              |
| 1:D:3211:LEU:HD23 | 1:D:3215:MET:HE1  | 1.89                     | 0.55              |
| 1:D:3285:TYR:CD1  | 1:D:3325:LYS:HG2  | 2.41                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4031:THR:O    | 1:A:4034:GLU:HG3  | 2.07                     | 0.55              |
| 2:G:80:ASP:OD1    | 2:G:81:VAL:N      | 2.40                     | 0.55              |
| 1:B:246:THR:HG21  | 1:B:267:VAL:HG21  | 1.89                     | 0.55              |
| 1:B:666:GLY:HA2   | 1:B:1012:ILE:HG21 | 1.87                     | 0.55              |
| 1:B:2619:LYS:HZ1  | 1:B:2627:TRP:CD1  | 2.24                     | 0.55              |
| 1:B:3019:ILE:H    | 1:B:3019:ILE:HD12 | 1.72                     | 0.55              |
| 1:C:254:GLU:CD    | 1:C:258:ARG:HE    | 2.14                     | 0.55              |
| 1:C:2360:ASP:OD2  | 1:C:2383:HIS:ND1  | 2.30                     | 0.55              |
| 1:C:2445:ILE:HG13 | 1:C:2865:GLY:HA2  | 1.88                     | 0.55              |
| 1:C:2644:LEU:O    | 1:C:2648:ILE:HG13 | 2.07                     | 0.55              |
| 1:C:2765:GLU:OE2  | 1:C:2772:ARG:NH2  | 2.38                     | 0.55              |
| 1:C:3211:LEU:HD23 | 1:C:3215:MET:HE1  | 1.88                     | 0.55              |
| 1:C:4120:GLU:HA   | 1:C:4123:GLU:OE2  | 2.05                     | 0.55              |
| 1:D:1757:LEU:HD22 | 1:D:2117:ILE:HD11 | 1.89                     | 0.55              |
| 1:D:4031:THR:O    | 1:D:4034:GLU:HG3  | 2.07                     | 0.55              |
| 1:D:4709:LYS:O    | 1:D:4713:VAL:HG23 | 2.06                     | 0.55              |
| 1:A:335:LYS:NZ    | 1:A:401:ASP:OD2   | 2.31                     | 0.55              |
| 1:A:3019:ILE:H    | 1:A:3019:ILE:HD12 | 1.72                     | 0.55              |
| 2:F:80:ASP:OD1    | 2:F:81:VAL:N      | 2.40                     | 0.55              |
| 1:B:879:GLU:HG3   | 1:B:937:LEU:HG    | 1.87                     | 0.55              |
| 1:B:2929:LEU:HD21 | 1:B:2971:ILE:HG12 | 1.89                     | 0.55              |
| 1:B:3109:PHE:CE1  | 1:B:3162:PHE:HD1  | 2.24                     | 0.55              |
| 1:C:2844:MET:O    | 1:C:2847:ASN:OD1  | 2.24                     | 0.55              |
| 1:D:3691:TYR:O    | 1:D:3695:MET:HG3  | 2.07                     | 0.55              |
| 1:D:3732:HIS:O    | 1:D:3776:LYS:NZ   | 2.36                     | 0.55              |
| 1:D:4673:ASP:HB3  | 1:D:4676:ALA:HB3  | 1.87                     | 0.55              |
| 1:A:1551:ASN:O    | 1:D:2830:ASN:ND2  | 2.35                     | 0.55              |
| 2:F:58:LYS:HE2    | 2:F:81:VAL:HG12   | 1.87                     | 0.55              |
| 1:C:2768:LYS:HB3  | 1:C:2772:ARG:HD3  | 1.87                     | 0.55              |
| 1:C:2857:LYS:O    | 1:C:2860:LEU:HG   | 2.06                     | 0.55              |
| 1:C:3691:TYR:O    | 1:C:3695:MET:HG3  | 2.07                     | 0.55              |
| 1:D:2142:MET:CE   | 1:D:2192:MET:HG2  | 2.37                     | 0.55              |
| 1:D:2844:MET:O    | 1:D:2847:ASN:OD1  | 2.25                     | 0.55              |
| 1:D:2929:LEU:HD21 | 1:D:2971:ILE:HG12 | 1.89                     | 0.55              |
| 1:D:3026:ALA:O    | 1:D:3030:VAL:HG23 | 2.05                     | 0.55              |
| 1:D:3065:ALA:O    | 1:D:3068:LEU:HG   | 2.05                     | 0.55              |
| 1:A:246:THR:HG21  | 1:A:267:VAL:HG21  | 1.89                     | 0.55              |
| 1:A:977:LYS:HB2   | 1:A:980:PRO:HG3   | 1.87                     | 0.55              |
| 1:A:2488:LEU:HD21 | 1:A:2548:LEU:HD22 | 1.88                     | 0.55              |
| 2:H:80:ASP:OD1    | 2:H:81:VAL:N      | 2.40                     | 0.55              |
| 1:B:2360:ASP:OD2  | 1:B:2383:HIS:ND1  | 2.30                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2537:GLY:O    | 1:B:2540:HIS:NE2  | 2.38                     | 0.55              |
| 1:C:2125:GLN:OE1  | 1:C:2144:ARG:NH1  | 2.39                     | 0.55              |
| 1:C:2719:TYR:HD2  | 1:C:2791:ARG:HH12 | 1.55                     | 0.55              |
| 1:C:3832:ASP:HB3  | 1:C:3835:PHE:HB3  | 1.89                     | 0.55              |
| 1:D:467:ASP:OD2   | 1:D:469:HIS:NE2   | 2.40                     | 0.55              |
| 1:A:467:ASP:OD2   | 1:A:469:HIS:NE2   | 2.40                     | 0.55              |
| 1:A:666:GLY:HA2   | 1:A:1012:ILE:HG21 | 1.87                     | 0.55              |
| 1:A:2420:ARG:HG2  | 1:A:2424:ARG:HD2  | 1.89                     | 0.55              |
| 1:A:2929:LEU:HD21 | 1:A:2971:ILE:HG12 | 1.89                     | 0.55              |
| 1:B:2640:LEU:HA   | 1:B:2643:LYS:HE2  | 1.89                     | 0.55              |
| 1:B:3193:ALA:HA   | 1:B:3199:THR:HG21 | 1.89                     | 0.55              |
| 1:C:4031:THR:O    | 1:C:4034:GLU:HG3  | 2.07                     | 0.55              |
| 1:D:2420:ARG:HG2  | 1:D:2424:ARG:HD2  | 1.89                     | 0.55              |
| 1:D:2659:GLN:O    | 1:D:2663:LYS:HG2  | 2.06                     | 0.55              |
| 1:D:3178:HIS:NE2  | 1:D:3262:GLU:O    | 2.40                     | 0.55              |
| 1:D:3193:ALA:HA   | 1:D:3199:THR:HG21 | 1.89                     | 0.55              |
| 1:D:4640:PHE:CD2  | 1:D:4641:PRO:HD3  | 2.42                     | 0.55              |
| 1:A:3109:PHE:CE1  | 1:A:3162:PHE:HD1  | 2.24                     | 0.55              |
| 1:A:3285:TYR:CD1  | 1:A:3325:LYS:HG2  | 2.41                     | 0.55              |
| 1:A:4082:GLU:HA   | 1:A:4085:LYS:HG2  | 1.89                     | 0.55              |
| 2:E:80:ASP:OD1    | 2:E:81:VAL:N      | 2.40                     | 0.55              |
| 1:B:3691:TYR:O    | 1:B:3695:MET:HG3  | 2.07                     | 0.55              |
| 1:C:246:THR:HG21  | 1:C:267:VAL:HG21  | 1.89                     | 0.55              |
| 1:C:2929:LEU:HD21 | 1:C:2971:ILE:HG12 | 1.89                     | 0.55              |
| 1:C:3257:ASN:HD21 | 1:C:3260:ARG:HH21 | 1.54                     | 0.55              |
| 1:C:4075:ASN:OD1  | 1:C:4077:THR:OG1  | 2.18                     | 0.55              |
| 1:A:2176:VAL:HG22 | 1:A:2220:TYR:CZ   | 2.41                     | 0.55              |
| 1:A:2644:LEU:O    | 1:A:2648:ILE:HG13 | 2.06                     | 0.55              |
| 1:A:3257:ASN:HD21 | 1:A:3260:ARG:HH21 | 1.54                     | 0.55              |
| 1:A:4640:PHE:CD2  | 1:A:4641:PRO:HD3  | 2.42                     | 0.55              |
| 1:B:755:ILE:HG13  | 1:B:770:ILE:HD13  | 1.88                     | 0.55              |
| 1:B:1226:TYR:HD1  | 1:B:1229:ILE:HD11 | 1.71                     | 0.55              |
| 1:B:2142:MET:CE   | 1:B:2192:MET:HG2  | 2.37                     | 0.55              |
| 1:B:2445:ILE:HG13 | 1:B:2865:GLY:HA2  | 1.88                     | 0.55              |
| 1:B:2729:HIS:N    | 1:B:2771:TYR:OH   | 2.40                     | 0.55              |
| 1:C:2581:ARG:HH21 | 1:C:2582:PRO:HG2  | 1.72                     | 0.55              |
| 1:C:3193:ALA:HA   | 1:C:3199:THR:HG21 | 1.89                     | 0.55              |
| 1:D:114:LEU:HB2   | 1:D:117:HIS:CD2   | 2.42                     | 0.55              |
| 1:D:1239:PHE:O    | 1:D:1807:ARG:NH1  | 2.40                     | 0.55              |
| 1:A:2640:LEU:HA   | 1:A:2643:LYS:HE2  | 1.89                     | 0.55              |
| 1:A:3193:ALA:HA   | 1:A:3199:THR:HG21 | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:719:GLY:H     | 1:B:724:SER:HB2   | 1.72                     | 0.55              |
| 1:B:2687:SER:C    | 1:B:2688:MET:HE2  | 2.31                     | 0.55              |
| 1:B:4640:PHE:CD2  | 1:B:4641:PRO:HD3  | 2.42                     | 0.55              |
| 1:D:254:GLU:CD    | 1:D:258:ARG:HE    | 2.14                     | 0.55              |
| 1:D:2644:LEU:O    | 1:D:2648:ILE:HG13 | 2.07                     | 0.55              |
| 1:A:114:LEU:HB2   | 1:A:117:HIS:CD2   | 2.42                     | 0.54              |
| 1:A:2729:HIS:N    | 1:A:2771:TYR:OH   | 2.40                     | 0.54              |
| 1:A:3211:LEU:HD23 | 1:A:3215:MET:HE1  | 1.89                     | 0.54              |
| 1:B:1757:LEU:HD22 | 1:B:2117:ILE:HD11 | 1.89                     | 0.54              |
| 1:B:2844:MET:O    | 1:B:2847:ASN:OD1  | 2.24                     | 0.54              |
| 1:B:2857:LYS:O    | 1:B:2860:LEU:HG   | 2.06                     | 0.54              |
| 1:B:3178:HIS:NE2  | 1:B:3262:GLU:O    | 2.40                     | 0.54              |
| 1:C:3019:ILE:H    | 1:C:3019:ILE:HD12 | 1.72                     | 0.54              |
| 1:C:3285:TYR:CD1  | 1:C:3325:LYS:HG2  | 2.41                     | 0.54              |
| 1:C:3986:LEU:HD12 | 1:C:4101:LEU:HD12 | 1.89                     | 0.54              |
| 1:C:4640:PHE:CD2  | 1:C:4641:PRO:HD3  | 2.42                     | 0.54              |
| 1:D:2537:GLY:O    | 1:D:2540:HIS:NE2  | 2.38                     | 0.54              |
| 1:D:3019:ILE:HD12 | 1:D:3019:ILE:H    | 1.72                     | 0.54              |
| 1:D:3986:LEU:HD12 | 1:D:4101:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:719:GLY:H     | 1:A:724:SER:HB2   | 1.72                     | 0.54              |
| 1:A:1010:ASP:OD1  | 1:A:1013:ARG:NH1  | 2.39                     | 0.54              |
| 1:A:4169:LYS:NZ   | 4:A:5002:ATP:O2A  | 2.38                     | 0.54              |
| 1:B:467:ASP:OD2   | 1:B:469:HIS:NE2   | 2.40                     | 0.54              |
| 1:B:4082:GLU:HA   | 1:B:4085:LYS:HG2  | 1.89                     | 0.54              |
| 1:C:905:GLY:HA3   | 1:C:914:GLN:CB    | 2.37                     | 0.54              |
| 1:D:131:CYS:SG    | 1:D:150:GLN:HB2   | 2.47                     | 0.54              |
| 1:D:2768:LYS:HB3  | 1:D:2772:ARG:HD3  | 1.87                     | 0.54              |
| 1:D:4854:VAL:HA   | 1:D:4858:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:2581:ARG:HH21 | 1:A:2582:PRO:HG2  | 1.72                     | 0.54              |
| 1:A:2846:GLU:HG2  | 1:A:2874:TYR:CD2  | 2.43                     | 0.54              |
| 1:B:114:LEU:HB2   | 1:B:117:HIS:CD2   | 2.42                     | 0.54              |
| 1:B:1010:ASP:OD1  | 1:B:1013:ARG:NH1  | 2.39                     | 0.54              |
| 1:B:2420:ARG:HG2  | 1:B:2424:ARG:HD2  | 1.89                     | 0.54              |
| 1:B:2719:TYR:HD2  | 1:B:2791:ARG:HH12 | 1.55                     | 0.54              |
| 1:B:4854:VAL:HA   | 1:B:4858:LEU:HD12 | 1.89                     | 0.54              |
| 1:C:2420:ARG:HG2  | 1:C:2424:ARG:HD2  | 1.89                     | 0.54              |
| 1:D:719:GLY:H     | 1:D:724:SER:HB2   | 1.72                     | 0.54              |
| 1:D:1645:THR:HG22 | 1:D:1695:PRO:HG3  | 1.90                     | 0.54              |
| 1:A:2844:MET:O    | 1:A:2847:ASN:OD1  | 2.24                     | 0.54              |
| 1:B:905:GLY:HA3   | 1:B:914:GLN:CB    | 2.37                     | 0.54              |
| 1:B:1645:THR:HG22 | 1:B:1695:PRO:HG3  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2443:PRO:HB3  | 1:B:2453:GLU:HA   | 1.87                     | 0.54              |
| 1:B:2581:ARG:HH21 | 1:B:2582:PRO:HG2  | 1.72                     | 0.54              |
| 1:B:2917:ILE:HD11 | 1:B:2999:LYS:HD2  | 1.90                     | 0.54              |
| 1:C:666:GLY:HA2   | 1:C:1012:ILE:HG21 | 1.87                     | 0.54              |
| 1:C:1757:LEU:HD22 | 1:C:2117:ILE:HD11 | 1.88                     | 0.54              |
| 1:D:1939:ASN:OD1  | 1:D:1940:GLN:N    | 2.41                     | 0.54              |
| 1:D:4023:LEU:HG   | 1:D:4084:VAL:HG12 | 1.90                     | 0.54              |
| 1:A:2836:ASP:OD1  | 1:A:2837:LEU:N    | 2.41                     | 0.54              |
| 1:A:2917:ILE:HD11 | 1:A:2999:LYS:HD2  | 1.90                     | 0.54              |
| 1:A:3691:TYR:O    | 1:A:3695:MET:HG3  | 2.07                     | 0.54              |
| 1:A:4116:GLN:HA   | 1:A:4119:LEU:HD12 | 1.90                     | 0.54              |
| 1:B:1939:ASN:OD1  | 1:B:1940:GLN:N    | 2.41                     | 0.54              |
| 1:C:131:CYS:SG    | 1:C:150:GLN:HB2   | 2.47                     | 0.54              |
| 1:C:1440:ASN:HB3  | 1:C:1546:GLN:HB3  | 1.90                     | 0.54              |
| 1:C:2142:MET:CE   | 1:C:2192:MET:HG2  | 2.37                     | 0.54              |
| 1:C:3178:HIS:NE2  | 1:C:3262:GLU:O    | 2.40                     | 0.54              |
| 1:D:246:THR:HG21  | 1:D:267:VAL:HG21  | 1.89                     | 0.54              |
| 1:D:4082:GLU:HA   | 1:D:4085:LYS:HG2  | 1.89                     | 0.54              |
| 1:A:1645:THR:HG22 | 1:A:1695:PRO:HG3  | 1.90                     | 0.54              |
| 1:A:3178:HIS:NE2  | 1:A:3262:GLU:O    | 2.40                     | 0.54              |
| 1:B:2975:PHE:HB3  | 1:B:3039:THR:HG21 | 1.89                     | 0.54              |
| 1:C:1010:ASP:OD1  | 1:C:1013:ARG:NH1  | 2.39                     | 0.54              |
| 1:C:1144:ARG:NH1  | 1:C:1191:ALA:O    | 2.33                     | 0.54              |
| 1:D:2179:LEU:HD23 | 1:D:2187:ILE:HD13 | 1.89                     | 0.54              |
| 1:D:2917:ILE:HD11 | 1:D:2999:LYS:HD2  | 1.90                     | 0.54              |
| 1:D:3283:ILE:HA   | 1:D:3286:ASN:ND2  | 2.23                     | 0.54              |
| 1:D:3832:ASP:HB3  | 1:D:3835:PHE:HB3  | 1.89                     | 0.54              |
| 1:D:4116:GLN:HA   | 1:D:4119:LEU:HD12 | 1.90                     | 0.54              |
| 1:A:755:ILE:HG13  | 1:A:770:ILE:HD13  | 1.89                     | 0.54              |
| 1:A:3283:ILE:HA   | 1:A:3286:ASN:ND2  | 2.23                     | 0.54              |
| 1:A:3832:ASP:HB3  | 1:A:3835:PHE:HB3  | 1.89                     | 0.54              |
| 1:B:1239:PHE:O    | 1:B:1807:ARG:NH1  | 2.40                     | 0.54              |
| 1:C:467:ASP:OD2   | 1:C:469:HIS:NE2   | 2.40                     | 0.54              |
| 1:C:3237:VAL:HG23 | 1:C:3238:ILE:HG23 | 1.90                     | 0.54              |
| 1:D:1440:ASN:HB3  | 1:D:1546:GLN:HB3  | 1.90                     | 0.54              |
| 1:D:2719:TYR:HD2  | 1:D:2791:ARG:HH12 | 1.55                     | 0.54              |
| 1:D:4169:LYS:NZ   | 4:D:5002:ATP:O2A  | 2.38                     | 0.54              |
| 1:A:2142:MET:CE   | 1:A:2192:MET:HG2  | 2.37                     | 0.54              |
| 1:B:254:GLU:OE2   | 1:B:258:ARG:NE    | 2.41                     | 0.54              |
| 1:B:1272:ARG:NH2  | 1:B:1582:CYS:SG   | 2.81                     | 0.54              |
| 1:B:3069:GLU:CD   | 1:B:3132:ARG:HH11 | 2.16                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3986:LEU:HD12 | 1:B:4101:LEU:HD12 | 1.89                     | 0.54              |
| 1:C:114:LEU:HB2   | 1:C:117:HIS:CD2   | 2.42                     | 0.54              |
| 1:C:1645:THR:HG22 | 1:C:1695:PRO:HG3  | 1.89                     | 0.54              |
| 1:C:1939:ASN:OD1  | 1:C:1940:GLN:N    | 2.41                     | 0.54              |
| 1:C:2711:ILE:HD12 | 1:C:2783:LEU:HB3  | 1.90                     | 0.54              |
| 1:C:2729:HIS:N    | 1:C:2771:TYR:OH   | 2.40                     | 0.54              |
| 1:C:2917:ILE:HD11 | 1:C:2999:LYS:HD2  | 1.90                     | 0.54              |
| 1:C:3109:PHE:CE1  | 1:C:3162:PHE:HD1  | 2.24                     | 0.54              |
| 1:D:857:LEU:HG    | 1:D:860:ALA:HB2   | 1.89                     | 0.54              |
| 1:D:1074:ARG:HH12 | 1:D:1078:CYS:H    | 1.56                     | 0.54              |
| 1:D:2640:LEU:HA   | 1:D:2643:LYS:HE2  | 1.89                     | 0.54              |
| 1:D:2852:TRP:O    | 1:D:2855:LYS:HG2  | 2.08                     | 0.54              |
| 1:D:3846:LEU:HB3  | 1:D:3854:PHE:CE2  | 2.43                     | 0.54              |
| 1:A:131:CYS:SG    | 1:A:150:GLN:HB2   | 2.47                     | 0.54              |
| 1:A:4854:VAL:HA   | 1:A:4858:LEU:HD12 | 1.89                     | 0.54              |
| 2:H:30:MET:HB2    | 2:H:99:ILE:HG13   | 1.90                     | 0.54              |
| 1:B:131:CYS:SG    | 1:B:150:GLN:HB2   | 2.47                     | 0.54              |
| 1:B:2443:PRO:HD3  | 1:B:2512:MET:HE2  | 1.90                     | 0.54              |
| 1:C:719:GLY:H     | 1:C:724:SER:HB2   | 1.72                     | 0.54              |
| 1:C:2443:PRO:HB3  | 1:C:2453:GLU:HA   | 1.88                     | 0.54              |
| 1:C:3069:GLU:CD   | 1:C:3132:ARG:HH11 | 2.16                     | 0.54              |
| 1:C:4854:VAL:HA   | 1:C:4858:LEU:HD12 | 1.89                     | 0.54              |
| 1:D:2836:ASP:OD1  | 1:D:2837:LEU:N    | 2.41                     | 0.54              |
| 1:A:1074:ARG:HH12 | 1:A:1078:CYS:H    | 1.56                     | 0.54              |
| 1:A:2905:ARG:NE   | 1:A:2906:GLY:H    | 2.00                     | 0.54              |
| 1:A:3237:VAL:HG23 | 1:A:3238:ILE:HG23 | 1.90                     | 0.54              |
| 1:B:3295:TRP:HA   | 1:B:3298:ARG:HG2  | 1.90                     | 0.54              |
| 1:B:3846:LEU:HB3  | 1:B:3854:PHE:CE2  | 2.43                     | 0.54              |
| 1:C:254:GLU:OE2   | 1:C:258:ARG:NE    | 2.41                     | 0.54              |
| 1:C:4082:GLU:HA   | 1:C:4085:LYS:HG2  | 1.89                     | 0.54              |
| 1:D:1010:ASP:OD1  | 1:D:1013:ARG:NH1  | 2.39                     | 0.54              |
| 1:D:1718:ARG:NH1  | 1:D:1831:MET:O    | 2.41                     | 0.54              |
| 1:D:2711:ILE:HD12 | 1:D:2783:LEU:HB3  | 1.90                     | 0.54              |
| 1:D:2729:HIS:N    | 1:D:2771:TYR:OH   | 2.40                     | 0.54              |
| 1:D:3008:PHE:HD1  | 1:D:3036:LEU:HD23 | 1.73                     | 0.54              |
| 1:D:3257:ASN:HD21 | 1:D:3260:ARG:HH21 | 1.54                     | 0.54              |
| 1:A:1939:ASN:OD1  | 1:A:1940:GLN:N    | 2.41                     | 0.53              |
| 1:A:3325:LYS:HA   | 1:A:3328:LYS:HG2  | 1.91                     | 0.53              |
| 1:A:3955:GLN:HG2  | 1:A:3972:MET:HE1  | 1.90                     | 0.53              |
| 2:G:30:MET:HB2    | 2:G:99:ILE:HG13   | 1.90                     | 0.53              |
| 1:B:919:VAL:HG21  | 1:B:923:LYS:HD2   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2836:ASP:OD1  | 1:B:2837:LEU:N    | 2.41                     | 0.53              |
| 1:B:3955:GLN:HG2  | 1:B:3972:MET:HE1  | 1.90                     | 0.53              |
| 1:C:1239:PHE:O    | 1:C:1807:ARG:NH1  | 2.40                     | 0.53              |
| 1:C:3034:HIS:CE1  | 1:C:3107:SER:HG   | 2.25                     | 0.53              |
| 1:C:3295:TRP:HA   | 1:C:3298:ARG:HG2  | 1.90                     | 0.53              |
| 1:D:304:LYS:HB2   | 1:D:316:LEU:HD23  | 1.90                     | 0.53              |
| 1:D:1685:LEU:HD22 | 1:D:1706:LEU:HB2  | 1.90                     | 0.53              |
| 1:D:1815:GLU:O    | 1:D:1819:VAL:HG12 | 2.08                     | 0.53              |
| 1:D:2679:ASP:HA   | 1:D:2920:ARG:HG2  | 1.90                     | 0.53              |
| 1:D:2720:PHE:HE2  | 1:D:2896:LEU:HA   | 1.74                     | 0.53              |
| 1:D:2846:GLU:HG2  | 1:D:2874:TYR:CD2  | 2.43                     | 0.53              |
| 1:D:3325:LYS:HA   | 1:D:3328:LYS:HG2  | 1.91                     | 0.53              |
| 1:D:3955:GLN:HG2  | 1:D:3972:MET:HE1  | 1.90                     | 0.53              |
| 1:A:1685:LEU:HD22 | 1:A:1706:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:1718:ARG:NH1  | 1:A:1831:MET:O    | 2.41                     | 0.53              |
| 1:A:2711:ILE:HD12 | 1:A:2783:LEU:HB3  | 1.90                     | 0.53              |
| 1:A:3986:LEU:HD12 | 1:A:4101:LEU:HD12 | 1.89                     | 0.53              |
| 1:B:857:LEU:HG    | 1:B:860:ALA:HB2   | 1.89                     | 0.53              |
| 1:C:1272:ARG:NH2  | 1:C:1582:CYS:SG   | 2.81                     | 0.53              |
| 1:C:1815:GLU:O    | 1:C:1819:VAL:HG12 | 2.08                     | 0.53              |
| 1:C:2975:PHE:HB3  | 1:C:3039:THR:HG21 | 1.90                     | 0.53              |
| 1:C:3285:TYR:HD1  | 1:C:3325:LYS:HG2  | 1.73                     | 0.53              |
| 1:C:3955:GLN:HG2  | 1:C:3972:MET:HE1  | 1.90                     | 0.53              |
| 1:C:4023:LEU:HG   | 1:C:4084:VAL:HG12 | 1.90                     | 0.53              |
| 1:D:3109:PHE:CE1  | 1:D:3162:PHE:HD1  | 2.24                     | 0.53              |
| 1:D:4238:ILE:HG23 | 1:D:4239:LEU:HD12 | 1.91                     | 0.53              |
| 1:A:304:LYS:HB2   | 1:A:316:LEU:HD23  | 1.90                     | 0.53              |
| 1:A:1239:PHE:O    | 1:A:1807:ARG:NH1  | 2.40                     | 0.53              |
| 1:A:3295:TRP:HA   | 1:A:3298:ARG:HG2  | 1.90                     | 0.53              |
| 1:B:1011:ARG:HH22 | 4:B:5003:ATP:PB   | 2.31                     | 0.53              |
| 1:B:1718:ARG:NH1  | 1:B:1831:MET:O    | 2.41                     | 0.53              |
| 1:B:1979:PHE:HZ   | 1:B:1996:LEU:HB3  | 1.73                     | 0.53              |
| 1:B:3233:HIS:O    | 1:B:3237:VAL:HG22 | 2.09                     | 0.53              |
| 1:C:304:LYS:HB2   | 1:C:316:LEU:HD23  | 1.90                     | 0.53              |
| 1:C:2179:LEU:HD23 | 1:C:2187:ILE:HD13 | 1.89                     | 0.53              |
| 1:C:2640:LEU:HA   | 1:C:2643:LYS:HE2  | 1.89                     | 0.53              |
| 1:C:4116:GLN:HA   | 1:C:4119:LEU:HD12 | 1.90                     | 0.53              |
| 1:D:3285:TYR:HD1  | 1:D:3325:LYS:HG2  | 1.73                     | 0.53              |
| 1:A:254:GLU:OE2   | 1:A:258:ARG:NE    | 2.41                     | 0.53              |
| 1:A:915:HIS:NE2   | 1:A:917:CYS:HB2   | 2.24                     | 0.53              |
| 1:A:2719:TYR:HD2  | 1:A:2791:ARG:HH12 | 1.55                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3008:PHE:HD1  | 1:A:3036:LEU:HD23 | 1.73                     | 0.53              |
| 1:A:3226:ILE:HD12 | 1:A:3230:GLN:HB2  | 1.91                     | 0.53              |
| 1:A:3846:LEU:HB3  | 1:A:3854:PHE:CE2  | 2.43                     | 0.53              |
| 1:A:4250:TYR:O    | 1:A:4254:THR:HG23 | 2.09                     | 0.53              |
| 1:B:1144:ARG:NH1  | 1:B:1191:ALA:O    | 2.33                     | 0.53              |
| 1:B:3008:PHE:HD1  | 1:B:3036:LEU:HD23 | 1.73                     | 0.53              |
| 1:B:3237:VAL:HG23 | 1:B:3238:ILE:HG23 | 1.90                     | 0.53              |
| 1:B:3832:ASP:HB3  | 1:B:3835:PHE:HB3  | 1.89                     | 0.53              |
| 1:B:4116:GLN:HA   | 1:B:4119:LEU:HD12 | 1.90                     | 0.53              |
| 1:B:4169:LYS:NZ   | 4:B:5002:ATP:O2A  | 2.38                     | 0.53              |
| 1:B:4238:ILE:HG23 | 1:B:4239:LEU:HD12 | 1.91                     | 0.53              |
| 1:C:582:SER:OG    | 1:C:584:GLU:OE1   | 2.26                     | 0.53              |
| 1:C:3008:PHE:HD1  | 1:C:3036:LEU:HD23 | 1.73                     | 0.53              |
| 1:D:2975:PHE:HB3  | 1:D:3039:THR:HG21 | 1.90                     | 0.53              |
| 1:A:1815:GLU:O    | 1:A:1819:VAL:HG12 | 2.08                     | 0.53              |
| 1:A:2720:PHE:HE2  | 1:A:2896:LEU:HA   | 1.74                     | 0.53              |
| 1:A:2852:TRP:O    | 1:A:2855:LYS:HG2  | 2.08                     | 0.53              |
| 1:A:3285:TYR:HD1  | 1:A:3325:LYS:HG2  | 1.73                     | 0.53              |
| 1:B:625:VAL:HG12  | 1:B:2133:ARG:HH11 | 1.74                     | 0.53              |
| 1:B:2846:GLU:HG2  | 1:B:2874:TYR:CD2  | 2.43                     | 0.53              |
| 1:B:3283:ILE:HA   | 1:B:3286:ASN:ND2  | 2.23                     | 0.53              |
| 1:B:3976:LYS:NZ   | 1:B:4093:ASP:O    | 2.42                     | 0.53              |
| 1:C:1718:ARG:NH1  | 1:C:1831:MET:O    | 2.41                     | 0.53              |
| 1:C:2758:LYS:HE3  | 1:C:2763:LEU:HD23 | 1.90                     | 0.53              |
| 1:C:2846:GLU:HG2  | 1:C:2874:TYR:CD2  | 2.43                     | 0.53              |
| 1:C:3226:ILE:HD12 | 1:C:3230:GLN:HB2  | 1.91                     | 0.53              |
| 1:C:3283:ILE:HA   | 1:C:3286:ASN:ND2  | 2.23                     | 0.53              |
| 1:D:2096:GLY:O    | 1:D:2100:ARG:NE   | 2.40                     | 0.53              |
| 1:D:2581:ARG:HH21 | 1:D:2582:PRO:HG2  | 1.72                     | 0.53              |
| 1:D:3233:HIS:O    | 1:D:3237:VAL:HG22 | 2.09                     | 0.53              |
| 1:A:582:SER:OG    | 1:A:584:GLU:OE1   | 2.26                     | 0.53              |
| 1:A:919:VAL:HG21  | 1:A:923:LYS:HD2   | 1.90                     | 0.53              |
| 1:A:1939:ASN:HD22 | 1:A:1992:ILE:HG13 | 1.74                     | 0.53              |
| 1:A:2423:LEU:HA   | 1:A:2426:LEU:HD12 | 1.90                     | 0.53              |
| 1:B:1711:LEU:HB2  | 1:B:1831:MET:SD   | 2.49                     | 0.53              |
| 1:B:1815:GLU:O    | 1:B:1819:VAL:HG12 | 2.08                     | 0.53              |
| 1:C:625:VAL:HG12  | 1:C:2133:ARG:HH11 | 1.74                     | 0.53              |
| 1:C:1014:GLN:C    | 1:C:1027:ARG:HH22 | 2.17                     | 0.53              |
| 1:C:2423:LEU:HA   | 1:C:2426:LEU:HD12 | 1.90                     | 0.53              |
| 1:C:3233:HIS:O    | 1:C:3237:VAL:HG22 | 2.09                     | 0.53              |
| 1:C:3846:LEU:HB3  | 1:C:3854:PHE:CE2  | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1718:ARG:CZ   | 1:D:1758:ARG:HD3  | 2.39                     | 0.53              |
| 1:D:2232:PRO:C    | 1:D:2234:MET:H    | 2.17                     | 0.53              |
| 1:A:1272:ARG:NH2  | 1:A:1582:CYS:SG   | 2.81                     | 0.53              |
| 1:A:2975:PHE:HB3  | 1:A:3039:THR:HG21 | 1.90                     | 0.53              |
| 1:B:304:LYS:HB2   | 1:B:316:LEU:HD23  | 1.90                     | 0.53              |
| 1:B:2244:ALA:O    | 1:B:2248:MET:HB2  | 2.08                     | 0.53              |
| 1:B:2834:SER:OG   | 1:B:2836:ASP:OD1  | 2.24                     | 0.53              |
| 1:B:2852:TRP:O    | 1:B:2855:LYS:HG2  | 2.08                     | 0.53              |
| 1:D:254:GLU:OE2   | 1:D:258:ARG:NE    | 2.41                     | 0.53              |
| 1:D:2758:LYS:HE3  | 1:D:2763:LEU:HD23 | 1.90                     | 0.53              |
| 1:A:857:LEU:HG    | 1:A:860:ALA:HB2   | 1.89                     | 0.53              |
| 1:A:1718:ARG:CZ   | 1:A:1758:ARG:HD3  | 2.39                     | 0.53              |
| 1:A:2004:MET:HE1  | 1:A:2095:ILE:HD13 | 1.91                     | 0.53              |
| 1:B:335:LYS:NZ    | 1:B:401:ASP:OD2   | 2.31                     | 0.53              |
| 1:B:874:LEU:HB2   | 1:B:880:ARG:NH1   | 2.24                     | 0.53              |
| 1:B:925:PRO:HB2   | 1:B:928:GLU:OE1   | 2.09                     | 0.53              |
| 1:B:1286:THR:OG1  | 1:B:1550:PRO:O    | 2.24                     | 0.53              |
| 1:B:1718:ARG:CZ   | 1:B:1758:ARG:HD3  | 2.39                     | 0.53              |
| 1:B:2004:MET:HE1  | 1:B:2095:ILE:HD13 | 1.91                     | 0.53              |
| 1:B:2711:ILE:HD12 | 1:B:2783:LEU:HB3  | 1.90                     | 0.53              |
| 1:B:2971:ILE:HG23 | 1:B:2975:PHE:CE2  | 2.44                     | 0.53              |
| 1:C:1074:ARG:HH12 | 1:C:1078:CYS:H    | 1.56                     | 0.53              |
| 1:C:2720:PHE:HE2  | 1:C:2896:LEU:HA   | 1.74                     | 0.53              |
| 1:C:2852:TRP:O    | 1:C:2855:LYS:HG2  | 2.08                     | 0.53              |
| 1:D:1011:ARG:HH22 | 4:D:5003:ATP:PB   | 2.31                     | 0.53              |
| 1:D:1272:ARG:NH2  | 1:D:1582:CYS:SG   | 2.81                     | 0.53              |
| 1:A:514:PHE:HD2   | 1:A:526:TRP:HB2   | 1.74                     | 0.53              |
| 1:A:625:VAL:HG12  | 1:A:2133:ARG:HH11 | 1.74                     | 0.53              |
| 1:A:1440:ASN:HB3  | 1:A:1546:GLN:HB3  | 1.90                     | 0.53              |
| 1:A:2244:ALA:O    | 1:A:2248:MET:HB2  | 2.08                     | 0.53              |
| 1:A:3944:VAL:HG13 | 1:A:3978:MET:HE2  | 1.91                     | 0.53              |
| 1:A:4023:LEU:HG   | 1:A:4084:VAL:HG12 | 1.90                     | 0.53              |
| 1:B:915:HIS:NE2   | 1:B:917:CYS:HB2   | 2.24                     | 0.53              |
| 1:B:1014:GLN:C    | 1:B:1027:ARG:HH22 | 2.17                     | 0.53              |
| 1:B:1440:ASN:HB3  | 1:B:1546:GLN:HB3  | 1.90                     | 0.53              |
| 1:B:1939:ASN:HD22 | 1:B:1992:ILE:HG13 | 1.74                     | 0.53              |
| 1:B:2179:LEU:HD23 | 1:B:2187:ILE:HD13 | 1.89                     | 0.53              |
| 1:B:2679:ASP:HA   | 1:B:2920:ARG:HG2  | 1.91                     | 0.53              |
| 1:D:625:VAL:HG12  | 1:D:2133:ARG:HH11 | 1.74                     | 0.53              |
| 1:D:1979:PHE:HZ   | 1:D:1996:LEU:HB3  | 1.73                     | 0.53              |
| 1:A:874:LEU:HB2   | 1:A:880:ARG:NH1   | 2.24                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:982:ASP:HB2   | 1:A:985:PHE:CE1   | 2.43                     | 0.53              |
| 1:A:2758:LYS:HE3  | 1:A:2763:LEU:HD23 | 1.90                     | 0.53              |
| 1:A:4569:GLU:HB3  | 1:A:4570:PRO:HD3  | 1.91                     | 0.53              |
| 2:H:22:THR:HA     | 2:H:50:ARG:HA     | 1.91                     | 0.53              |
| 1:B:3226:ILE:HD12 | 1:B:3230:GLN:HB2  | 1.91                     | 0.53              |
| 1:C:857:LEU:HG    | 1:C:860:ALA:HB2   | 1.89                     | 0.53              |
| 1:C:910:ASP:OD1   | 1:C:911:ASN:N     | 2.42                     | 0.53              |
| 1:C:919:VAL:HG21  | 1:C:923:LYS:HD2   | 1.90                     | 0.53              |
| 1:C:1979:PHE:HZ   | 1:C:1996:LEU:HB3  | 1.73                     | 0.53              |
| 1:C:2679:ASP:HA   | 1:C:2920:ARG:HG2  | 1.90                     | 0.53              |
| 1:C:3976:LYS:NZ   | 1:C:4093:ASP:O    | 2.42                     | 0.53              |
| 1:D:2244:ALA:O    | 1:D:2248:MET:HB2  | 2.08                     | 0.53              |
| 1:D:2999:LYS:HA   | 1:D:3002:GLU:CD   | 2.34                     | 0.53              |
| 1:D:3069:GLU:CD   | 1:D:3132:ARG:HH11 | 2.16                     | 0.53              |
| 1:D:3226:ILE:HD12 | 1:D:3230:GLN:HB2  | 1.91                     | 0.53              |
| 1:A:218:SER:HB2   | 1:A:286:GLY:HA3   | 1.91                     | 0.52              |
| 1:A:1011:ARG:HH22 | 4:A:5003:ATP:PB   | 2.32                     | 0.52              |
| 1:A:2149:ILE:HG21 | 1:A:2167:MET:HE1  | 1.91                     | 0.52              |
| 1:A:4829:ASP:N    | 1:D:4822:ARG:HH12 | 2.07                     | 0.52              |
| 2:E:30:MET:HB2    | 2:E:99:ILE:HG13   | 1.90                     | 0.52              |
| 1:B:514:PHE:HD2   | 1:B:526:TRP:HB2   | 1.74                     | 0.52              |
| 1:B:2096:GLY:O    | 1:B:2100:ARG:NE   | 2.40                     | 0.52              |
| 1:B:2668:CYS:O    | 1:B:2672:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:4023:LEU:HG   | 1:B:4084:VAL:HG12 | 1.90                     | 0.52              |
| 1:C:874:LEU:HB2   | 1:C:880:ARG:NH1   | 2.24                     | 0.52              |
| 1:C:2244:ALA:O    | 1:C:2248:MET:HB2  | 2.08                     | 0.52              |
| 1:C:2537:GLY:O    | 1:C:2540:HIS:NE2  | 2.38                     | 0.52              |
| 1:C:2668:CYS:O    | 1:C:2672:VAL:HG23 | 2.09                     | 0.52              |
| 1:D:982:ASP:HB2   | 1:D:985:PHE:CE1   | 2.44                     | 0.52              |
| 1:D:1014:GLN:C    | 1:D:1027:ARG:HH22 | 2.17                     | 0.52              |
| 1:D:3976:LYS:NZ   | 1:D:4093:ASP:O    | 2.41                     | 0.52              |
| 1:A:1711:LEU:HB2  | 1:A:1831:MET:SD   | 2.49                     | 0.52              |
| 1:A:2971:ILE:HG23 | 1:A:2975:PHE:CE2  | 2.44                     | 0.52              |
| 1:A:3015:VAL:HB   | 1:A:3029:ILE:HG21 | 1.91                     | 0.52              |
| 1:A:3069:GLU:CD   | 1:A:3132:ARG:HH11 | 2.16                     | 0.52              |
| 1:A:3986:LEU:HD11 | 1:A:4105:LEU:HG   | 1.92                     | 0.52              |
| 2:F:24:VAL:HG12   | 2:F:48:LYS:HG2    | 1.91                     | 0.52              |
| 2:H:63:GLY:O      | 2:H:67:MET:HG3    | 2.10                     | 0.52              |
| 1:B:663:VAL:HG23  | 1:B:671:LYS:HE3   | 1.91                     | 0.52              |
| 1:B:910:ASP:OD1   | 1:B:911:ASN:N     | 2.42                     | 0.52              |
| 1:B:2720:PHE:HE2  | 1:B:2896:LEU:HA   | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2758:LYS:HE3  | 1:B:2763:LEU:HD23 | 1.90                     | 0.52              |
| 1:B:3285:TYR:HD1  | 1:B:3325:LYS:HG2  | 1.73                     | 0.52              |
| 1:B:3325:LYS:HA   | 1:B:3328:LYS:HG2  | 1.91                     | 0.52              |
| 1:C:1011:ARG:HH22 | 4:C:5003:ATP:PB   | 2.31                     | 0.52              |
| 1:C:1286:THR:OG1  | 1:C:1550:PRO:O    | 2.24                     | 0.52              |
| 1:C:1718:ARG:CZ   | 1:C:1758:ARG:HD3  | 2.39                     | 0.52              |
| 1:C:4250:TYR:O    | 1:C:4254:THR:HG23 | 2.09                     | 0.52              |
| 1:D:905:GLY:HA3   | 1:D:914:GLN:CB    | 2.37                     | 0.52              |
| 1:D:915:HIS:NE2   | 1:D:917:CYS:HB2   | 2.24                     | 0.52              |
| 1:D:2004:MET:HE1  | 1:D:2095:ILE:HD13 | 1.91                     | 0.52              |
| 1:D:3098:THR:HA   | 1:D:3102:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:905:GLY:HA3   | 1:A:914:GLN:CB    | 2.37                     | 0.52              |
| 1:A:910:ASP:OD1   | 1:A:911:ASN:N     | 2.42                     | 0.52              |
| 1:A:2443:PRO:HD3  | 1:A:2512:MET:HE2  | 1.90                     | 0.52              |
| 1:A:2542:ALA:HA   | 1:A:2545:ILE:HG12 | 1.92                     | 0.52              |
| 1:A:3002:GLU:HB3  | 1:A:3045:VAL:HG13 | 1.92                     | 0.52              |
| 1:A:3976:LYS:NZ   | 1:A:4093:ASP:O    | 2.42                     | 0.52              |
| 2:G:22:THR:HA     | 2:G:50:ARG:HA     | 1.91                     | 0.52              |
| 1:B:982:ASP:HB2   | 1:B:985:PHE:CE1   | 2.43                     | 0.52              |
| 1:B:1685:LEU:HD22 | 1:B:1706:LEU:HB2  | 1.90                     | 0.52              |
| 1:B:3944:VAL:HG13 | 1:B:3978:MET:HE2  | 1.91                     | 0.52              |
| 1:B:4250:TYR:O    | 1:B:4254:THR:HG23 | 2.09                     | 0.52              |
| 1:C:1685:LEU:HD22 | 1:C:1706:LEU:HB2  | 1.90                     | 0.52              |
| 1:C:2096:GLY:O    | 1:C:2100:ARG:NE   | 2.40                     | 0.52              |
| 1:C:3325:LYS:HA   | 1:C:3328:LYS:HG2  | 1.91                     | 0.52              |
| 1:D:514:PHE:HD2   | 1:D:526:TRP:HB2   | 1.74                     | 0.52              |
| 1:D:2443:PRO:HD3  | 1:D:2512:MET:HE2  | 1.90                     | 0.52              |
| 1:D:3002:GLU:HB3  | 1:D:3045:VAL:HG13 | 1.92                     | 0.52              |
| 1:D:3237:VAL:HG23 | 1:D:3238:ILE:HG23 | 1.90                     | 0.52              |
| 1:D:3284:ILE:O    | 1:D:3288:LEU:HG   | 2.10                     | 0.52              |
| 1:D:4250:TYR:O    | 1:D:4254:THR:HG23 | 2.09                     | 0.52              |
| 1:A:1014:GLN:C    | 1:A:1027:ARG:HH22 | 2.17                     | 0.52              |
| 1:A:2179:LEU:HD23 | 1:A:2187:ILE:HD13 | 1.89                     | 0.52              |
| 1:A:2232:PRO:C    | 1:A:2234:MET:H    | 2.17                     | 0.52              |
| 1:A:2537:GLY:O    | 1:A:2540:HIS:NE2  | 2.38                     | 0.52              |
| 1:A:3098:THR:HA   | 1:A:3102:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:3233:HIS:O    | 1:A:3237:VAL:HG22 | 2.09                     | 0.52              |
| 2:E:22:THR:HA     | 2:E:50:ARG:HA     | 1.91                     | 0.52              |
| 2:G:24:VAL:HG12   | 2:G:48:LYS:HG2    | 1.91                     | 0.52              |
| 1:B:2923:TYR:HE1  | 1:B:2999:LYS:HG3  | 1.74                     | 0.52              |
| 1:B:2999:LYS:HA   | 1:B:3002:GLU:CD   | 2.34                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:925:PRO:HB2   | 1:C:928:GLU:OE1   | 2.09                     | 0.52              |
| 1:C:982:ASP:HB2   | 1:C:985:PHE:CE1   | 2.43                     | 0.52              |
| 1:C:1939:ASN:HD22 | 1:C:1992:ILE:HG13 | 1.74                     | 0.52              |
| 1:C:2004:MET:HE1  | 1:C:2095:ILE:HD13 | 1.91                     | 0.52              |
| 1:C:2836:ASP:OD1  | 1:C:2837:LEU:N    | 2.41                     | 0.52              |
| 1:D:218:SER:HB2   | 1:D:286:GLY:HA3   | 1.91                     | 0.52              |
| 1:D:874:LEU:HB2   | 1:D:880:ARG:NH1   | 2.24                     | 0.52              |
| 1:D:1113:MET:HB2  | 1:D:1156:TRP:CZ2  | 2.45                     | 0.52              |
| 1:D:2542:ALA:HA   | 1:D:2545:ILE:HG12 | 1.92                     | 0.52              |
| 1:D:2549:LEU:HB3  | 1:D:2588:LEU:HD22 | 1.91                     | 0.52              |
| 1:D:2668:CYS:O    | 1:D:2672:VAL:HG23 | 2.09                     | 0.52              |
| 1:D:2971:ILE:HG23 | 1:D:2975:PHE:CE2  | 2.44                     | 0.52              |
| 1:D:3729:ALA:HA   | 1:D:3732:HIS:CD2  | 2.45                     | 0.52              |
| 1:D:3986:LEU:HD11 | 1:D:4105:LEU:HG   | 1.92                     | 0.52              |
| 1:D:4896:ASP:OD2  | 1:D:4897:TYR:N    | 2.43                     | 0.52              |
| 1:A:194:LEU:HD21  | 1:A:201:LEU:HD23  | 1.92                     | 0.52              |
| 1:A:2681:MET:SD   | 1:A:2919:LYS:HB2  | 2.49                     | 0.52              |
| 1:A:3284:ILE:O    | 1:A:3288:LEU:HG   | 2.10                     | 0.52              |
| 1:A:3729:ALA:HA   | 1:A:3732:HIS:CD2  | 2.44                     | 0.52              |
| 1:A:4279:MET:HE2  | 1:B:4484:ILE:HG22 | 1.90                     | 0.52              |
| 1:A:4827:ILE:O    | 1:A:4831:ILE:HG12 | 2.10                     | 0.52              |
| 1:A:4840:GLU:O    | 1:A:4844:ILE:HG12 | 2.10                     | 0.52              |
| 2:E:24:VAL:HG12   | 2:E:48:LYS:HG2    | 1.91                     | 0.52              |
| 2:E:63:GLY:O      | 2:E:67:MET:HG3    | 2.10                     | 0.52              |
| 2:F:30:MET:HB2    | 2:F:99:ILE:HG13   | 1.90                     | 0.52              |
| 2:G:63:GLY:O      | 2:G:67:MET:HG3    | 2.10                     | 0.52              |
| 1:B:2232:PRO:C    | 1:B:2234:MET:H    | 2.17                     | 0.52              |
| 1:B:2423:LEU:HA   | 1:B:2426:LEU:HD12 | 1.90                     | 0.52              |
| 1:B:2926:LEU:O    | 1:B:2930:ILE:HG12 | 2.10                     | 0.52              |
| 1:B:3034:HIS:CE1  | 1:B:3107:SER:HG   | 2.24                     | 0.52              |
| 1:C:915:HIS:NE2   | 1:C:917:CYS:HB2   | 2.24                     | 0.52              |
| 1:C:3015:VAL:HB   | 1:C:3029:ILE:HG21 | 1.91                     | 0.52              |
| 1:D:925:PRO:HB2   | 1:D:928:GLU:OE1   | 2.09                     | 0.52              |
| 1:D:2127:ARG:NH2  | 1:D:2165:LEU:O    | 2.43                     | 0.52              |
| 1:D:2175:MET:SD   | 1:D:2193:VAL:HG13 | 2.50                     | 0.52              |
| 1:D:2926:LEU:O    | 1:D:2930:ILE:HG12 | 2.10                     | 0.52              |
| 1:A:663:VAL:HG23  | 1:A:671:LYS:HE3   | 1.91                     | 0.52              |
| 1:B:4896:ASP:OD2  | 1:B:4897:TYR:N    | 2.43                     | 0.52              |
| 1:C:625:VAL:HG23  | 1:C:628:ASN:HB2   | 1.92                     | 0.52              |
| 1:C:663:VAL:HG23  | 1:C:671:LYS:HE3   | 1.91                     | 0.52              |
| 1:C:1711:LEU:HB2  | 1:C:1831:MET:SD   | 2.49                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1894:LEU:O    | 1:C:2068:ARG:NH2  | 2.43                     | 0.52              |
| 1:C:2681:MET:SD   | 1:C:2919:LYS:HB2  | 2.49                     | 0.52              |
| 1:C:2971:ILE:HG23 | 1:C:2975:PHE:CE2  | 2.44                     | 0.52              |
| 1:C:2999:LYS:HA   | 1:C:3002:GLU:CD   | 2.34                     | 0.52              |
| 1:C:3986:LEU:HD11 | 1:C:4105:LEU:HG   | 1.92                     | 0.52              |
| 1:D:3295:TRP:HA   | 1:D:3298:ARG:HG2  | 1.90                     | 0.52              |
| 1:A:2785:TRP:HB2  | 1:A:2787:TRP:CZ3  | 2.45                     | 0.52              |
| 1:A:2999:LYS:HA   | 1:A:3002:GLU:CD   | 2.34                     | 0.52              |
| 1:B:625:VAL:HG23  | 1:B:628:ASN:HB2   | 1.92                     | 0.52              |
| 1:B:4827:ILE:O    | 1:B:4831:ILE:HG12 | 2.10                     | 0.52              |
| 1:C:2443:PRO:HD3  | 1:C:2512:MET:HE2  | 1.90                     | 0.52              |
| 1:C:2923:TYR:HE1  | 1:C:2999:LYS:HG3  | 1.74                     | 0.52              |
| 1:C:2926:LEU:O    | 1:C:2930:ILE:HG12 | 2.10                     | 0.52              |
| 1:C:3944:VAL:HG13 | 1:C:3978:MET:HE2  | 1.91                     | 0.52              |
| 1:C:4238:ILE:HG23 | 1:C:4239:LEU:HD12 | 1.90                     | 0.52              |
| 1:D:194:LEU:HD21  | 1:D:201:LEU:HD23  | 1.92                     | 0.52              |
| 1:D:962:LYS:C     | 1:D:963:LYS:HD3   | 2.35                     | 0.52              |
| 1:D:2423:LEU:HA   | 1:D:2426:LEU:HD12 | 1.90                     | 0.52              |
| 1:D:3317:THR:O    | 1:D:3321:PRO:HD2  | 2.10                     | 0.52              |
| 1:D:3944:VAL:HG13 | 1:D:3978:MET:HE2  | 1.91                     | 0.52              |
| 1:A:882:ARG:NH2   | 1:A:1057:LEU:O    | 2.43                     | 0.52              |
| 1:A:2581:ARG:NH2  | 1:A:2582:PRO:HG2  | 2.25                     | 0.52              |
| 1:A:2668:CYS:O    | 1:A:2672:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:582:SER:OG    | 1:B:584:GLU:OE1   | 2.26                     | 0.52              |
| 1:B:1911:GLN:HG3  | 1:B:2090:ARG:HH11 | 1.75                     | 0.52              |
| 1:B:2549:LEU:HB3  | 1:B:2588:LEU:HD22 | 1.91                     | 0.52              |
| 1:B:3176:ASP:HA   | 1:B:3265:CYS:SG   | 2.50                     | 0.52              |
| 1:B:3284:ILE:O    | 1:B:3288:LEU:HG   | 2.10                     | 0.52              |
| 1:C:335:LYS:NZ    | 1:C:401:ASP:OD2   | 2.31                     | 0.52              |
| 1:C:514:PHE:HD2   | 1:C:526:TRP:HB2   | 1.74                     | 0.52              |
| 1:C:2542:ALA:HA   | 1:C:2545:ILE:HG12 | 1.92                     | 0.52              |
| 1:C:2549:LEU:HB3  | 1:C:2588:LEU:HD22 | 1.91                     | 0.52              |
| 1:C:3002:GLU:HB3  | 1:C:3045:VAL:HG13 | 1.92                     | 0.52              |
| 1:D:882:ARG:NH2   | 1:D:1057:LEU:O    | 2.43                     | 0.52              |
| 1:D:919:VAL:HG21  | 1:D:923:LYS:HD2   | 1.90                     | 0.52              |
| 1:D:2785:TRP:HB2  | 1:D:2787:TRP:CZ3  | 2.45                     | 0.52              |
| 1:D:3015:VAL:HB   | 1:D:3029:ILE:HG21 | 1.91                     | 0.52              |
| 1:A:962:LYS:C     | 1:A:963:LYS:HD3   | 2.35                     | 0.52              |
| 2:F:63:GLY:O      | 2:F:67:MET:HG3    | 2.10                     | 0.52              |
| 1:B:1074:ARG:HH12 | 1:B:1078:CYS:H    | 1.56                     | 0.52              |
| 1:B:2175:MET:SD   | 1:B:2193:VAL:HG13 | 2.50                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2581:ARG:NH2  | 1:B:2582:PRO:HG2  | 2.25                     | 0.52              |
| 1:B:3019:ILE:HD11 | 1:B:3096:TYR:HB2  | 1.92                     | 0.52              |
| 1:B:4840:GLU:O    | 1:B:4844:ILE:HG12 | 2.10                     | 0.52              |
| 1:C:218:SER:HB2   | 1:C:286:GLY:HA3   | 1.91                     | 0.52              |
| 1:C:996:VAL:HB    | 1:C:1051:ARG:HE   | 1.75                     | 0.52              |
| 1:C:1113:MET:HB2  | 1:C:1156:TRP:CZ2  | 2.45                     | 0.52              |
| 1:C:3882:GLN:NE2  | 1:C:3946:GLY:HA3  | 2.25                     | 0.52              |
| 1:D:625:VAL:HG23  | 1:D:628:ASN:HB2   | 1.92                     | 0.52              |
| 1:D:1711:LEU:HB2  | 1:D:1831:MET:SD   | 2.49                     | 0.52              |
| 1:A:375:GLN:N     | 1:A:390:LYS:O     | 2.34                     | 0.52              |
| 1:A:2923:TYR:HE1  | 1:A:2999:LYS:HG3  | 1.74                     | 0.52              |
| 2:F:22:THR:HA     | 2:F:50:ARG:HA     | 1.91                     | 0.52              |
| 1:B:1113:MET:HB2  | 1:B:1156:TRP:CZ2  | 2.45                     | 0.52              |
| 1:B:2785:TRP:HB2  | 1:B:2787:TRP:CZ3  | 2.45                     | 0.52              |
| 1:B:3015:VAL:HB   | 1:B:3029:ILE:HG21 | 1.91                     | 0.52              |
| 1:B:3650:GLU:HB2  | 1:B:3651:PRO:HD3  | 1.92                     | 0.52              |
| 1:C:1948:MET:HA   | 1:C:1951:LEU:HD23 | 1.91                     | 0.52              |
| 1:C:2149:ILE:HG21 | 1:C:2167:MET:HE1  | 1.91                     | 0.52              |
| 1:C:3176:ASP:HA   | 1:C:3265:CYS:SG   | 2.50                     | 0.52              |
| 1:D:614:LEU:HD22  | 1:D:632:ILE:HG12  | 1.92                     | 0.52              |
| 1:A:625:VAL:HG23  | 1:A:628:ASN:HB2   | 1.92                     | 0.51              |
| 1:A:917:CYS:HA    | 1:A:924:LEU:HG    | 1.93                     | 0.51              |
| 1:A:1219:LYS:NZ   | 1:A:1243:THR:O    | 2.43                     | 0.51              |
| 1:A:1979:PHE:HZ   | 1:A:1996:LEU:HB3  | 1.73                     | 0.51              |
| 1:A:2926:LEU:O    | 1:A:2930:ILE:HG12 | 2.10                     | 0.51              |
| 1:A:3176:ASP:HA   | 1:A:3265:CYS:SG   | 2.50                     | 0.51              |
| 1:A:3317:THR:O    | 1:A:3321:PRO:HD2  | 2.10                     | 0.51              |
| 2:G:26:HIS:CE1    | 2:G:46:PRO:HA     | 2.45                     | 0.51              |
| 1:B:614:LEU:HD22  | 1:B:632:ILE:HG12  | 1.92                     | 0.51              |
| 1:B:996:VAL:HB    | 1:B:1051:ARG:HE   | 1.75                     | 0.51              |
| 1:B:2149:ILE:HG21 | 1:B:2167:MET:HE1  | 1.91                     | 0.51              |
| 1:B:3002:GLU:HB3  | 1:B:3045:VAL:HG13 | 1.92                     | 0.51              |
| 1:C:2581:ARG:NH2  | 1:C:2582:PRO:HG2  | 2.25                     | 0.51              |
| 1:C:3284:ILE:O    | 1:C:3288:LEU:HG   | 2.10                     | 0.51              |
| 1:C:3650:GLU:HB2  | 1:C:3651:PRO:HD3  | 1.92                     | 0.51              |
| 1:D:1428:TYR:OH   | 1:D:1444:GLY:O    | 2.28                     | 0.51              |
| 1:D:2635:GLU:HA   | 1:D:2638:LEU:HB2  | 1.92                     | 0.51              |
| 1:D:2923:TYR:HE1  | 1:D:2999:LYS:HG3  | 1.74                     | 0.51              |
| 1:D:3019:ILE:HD11 | 1:D:3096:TYR:HB2  | 1.92                     | 0.51              |
| 1:D:3176:ASP:HA   | 1:D:3265:CYS:SG   | 2.50                     | 0.51              |
| 1:D:3882:GLN:NE2  | 1:D:3946:GLY:HA3  | 2.25                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:4827:ILE:O    | 1:D:4831:ILE:HG12 | 2.10                     | 0.51              |
| 1:A:1911:GLN:HG3  | 1:A:2090:ARG:HH11 | 1.75                     | 0.51              |
| 1:A:2549:LEU:HB3  | 1:A:2588:LEU:HD22 | 1.91                     | 0.51              |
| 1:A:2557:LYS:HA   | 1:A:2602:HIS:CE1  | 2.45                     | 0.51              |
| 1:A:3882:GLN:NE2  | 1:A:3946:GLY:HA3  | 2.25                     | 0.51              |
| 1:A:4238:ILE:HG23 | 1:A:4239:LEU:HD12 | 1.90                     | 0.51              |
| 1:A:4896:ASP:OD2  | 1:A:4897:TYR:N    | 2.43                     | 0.51              |
| 2:F:83:TYR:OH     | 1:B:1768:PHE:O    | 2.17                     | 0.51              |
| 1:B:882:ARG:NH2   | 1:B:1057:LEU:O    | 2.43                     | 0.51              |
| 1:B:1894:LEU:O    | 1:B:2068:ARG:NH2  | 2.43                     | 0.51              |
| 1:B:2542:ALA:HA   | 1:B:2545:ILE:HG12 | 1.92                     | 0.51              |
| 1:B:2681:MET:SD   | 1:B:2919:LYS:HB2  | 2.49                     | 0.51              |
| 1:B:2905:ARG:NE   | 1:B:2906:GLY:H    | 2.00                     | 0.51              |
| 1:B:3317:THR:O    | 1:B:3321:PRO:HD2  | 2.10                     | 0.51              |
| 1:B:3986:LEU:HD11 | 1:B:4105:LEU:HG   | 1.92                     | 0.51              |
| 1:B:4569:GLU:HB3  | 1:B:4570:PRO:HD3  | 1.91                     | 0.51              |
| 1:C:614:LEU:HD22  | 1:C:632:ILE:HG12  | 1.92                     | 0.51              |
| 1:C:4492:LEU:HD13 | 1:C:4592:CYS:SG   | 2.51                     | 0.51              |
| 1:D:1788:LYS:HG3  | 1:D:1834:PHE:CE1  | 2.46                     | 0.51              |
| 1:D:2557:LYS:HA   | 1:D:2602:HIS:CE1  | 2.45                     | 0.51              |
| 1:D:3914:LYS:HZ1  | 1:D:3973:ASP:CG   | 2.19                     | 0.51              |
| 1:D:4492:LEU:HD13 | 1:D:4592:CYS:SG   | 2.51                     | 0.51              |
| 1:D:4569:GLU:HB3  | 1:D:4570:PRO:HD3  | 1.91                     | 0.51              |
| 1:A:1113:MET:HB2  | 1:A:1156:TRP:CZ2  | 2.45                     | 0.51              |
| 1:A:3655:ASP:OD1  | 1:A:3656:GLU:N    | 2.44                     | 0.51              |
| 2:F:78:THR:OG1    | 2:F:80:ASP:OD1    | 2.26                     | 0.51              |
| 1:B:218:SER:HB2   | 1:B:286:GLY:HA3   | 1.91                     | 0.51              |
| 1:B:1457:PHE:HD1  | 1:B:1461:ARG:HH21 | 1.59                     | 0.51              |
| 1:B:1948:MET:HA   | 1:B:1951:LEU:HD23 | 1.91                     | 0.51              |
| 1:B:2651:ALA:O    | 1:B:2655:LYS:HB2  | 2.11                     | 0.51              |
| 1:B:3211:LEU:CD2  | 1:B:3215:MET:HE1  | 2.41                     | 0.51              |
| 1:B:4492:LEU:HD13 | 1:B:4592:CYS:SG   | 2.51                     | 0.51              |
| 1:C:917:CYS:HA    | 1:C:924:LEU:HG    | 1.92                     | 0.51              |
| 1:C:1114:ARG:HB2  | 1:C:1206:SER:HB3  | 1.92                     | 0.51              |
| 1:D:582:SER:OG    | 1:D:584:GLU:OE1   | 2.26                     | 0.51              |
| 1:D:910:ASP:OD1   | 1:D:911:ASN:N     | 2.42                     | 0.51              |
| 1:D:2681:MET:SD   | 1:D:2919:LYS:HB2  | 2.49                     | 0.51              |
| 1:D:4840:GLU:O    | 1:D:4844:ILE:HG12 | 2.10                     | 0.51              |
| 1:A:882:ARG:NH2   | 1:A:1057:LEU:HD12 | 2.26                     | 0.51              |
| 1:A:1894:LEU:O    | 1:A:2068:ARG:NH2  | 2.43                     | 0.51              |
| 1:A:2175:MET:SD   | 1:A:2193:VAL:HG13 | 2.50                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2679:ASP:HA   | 1:A:2920:ARG:HG2  | 1.91                     | 0.51              |
| 1:A:3211:LEU:CD2  | 1:A:3215:MET:HE1  | 2.41                     | 0.51              |
| 1:C:882:ARG:NH2   | 1:C:1057:LEU:O    | 2.43                     | 0.51              |
| 1:C:2175:MET:SD   | 1:C:2193:VAL:HG13 | 2.50                     | 0.51              |
| 1:C:2557:LYS:HA   | 1:C:2602:HIS:CE1  | 2.45                     | 0.51              |
| 1:C:3729:ALA:HA   | 1:C:3732:HIS:CD2  | 2.45                     | 0.51              |
| 1:D:1894:LEU:O    | 1:D:2068:ARG:NH2  | 2.43                     | 0.51              |
| 1:D:1911:GLN:HG3  | 1:D:2090:ARG:HH11 | 1.75                     | 0.51              |
| 1:D:3122:ILE:HA   | 1:D:3126:VAL:HB   | 1.93                     | 0.51              |
| 1:A:2621:TYR:HD2  | 1:A:2675:ALA:HB1  | 1.75                     | 0.51              |
| 2:F:58:LYS:NZ     | 2:F:81:VAL:HA     | 2.25                     | 0.51              |
| 2:G:58:LYS:NZ     | 2:G:81:VAL:HA     | 2.25                     | 0.51              |
| 1:B:194:LEU:HD21  | 1:B:201:LEU:HD23  | 1.92                     | 0.51              |
| 1:B:1428:TYR:OH   | 1:B:1444:GLY:O    | 2.28                     | 0.51              |
| 1:B:3098:THR:HA   | 1:B:3102:LEU:HD12 | 1.91                     | 0.51              |
| 1:B:3168:VAL:HG13 | 1:B:3179:ASN:HD22 | 1.76                     | 0.51              |
| 1:B:3729:ALA:HA   | 1:B:3732:HIS:CD2  | 2.45                     | 0.51              |
| 1:C:194:LEU:HD21  | 1:C:201:LEU:HD23  | 1.92                     | 0.51              |
| 1:C:2785:TRP:HB2  | 1:C:2787:TRP:CZ3  | 2.45                     | 0.51              |
| 1:C:3168:VAL:HG13 | 1:C:3179:ASN:HD22 | 1.76                     | 0.51              |
| 1:C:4569:GLU:HB3  | 1:C:4570:PRO:HD3  | 1.91                     | 0.51              |
| 1:C:4827:ILE:O    | 1:C:4831:ILE:HG12 | 2.10                     | 0.51              |
| 1:D:663:VAL:HG23  | 1:D:671:LYS:HE3   | 1.91                     | 0.51              |
| 1:D:2149:ILE:HG21 | 1:D:2167:MET:HE1  | 1.91                     | 0.51              |
| 1:A:614:LEU:HD22  | 1:A:632:ILE:HG12  | 1.92                     | 0.51              |
| 1:A:925:PRO:HB2   | 1:A:928:GLU:OE1   | 2.09                     | 0.51              |
| 1:A:996:VAL:HB    | 1:A:1051:ARG:HE   | 1.75                     | 0.51              |
| 1:A:3650:GLU:HB2  | 1:A:3651:PRO:HD3  | 1.92                     | 0.51              |
| 1:B:2087:LEU:O    | 1:B:2091:GLN:HG2  | 2.11                     | 0.51              |
| 1:B:3882:GLN:NE2  | 1:B:3946:GLY:HA3  | 2.25                     | 0.51              |
| 1:C:1457:PHE:HD1  | 1:C:1461:ARG:HH21 | 1.59                     | 0.51              |
| 1:C:1690:GLU:OE1  | 1:C:1790:LYS:NZ   | 2.44                     | 0.51              |
| 1:C:1788:LYS:HG3  | 1:C:1834:PHE:CE1  | 2.46                     | 0.51              |
| 1:C:1911:GLN:HG3  | 1:C:2090:ARG:HH11 | 1.75                     | 0.51              |
| 1:C:2232:PRO:C    | 1:C:2234:MET:H    | 2.17                     | 0.51              |
| 1:C:2621:TYR:HD2  | 1:C:2675:ALA:HB1  | 1.75                     | 0.51              |
| 1:C:2729:HIS:HE1  | 1:C:2756:LEU:HG   | 1.76                     | 0.51              |
| 1:C:3317:THR:O    | 1:C:3321:PRO:HD2  | 2.10                     | 0.51              |
| 1:D:996:VAL:HB    | 1:D:1051:ARG:HE   | 1.75                     | 0.51              |
| 1:D:2403:ALA:O    | 1:D:2474:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:1286:THR:OG1  | 1:A:1550:PRO:O    | 2.24                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1428:TYR:OH   | 1:A:1444:GLY:O    | 2.28                     | 0.51              |
| 1:A:3019:ILE:HD11 | 1:A:3096:TYR:HB2  | 1.92                     | 0.51              |
| 1:B:2127:ARG:NH2  | 1:B:2165:LEU:O    | 2.43                     | 0.51              |
| 1:C:962:LYS:C     | 1:C:963:LYS:HD3   | 2.35                     | 0.51              |
| 1:C:1428:TYR:OH   | 1:C:1444:GLY:O    | 2.28                     | 0.51              |
| 1:C:3098:THR:HA   | 1:C:3102:LEU:HD12 | 1.91                     | 0.51              |
| 1:D:1939:ASN:HD22 | 1:D:1992:ILE:HG13 | 1.74                     | 0.51              |
| 1:D:2651:ALA:O    | 1:D:2655:LYS:HB2  | 2.11                     | 0.51              |
| 1:D:3655:ASP:OD1  | 1:D:3656:GLU:N    | 2.44                     | 0.51              |
| 1:A:2087:LEU:O    | 1:A:2091:GLN:HG2  | 2.11                     | 0.51              |
| 1:A:3122:ILE:HA   | 1:A:3126:VAL:HB   | 1.93                     | 0.51              |
| 1:A:3914:LYS:HZ1  | 1:A:3973:ASP:CG   | 2.19                     | 0.51              |
| 2:H:24:VAL:HG12   | 2:H:48:LYS:HG2    | 1.91                     | 0.51              |
| 1:B:902:TRP:HE1   | 1:B:915:HIS:CG    | 2.29                     | 0.51              |
| 1:B:1690:GLU:OE1  | 1:B:1790:LYS:NZ   | 2.44                     | 0.51              |
| 1:B:2426:LEU:HD23 | 1:C:143:LEU:HD11  | 1.93                     | 0.51              |
| 1:B:3805:LEU:HD21 | 1:B:3891:TYR:HB2  | 1.93                     | 0.51              |
| 1:C:1219:LYS:NZ   | 1:C:1243:THR:O    | 2.43                     | 0.51              |
| 1:C:2641:SER:HB2  | 1:C:2676:LEU:HD21 | 1.92                     | 0.51              |
| 1:C:3122:ILE:HA   | 1:C:3126:VAL:HB   | 1.93                     | 0.51              |
| 1:C:4840:GLU:O    | 1:C:4844:ILE:HG12 | 2.10                     | 0.51              |
| 1:C:4896:ASP:OD2  | 1:C:4897:TYR:N    | 2.43                     | 0.51              |
| 1:D:882:ARG:NH2   | 1:D:1057:LEU:HD12 | 2.26                     | 0.51              |
| 1:D:1114:ARG:HB2  | 1:D:1206:SER:HB3  | 1.92                     | 0.51              |
| 1:D:1948:MET:HA   | 1:D:1951:LEU:HD23 | 1.92                     | 0.51              |
| 1:D:2621:TYR:HD2  | 1:D:2675:ALA:HB1  | 1.75                     | 0.51              |
| 1:D:3211:LEU:CD2  | 1:D:3215:MET:HE1  | 2.41                     | 0.51              |
| 1:A:2127:ARG:NH2  | 1:A:2165:LEU:O    | 2.43                     | 0.51              |
| 1:A:3168:VAL:HG13 | 1:A:3179:ASN:HD22 | 1.76                     | 0.51              |
| 1:A:4492:LEU:HD13 | 1:A:4592:CYS:SG   | 2.51                     | 0.51              |
| 2:E:58:LYS:NZ     | 2:E:81:VAL:HA     | 2.25                     | 0.51              |
| 1:B:821:PRO:HB2   | 1:B:823:TYR:HD1   | 1.76                     | 0.51              |
| 1:B:2202:TYR:O    | 1:B:2206:ILE:HG12 | 2.11                     | 0.51              |
| 1:B:3122:ILE:HD13 | 1:B:3167:PRO:HD3  | 1.92                     | 0.51              |
| 1:B:3238:ILE:O    | 1:B:3242:LEU:N    | 2.29                     | 0.51              |
| 1:C:2651:ALA:O    | 1:C:2655:LYS:HB2  | 2.11                     | 0.51              |
| 1:A:2729:HIS:HE1  | 1:A:2756:LEU:HG   | 1.76                     | 0.51              |
| 1:B:892:LEU:HA    | 1:B:895:MET:CE    | 2.41                     | 0.51              |
| 1:B:917:CYS:HA    | 1:B:924:LEU:HG    | 1.92                     | 0.51              |
| 1:B:4264:LEU:O    | 1:B:4268:MET:HG2  | 2.12                     | 0.51              |
| 1:C:2635:GLU:HA   | 1:C:2638:LEU:HB2  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3211:LEU:CD2  | 1:C:3215:MET:HE1  | 2.41                     | 0.51              |
| 1:C:4867:ILE:HG12 | 1:D:4864:GLY:HA2  | 1.92                     | 0.51              |
| 1:D:892:LEU:HA    | 1:D:895:MET:CE    | 2.41                     | 0.51              |
| 1:D:1219:LYS:NZ   | 1:D:1243:THR:O    | 2.43                     | 0.51              |
| 1:D:2622:CYS:SG   | 1:D:2623:LEU:N    | 2.84                     | 0.51              |
| 1:D:2729:HIS:HE1  | 1:D:2756:LEU:HG   | 1.76                     | 0.51              |
| 1:D:3122:ILE:HD13 | 1:D:3167:PRO:HD3  | 1.92                     | 0.51              |
| 1:D:3650:GLU:HB2  | 1:D:3651:PRO:HD3  | 1.92                     | 0.51              |
| 1:A:892:LEU:HA    | 1:A:895:MET:CE    | 2.41                     | 0.50              |
| 1:A:2635:GLU:HA   | 1:A:2638:LEU:HB2  | 1.92                     | 0.50              |
| 1:A:2651:ALA:O    | 1:A:2655:LYS:HB2  | 2.11                     | 0.50              |
| 2:H:58:LYS:NZ     | 2:H:81:VAL:HA     | 2.25                     | 0.50              |
| 1:B:2557:LYS:HA   | 1:B:2602:HIS:CE1  | 2.45                     | 0.50              |
| 1:B:2621:TYR:HD2  | 1:B:2675:ALA:HB1  | 1.75                     | 0.50              |
| 1:B:3122:ILE:HA   | 1:B:3126:VAL:HB   | 1.93                     | 0.50              |
| 1:C:2127:ARG:NH2  | 1:C:2165:LEU:O    | 2.43                     | 0.50              |
| 1:C:2403:ALA:O    | 1:C:2474:ARG:NH2  | 2.44                     | 0.50              |
| 1:C:2673:ALA:HB1  | 1:C:2974:TYR:HD1  | 1.77                     | 0.50              |
| 1:C:3019:ILE:HD11 | 1:C:3096:TYR:HB2  | 1.92                     | 0.50              |
| 1:C:3805:LEU:HD21 | 1:C:3891:TYR:HB2  | 1.93                     | 0.50              |
| 1:D:2581:ARG:NH2  | 1:D:2582:PRO:HG2  | 2.25                     | 0.50              |
| 1:D:3282:LYS:HD3  | 1:D:3286:ASN:HD22 | 1.76                     | 0.50              |
| 1:A:902:TRP:HE1   | 1:A:915:HIS:CG    | 2.29                     | 0.50              |
| 1:A:1457:PHE:HD1  | 1:A:1461:ARG:HH21 | 1.59                     | 0.50              |
| 1:A:1788:LYS:HG3  | 1:A:1834:PHE:CE1  | 2.45                     | 0.50              |
| 1:A:3932:GLN:O    | 1:A:3985:MET:HE1  | 2.11                     | 0.50              |
| 2:G:8:ILE:HA      | 1:C:730:LEU:HD11  | 1.93                     | 0.50              |
| 1:B:1788:LYS:HG3  | 1:B:1834:PHE:CE1  | 2.46                     | 0.50              |
| 1:B:2726:GLU:OE1  | 1:B:2726:GLU:N    | 2.45                     | 0.50              |
| 1:C:892:LEU:HA    | 1:C:895:MET:CE    | 2.41                     | 0.50              |
| 1:C:1041:ARG:O    | 1:C:1044:LYS:HG3  | 2.12                     | 0.50              |
| 1:C:2087:LEU:O    | 1:C:2091:GLN:HG2  | 2.11                     | 0.50              |
| 1:D:917:CYS:HA    | 1:D:924:LEU:HG    | 1.92                     | 0.50              |
| 1:D:2834:SER:OG   | 1:D:2836:ASP:OD1  | 2.24                     | 0.50              |
| 1:A:1041:ARG:O    | 1:A:1044:LYS:HG3  | 2.12                     | 0.50              |
| 1:A:1948:MET:HA   | 1:A:1951:LEU:HD23 | 1.91                     | 0.50              |
| 1:A:2622:CYS:SG   | 1:A:2623:LEU:N    | 2.84                     | 0.50              |
| 1:B:962:LYS:C     | 1:B:963:LYS:HD3   | 2.35                     | 0.50              |
| 1:B:1114:ARG:HB2  | 1:B:1206:SER:HB3  | 1.92                     | 0.50              |
| 1:B:2635:GLU:HA   | 1:B:2638:LEU:HB2  | 1.92                     | 0.50              |
| 1:C:816:PRO:HB2   | 1:C:819:TYR:CD1   | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:821:PRO:HB2   | 1:C:823:TYR:HD1   | 1.76                     | 0.50              |
| 1:C:902:TRP:HE1   | 1:C:915:HIS:CG    | 2.29                     | 0.50              |
| 1:D:2726:GLU:OE1  | 1:D:2726:GLU:N    | 2.45                     | 0.50              |
| 1:D:3010:LYS:O    | 1:D:3014:LEU:HD23 | 2.12                     | 0.50              |
| 1:D:3168:VAL:HG13 | 1:D:3179:ASN:HD22 | 1.76                     | 0.50              |
| 1:A:1788:LYS:HD3  | 1:A:1833:ILE:HG22 | 1.93                     | 0.50              |
| 1:A:2202:TYR:O    | 1:A:2206:ILE:HG12 | 2.11                     | 0.50              |
| 1:A:2726:GLU:OE1  | 1:A:2726:GLU:N    | 2.45                     | 0.50              |
| 1:B:1041:ARG:O    | 1:B:1044:LYS:HG3  | 2.12                     | 0.50              |
| 1:B:2622:CYS:SG   | 1:B:2623:LEU:N    | 2.84                     | 0.50              |
| 1:D:1041:ARG:O    | 1:D:1044:LYS:HG3  | 2.12                     | 0.50              |
| 1:D:2087:LEU:O    | 1:D:2091:GLN:HG2  | 2.11                     | 0.50              |
| 1:A:4264:LEU:O    | 1:A:4268:MET:HG2  | 2.12                     | 0.50              |
| 1:B:816:PRO:HB2   | 1:B:819:TYR:CD1   | 2.46                     | 0.50              |
| 1:B:2403:ALA:O    | 1:B:2474:ARG:NH2  | 2.44                     | 0.50              |
| 1:B:2729:HIS:HE1  | 1:B:2756:LEU:HG   | 1.76                     | 0.50              |
| 1:C:2718:GLU:HA   | 1:C:2721:ILE:HG12 | 1.94                     | 0.50              |
| 1:C:3932:GLN:O    | 1:C:3985:MET:HE1  | 2.12                     | 0.50              |
| 1:D:365:HIS:HB2   | 1:D:393:MET:HE2   | 1.93                     | 0.50              |
| 1:D:902:TRP:HE1   | 1:D:915:HIS:CG    | 2.29                     | 0.50              |
| 1:A:2403:ALA:O    | 1:A:2474:ARG:NH2  | 2.44                     | 0.50              |
| 1:A:3282:LYS:HD3  | 1:A:3286:ASN:HD22 | 1.76                     | 0.50              |
| 1:A:3947:PHE:HB2  | 1:A:3978:MET:HE1  | 1.93                     | 0.50              |
| 1:A:4253:LEU:O    | 1:A:4257:ARG:HG2  | 2.11                     | 0.50              |
| 1:B:1219:LYS:NZ   | 1:B:1243:THR:O    | 2.43                     | 0.50              |
| 1:B:2718:GLU:HA   | 1:B:2721:ILE:HG12 | 1.94                     | 0.50              |
| 1:B:3851:ASN:O    | 1:B:3855:GLN:HG3  | 2.12                     | 0.50              |
| 1:C:1611:ILE:H    | 1:C:1611:ILE:HD12 | 1.77                     | 0.50              |
| 1:C:2905:ARG:NE   | 1:C:2906:GLY:H    | 2.01                     | 0.50              |
| 1:C:4607:ALA:HB1  | 1:C:4649:VAL:HG21 | 1.94                     | 0.50              |
| 1:D:1690:GLU:OE1  | 1:D:1790:LYS:NZ   | 2.44                     | 0.50              |
| 1:D:2718:GLU:HA   | 1:D:2721:ILE:HG12 | 1.94                     | 0.50              |
| 1:A:2641:SER:HB2  | 1:A:2676:LEU:HD21 | 1.92                     | 0.50              |
| 1:A:3023:GLY:N    | 1:A:3025:ASP:OD2  | 2.45                     | 0.50              |
| 1:A:3661:VAL:HG23 | 1:A:3666:GLN:HG2  | 1.94                     | 0.50              |
| 1:B:1611:ILE:H    | 1:B:1611:ILE:HD12 | 1.77                     | 0.50              |
| 1:B:2641:SER:HB2  | 1:B:2676:LEU:HD21 | 1.92                     | 0.50              |
| 1:B:3655:ASP:OD1  | 1:B:3656:GLU:N    | 2.44                     | 0.50              |
| 1:B:4607:ALA:HB1  | 1:B:4649:VAL:HG21 | 1.94                     | 0.50              |
| 1:C:2834:SER:OG   | 1:C:2836:ASP:OD1  | 2.24                     | 0.50              |
| 1:C:3305:PRO:HB2  | 1:C:3309:LYS:NZ   | 2.27                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4264:LEU:O    | 1:C:4268:MET:HG2  | 2.12                     | 0.50              |
| 1:D:1457:PHE:HD1  | 1:D:1461:ARG:HH21 | 1.59                     | 0.50              |
| 1:D:1937:GLN:HG2  | 1:D:3609:TYR:HA   | 1.94                     | 0.50              |
| 1:D:2202:TYR:O    | 1:D:2206:ILE:HG12 | 2.11                     | 0.50              |
| 1:D:2409:ILE:HG21 | 1:D:2420:ARG:NH2  | 2.27                     | 0.50              |
| 1:D:3986:LEU:HG   | 1:D:3999:MET:SD   | 2.51                     | 0.50              |
| 1:A:3986:LEU:HG   | 1:A:3999:MET:SD   | 2.52                     | 0.50              |
| 1:B:365:HIS:HB2   | 1:B:393:MET:HE2   | 1.93                     | 0.50              |
| 1:B:4253:LEU:O    | 1:B:4257:ARG:HG2  | 2.11                     | 0.50              |
| 1:C:375:GLN:N     | 1:C:390:LYS:O     | 2.34                     | 0.50              |
| 1:C:1221:VAL:HG12 | 1:C:1238:PRO:HG2  | 1.94                     | 0.50              |
| 1:C:3655:ASP:OD1  | 1:C:3656:GLU:N    | 2.44                     | 0.50              |
| 1:C:3851:ASN:O    | 1:C:3855:GLN:HG3  | 2.12                     | 0.50              |
| 1:C:3986:LEU:HG   | 1:C:3999:MET:SD   | 2.52                     | 0.50              |
| 1:D:3932:GLN:O    | 1:D:3985:MET:HE1  | 2.12                     | 0.50              |
| 1:A:821:PRO:HB2   | 1:A:823:TYR:CD1   | 2.47                     | 0.50              |
| 1:A:1114:ARG:HB2  | 1:A:1206:SER:HB3  | 1.92                     | 0.50              |
| 1:A:3122:ILE:HD13 | 1:A:3167:PRO:HD3  | 1.92                     | 0.50              |
| 1:A:4287:TYR:CD2  | 1:B:4588:ILE:HG12 | 2.47                     | 0.50              |
| 1:B:28:ILE:HG22   | 1:B:29:HIS:HD2    | 1.77                     | 0.50              |
| 1:B:2180:GLY:HA2  | 1:B:2183:GLU:HG2  | 1.94                     | 0.50              |
| 1:C:290:ARG:NH2   | 1:C:351:THR:OG1   | 2.45                     | 0.50              |
| 1:C:882:ARG:NH2   | 1:C:1057:LEU:HD12 | 2.26                     | 0.50              |
| 1:D:816:PRO:HB2   | 1:D:819:TYR:CD1   | 2.46                     | 0.50              |
| 1:D:2641:SER:HB2  | 1:D:2676:LEU:HD21 | 1.92                     | 0.50              |
| 1:D:4253:LEU:O    | 1:D:4257:ARG:HG2  | 2.11                     | 0.50              |
| 1:A:365:HIS:HB2   | 1:A:393:MET:HE2   | 1.93                     | 0.49              |
| 1:A:816:PRO:HB2   | 1:A:819:TYR:CD1   | 2.46                     | 0.49              |
| 1:A:1611:ILE:H    | 1:A:1611:ILE:HD12 | 1.77                     | 0.49              |
| 1:A:2893:LEU:HD23 | 1:A:2896:LEU:HD21 | 1.94                     | 0.49              |
| 1:B:882:ARG:NH2   | 1:B:1057:LEU:HD12 | 2.26                     | 0.49              |
| 1:B:3305:PRO:HB2  | 1:B:3309:LYS:NZ   | 2.27                     | 0.49              |
| 1:B:3986:LEU:HG   | 1:B:3999:MET:SD   | 2.51                     | 0.49              |
| 1:C:814:LEU:HD23  | 1:C:815:PRO:O     | 2.12                     | 0.49              |
| 1:C:3228:TYR:OH   | 1:C:3236:GLU:HB3  | 2.12                     | 0.49              |
| 1:C:4137:GLU:HG2  | 1:C:4147:ARG:HG2  | 1.94                     | 0.49              |
| 1:D:1221:VAL:HG12 | 1:D:1238:PRO:HG2  | 1.94                     | 0.49              |
| 1:D:1611:ILE:HD12 | 1:D:1611:ILE:H    | 1.77                     | 0.49              |
| 1:D:2905:ARG:NE   | 1:D:2906:GLY:H    | 2.01                     | 0.49              |
| 1:A:1690:GLU:OE1  | 1:A:1790:LYS:NZ   | 2.44                     | 0.49              |
| 1:A:1937:GLN:HG2  | 1:A:3609:TYR:HA   | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2119:LEU:HD13 | 1:A:2154:VAL:HG23 | 1.94                     | 0.49              |
| 1:A:3010:LYS:O    | 1:A:3014:LEU:HD23 | 2.12                     | 0.49              |
| 1:A:3851:ASN:O    | 1:A:3855:GLN:HG3  | 2.12                     | 0.49              |
| 1:A:4607:ALA:HB1  | 1:A:4649:VAL:HG21 | 1.94                     | 0.49              |
| 1:B:1937:GLN:HG2  | 1:B:3609:TYR:HA   | 1.94                     | 0.49              |
| 1:B:2409:ILE:HG21 | 1:B:2420:ARG:NH2  | 2.27                     | 0.49              |
| 1:C:365:HIS:HB2   | 1:C:393:MET:HE2   | 1.93                     | 0.49              |
| 1:C:1963:LYS:HB3  | 1:C:1966:ARG:HH21 | 1.77                     | 0.49              |
| 1:C:2202:TYR:O    | 1:C:2206:ILE:HG12 | 2.11                     | 0.49              |
| 1:C:2232:PRO:HD2  | 1:C:2379:ASP:HA   | 1.95                     | 0.49              |
| 1:C:2622:CYS:SG   | 1:C:2623:LEU:N    | 2.84                     | 0.49              |
| 1:D:821:PRO:HB2   | 1:D:823:TYR:CD1   | 2.47                     | 0.49              |
| 1:D:3947:PHE:HB2  | 1:D:3978:MET:HE1  | 1.93                     | 0.49              |
| 1:A:2718:GLU:HA   | 1:A:2721:ILE:HG12 | 1.94                     | 0.49              |
| 1:B:434:ASP:HB3   | 1:B:438:LYS:NZ    | 2.28                     | 0.49              |
| 1:B:3947:PHE:HB2  | 1:B:3978:MET:HE1  | 1.93                     | 0.49              |
| 1:B:4964:ASP:OD2  | 1:B:4965:GLN:N    | 2.46                     | 0.49              |
| 1:C:3065:ALA:HB1  | 1:C:3132:ARG:NH1  | 2.21                     | 0.49              |
| 1:C:3122:ILE:HD13 | 1:C:3167:PRO:HD3  | 1.92                     | 0.49              |
| 1:C:4253:LEU:O    | 1:C:4257:ARG:HG2  | 2.11                     | 0.49              |
| 1:D:889:ILE:HG22  | 1:D:893:TRP:CZ3   | 2.48                     | 0.49              |
| 1:D:2893:LEU:HD23 | 1:D:2896:LEU:HD21 | 1.94                     | 0.49              |
| 1:D:3305:PRO:HB2  | 1:D:3309:LYS:NZ   | 2.27                     | 0.49              |
| 1:A:889:ILE:HG22  | 1:A:893:TRP:CZ3   | 2.48                     | 0.49              |
| 1:A:2673:ALA:HB1  | 1:A:2974:TYR:HD1  | 1.77                     | 0.49              |
| 1:A:2834:SER:OG   | 1:A:2836:ASP:OD1  | 2.24                     | 0.49              |
| 1:A:3124:GLU:C    | 1:A:3126:VAL:H    | 2.20                     | 0.49              |
| 1:A:3305:PRO:HB2  | 1:A:3309:LYS:NZ   | 2.27                     | 0.49              |
| 1:A:4767:LEU:O    | 1:A:4771:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:371:TRP:O     | 1:B:394:HIS:N     | 2.45                     | 0.49              |
| 1:B:3023:GLY:N    | 1:B:3025:ASP:OD2  | 2.45                     | 0.49              |
| 1:B:3124:GLU:C    | 1:B:3126:VAL:H    | 2.20                     | 0.49              |
| 1:C:28:ILE:HG22   | 1:C:29:HIS:HD2    | 1.77                     | 0.49              |
| 1:C:1788:LYS:HD3  | 1:C:1833:ILE:HG22 | 1.93                     | 0.49              |
| 1:C:3947:PHE:HB2  | 1:C:3978:MET:HE1  | 1.93                     | 0.49              |
| 1:D:3228:TYR:OH   | 1:D:3236:GLU:HB3  | 2.12                     | 0.49              |
| 1:D:3661:VAL:HG23 | 1:D:3666:GLN:HG2  | 1.94                     | 0.49              |
| 1:A:2058:LEU:O    | 1:A:2062:ILE:HG12 | 2.13                     | 0.49              |
| 1:A:3805:LEU:HD21 | 1:A:3891:TYR:HB2  | 1.93                     | 0.49              |
| 1:B:3010:LYS:O    | 1:B:3014:LEU:HD23 | 2.11                     | 0.49              |
| 1:B:3661:VAL:HG23 | 1:B:3666:GLN:HG2  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4867:ILE:HG12 | 1:C:4864:GLY:HA2  | 1.94                     | 0.49              |
| 1:C:3010:LYS:O    | 1:C:3014:LEU:HD23 | 2.11                     | 0.49              |
| 1:D:290:ARG:NH2   | 1:D:351:THR:OG1   | 2.45                     | 0.49              |
| 1:D:821:PRO:HB2   | 1:D:823:TYR:HD1   | 1.76                     | 0.49              |
| 1:D:853:PRO:HB3   | 1:D:1083:GLU:OE2  | 2.12                     | 0.49              |
| 1:D:1040:ASP:HA   | 1:D:1043:LYS:HG2  | 1.95                     | 0.49              |
| 1:D:2232:PRO:HD2  | 1:D:2379:ASP:HA   | 1.95                     | 0.49              |
| 1:D:3851:ASN:O    | 1:D:3855:GLN:HG3  | 2.12                     | 0.49              |
| 1:A:28:ILE:HG22   | 1:A:29:HIS:HD2    | 1.77                     | 0.49              |
| 1:A:853:PRO:HB3   | 1:A:1083:GLU:OE2  | 2.12                     | 0.49              |
| 1:B:853:PRO:HB3   | 1:B:1083:GLU:OE2  | 2.12                     | 0.49              |
| 1:B:1788:LYS:HD3  | 1:B:1833:ILE:HG22 | 1.93                     | 0.49              |
| 1:B:1959:ALA:O    | 1:B:1966:ARG:NH2  | 2.46                     | 0.49              |
| 1:B:1963:LYS:HB3  | 1:B:1966:ARG:HH21 | 1.78                     | 0.49              |
| 1:B:2322:ARG:O    | 1:B:2326:ARG:HG2  | 2.13                     | 0.49              |
| 1:B:2673:ALA:HB1  | 1:B:2974:TYR:HD1  | 1.77                     | 0.49              |
| 1:B:3228:TYR:OH   | 1:B:3236:GLU:HB3  | 2.12                     | 0.49              |
| 1:C:1040:ASP:HA   | 1:C:1043:LYS:HG2  | 1.95                     | 0.49              |
| 1:C:2409:ILE:HG21 | 1:C:2420:ARG:NH2  | 2.27                     | 0.49              |
| 1:C:2500:ALA:HB1  | 1:C:2554:ARG:HG2  | 1.94                     | 0.49              |
| 1:C:3124:GLU:C    | 1:C:3126:VAL:H    | 2.20                     | 0.49              |
| 1:D:176:ARG:N     | 1:D:179:ASP:OD2   | 2.37                     | 0.49              |
| 1:D:1788:LYS:HD3  | 1:D:1833:ILE:HG22 | 1.93                     | 0.49              |
| 1:D:4264:LEU:O    | 1:D:4268:MET:HG2  | 2.12                     | 0.49              |
| 1:A:2156:TYR:HE1  | 1:A:2202:TYR:HE2  | 1.61                     | 0.49              |
| 1:A:2409:ILE:HG21 | 1:A:2420:ARG:NH2  | 2.27                     | 0.49              |
| 1:B:176:ARG:N     | 1:B:179:ASP:OD2   | 2.37                     | 0.49              |
| 1:B:965:LYS:HE3   | 1:B:977:LYS:HG3   | 1.94                     | 0.49              |
| 1:B:1040:ASP:HA   | 1:B:1043:LYS:HG2  | 1.95                     | 0.49              |
| 1:B:4079:ASP:O    | 1:B:4082:GLU:HG3  | 2.13                     | 0.49              |
| 1:C:434:ASP:HB3   | 1:C:438:LYS:NZ    | 2.28                     | 0.49              |
| 1:C:821:PRO:HB2   | 1:C:823:TYR:CD1   | 2.47                     | 0.49              |
| 1:C:2119:LEU:HD13 | 1:C:2154:VAL:HG23 | 1.94                     | 0.49              |
| 1:C:4964:ASP:OD2  | 1:C:4965:GLN:N    | 2.46                     | 0.49              |
| 1:D:814:LEU:HD23  | 1:D:815:PRO:O     | 2.12                     | 0.49              |
| 1:D:1959:ALA:O    | 1:D:1966:ARG:NH2  | 2.46                     | 0.49              |
| 1:D:1963:LYS:HB3  | 1:D:1966:ARG:HH21 | 1.78                     | 0.49              |
| 1:D:4137:GLU:HG2  | 1:D:4147:ARG:HG2  | 1.94                     | 0.49              |
| 1:D:4607:ALA:HB1  | 1:D:4649:VAL:HG21 | 1.94                     | 0.49              |
| 1:A:371:TRP:O     | 1:A:394:HIS:N     | 2.45                     | 0.49              |
| 1:A:655:MET:HG2   | 1:A:794:PHE:HE1   | 1.78                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:821:PRO:HB2   | 1:A:823:TYR:HD1   | 1.76                     | 0.49              |
| 1:A:1221:VAL:HG12 | 1:A:1238:PRO:HG2  | 1.94                     | 0.49              |
| 1:A:1963:LYS:HB3  | 1:A:1966:ARG:HH21 | 1.78                     | 0.49              |
| 1:A:3034:HIS:CE1  | 1:A:3107:SER:HG   | 2.26                     | 0.49              |
| 1:A:3238:ILE:O    | 1:A:3242:LEU:N    | 2.29                     | 0.49              |
| 1:B:1221:VAL:HG12 | 1:B:1238:PRO:HG2  | 1.94                     | 0.49              |
| 1:B:2058:LEU:O    | 1:B:2062:ILE:HG12 | 2.13                     | 0.49              |
| 1:B:2720:PHE:CE2  | 1:B:2896:LEU:HA   | 2.48                     | 0.49              |
| 1:C:1038:LEU:HD22 | 1:C:1043:LYS:HB3  | 1.95                     | 0.49              |
| 1:C:2156:TYR:HE1  | 1:C:2202:TYR:HE2  | 1.61                     | 0.49              |
| 1:C:2180:GLY:HA2  | 1:C:2183:GLU:HG2  | 1.94                     | 0.49              |
| 1:C:4113:THR:O    | 1:C:4117:THR:HG23 | 2.13                     | 0.49              |
| 1:C:4587:ILE:HD13 | 1:C:4722:LEU:HB3  | 1.95                     | 0.49              |
| 1:D:4587:ILE:HD13 | 1:D:4722:LEU:HB3  | 1.95                     | 0.49              |
| 1:D:4964:ASP:OD2  | 1:D:4965:GLN:N    | 2.46                     | 0.49              |
| 1:A:1959:ALA:O    | 1:A:1966:ARG:NH2  | 2.46                     | 0.49              |
| 1:A:2322:ARG:O    | 1:A:2326:ARG:HG2  | 2.13                     | 0.49              |
| 1:A:4964:ASP:OD2  | 1:A:4965:GLN:N    | 2.46                     | 0.49              |
| 1:B:290:ARG:NH2   | 1:B:351:THR:OG1   | 2.45                     | 0.49              |
| 1:B:889:ILE:HG22  | 1:B:893:TRP:CZ3   | 2.48                     | 0.49              |
| 1:B:2893:LEU:HD23 | 1:B:2896:LEU:HD21 | 1.94                     | 0.49              |
| 1:D:19:GLU:HG2    | 1:D:66:THR:HB     | 1.95                     | 0.49              |
| 1:D:2156:TYR:HE1  | 1:D:2202:TYR:HE2  | 1.61                     | 0.49              |
| 1:D:2673:ALA:HB1  | 1:D:2974:TYR:HD1  | 1.77                     | 0.49              |
| 1:D:2720:PHE:CE2  | 1:D:2896:LEU:HA   | 2.48                     | 0.49              |
| 1:D:3124:GLU:C    | 1:D:3126:VAL:H    | 2.20                     | 0.49              |
| 1:D:3314:LEU:HA   | 1:D:3318:HIS:HD1  | 1.78                     | 0.49              |
| 1:D:3805:LEU:HD21 | 1:D:3891:TYR:HB2  | 1.93                     | 0.49              |
| 1:D:4079:ASP:O    | 1:D:4082:GLU:HG3  | 2.13                     | 0.49              |
| 1:D:4767:LEU:O    | 1:D:4771:VAL:HG23 | 2.13                     | 0.49              |
| 1:A:434:ASP:HB3   | 1:A:438:LYS:NZ    | 2.28                     | 0.49              |
| 1:A:1671:ARG:NH2  | 2:E:89:PRO:HB2    | 2.28                     | 0.49              |
| 1:A:4503:ARG:NH2  | 1:A:4721:TYR:HE2  | 2.11                     | 0.49              |
| 1:B:480:ARG:NH2   | 1:B:3678:GLU:OE2  | 2.45                     | 0.49              |
| 1:B:814:LEU:HD23  | 1:B:815:PRO:O     | 2.12                     | 0.49              |
| 1:B:2119:LEU:HD13 | 1:B:2154:VAL:HG23 | 1.94                     | 0.49              |
| 1:B:2156:TYR:HE1  | 1:B:2202:TYR:HE2  | 1.61                     | 0.49              |
| 1:B:2409:ILE:HG12 | 1:B:2420:ARG:CZ   | 2.43                     | 0.49              |
| 1:B:2652:LEU:HD22 | 1:B:2669:LEU:HD11 | 1.94                     | 0.49              |
| 1:B:3932:GLN:O    | 1:B:3985:MET:HE1  | 2.11                     | 0.49              |
| 1:C:1937:GLN:HG2  | 1:C:3609:TYR:HA   | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3642:GLU:HG3  | 1:C:3646:LYS:NZ   | 2.28                     | 0.49              |
| 1:D:2652:LEU:HD22 | 1:D:2669:LEU:HD11 | 1.95                     | 0.49              |
| 1:D:2957:GLU:O    | 1:D:2961:LYS:HG3  | 2.13                     | 0.49              |
| 1:D:3065:ALA:HB1  | 1:D:3132:ARG:NH1  | 2.21                     | 0.49              |
| 1:D:3238:ILE:O    | 1:D:3242:LEU:N    | 2.29                     | 0.49              |
| 1:A:585:ALA:O     | 1:A:589:ILE:HG12  | 2.12                     | 0.48              |
| 1:A:902:TRP:CZ3   | 1:A:913:ARG:HD2   | 2.48                     | 0.48              |
| 1:A:2180:GLY:HA2  | 1:A:2183:GLU:HG2  | 1.94                     | 0.48              |
| 1:A:4113:THR:O    | 1:A:4117:THR:HG23 | 2.13                     | 0.48              |
| 1:B:821:PRO:HB2   | 1:B:823:TYR:CD1   | 2.47                     | 0.48              |
| 1:B:4137:GLU:HG2  | 1:B:4147:ARG:HG2  | 1.94                     | 0.48              |
| 1:C:546:LYS:O     | 1:C:550:GLN:HG2   | 2.13                     | 0.48              |
| 1:C:585:ALA:O     | 1:C:589:ILE:HG12  | 2.12                     | 0.48              |
| 1:C:889:ILE:HG22  | 1:C:893:TRP:CZ3   | 2.48                     | 0.48              |
| 1:C:902:TRP:CZ3   | 1:C:913:ARG:HD2   | 2.48                     | 0.48              |
| 1:C:965:LYS:HE3   | 1:C:977:LYS:HG3   | 1.94                     | 0.48              |
| 1:C:1959:ALA:O    | 1:C:1966:ARG:NH2  | 2.46                     | 0.48              |
| 1:C:2270:ALA:HB2  | 1:C:2327:ARG:HD3  | 1.95                     | 0.48              |
| 1:C:2720:PHE:CE2  | 1:C:2896:LEU:HA   | 2.48                     | 0.48              |
| 1:C:4114:ARG:O    | 1:C:4117:THR:OG1  | 2.28                     | 0.48              |
| 1:D:902:TRP:CZ3   | 1:D:913:ARG:HD2   | 2.48                     | 0.48              |
| 1:D:2180:GLY:HA2  | 1:D:2183:GLU:HG2  | 1.94                     | 0.48              |
| 1:A:176:ARG:N     | 1:A:179:ASP:OD2   | 2.37                     | 0.48              |
| 1:A:965:LYS:HE3   | 1:A:977:LYS:HG3   | 1.94                     | 0.48              |
| 1:A:1040:ASP:HA   | 1:A:1043:LYS:HG2  | 1.94                     | 0.48              |
| 1:A:2265:VAL:HG21 | 1:A:2301:PHE:CE2  | 2.49                     | 0.48              |
| 1:A:2720:PHE:CE2  | 1:A:2896:LEU:HA   | 2.48                     | 0.48              |
| 1:A:2957:GLU:O    | 1:A:2961:LYS:HG3  | 2.13                     | 0.48              |
| 1:A:3314:LEU:HA   | 1:A:3318:HIS:HD1  | 1.78                     | 0.48              |
| 1:B:585:ALA:O     | 1:B:589:ILE:HG12  | 2.12                     | 0.48              |
| 1:B:4767:LEU:O    | 1:B:4771:VAL:HG23 | 2.13                     | 0.48              |
| 1:C:853:PRO:HB3   | 1:C:1083:GLU:OE2  | 2.12                     | 0.48              |
| 1:C:2582:PRO:HA   | 1:C:2585:MET:HE2  | 1.95                     | 0.48              |
| 1:C:3282:LYS:HD3  | 1:C:3286:ASN:HD22 | 1.76                     | 0.48              |
| 1:C:4079:ASP:O    | 1:C:4082:GLU:HG3  | 2.13                     | 0.48              |
| 1:C:4767:LEU:O    | 1:C:4771:VAL:HG23 | 2.13                     | 0.48              |
| 1:D:28:ILE:HG22   | 1:D:29:HIS:HD2    | 1.77                     | 0.48              |
| 1:D:585:ALA:O     | 1:D:589:ILE:HG12  | 2.12                     | 0.48              |
| 1:D:2582:PRO:HA   | 1:D:2585:MET:HE2  | 1.95                     | 0.48              |
| 1:D:3007:LEU:HA   | 1:D:3010:LYS:HE2  | 1.95                     | 0.48              |
| 1:A:546:LYS:O     | 1:A:550:GLN:HG2   | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2396:ILE:HG13 | 1:A:2468:MET:HE1  | 1.95                     | 0.48              |
| 1:A:2500:ALA:HB1  | 1:A:2554:ARG:HG2  | 1.94                     | 0.48              |
| 1:A:2582:PRO:HA   | 1:A:2585:MET:HE2  | 1.95                     | 0.48              |
| 1:B:3282:LYS:HD3  | 1:B:3286:ASN:HD22 | 1.76                     | 0.48              |
| 1:C:394:HIS:CE1   | 1:C:396:GLU:HG3   | 2.49                     | 0.48              |
| 1:C:1911:GLN:HG3  | 1:C:2090:ARG:NH1  | 2.29                     | 0.48              |
| 1:C:2893:LEU:HD23 | 1:C:2896:LEU:HD21 | 1.94                     | 0.48              |
| 1:C:2957:GLU:O    | 1:C:2961:LYS:HG3  | 2.13                     | 0.48              |
| 1:C:3023:GLY:N    | 1:C:3025:ASP:OD2  | 2.45                     | 0.48              |
| 1:D:655:MET:HG2   | 1:D:794:PHE:HE1   | 1.78                     | 0.48              |
| 1:D:2119:LEU:HD13 | 1:D:2154:VAL:HG23 | 1.94                     | 0.48              |
| 1:A:19:GLU:HG2    | 1:A:66:THR:HB     | 1.95                     | 0.48              |
| 1:A:290:ARG:NH2   | 1:A:351:THR:OG1   | 2.45                     | 0.48              |
| 1:A:3228:TYR:OH   | 1:A:3236:GLU:HB3  | 2.12                     | 0.48              |
| 1:B:2243:ALA:O    | 1:B:2247:VAL:HG22 | 2.14                     | 0.48              |
| 1:B:2265:VAL:HG21 | 1:B:2301:PHE:CE2  | 2.48                     | 0.48              |
| 1:B:2396:ILE:HG13 | 1:B:2468:MET:HE1  | 1.95                     | 0.48              |
| 1:B:2424:ARG:HG2  | 1:B:2476:TYR:CE1  | 2.49                     | 0.48              |
| 1:B:2582:PRO:HA   | 1:B:2585:MET:HE2  | 1.95                     | 0.48              |
| 1:B:2852:TRP:CH2  | 1:B:2868:HIS:HE1  | 2.32                     | 0.48              |
| 1:B:3198:PRO:HB3  | 1:B:3203:ASP:HB3  | 1.96                     | 0.48              |
| 1:C:2426:LEU:HD23 | 1:D:143:LEU:HD11  | 1.94                     | 0.48              |
| 1:C:2716:LYS:O    | 1:C:2901:TYR:OH   | 2.31                     | 0.48              |
| 1:D:434:ASP:HB3   | 1:D:438:LYS:NZ    | 2.28                     | 0.48              |
| 1:D:2322:ARG:O    | 1:D:2326:ARG:HG2  | 2.13                     | 0.48              |
| 1:D:2500:ALA:HB1  | 1:D:2554:ARG:HG2  | 1.94                     | 0.48              |
| 1:D:2717:LEU:HD12 | 1:D:2779:LEU:HD13 | 1.96                     | 0.48              |
| 1:D:3108:LEU:HD23 | 1:D:3109:PHE:HE2  | 1.78                     | 0.48              |
| 1:A:1911:GLN:HG3  | 1:A:2090:ARG:NH1  | 2.29                     | 0.48              |
| 1:A:1956:ALA:O    | 1:A:1960:ARG:NH1  | 2.46                     | 0.48              |
| 1:A:2096:GLY:O    | 1:A:2100:ARG:NE   | 2.40                     | 0.48              |
| 1:A:4079:ASP:O    | 1:A:4082:GLU:HG3  | 2.13                     | 0.48              |
| 1:A:4137:GLU:HG2  | 1:A:4147:ARG:HG2  | 1.94                     | 0.48              |
| 1:B:546:LYS:O     | 1:B:550:GLN:HG2   | 2.13                     | 0.48              |
| 1:B:2500:ALA:HB1  | 1:B:2554:ARG:HG2  | 1.94                     | 0.48              |
| 1:B:4053:GLU:OE2  | 1:B:4063:THR:OG1  | 2.32                     | 0.48              |
| 1:C:1113:MET:HG2  | 1:C:1207:LEU:HD23 | 1.96                     | 0.48              |
| 1:C:2409:ILE:HG12 | 1:C:2420:ARG:CZ   | 2.43                     | 0.48              |
| 1:C:3007:LEU:HA   | 1:C:3010:LYS:HE2  | 1.95                     | 0.48              |
| 1:C:3138:TYR:CG   | 1:C:3208:ILE:HG13 | 2.49                     | 0.48              |
| 1:C:3661:VAL:HG23 | 1:C:3666:GLN:HG2  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3900:GLU:OE1  | 1:C:3901:GLN:NE2  | 2.44                     | 0.48              |
| 1:A:2232:PRO:HD2  | 1:A:2379:ASP:HA   | 1.95                     | 0.48              |
| 1:A:2424:ARG:HG2  | 1:A:2476:TYR:CE1  | 2.49                     | 0.48              |
| 1:A:2852:TRP:CH2  | 1:A:2868:HIS:HE1  | 2.32                     | 0.48              |
| 1:A:3138:TYR:CG   | 1:A:3208:ILE:HG13 | 2.49                     | 0.48              |
| 1:B:137:ARG:NH2   | 1:B:203:VAL:O     | 2.36                     | 0.48              |
| 1:B:885:LEU:HD13  | 1:B:1060:TYR:CD1  | 2.49                     | 0.48              |
| 1:B:3138:TYR:CG   | 1:B:3208:ILE:HG13 | 2.49                     | 0.48              |
| 1:B:3642:GLU:HG3  | 1:B:3646:LYS:NZ   | 2.28                     | 0.48              |
| 1:C:19:GLU:HG2    | 1:C:66:THR:HB     | 1.95                     | 0.48              |
| 1:C:2243:ALA:O    | 1:C:2247:VAL:HG22 | 2.14                     | 0.48              |
| 1:C:3108:LEU:HD23 | 1:C:3109:PHE:HE2  | 1.78                     | 0.48              |
| 1:C:4053:GLU:OE2  | 1:C:4063:THR:OG1  | 2.32                     | 0.48              |
| 1:D:227:TYR:CG    | 1:D:352:SER:HB2   | 2.48                     | 0.48              |
| 1:D:546:LYS:O     | 1:D:550:GLN:HG2   | 2.13                     | 0.48              |
| 1:D:2265:VAL:HG21 | 1:D:2301:PHE:CE2  | 2.48                     | 0.48              |
| 1:D:2913:ASP:HB2  | 1:D:2919:LYS:NZ   | 2.28                     | 0.48              |
| 1:D:3642:GLU:HG3  | 1:D:3646:LYS:NZ   | 2.28                     | 0.48              |
| 1:A:227:TYR:CG    | 1:A:352:SER:HB2   | 2.48                     | 0.48              |
| 1:A:2270:ALA:HB2  | 1:A:2327:ARG:HD3  | 1.95                     | 0.48              |
| 1:A:2717:LEU:HD12 | 1:A:2779:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:2913:ASP:HB2  | 1:A:2919:LYS:NZ   | 2.28                     | 0.48              |
| 1:A:3198:PRO:HB3  | 1:A:3203:ASP:HB3  | 1.96                     | 0.48              |
| 1:A:3642:GLU:HG3  | 1:A:3646:LYS:NZ   | 2.28                     | 0.48              |
| 1:A:4114:ARG:O    | 1:A:4117:THR:OG1  | 2.28                     | 0.48              |
| 1:A:4587:ILE:HD13 | 1:A:4722:LEU:HB3  | 1.95                     | 0.48              |
| 1:B:54:ASN:HB2    | 1:B:57:ASN:HB2    | 1.96                     | 0.48              |
| 1:B:1038:LEU:HD22 | 1:B:1043:LYS:HB3  | 1.95                     | 0.48              |
| 1:B:3312:PRO:HA   | 1:B:3315:LEU:HD12 | 1.96                     | 0.48              |
| 1:B:3314:LEU:HA   | 1:B:3318:HIS:HD1  | 1.78                     | 0.48              |
| 1:B:4113:THR:O    | 1:B:4117:THR:HG23 | 2.13                     | 0.48              |
| 1:B:4292:MET:HA   | 1:B:4292:MET:CE   | 2.44                     | 0.48              |
| 1:C:371:TRP:O     | 1:C:394:HIS:N     | 2.45                     | 0.48              |
| 1:C:2652:LEU:HD23 | 1:C:2962:PHE:HE1  | 1.79                     | 0.48              |
| 1:D:394:HIS:CE1   | 1:D:396:GLU:HG3   | 2.49                     | 0.48              |
| 1:D:965:LYS:HE3   | 1:D:977:LYS:HG3   | 1.94                     | 0.48              |
| 1:D:2409:ILE:HG12 | 1:D:2420:ARG:CZ   | 2.43                     | 0.48              |
| 1:D:2742:ILE:O    | 1:D:2754:GLN:N    | 2.33                     | 0.48              |
| 1:D:3137:LEU:HD23 | 1:D:3140:LEU:HD12 | 1.96                     | 0.48              |
| 1:A:514:PHE:CD2   | 1:A:526:TRP:HB2   | 2.49                     | 0.48              |
| 1:A:814:LEU:HD23  | 1:A:815:PRO:O     | 2.12                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:885:LEU:HD13  | 1:A:1060:TYR:CD1  | 2.49                     | 0.48              |
| 1:A:1009:ARG:NH1  | 1:A:1013:ARG:HG3  | 2.29                     | 0.48              |
| 1:A:2295:GLY:HA3  | 1:A:2391:PHE:HE2  | 1.79                     | 0.48              |
| 1:A:2652:LEU:HD22 | 1:A:2669:LEU:HD11 | 1.95                     | 0.48              |
| 2:G:78:THR:OG1    | 2:G:80:ASP:OD1    | 2.26                     | 0.48              |
| 1:B:1113:MET:HG2  | 1:B:1207:LEU:HD23 | 1.96                     | 0.48              |
| 1:B:4587:ILE:HD13 | 1:B:4722:LEU:HB3  | 1.95                     | 0.48              |
| 1:C:137:ARG:NH2   | 1:C:203:VAL:O     | 2.36                     | 0.48              |
| 1:C:1009:ARG:NH1  | 1:C:1013:ARG:HG3  | 2.29                     | 0.48              |
| 1:C:3137:LEU:HD23 | 1:C:3140:LEU:HD12 | 1.96                     | 0.48              |
| 1:D:419:ILE:HG21  | 1:D:492:GLU:HG3   | 1.96                     | 0.48              |
| 1:D:2424:ARG:HG2  | 1:D:2476:TYR:CE1  | 2.49                     | 0.48              |
| 1:A:394:HIS:CE1   | 1:A:396:GLU:HG3   | 2.49                     | 0.48              |
| 1:A:419:ILE:HG21  | 1:A:492:GLU:HG3   | 1.96                     | 0.48              |
| 1:A:2409:ILE:HG12 | 1:A:2420:ARG:CZ   | 2.43                     | 0.48              |
| 1:A:2460:PHE:HE2  | 1:A:2465:LYS:HD2  | 1.79                     | 0.48              |
| 1:A:2716:LYS:O    | 1:A:2901:TYR:OH   | 2.31                     | 0.48              |
| 1:A:3261:ALA:C    | 1:A:3263:MET:H    | 2.22                     | 0.48              |
| 1:A:3312:PRO:HA   | 1:A:3315:LEU:HD12 | 1.96                     | 0.48              |
| 1:B:2295:GLY:HA3  | 1:B:2391:PHE:HE2  | 1.79                     | 0.48              |
| 1:B:2957:GLU:O    | 1:B:2961:LYS:HG3  | 2.13                     | 0.48              |
| 1:B:3108:LEU:HD23 | 1:B:3109:PHE:HE2  | 1.78                     | 0.48              |
| 1:B:3238:ILE:HG13 | 1:B:3239:LEU:N    | 2.29                     | 0.48              |
| 1:B:3250:TRP:HA   | 1:B:3255:GLU:OE2  | 2.14                     | 0.48              |
| 1:B:4503:ARG:NH2  | 1:B:4721:TYR:HE2  | 2.11                     | 0.48              |
| 1:C:680:ASP:OD2   | 1:C:801:ARG:HG3   | 2.14                     | 0.48              |
| 1:C:2742:ILE:O    | 1:C:2754:GLN:N    | 2.33                     | 0.48              |
| 1:C:2852:TRP:CH2  | 1:C:2868:HIS:HE1  | 2.32                     | 0.48              |
| 1:C:2913:ASP:HB2  | 1:C:2919:LYS:NZ   | 2.28                     | 0.48              |
| 1:D:54:ASN:HB2    | 1:D:57:ASN:HB2    | 1.96                     | 0.48              |
| 1:D:680:ASP:OD2   | 1:D:801:ARG:HG3   | 2.14                     | 0.48              |
| 1:D:2278:GLN:HA   | 1:D:2281:VAL:HG22 | 1.96                     | 0.48              |
| 1:D:2460:PHE:HE2  | 1:D:2465:LYS:HD2  | 1.79                     | 0.48              |
| 1:D:3312:PRO:HA   | 1:D:3315:LEU:HD12 | 1.96                     | 0.48              |
| 1:D:4292:MET:HA   | 1:D:4292:MET:CE   | 2.44                     | 0.48              |
| 1:A:680:ASP:OD2   | 1:A:801:ARG:HG3   | 2.14                     | 0.48              |
| 1:A:1038:LEU:HD22 | 1:A:1043:LYS:HB3  | 1.95                     | 0.48              |
| 1:A:2742:ILE:O    | 1:A:2754:GLN:N    | 2.33                     | 0.48              |
| 1:A:3946:GLY:O    | 1:A:3950:VAL:HG23 | 2.14                     | 0.48              |
| 2:E:78:THR:OG1    | 2:E:80:ASP:OD1    | 2.26                     | 0.48              |
| 1:B:227:TYR:CG    | 1:B:352:SER:HB2   | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:394:HIS:CE1   | 1:B:396:GLU:HG3   | 2.49                     | 0.48              |
| 1:B:419:ILE:HG21  | 1:B:492:GLU:HG3   | 1.96                     | 0.48              |
| 1:B:655:MET:HG2   | 1:B:794:PHE:HE1   | 1.78                     | 0.48              |
| 1:B:680:ASP:OD2   | 1:B:801:ARG:HG3   | 2.14                     | 0.48              |
| 1:B:850:LEU:HD11  | 1:B:1249:MET:HE1  | 1.96                     | 0.48              |
| 1:B:1911:GLN:HG3  | 1:B:2090:ARG:NH1  | 2.29                     | 0.48              |
| 1:B:2270:ALA:HB2  | 1:B:2327:ARG:HD3  | 1.95                     | 0.48              |
| 1:B:2460:PHE:HE2  | 1:B:2465:LYS:HD2  | 1.79                     | 0.48              |
| 1:B:3076:LYS:HA   | 1:B:3079:GLN:HB2  | 1.96                     | 0.48              |
| 1:B:3311:LYS:HZ3  | 1:B:3313:GLN:H    | 1.62                     | 0.48              |
| 1:C:514:PHE:CD2   | 1:C:526:TRP:HB2   | 2.49                     | 0.48              |
| 1:C:1103:PHE:CE1  | 1:C:1164:CYS:HB2  | 2.49                     | 0.48              |
| 1:C:2471:PHE:CE1  | 1:C:2475:VAL:HG21 | 2.49                     | 0.48              |
| 1:D:1009:ARG:NH1  | 1:D:1013:ARG:HG3  | 2.29                     | 0.48              |
| 1:D:1113:MET:HG2  | 1:D:1207:LEU:HD23 | 1.96                     | 0.48              |
| 1:D:2058:LEU:O    | 1:D:2062:ILE:HG12 | 2.13                     | 0.48              |
| 1:D:2652:LEU:HD23 | 1:D:2962:PHE:HE1  | 1.79                     | 0.48              |
| 1:D:3034:HIS:CE1  | 1:D:3107:SER:HG   | 2.25                     | 0.48              |
| 1:D:3138:TYR:CG   | 1:D:3208:ILE:HG13 | 2.49                     | 0.48              |
| 1:A:54:ASN:HB2    | 1:A:57:ASN:HB2    | 1.96                     | 0.47              |
| 1:A:634:ASP:OD1   | 1:A:1671:ARG:NH2  | 2.37                     | 0.47              |
| 1:A:655:MET:HE1   | 1:A:836:HIS:CG    | 2.49                     | 0.47              |
| 1:A:1113:MET:HG2  | 1:A:1207:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:2243:ALA:O    | 1:A:2247:VAL:HG22 | 2.14                     | 0.47              |
| 1:A:4274:MET:HE2  | 1:A:4274:MET:HB2  | 1.70                     | 0.47              |
| 1:A:4640:PHE:CG   | 1:A:4641:PRO:HD3  | 2.49                     | 0.47              |
| 1:B:675:TYR:HB3   | 1:B:822:CYS:SG    | 2.54                     | 0.47              |
| 1:B:890:HIS:HA    | 1:B:893:TRP:CE3   | 2.45                     | 0.47              |
| 1:B:902:TRP:CZ3   | 1:B:913:ARG:HD2   | 2.48                     | 0.47              |
| 1:B:2403:ALA:HB2  | 1:B:2475:VAL:HG12 | 1.96                     | 0.47              |
| 1:B:3946:GLY:O    | 1:B:3950:VAL:HG23 | 2.14                     | 0.47              |
| 1:C:2322:ARG:O    | 1:C:2326:ARG:HG2  | 2.13                     | 0.47              |
| 1:C:2424:ARG:HG2  | 1:C:2476:TYR:CE1  | 2.49                     | 0.47              |
| 1:C:2725:ALA:HB1  | 1:C:2771:TYR:HE2  | 1.79                     | 0.47              |
| 1:C:3076:LYS:HA   | 1:C:3079:GLN:HB2  | 1.96                     | 0.47              |
| 1:C:3312:PRO:HA   | 1:C:3315:LEU:HD12 | 1.96                     | 0.47              |
| 1:C:3314:LEU:HA   | 1:C:3318:HIS:HD1  | 1.78                     | 0.47              |
| 1:D:514:PHE:CD2   | 1:D:526:TRP:HB2   | 2.49                     | 0.47              |
| 1:D:766:ILE:HB    | 1:D:779:PHE:HB2   | 1.96                     | 0.47              |
| 1:D:2270:ALA:HB2  | 1:D:2327:ARG:HD3  | 1.95                     | 0.47              |
| 1:D:2396:ILE:HG13 | 1:D:2468:MET:HE1  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2795:GLY:HA2  | 1:A:2798:MET:HE2  | 1.96                     | 0.47              |
| 1:B:766:ILE:HB    | 1:B:779:PHE:HB2   | 1.96                     | 0.47              |
| 1:B:1103:PHE:CE1  | 1:B:1164:CYS:HB2  | 2.49                     | 0.47              |
| 1:B:3007:LEU:HA   | 1:B:3010:LYS:HE2  | 1.95                     | 0.47              |
| 1:B:3065:ALA:HB1  | 1:B:3132:ARG:NH1  | 2.21                     | 0.47              |
| 1:C:850:LEU:HD11  | 1:C:1249:MET:HE1  | 1.96                     | 0.47              |
| 1:C:885:LEU:HD13  | 1:C:1060:TYR:CD1  | 2.49                     | 0.47              |
| 1:C:2652:LEU:HD22 | 1:C:2669:LEU:HD11 | 1.94                     | 0.47              |
| 1:D:2787:TRP:HE1  | 1:D:2840:MET:HE2  | 1.80                     | 0.47              |
| 1:D:4503:ARG:NH2  | 1:D:4721:TYR:HE2  | 2.11                     | 0.47              |
| 1:A:2725:ALA:HB1  | 1:A:2771:TYR:HE2  | 1.79                     | 0.47              |
| 1:A:3235:MET:HG3  | 1:A:3239:LEU:HD12 | 1.95                     | 0.47              |
| 1:A:4292:MET:HA   | 1:A:4292:MET:CE   | 2.44                     | 0.47              |
| 2:H:78:THR:OG1    | 2:H:80:ASP:OD1    | 2.26                     | 0.47              |
| 1:B:2723:LYS:HA   | 1:B:2726:GLU:HB2  | 1.96                     | 0.47              |
| 1:B:2831:VAL:HG13 | 1:B:2894:LYS:HD3  | 1.97                     | 0.47              |
| 1:B:2913:ASP:HB2  | 1:B:2919:LYS:NZ   | 2.28                     | 0.47              |
| 1:B:4640:PHE:CG   | 1:B:4641:PRO:HD3  | 2.49                     | 0.47              |
| 1:C:54:ASN:HB2    | 1:C:57:ASN:HB2    | 1.96                     | 0.47              |
| 1:C:2058:LEU:O    | 1:C:2062:ILE:HG12 | 2.13                     | 0.47              |
| 1:C:2265:VAL:HG21 | 1:C:2301:PHE:CE2  | 2.48                     | 0.47              |
| 1:C:2396:ILE:HG13 | 1:C:2468:MET:HE1  | 1.95                     | 0.47              |
| 1:C:3198:PRO:HB3  | 1:C:3203:ASP:HB3  | 1.96                     | 0.47              |
| 1:C:3235:MET:HG3  | 1:C:3239:LEU:HD12 | 1.95                     | 0.47              |
| 1:D:371:TRP:O     | 1:D:394:HIS:N     | 2.46                     | 0.47              |
| 1:D:480:ARG:NH2   | 1:D:3678:GLU:OE2  | 2.45                     | 0.47              |
| 1:D:514:PHE:HA    | 1:D:517:VAL:HG12  | 1.96                     | 0.47              |
| 1:D:675:TYR:HB3   | 1:D:822:CYS:SG    | 2.54                     | 0.47              |
| 1:D:1956:ALA:O    | 1:D:1960:ARG:NH1  | 2.46                     | 0.47              |
| 1:D:2295:GLY:HA3  | 1:D:2391:PHE:HE2  | 1.79                     | 0.47              |
| 1:D:2403:ALA:HB2  | 1:D:2475:VAL:HG12 | 1.96                     | 0.47              |
| 1:D:2719:TYR:HD2  | 1:D:2791:ARG:NH1  | 2.12                     | 0.47              |
| 1:D:3235:MET:HG3  | 1:D:3239:LEU:HD12 | 1.95                     | 0.47              |
| 1:D:3261:ALA:C    | 1:D:3263:MET:H    | 2.22                     | 0.47              |
| 1:D:3304:GLN:HA   | 1:D:3307:ILE:HG12 | 1.97                     | 0.47              |
| 1:D:4113:THR:O    | 1:D:4117:THR:HG23 | 2.13                     | 0.47              |
| 1:A:675:TYR:HB3   | 1:A:822:CYS:SG    | 2.54                     | 0.47              |
| 1:A:1103:PHE:CE1  | 1:A:1164:CYS:HB2  | 2.49                     | 0.47              |
| 1:A:2723:LYS:HA   | 1:A:2726:GLU:HB2  | 1.96                     | 0.47              |
| 1:A:2728:SER:HB2  | 1:A:2771:TYR:OH   | 2.14                     | 0.47              |
| 1:A:3238:ILE:HG13 | 1:A:3239:LEU:N    | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3304:GLN:HA   | 1:A:3307:ILE:HG12 | 1.96                     | 0.47              |
| 1:A:4518:LEU:HA   | 1:B:4809:MET:HE2  | 1.96                     | 0.47              |
| 1:B:19:GLU:HG2    | 1:B:66:THR:HB     | 1.95                     | 0.47              |
| 1:B:514:PHE:CD2   | 1:B:526:TRP:HB2   | 2.49                     | 0.47              |
| 1:B:655:MET:HE1   | 1:B:836:HIS:CG    | 2.49                     | 0.47              |
| 1:B:1956:ALA:O    | 1:B:1960:ARG:NH1  | 2.46                     | 0.47              |
| 1:B:2134:MET:HE2  | 1:B:2192:MET:HG3  | 1.97                     | 0.47              |
| 1:B:2232:PRO:HD2  | 1:B:2379:ASP:HA   | 1.95                     | 0.47              |
| 1:B:2418:ARG:NH2  | 1:C:156:GLU:OE1   | 2.41                     | 0.47              |
| 1:B:2853:ALA:O    | 1:B:2857:LYS:HG3  | 2.15                     | 0.47              |
| 1:B:2973:GLN:HA   | 1:B:2976:LYS:HE2  | 1.96                     | 0.47              |
| 1:B:4276:VAL:HG23 | 1:C:4487:TYR:CE2  | 2.50                     | 0.47              |
| 1:C:227:TYR:CG    | 1:C:352:SER:HB2   | 2.48                     | 0.47              |
| 1:C:674:TYR:CE1   | 1:C:756:SER:HB2   | 2.50                     | 0.47              |
| 1:C:2295:GLY:HA3  | 1:C:2391:PHE:HE2  | 1.79                     | 0.47              |
| 1:C:2447:LYS:HD2  | 1:C:2864:GLY:HA3  | 1.97                     | 0.47              |
| 1:C:2717:LEU:HD12 | 1:C:2779:LEU:HD13 | 1.96                     | 0.47              |
| 1:C:4292:MET:CE   | 1:C:4292:MET:HA   | 2.44                     | 0.47              |
| 1:C:4503:ARG:NH2  | 1:C:4721:TYR:HE2  | 2.11                     | 0.47              |
| 1:D:655:MET:HE1   | 1:D:836:HIS:CG    | 2.49                     | 0.47              |
| 1:D:850:LEU:HD11  | 1:D:1249:MET:HE1  | 1.96                     | 0.47              |
| 1:D:885:LEU:HD13  | 1:D:1060:TYR:CD1  | 2.49                     | 0.47              |
| 1:D:2471:PHE:O    | 1:D:2475:VAL:HG22 | 2.14                     | 0.47              |
| 1:D:3064:ALA:HB1  | 1:D:3101:LEU:HD11 | 1.97                     | 0.47              |
| 1:D:3946:GLY:O    | 1:D:3950:VAL:HG23 | 2.14                     | 0.47              |
| 1:D:4000:VAL:HG12 | 1:D:4114:ARG:NH1  | 2.30                     | 0.47              |
| 1:D:4640:PHE:CG   | 1:D:4641:PRO:HD3  | 2.49                     | 0.47              |
| 1:A:2134:MET:HE2  | 1:A:2192:MET:HG3  | 1.97                     | 0.47              |
| 1:A:2444:THR:HB   | 1:A:2866:GLY:HA2  | 1.97                     | 0.47              |
| 1:A:2471:PHE:CE1  | 1:A:2475:VAL:HG21 | 2.49                     | 0.47              |
| 1:A:2666:LEU:HD13 | 1:A:2966:VAL:HA   | 1.97                     | 0.47              |
| 1:A:2973:GLN:HA   | 1:A:2976:LYS:HE2  | 1.96                     | 0.47              |
| 1:B:514:PHE:HA    | 1:B:517:VAL:HG12  | 1.96                     | 0.47              |
| 1:B:2652:LEU:HD23 | 1:B:2962:PHE:HE1  | 1.79                     | 0.47              |
| 1:B:2787:TRP:HE1  | 1:B:2840:MET:HE2  | 1.80                     | 0.47              |
| 1:B:3137:LEU:HD23 | 1:B:3140:LEU:HD12 | 1.96                     | 0.47              |
| 1:B:3261:ALA:C    | 1:B:3263:MET:H    | 2.22                     | 0.47              |
| 1:B:4000:VAL:HG12 | 1:B:4114:ARG:NH1  | 2.30                     | 0.47              |
| 1:B:4027:THR:HA   | 1:B:4032:PHE:CD1  | 2.50                     | 0.47              |
| 1:C:419:ILE:HG21  | 1:C:492:GLU:HG3   | 1.96                     | 0.47              |
| 1:C:655:MET:HE1   | 1:C:836:HIS:CG    | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:675:TYR:HB3   | 1:C:822:CYS:SG    | 2.54                     | 0.47              |
| 1:C:2403:ALA:HB2  | 1:C:2475:VAL:HG12 | 1.96                     | 0.47              |
| 1:C:2831:VAL:HG13 | 1:C:2894:LYS:HD3  | 1.97                     | 0.47              |
| 1:C:2853:ALA:O    | 1:C:2857:LYS:HG3  | 2.15                     | 0.47              |
| 1:C:3304:GLN:HA   | 1:C:3307:ILE:HG12 | 1.97                     | 0.47              |
| 1:C:4274:MET:HE2  | 1:C:4274:MET:HB2  | 1.70                     | 0.47              |
| 1:D:988:LEU:HB3   | 1:D:993:GLU:OE2   | 2.15                     | 0.47              |
| 1:D:1718:ARG:HH12 | 1:D:1832:GLY:HA3  | 1.79                     | 0.47              |
| 1:D:2243:ALA:O    | 1:D:2247:VAL:HG22 | 2.14                     | 0.47              |
| 1:D:2723:LYS:HA   | 1:D:2726:GLU:HB2  | 1.96                     | 0.47              |
| 1:D:2985:ALA:HB2  | 1:D:3001:LYS:HZ2  | 1.80                     | 0.47              |
| 1:D:4027:THR:HA   | 1:D:4032:PHE:CD1  | 2.50                     | 0.47              |
| 1:A:3007:LEU:HA   | 1:A:3010:LYS:HE2  | 1.95                     | 0.47              |
| 1:A:3076:LYS:HA   | 1:A:3079:GLN:HB2  | 1.96                     | 0.47              |
| 1:A:3722:GLN:HB3  | 1:A:4681:ASP:OD1  | 2.15                     | 0.47              |
| 1:B:2471:PHE:CE1  | 1:B:2475:VAL:HG21 | 2.49                     | 0.47              |
| 1:B:3235:MET:HG3  | 1:B:3239:LEU:HD12 | 1.95                     | 0.47              |
| 1:C:655:MET:HG2   | 1:C:794:PHE:HE1   | 1.78                     | 0.47              |
| 1:C:2471:PHE:O    | 1:C:2475:VAL:HG22 | 2.14                     | 0.47              |
| 1:C:2698:GLU:O    | 1:C:2698:GLU:HG2  | 2.15                     | 0.47              |
| 1:C:4640:PHE:CG   | 1:C:4641:PRO:HD3  | 2.49                     | 0.47              |
| 1:D:1038:LEU:HD22 | 1:D:1043:LYS:HB3  | 1.95                     | 0.47              |
| 1:D:2471:PHE:CE1  | 1:D:2475:VAL:HG21 | 2.49                     | 0.47              |
| 1:D:3076:LYS:HA   | 1:D:3079:GLN:HB2  | 1.96                     | 0.47              |
| 1:D:3198:PRO:HB3  | 1:D:3203:ASP:HB3  | 1.96                     | 0.47              |
| 1:D:3250:TRP:HA   | 1:D:3255:GLU:OE2  | 2.14                     | 0.47              |
| 1:A:128:MET:HG2   | 1:A:151:GLU:HA    | 1.97                     | 0.47              |
| 1:A:2403:ALA:HB2  | 1:A:2475:VAL:HG12 | 1.96                     | 0.47              |
| 1:A:2719:TYR:HD2  | 1:A:2791:ARG:NH1  | 2.12                     | 0.47              |
| 1:A:2918:GLU:HG3  | 1:A:2923:TYR:CE2  | 2.50                     | 0.47              |
| 1:A:3064:ALA:HB1  | 1:A:3101:LEU:HD11 | 1.97                     | 0.47              |
| 1:A:3137:LEU:HD23 | 1:A:3140:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:4522:VAL:HG23 | 1:B:4786:PHE:CZ   | 2.49                     | 0.47              |
| 2:E:8:ILE:HD11    | 2:E:74:LYS:HB2    | 1.97                     | 0.47              |
| 1:B:2278:GLN:HA   | 1:B:2281:VAL:HG22 | 1.96                     | 0.47              |
| 1:B:2447:LYS:HD2  | 1:B:2864:GLY:HA3  | 1.97                     | 0.47              |
| 1:B:2471:PHE:O    | 1:B:2475:VAL:HG22 | 2.14                     | 0.47              |
| 1:B:2666:LEU:HD13 | 1:B:2966:VAL:HA   | 1.97                     | 0.47              |
| 1:B:2716:LYS:O    | 1:B:2901:TYR:OH   | 2.31                     | 0.47              |
| 1:B:2717:LEU:HD12 | 1:B:2779:LEU:HD13 | 1.95                     | 0.47              |
| 1:B:2725:ALA:HB1  | 1:B:2771:TYR:HE2  | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2728:SER:HB2  | 1:B:2771:TYR:OH   | 2.14                     | 0.47              |
| 1:B:2831:VAL:HB   | 1:C:1435:GLY:HA2  | 1.97                     | 0.47              |
| 1:B:2985:ALA:HB2  | 1:B:3001:LYS:HZ2  | 1.80                     | 0.47              |
| 1:B:3064:ALA:HB1  | 1:B:3101:LEU:HD11 | 1.97                     | 0.47              |
| 1:B:3914:LYS:HZ1  | 1:B:3973:ASP:CG   | 2.22                     | 0.47              |
| 1:B:3956:MET:HG3  | 1:B:4065:PHE:CZ   | 2.50                     | 0.47              |
| 1:B:4522:VAL:HG23 | 1:C:4786:PHE:CZ   | 2.50                     | 0.47              |
| 1:C:1718:ARG:HH12 | 1:C:1832:GLY:HA3  | 1.79                     | 0.47              |
| 1:C:2460:PHE:HE2  | 1:C:2465:LYS:HD2  | 1.79                     | 0.47              |
| 1:C:2585:MET:HE3  | 1:C:2616:ARG:NH2  | 2.21                     | 0.47              |
| 1:C:2742:ILE:HB   | 1:C:2753:VAL:HG12 | 1.96                     | 0.47              |
| 1:C:2918:GLU:HG3  | 1:C:2923:TYR:CE2  | 2.50                     | 0.47              |
| 1:C:3122:ILE:HG12 | 1:C:3127:GLN:HG2  | 1.97                     | 0.47              |
| 1:C:3178:HIS:ND1  | 1:C:3178:HIS:O    | 2.48                     | 0.47              |
| 1:C:3238:ILE:HG13 | 1:C:3239:LEU:N    | 2.29                     | 0.47              |
| 1:C:3261:ALA:C    | 1:C:3263:MET:H    | 2.22                     | 0.47              |
| 1:C:4000:VAL:HG12 | 1:C:4114:ARG:NH1  | 2.30                     | 0.47              |
| 1:D:128:MET:HG2   | 1:D:151:GLU:HA    | 1.97                     | 0.47              |
| 1:D:1038:LEU:HD23 | 1:D:1039:ASP:N    | 2.30                     | 0.47              |
| 1:D:1911:GLN:HG3  | 1:D:2090:ARG:NH1  | 2.29                     | 0.47              |
| 1:D:2134:MET:HE2  | 1:D:2192:MET:HG3  | 1.97                     | 0.47              |
| 1:D:2444:THR:HB   | 1:D:2866:GLY:HA2  | 1.97                     | 0.47              |
| 1:D:2742:ILE:HB   | 1:D:2753:VAL:HG12 | 1.96                     | 0.47              |
| 1:D:2852:TRP:CH2  | 1:D:2868:HIS:HE1  | 2.32                     | 0.47              |
| 1:D:3238:ILE:HG13 | 1:D:3239:LEU:N    | 2.29                     | 0.47              |
| 1:A:514:PHE:HA    | 1:A:517:VAL:HG12  | 1.96                     | 0.47              |
| 1:A:2696:ASP:HB3  | 1:A:2700:ASN:HA   | 1.97                     | 0.47              |
| 1:A:2853:ALA:O    | 1:A:2857:LYS:HG3  | 2.15                     | 0.47              |
| 1:A:3108:LEU:HD23 | 1:A:3109:PHE:HE2  | 1.78                     | 0.47              |
| 1:A:3250:TRP:HA   | 1:A:3255:GLU:OE2  | 2.14                     | 0.47              |
| 1:B:370:LEU:HB2   | 1:B:393:MET:HG3   | 1.97                     | 0.47              |
| 1:B:674:TYR:CE1   | 1:B:756:SER:HB2   | 2.50                     | 0.47              |
| 1:B:756:SER:OG    | 1:B:769:ARG:HB3   | 2.15                     | 0.47              |
| 1:B:1144:ARG:HD2  | 1:B:1192:PHE:CE1  | 2.50                     | 0.47              |
| 1:B:3122:ILE:HG12 | 1:B:3127:GLN:HG2  | 1.97                     | 0.47              |
| 1:C:514:PHE:HA    | 1:C:517:VAL:HG12  | 1.95                     | 0.47              |
| 1:C:634:ASP:OD1   | 1:C:1671:ARG:NH2  | 2.37                     | 0.47              |
| 1:C:1956:ALA:O    | 1:C:1960:ARG:NH1  | 2.46                     | 0.47              |
| 1:C:2726:GLU:N    | 1:C:2726:GLU:OE1  | 2.45                     | 0.47              |
| 1:C:3089:GLY:O    | 1:C:3092:GLN:HG3  | 2.15                     | 0.47              |
| 1:C:3250:TRP:HA   | 1:C:3255:GLU:OE2  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3311:LYS:HZ3  | 1:C:3313:GLN:H    | 1.63                     | 0.47              |
| 1:D:1145:TRP:CE2  | 1:D:1149:ASN:HB3  | 2.50                     | 0.47              |
| 1:D:2795:GLY:HA2  | 1:D:2798:MET:HE2  | 1.96                     | 0.47              |
| 1:D:2973:GLN:HA   | 1:D:2976:LYS:HE2  | 1.96                     | 0.47              |
| 1:D:3097:THR:HG23 | 1:D:3101:LEU:HD23 | 1.97                     | 0.47              |
| 1:D:3178:HIS:ND1  | 1:D:3178:HIS:O    | 2.48                     | 0.47              |
| 1:A:850:LEU:HD11  | 1:A:1249:MET:HE1  | 1.96                     | 0.47              |
| 1:A:988:LEU:HB3   | 1:A:993:GLU:OE2   | 2.15                     | 0.47              |
| 1:A:1931:ASP:OD1  | 1:A:1932:PHE:N    | 2.48                     | 0.47              |
| 1:A:2431:ASP:O    | 1:A:2435:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:2447:LYS:HD2  | 1:A:2864:GLY:HA3  | 1.97                     | 0.47              |
| 1:A:3271:GLU:HA   | 1:A:3274:ASN:HB2  | 1.97                     | 0.47              |
| 1:A:4000:VAL:HG12 | 1:A:4114:ARG:NH1  | 2.30                     | 0.47              |
| 2:F:8:ILE:HA      | 1:B:730:LEU:HD11  | 1.96                     | 0.47              |
| 1:B:996:VAL:HG11  | 1:B:1051:ARG:HG2  | 1.97                     | 0.47              |
| 1:B:1009:ARG:NH1  | 1:B:1013:ARG:HG3  | 2.29                     | 0.47              |
| 1:B:2406:MET:O    | 1:B:2409:ILE:HG22 | 2.15                     | 0.47              |
| 1:B:2719:TYR:HD2  | 1:B:2791:ARG:NH1  | 2.12                     | 0.47              |
| 1:B:4891:CYS:HB3  | 1:B:4913:HIS:CE1  | 2.50                     | 0.47              |
| 1:C:1144:ARG:HD2  | 1:C:1192:PHE:CE1  | 2.50                     | 0.47              |
| 1:C:2719:TYR:HD2  | 1:C:2791:ARG:NH1  | 2.12                     | 0.47              |
| 1:C:2973:GLN:HA   | 1:C:2976:LYS:HE2  | 1.96                     | 0.47              |
| 1:C:3215:MET:HA   | 1:C:3218:ILE:HG12 | 1.97                     | 0.47              |
| 1:C:3249:TRP:HA   | 1:C:3252:HIS:ND1  | 2.30                     | 0.47              |
| 1:C:3722:GLN:HB3  | 1:C:4681:ASP:OD1  | 2.15                     | 0.47              |
| 1:C:3956:MET:HG3  | 1:C:4065:PHE:CZ   | 2.50                     | 0.47              |
| 1:C:4027:THR:HA   | 1:C:4032:PHE:CD1  | 2.50                     | 0.47              |
| 1:D:28:ILE:O      | 1:D:31:GLU:HG3    | 2.15                     | 0.47              |
| 1:D:674:TYR:CE1   | 1:D:756:SER:HB2   | 2.49                     | 0.47              |
| 1:D:1103:PHE:CE1  | 1:D:1164:CYS:HB2  | 2.49                     | 0.47              |
| 1:D:1118:SER:HB3  | 1:D:1204:VAL:HG11 | 1.97                     | 0.47              |
| 1:D:2178:VAL:HG21 | 1:D:2192:MET:CE   | 2.45                     | 0.47              |
| 1:D:2728:SER:HB2  | 1:D:2771:TYR:OH   | 2.14                     | 0.47              |
| 1:A:1038:LEU:HD23 | 1:A:1039:ASP:N    | 2.30                     | 0.47              |
| 1:A:2742:ILE:HB   | 1:A:2753:VAL:HG12 | 1.96                     | 0.47              |
| 1:A:2830:ASN:CG   | 1:B:1549:SER:HB2  | 2.40                     | 0.47              |
| 1:A:3956:MET:HG3  | 1:A:4065:PHE:CZ   | 2.50                     | 0.47              |
| 2:F:8:ILE:HD11    | 2:F:74:LYS:HB2    | 1.97                     | 0.47              |
| 1:B:634:ASP:OD1   | 1:B:1671:ARG:NH2  | 2.37                     | 0.47              |
| 1:B:2431:ASP:O    | 1:B:2435:VAL:HG23 | 2.15                     | 0.47              |
| 1:B:2566:ARG:O    | 1:B:2570:GLU:HG3  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2698:GLU:HG2  | 1:B:2698:GLU:O    | 2.15                     | 0.47              |
| 1:B:2971:ILE:HG23 | 1:B:2975:PHE:HE2  | 1.80                     | 0.47              |
| 1:B:3178:HIS:ND1  | 1:B:3178:HIS:O    | 2.48                     | 0.47              |
| 1:B:3304:GLN:HA   | 1:B:3307:ILE:HG12 | 1.97                     | 0.47              |
| 1:B:3722:GLN:HB3  | 1:B:4681:ASP:OD1  | 2.15                     | 0.47              |
| 1:B:4631:ASP:HA   | 1:B:4708:TRP:HE1  | 1.80                     | 0.47              |
| 1:C:480:ARG:NH2   | 1:C:3678:GLU:OE2  | 2.45                     | 0.47              |
| 1:C:606:ARG:HH21  | 1:C:1633:PRO:HD2  | 1.81                     | 0.47              |
| 1:C:766:ILE:HB    | 1:C:779:PHE:HB2   | 1.96                     | 0.47              |
| 1:C:1145:TRP:CE2  | 1:C:1149:ASN:HB3  | 2.50                     | 0.47              |
| 1:C:2134:MET:HE2  | 1:C:2192:MET:HG3  | 1.97                     | 0.47              |
| 1:C:2566:ARG:O    | 1:C:2570:GLU:HG3  | 2.15                     | 0.47              |
| 1:C:4631:ASP:HA   | 1:C:4708:TRP:HE1  | 1.80                     | 0.47              |
| 1:D:4053:GLU:OE2  | 1:D:4063:THR:OG1  | 2.32                     | 0.47              |
| 1:D:4891:CYS:HB3  | 1:D:4913:HIS:CE1  | 2.50                     | 0.47              |
| 1:A:766:ILE:HB    | 1:A:779:PHE:HB2   | 1.96                     | 0.46              |
| 1:A:1118:SER:HB3  | 1:A:1204:VAL:HG11 | 1.97                     | 0.46              |
| 1:A:2278:GLN:HA   | 1:A:2281:VAL:HG22 | 1.96                     | 0.46              |
| 1:A:2769:GLU:C    | 1:A:2771:TYR:H    | 2.24                     | 0.46              |
| 1:A:2787:TRP:HE1  | 1:A:2840:MET:HE2  | 1.80                     | 0.46              |
| 1:A:3097:THR:HG23 | 1:A:3101:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:4053:GLU:OE2  | 1:A:4063:THR:OG1  | 2.32                     | 0.46              |
| 1:B:1718:ARG:HH12 | 1:B:1832:GLY:HA3  | 1.79                     | 0.46              |
| 1:B:1848:PRO:HG3  | 1:B:1890:LYS:O    | 2.15                     | 0.46              |
| 1:B:2742:ILE:HB   | 1:B:2753:VAL:HG12 | 1.96                     | 0.46              |
| 1:B:3249:TRP:HA   | 1:B:3252:HIS:ND1  | 2.30                     | 0.46              |
| 1:C:128:MET:HG2   | 1:C:151:GLU:HA    | 1.97                     | 0.46              |
| 1:C:2696:ASP:HB3  | 1:C:2700:ASN:HA   | 1.97                     | 0.46              |
| 1:C:3946:GLY:O    | 1:C:3950:VAL:HG23 | 2.14                     | 0.46              |
| 1:D:1761:MET:HE3  | 1:D:1761:MET:HB3  | 1.83                     | 0.46              |
| 1:D:1931:ASP:OD1  | 1:D:1932:PHE:N    | 2.48                     | 0.46              |
| 1:D:2698:GLU:O    | 1:D:2698:GLU:HG2  | 2.14                     | 0.46              |
| 1:D:3122:ILE:HG12 | 1:D:3127:GLN:HG2  | 1.97                     | 0.46              |
| 1:A:28:ILE:O      | 1:A:31:GLU:HG3    | 2.15                     | 0.46              |
| 1:A:1145:TRP:CE2  | 1:A:1149:ASN:HB3  | 2.50                     | 0.46              |
| 1:A:2585:MET:HE3  | 1:A:2616:ARG:NH2  | 2.21                     | 0.46              |
| 1:B:128:MET:HG2   | 1:B:151:GLU:HA    | 1.97                     | 0.46              |
| 1:B:988:LEU:HB3   | 1:B:993:GLU:OE2   | 2.15                     | 0.46              |
| 1:B:1145:TRP:CE2  | 1:B:1149:ASN:HB3  | 2.50                     | 0.46              |
| 1:B:2444:THR:HB   | 1:B:2866:GLY:HA2  | 1.97                     | 0.46              |
| 1:C:227:TYR:CD2   | 1:C:352:SER:HB2   | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1442:TRP:CD1  | 1:C:1489:CYS:HB2  | 2.50                     | 0.46              |
| 1:C:2278:GLN:HA   | 1:C:2281:VAL:HG22 | 1.96                     | 0.46              |
| 1:C:2431:ASP:O    | 1:C:2435:VAL:HG23 | 2.15                     | 0.46              |
| 1:C:2795:GLY:HA2  | 1:C:2798:MET:HE2  | 1.96                     | 0.46              |
| 1:D:1442:TRP:CD1  | 1:D:1489:CYS:HB2  | 2.51                     | 0.46              |
| 1:D:3089:GLY:O    | 1:D:3092:GLN:HG3  | 2.15                     | 0.46              |
| 1:A:370:LEU:HB2   | 1:A:393:MET:HG3   | 1.97                     | 0.46              |
| 1:A:748:LEU:HB2   | 2:E:8:ILE:HG23    | 1.97                     | 0.46              |
| 1:A:1664:VAL:HG23 | 1:A:1676:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:2507:LEU:HA   | 1:A:2510:THR:HG23 | 1.97                     | 0.46              |
| 1:A:4631:ASP:HA   | 1:A:4708:TRP:HE1  | 1.80                     | 0.46              |
| 1:B:2795:GLY:HA2  | 1:B:2798:MET:HE2  | 1.96                     | 0.46              |
| 1:B:4518:LEU:HD23 | 1:C:4809:MET:HE3  | 1.96                     | 0.46              |
| 1:C:1118:SER:HB3  | 1:C:1204:VAL:HG11 | 1.97                     | 0.46              |
| 1:C:2723:LYS:HA   | 1:C:2726:GLU:HB2  | 1.96                     | 0.46              |
| 1:C:2728:SER:HB2  | 1:C:2771:TYR:OH   | 2.14                     | 0.46              |
| 1:C:2971:ILE:HG23 | 1:C:2975:PHE:HE2  | 1.80                     | 0.46              |
| 1:C:3064:ALA:HB1  | 1:C:3101:LEU:HD11 | 1.97                     | 0.46              |
| 1:C:4522:VAL:HG23 | 1:D:4786:PHE:CZ   | 2.50                     | 0.46              |
| 1:D:1664:VAL:HG23 | 1:D:1676:LEU:HD11 | 1.97                     | 0.46              |
| 1:D:1932:PHE:CE1  | 1:D:1996:LEU:HB2  | 2.51                     | 0.46              |
| 1:D:2447:LYS:HD2  | 1:D:2864:GLY:HA3  | 1.97                     | 0.46              |
| 1:D:3023:GLY:N    | 1:D:3025:ASP:OD2  | 2.45                     | 0.46              |
| 1:D:3944:VAL:HG11 | 1:D:4002:MET:HE2  | 1.96                     | 0.46              |
| 1:D:4631:ASP:HA   | 1:D:4708:TRP:HE1  | 1.81                     | 0.46              |
| 1:A:447:LEU:HD12  | 1:A:447:LEU:HA    | 1.83                     | 0.46              |
| 1:A:756:SER:OG    | 1:A:769:ARG:HB3   | 2.15                     | 0.46              |
| 1:A:1219:LYS:NZ   | 1:A:1243:THR:OG1  | 2.42                     | 0.46              |
| 1:A:1610:ARG:HH21 | 1:A:1617:TRP:HZ2  | 1.64                     | 0.46              |
| 1:A:2698:GLU:O    | 1:A:2698:GLU:HG2  | 2.15                     | 0.46              |
| 1:A:2831:VAL:HG13 | 1:A:2894:LYS:HD3  | 1.97                     | 0.46              |
| 1:A:2954:PHE:HB2  | 1:A:2957:GLU:HG2  | 1.98                     | 0.46              |
| 1:A:3249:TRP:HA   | 1:A:3252:HIS:ND1  | 2.30                     | 0.46              |
| 2:H:8:ILE:HD11    | 2:H:74:LYS:HB2    | 1.97                     | 0.46              |
| 1:B:2918:GLU:HG3  | 1:B:2923:TYR:CE2  | 2.50                     | 0.46              |
| 1:B:3019:ILE:HD11 | 1:B:3096:TYR:CD1  | 2.51                     | 0.46              |
| 1:B:3215:MET:HA   | 1:B:3218:ILE:HG12 | 1.97                     | 0.46              |
| 1:C:932:ASN:O     | 1:C:935:MET:HG3   | 2.16                     | 0.46              |
| 1:C:1610:ARG:HH21 | 1:C:1617:TRP:HZ2  | 1.64                     | 0.46              |
| 1:C:1931:ASP:OD1  | 1:C:1932:PHE:N    | 2.48                     | 0.46              |
| 1:C:2080:LEU:O    | 1:C:2084:MET:HG3  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2918:GLU:HA   | 1:C:2923:TYR:CD2  | 2.51                     | 0.46              |
| 1:C:3019:ILE:HD11 | 1:C:3096:TYR:CD1  | 2.51                     | 0.46              |
| 1:C:4891:CYS:HB3  | 1:C:4913:HIS:CE1  | 2.50                     | 0.46              |
| 1:D:2406:MET:O    | 1:D:2409:ILE:HG22 | 2.15                     | 0.46              |
| 1:D:2623:LEU:HD12 | 1:D:2624:PRO:HD2  | 1.98                     | 0.46              |
| 1:D:2971:ILE:HG23 | 1:D:2975:PHE:HE2  | 1.80                     | 0.46              |
| 1:A:290:ARG:NH1   | 1:A:353:GLU:HG2   | 2.31                     | 0.46              |
| 1:A:1442:TRP:CD1  | 1:A:1489:CYS:HB2  | 2.51                     | 0.46              |
| 1:A:3178:HIS:ND1  | 1:A:3178:HIS:O    | 2.48                     | 0.46              |
| 1:A:4891:CYS:HB3  | 1:A:4913:HIS:CE1  | 2.50                     | 0.46              |
| 1:B:932:ASN:O     | 1:B:935:MET:HG3   | 2.16                     | 0.46              |
| 1:B:1931:ASP:OD1  | 1:B:1932:PHE:N    | 2.48                     | 0.46              |
| 1:B:3089:GLY:O    | 1:B:3092:GLN:HG3  | 2.15                     | 0.46              |
| 1:B:3944:VAL:HG11 | 1:B:4002:MET:HE2  | 1.96                     | 0.46              |
| 1:C:756:SER:OG    | 1:C:769:ARG:HB3   | 2.15                     | 0.46              |
| 1:C:2778:SER:O    | 1:C:2781:THR:OG1  | 2.31                     | 0.46              |
| 1:D:2507:LEU:HA   | 1:D:2510:THR:HG23 | 1.97                     | 0.46              |
| 1:D:2918:GLU:HA   | 1:D:2923:TYR:CD2  | 2.51                     | 0.46              |
| 1:D:3271:GLU:HA   | 1:D:3274:ASN:HB2  | 1.97                     | 0.46              |
| 1:A:674:TYR:CE1   | 1:A:756:SER:HB2   | 2.49                     | 0.46              |
| 1:A:1144:ARG:HD2  | 1:A:1192:PHE:CE1  | 2.50                     | 0.46              |
| 1:A:1718:ARG:HH12 | 1:A:1832:GLY:HA3  | 1.79                     | 0.46              |
| 1:A:2080:LEU:O    | 1:A:2084:MET:HG3  | 2.16                     | 0.46              |
| 1:A:2918:GLU:HA   | 1:A:2923:TYR:CD2  | 2.51                     | 0.46              |
| 1:A:3217:GLU:O    | 1:A:3220:GLU:HG3  | 2.16                     | 0.46              |
| 2:G:8:ILE:HD11    | 2:G:74:LYS:HB2    | 1.97                     | 0.46              |
| 1:B:1442:TRP:CD1  | 1:B:1489:CYS:HB2  | 2.51                     | 0.46              |
| 1:B:2586:GLN:HA   | 1:B:2589:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:2787:TRP:CD1  | 1:B:2905:ARG:HA   | 2.51                     | 0.46              |
| 1:B:2918:GLU:HA   | 1:B:2923:TYR:CD2  | 2.51                     | 0.46              |
| 1:C:28:ILE:O      | 1:C:31:GLU:HG3    | 2.15                     | 0.46              |
| 1:C:1848:PRO:HG3  | 1:C:1890:LYS:O    | 2.15                     | 0.46              |
| 1:C:2157:GLN:O    | 1:C:3615:ARG:NH2  | 2.25                     | 0.46              |
| 1:D:756:SER:OG    | 1:D:769:ARG:HB3   | 2.15                     | 0.46              |
| 1:D:1610:ARG:HH21 | 1:D:1617:TRP:HZ2  | 1.64                     | 0.46              |
| 1:D:2566:ARG:O    | 1:D:2570:GLU:HG3  | 2.15                     | 0.46              |
| 1:D:2725:ALA:HB1  | 1:D:2771:TYR:HE2  | 1.79                     | 0.46              |
| 1:D:2787:TRP:CD1  | 1:D:2905:ARG:HA   | 2.51                     | 0.46              |
| 1:D:2918:GLU:HG3  | 1:D:2923:TYR:CE2  | 2.50                     | 0.46              |
| 1:D:3956:MET:HG3  | 1:D:4065:PHE:CZ   | 2.50                     | 0.46              |
| 1:A:2593:VAL:HG12 | 1:A:2644:LEU:HD22 | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3215:MET:HA   | 1:A:3218:ILE:HG12 | 1.97                     | 0.46              |
| 1:B:744:PRO:HD2   | 1:B:773:GLN:OE1   | 2.15                     | 0.46              |
| 1:B:2623:LEU:HD12 | 1:B:2624:PRO:HD2  | 1.98                     | 0.46              |
| 1:C:370:LEU:HB2   | 1:C:393:MET:HG3   | 1.97                     | 0.46              |
| 1:C:1664:VAL:HG23 | 1:C:1676:LEU:HD11 | 1.97                     | 0.46              |
| 1:C:1932:PHE:CE1  | 1:C:1996:LEU:HB2  | 2.51                     | 0.46              |
| 1:C:2150:MET:O    | 1:C:2156:TYR:OH   | 2.21                     | 0.46              |
| 1:C:2406:MET:O    | 1:C:2409:ILE:HG22 | 2.15                     | 0.46              |
| 1:C:2507:LEU:HA   | 1:C:2510:THR:HG23 | 1.97                     | 0.46              |
| 1:C:2623:LEU:HD12 | 1:C:2624:PRO:HD2  | 1.98                     | 0.46              |
| 1:C:3097:THR:HG23 | 1:C:3101:LEU:HD23 | 1.97                     | 0.46              |
| 1:C:3257:ASN:OD1  | 1:C:3260:ARG:NH2  | 2.49                     | 0.46              |
| 1:D:290:ARG:NH1   | 1:D:353:GLU:HG2   | 2.31                     | 0.46              |
| 1:D:370:LEU:HB2   | 1:D:393:MET:HG3   | 1.97                     | 0.46              |
| 1:D:1144:ARG:HD2  | 1:D:1192:PHE:CE1  | 2.50                     | 0.46              |
| 1:D:3249:TRP:HA   | 1:D:3252:HIS:ND1  | 2.30                     | 0.46              |
| 1:D:3257:ASN:OD1  | 1:D:3260:ARG:NH2  | 2.49                     | 0.46              |
| 1:D:4697:VAL:O    | 1:D:4701:ILE:HG23 | 2.16                     | 0.46              |
| 1:A:480:ARG:NH2   | 1:A:3678:GLU:OE2  | 2.45                     | 0.46              |
| 1:A:744:PRO:HD2   | 1:A:773:GLN:OE1   | 2.15                     | 0.46              |
| 1:A:2566:ARG:O    | 1:A:2570:GLU:HG3  | 2.15                     | 0.46              |
| 1:A:2623:LEU:HD12 | 1:A:2624:PRO:HD2  | 1.98                     | 0.46              |
| 1:A:2787:TRP:CD1  | 1:A:2905:ARG:HA   | 2.51                     | 0.46              |
| 1:A:3065:ALA:HB1  | 1:A:3132:ARG:NH1  | 2.21                     | 0.46              |
| 1:A:4194:GLU:HG2  | 1:A:4645:TRP:HZ3  | 1.80                     | 0.46              |
| 1:B:1038:LEU:HD23 | 1:B:1039:ASP:N    | 2.30                     | 0.46              |
| 1:B:3217:GLU:O    | 1:B:3220:GLU:HG3  | 2.16                     | 0.46              |
| 1:B:4194:GLU:HG2  | 1:B:4645:TRP:HZ3  | 1.80                     | 0.46              |
| 1:C:176:ARG:N     | 1:C:179:ASP:OD2   | 2.37                     | 0.46              |
| 1:C:2418:ARG:NH2  | 1:D:156:GLU:OE1   | 2.42                     | 0.46              |
| 1:C:2985:ALA:HB2  | 1:C:3001:LYS:HZ2  | 1.80                     | 0.46              |
| 1:D:227:TYR:CD2   | 1:D:352:SER:HB2   | 2.51                     | 0.46              |
| 1:D:606:ARG:HH21  | 1:D:1633:PRO:HD2  | 1.80                     | 0.46              |
| 1:D:2431:ASP:O    | 1:D:2435:VAL:HG23 | 2.15                     | 0.46              |
| 1:D:2853:ALA:O    | 1:D:2857:LYS:HG3  | 2.15                     | 0.46              |
| 1:D:3215:MET:HA   | 1:D:3218:ILE:HG12 | 1.97                     | 0.46              |
| 1:D:3217:GLU:O    | 1:D:3220:GLU:HG3  | 2.16                     | 0.46              |
| 1:A:996:VAL:HG11  | 1:A:1051:ARG:HG2  | 1.97                     | 0.46              |
| 1:A:2000:HIS:O    | 1:A:2004:MET:HG2  | 2.16                     | 0.46              |
| 1:A:2652:LEU:HD23 | 1:A:2962:PHE:HE1  | 1.79                     | 0.46              |
| 1:A:3122:ILE:HG12 | 1:A:3127:GLN:HG2  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3311:LYS:NZ   | 1:A:3313:GLN:H    | 2.14                     | 0.46              |
| 1:A:4287:TYR:CE2  | 1:B:4588:ILE:HG23 | 2.51                     | 0.46              |
| 1:B:227:TYR:CD2   | 1:B:352:SER:HB2   | 2.50                     | 0.46              |
| 1:B:606:ARG:HH21  | 1:B:1633:PRO:HD2  | 1.81                     | 0.46              |
| 1:B:2080:LEU:O    | 1:B:2084:MET:HG3  | 2.16                     | 0.46              |
| 1:B:2769:GLU:C    | 1:B:2771:TYR:H    | 2.24                     | 0.46              |
| 1:B:3097:THR:HG23 | 1:B:3101:LEU:HD23 | 1.97                     | 0.46              |
| 1:C:810:GLU:OE1   | 1:C:810:GLU:N     | 2.49                     | 0.46              |
| 1:C:952:ILE:HG13  | 1:C:1061:GLY:O    | 2.16                     | 0.46              |
| 1:C:1038:LEU:HD23 | 1:C:1039:ASP:N    | 2.30                     | 0.46              |
| 1:C:2666:LEU:HD13 | 1:C:2966:VAL:HA   | 1.97                     | 0.46              |
| 1:C:2787:TRP:HE1  | 1:C:2840:MET:HE2  | 1.80                     | 0.46              |
| 1:C:3944:VAL:HG11 | 1:C:4002:MET:HE2  | 1.96                     | 0.46              |
| 1:D:2831:VAL:HG13 | 1:D:2894:LYS:HD3  | 1.97                     | 0.46              |
| 1:D:2904:SER:OG   | 1:D:2905:ARG:N    | 2.49                     | 0.46              |
| 1:D:3311:LYS:NZ   | 1:D:3313:GLN:H    | 2.14                     | 0.46              |
| 1:D:3722:GLN:HB3  | 1:D:4681:ASP:OD1  | 2.15                     | 0.46              |
| 1:D:4004:VAL:HA   | 1:D:4118:PHE:HZ   | 1.81                     | 0.46              |
| 1:A:58:VAL:HG13   | 1:A:319:LYS:HG2   | 1.98                     | 0.46              |
| 1:A:472:HIS:O     | 1:A:476:GLN:HG2   | 2.16                     | 0.46              |
| 1:A:487:ASN:O     | 1:A:491:GLU:HG2   | 2.16                     | 0.46              |
| 1:A:890:HIS:HA    | 1:A:893:TRP:CE3   | 2.45                     | 0.46              |
| 1:A:1289:SER:O    | 1:A:1295:SER:OG   | 2.24                     | 0.46              |
| 1:A:2471:PHE:O    | 1:A:2475:VAL:HG22 | 2.14                     | 0.46              |
| 1:A:3257:ASN:OD1  | 1:A:3260:ARG:NH2  | 2.49                     | 0.46              |
| 2:G:9:SER:HB3     | 2:G:72:ARG:HB3    | 1.97                     | 0.46              |
| 1:B:58:VAL:HG13   | 1:B:319:LYS:HG2   | 1.98                     | 0.46              |
| 1:B:487:ASN:O     | 1:B:491:GLU:HG2   | 2.16                     | 0.46              |
| 1:B:1118:SER:HB3  | 1:B:1204:VAL:HG11 | 1.97                     | 0.46              |
| 1:B:1464:THR:HG22 | 1:B:1483:SER:HB2  | 1.98                     | 0.46              |
| 1:B:1610:ARG:HH21 | 1:B:1617:TRP:HZ2  | 1.64                     | 0.46              |
| 1:C:35:LEU:HD23   | 1:C:51:SER:HA     | 1.98                     | 0.46              |
| 1:C:181:LEU:N     | 1:C:212:TRP:O     | 2.45                     | 0.46              |
| 1:C:3246:MET:HE2  | 1:C:3246:MET:HB3  | 1.80                     | 0.46              |
| 1:C:4697:VAL:O    | 1:C:4701:ILE:HG23 | 2.16                     | 0.46              |
| 1:D:890:HIS:HA    | 1:D:893:TRP:CE3   | 2.45                     | 0.46              |
| 1:D:996:VAL:HG11  | 1:D:1051:ARG:HG2  | 1.97                     | 0.46              |
| 1:D:2666:LEU:HD13 | 1:D:2966:VAL:HA   | 1.97                     | 0.46              |
| 1:D:2696:ASP:HB3  | 1:D:2700:ASN:HA   | 1.97                     | 0.46              |
| 1:A:227:TYR:CD2   | 1:A:352:SER:HB2   | 2.51                     | 0.45              |
| 1:A:2406:MET:O    | 1:A:2409:ILE:HG22 | 2.15                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3019:ILE:HD11 | 1:A:3096:TYR:CD1  | 2.50                     | 0.45              |
| 1:B:290:ARG:NH1   | 1:B:353:GLU:HG2   | 2.31                     | 0.45              |
| 1:B:679:VAL:HA    | 1:B:800:VAL:HG12  | 1.98                     | 0.45              |
| 1:B:897:LYS:HA    | 1:B:900:LEU:HD12  | 1.98                     | 0.45              |
| 1:B:2250:ASN:HB3  | 1:B:2253:LEU:HB2  | 1.99                     | 0.45              |
| 1:B:2954:PHE:HB2  | 1:B:2957:GLU:HG2  | 1.98                     | 0.45              |
| 1:B:3271:GLU:HA   | 1:B:3274:ASN:HB2  | 1.98                     | 0.45              |
| 1:C:2444:THR:HB   | 1:C:2866:GLY:HA2  | 1.97                     | 0.45              |
| 1:C:3192:ARG:NH1  | 1:C:3195:LEU:HD13 | 2.32                     | 0.45              |
| 1:C:3217:GLU:O    | 1:C:3220:GLU:HG3  | 2.16                     | 0.45              |
| 1:D:744:PRO:HD2   | 1:D:773:GLN:OE1   | 2.15                     | 0.45              |
| 1:D:1464:THR:HG22 | 1:D:1483:SER:HB2  | 1.98                     | 0.45              |
| 1:A:503:ASP:O     | 1:A:507:VAL:HG23  | 2.16                     | 0.45              |
| 1:A:897:LYS:HA    | 1:A:900:LEU:HD12  | 1.98                     | 0.45              |
| 1:A:932:ASN:O     | 1:A:935:MET:HG3   | 2.16                     | 0.45              |
| 1:A:1848:PRO:HG3  | 1:A:1890:LYS:O    | 2.16                     | 0.45              |
| 1:A:1932:PHE:CE1  | 1:A:1996:LEU:HB2  | 2.51                     | 0.45              |
| 1:A:3089:GLY:O    | 1:A:3092:GLN:HG3  | 2.15                     | 0.45              |
| 1:A:3944:VAL:HG11 | 1:A:4002:MET:HE2  | 1.97                     | 0.45              |
| 1:A:4276:VAL:HG23 | 1:B:4487:TYR:CE2  | 2.51                     | 0.45              |
| 1:A:4697:VAL:O    | 1:A:4701:ILE:HG23 | 2.16                     | 0.45              |
| 1:B:28:ILE:O      | 1:B:31:GLU:HG3    | 2.15                     | 0.45              |
| 1:B:1058:LEU:HG   | 1:B:1064:LEU:H    | 1.82                     | 0.45              |
| 1:B:1932:PHE:CE1  | 1:B:1996:LEU:HB2  | 2.51                     | 0.45              |
| 1:B:2150:MET:O    | 1:B:2156:TYR:OH   | 2.21                     | 0.45              |
| 1:B:2507:LEU:HA   | 1:B:2510:THR:HG23 | 1.97                     | 0.45              |
| 1:C:487:ASN:O     | 1:C:491:GLU:HG2   | 2.16                     | 0.45              |
| 1:C:988:LEU:HB3   | 1:C:993:GLU:OE2   | 2.15                     | 0.45              |
| 1:C:2713:ILE:HG22 | 1:C:2779:LEU:HD21 | 1.98                     | 0.45              |
| 1:C:2904:SER:OG   | 1:C:2905:ARG:N    | 2.49                     | 0.45              |
| 1:C:4488:GLN:O    | 1:C:4492:LEU:HD23 | 2.17                     | 0.45              |
| 1:C:4518:LEU:HD23 | 1:D:4809:MET:HE3  | 1.97                     | 0.45              |
| 1:D:876:PRO:O     | 1:D:881:ILE:HG12  | 2.17                     | 0.45              |
| 1:D:1248:THR:HG21 | 1:D:1598:ARG:NE   | 2.32                     | 0.45              |
| 1:D:1433:PHE:CD2  | 1:D:1551:ASN:HB3  | 2.52                     | 0.45              |
| 1:D:2769:GLU:C    | 1:D:2771:TYR:H    | 2.24                     | 0.45              |
| 1:D:4488:GLN:O    | 1:D:4492:LEU:HD23 | 2.17                     | 0.45              |
| 1:A:1248:THR:HG21 | 1:A:1598:ARG:NE   | 2.32                     | 0.45              |
| 1:A:2614:TYR:CE2  | 1:A:2672:VAL:HG22 | 2.51                     | 0.45              |
| 1:A:2985:ALA:HB2  | 1:A:3001:LYS:HZ2  | 1.81                     | 0.45              |
| 2:H:9:SER:HB3     | 2:H:72:ARG:HB3    | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1664:VAL:HG23 | 1:B:1676:LEU:HD11 | 1.97                     | 0.45              |
| 1:B:2614:TYR:CE2  | 1:B:2672:VAL:HG22 | 2.51                     | 0.45              |
| 1:B:4488:GLN:O    | 1:B:4492:LEU:HD23 | 2.17                     | 0.45              |
| 1:C:503:ASP:O     | 1:C:507:VAL:HG23  | 2.16                     | 0.45              |
| 1:C:744:PRO:HD2   | 1:C:773:GLN:OE1   | 2.15                     | 0.45              |
| 1:C:1433:PHE:CD2  | 1:C:1551:ASN:HB3  | 2.52                     | 0.45              |
| 1:C:2954:PHE:HB2  | 1:C:2957:GLU:HG2  | 1.97                     | 0.45              |
| 1:C:3131:TYR:HB3  | 1:C:3204:VAL:HG11 | 1.99                     | 0.45              |
| 1:C:4169:LYS:NZ   | 4:C:5002:ATP:O2A  | 2.38                     | 0.45              |
| 1:D:952:ILE:HG13  | 1:D:1061:GLY:O    | 2.16                     | 0.45              |
| 1:D:3131:TYR:HB3  | 1:D:3204:VAL:HG11 | 1.99                     | 0.45              |
| 1:D:3192:ARG:NH1  | 1:D:3195:LEU:HD13 | 2.32                     | 0.45              |
| 1:A:35:LEU:HD23   | 1:A:51:SER:HA     | 1.98                     | 0.45              |
| 1:A:810:GLU:OE1   | 1:A:810:GLU:N     | 2.49                     | 0.45              |
| 1:A:1058:LEU:HG   | 1:A:1064:LEU:H    | 1.82                     | 0.45              |
| 1:A:1152:TYR:HD1  | 1:A:1184:ASP:HA   | 1.82                     | 0.45              |
| 1:A:2884:LYS:O    | 1:A:2887:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:3043:ARG:HH22 | 1:A:3119:GLU:HB2  | 1.82                     | 0.45              |
| 1:A:4004:VAL:HA   | 1:A:4118:PHE:HZ   | 1.81                     | 0.45              |
| 1:B:472:HIS:O     | 1:B:476:GLN:HG2   | 2.16                     | 0.45              |
| 1:B:611:LEU:HD22  | 1:B:1660:LEU:HD22 | 1.99                     | 0.45              |
| 1:B:2000:HIS:O    | 1:B:2004:MET:HG2  | 2.16                     | 0.45              |
| 1:B:3311:LYS:NZ   | 1:B:3313:GLN:H    | 2.14                     | 0.45              |
| 1:C:611:LEU:HD22  | 1:C:1660:LEU:HD22 | 1.99                     | 0.45              |
| 1:C:2114:GLU:HG2  | 1:C:2115:ASP:N    | 2.32                     | 0.45              |
| 1:C:3213:LYS:HA   | 1:C:3216:GLU:HG3  | 1.99                     | 0.45              |
| 1:D:137:ARG:NH2   | 1:D:203:VAL:O     | 2.36                     | 0.45              |
| 1:D:2080:LEU:O    | 1:D:2084:MET:HG3  | 2.16                     | 0.45              |
| 1:D:2610:LEU:HD12 | 1:D:2614:TYR:HE2  | 1.81                     | 0.45              |
| 1:A:423:VAL:HG22  | 1:A:494:MET:HE1   | 1.99                     | 0.45              |
| 1:A:3242:LEU:O    | 1:A:3246:MET:HG2  | 2.17                     | 0.45              |
| 1:A:4786:PHE:CZ   | 1:D:4522:VAL:HG23 | 2.52                     | 0.45              |
| 2:E:9:SER:HB3     | 2:E:72:ARG:HB3    | 1.97                     | 0.45              |
| 1:B:986:ILE:HB    | 1:B:1055:ARG:HG2  | 1.99                     | 0.45              |
| 1:B:1248:THR:HG21 | 1:B:1598:ARG:NE   | 2.32                     | 0.45              |
| 1:B:2353:ILE:HG23 | 1:B:2359:ARG:HB3  | 1.99                     | 0.45              |
| 1:B:3257:ASN:OD1  | 1:B:3260:ARG:NH2  | 2.49                     | 0.45              |
| 1:C:876:PRO:O     | 1:C:881:ILE:HG12  | 2.17                     | 0.45              |
| 1:C:1058:LEU:HG   | 1:C:1064:LEU:H    | 1.82                     | 0.45              |
| 1:C:1464:THR:HG22 | 1:C:1483:SER:HB2  | 1.99                     | 0.45              |
| 1:C:2000:HIS:O    | 1:C:2004:MET:HG2  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2379:ASP:OD1  | 1:C:2380:ASP:N    | 2.50                     | 0.45              |
| 1:C:2586:GLN:HA   | 1:C:2589:LEU:HD12 | 1.98                     | 0.45              |
| 1:C:2884:LYS:O    | 1:C:2887:GLU:HG3  | 2.17                     | 0.45              |
| 1:C:3043:ARG:HH22 | 1:C:3119:GLU:HB2  | 1.82                     | 0.45              |
| 1:C:3271:GLU:HA   | 1:C:3274:ASN:HB2  | 1.97                     | 0.45              |
| 1:C:3311:LYS:NZ   | 1:C:3313:GLN:H    | 2.14                     | 0.45              |
| 1:D:472:HIS:O     | 1:D:476:GLN:HG2   | 2.16                     | 0.45              |
| 1:D:487:ASN:O     | 1:D:491:GLU:HG2   | 2.16                     | 0.45              |
| 1:D:986:ILE:HB    | 1:D:1055:ARG:HG2  | 1.99                     | 0.45              |
| 1:D:2114:GLU:HG2  | 1:D:2115:ASP:N    | 2.32                     | 0.45              |
| 1:D:2250:ASN:HB3  | 1:D:2253:LEU:HB2  | 1.99                     | 0.45              |
| 1:D:2379:ASP:OD1  | 1:D:2380:ASP:N    | 2.50                     | 0.45              |
| 1:D:3019:ILE:HD11 | 1:D:3096:TYR:CD1  | 2.51                     | 0.45              |
| 1:D:3242:LEU:O    | 1:D:3246:MET:HG2  | 2.17                     | 0.45              |
| 1:D:3307:ILE:HA   | 1:D:3310:VAL:HG12 | 1.99                     | 0.45              |
| 1:A:679:VAL:HA    | 1:A:800:VAL:HG12  | 1.98                     | 0.45              |
| 1:A:876:PRO:O     | 1:A:881:ILE:HG12  | 2.17                     | 0.45              |
| 1:A:1464:THR:HG22 | 1:A:1483:SER:HB2  | 1.99                     | 0.45              |
| 1:A:1761:MET:HE3  | 1:A:1761:MET:HB3  | 1.84                     | 0.45              |
| 1:A:2250:ASN:HB3  | 1:A:2253:LEU:HB2  | 1.99                     | 0.45              |
| 1:A:2441:GLN:NE2  | 1:A:2442:MET:O    | 2.50                     | 0.45              |
| 1:A:2586:GLN:HA   | 1:A:2589:LEU:HD12 | 1.98                     | 0.45              |
| 1:A:2610:LEU:HD12 | 1:A:2614:TYR:HE2  | 1.82                     | 0.45              |
| 1:A:2715:GLU:O    | 1:A:2718:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:2904:SER:OG   | 1:A:2905:ARG:N    | 2.49                     | 0.45              |
| 1:A:2971:ILE:HG23 | 1:A:2975:PHE:HE2  | 1.80                     | 0.45              |
| 1:A:3307:ILE:HA   | 1:A:3310:VAL:HG12 | 1.99                     | 0.45              |
| 1:B:35:LEU:HD23   | 1:B:51:SER:HA     | 1.98                     | 0.45              |
| 1:B:503:ASP:O     | 1:B:507:VAL:HG23  | 2.16                     | 0.45              |
| 1:B:810:GLU:N     | 1:B:810:GLU:OE1   | 2.49                     | 0.45              |
| 1:B:876:PRO:O     | 1:B:881:ILE:HG12  | 2.17                     | 0.45              |
| 1:B:2593:VAL:HG12 | 1:B:2644:LEU:HD22 | 1.98                     | 0.45              |
| 1:B:3099:VAL:O    | 1:B:3103:PRO:HG2  | 2.17                     | 0.45              |
| 1:B:3246:MET:HE2  | 1:B:3246:MET:HB3  | 1.80                     | 0.45              |
| 1:C:897:LYS:HA    | 1:C:900:LEU:HD12  | 1.98                     | 0.45              |
| 1:C:2610:LEU:HD12 | 1:C:2614:TYR:HE2  | 1.82                     | 0.45              |
| 1:C:2769:GLU:C    | 1:C:2771:TYR:H    | 2.24                     | 0.45              |
| 1:C:4004:VAL:HA   | 1:C:4118:PHE:HZ   | 1.81                     | 0.45              |
| 1:C:4276:VAL:HG23 | 1:D:4487:TYR:CE2  | 2.50                     | 0.45              |
| 1:D:810:GLU:OE1   | 1:D:810:GLU:N     | 2.49                     | 0.45              |
| 1:D:2150:MET:O    | 1:D:2156:TYR:OH   | 2.21                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2353:ILE:HG23 | 1:D:2359:ARG:HB3  | 1.99                     | 0.45              |
| 1:D:4194:GLU:HG2  | 1:D:4645:TRP:HZ3  | 1.80                     | 0.45              |
| 1:A:2353:ILE:HG23 | 1:A:2359:ARG:HB3  | 1.99                     | 0.45              |
| 1:A:3050:LEU:HD23 | 1:A:3053:VAL:HG23 | 1.98                     | 0.45              |
| 1:A:3900:GLU:OE1  | 1:A:3901:GLN:NE2  | 2.44                     | 0.45              |
| 1:A:4810:LEU:HB2  | 1:D:4518:LEU:O    | 2.16                     | 0.45              |
| 1:B:198:ASN:OD1   | 1:B:199:GLY:N     | 2.50                     | 0.45              |
| 1:B:423:VAL:HG22  | 1:B:494:MET:HE1   | 1.99                     | 0.45              |
| 1:B:2441:GLN:NE2  | 1:B:2442:MET:O    | 2.50                     | 0.45              |
| 1:B:2980:LEU:O    | 1:B:2984:SER:N    | 2.50                     | 0.45              |
| 1:B:3043:ARG:HH22 | 1:B:3119:GLU:HB2  | 1.82                     | 0.45              |
| 1:B:4697:VAL:O    | 1:B:4701:ILE:HG23 | 2.16                     | 0.45              |
| 1:C:996:VAL:HG11  | 1:C:1051:ARG:HG2  | 1.97                     | 0.45              |
| 1:C:2386:ASN:HA   | 1:C:2389:MET:HE3  | 1.99                     | 0.45              |
| 1:C:2980:LEU:O    | 1:C:2984:SER:N    | 2.50                     | 0.45              |
| 1:C:3242:LEU:O    | 1:C:3246:MET:HG2  | 2.17                     | 0.45              |
| 1:C:4908:HIS:CE1  | 1:C:4913:HIS:ND1  | 2.85                     | 0.45              |
| 1:D:611:LEU:HD22  | 1:D:1660:LEU:HD22 | 1.99                     | 0.45              |
| 1:D:869:THR:HB    | 1:D:941:LYS:HB3   | 1.98                     | 0.45              |
| 1:D:2593:VAL:HG12 | 1:D:2644:LEU:HD22 | 1.98                     | 0.45              |
| 1:D:2954:PHE:HB2  | 1:D:2957:GLU:HG2  | 1.97                     | 0.45              |
| 1:D:4117:THR:O    | 1:D:4121:LEU:HD13 | 2.17                     | 0.45              |
| 1:A:606:ARG:HH21  | 1:A:1633:PRO:HD2  | 1.80                     | 0.45              |
| 1:A:988:LEU:HB2   | 1:A:1055:ARG:NE   | 2.27                     | 0.45              |
| 1:A:1718:ARG:HH21 | 1:A:1758:ARG:NH1  | 2.15                     | 0.45              |
| 1:A:2644:LEU:HD11 | 1:A:2648:ILE:HD11 | 1.99                     | 0.45              |
| 1:A:3853:ASP:OD1  | 1:A:3854:PHE:N    | 2.50                     | 0.45              |
| 2:F:9:SER:HB3     | 2:F:72:ARG:HB3    | 1.97                     | 0.45              |
| 1:B:2696:ASP:HB3  | 1:B:2700:ASN:HA   | 1.97                     | 0.45              |
| 1:B:3131:TYR:HB3  | 1:B:3204:VAL:HG11 | 1.99                     | 0.45              |
| 1:B:3307:ILE:HA   | 1:B:3310:VAL:HG12 | 1.99                     | 0.45              |
| 1:B:3642:GLU:HG3  | 1:B:3646:LYS:HZ2  | 1.82                     | 0.45              |
| 1:B:4174:PHE:HA   | 1:B:4880:VAL:HG21 | 1.99                     | 0.45              |
| 1:C:290:ARG:NH1   | 1:C:353:GLU:HG2   | 2.31                     | 0.45              |
| 1:C:472:HIS:O     | 1:C:476:GLN:HG2   | 2.16                     | 0.45              |
| 1:C:869:THR:HB    | 1:C:941:LYS:HB3   | 1.98                     | 0.45              |
| 1:C:1718:ARG:NE   | 1:C:1758:ARG:HD3  | 2.32                     | 0.45              |
| 1:C:2441:GLN:NE2  | 1:C:2442:MET:O    | 2.50                     | 0.45              |
| 1:C:2645:PHE:HE2  | 1:C:2925:PHE:CE1  | 2.35                     | 0.45              |
| 1:C:2787:TRP:CD1  | 1:C:2905:ARG:HA   | 2.51                     | 0.45              |
| 1:C:2791:ARG:O    | 1:C:2793:ARG:NH2  | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3272:HIS:O    | 1:C:3276:LEU:HG   | 2.17                     | 0.45              |
| 1:C:4194:GLU:HG2  | 1:C:4645:TRP:HZ3  | 1.80                     | 0.45              |
| 1:D:1848:PRO:HG3  | 1:D:1890:LYS:O    | 2.15                     | 0.45              |
| 1:D:2884:LYS:O    | 1:D:2887:GLU:HG3  | 2.17                     | 0.45              |
| 1:D:2980:LEU:O    | 1:D:2984:SER:N    | 2.50                     | 0.45              |
| 1:D:4264:LEU:HG   | 1:D:4268:MET:HE3  | 1.99                     | 0.45              |
| 1:A:611:LEU:HD22  | 1:A:1660:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:1433:PHE:CD2  | 1:A:1551:ASN:HB3  | 2.52                     | 0.45              |
| 1:A:2645:PHE:HE2  | 1:A:2925:PHE:CE1  | 2.35                     | 0.45              |
| 1:A:2791:ARG:O    | 1:A:2793:ARG:NH2  | 2.50                     | 0.45              |
| 1:A:3272:HIS:O    | 1:A:3276:LEU:HG   | 2.17                     | 0.45              |
| 1:B:1289:SER:O    | 1:B:1295:SER:OG   | 2.24                     | 0.45              |
| 1:B:2619:LYS:HZ1  | 1:B:2627:TRP:CG   | 2.35                     | 0.45              |
| 1:B:3050:LEU:HD23 | 1:B:3053:VAL:HG23 | 1.98                     | 0.45              |
| 1:B:3975:GLN:O    | 1:B:3979:VAL:HG23 | 2.17                     | 0.45              |
| 1:C:2614:TYR:CE2  | 1:C:2672:VAL:HG22 | 2.52                     | 0.45              |
| 1:C:2674:GLY:HA2  | 1:C:2978:HIS:CE1  | 2.52                     | 0.45              |
| 1:C:3307:ILE:HA   | 1:C:3310:VAL:HG12 | 1.99                     | 0.45              |
| 1:C:3314:LEU:HA   | 1:C:3318:HIS:ND1  | 2.32                     | 0.45              |
| 1:C:4253:LEU:HD22 | 1:C:4257:ARG:HH12 | 1.82                     | 0.45              |
| 1:D:188:SER:HB2   | 1:D:190:ARG:NH1   | 2.30                     | 0.45              |
| 1:D:423:VAL:HG22  | 1:D:494:MET:HE1   | 1.99                     | 0.45              |
| 1:D:447:LEU:O     | 1:D:449:ILE:N     | 2.50                     | 0.45              |
| 1:D:2000:HIS:O    | 1:D:2004:MET:HG2  | 2.16                     | 0.45              |
| 1:D:2441:GLN:NE2  | 1:D:2442:MET:O    | 2.50                     | 0.45              |
| 1:D:2715:GLU:O    | 1:D:2718:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:2379:ASP:OD1  | 1:A:2380:ASP:N    | 2.50                     | 0.45              |
| 1:A:2713:ILE:HG22 | 1:A:2779:LEU:HD21 | 1.98                     | 0.45              |
| 1:A:3131:TYR:HB3  | 1:A:3204:VAL:HG11 | 1.99                     | 0.45              |
| 1:A:3192:ARG:NH1  | 1:A:3195:LEU:HD13 | 2.32                     | 0.45              |
| 1:A:4174:PHE:HA   | 1:A:4880:VAL:HG21 | 1.99                     | 0.45              |
| 1:B:952:ILE:HG13  | 1:B:1061:GLY:O    | 2.16                     | 0.45              |
| 1:B:1718:ARG:NE   | 1:B:1758:ARG:HD3  | 2.32                     | 0.45              |
| 1:B:3192:ARG:NH1  | 1:B:3195:LEU:HD13 | 2.32                     | 0.45              |
| 1:C:1152:TYR:HD1  | 1:C:1184:ASP:HA   | 1.82                     | 0.45              |
| 1:C:2681:MET:HE1  | 1:C:2917:ILE:HA   | 1.99                     | 0.45              |
| 1:C:2715:GLU:O    | 1:C:2718:GLU:HG3  | 2.17                     | 0.45              |
| 1:C:2831:VAL:HB   | 1:D:1435:GLY:HA2  | 1.98                     | 0.45              |
| 1:C:3050:LEU:HD23 | 1:C:3053:VAL:HG23 | 1.98                     | 0.45              |
| 1:C:3914:LYS:HZ1  | 1:C:3973:ASP:CG   | 2.24                     | 0.45              |
| 1:D:35:LEU:HD23   | 1:D:51:SER:HA     | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:829:LYS:NZ    | 1:D:1037:LEU:O    | 2.49                     | 0.45              |
| 1:D:3695:MET:HB3  | 1:D:3731:LEU:HD11 | 1.99                     | 0.45              |
| 1:D:3900:GLU:OE1  | 1:D:3901:GLN:NE2  | 2.44                     | 0.45              |
| 1:A:198:ASN:OD1   | 1:A:199:GLY:N     | 2.50                     | 0.44              |
| 1:A:447:LEU:O     | 1:A:449:ILE:N     | 2.50                     | 0.44              |
| 1:A:2418:ARG:NH2  | 1:B:156:GLU:OE1   | 2.41                     | 0.44              |
| 1:A:4488:GLN:O    | 1:A:4492:LEU:HD23 | 2.17                     | 0.44              |
| 1:B:1152:TYR:HD1  | 1:B:1184:ASP:HA   | 1.82                     | 0.44              |
| 1:B:2604:LYS:HD3  | 1:B:2664:LEU:HD13 | 2.00                     | 0.44              |
| 1:B:2644:LEU:HD11 | 1:B:2648:ILE:HD11 | 1.99                     | 0.44              |
| 1:B:2645:PHE:HE2  | 1:B:2925:PHE:CE1  | 2.35                     | 0.44              |
| 1:B:2852:TRP:HA   | 1:B:2855:LYS:HE3  | 2.00                     | 0.44              |
| 1:B:2905:ARG:HE   | 1:B:2906:GLY:N    | 2.03                     | 0.44              |
| 1:B:3242:LEU:O    | 1:B:3246:MET:HG2  | 2.17                     | 0.44              |
| 1:C:826:VAL:HG21  | 1:C:832:LEU:HB2   | 1.99                     | 0.44              |
| 1:C:928:GLU:O     | 1:C:932:ASN:ND2   | 2.50                     | 0.44              |
| 1:C:1248:THR:HG21 | 1:C:1598:ARG:NE   | 2.32                     | 0.44              |
| 1:C:3099:VAL:O    | 1:C:3103:PRO:HG2  | 2.17                     | 0.44              |
| 1:D:932:ASN:O     | 1:D:935:MET:HG3   | 2.15                     | 0.44              |
| 1:D:1289:SER:O    | 1:D:1295:SER:OG   | 2.24                     | 0.44              |
| 1:D:2645:PHE:HE2  | 1:D:2925:PHE:CE1  | 2.35                     | 0.44              |
| 1:A:928:GLU:O     | 1:A:932:ASN:ND2   | 2.50                     | 0.44              |
| 1:A:4117:THR:O    | 1:A:4121:LEU:HD13 | 2.17                     | 0.44              |
| 2:H:50:ARG:HH21   | 2:H:53:LYS:HZ3    | 1.66                     | 0.44              |
| 1:B:1433:PHE:CD2  | 1:B:1551:ASN:HB3  | 2.52                     | 0.44              |
| 1:B:2379:ASP:OD1  | 1:B:2380:ASP:N    | 2.50                     | 0.44              |
| 1:B:2386:ASN:HA   | 1:B:2389:MET:HE3  | 1.99                     | 0.44              |
| 1:B:2681:MET:HE1  | 1:B:2917:ILE:HA   | 1.99                     | 0.44              |
| 1:B:2714:PRO:HD2  | 1:B:2717:LEU:HB2  | 1.99                     | 0.44              |
| 1:B:2715:GLU:O    | 1:B:2718:GLU:HG3  | 2.17                     | 0.44              |
| 1:B:2742:ILE:O    | 1:B:2754:GLN:N    | 2.33                     | 0.44              |
| 1:B:2904:SER:OG   | 1:B:2905:ARG:N    | 2.49                     | 0.44              |
| 1:B:4117:THR:O    | 1:B:4121:LEU:HD13 | 2.17                     | 0.44              |
| 1:B:4253:LEU:HD22 | 1:B:4257:ARG:HH12 | 1.82                     | 0.44              |
| 1:C:2250:ASN:HB3  | 1:C:2253:LEU:HB2  | 1.98                     | 0.44              |
| 1:C:2605:MET:HB3  | 1:C:2606:PRO:HD3  | 2.00                     | 0.44              |
| 1:C:2878:THR:O    | 1:C:2882:LYS:HG3  | 2.17                     | 0.44              |
| 1:C:3975:GLN:O    | 1:C:3979:VAL:HG23 | 2.17                     | 0.44              |
| 1:D:3099:VAL:O    | 1:D:3103:PRO:HG2  | 2.17                     | 0.44              |
| 1:A:986:ILE:HB    | 1:A:1055:ARG:HG2  | 1.99                     | 0.44              |
| 1:A:1035:TYR:CZ   | 1:A:1043:LYS:HB2  | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1557:LEU:HD22 | 1:A:1566:LEU:HD23 | 2.00                     | 0.44              |
| 1:A:2426:LEU:HD23 | 1:B:143:LEU:HD11  | 1.98                     | 0.44              |
| 1:A:4253:LEU:HD22 | 1:A:4257:ARG:HH12 | 1.82                     | 0.44              |
| 1:B:869:THR:HB    | 1:B:941:LYS:HB3   | 1.98                     | 0.44              |
| 1:B:1557:LEU:HD22 | 1:B:1566:LEU:HD23 | 1.99                     | 0.44              |
| 1:B:1694:MET:SD   | 1:B:1695:PRO:HD2  | 2.58                     | 0.44              |
| 1:B:1718:ARG:HH21 | 1:B:1758:ARG:NH1  | 2.15                     | 0.44              |
| 1:B:2884:LYS:O    | 1:B:2887:GLU:HG3  | 2.17                     | 0.44              |
| 1:B:3213:LYS:HA   | 1:B:3216:GLU:HG3  | 1.99                     | 0.44              |
| 1:B:4908:HIS:CE1  | 1:B:4913:HIS:ND1  | 2.85                     | 0.44              |
| 1:C:423:VAL:HG22  | 1:C:494:MET:HE1   | 1.99                     | 0.44              |
| 1:C:986:ILE:HB    | 1:C:1055:ARG:HG2  | 1.99                     | 0.44              |
| 1:C:2613:HIS:HA   | 1:C:2616:ARG:NE   | 2.33                     | 0.44              |
| 1:C:2644:LEU:HD11 | 1:C:2648:ILE:HD11 | 1.99                     | 0.44              |
| 1:C:4117:THR:O    | 1:C:4121:LEU:HD13 | 2.17                     | 0.44              |
| 1:D:58:VAL:HG13   | 1:D:319:LYS:HG2   | 1.98                     | 0.44              |
| 1:D:503:ASP:O     | 1:D:507:VAL:HG23  | 2.16                     | 0.44              |
| 1:D:1557:LEU:HD22 | 1:D:1566:LEU:HD23 | 1.99                     | 0.44              |
| 1:D:2456:MET:CE   | 1:D:2462:PRO:HD3  | 2.46                     | 0.44              |
| 1:D:2580:LEU:HD23 | 1:D:2581:ARG:N    | 2.33                     | 0.44              |
| 1:D:2644:LEU:HD11 | 1:D:2648:ILE:HD11 | 1.99                     | 0.44              |
| 1:D:2713:ILE:HG22 | 1:D:2779:LEU:HD21 | 1.98                     | 0.44              |
| 1:D:2852:TRP:HA   | 1:D:2855:LYS:HE3  | 2.00                     | 0.44              |
| 1:D:2878:THR:O    | 1:D:2882:LYS:HG3  | 2.17                     | 0.44              |
| 1:D:3043:ARG:HH22 | 1:D:3119:GLU:HB2  | 1.82                     | 0.44              |
| 1:D:3272:HIS:O    | 1:D:3276:LEU:HG   | 2.17                     | 0.44              |
| 1:D:3853:ASP:OD1  | 1:D:3854:PHE:N    | 2.50                     | 0.44              |
| 1:D:4253:LEU:HD22 | 1:D:4257:ARG:HH12 | 1.82                     | 0.44              |
| 1:A:952:ILE:HG13  | 1:A:1061:GLY:O    | 2.16                     | 0.44              |
| 1:A:1156:TRP:HB2  | 1:A:1160:ASP:HB2  | 2.00                     | 0.44              |
| 1:A:2178:VAL:HG21 | 1:A:2192:MET:CE   | 2.45                     | 0.44              |
| 1:A:2604:LYS:HD3  | 1:A:2664:LEU:HD13 | 2.00                     | 0.44              |
| 1:A:2612:ASN:O    | 1:A:2616:ARG:HG2  | 2.18                     | 0.44              |
| 1:A:2930:ILE:HG23 | 1:A:3010:LYS:HE3  | 2.00                     | 0.44              |
| 1:A:3273:MET:HA   | 1:A:3276:LEU:HB2  | 1.99                     | 0.44              |
| 1:B:765:SER:HA    | 1:B:779:PHE:O     | 2.18                     | 0.44              |
| 1:B:2580:LEU:HD23 | 1:B:2581:ARG:N    | 2.33                     | 0.44              |
| 1:B:2674:GLY:HA2  | 1:B:2978:HIS:CE1  | 2.52                     | 0.44              |
| 1:B:2791:ARG:O    | 1:B:2793:ARG:NH2  | 2.50                     | 0.44              |
| 1:B:3233:HIS:HA   | 1:B:3236:GLU:HG2  | 2.00                     | 0.44              |
| 1:B:4004:VAL:HA   | 1:B:4118:PHE:CZ   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4004:VAL:HA   | 1:B:4118:PHE:HZ   | 1.81                     | 0.44              |
| 1:C:3608:LEU:H    | 1:C:3608:LEU:HD23 | 1.83                     | 0.44              |
| 1:D:508:TYR:CE1   | 1:D:517:VAL:HG11  | 2.53                     | 0.44              |
| 1:D:897:LYS:HA    | 1:D:900:LEU:HD12  | 1.98                     | 0.44              |
| 1:D:1035:TYR:CZ   | 1:D:1043:LYS:HB2  | 2.53                     | 0.44              |
| 1:D:1718:ARG:NE   | 1:D:1758:ARG:HD3  | 2.32                     | 0.44              |
| 1:D:2613:HIS:HA   | 1:D:2616:ARG:NE   | 2.33                     | 0.44              |
| 1:D:2614:TYR:CE2  | 1:D:2672:VAL:HG22 | 2.52                     | 0.44              |
| 1:D:2681:MET:HE1  | 1:D:2917:ILE:HA   | 1.99                     | 0.44              |
| 1:D:2791:ARG:O    | 1:D:2793:ARG:NH2  | 2.50                     | 0.44              |
| 1:D:2894:LYS:O    | 1:D:2898:ILE:HG12 | 2.17                     | 0.44              |
| 1:D:3213:LYS:HA   | 1:D:3216:GLU:HG3  | 1.99                     | 0.44              |
| 1:D:4177:VAL:HB   | 1:D:4880:VAL:HG22 | 2.00                     | 0.44              |
| 1:A:826:VAL:HG21  | 1:A:832:LEU:HB2   | 1.99                     | 0.44              |
| 1:A:1115:VAL:HG11 | 1:A:1162:VAL:HG11 | 2.00                     | 0.44              |
| 1:A:2114:GLU:HG2  | 1:A:2115:ASP:N    | 2.32                     | 0.44              |
| 1:A:2619:LYS:HZ1  | 1:A:2627:TRP:CG   | 2.35                     | 0.44              |
| 1:A:3099:VAL:O    | 1:A:3103:PRO:HG2  | 2.17                     | 0.44              |
| 1:A:3975:GLN:O    | 1:A:3979:VAL:HG23 | 2.17                     | 0.44              |
| 1:B:308:LEU:HD23  | 1:B:368:THR:HG21  | 1.99                     | 0.44              |
| 1:B:1156:TRP:HB2  | 1:B:1160:ASP:HB2  | 2.00                     | 0.44              |
| 1:B:2930:ILE:HG23 | 1:B:3010:LYS:HE3  | 2.00                     | 0.44              |
| 1:B:2936:ALA:HA   | 1:B:2939:TYR:HD2  | 1.83                     | 0.44              |
| 1:B:3853:ASP:OD1  | 1:B:3854:PHE:N    | 2.50                     | 0.44              |
| 1:C:654:SER:O     | 1:C:655:MET:HE2   | 2.18                     | 0.44              |
| 1:C:1557:LEU:HD22 | 1:C:1566:LEU:HD23 | 2.00                     | 0.44              |
| 1:C:1963:LYS:HA   | 1:C:1966:ARG:HE   | 1.83                     | 0.44              |
| 1:C:2353:ILE:HG23 | 1:C:2359:ARG:HB3  | 1.99                     | 0.44              |
| 1:C:2604:LYS:HD3  | 1:C:2664:LEU:HD13 | 2.00                     | 0.44              |
| 1:C:3695:MET:HB3  | 1:C:3731:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:4831:ILE:HD12 | 1:C:4843:ARG:HH21 | 1.82                     | 0.44              |
| 1:D:679:VAL:HA    | 1:D:800:VAL:HG12  | 1.98                     | 0.44              |
| 1:D:1446:ILE:HG12 | 1:D:1542:ALA:HB2  | 1.99                     | 0.44              |
| 1:D:1825:PHE:CE1  | 1:D:1842:ILE:HG12 | 2.53                     | 0.44              |
| 1:D:2586:GLN:HA   | 1:D:2589:LEU:HD12 | 1.98                     | 0.44              |
| 1:D:2612:ASN:O    | 1:D:2616:ARG:HG2  | 2.18                     | 0.44              |
| 1:D:2857:LYS:HA   | 1:D:2860:LEU:HG   | 1.99                     | 0.44              |
| 1:D:3050:LEU:HD23 | 1:D:3053:VAL:HG23 | 1.98                     | 0.44              |
| 1:D:3273:MET:HA   | 1:D:3276:LEU:HB2  | 1.99                     | 0.44              |
| 1:D:4174:PHE:HA   | 1:D:4880:VAL:HG21 | 1.99                     | 0.44              |
| 1:D:4908:HIS:CE1  | 1:D:4913:HIS:ND1  | 2.85                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:869:THR:HB    | 1:A:941:LYS:HB3   | 1.98                     | 0.44              |
| 1:A:2980:LEU:O    | 1:A:2984:SER:N    | 2.50                     | 0.44              |
| 1:A:3043:ARG:HG2  | 1:A:3047:LYS:NZ   | 2.33                     | 0.44              |
| 1:A:3233:HIS:HA   | 1:A:3236:GLU:HG2  | 2.00                     | 0.44              |
| 1:A:4831:ILE:HD12 | 1:A:4843:ARG:HH21 | 1.82                     | 0.44              |
| 1:A:4908:HIS:CE1  | 1:A:4913:HIS:ND1  | 2.85                     | 0.44              |
| 1:B:826:VAL:HG21  | 1:B:832:LEU:HB2   | 1.99                     | 0.44              |
| 1:B:1035:TYR:CZ   | 1:B:1043:LYS:HB2  | 2.53                     | 0.44              |
| 1:B:1825:PHE:CE1  | 1:B:1842:ILE:HG12 | 2.53                     | 0.44              |
| 1:B:1963:LYS:HA   | 1:B:1966:ARG:HE   | 1.83                     | 0.44              |
| 1:B:2610:LEU:HD12 | 1:B:2614:TYR:HE2  | 1.82                     | 0.44              |
| 1:B:3046:MET:SD   | 1:B:3058:ARG:NH2  | 2.89                     | 0.44              |
| 1:B:3608:LEU:HD23 | 1:B:3608:LEU:H    | 1.83                     | 0.44              |
| 1:B:4089:GLU:OE1  | 1:B:4089:GLU:N    | 2.48                     | 0.44              |
| 1:C:1446:ILE:HG12 | 1:C:1542:ALA:HB2  | 1.99                     | 0.44              |
| 1:C:1825:PHE:CE1  | 1:C:1842:ILE:HG12 | 2.53                     | 0.44              |
| 1:C:3043:ARG:HG2  | 1:C:3047:LYS:NZ   | 2.33                     | 0.44              |
| 1:C:4264:LEU:HG   | 1:C:4268:MET:HE3  | 1.99                     | 0.44              |
| 1:D:467:ASP:OD1   | 1:D:468:GLU:N     | 2.51                     | 0.44              |
| 1:D:2115:ASP:OD1  | 1:D:2152:ASN:ND2  | 2.51                     | 0.44              |
| 1:D:4274:MET:HE2  | 1:D:4274:MET:HB2  | 1.70                     | 0.44              |
| 1:A:1446:ILE:HG12 | 1:A:1542:ALA:HB2  | 1.99                     | 0.44              |
| 1:A:1614:ARG:HG2  | 1:A:1615:GLN:NE2  | 2.33                     | 0.44              |
| 1:A:2062:ILE:HG21 | 1:A:2087:LEU:HG   | 2.00                     | 0.44              |
| 1:A:2790:GLU:O    | 1:A:2902:ALA:N    | 2.41                     | 0.44              |
| 1:A:2824:ARG:HH11 | 1:A:2825:ALA:H    | 1.65                     | 0.44              |
| 1:A:2852:TRP:HA   | 1:A:2855:LYS:HE3  | 2.00                     | 0.44              |
| 1:A:2894:LYS:O    | 1:A:2898:ILE:HG12 | 2.17                     | 0.44              |
| 1:B:1115:VAL:HG11 | 1:B:1162:VAL:HG11 | 2.00                     | 0.44              |
| 1:B:2114:GLU:HG2  | 1:B:2115:ASP:N    | 2.32                     | 0.44              |
| 1:B:2673:ALA:HB1  | 1:B:2974:TYR:CD1  | 2.53                     | 0.44              |
| 1:B:3272:HIS:O    | 1:B:3276:LEU:HG   | 2.17                     | 0.44              |
| 1:B:3290:ILE:HG13 | 1:B:3291:ASP:N    | 2.33                     | 0.44              |
| 1:B:3728:GLN:HG2  | 1:B:3765:ILE:HA   | 2.00                     | 0.44              |
| 1:C:58:VAL:HG13   | 1:C:319:LYS:HG2   | 1.98                     | 0.44              |
| 1:C:198:ASN:OD1   | 1:C:199:GLY:N     | 2.50                     | 0.44              |
| 1:C:447:LEU:O     | 1:C:449:ILE:N     | 2.50                     | 0.44              |
| 1:C:1438:PRO:HB3  | 1:C:1505:LEU:HD23 | 1.99                     | 0.44              |
| 1:C:2852:TRP:HA   | 1:C:2855:LYS:HE3  | 2.00                     | 0.44              |
| 1:C:2894:LYS:O    | 1:C:2898:ILE:HG12 | 2.17                     | 0.44              |
| 1:C:3853:ASP:OD1  | 1:C:3854:PHE:N    | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4004:VAL:HA   | 1:C:4118:PHE:CZ   | 2.53                     | 0.44              |
| 1:C:4155:SER:O    | 1:C:4159:GLN:HG2  | 2.18                     | 0.44              |
| 1:C:4174:PHE:HA   | 1:C:4880:VAL:HG21 | 1.99                     | 0.44              |
| 1:D:1152:TYR:HD1  | 1:D:1184:ASP:HA   | 1.82                     | 0.44              |
| 1:D:1512:ASP:O    | 1:D:1516:GLY:N    | 2.44                     | 0.44              |
| 1:D:1614:ARG:HG2  | 1:D:1615:GLN:NE2  | 2.33                     | 0.44              |
| 1:D:2936:ALA:HA   | 1:D:2939:TYR:HD2  | 1.83                     | 0.44              |
| 1:D:3314:LEU:HA   | 1:D:3318:HIS:ND1  | 2.32                     | 0.44              |
| 1:A:1694:MET:SD   | 1:A:1695:PRO:HD2  | 2.58                     | 0.44              |
| 1:A:1825:PHE:CE1  | 1:A:1842:ILE:HG12 | 2.53                     | 0.44              |
| 1:A:1963:LYS:HA   | 1:A:1966:ARG:HE   | 1.83                     | 0.44              |
| 1:A:2681:MET:HE1  | 1:A:2917:ILE:HA   | 1.99                     | 0.44              |
| 1:A:2768:LYS:O    | 1:A:2772:ARG:N    | 2.47                     | 0.44              |
| 1:A:2878:THR:O    | 1:A:2882:LYS:HG3  | 2.17                     | 0.44              |
| 1:A:3046:MET:SD   | 1:A:3058:ARG:NH2  | 2.89                     | 0.44              |
| 1:A:3314:LEU:HA   | 1:A:3318:HIS:ND1  | 2.32                     | 0.44              |
| 1:B:44:ASN:ND2    | 1:B:46:LEU:HB2    | 2.33                     | 0.44              |
| 1:B:1438:PRO:HB3  | 1:B:1505:LEU:HD23 | 1.99                     | 0.44              |
| 1:B:2258:ARG:HB3  | 1:B:2260:PRO:HD2  | 1.99                     | 0.44              |
| 1:B:3940:LEU:HD11 | 1:B:3981:MET:HE1  | 2.00                     | 0.44              |
| 1:C:679:VAL:HA    | 1:C:800:VAL:HG12  | 1.98                     | 0.44              |
| 1:C:1732:GLU:HB2  | 1:C:1753:LEU:HD21 | 2.00                     | 0.44              |
| 1:C:2593:VAL:HG12 | 1:C:2644:LEU:HD22 | 1.98                     | 0.44              |
| 1:C:2714:PRO:HD2  | 1:C:2717:LEU:HB2  | 1.99                     | 0.44              |
| 1:C:2794:GLU:HA   | 1:C:2797:SER:OG   | 2.18                     | 0.44              |
| 1:C:2824:ARG:HH11 | 1:C:2825:ALA:H    | 1.65                     | 0.44              |
| 1:C:3210:SER:H    | 1:C:3213:LYS:NZ   | 2.16                     | 0.44              |
| 1:C:3290:ILE:HG13 | 1:C:3291:ASP:N    | 2.33                     | 0.44              |
| 1:D:308:LEU:HD23  | 1:D:368:THR:HG21  | 1.99                     | 0.44              |
| 1:D:988:LEU:HB2   | 1:D:1055:ARG:NE   | 2.27                     | 0.44              |
| 1:D:1058:LEU:HG   | 1:D:1064:LEU:H    | 1.82                     | 0.44              |
| 1:D:1292:SER:O    | 1:D:1295:SER:OG   | 2.36                     | 0.44              |
| 1:D:2794:GLU:HA   | 1:D:2797:SER:OG   | 2.18                     | 0.44              |
| 1:D:3043:ARG:HG2  | 1:D:3047:LYS:NZ   | 2.33                     | 0.44              |
| 1:D:3650:GLU:CD   | 1:D:3660:ARG:HH21 | 2.26                     | 0.44              |
| 1:D:3975:GLN:O    | 1:D:3979:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:28:ILE:HD11   | 1:A:201:LEU:HD11  | 2.00                     | 0.44              |
| 1:A:29:HIS:CE1    | 1:A:31:GLU:HG2    | 2.53                     | 0.44              |
| 1:A:1427:TYR:HB2  | 1:A:1563:VAL:HG11 | 2.00                     | 0.44              |
| 1:A:1718:ARG:NE   | 1:A:1758:ARG:HD3  | 2.32                     | 0.44              |
| 1:A:2258:ARG:HB3  | 1:A:2260:PRO:HD2  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2580:LEU:HD23 | 1:A:2581:ARG:N    | 2.32                     | 0.44              |
| 1:A:2714:PRO:HD2  | 1:A:2717:LEU:HB2  | 1.99                     | 0.44              |
| 1:A:4177:VAL:HB   | 1:A:4880:VAL:HG22 | 2.00                     | 0.44              |
| 1:A:4617:ILE:HA   | 1:A:4665:ARG:HH12 | 1.82                     | 0.44              |
| 2:E:26:HIS:CD2    | 2:E:46:PRO:HA     | 2.53                     | 0.44              |
| 1:B:28:ILE:HD11   | 1:B:201:LEU:HD11  | 2.00                     | 0.44              |
| 1:B:928:GLU:O     | 1:B:932:ASN:ND2   | 2.50                     | 0.44              |
| 1:B:1113:MET:HB2  | 1:B:1156:TRP:HZ2  | 1.83                     | 0.44              |
| 1:B:1614:ARG:HG2  | 1:B:1615:GLN:NE2  | 2.33                     | 0.44              |
| 1:B:2585:MET:HE3  | 1:B:2616:ARG:NH2  | 2.21                     | 0.44              |
| 1:B:2794:GLU:HA   | 1:B:2797:SER:OG   | 2.18                     | 0.44              |
| 1:B:2857:LYS:HA   | 1:B:2860:LEU:HG   | 1.99                     | 0.44              |
| 1:B:3293:GLY:N    | 1:B:3296:MET:HE1  | 2.32                     | 0.44              |
| 1:B:3713:SER:OG   | 1:B:3716:GLU:OE1  | 2.29                     | 0.44              |
| 1:C:548:CYS:HB3   | 1:C:582:SER:HB2   | 2.00                     | 0.44              |
| 1:C:765:SER:HA    | 1:C:779:PHE:O     | 2.18                     | 0.44              |
| 1:C:2258:ARG:HB3  | 1:C:2260:PRO:HD2  | 1.99                     | 0.44              |
| 1:C:2612:ASN:O    | 1:C:2616:ARG:HG2  | 2.18                     | 0.44              |
| 1:C:2957:GLU:O    | 1:C:2960:ILE:HG22 | 2.18                     | 0.44              |
| 1:C:3940:LEU:HD11 | 1:C:3981:MET:HE1  | 2.00                     | 0.44              |
| 1:C:4291:PHE:CZ   | 1:C:4295:LEU:HD11 | 2.53                     | 0.44              |
| 1:C:4617:ILE:HA   | 1:C:4665:ARG:HH12 | 1.83                     | 0.44              |
| 1:C:4625:ASP:OD1  | 1:C:4625:ASP:N    | 2.46                     | 0.44              |
| 1:D:44:ASN:ND2    | 1:D:46:LEU:HB2    | 2.33                     | 0.44              |
| 1:D:765:SER:HA    | 1:D:779:PHE:O     | 2.18                     | 0.44              |
| 1:D:1718:ARG:HH21 | 1:D:1758:ARG:NH1  | 2.15                     | 0.44              |
| 1:D:2415:GLU:OE1  | 1:D:2418:ARG:NH1  | 2.51                     | 0.44              |
| 1:D:2674:GLY:HA2  | 1:D:2978:HIS:CE1  | 2.52                     | 0.44              |
| 1:D:4898:PHE:O    | 1:D:4904:GLY:HA3  | 2.18                     | 0.44              |
| 1:A:44:ASN:ND2    | 1:A:46:LEU:HB2    | 2.33                     | 0.43              |
| 1:A:376:SER:O     | 1:A:376:SER:OG    | 2.36                     | 0.43              |
| 1:A:467:ASP:OD1   | 1:A:468:GLU:N     | 2.51                     | 0.43              |
| 1:A:508:TYR:CE1   | 1:A:517:VAL:HG11  | 2.53                     | 0.43              |
| 1:A:2678:PRO:HB3  | 1:A:2922:ALA:HB2  | 2.00                     | 0.43              |
| 1:A:2957:GLU:HA   | 1:A:2960:ILE:HG22 | 1.99                     | 0.43              |
| 1:A:4507:LEU:HD12 | 1:A:4507:LEU:HA   | 1.79                     | 0.43              |
| 1:B:392:ILE:HG13  | 1:B:393:MET:H     | 1.83                     | 0.43              |
| 1:B:447:LEU:O     | 1:B:449:ILE:N     | 2.50                     | 0.43              |
| 1:B:548:CYS:HB3   | 1:B:582:SER:HB2   | 2.00                     | 0.43              |
| 1:B:654:SER:O     | 1:B:655:MET:HE2   | 2.18                     | 0.43              |
| 1:B:2878:THR:O    | 1:B:2882:LYS:HG3  | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2972:ASP:O    | 1:B:2976:LYS:HG3  | 2.18                     | 0.43              |
| 1:B:4155:SER:O    | 1:B:4159:GLN:HG2  | 2.18                     | 0.43              |
| 1:B:4617:ILE:HA   | 1:B:4665:ARG:HH12 | 1.83                     | 0.43              |
| 1:C:44:ASN:ND2    | 1:C:46:LEU:HB2    | 2.33                     | 0.43              |
| 1:C:508:TYR:CE1   | 1:C:517:VAL:HG11  | 2.53                     | 0.43              |
| 1:C:785:ASP:OD1   | 1:C:786:GLY:N     | 2.51                     | 0.43              |
| 1:C:1292:SER:O    | 1:C:1295:SER:OG   | 2.36                     | 0.43              |
| 1:C:1614:ARG:HG2  | 1:C:1615:GLN:NE2  | 2.33                     | 0.43              |
| 1:C:1694:MET:SD   | 1:C:1695:PRO:HD2  | 2.58                     | 0.43              |
| 1:C:1718:ARG:HH21 | 1:C:1758:ARG:NH1  | 2.15                     | 0.43              |
| 1:C:2894:LYS:HA   | 1:C:2897:GLN:HG3  | 2.00                     | 0.43              |
| 1:D:2787:TRP:HD1  | 1:D:2905:ARG:HA   | 1.83                     | 0.43              |
| 1:D:2905:ARG:HE   | 1:D:2906:GLY:N    | 2.03                     | 0.43              |
| 1:D:2957:GLU:O    | 1:D:2960:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:731:HIS:HB3   | 1:A:738:ALA:HB1   | 2.00                     | 0.43              |
| 1:A:1284:LYS:HZ3  | 1:A:1286:THR:HB   | 1.82                     | 0.43              |
| 1:A:2332:GLY:O    | 1:A:2336:ARG:HG3  | 2.18                     | 0.43              |
| 1:A:2386:ASN:HA   | 1:A:2389:MET:HE3  | 1.99                     | 0.43              |
| 1:A:2857:LYS:HA   | 1:A:2860:LEU:HG   | 1.99                     | 0.43              |
| 1:A:3008:PHE:CE2  | 1:A:3060:PHE:HE2  | 2.37                     | 0.43              |
| 1:A:3293:GLY:N    | 1:A:3296:MET:HE1  | 2.32                     | 0.43              |
| 1:A:3608:LEU:HD23 | 1:A:3608:LEU:H    | 1.83                     | 0.43              |
| 1:A:4021:LEU:HD22 | 1:A:4128:TYR:CE2  | 2.53                     | 0.43              |
| 1:A:4264:LEU:HG   | 1:A:4268:MET:HE3  | 1.99                     | 0.43              |
| 1:B:370:LEU:HD23  | 1:B:395:HIS:HA    | 2.01                     | 0.43              |
| 1:B:508:TYR:CE1   | 1:B:517:VAL:HG11  | 2.53                     | 0.43              |
| 1:B:731:HIS:HB3   | 1:B:738:ALA:HB1   | 2.00                     | 0.43              |
| 1:B:1292:SER:O    | 1:B:1295:SER:OG   | 2.36                     | 0.43              |
| 1:B:2332:GLY:O    | 1:B:2336:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:2612:ASN:O    | 1:B:2616:ARG:HG2  | 2.18                     | 0.43              |
| 1:B:2713:ILE:HG22 | 1:B:2779:LEU:HD21 | 1.98                     | 0.43              |
| 1:B:2929:LEU:HD11 | 1:B:2967:VAL:HG13 | 2.00                     | 0.43              |
| 1:B:3277:LEU:O    | 1:B:3281:LEU:HG   | 2.18                     | 0.43              |
| 1:B:3920:LEU:HD22 | 1:B:3935:LEU:HD11 | 2.00                     | 0.43              |
| 1:C:1113:MET:HB2  | 1:C:1156:TRP:HZ2  | 1.83                     | 0.43              |
| 1:C:2482:ASP:O    | 1:C:2485:LEU:HG   | 2.18                     | 0.43              |
| 1:C:2580:LEU:HD23 | 1:C:2581:ARG:N    | 2.33                     | 0.43              |
| 1:C:2581:ARG:HG3  | 1:C:2583:SER:H    | 1.83                     | 0.43              |
| 1:C:2593:VAL:HG12 | 1:C:2644:LEU:HD13 | 1.99                     | 0.43              |
| 1:C:2936:ALA:HA   | 1:C:2939:TYR:HD2  | 1.83                     | 0.43              |
| 1:C:2957:GLU:HA   | 1:C:2960:ILE:HG22 | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3277:LEU:O    | 1:C:3281:LEU:HG   | 2.18                     | 0.43              |
| 1:C:4898:PHE:O    | 1:C:4904:GLY:HA3  | 2.18                     | 0.43              |
| 1:D:370:LEU:HD23  | 1:D:395:HIS:HA    | 2.00                     | 0.43              |
| 1:D:1115:VAL:HG11 | 1:D:1162:VAL:HG11 | 2.00                     | 0.43              |
| 1:D:2157:GLN:O    | 1:D:3615:ARG:NH2  | 2.25                     | 0.43              |
| 1:D:2604:LYS:HD3  | 1:D:2664:LEU:HD13 | 2.00                     | 0.43              |
| 1:D:2619:LYS:HZ1  | 1:D:2627:TRP:CG   | 2.35                     | 0.43              |
| 1:D:3210:SER:H    | 1:D:3213:LYS:NZ   | 2.16                     | 0.43              |
| 1:A:308:LEU:HD23  | 1:A:368:THR:HG21  | 1.99                     | 0.43              |
| 1:A:548:CYS:HB3   | 1:A:582:SER:HB2   | 2.00                     | 0.43              |
| 1:A:2936:ALA:HA   | 1:A:2939:TYR:HD2  | 1.83                     | 0.43              |
| 1:A:4116:GLN:O    | 1:A:4120:GLU:OE1  | 2.36                     | 0.43              |
| 1:B:467:ASP:OD1   | 1:B:468:GLU:N     | 2.51                     | 0.43              |
| 1:B:655:MET:HG3   | 1:B:1619:VAL:HG11 | 2.01                     | 0.43              |
| 1:B:2115:ASP:OD1  | 1:B:2152:ASN:ND2  | 2.51                     | 0.43              |
| 1:B:2957:GLU:HA   | 1:B:2960:ILE:HG22 | 1.99                     | 0.43              |
| 1:B:3043:ARG:HG3  | 1:B:3120:ASP:CG   | 2.44                     | 0.43              |
| 1:B:4792:PHE:HB3  | 1:B:4843:ARG:NH2  | 2.33                     | 0.43              |
| 1:C:1115:VAL:HG11 | 1:C:1162:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:2415:GLU:OE1  | 1:C:2418:ARG:NH1  | 2.51                     | 0.43              |
| 1:C:2581:ARG:HB3  | 1:C:2584:MET:CE   | 2.48                     | 0.43              |
| 1:C:2673:ALA:HB1  | 1:C:2974:TYR:CD1  | 2.53                     | 0.43              |
| 1:C:2873:PRO:O    | 1:C:2877:LEU:HG   | 2.19                     | 0.43              |
| 1:C:3106:SER:O    | 1:C:3110:GLU:HG2  | 2.18                     | 0.43              |
| 1:D:537:LEU:O     | 1:D:541:ILE:HG12  | 2.19                     | 0.43              |
| 1:D:654:SER:O     | 1:D:655:MET:HE2   | 2.18                     | 0.43              |
| 1:D:3046:MET:SD   | 1:D:3058:ARG:NH2  | 2.89                     | 0.43              |
| 1:D:3106:SER:O    | 1:D:3110:GLU:HG2  | 2.18                     | 0.43              |
| 1:D:3213:LYS:O    | 1:D:3216:GLU:HG3  | 2.19                     | 0.43              |
| 1:D:3920:LEU:HD22 | 1:D:3935:LEU:HD11 | 2.01                     | 0.43              |
| 1:D:4004:VAL:HA   | 1:D:4118:PHE:CZ   | 2.53                     | 0.43              |
| 1:D:4116:GLN:O    | 1:D:4120:GLU:OE1  | 2.36                     | 0.43              |
| 1:D:4831:ILE:HD12 | 1:D:4843:ARG:HH21 | 1.82                     | 0.43              |
| 1:A:392:ILE:HG13  | 1:A:393:MET:H     | 1.83                     | 0.43              |
| 1:A:785:ASP:OD1   | 1:A:786:GLY:N     | 2.51                     | 0.43              |
| 1:A:1438:PRO:HB3  | 1:A:1505:LEU:HD23 | 1.99                     | 0.43              |
| 1:A:2619:LYS:HA   | 1:A:2622:CYS:SG   | 2.58                     | 0.43              |
| 1:A:2674:GLY:HA2  | 1:A:2978:HIS:CE1  | 2.52                     | 0.43              |
| 1:A:3213:LYS:HA   | 1:A:3216:GLU:HG3  | 1.99                     | 0.43              |
| 1:A:4004:VAL:HA   | 1:A:4118:PHE:CZ   | 2.53                     | 0.43              |
| 1:A:4089:GLU:OE1  | 1:A:4089:GLU:N    | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:26:HIS:CD2    | 2:H:46:PRO:HA     | 2.53                     | 0.43              |
| 1:B:188:SER:HB2   | 1:B:190:ARG:NH1   | 2.30                     | 0.43              |
| 1:B:1446:ILE:HG12 | 1:B:1542:ALA:HB2  | 1.99                     | 0.43              |
| 1:B:2605:MET:HB3  | 1:B:2606:PRO:HD3  | 2.00                     | 0.43              |
| 1:B:2894:LYS:O    | 1:B:2898:ILE:HG12 | 2.17                     | 0.43              |
| 1:C:392:ILE:HG13  | 1:C:393:MET:H     | 1.83                     | 0.43              |
| 1:C:467:ASP:OD1   | 1:C:468:GLU:N     | 2.51                     | 0.43              |
| 1:C:1289:SER:O    | 1:C:1295:SER:OG   | 2.24                     | 0.43              |
| 1:C:2930:ILE:HG23 | 1:C:3010:LYS:HE3  | 2.00                     | 0.43              |
| 1:C:3213:LYS:O    | 1:C:3216:GLU:HG3  | 2.19                     | 0.43              |
| 1:C:3951:PHE:O    | 1:C:3955:GLN:HG3  | 2.19                     | 0.43              |
| 1:C:4021:LEU:HD22 | 1:C:4128:TYR:CE2  | 2.53                     | 0.43              |
| 1:D:655:MET:HG3   | 1:D:1619:VAL:HG11 | 2.01                     | 0.43              |
| 1:D:826:VAL:HG21  | 1:D:832:LEU:HB2   | 1.99                     | 0.43              |
| 1:D:928:GLU:O     | 1:D:932:ASN:ND2   | 2.50                     | 0.43              |
| 1:D:1113:MET:HB2  | 1:D:1156:TRP:HZ2  | 1.83                     | 0.43              |
| 1:D:1694:MET:SD   | 1:D:1695:PRO:HD2  | 2.58                     | 0.43              |
| 1:D:2258:ARG:HB3  | 1:D:2260:PRO:HD2  | 1.99                     | 0.43              |
| 1:D:2581:ARG:HG3  | 1:D:2583:SER:H    | 1.83                     | 0.43              |
| 1:D:2873:PRO:O    | 1:D:2877:LEU:HG   | 2.19                     | 0.43              |
| 1:D:2930:ILE:HG23 | 1:D:3010:LYS:HE3  | 2.00                     | 0.43              |
| 1:D:3233:HIS:HA   | 1:D:3236:GLU:HG2  | 2.00                     | 0.43              |
| 1:D:4291:PHE:CZ   | 1:D:4295:LEU:HD11 | 2.53                     | 0.43              |
| 1:D:4617:ILE:HA   | 1:D:4665:ARG:HH12 | 1.83                     | 0.43              |
| 1:A:137:ARG:NH2   | 1:A:203:VAL:O     | 2.36                     | 0.43              |
| 1:A:974:SER:HB3   | 1:A:976:TYR:CD2   | 2.52                     | 0.43              |
| 1:A:2620:TYR:HB2  | 1:A:2627:TRP:CZ3  | 2.54                     | 0.43              |
| 1:A:2972:ASP:O    | 1:A:2976:LYS:HG3  | 2.18                     | 0.43              |
| 1:A:4291:PHE:CZ   | 1:A:4295:LEU:HD11 | 2.53                     | 0.43              |
| 2:F:26:HIS:CD2    | 2:F:46:PRO:HA     | 2.53                     | 0.43              |
| 1:B:728:ASP:OD1   | 1:B:731:HIS:N     | 2.41                     | 0.43              |
| 1:B:1282:CYS:SG   | 1:B:1556:GLU:HG3  | 2.58                     | 0.43              |
| 1:B:1427:TYR:HB2  | 1:B:1563:VAL:HG11 | 2.00                     | 0.43              |
| 1:B:2581:ARG:HB3  | 1:B:2584:MET:CE   | 2.48                     | 0.43              |
| 1:B:3008:PHE:CE2  | 1:B:3060:PHE:HE2  | 2.37                     | 0.43              |
| 1:B:3043:ARG:HG2  | 1:B:3047:LYS:NZ   | 2.33                     | 0.43              |
| 1:B:3254:PRO:HB3  | 1:B:3258:PRO:HA   | 2.00                     | 0.43              |
| 1:B:3273:MET:HA   | 1:B:3276:LEU:HB2  | 1.99                     | 0.43              |
| 1:B:3650:GLU:CD   | 1:B:3660:ARG:HH21 | 2.26                     | 0.43              |
| 1:B:3695:MET:HB3  | 1:B:3731:LEU:HD11 | 1.99                     | 0.43              |
| 1:B:4177:VAL:HB   | 1:B:4880:VAL:HG22 | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4605:GLU:HB3  | 1:B:4609:LYS:NZ   | 2.34                     | 0.43              |
| 1:C:537:LEU:O     | 1:C:541:ILE:HG12  | 2.19                     | 0.43              |
| 1:C:1035:TYR:CZ   | 1:C:1043:LYS:HB2  | 2.53                     | 0.43              |
| 1:C:1219:LYS:HZ3  | 1:C:1245:ARG:C    | 2.26                     | 0.43              |
| 1:C:3233:HIS:HA   | 1:C:3236:GLU:HG2  | 2.00                     | 0.43              |
| 1:D:548:CYS:HB3   | 1:D:582:SER:HB2   | 2.00                     | 0.43              |
| 1:D:2332:GLY:O    | 1:D:2336:ARG:HG3  | 2.18                     | 0.43              |
| 1:D:2714:PRO:HD2  | 1:D:2717:LEU:HB2  | 1.99                     | 0.43              |
| 1:A:896:ASN:HA    | 1:A:899:GLU:CD    | 2.44                     | 0.43              |
| 1:A:1292:SER:O    | 1:A:1295:SER:OG   | 2.36                     | 0.43              |
| 1:A:3098:THR:OG1  | 1:A:3147:TYR:OH   | 2.12                     | 0.43              |
| 1:A:3920:LEU:HD22 | 1:A:3935:LEU:HD11 | 2.00                     | 0.43              |
| 1:A:4023:LEU:HD12 | 1:A:4026:LEU:HD23 | 2.00                     | 0.43              |
| 1:B:29:HIS:CE1    | 1:B:31:GLU:HG2    | 2.53                     | 0.43              |
| 1:B:1308:ILE:HD12 | 1:B:1445:TRP:CH2  | 2.54                     | 0.43              |
| 1:B:2873:PRO:O    | 1:B:2877:LEU:HG   | 2.19                     | 0.43              |
| 1:B:4023:LEU:HD12 | 1:B:4026:LEU:HD23 | 2.01                     | 0.43              |
| 1:C:1538:LYS:NZ   | 1:C:1636:ASN:OD1  | 2.52                     | 0.43              |
| 1:C:2593:VAL:HA   | 1:C:2644:LEU:HD13 | 2.01                     | 0.43              |
| 1:C:2619:LYS:HA   | 1:C:2622:CYS:SG   | 2.58                     | 0.43              |
| 1:C:2787:TRP:HD1  | 1:C:2905:ARG:HA   | 1.83                     | 0.43              |
| 1:C:2857:LYS:HA   | 1:C:2860:LEU:HG   | 1.99                     | 0.43              |
| 1:C:3273:MET:HA   | 1:C:3276:LEU:HB2  | 1.99                     | 0.43              |
| 1:C:3728:GLN:HG2  | 1:C:3765:ILE:HA   | 2.00                     | 0.43              |
| 1:C:3858:LEU:HD23 | 1:C:3858:LEU:HA   | 1.88                     | 0.43              |
| 1:C:4116:GLN:O    | 1:C:4120:GLU:OE1  | 2.36                     | 0.43              |
| 1:D:28:ILE:HD11   | 1:D:201:LEU:HD11  | 2.00                     | 0.43              |
| 1:D:785:ASP:OD1   | 1:D:786:GLY:N     | 2.51                     | 0.43              |
| 1:D:2768:LYS:O    | 1:D:2772:ARG:N    | 2.47                     | 0.43              |
| 1:D:2824:ARG:HH11 | 1:D:2825:ALA:H    | 1.65                     | 0.43              |
| 1:D:2868:HIS:HB3  | 1:D:2871:LEU:HB3  | 2.01                     | 0.43              |
| 1:A:2593:VAL:HG12 | 1:A:2644:LEU:HD13 | 1.99                     | 0.43              |
| 1:A:2794:GLU:HA   | 1:A:2797:SER:OG   | 2.18                     | 0.43              |
| 1:A:2957:GLU:O    | 1:A:2960:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:3650:GLU:CD   | 1:A:3660:ARG:HH21 | 2.26                     | 0.43              |
| 1:A:3713:SER:OG   | 1:A:3716:GLU:OE1  | 2.28                     | 0.43              |
| 1:A:3728:GLN:HG2  | 1:A:3765:ILE:HA   | 2.00                     | 0.43              |
| 1:B:1732:GLU:HB2  | 1:B:1753:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:3018:ARG:HD3  | 1:B:3021:LEU:HD22 | 2.01                     | 0.43              |
| 1:B:3213:LYS:O    | 1:B:3216:GLU:HG3  | 2.18                     | 0.43              |
| 1:B:3255:GLU:HB3  | 1:B:3269:ASN:HA   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3306:ILE:HA   | 1:B:3309:LYS:HE2  | 2.01                     | 0.43              |
| 1:B:3329:LYS:HD3  | 1:B:3329:LYS:HA   | 1.86                     | 0.43              |
| 1:B:3951:PHE:O    | 1:B:3955:GLN:HG3  | 2.18                     | 0.43              |
| 1:B:4021:LEU:HD22 | 1:B:4128:TYR:CE2  | 2.53                     | 0.43              |
| 1:B:4264:LEU:HG   | 1:B:4268:MET:HE3  | 1.99                     | 0.43              |
| 1:C:29:HIS:CE1    | 1:C:31:GLU:HG2    | 2.53                     | 0.43              |
| 1:C:137:ARG:NH2   | 1:C:202:HIS:HB3   | 2.34                     | 0.43              |
| 1:C:308:LEU:HD23  | 1:C:368:THR:HG21  | 1.99                     | 0.43              |
| 1:C:2115:ASP:OD1  | 1:C:2152:ASN:ND2  | 2.51                     | 0.43              |
| 1:C:2332:GLY:O    | 1:C:2336:ARG:HG3  | 2.18                     | 0.43              |
| 1:C:2929:LEU:HD11 | 1:C:2967:VAL:HG13 | 2.00                     | 0.43              |
| 1:C:3018:ARG:HD3  | 1:C:3021:LEU:HD22 | 2.01                     | 0.43              |
| 1:C:3238:ILE:O    | 1:C:3242:LEU:N    | 2.29                     | 0.43              |
| 1:C:3306:ILE:HA   | 1:C:3309:LYS:HE2  | 2.01                     | 0.43              |
| 1:C:3650:GLU:CD   | 1:C:3660:ARG:HH21 | 2.26                     | 0.43              |
| 1:D:29:HIS:CE1    | 1:D:31:GLU:HG2    | 2.53                     | 0.43              |
| 1:D:198:ASN:OD1   | 1:D:199:GLY:N     | 2.50                     | 0.43              |
| 1:D:392:ILE:HG13  | 1:D:393:MET:H     | 1.84                     | 0.43              |
| 1:D:1156:TRP:HB2  | 1:D:1160:ASP:HB2  | 2.00                     | 0.43              |
| 1:D:1438:PRO:HB3  | 1:D:1505:LEU:HD23 | 1.99                     | 0.43              |
| 1:D:2386:ASN:HA   | 1:D:2389:MET:HE3  | 1.99                     | 0.43              |
| 1:D:2581:ARG:HB3  | 1:D:2584:MET:CE   | 2.48                     | 0.43              |
| 1:D:3608:LEU:HD23 | 1:D:3608:LEU:H    | 1.83                     | 0.43              |
| 1:A:27:THR:HA     | 1:A:31:GLU:O      | 2.19                     | 0.43              |
| 1:A:654:SER:O     | 1:A:655:MET:HE2   | 2.18                     | 0.43              |
| 1:A:827:LEU:HD23  | 1:A:827:LEU:HA    | 1.86                     | 0.43              |
| 1:A:947:GLY:C     | 1:A:1067:PRO:HB3  | 2.44                     | 0.43              |
| 1:A:2178:VAL:HG11 | 1:A:2192:MET:HE1  | 2.00                     | 0.43              |
| 1:A:2415:GLU:OE1  | 1:A:2418:ARG:NH1  | 2.51                     | 0.43              |
| 1:A:2868:HIS:HB3  | 1:A:2871:LEU:HB3  | 2.01                     | 0.43              |
| 1:A:3255:GLU:HB3  | 1:A:3269:ASN:HA   | 2.01                     | 0.43              |
| 1:A:4155:SER:O    | 1:A:4159:GLN:HG2  | 2.18                     | 0.43              |
| 1:A:4898:PHE:O    | 1:A:4904:GLY:HA3  | 2.18                     | 0.43              |
| 1:B:448:PRO:HB2   | 1:B:451:SER:OG    | 2.19                     | 0.43              |
| 1:B:712:GLU:HA    | 1:B:838:ARG:HG3   | 2.00                     | 0.43              |
| 1:B:2178:VAL:HG11 | 1:B:2192:MET:HE1  | 2.00                     | 0.43              |
| 1:B:2856:LYS:HG2  | 1:B:2859:GLU:OE1  | 2.19                     | 0.43              |
| 1:B:2893:LEU:O    | 1:B:2896:LEU:HG   | 2.19                     | 0.43              |
| 1:B:2914:THR:N    | 1:B:2915:PRO:HD2  | 2.33                     | 0.43              |
| 1:B:4116:GLN:O    | 1:B:4120:GLU:OE1  | 2.36                     | 0.43              |
| 1:B:4831:ILE:HD12 | 1:B:4843:ARG:HH21 | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:23:GLN:HB3    | 1:C:36:CYS:SG     | 2.59                     | 0.43              |
| 1:C:28:ILE:HD11   | 1:C:201:LEU:HD11  | 2.00                     | 0.43              |
| 1:C:470:LEU:HB2   | 1:C:475:LYS:HG3   | 2.01                     | 0.43              |
| 1:C:968:LYS:HA    | 1:C:971:GLN:HG2   | 2.01                     | 0.43              |
| 1:C:1100:ARG:HB2  | 1:C:1236:TYR:CD1  | 2.54                     | 0.43              |
| 1:C:1427:TYR:HB2  | 1:C:1563:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:1711:LEU:HG   | 1:C:1711:LEU:O    | 2.19                     | 0.43              |
| 1:C:2434:GLY:O    | 1:C:2438:ILE:HG13 | 2.19                     | 0.43              |
| 1:C:2893:LEU:O    | 1:C:2896:LEU:HG   | 2.19                     | 0.43              |
| 1:C:2914:THR:N    | 1:C:2915:PRO:HD2  | 2.33                     | 0.43              |
| 1:C:2972:ASP:O    | 1:C:2976:LYS:HG3  | 2.18                     | 0.43              |
| 1:C:4023:LEU:HD12 | 1:C:4026:LEU:HD23 | 2.00                     | 0.43              |
| 1:D:447:LEU:HD12  | 1:D:447:LEU:HA    | 1.83                     | 0.43              |
| 1:D:1896:MET:O    | 1:D:1896:MET:HG2  | 2.19                     | 0.43              |
| 1:D:2178:VAL:HG11 | 1:D:2192:MET:HE1  | 2.00                     | 0.43              |
| 1:D:2434:GLY:O    | 1:D:2438:ILE:HG13 | 2.19                     | 0.43              |
| 1:D:2589:LEU:HA   | 1:D:2592:LEU:HD12 | 2.01                     | 0.43              |
| 1:D:2593:VAL:HG12 | 1:D:2644:LEU:HD13 | 2.00                     | 0.43              |
| 1:D:2610:LEU:HD12 | 1:D:2614:TYR:CE2  | 2.54                     | 0.43              |
| 1:D:2673:ALA:HB1  | 1:D:2974:TYR:CD1  | 2.53                     | 0.43              |
| 1:D:3277:LEU:O    | 1:D:3281:LEU:HG   | 2.18                     | 0.43              |
| 1:D:3940:LEU:HD11 | 1:D:3981:MET:HE1  | 2.00                     | 0.43              |
| 1:D:4030:ASP:OD1  | 1:D:4031:THR:N    | 2.52                     | 0.43              |
| 1:A:765:SER:HA    | 1:A:779:PHE:O     | 2.18                     | 0.43              |
| 1:A:2115:ASP:OD1  | 1:A:2152:ASN:ND2  | 2.51                     | 0.43              |
| 1:A:2456:MET:CE   | 1:A:2462:PRO:HD3  | 2.46                     | 0.43              |
| 1:A:2482:ASP:O    | 1:A:2485:LEU:HG   | 2.18                     | 0.43              |
| 1:A:2610:LEU:HD12 | 1:A:2614:TYR:CE2  | 2.54                     | 0.43              |
| 1:A:2613:HIS:HA   | 1:A:2616:ARG:NE   | 2.33                     | 0.43              |
| 1:A:2837:LEU:HD11 | 1:A:2903:VAL:HG13 | 2.01                     | 0.43              |
| 1:A:2873:PRO:O    | 1:A:2877:LEU:HG   | 2.19                     | 0.43              |
| 1:A:3290:ILE:HG13 | 1:A:3291:ASP:N    | 2.33                     | 0.43              |
| 1:A:4792:PHE:HB3  | 1:A:4843:ARG:NH2  | 2.33                     | 0.43              |
| 1:B:240:HIS:O     | 1:C:167:LYS:NZ    | 2.27                     | 0.43              |
| 1:B:785:ASP:OD1   | 1:B:786:GLY:N     | 2.51                     | 0.43              |
| 1:B:1100:ARG:HB2  | 1:B:1236:TYR:CD1  | 2.54                     | 0.43              |
| 1:B:2062:ILE:HG21 | 1:B:2087:LEU:HG   | 2.00                     | 0.43              |
| 1:B:2415:GLU:OE1  | 1:B:2418:ARG:NH1  | 2.51                     | 0.43              |
| 1:B:2456:MET:CE   | 1:B:2462:PRO:HD3  | 2.46                     | 0.43              |
| 1:B:2589:LEU:HA   | 1:B:2592:LEU:HD12 | 2.01                     | 0.43              |
| 1:B:2613:HIS:HA   | 1:B:2616:ARG:NE   | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2728:SER:O    | 1:B:2731:LYS:HG3  | 2.19                     | 0.43              |
| 1:B:2868:HIS:HB3  | 1:B:2871:LEU:HB3  | 2.01                     | 0.43              |
| 1:B:3314:LEU:HA   | 1:B:3318:HIS:ND1  | 2.32                     | 0.43              |
| 1:C:655:MET:HG3   | 1:C:1619:VAL:HG11 | 2.01                     | 0.43              |
| 1:C:1088:PHE:CE1  | 1:C:1207:LEU:HD12 | 2.54                     | 0.43              |
| 1:C:2759:PRO:HD2  | 1:C:2762:LEU:HD13 | 2.01                     | 0.43              |
| 1:C:2868:HIS:HB3  | 1:C:2871:LEU:HB3  | 2.01                     | 0.43              |
| 1:C:3920:LEU:HD22 | 1:C:3935:LEU:HD11 | 2.01                     | 0.43              |
| 1:C:4605:GLU:HB3  | 1:C:4609:LYS:NZ   | 2.34                     | 0.43              |
| 1:D:968:LYS:HA    | 1:D:971:GLN:HG2   | 2.01                     | 0.43              |
| 1:D:1282:CYS:SG   | 1:D:1556:GLU:HG3  | 2.58                     | 0.43              |
| 1:D:1711:LEU:HG   | 1:D:1711:LEU:O    | 2.19                     | 0.43              |
| 1:D:1732:GLU:HB2  | 1:D:1753:LEU:HD21 | 2.00                     | 0.43              |
| 1:D:2062:ILE:HG21 | 1:D:2087:LEU:HG   | 2.00                     | 0.43              |
| 1:D:2605:MET:HB3  | 1:D:2606:PRO:HD3  | 2.00                     | 0.43              |
| 1:D:2893:LEU:O    | 1:D:2896:LEU:HG   | 2.19                     | 0.43              |
| 1:D:2914:THR:N    | 1:D:2915:PRO:HD2  | 2.33                     | 0.43              |
| 1:D:3008:PHE:CE2  | 1:D:3060:PHE:HE2  | 2.37                     | 0.43              |
| 1:D:3254:PRO:HB3  | 1:D:3258:PRO:HA   | 2.00                     | 0.43              |
| 1:D:4021:LEU:HD22 | 1:D:4128:TYR:CE2  | 2.53                     | 0.43              |
| 1:A:537:LEU:O     | 1:A:541:ILE:HG12  | 2.19                     | 0.43              |
| 1:A:655:MET:HG3   | 1:A:1619:VAL:HG11 | 2.01                     | 0.43              |
| 1:A:1139:GLY:HA3  | 1:A:1156:TRP:CZ3  | 2.54                     | 0.43              |
| 1:A:1847:GLU:OE2  | 1:A:1849:SER:OG   | 2.32                     | 0.43              |
| 1:A:2511:ASP:OD2  | 1:A:2512:MET:N    | 2.52                     | 0.43              |
| 1:A:2581:ARG:HB3  | 1:A:2584:MET:CE   | 2.48                     | 0.43              |
| 1:A:2605:MET:HB3  | 1:A:2606:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:2905:ARG:HE   | 1:A:2906:GLY:N    | 2.03                     | 0.43              |
| 1:A:3695:MET:HB3  | 1:A:3731:LEU:HD11 | 1.99                     | 0.43              |
| 1:A:3940:LEU:HD11 | 1:A:3981:MET:HE1  | 2.00                     | 0.43              |
| 1:A:4583:SER:O    | 1:A:4587:ILE:HG12 | 2.19                     | 0.43              |
| 1:B:974:SER:HB3   | 1:B:976:TYR:CD2   | 2.52                     | 0.43              |
| 1:B:2482:ASP:O    | 1:B:2485:LEU:HG   | 2.18                     | 0.43              |
| 1:B:2593:VAL:HG12 | 1:B:2644:LEU:HD13 | 2.00                     | 0.43              |
| 1:B:2593:VAL:HA   | 1:B:2644:LEU:HD13 | 2.01                     | 0.43              |
| 1:B:2610:LEU:HD12 | 1:B:2614:TYR:CE2  | 2.54                     | 0.43              |
| 1:B:2619:LYS:HA   | 1:B:2622:CYS:SG   | 2.58                     | 0.43              |
| 1:B:2894:LYS:HA   | 1:B:2897:GLN:HG3  | 2.00                     | 0.43              |
| 1:B:4291:PHE:CZ   | 1:B:4295:LEU:HD11 | 2.53                     | 0.43              |
| 1:C:731:HIS:HB3   | 1:C:738:ALA:HB1   | 2.00                     | 0.43              |
| 1:C:1014:GLN:HB3  | 1:C:1027:ARG:NH2  | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1139:GLY:HA3  | 1:C:1156:TRP:CZ3  | 2.54                     | 0.43              |
| 1:C:1156:TRP:HB2  | 1:C:1160:ASP:HB2  | 2.00                     | 0.43              |
| 1:C:1757:LEU:HD11 | 1:C:2108:ILE:HD11 | 2.01                     | 0.43              |
| 1:C:1896:MET:HG2  | 1:C:1896:MET:O    | 2.19                     | 0.43              |
| 1:C:2061:LEU:O    | 1:C:2065:THR:HG23 | 2.19                     | 0.43              |
| 1:C:2062:ILE:HG21 | 1:C:2087:LEU:HG   | 2.00                     | 0.43              |
| 1:C:2511:ASP:OD2  | 1:C:2512:MET:N    | 2.52                     | 0.43              |
| 1:C:3171:LEU:CB   | 1:C:3211:LEU:HB2  | 2.49                     | 0.43              |
| 1:C:4792:PHE:HB3  | 1:C:4843:ARG:NH2  | 2.33                     | 0.43              |
| 1:D:23:GLN:HB3    | 1:D:36:CYS:SG     | 2.59                     | 0.43              |
| 1:D:634:ASP:OD1   | 1:D:1671:ARG:NH2  | 2.37                     | 0.43              |
| 1:D:712:GLU:HA    | 1:D:838:ARG:HG3   | 2.01                     | 0.43              |
| 1:D:731:HIS:HB3   | 1:D:738:ALA:HB1   | 2.00                     | 0.43              |
| 1:D:2061:LEU:O    | 1:D:2065:THR:HG23 | 2.19                     | 0.43              |
| 1:D:2482:ASP:O    | 1:D:2485:LEU:HG   | 2.18                     | 0.43              |
| 1:D:2664:LEU:O    | 1:D:2667:PRO:HD2  | 2.19                     | 0.43              |
| 1:D:2790:GLU:O    | 1:D:2902:ALA:N    | 2.41                     | 0.43              |
| 1:D:2957:GLU:HA   | 1:D:2960:ILE:HG22 | 1.99                     | 0.43              |
| 1:D:3235:MET:HA   | 1:D:3239:LEU:HD12 | 2.01                     | 0.43              |
| 1:D:4023:LEU:HD12 | 1:D:4026:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:23:GLN:HB3    | 1:A:36:CYS:SG     | 2.59                     | 0.42              |
| 1:A:448:PRO:HB2   | 1:A:451:SER:OG    | 2.19                     | 0.42              |
| 1:A:1678:SER:HB3  | 1:A:1768:PHE:CE2  | 2.54                     | 0.42              |
| 1:A:2061:LEU:O    | 1:A:2065:THR:HG23 | 2.19                     | 0.42              |
| 1:A:2525:LEU:O    | 1:A:2529:THR:OG1  | 2.32                     | 0.42              |
| 1:A:2893:LEU:O    | 1:A:2896:LEU:HG   | 2.19                     | 0.42              |
| 1:A:3043:ARG:HG3  | 1:A:3120:ASP:CG   | 2.44                     | 0.42              |
| 1:A:3171:LEU:CB   | 1:A:3211:LEU:HB2  | 2.49                     | 0.42              |
| 2:F:22:THR:HG22   | 2:F:50:ARG:HB2    | 2.01                     | 0.42              |
| 1:B:1088:PHE:CE1  | 1:B:1207:LEU:HD12 | 2.54                     | 0.42              |
| 1:B:4583:SER:O    | 1:B:4587:ILE:HG12 | 2.19                     | 0.42              |
| 1:C:2678:PRO:HB3  | 1:C:2922:ALA:HB2  | 2.00                     | 0.42              |
| 1:C:3254:PRO:HB3  | 1:C:3258:PRO:HA   | 2.00                     | 0.42              |
| 1:C:3323:MET:HE3  | 1:C:3327:LYS:NZ   | 2.34                     | 0.42              |
| 1:C:4030:ASP:OD1  | 1:C:4031:THR:N    | 2.52                     | 0.42              |
| 1:D:27:THR:HA     | 1:D:31:GLU:O      | 2.19                     | 0.42              |
| 1:D:896:ASN:HA    | 1:D:899:GLU:CD    | 2.44                     | 0.42              |
| 1:D:1088:PHE:CE1  | 1:D:1207:LEU:HD12 | 2.54                     | 0.42              |
| 1:D:1139:GLY:HA3  | 1:D:1156:TRP:CZ3  | 2.54                     | 0.42              |
| 1:D:1219:LYS:HZ3  | 1:D:1245:ARG:C    | 2.27                     | 0.42              |
| 1:D:2620:TYR:HB2  | 1:D:2627:TRP:CZ3  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2649:PHE:HE2  | 1:D:2962:PHE:HZ   | 1.67                     | 0.42              |
| 1:D:4583:SER:O    | 1:D:4587:ILE:HG12 | 2.19                     | 0.42              |
| 1:A:712:GLU:HA    | 1:A:838:ARG:HG3   | 2.00                     | 0.42              |
| 1:A:1494:MET:SD   | 1:A:1497:GLY:HA2  | 2.60                     | 0.42              |
| 1:A:1711:LEU:HG   | 1:A:1711:LEU:O    | 2.19                     | 0.42              |
| 1:A:1732:GLU:HB2  | 1:A:1753:LEU:HD21 | 2.00                     | 0.42              |
| 1:A:2589:LEU:HA   | 1:A:2592:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:2787:TRP:HD1  | 1:A:2905:ARG:HA   | 1.84                     | 0.42              |
| 1:A:2914:THR:N    | 1:A:2915:PRO:HD2  | 2.33                     | 0.42              |
| 1:A:3235:MET:HA   | 1:A:3239:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:3277:LEU:O    | 1:A:3281:LEU:HG   | 2.18                     | 0.42              |
| 1:A:3613:ARG:O    | 1:A:3617:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:3958:LEU:HB2  | 1:A:3968:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:4030:ASP:OD1  | 1:A:4031:THR:N    | 2.52                     | 0.42              |
| 1:A:4197:ILE:HG12 | 1:A:4923:MET:HE3  | 2.01                     | 0.42              |
| 1:A:4625:ASP:OD1  | 1:A:4625:ASP:N    | 2.46                     | 0.42              |
| 1:B:947:GLY:C     | 1:B:1067:PRO:HB3  | 2.44                     | 0.42              |
| 1:B:1270:VAL:HG22 | 1:B:1285:VAL:HG22 | 2.01                     | 0.42              |
| 1:B:1711:LEU:O    | 1:B:1711:LEU:HG   | 2.19                     | 0.42              |
| 1:B:1977:LEU:HD23 | 1:B:1977:LEU:O    | 2.20                     | 0.42              |
| 1:B:2511:ASP:OD2  | 1:B:2512:MET:N    | 2.52                     | 0.42              |
| 1:B:2620:TYR:HB2  | 1:B:2627:TRP:CZ3  | 2.54                     | 0.42              |
| 1:B:2759:PRO:HD2  | 1:B:2762:LEU:HD13 | 2.01                     | 0.42              |
| 1:B:2824:ARG:HH11 | 1:B:2825:ALA:H    | 1.65                     | 0.42              |
| 1:B:2837:LEU:HD11 | 1:B:2903:VAL:HG13 | 2.01                     | 0.42              |
| 1:B:2957:GLU:O    | 1:B:2960:ILE:HG22 | 2.18                     | 0.42              |
| 1:B:3106:SER:O    | 1:B:3110:GLU:HG2  | 2.19                     | 0.42              |
| 1:C:1282:CYS:SG   | 1:C:1556:GLU:HG3  | 2.58                     | 0.42              |
| 1:C:1287:GLN:OE1  | 1:C:1290:PHE:N    | 2.52                     | 0.42              |
| 1:C:2619:LYS:HZ1  | 1:C:2627:TRP:CG   | 2.37                     | 0.42              |
| 1:C:2837:LEU:HD11 | 1:C:2903:VAL:HG13 | 2.01                     | 0.42              |
| 1:C:2905:ARG:HE   | 1:C:2906:GLY:N    | 2.03                     | 0.42              |
| 1:C:3613:ARG:O    | 1:C:3617:VAL:HG23 | 2.20                     | 0.42              |
| 1:C:4177:VAL:HB   | 1:C:4880:VAL:HG22 | 1.99                     | 0.42              |
| 1:D:1011:ARG:O    | 1:D:1014:GLN:HB2  | 2.20                     | 0.42              |
| 1:D:1058:LEU:HA   | 1:D:1062:TYR:O    | 2.19                     | 0.42              |
| 1:D:1270:VAL:HG22 | 1:D:1285:VAL:HG22 | 2.01                     | 0.42              |
| 1:D:1829:LEU:HD12 | 1:D:1829:LEU:HA   | 1.92                     | 0.42              |
| 1:D:2222:LEU:HD23 | 1:D:2222:LEU:HA   | 1.84                     | 0.42              |
| 1:D:2525:LEU:O    | 1:D:2529:THR:OG1  | 2.32                     | 0.42              |
| 1:D:2619:LYS:HA   | 1:D:2622:CYS:SG   | 2.58                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2678:PRO:HB3  | 1:D:2922:ALA:HB2  | 2.00                     | 0.42              |
| 1:D:2778:SER:O    | 1:D:2781:THR:OG1  | 2.31                     | 0.42              |
| 1:D:2837:LEU:HD11 | 1:D:2903:VAL:HG13 | 2.01                     | 0.42              |
| 1:D:2972:ASP:O    | 1:D:2976:LYS:HG3  | 2.18                     | 0.42              |
| 1:D:3951:PHE:O    | 1:D:3955:GLN:HG3  | 2.18                     | 0.42              |
| 1:D:3958:LEU:HB2  | 1:D:3968:LEU:HD13 | 2.01                     | 0.42              |
| 1:D:4197:ILE:HG12 | 1:D:4923:MET:HE3  | 2.01                     | 0.42              |
| 1:A:996:VAL:HA    | 1:A:999:LEU:HD12  | 2.02                     | 0.42              |
| 1:A:1023:ASP:OD1  | 1:A:1025:LYS:HG3  | 2.19                     | 0.42              |
| 1:A:1113:MET:HB2  | 1:A:1156:TRP:HZ2  | 1.83                     | 0.42              |
| 1:A:2856:LYS:HG2  | 1:A:2859:GLU:OE1  | 2.19                     | 0.42              |
| 1:A:2929:LEU:HD11 | 1:A:2967:VAL:HG13 | 2.00                     | 0.42              |
| 1:A:3106:SER:O    | 1:A:3110:GLU:HG2  | 2.19                     | 0.42              |
| 1:A:3311:LYS:HD2  | 1:A:3312:PRO:HD2  | 2.00                     | 0.42              |
| 1:B:23:GLN:HB3    | 1:B:36:CYS:SG     | 2.59                     | 0.42              |
| 1:B:827:LEU:HD23  | 1:B:827:LEU:HA    | 1.86                     | 0.42              |
| 1:B:1594:VAL:O    | 1:B:1594:VAL:HG13 | 2.20                     | 0.42              |
| 1:B:1757:LEU:HD11 | 1:B:2108:ILE:HD11 | 2.01                     | 0.42              |
| 1:B:1795:LEU:O    | 1:B:1799:VAL:HG23 | 2.20                     | 0.42              |
| 1:B:2061:LEU:O    | 1:B:2065:THR:HG23 | 2.19                     | 0.42              |
| 1:B:2525:LEU:O    | 1:B:2529:THR:OG1  | 2.32                     | 0.42              |
| 1:B:2678:PRO:HB3  | 1:B:2922:ALA:HB2  | 2.00                     | 0.42              |
| 1:B:3135:THR:HA   | 1:B:3208:ILE:HD11 | 2.02                     | 0.42              |
| 1:B:3276:LEU:O    | 1:B:3280:ILE:HG12 | 2.20                     | 0.42              |
| 1:B:4030:ASP:OD1  | 1:B:4031:THR:N    | 2.52                     | 0.42              |
| 1:B:4114:ARG:O    | 1:B:4117:THR:OG1  | 2.28                     | 0.42              |
| 1:C:139:SER:O     | 1:C:140:THR:OG1   | 2.33                     | 0.42              |
| 1:C:448:PRO:HB2   | 1:C:451:SER:OG    | 2.19                     | 0.42              |
| 1:C:769:ARG:HG3   | 1:C:773:GLN:C     | 2.45                     | 0.42              |
| 1:C:1947:VAL:HG12 | 1:C:1948:MET:HE2  | 2.02                     | 0.42              |
| 1:C:2000:HIS:CE1  | 1:C:3628:TRP:HB3  | 2.54                     | 0.42              |
| 1:C:3723:LYS:NZ   | 1:C:4682:ALA:O    | 2.52                     | 0.42              |
| 1:D:919:VAL:HG21  | 1:D:923:LYS:CD    | 2.50                     | 0.42              |
| 1:D:1594:VAL:O    | 1:D:1594:VAL:HG13 | 2.20                     | 0.42              |
| 1:D:1963:LYS:HA   | 1:D:1966:ARG:HE   | 1.83                     | 0.42              |
| 1:D:2511:ASP:OD2  | 1:D:2512:MET:N    | 2.52                     | 0.42              |
| 1:D:3255:GLU:HB3  | 1:D:3269:ASN:HA   | 2.01                     | 0.42              |
| 1:D:3276:LEU:O    | 1:D:3280:ILE:HG12 | 2.20                     | 0.42              |
| 1:D:3293:GLY:N    | 1:D:3296:MET:HE1  | 2.32                     | 0.42              |
| 1:A:1088:PHE:CE1  | 1:A:1207:LEU:HD12 | 2.54                     | 0.42              |
| 1:A:1282:CYS:SG   | 1:A:1556:GLU:HG3  | 2.58                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2581:ARG:HG3  | 1:A:2583:SER:H    | 1.83                     | 0.42              |
| 1:A:2593:VAL:HA   | 1:A:2644:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:2664:LEU:O    | 1:A:2667:PRO:HD2  | 2.19                     | 0.42              |
| 1:A:4265:LYS:HE3  | 1:B:4694:LEU:HB3  | 2.01                     | 0.42              |
| 2:G:22:THR:HG22   | 2:G:50:ARG:HB2    | 2.01                     | 0.42              |
| 1:B:808:HIS:O     | 1:B:1616:GLY:HA2  | 2.20                     | 0.42              |
| 1:B:1686:LEU:HD23 | 1:B:1686:LEU:HA   | 1.91                     | 0.42              |
| 1:B:2434:GLY:O    | 1:B:2438:ILE:HG13 | 2.19                     | 0.42              |
| 1:B:2787:TRP:HD1  | 1:B:2905:ARG:HA   | 1.84                     | 0.42              |
| 1:B:4120:GLU:HA   | 1:B:4123:GLU:CD   | 2.45                     | 0.42              |
| 1:C:625:VAL:CG1   | 1:C:2133:ARG:HD3  | 2.50                     | 0.42              |
| 1:C:712:GLU:HA    | 1:C:838:ARG:HG3   | 2.00                     | 0.42              |
| 1:C:919:VAL:HG21  | 1:C:923:LYS:CD    | 2.50                     | 0.42              |
| 1:C:988:LEU:HB2   | 1:C:1055:ARG:NE   | 2.27                     | 0.42              |
| 1:C:1308:ILE:HD12 | 1:C:1445:TRP:CH2  | 2.54                     | 0.42              |
| 1:C:1795:LEU:O    | 1:C:1799:VAL:HG23 | 2.20                     | 0.42              |
| 1:C:2127:ARG:O    | 1:C:2130:LEU:HB2  | 2.20                     | 0.42              |
| 1:C:3043:ARG:HG3  | 1:C:3120:ASP:CG   | 2.44                     | 0.42              |
| 1:C:3255:GLU:HB3  | 1:C:3269:ASN:HA   | 2.01                     | 0.42              |
| 1:C:4107:GLU:OE1  | 1:C:4149:TYR:OH   | 2.27                     | 0.42              |
| 1:C:4583:SER:O    | 1:C:4587:ILE:HG12 | 2.19                     | 0.42              |
| 1:D:448:PRO:HB2   | 1:D:451:SER:OG    | 2.19                     | 0.42              |
| 1:D:692:HIS:O     | 1:D:794:PHE:HA    | 2.20                     | 0.42              |
| 1:D:804:LEU:HD13  | 1:D:832:LEU:HD21  | 2.02                     | 0.42              |
| 1:D:1100:ARG:HB2  | 1:D:1236:TYR:CD1  | 2.54                     | 0.42              |
| 1:D:1608:VAL:HA   | 1:D:1618:LEU:O    | 2.20                     | 0.42              |
| 1:D:1977:LEU:O    | 1:D:1977:LEU:HD23 | 2.20                     | 0.42              |
| 1:D:2127:ARG:O    | 1:D:2130:LEU:HB2  | 2.20                     | 0.42              |
| 1:D:2788:ARG:NH1  | 1:D:2904:SER:HB3  | 2.35                     | 0.42              |
| 1:D:2894:LYS:HA   | 1:D:2897:GLN:HG3  | 2.00                     | 0.42              |
| 1:D:3723:LYS:NZ   | 1:D:4682:ALA:O    | 2.52                     | 0.42              |
| 1:D:4155:SER:O    | 1:D:4159:GLN:HG2  | 2.18                     | 0.42              |
| 1:A:1058:LEU:HA   | 1:A:1062:TYR:O    | 2.19                     | 0.42              |
| 1:A:1100:ARG:HB2  | 1:A:1236:TYR:CD1  | 2.54                     | 0.42              |
| 1:A:1308:ILE:HD12 | 1:A:1445:TRP:CH2  | 2.54                     | 0.42              |
| 1:A:1795:LEU:O    | 1:A:1799:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:2649:PHE:HE2  | 1:A:2962:PHE:HZ   | 1.67                     | 0.42              |
| 1:A:2673:ALA:HB1  | 1:A:2974:TYR:CD1  | 2.53                     | 0.42              |
| 1:A:2728:SER:O    | 1:A:2731:LYS:HG3  | 2.19                     | 0.42              |
| 1:A:3254:PRO:HB3  | 1:A:3258:PRO:HA   | 2.00                     | 0.42              |
| 1:A:3323:MET:HB3  | 1:A:3327:LYS:NZ   | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3723:LYS:NZ   | 1:A:4682:ALA:O    | 2.52                     | 0.42              |
| 1:A:3951:PHE:O    | 1:A:3955:GLN:HG3  | 2.19                     | 0.42              |
| 1:B:137:ARG:NH2   | 1:B:202:HIS:HB3   | 2.34                     | 0.42              |
| 1:B:470:LEU:HB2   | 1:B:475:LYS:HG3   | 2.01                     | 0.42              |
| 1:B:677:LEU:HD12  | 1:B:801:ARG:O     | 2.20                     | 0.42              |
| 1:B:804:LEU:HD13  | 1:B:832:LEU:HD21  | 2.02                     | 0.42              |
| 1:B:1014:GLN:HB3  | 1:B:1027:ARG:NH2  | 2.34                     | 0.42              |
| 1:B:2729:HIS:CD2  | 1:B:2763:LEU:HD11 | 2.55                     | 0.42              |
| 1:B:3323:MET:HB3  | 1:B:3327:LYS:NZ   | 2.34                     | 0.42              |
| 1:B:3958:LEU:HB2  | 1:B:3968:LEU:HD13 | 2.01                     | 0.42              |
| 1:B:4898:PHE:O    | 1:B:4904:GLY:HA3  | 2.18                     | 0.42              |
| 1:C:829:LYS:NZ    | 1:C:1037:LEU:O    | 2.49                     | 0.42              |
| 1:C:875:PRO:HD2   | 1:C:878:LEU:HD12  | 2.01                     | 0.42              |
| 1:C:1011:ARG:O    | 1:C:1014:GLN:HB2  | 2.19                     | 0.42              |
| 1:C:1494:MET:SD   | 1:C:1497:GLY:HA2  | 2.59                     | 0.42              |
| 1:C:2589:LEU:HA   | 1:C:2592:LEU:HD12 | 2.01                     | 0.42              |
| 1:C:2728:SER:O    | 1:C:2731:LYS:HG3  | 2.19                     | 0.42              |
| 1:D:137:ARG:NH2   | 1:D:202:HIS:HB3   | 2.34                     | 0.42              |
| 1:D:947:GLY:C     | 1:D:1067:PRO:HB3  | 2.44                     | 0.42              |
| 1:D:1308:ILE:HD12 | 1:D:1445:TRP:CH2  | 2.54                     | 0.42              |
| 1:D:1427:TYR:HB2  | 1:D:1563:VAL:HG11 | 2.00                     | 0.42              |
| 1:D:1998:ASP:O    | 1:D:2001:GLU:HG3  | 2.20                     | 0.42              |
| 1:D:2307:PHE:CG   | 1:D:2401:ARG:HD3  | 2.55                     | 0.42              |
| 1:D:2759:PRO:HD2  | 1:D:2762:LEU:HD13 | 2.01                     | 0.42              |
| 1:D:3276:LEU:HA   | 1:D:3276:LEU:HD23 | 1.85                     | 0.42              |
| 1:D:3728:GLN:HG2  | 1:D:3765:ILE:HA   | 2.00                     | 0.42              |
| 1:A:137:ARG:NH2   | 1:A:202:HIS:HB3   | 2.34                     | 0.42              |
| 1:A:804:LEU:HD13  | 1:A:832:LEU:HD21  | 2.02                     | 0.42              |
| 1:A:887:GLU:O     | 1:A:890:HIS:ND1   | 2.52                     | 0.42              |
| 1:A:1023:ASP:OD1  | 1:A:1024:VAL:N    | 2.53                     | 0.42              |
| 1:A:2420:ARG:HD3  | 1:A:2424:ARG:NH1  | 2.35                     | 0.42              |
| 1:A:2705:PRO:HD3  | 1:A:2854:LYS:HG3  | 2.02                     | 0.42              |
| 1:A:3213:LYS:O    | 1:A:3216:GLU:HG3  | 2.19                     | 0.42              |
| 1:A:4027:THR:HA   | 1:A:4032:PHE:CD1  | 2.50                     | 0.42              |
| 1:A:4605:GLU:HB3  | 1:A:4609:LYS:NZ   | 2.34                     | 0.42              |
| 1:B:769:ARG:HG3   | 1:B:773:GLN:C     | 2.45                     | 0.42              |
| 1:B:996:VAL:HA    | 1:B:999:LEU:HD12  | 2.02                     | 0.42              |
| 1:B:2420:ARG:HD3  | 1:B:2424:ARG:NH1  | 2.35                     | 0.42              |
| 1:B:2649:PHE:HE2  | 1:B:2962:PHE:HZ   | 1.67                     | 0.42              |
| 1:B:2788:ARG:HD3  | 1:B:2788:ARG:H    | 1.84                     | 0.42              |
| 1:B:2857:LYS:O    | 1:B:2861:GLU:OE1  | 2.38                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3210:SER:H    | 1:B:3213:LYS:NZ   | 2.16                     | 0.42              |
| 1:C:174:LYS:O     | 1:C:176:ARG:NH1   | 2.53                     | 0.42              |
| 1:C:370:LEU:HD23  | 1:C:395:HIS:HA    | 2.01                     | 0.42              |
| 1:C:677:LEU:HD12  | 1:C:801:ARG:O     | 2.20                     | 0.42              |
| 1:C:887:GLU:O     | 1:C:890:HIS:ND1   | 2.52                     | 0.42              |
| 1:C:890:HIS:HA    | 1:C:893:TRP:CE3   | 2.45                     | 0.42              |
| 1:C:1423:THR:HG23 | 1:C:1564:MET:HG2  | 2.02                     | 0.42              |
| 1:C:1594:VAL:HG13 | 1:C:1594:VAL:O    | 2.20                     | 0.42              |
| 1:C:1998:ASP:O    | 1:C:2001:GLU:HG3  | 2.20                     | 0.42              |
| 1:C:2135:GLY:H    | 1:C:2138:GLU:HB2  | 1.84                     | 0.42              |
| 1:C:2620:TYR:HB2  | 1:C:2627:TRP:CZ3  | 2.54                     | 0.42              |
| 1:C:3235:MET:HA   | 1:C:3239:LEU:HD12 | 2.01                     | 0.42              |
| 1:C:4089:GLU:OE1  | 1:C:4089:GLU:N    | 2.48                     | 0.42              |
| 1:D:174:LYS:O     | 1:D:176:ARG:NH1   | 2.53                     | 0.42              |
| 1:D:370:LEU:C     | 1:D:393:MET:HE3   | 2.45                     | 0.42              |
| 1:D:871:GLN:OE1   | 1:D:871:GLN:N     | 2.43                     | 0.42              |
| 1:D:1287:GLN:OE1  | 1:D:1290:PHE:N    | 2.52                     | 0.42              |
| 1:D:1423:THR:HG23 | 1:D:1564:MET:HG2  | 2.02                     | 0.42              |
| 1:D:2705:PRO:HD3  | 1:D:2854:LYS:HG3  | 2.02                     | 0.42              |
| 1:D:2856:LYS:HG2  | 1:D:2859:GLU:OE1  | 2.19                     | 0.42              |
| 1:D:3135:THR:HA   | 1:D:3208:ILE:HD11 | 2.01                     | 0.42              |
| 1:D:3290:ILE:HG13 | 1:D:3291:ASP:N    | 2.33                     | 0.42              |
| 1:D:4089:GLU:OE1  | 1:D:4089:GLU:N    | 2.48                     | 0.42              |
| 1:D:4237:SER:O    | 1:D:4241:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:4792:PHE:HB3  | 1:D:4843:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:125:TYR:CE1   | 1:A:417:ARG:HD3   | 2.55                     | 0.42              |
| 1:A:370:LEU:C     | 1:A:393:MET:HE3   | 2.45                     | 0.42              |
| 1:A:1538:LYS:NZ   | 1:A:1636:ASN:OD1  | 2.52                     | 0.42              |
| 1:A:1896:MET:HG2  | 1:A:1896:MET:O    | 2.19                     | 0.42              |
| 1:A:2135:GLY:H    | 1:A:2138:GLU:HB2  | 1.84                     | 0.42              |
| 1:A:2434:GLY:O    | 1:A:2438:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:2894:LYS:HA   | 1:A:2897:GLN:HG3  | 2.01                     | 0.42              |
| 1:A:4120:GLU:HA   | 1:A:4123:GLU:CD   | 2.45                     | 0.42              |
| 1:A:4617:ILE:HG13 | 1:A:4665:ARG:HH12 | 1.85                     | 0.42              |
| 1:B:174:LYS:O     | 1:B:176:ARG:NH1   | 2.53                     | 0.42              |
| 1:B:447:LEU:HD12  | 1:B:447:LEU:HA    | 1.83                     | 0.42              |
| 1:B:968:LYS:HA    | 1:B:971:GLN:HG2   | 2.01                     | 0.42              |
| 1:B:1139:GLY:HA3  | 1:B:1156:TRP:CZ3  | 2.54                     | 0.42              |
| 1:B:1678:SER:HB3  | 1:B:1768:PHE:CE2  | 2.54                     | 0.42              |
| 1:B:1998:ASP:O    | 1:B:2001:GLU:HG3  | 2.19                     | 0.42              |
| 1:B:2157:GLN:O    | 1:B:3615:ARG:NH2  | 2.25                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2607:LEU:HD12 | 1:B:2607:LEU:HA   | 1.95                     | 0.42              |
| 1:B:2646:TRP:CH2  | 1:B:2925:PHE:HA   | 2.55                     | 0.42              |
| 1:B:3739:MET:HE2  | 1:B:3739:MET:HB3  | 1.87                     | 0.42              |
| 1:C:272:ARG:C     | 1:C:299:HIS:HE2   | 2.28                     | 0.42              |
| 1:C:896:ASN:HA    | 1:C:899:GLU:CD    | 2.44                     | 0.42              |
| 1:C:1058:LEU:HA   | 1:C:1062:TYR:O    | 2.19                     | 0.42              |
| 1:C:1205:CYS:SG   | 1:C:1215:MET:HE3  | 2.60                     | 0.42              |
| 1:C:2086:VAL:HG22 | 1:C:3687:LEU:HD13 | 2.02                     | 0.42              |
| 1:C:2222:LEU:HB3  | 1:C:2264:LYS:HD2  | 2.02                     | 0.42              |
| 1:C:2420:ARG:HD3  | 1:C:2424:ARG:NH1  | 2.35                     | 0.42              |
| 1:C:3109:PHE:HE1  | 1:C:3162:PHE:CD1  | 2.31                     | 0.42              |
| 1:C:3135:THR:HA   | 1:C:3208:ILE:HD11 | 2.02                     | 0.42              |
| 1:C:3311:LYS:HD2  | 1:C:3312:PRO:HD2  | 2.00                     | 0.42              |
| 1:D:769:ARG:HG3   | 1:D:773:GLN:C     | 2.45                     | 0.42              |
| 1:D:911:ASN:OD1   | 1:D:912:LYS:N     | 2.53                     | 0.42              |
| 1:D:1023:ASP:OD1  | 1:D:1024:VAL:N    | 2.53                     | 0.42              |
| 1:D:1205:CYS:SG   | 1:D:1215:MET:HE3  | 2.60                     | 0.42              |
| 1:D:1494:MET:SD   | 1:D:1497:GLY:HA2  | 2.60                     | 0.42              |
| 1:D:1757:LEU:HD11 | 1:D:2108:ILE:HD11 | 2.01                     | 0.42              |
| 1:D:1947:VAL:HG12 | 1:D:1948:MET:HE2  | 2.02                     | 0.42              |
| 1:D:2424:ARG:HG2  | 1:D:2476:TYR:CD1  | 2.55                     | 0.42              |
| 1:D:2716:LYS:O    | 1:D:2901:TYR:OH   | 2.31                     | 0.42              |
| 1:D:3043:ARG:HG3  | 1:D:3120:ASP:CG   | 2.44                     | 0.42              |
| 1:D:3323:MET:HB3  | 1:D:3327:LYS:HZ3  | 1.84                     | 0.42              |
| 1:D:3323:MET:HE3  | 1:D:3327:LYS:NZ   | 2.35                     | 0.42              |
| 1:A:643:LEU:HD13  | 1:A:1657:THR:HG23 | 2.02                     | 0.42              |
| 1:A:2585:MET:O    | 1:A:2589:LEU:HG   | 2.20                     | 0.42              |
| 1:A:3001:LYS:NZ   | 1:A:3041:ASP:OD2  | 2.37                     | 0.42              |
| 1:A:4255:LEU:HD23 | 1:B:4710:LEU:HD13 | 2.01                     | 0.42              |
| 1:B:896:ASN:HA    | 1:B:899:GLU:CD    | 2.44                     | 0.42              |
| 1:B:1023:ASP:OD1  | 1:B:1025:LYS:HG3  | 2.19                     | 0.42              |
| 1:B:1287:GLN:OE1  | 1:B:1290:PHE:N    | 2.52                     | 0.42              |
| 1:B:1494:MET:SD   | 1:B:1497:GLY:HA2  | 2.59                     | 0.42              |
| 1:B:2580:LEU:O    | 1:B:2585:MET:HE1  | 2.19                     | 0.42              |
| 1:B:2581:ARG:HG3  | 1:B:2583:SER:H    | 1.83                     | 0.42              |
| 1:B:2591:ARG:HH22 | 1:B:2875:ASP:HB2  | 1.85                     | 0.42              |
| 1:B:2664:LEU:O    | 1:B:2667:PRO:HD2  | 2.19                     | 0.42              |
| 1:B:3171:LEU:CB   | 1:B:3211:LEU:HB2  | 2.49                     | 0.42              |
| 1:B:3699:CYS:SG   | 1:B:3731:LEU:HD12 | 2.60                     | 0.42              |
| 1:C:370:LEU:C     | 1:C:393:MET:HE3   | 2.45                     | 0.42              |
| 1:C:3008:PHE:CE2  | 1:C:3060:PHE:HE2  | 2.37                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3323:MET:HB3  | 1:C:3327:LYS:NZ   | 2.34                     | 0.42              |
| 1:C:4107:GLU:OE2  | 1:C:4135:ARG:NE   | 2.53                     | 0.42              |
| 1:C:4631:ASP:O    | 1:C:4634:VAL:HG12 | 2.20                     | 0.42              |
| 1:D:470:LEU:HB2   | 1:D:475:LYS:HG3   | 2.01                     | 0.42              |
| 1:D:1014:GLN:HB3  | 1:D:1027:ARG:NH2  | 2.34                     | 0.42              |
| 1:D:1138:ASP:HB2  | 1:D:1145:TRP:CD1  | 2.55                     | 0.42              |
| 1:D:1991:GLU:HG2  | 1:D:1992:ILE:N    | 2.35                     | 0.42              |
| 1:D:2000:HIS:CE1  | 1:D:3628:TRP:HB3  | 2.54                     | 0.42              |
| 1:D:2086:VAL:HG22 | 1:D:3687:LEU:HD13 | 2.02                     | 0.42              |
| 1:D:2420:ARG:HD3  | 1:D:2424:ARG:NH1  | 2.35                     | 0.42              |
| 1:D:2929:LEU:HD11 | 1:D:2967:VAL:HG13 | 2.00                     | 0.42              |
| 1:D:3129:SER:O    | 1:D:3133:ILE:HG13 | 2.20                     | 0.42              |
| 1:D:4190:VAL:HG11 | 1:D:4949:TRP:CH2  | 2.55                     | 0.42              |
| 1:A:692:HIS:O     | 1:A:794:PHE:HA    | 2.20                     | 0.42              |
| 1:A:891:GLU:O     | 1:A:894:VAL:HG22  | 2.20                     | 0.42              |
| 1:A:968:LYS:HA    | 1:A:971:GLN:HG2   | 2.01                     | 0.42              |
| 1:A:1011:ARG:O    | 1:A:1014:GLN:HB2  | 2.19                     | 0.42              |
| 1:A:1608:VAL:HA   | 1:A:1618:LEU:O    | 2.20                     | 0.42              |
| 1:A:2127:ARG:O    | 1:A:2130:LEU:HB2  | 2.20                     | 0.42              |
| 1:A:2729:HIS:CD2  | 1:A:2763:LEU:HD11 | 2.55                     | 0.42              |
| 1:A:3129:SER:O    | 1:A:3133:ILE:HG13 | 2.20                     | 0.42              |
| 1:A:3210:SER:H    | 1:A:3213:LYS:NZ   | 2.16                     | 0.42              |
| 1:A:3234:VAL:HG13 | 1:A:3238:ILE:HD11 | 2.02                     | 0.42              |
| 1:A:3306:ILE:HA   | 1:A:3309:LYS:HE2  | 2.01                     | 0.42              |
| 1:A:4190:VAL:HG11 | 1:A:4949:TRP:CH2  | 2.55                     | 0.42              |
| 1:A:4237:SER:O    | 1:A:4241:VAL:HG23 | 2.20                     | 0.42              |
| 1:B:230:GLY:HA2   | 1:B:289:ILE:HD11  | 2.02                     | 0.42              |
| 1:B:537:LEU:O     | 1:B:541:ILE:HG12  | 2.19                     | 0.42              |
| 1:B:829:LYS:NZ    | 1:B:1037:LEU:O    | 2.49                     | 0.42              |
| 1:B:887:GLU:O     | 1:B:890:HIS:ND1   | 2.52                     | 0.42              |
| 1:B:1058:LEU:HA   | 1:B:1062:TYR:O    | 2.19                     | 0.42              |
| 1:B:2565:GLN:O    | 1:B:2568:SER:OG   | 2.21                     | 0.42              |
| 1:B:3723:LYS:NZ   | 1:B:4682:ALA:O    | 2.52                     | 0.42              |
| 1:B:3929:THR:O    | 1:B:3933:GLN:HG2  | 2.20                     | 0.42              |
| 1:C:804:LEU:HD13  | 1:C:832:LEU:HD21  | 2.02                     | 0.42              |
| 1:C:808:HIS:O     | 1:C:1616:GLY:HA2  | 2.20                     | 0.42              |
| 1:C:911:ASN:OD1   | 1:C:912:LYS:N     | 2.53                     | 0.42              |
| 1:C:1502:ASN:OD1  | 1:C:1503:ASN:N    | 2.53                     | 0.42              |
| 1:C:1678:SER:HB3  | 1:C:1768:PHE:CE2  | 2.54                     | 0.42              |
| 1:C:3046:MET:SD   | 1:C:3058:ARG:NH2  | 2.89                     | 0.42              |
| 1:C:3958:LEU:HB2  | 1:C:3968:LEU:HD13 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4242:ARG:HH22 | 1:C:4249:ARG:NH1  | 2.18                     | 0.42              |
| 1:D:1010:ASP:HA   | 1:D:1013:ARG:HD2  | 2.02                     | 0.42              |
| 1:D:1678:SER:HB3  | 1:D:1768:PHE:CE2  | 2.54                     | 0.42              |
| 1:D:2407:HIS:CG   | 1:D:2408:LEU:N    | 2.88                     | 0.42              |
| 1:D:3171:LEU:CB   | 1:D:3211:LEU:HB2  | 2.49                     | 0.42              |
| 1:D:3613:ARG:O    | 1:D:3617:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:875:PRO:HD2   | 1:A:878:LEU:HD12  | 2.01                     | 0.42              |
| 1:A:1205:CYS:SG   | 1:A:1215:MET:HE3  | 2.60                     | 0.42              |
| 1:A:1219:LYS:HZ3  | 1:A:1245:ARG:C    | 2.27                     | 0.42              |
| 1:A:2071:GLN:O    | 1:A:3660:ARG:NH2  | 2.53                     | 0.42              |
| 1:A:2580:LEU:O    | 1:A:2585:MET:HE1  | 2.19                     | 0.42              |
| 1:A:2591:ARG:HH22 | 1:A:2875:ASP:HB2  | 1.85                     | 0.42              |
| 1:A:3311:LYS:HG3  | 1:A:3313:GLN:N    | 2.34                     | 0.42              |
| 1:A:3699:CYS:SG   | 1:A:3731:LEU:HD12 | 2.60                     | 0.42              |
| 1:A:4107:GLU:OE2  | 1:A:4135:ARG:NE   | 2.53                     | 0.42              |
| 2:H:8:ILE:HG23    | 1:D:748:LEU:HB2   | 2.02                     | 0.42              |
| 1:B:27:THR:HA     | 1:B:31:GLU:O      | 2.19                     | 0.42              |
| 1:B:891:GLU:O     | 1:B:894:VAL:HG22  | 2.20                     | 0.42              |
| 1:B:1608:VAL:HA   | 1:B:1618:LEU:O    | 2.20                     | 0.42              |
| 1:B:1947:VAL:HG12 | 1:B:1948:MET:HE2  | 2.02                     | 0.42              |
| 1:B:2407:HIS:CG   | 1:B:2408:LEU:N    | 2.88                     | 0.42              |
| 1:B:3613:ARG:O    | 1:B:3617:VAL:HG23 | 2.20                     | 0.42              |
| 1:B:4197:ILE:HG12 | 1:B:4923:MET:HE3  | 2.02                     | 0.42              |
| 1:C:692:HIS:O     | 1:C:794:PHE:HA    | 2.20                     | 0.42              |
| 1:C:947:GLY:C     | 1:C:1067:PRO:HB3  | 2.44                     | 0.42              |
| 1:C:1608:VAL:HA   | 1:C:1618:LEU:O    | 2.20                     | 0.42              |
| 1:C:2424:ARG:HG2  | 1:C:2476:TYR:CD1  | 2.55                     | 0.42              |
| 1:C:2525:LEU:HB2  | 1:C:2526:PRO:HD3  | 2.02                     | 0.42              |
| 1:C:2610:LEU:HD12 | 1:C:2614:TYR:CE2  | 2.54                     | 0.42              |
| 1:C:2646:TRP:CH2  | 1:C:2925:PHE:HA   | 2.55                     | 0.42              |
| 1:C:2649:PHE:HE2  | 1:C:2962:PHE:HZ   | 1.67                     | 0.42              |
| 1:D:875:PRO:HD2   | 1:D:878:LEU:HD12  | 2.01                     | 0.42              |
| 1:D:891:GLU:O     | 1:D:894:VAL:HG22  | 2.20                     | 0.42              |
| 1:D:996:VAL:HA    | 1:D:999:LEU:HD12  | 2.02                     | 0.42              |
| 1:D:2303:ARG:HH11 | 1:D:2304:PHE:HA   | 1.85                     | 0.42              |
| 1:D:2525:LEU:HB2  | 1:D:2526:PRO:HD3  | 2.02                     | 0.42              |
| 1:D:3173:THR:OG1  | 1:D:3201:VAL:HG13 | 2.20                     | 0.42              |
| 1:D:3191:GLU:OE2  | 1:D:3192:ARG:HG2  | 2.20                     | 0.42              |
| 1:D:4107:GLU:OE2  | 1:D:4135:ARG:NE   | 2.53                     | 0.42              |
| 1:D:4120:GLU:HA   | 1:D:4123:GLU:CD   | 2.45                     | 0.42              |
| 1:A:1014:GLN:HB3  | 1:A:1027:ARG:NH2  | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1138:ASP:HB2  | 1:A:1145:TRP:CD1  | 2.55                     | 0.41              |
| 1:A:1270:VAL:HG22 | 1:A:1285:VAL:HG22 | 2.01                     | 0.41              |
| 1:A:1998:ASP:O    | 1:A:2001:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:2307:PHE:CG   | 1:A:2401:ARG:HD3  | 2.55                     | 0.41              |
| 1:A:2581:ARG:HB3  | 1:A:2584:MET:HE2  | 2.02                     | 0.41              |
| 1:A:3323:MET:HE3  | 1:A:3327:LYS:NZ   | 2.35                     | 0.41              |
| 1:A:3929:THR:O    | 1:A:3933:GLN:HG2  | 2.20                     | 0.41              |
| 1:B:875:PRO:HD2   | 1:B:878:LEU:HD12  | 2.01                     | 0.41              |
| 1:B:911:ASN:OD1   | 1:B:912:LYS:N     | 2.53                     | 0.41              |
| 1:B:1011:ARG:O    | 1:B:1014:GLN:HB2  | 2.19                     | 0.41              |
| 1:B:2000:HIS:CE1  | 1:B:3628:TRP:HB3  | 2.54                     | 0.41              |
| 1:B:2135:GLY:H    | 1:B:2138:GLU:HB2  | 1.84                     | 0.41              |
| 1:B:2172:MET:HE2  | 1:B:2172:MET:HB2  | 1.93                     | 0.41              |
| 1:B:2303:ARG:HH11 | 1:B:2304:PHE:HA   | 1.84                     | 0.41              |
| 1:B:2406:MET:HE1  | 1:B:2420:ARG:HH21 | 1.85                     | 0.41              |
| 1:B:2525:LEU:HB2  | 1:B:2526:PRO:HD3  | 2.02                     | 0.41              |
| 1:B:2788:ARG:NH1  | 1:B:2904:SER:HB3  | 2.35                     | 0.41              |
| 1:B:2891:ASP:OD1  | 1:B:2892:ILE:N    | 2.53                     | 0.41              |
| 1:B:4107:GLU:OE2  | 1:B:4135:ARG:NE   | 2.53                     | 0.41              |
| 1:C:2141:LEU:O    | 1:C:2144:ARG:HG3  | 2.20                     | 0.41              |
| 1:C:2307:PHE:CG   | 1:C:2401:ARG:HD3  | 2.55                     | 0.41              |
| 1:C:2580:LEU:O    | 1:C:2585:MET:HE1  | 2.19                     | 0.41              |
| 1:C:2585:MET:O    | 1:C:2589:LEU:HG   | 2.20                     | 0.41              |
| 1:C:2856:LYS:HG2  | 1:C:2859:GLU:OE1  | 2.19                     | 0.41              |
| 1:C:2926:LEU:HG   | 1:C:3003:MET:HE2  | 2.02                     | 0.41              |
| 1:C:3276:LEU:O    | 1:C:3280:ILE:HG12 | 2.20                     | 0.41              |
| 1:C:4863:GLN:HG3  | 1:D:4860:ALA:CB   | 2.50                     | 0.41              |
| 1:D:49:LEU:HD11   | 1:D:203:VAL:HG13  | 2.02                     | 0.41              |
| 1:D:625:VAL:CG1   | 1:D:2133:ARG:HD3  | 2.50                     | 0.41              |
| 1:D:878:LEU:HB3   | 1:D:879:GLU:H     | 1.77                     | 0.41              |
| 1:D:1023:ASP:OD1  | 1:D:1025:LYS:HG3  | 2.19                     | 0.41              |
| 1:D:1100:ARG:HB2  | 1:D:1236:TYR:CE1  | 2.55                     | 0.41              |
| 1:D:1538:LYS:NZ   | 1:D:1636:ASN:OD1  | 2.51                     | 0.41              |
| 1:D:2222:LEU:HB3  | 1:D:2264:LYS:HD2  | 2.02                     | 0.41              |
| 1:D:2581:ARG:HB3  | 1:D:2584:MET:HE2  | 2.02                     | 0.41              |
| 1:D:2585:MET:O    | 1:D:2589:LEU:HG   | 2.20                     | 0.41              |
| 1:D:3311:LYS:HD2  | 1:D:3312:PRO:HD2  | 2.00                     | 0.41              |
| 1:D:3328:LYS:NZ   | 1:D:3329:LYS:HE3  | 2.35                     | 0.41              |
| 1:A:21:VAL:HG13   | 1:A:217:ILE:HG13  | 2.02                     | 0.41              |
| 1:A:370:LEU:HD23  | 1:A:395:HIS:HA    | 2.01                     | 0.41              |
| 1:A:394:HIS:HE1   | 1:A:396:GLU:HG3   | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:470:LEU:HB2   | 1:A:475:LYS:HG3   | 2.01                     | 0.41              |
| 1:A:769:ARG:HG3   | 1:A:773:GLN:C     | 2.45                     | 0.41              |
| 1:A:928:GLU:HG3   | 4:A:5003:ATP:C8   | 2.55                     | 0.41              |
| 1:A:1287:GLN:OE1  | 1:A:1290:PHE:N    | 2.52                     | 0.41              |
| 1:A:1757:LEU:HD11 | 1:A:2108:ILE:HD11 | 2.01                     | 0.41              |
| 1:A:2141:LEU:O    | 1:A:2144:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:2759:PRO:HD2  | 1:A:2762:LEU:HD13 | 2.01                     | 0.41              |
| 1:A:3187:LYS:O    | 1:A:3187:LYS:HG2  | 2.21                     | 0.41              |
| 1:A:3276:LEU:O    | 1:A:3280:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:3773:VAL:HG12 | 1:A:3777:MET:HE3  | 2.02                     | 0.41              |
| 1:A:4242:ARG:HH22 | 1:A:4249:ARG:NH1  | 2.18                     | 0.41              |
| 1:B:125:TYR:CE1   | 1:B:417:ARG:HD3   | 2.55                     | 0.41              |
| 1:B:314:LEU:HD21  | 1:B:393:MET:HB2   | 2.02                     | 0.41              |
| 1:B:1023:ASP:OD1  | 1:B:1024:VAL:N    | 2.53                     | 0.41              |
| 1:B:3311:LYS:HD2  | 1:B:3312:PRO:HD2  | 2.00                     | 0.41              |
| 1:B:4190:VAL:HG11 | 1:B:4949:TRP:CH2  | 2.55                     | 0.41              |
| 1:B:4242:ARG:HH22 | 1:B:4249:ARG:NH1  | 2.18                     | 0.41              |
| 1:B:4507:LEU:HD12 | 1:B:4507:LEU:HA   | 1.79                     | 0.41              |
| 1:C:125:TYR:CE1   | 1:C:417:ARG:HD3   | 2.55                     | 0.41              |
| 1:C:364:GLN:HG3   | 1:C:370:LEU:O     | 2.20                     | 0.41              |
| 1:C:1105:PHE:HB3  | 1:C:1162:VAL:HG13 | 2.02                     | 0.41              |
| 1:C:1138:ASP:HB2  | 1:C:1145:TRP:CD1  | 2.55                     | 0.41              |
| 1:C:2178:VAL:HG11 | 1:C:2192:MET:HE1  | 2.00                     | 0.41              |
| 1:C:2486:HIS:O    | 1:C:2490:VAL:HG22 | 2.20                     | 0.41              |
| 1:C:2565:GLN:O    | 1:C:2568:SER:OG   | 2.21                     | 0.41              |
| 1:C:2730:ASP:OD1  | 1:C:2824:ARG:HA   | 2.20                     | 0.41              |
| 1:C:3187:LYS:O    | 1:C:3187:LYS:HG2  | 2.20                     | 0.41              |
| 1:C:4237:SER:O    | 1:C:4241:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:4587:ILE:HG13 | 1:C:4726:MET:HE2  | 2.02                     | 0.41              |
| 1:D:887:GLU:O     | 1:D:890:HIS:ND1   | 2.52                     | 0.41              |
| 1:D:902:TRP:NE1   | 1:D:915:HIS:HB2   | 2.35                     | 0.41              |
| 1:D:974:SER:HB3   | 1:D:976:TYR:CD2   | 2.52                     | 0.41              |
| 1:D:2593:VAL:HA   | 1:D:2644:LEU:HD13 | 2.01                     | 0.41              |
| 1:D:2691:LYS:HG3  | 1:D:2693:SER:H    | 1.86                     | 0.41              |
| 1:D:2728:SER:O    | 1:D:2731:LYS:HG3  | 2.19                     | 0.41              |
| 1:D:2730:ASP:OD1  | 1:D:2824:ARG:HA   | 2.20                     | 0.41              |
| 1:D:2857:LYS:O    | 1:D:2861:GLU:OE1  | 2.38                     | 0.41              |
| 1:D:4605:GLU:HB3  | 1:D:4609:LYS:NZ   | 2.34                     | 0.41              |
| 1:A:364:GLN:HG3   | 1:A:370:LEU:O     | 2.20                     | 0.41              |
| 1:A:1100:ARG:HB2  | 1:A:1236:TYR:CE1  | 2.56                     | 0.41              |
| 1:A:1594:VAL:HG13 | 1:A:1594:VAL:O    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2000:HIS:CE1  | 1:A:3628:TRP:HB3  | 2.54                     | 0.41              |
| 1:A:2646:TRP:CH2  | 1:A:2925:PHE:HA   | 2.55                     | 0.41              |
| 1:A:4517:LEU:O    | 1:B:4809:MET:HE2  | 2.20                     | 0.41              |
| 1:A:4737:PHE:CD1  | 1:B:4783:VAL:HG13 | 2.55                     | 0.41              |
| 1:B:49:LEU:HD11   | 1:B:203:VAL:HG13  | 2.02                     | 0.41              |
| 1:B:988:LEU:HB2   | 1:B:1055:ARG:NE   | 2.27                     | 0.41              |
| 1:B:1138:ASP:HB2  | 1:B:1145:TRP:CD1  | 2.55                     | 0.41              |
| 1:B:2127:ARG:O    | 1:B:2130:LEU:HB2  | 2.20                     | 0.41              |
| 1:B:2486:HIS:O    | 1:B:2490:VAL:HG22 | 2.21                     | 0.41              |
| 1:B:3773:VAL:HG12 | 1:B:3777:MET:HE3  | 2.03                     | 0.41              |
| 1:B:4237:SER:O    | 1:B:4241:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:4631:ASP:O    | 1:B:4634:VAL:HG12 | 2.20                     | 0.41              |
| 1:C:21:VAL:HG13   | 1:C:217:ILE:HG13  | 2.02                     | 0.41              |
| 1:C:365:HIS:HE1   | 1:C:367:ASP:HB2   | 1.86                     | 0.41              |
| 1:C:728:ASP:OD1   | 1:C:731:HIS:N     | 2.41                     | 0.41              |
| 1:C:928:GLU:HG3   | 4:C:5003:ATP:C8   | 2.55                     | 0.41              |
| 1:C:1977:LEU:O    | 1:C:1977:LEU:HD23 | 2.20                     | 0.41              |
| 1:C:1991:GLU:HG2  | 1:C:1992:ILE:N    | 2.35                     | 0.41              |
| 1:C:2071:GLN:O    | 1:C:3660:ARG:NH2  | 2.53                     | 0.41              |
| 1:C:2338:GLU:N    | 1:C:2338:GLU:OE1  | 2.54                     | 0.41              |
| 1:C:2842:GLU:O    | 1:C:2846:GLU:HG3  | 2.21                     | 0.41              |
| 1:C:2891:ASP:OD1  | 1:C:2892:ILE:N    | 2.54                     | 0.41              |
| 1:C:3173:THR:OG1  | 1:C:3201:VAL:HG13 | 2.20                     | 0.41              |
| 1:C:4044:SER:HA   | 1:C:4077:THR:HA   | 2.02                     | 0.41              |
| 1:C:4120:GLU:HA   | 1:C:4123:GLU:CD   | 2.45                     | 0.41              |
| 1:D:21:VAL:HG13   | 1:D:217:ILE:HG13  | 2.02                     | 0.41              |
| 1:D:677:LEU:HD12  | 1:D:801:ARG:O     | 2.20                     | 0.41              |
| 1:D:1154:ARG:H    | 1:D:1182:LEU:HD22 | 1.85                     | 0.41              |
| 1:D:2649:PHE:CE2  | 1:D:2962:PHE:HZ   | 2.38                     | 0.41              |
| 1:D:3187:LYS:HG2  | 1:D:3187:LYS:O    | 2.21                     | 0.41              |
| 1:D:3323:MET:HB3  | 1:D:3327:LYS:NZ   | 2.34                     | 0.41              |
| 1:D:4242:ARG:HH22 | 1:D:4249:ARG:NH1  | 2.18                     | 0.41              |
| 1:A:1257:GLN:HB2  | 1:A:1595:LEU:HD12 | 2.03                     | 0.41              |
| 1:A:2086:VAL:HG22 | 1:A:3687:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:2303:ARG:HH11 | 1:A:2304:PHE:HA   | 1.84                     | 0.41              |
| 1:A:2691:LYS:HG3  | 1:A:2693:SER:H    | 1.86                     | 0.41              |
| 1:A:2788:ARG:NH1  | 1:A:2904:SER:HB3  | 2.35                     | 0.41              |
| 1:A:3007:LEU:O    | 1:A:3011:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:3163:ALA:HB3  | 1:A:3244:SER:OG   | 2.21                     | 0.41              |
| 1:A:3191:GLU:OE2  | 1:A:3192:ARG:HG2  | 2.20                     | 0.41              |
| 1:A:3912:VAL:O    | 1:A:3916:VAL:HG23 | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4038:ASP:O    | 1:A:4040:LYS:N    | 2.49                     | 0.41              |
| 2:E:22:THR:HG22   | 2:E:50:ARG:HB2    | 2.01                     | 0.41              |
| 1:B:643:LEU:HD13  | 1:B:1657:THR:HG23 | 2.02                     | 0.41              |
| 1:B:1257:GLN:HB2  | 1:B:1595:LEU:HD12 | 2.03                     | 0.41              |
| 1:B:2071:GLN:O    | 1:B:3660:ARG:NH2  | 2.53                     | 0.41              |
| 1:B:2178:VAL:HG21 | 1:B:2192:MET:CE   | 2.45                     | 0.41              |
| 1:B:2255:LEU:O    | 1:B:3810:ARG:NH2  | 2.49                     | 0.41              |
| 1:B:2649:PHE:CE2  | 1:B:2962:PHE:HZ   | 2.38                     | 0.41              |
| 1:B:2705:PRO:HD3  | 1:B:2854:LYS:HG3  | 2.02                     | 0.41              |
| 1:B:2842:GLU:O    | 1:B:2846:GLU:HG3  | 2.21                     | 0.41              |
| 1:B:3173:THR:OG1  | 1:B:3201:VAL:HG13 | 2.20                     | 0.41              |
| 1:B:3235:MET:HA   | 1:B:3239:LEU:HD12 | 2.01                     | 0.41              |
| 1:B:4044:SER:HA   | 1:B:4077:THR:HA   | 2.02                     | 0.41              |
| 1:C:230:GLY:HA2   | 1:C:289:ILE:HD11  | 2.02                     | 0.41              |
| 1:C:1010:ASP:HA   | 1:C:1013:ARG:HD2  | 2.02                     | 0.41              |
| 1:C:2303:ARG:HH11 | 1:C:2304:PHE:HA   | 1.85                     | 0.41              |
| 1:C:2406:MET:HE1  | 1:C:2420:ARG:HH21 | 1.85                     | 0.41              |
| 1:C:3276:LEU:HA   | 1:C:3276:LEU:HD23 | 1.85                     | 0.41              |
| 1:D:365:HIS:HE1   | 1:D:367:ASP:HB2   | 1.85                     | 0.41              |
| 1:D:643:LEU:HD13  | 1:D:1657:THR:HG23 | 2.02                     | 0.41              |
| 1:D:1795:LEU:O    | 1:D:1799:VAL:HG23 | 2.20                     | 0.41              |
| 1:D:2172:MET:HE2  | 1:D:2172:MET:HB2  | 1.93                     | 0.41              |
| 1:D:3306:ILE:HA   | 1:D:3309:LYS:HE2  | 2.01                     | 0.41              |
| 1:A:174:LYS:O     | 1:A:176:ARG:NH1   | 2.53                     | 0.41              |
| 1:A:1135:PHE:HB3  | 1:A:1192:PHE:CE2  | 2.56                     | 0.41              |
| 1:A:1154:ARG:H    | 1:A:1182:LEU:HD22 | 1.85                     | 0.41              |
| 1:A:1977:LEU:O    | 1:A:1977:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:2788:ARG:H    | 1:A:2788:ARG:HD3  | 1.85                     | 0.41              |
| 1:A:2842:GLU:O    | 1:A:2846:GLU:HG3  | 2.21                     | 0.41              |
| 1:A:3109:PHE:N    | 1:A:3109:PHE:CD2  | 2.88                     | 0.41              |
| 1:A:3926:GLY:O    | 1:A:3927:PRO:C    | 2.63                     | 0.41              |
| 1:B:272:ARG:C     | 1:B:299:HIS:HE2   | 2.28                     | 0.41              |
| 1:B:928:GLU:HG3   | 4:B:5003:ATP:C8   | 2.55                     | 0.41              |
| 1:B:1219:LYS:NZ   | 1:B:1243:THR:OG1  | 2.42                     | 0.41              |
| 1:B:1220:ASP:CG   | 1:B:1222:SER:HG   | 2.28                     | 0.41              |
| 1:B:1682:GLU:HB3  | 1:B:1683:PRO:HD3  | 2.03                     | 0.41              |
| 1:B:2778:SER:O    | 1:B:2781:THR:OG1  | 2.31                     | 0.41              |
| 1:B:2926:LEU:HG   | 1:B:3003:MET:HE2  | 2.02                     | 0.41              |
| 1:B:3129:SER:O    | 1:B:3133:ILE:HG13 | 2.20                     | 0.41              |
| 1:B:3323:MET:HE3  | 1:B:3327:LYS:NZ   | 2.34                     | 0.41              |
| 1:C:27:THR:HA     | 1:C:31:GLU:O      | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1023:ASP:OD1  | 1:C:1025:LYS:HG3  | 2.19                     | 0.41              |
| 1:C:1154:ARG:H    | 1:C:1182:LEU:HD22 | 1.85                     | 0.41              |
| 1:C:2407:HIS:CG   | 1:C:2408:LEU:N    | 2.88                     | 0.41              |
| 1:C:2413:LYS:HD3  | 1:C:2415:GLU:HB3  | 2.03                     | 0.41              |
| 1:C:2691:LYS:HG3  | 1:C:2693:SER:H    | 1.86                     | 0.41              |
| 1:C:2788:ARG:NH1  | 1:C:2904:SER:HB3  | 2.35                     | 0.41              |
| 1:C:2791:ARG:HD2  | 1:C:2901:TYR:CZ   | 2.55                     | 0.41              |
| 1:C:3234:VAL:HG13 | 1:C:3238:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:3912:VAL:O    | 1:C:3916:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:4190:VAL:HG11 | 1:C:4949:TRP:CH2  | 2.55                     | 0.41              |
| 1:C:4197:ILE:HG12 | 1:C:4923:MET:HE3  | 2.01                     | 0.41              |
| 1:D:808:HIS:O     | 1:D:1616:GLY:HA2  | 2.20                     | 0.41              |
| 1:D:2729:HIS:CD2  | 1:D:2763:LEU:HD11 | 2.55                     | 0.41              |
| 1:D:3018:ARG:HD3  | 1:D:3021:LEU:HD22 | 2.01                     | 0.41              |
| 1:D:3773:VAL:HG12 | 1:D:3777:MET:HE3  | 2.02                     | 0.41              |
| 1:D:3926:GLY:O    | 1:D:3927:PRO:C    | 2.63                     | 0.41              |
| 1:A:227:TYR:HA    | 1:A:355:LYS:HA    | 2.03                     | 0.41              |
| 1:A:371:TRP:N     | 1:A:394:HIS:O     | 2.42                     | 0.41              |
| 1:A:375:GLN:HB2   | 1:A:392:ILE:HB    | 2.03                     | 0.41              |
| 1:A:911:ASN:OD1   | 1:A:912:LYS:N     | 2.53                     | 0.41              |
| 1:A:2406:MET:HE1  | 1:A:2420:ARG:HH21 | 1.85                     | 0.41              |
| 1:A:2424:ARG:HG2  | 1:A:2476:TYR:CD1  | 2.55                     | 0.41              |
| 1:A:2891:ASP:OD1  | 1:A:2892:ILE:N    | 2.53                     | 0.41              |
| 1:A:3018:ARG:HD3  | 1:A:3021:LEU:HD22 | 2.01                     | 0.41              |
| 1:A:3135:THR:HA   | 1:A:3208:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:3328:LYS:NZ   | 1:A:3329:LYS:HE3  | 2.35                     | 0.41              |
| 1:A:3329:LYS:HA   | 1:A:3329:LYS:HD3  | 1.86                     | 0.41              |
| 1:B:364:GLN:HG3   | 1:B:370:LEU:O     | 2.20                     | 0.41              |
| 1:B:1135:PHE:HB3  | 1:B:1192:PHE:CE2  | 2.56                     | 0.41              |
| 1:B:1896:MET:O    | 1:B:1896:MET:HG2  | 2.19                     | 0.41              |
| 1:B:1991:GLU:HG2  | 1:B:1992:ILE:N    | 2.35                     | 0.41              |
| 1:B:2581:ARG:HB3  | 1:B:2584:MET:HE2  | 2.02                     | 0.41              |
| 1:B:2888:LYS:HA   | 1:B:2891:ASP:OD2  | 2.21                     | 0.41              |
| 1:B:3234:VAL:HG13 | 1:B:3238:ILE:HD11 | 2.02                     | 0.41              |
| 1:B:4617:ILE:HG13 | 1:B:4665:ARG:HH12 | 1.85                     | 0.41              |
| 1:C:49:LEU:HD11   | 1:C:203:VAL:HG13  | 2.02                     | 0.41              |
| 1:C:375:GLN:HB2   | 1:C:392:ILE:HB    | 2.03                     | 0.41              |
| 1:C:969:ASN:OD1   | 1:C:970:TYR:N     | 2.54                     | 0.41              |
| 1:C:1100:ARG:HB2  | 1:C:1236:TYR:CE1  | 2.56                     | 0.41              |
| 1:C:1257:GLN:HB2  | 1:C:1595:LEU:HD12 | 2.03                     | 0.41              |
| 1:C:1270:VAL:HG22 | 1:C:1285:VAL:HG22 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1682:GLU:HB3  | 1:C:1683:PRO:HD3  | 2.03                     | 0.41              |
| 1:C:2664:LEU:O    | 1:C:2667:PRO:HD2  | 2.19                     | 0.41              |
| 1:C:2788:ARG:HD3  | 1:C:2788:ARG:H    | 1.85                     | 0.41              |
| 1:C:3642:GLU:O    | 1:C:3646:LYS:HG3  | 2.20                     | 0.41              |
| 1:C:3699:CYS:SG   | 1:C:3731:LEU:HD12 | 2.60                     | 0.41              |
| 1:D:314:LEU:HD21  | 1:D:393:MET:HB2   | 2.02                     | 0.41              |
| 1:D:969:ASN:OD1   | 1:D:970:TYR:N     | 2.54                     | 0.41              |
| 1:D:1105:PHE:HB3  | 1:D:1162:VAL:HG13 | 2.02                     | 0.41              |
| 1:D:1135:PHE:HB3  | 1:D:1192:PHE:CE2  | 2.55                     | 0.41              |
| 1:D:1177:LEU:HD12 | 1:D:1177:LEU:HA   | 1.89                     | 0.41              |
| 1:D:1257:GLN:HB2  | 1:D:1595:LEU:HD12 | 2.03                     | 0.41              |
| 1:D:1502:ASN:OD1  | 1:D:1503:ASN:N    | 2.53                     | 0.41              |
| 1:D:2580:LEU:O    | 1:D:2585:MET:HE1  | 2.19                     | 0.41              |
| 1:D:2646:TRP:CH2  | 1:D:2925:PHE:HA   | 2.55                     | 0.41              |
| 1:D:2888:LYS:HA   | 1:D:2891:ASP:OD2  | 2.21                     | 0.41              |
| 1:D:3642:GLU:O    | 1:D:3646:LYS:HG3  | 2.20                     | 0.41              |
| 1:D:4617:ILE:HG13 | 1:D:4665:ARG:HH12 | 1.85                     | 0.41              |
| 1:A:677:LEU:HD12  | 1:A:801:ARG:O     | 2.20                     | 0.41              |
| 1:A:902:TRP:NE1   | 1:A:915:HIS:HB2   | 2.35                     | 0.41              |
| 1:A:919:VAL:HG21  | 1:A:923:LYS:CD    | 2.50                     | 0.41              |
| 1:A:1423:THR:HG23 | 1:A:1564:MET:HG2  | 2.02                     | 0.41              |
| 1:A:2338:GLU:N    | 1:A:2338:GLU:OE1  | 2.54                     | 0.41              |
| 1:A:3739:MET:HE2  | 1:A:3739:MET:HB3  | 1.87                     | 0.41              |
| 1:A:4631:ASP:O    | 1:A:4634:VAL:HG12 | 2.20                     | 0.41              |
| 2:G:88:HIS:HA     | 2:G:89:PRO:HD3    | 1.94                     | 0.41              |
| 1:B:370:LEU:C     | 1:B:393:MET:HE3   | 2.45                     | 0.41              |
| 1:B:456:LEU:O     | 1:B:460:ILE:HG12  | 2.21                     | 0.41              |
| 1:B:1205:CYS:SG   | 1:B:1215:MET:HE3  | 2.60                     | 0.41              |
| 1:B:1423:THR:HG23 | 1:B:1564:MET:HG2  | 2.02                     | 0.41              |
| 1:B:1686:LEU:HD22 | 1:B:1790:LYS:HE2  | 2.03                     | 0.41              |
| 1:B:2141:LEU:O    | 1:B:2144:ARG:HG3  | 2.20                     | 0.41              |
| 1:B:2307:PHE:CG   | 1:B:2401:ARG:HD3  | 2.55                     | 0.41              |
| 1:B:3243:CYS:HA   | 1:B:3246:MET:SD   | 2.61                     | 0.41              |
| 1:C:996:VAL:HA    | 1:C:999:LEU:HD12  | 2.02                     | 0.41              |
| 1:C:2888:LYS:HA   | 1:C:2891:ASP:OD2  | 2.21                     | 0.41              |
| 1:C:3986:LEU:HG   | 1:C:3999:MET:HE1  | 2.03                     | 0.41              |
| 1:C:4055:HIS:CD2  | 1:C:4057:HIS:HD1  | 2.38                     | 0.41              |
| 1:D:227:TYR:HA    | 1:D:355:LYS:HA    | 2.03                     | 0.41              |
| 1:D:1682:GLU:HB3  | 1:D:1683:PRO:HD3  | 2.03                     | 0.41              |
| 1:D:2135:GLY:H    | 1:D:2138:GLU:HB2  | 1.84                     | 0.41              |
| 1:D:2791:ARG:HD2  | 1:D:2901:TYR:CZ   | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:964:MET:SD    | 1:A:979:ALA:HB3   | 2.61                     | 0.41              |
| 1:A:1757:LEU:HD21 | 1:A:2113:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:1947:VAL:HG12 | 1:A:1948:MET:HE2  | 2.02                     | 0.41              |
| 1:A:1991:GLU:HG2  | 1:A:1992:ILE:N    | 2.35                     | 0.41              |
| 1:A:2157:GLN:O    | 1:A:3615:ARG:NH2  | 2.25                     | 0.41              |
| 1:A:2290:TRP:CZ3  | 1:A:2292:PRO:HB3  | 2.56                     | 0.41              |
| 1:A:2857:LYS:O    | 1:A:2861:GLU:OE1  | 2.38                     | 0.41              |
| 2:H:22:THR:HG22   | 2:H:50:ARG:HB2    | 2.01                     | 0.41              |
| 1:B:692:HIS:O     | 1:B:794:PHE:HA    | 2.20                     | 0.41              |
| 1:B:1010:ASP:HA   | 1:B:1013:ARG:HD2  | 2.02                     | 0.41              |
| 1:B:1100:ARG:HB2  | 1:B:1236:TYR:CE1  | 2.56                     | 0.41              |
| 1:B:2790:GLU:O    | 1:B:2902:ALA:N    | 2.41                     | 0.41              |
| 1:B:3109:PHE:HE1  | 1:B:3162:PHE:CD1  | 2.31                     | 0.41              |
| 1:B:3187:LYS:HG2  | 1:B:3187:LYS:O    | 2.21                     | 0.41              |
| 1:C:240:HIS:O     | 1:D:167:LYS:NZ    | 2.28                     | 0.41              |
| 1:C:2290:TRP:CZ3  | 1:C:2292:PRO:HB3  | 2.56                     | 0.41              |
| 1:C:2729:HIS:CD2  | 1:C:2763:LEU:HD11 | 2.55                     | 0.41              |
| 1:C:2768:LYS:O    | 1:C:2772:ARG:N    | 2.47                     | 0.41              |
| 1:C:2953:HIS:ND1  | 1:C:2953:HIS:O    | 2.54                     | 0.41              |
| 1:C:3163:ALA:HB3  | 1:C:3244:SER:OG   | 2.21                     | 0.41              |
| 1:C:3929:THR:O    | 1:C:3933:GLN:HG2  | 2.20                     | 0.41              |
| 1:D:125:TYR:CE1   | 1:D:417:ARG:HD3   | 2.55                     | 0.41              |
| 1:D:964:MET:SD    | 1:D:979:ALA:HB3   | 2.61                     | 0.41              |
| 1:D:1115:VAL:HG22 | 1:D:1164:CYS:SG   | 2.61                     | 0.41              |
| 1:D:2125:GLN:O    | 1:D:2129:LEU:HD23 | 2.21                     | 0.41              |
| 1:D:2290:TRP:CZ3  | 1:D:2292:PRO:HB3  | 2.56                     | 0.41              |
| 1:D:2591:ARG:HH22 | 1:D:2875:ASP:HB2  | 1.85                     | 0.41              |
| 1:D:2842:GLU:O    | 1:D:2846:GLU:HG3  | 2.21                     | 0.41              |
| 1:D:3929:THR:O    | 1:D:3933:GLN:HG2  | 2.20                     | 0.41              |
| 1:A:230:GLY:HA2   | 1:A:289:ILE:HD11  | 2.02                     | 0.41              |
| 1:A:625:VAL:CG1   | 1:A:2133:ARG:HD3  | 2.50                     | 0.41              |
| 1:A:732:LEU:HD23  | 1:A:732:LEU:HA    | 1.91                     | 0.41              |
| 1:A:808:HIS:O     | 1:A:1616:GLY:HA2  | 2.20                     | 0.41              |
| 1:A:1682:GLU:HB3  | 1:A:1683:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:1729:MET:HG3  | 1:A:1729:MET:O    | 2.21                     | 0.41              |
| 1:A:2222:LEU:HB3  | 1:A:2264:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:2451:VAL:HG11 | 1:A:2510:THR:HG22 | 2.03                     | 0.41              |
| 1:A:2465:LYS:O    | 1:A:2469:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:2525:LEU:HB2  | 1:A:2526:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:2554:ARG:NH1  | 1:A:2699:GLY:HA2  | 2.33                     | 0.41              |
| 1:A:2589:LEU:O    | 1:A:2593:VAL:HG13 | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2730:ASP:OD1  | 1:A:2824:ARG:HA   | 2.20                     | 0.41              |
| 1:A:2769:GLU:C    | 1:A:2771:TYR:N    | 2.79                     | 0.41              |
| 1:A:2953:HIS:ND1  | 1:A:2953:HIS:O    | 2.54                     | 0.41              |
| 1:A:3173:THR:OG1  | 1:A:3201:VAL:HG13 | 2.20                     | 0.41              |
| 1:A:3642:GLU:O    | 1:A:3646:LYS:HG3  | 2.20                     | 0.41              |
| 1:A:3858:LEU:HD23 | 1:A:3858:LEU:HA   | 1.88                     | 0.41              |
| 1:A:4032:PHE:HE2  | 1:A:4043:ILE:HG12 | 1.86                     | 0.41              |
| 1:A:4044:SER:HA   | 1:A:4077:THR:HA   | 2.02                     | 0.41              |
| 1:A:4059:THR:O    | 1:A:4063:THR:OG1  | 2.31                     | 0.41              |
| 1:B:21:VAL:HG13   | 1:B:217:ILE:HG13  | 2.02                     | 0.41              |
| 1:B:394:HIS:HE1   | 1:B:396:GLU:HG3   | 1.85                     | 0.41              |
| 1:B:992:GLN:OE1   | 1:B:992:GLN:N     | 2.54                     | 0.41              |
| 1:B:2086:VAL:HG22 | 1:B:3687:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:2413:LYS:HD3  | 1:B:2415:GLU:HB3  | 2.03                     | 0.41              |
| 1:B:2424:ARG:HG2  | 1:B:2476:TYR:CD1  | 2.55                     | 0.41              |
| 1:B:2722:ASN:C    | 1:B:2724:TYR:H    | 2.29                     | 0.41              |
| 1:B:2730:ASP:OD1  | 1:B:2824:ARG:HA   | 2.20                     | 0.41              |
| 1:B:2953:HIS:ND1  | 1:B:2953:HIS:O    | 2.54                     | 0.41              |
| 1:B:3109:PHE:N    | 1:B:3109:PHE:CD2  | 2.88                     | 0.41              |
| 1:B:3191:GLU:OE2  | 1:B:3192:ARG:HG2  | 2.20                     | 0.41              |
| 1:B:3297:LYS:HD2  | 1:B:3335:SER:O    | 2.21                     | 0.41              |
| 1:B:3328:LYS:NZ   | 1:B:3329:LYS:HE3  | 2.35                     | 0.41              |
| 1:B:3900:GLU:OE1  | 1:B:3901:GLN:NE2  | 2.44                     | 0.41              |
| 1:B:3912:VAL:O    | 1:B:3916:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:3926:GLY:O    | 1:B:3927:PRO:C    | 2.63                     | 0.41              |
| 1:B:4032:PHE:HE2  | 1:B:4043:ILE:HG12 | 1.86                     | 0.41              |
| 1:B:4055:HIS:CD2  | 1:B:4057:HIS:HD1  | 2.38                     | 0.41              |
| 1:B:4863:GLN:HG3  | 1:C:4860:ALA:CB   | 2.51                     | 0.41              |
| 1:B:4895:ASN:HA   | 1:B:4905:PHE:CD1  | 2.56                     | 0.41              |
| 1:C:188:SER:HB2   | 1:C:190:ARG:NH1   | 2.30                     | 0.41              |
| 1:C:272:ARG:O     | 1:C:299:HIS:NE2   | 2.46                     | 0.41              |
| 1:C:394:HIS:HE1   | 1:C:396:GLU:HG3   | 1.85                     | 0.41              |
| 1:C:456:LEU:O     | 1:C:460:ILE:HG12  | 2.21                     | 0.41              |
| 1:C:810:GLU:OE1   | 1:C:1614:ARG:HA   | 2.21                     | 0.41              |
| 1:C:1023:ASP:OD1  | 1:C:1024:VAL:N    | 2.53                     | 0.41              |
| 1:C:1115:VAL:HG22 | 1:C:1164:CYS:SG   | 2.61                     | 0.41              |
| 1:C:1686:LEU:HD22 | 1:C:1790:LYS:HE2  | 2.03                     | 0.41              |
| 1:C:2465:LYS:O    | 1:C:2469:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:2649:PHE:CE2  | 1:C:2962:PHE:HZ   | 2.38                     | 0.41              |
| 1:C:3243:CYS:HA   | 1:C:3246:MET:SD   | 2.61                     | 0.41              |
| 1:C:4507:LEU:HD12 | 1:C:4507:LEU:HA   | 1.79                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:364:GLN:HG3   | 1:D:370:LEU:O     | 2.20                     | 0.41              |
| 1:D:375:GLN:HB2   | 1:D:392:ILE:HB    | 2.03                     | 0.41              |
| 1:D:434:ASP:HB3   | 1:D:438:LYS:HZ3   | 1.85                     | 0.41              |
| 1:D:928:GLU:HG3   | 4:D:5003:ATP:C8   | 2.55                     | 0.41              |
| 1:D:965:LYS:HA    | 1:D:978:PRO:HD2   | 2.03                     | 0.41              |
| 1:D:1729:MET:HG3  | 1:D:1729:MET:O    | 2.21                     | 0.41              |
| 1:D:2071:GLN:O    | 1:D:3660:ARG:NH2  | 2.53                     | 0.41              |
| 1:D:2465:LYS:O    | 1:D:2469:VAL:HG23 | 2.21                     | 0.41              |
| 1:D:2926:LEU:HG   | 1:D:3003:MET:HE2  | 2.02                     | 0.41              |
| 1:D:2972:ASP:HA   | 1:D:3035:ILE:HD11 | 2.03                     | 0.41              |
| 1:D:2984:SER:OG   | 1:D:2989:PRO:HB2  | 2.21                     | 0.41              |
| 1:D:3007:LEU:O    | 1:D:3011:LEU:HD23 | 2.20                     | 0.41              |
| 1:D:3234:VAL:HG13 | 1:D:3238:ILE:HD11 | 2.02                     | 0.41              |
| 1:D:3699:CYS:SG   | 1:D:3731:LEU:HD12 | 2.60                     | 0.41              |
| 1:D:3912:VAL:O    | 1:D:3916:VAL:HG23 | 2.21                     | 0.41              |
| 1:D:4059:THR:O    | 1:D:4063:THR:OG1  | 2.31                     | 0.41              |
| 1:A:314:LEU:HD21  | 1:A:393:MET:HB2   | 2.02                     | 0.41              |
| 1:A:456:LEU:O     | 1:A:460:ILE:HG12  | 2.21                     | 0.41              |
| 1:A:1010:ASP:HA   | 1:A:1013:ARG:HD2  | 2.02                     | 0.41              |
| 1:A:1502:ASN:OD1  | 1:A:1503:ASN:N    | 2.53                     | 0.41              |
| 1:A:2222:LEU:HD23 | 1:A:2222:LEU:HA   | 1.84                     | 0.41              |
| 1:A:2407:HIS:CG   | 1:A:2408:LEU:N    | 2.88                     | 0.41              |
| 1:A:2984:SER:OG   | 1:A:2989:PRO:HB2  | 2.21                     | 0.41              |
| 1:A:3069:GLU:OE1  | 1:A:3132:ARG:NH1  | 2.54                     | 0.41              |
| 1:A:4875:ASP:OD2  | 1:D:4874:ARG:NH2  | 2.53                     | 0.41              |
| 1:A:4895:ASN:HA   | 1:A:4905:PHE:CD1  | 2.56                     | 0.41              |
| 1:B:919:VAL:HG21  | 1:B:923:LYS:CD    | 2.50                     | 0.41              |
| 1:B:969:ASN:OD1   | 1:B:970:TYR:N     | 2.54                     | 0.41              |
| 1:B:1796:THR:OG1  | 1:B:1845:LEU:HD11 | 2.21                     | 0.41              |
| 1:B:2338:GLU:OE1  | 1:B:2338:GLU:N    | 2.54                     | 0.41              |
| 1:B:2465:LYS:O    | 1:B:2469:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:2585:MET:O    | 1:B:2589:LEU:HG   | 2.20                     | 0.41              |
| 1:B:2769:GLU:C    | 1:B:2771:TYR:N    | 2.79                     | 0.41              |
| 1:B:2791:ARG:HD2  | 1:B:2901:TYR:CZ   | 2.56                     | 0.41              |
| 1:B:3007:LEU:O    | 1:B:3011:LEU:HD23 | 2.20                     | 0.41              |
| 1:B:3163:ALA:HB3  | 1:B:3244:SER:OG   | 2.21                     | 0.41              |
| 1:B:3986:LEU:HG   | 1:B:3999:MET:HE1  | 2.03                     | 0.41              |
| 1:C:114:LEU:HB2   | 1:C:117:HIS:HD2   | 1.84                     | 0.41              |
| 1:C:1757:LEU:HD21 | 1:C:2113:VAL:HG13 | 2.03                     | 0.41              |
| 1:C:2581:ARG:HB3  | 1:C:2584:MET:HE2  | 2.02                     | 0.41              |
| 1:C:2589:LEU:O    | 1:C:2593:VAL:HG13 | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2705:PRO:HD3  | 1:C:2854:LYS:HG3  | 2.02                     | 0.41              |
| 1:C:2769:GLU:C    | 1:C:2771:TYR:N    | 2.79                     | 0.41              |
| 1:C:3773:VAL:HG12 | 1:C:3777:MET:HE3  | 2.02                     | 0.41              |
| 1:D:230:GLY:HA2   | 1:D:289:ILE:HD11  | 2.02                     | 0.41              |
| 1:D:1219:LYS:NZ   | 1:D:1243:THR:OG1  | 2.42                     | 0.41              |
| 1:D:2141:LEU:O    | 1:D:2144:ARG:HG3  | 2.20                     | 0.41              |
| 1:D:2788:ARG:H    | 1:D:2788:ARG:HD3  | 1.84                     | 0.41              |
| 1:D:2891:ASP:OD1  | 1:D:2892:ILE:N    | 2.53                     | 0.41              |
| 1:D:3069:GLU:OE1  | 1:D:3132:ARG:NH1  | 2.54                     | 0.41              |
| 1:D:3163:ALA:HB3  | 1:D:3244:SER:OG   | 2.21                     | 0.41              |
| 1:D:3243:CYS:HA   | 1:D:3246:MET:SD   | 2.61                     | 0.41              |
| 1:D:4044:SER:HA   | 1:D:4077:THR:HA   | 2.02                     | 0.41              |
| 1:D:4055:HIS:CD2  | 1:D:4057:HIS:HD1  | 2.38                     | 0.41              |
| 1:A:13:PHE:CD1    | 1:A:174:LYS:HG3   | 2.56                     | 0.40              |
| 1:A:703:TYR:CD2   | 1:A:858:THR:HA    | 2.57                     | 0.40              |
| 1:A:829:LYS:NZ    | 1:A:1037:LEU:O    | 2.49                     | 0.40              |
| 1:A:965:LYS:HA    | 1:A:978:PRO:HD2   | 2.03                     | 0.40              |
| 1:A:2514:LEU:HB2  | 1:A:2518:ARG:HH21 | 1.86                     | 0.40              |
| 1:A:2736:LYS:HZ1  | 1:A:2756:LEU:HB3  | 1.86                     | 0.40              |
| 1:A:3305:PRO:HB2  | 1:A:3309:LYS:HZ3  | 1.86                     | 0.40              |
| 1:A:4622:SER:C    | 1:A:4624:ASP:H    | 2.30                     | 0.40              |
| 1:B:270:HIS:CE1   | 1:B:491:GLU:HG3   | 2.56                     | 0.40              |
| 1:B:375:GLN:HB2   | 1:B:392:ILE:HB    | 2.03                     | 0.40              |
| 1:B:1054:VAL:O    | 1:B:1057:LEU:HB3  | 2.21                     | 0.40              |
| 1:B:1105:PHE:HB3  | 1:B:1162:VAL:HG13 | 2.02                     | 0.40              |
| 1:B:1502:ASN:OD1  | 1:B:1503:ASN:N    | 2.53                     | 0.40              |
| 1:B:2222:LEU:HB3  | 1:B:2264:LYS:HD2  | 2.02                     | 0.40              |
| 1:C:891:GLU:O     | 1:C:894:VAL:HG22  | 2.20                     | 0.40              |
| 1:C:964:MET:SD    | 1:C:979:ALA:HB3   | 2.61                     | 0.40              |
| 1:C:1796:THR:OG1  | 1:C:1845:LEU:HD11 | 2.21                     | 0.40              |
| 1:C:3191:GLU:OE2  | 1:C:3192:ARG:HG2  | 2.20                     | 0.40              |
| 1:D:13:PHE:CD1    | 1:D:174:LYS:HG3   | 2.56                     | 0.40              |
| 1:D:62:LEU:O      | 1:D:66:THR:HG23   | 2.22                     | 0.40              |
| 1:D:394:HIS:HE1   | 1:D:396:GLU:HG3   | 1.85                     | 0.40              |
| 1:D:794:PHE:HB2   | 1:D:798:ILE:HG13  | 2.03                     | 0.40              |
| 1:D:1686:LEU:HD23 | 1:D:1686:LEU:HA   | 1.92                     | 0.40              |
| 1:D:2338:GLU:OE1  | 1:D:2338:GLU:N    | 2.54                     | 0.40              |
| 1:D:2406:MET:HE1  | 1:D:2420:ARG:HH21 | 1.85                     | 0.40              |
| 1:D:2413:LYS:HD3  | 1:D:2415:GLU:HB3  | 2.03                     | 0.40              |
| 1:D:2722:ASN:C    | 1:D:2724:TYR:H    | 2.29                     | 0.40              |
| 1:A:14:LEU:HG     | 1:A:177:VAL:HG12  | 2.04                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:992:GLN:OE1   | 1:A:992:GLN:N     | 2.54                     | 0.40              |
| 1:A:1115:VAL:HG22 | 1:A:1164:CYS:SG   | 2.61                     | 0.40              |
| 1:A:1796:THR:OG1  | 1:A:1845:LEU:HD11 | 2.21                     | 0.40              |
| 1:A:1929:SER:OG   | 1:A:3617:VAL:HG13 | 2.22                     | 0.40              |
| 1:A:2856:LYS:HD3  | 1:A:2868:HIS:CE1  | 2.56                     | 0.40              |
| 1:A:2926:LEU:HG   | 1:A:3003:MET:HE2  | 2.02                     | 0.40              |
| 1:A:3297:LYS:HD2  | 1:A:3335:SER:O    | 2.21                     | 0.40              |
| 1:A:4054:SER:O    | 1:A:4056:LYS:NZ   | 2.34                     | 0.40              |
| 1:A:4055:HIS:CD2  | 1:A:4057:HIS:HD1  | 2.38                     | 0.40              |
| 1:B:365:HIS:HE1   | 1:B:367:ASP:HB2   | 1.86                     | 0.40              |
| 1:B:794:PHE:HB2   | 1:B:798:ILE:HG13  | 2.03                     | 0.40              |
| 1:B:891:GLU:O     | 1:B:895:MET:HE2   | 2.22                     | 0.40              |
| 1:B:1115:VAL:HG22 | 1:B:1164:CYS:SG   | 2.61                     | 0.40              |
| 1:B:1979:PHE:CZ   | 1:B:1996:LEU:HD23 | 2.57                     | 0.40              |
| 1:B:2290:TRP:CZ3  | 1:B:2292:PRO:HB3  | 2.56                     | 0.40              |
| 1:B:2451:VAL:HG11 | 1:B:2510:THR:HG22 | 2.03                     | 0.40              |
| 1:B:2691:LYS:HG3  | 1:B:2693:SER:H    | 1.86                     | 0.40              |
| 1:B:2984:SER:OG   | 1:B:2989:PRO:HB2  | 2.21                     | 0.40              |
| 1:B:3138:TYR:OH   | 1:B:3209:PRO:HD3  | 2.22                     | 0.40              |
| 1:B:3642:GLU:O    | 1:B:3646:LYS:HG3  | 2.20                     | 0.40              |
| 1:B:4587:ILE:HG13 | 1:B:4726:MET:HE2  | 2.03                     | 0.40              |
| 1:B:4625:ASP:OD1  | 1:B:4625:ASP:N    | 2.46                     | 0.40              |
| 1:C:62:LEU:O      | 1:C:66:THR:HG23   | 2.21                     | 0.40              |
| 1:C:227:TYR:HA    | 1:C:355:LYS:HA    | 2.03                     | 0.40              |
| 1:C:974:SER:HB3   | 1:C:976:TYR:CD2   | 2.52                     | 0.40              |
| 1:C:999:LEU:CB    | 1:C:1050:LEU:HD21 | 2.51                     | 0.40              |
| 1:C:1135:PHE:HB3  | 1:C:1192:PHE:CE2  | 2.55                     | 0.40              |
| 1:C:2591:ARG:HH22 | 1:C:2875:ASP:HB2  | 1.85                     | 0.40              |
| 1:C:2722:ASN:C    | 1:C:2724:TYR:H    | 2.29                     | 0.40              |
| 1:C:2759:PRO:HD2  | 1:C:2762:LEU:HD22 | 2.03                     | 0.40              |
| 1:C:2788:ARG:HD2  | 1:C:2906:GLY:HA2  | 2.03                     | 0.40              |
| 1:C:2998:ASN:OD1  | 1:C:2999:LYS:N    | 2.55                     | 0.40              |
| 1:C:3138:TYR:OH   | 1:C:3209:PRO:HD3  | 2.22                     | 0.40              |
| 1:C:3328:LYS:NZ   | 1:C:3329:LYS:HE3  | 2.35                     | 0.40              |
| 1:C:3948:LEU:HD23 | 1:C:3948:LEU:HA   | 1.83                     | 0.40              |
| 1:D:999:LEU:CB    | 1:D:1050:LEU:HD21 | 2.51                     | 0.40              |
| 1:D:2589:LEU:O    | 1:D:2593:VAL:HG13 | 2.21                     | 0.40              |
| 1:D:3986:LEU:HG   | 1:D:3999:MET:HE1  | 2.03                     | 0.40              |
| 1:D:4631:ASP:O    | 1:D:4634:VAL:HG12 | 2.20                     | 0.40              |
| 1:A:49:LEU:HD11   | 1:A:203:VAL:HG13  | 2.02                     | 0.40              |
| 1:A:704:SER:HA    | 1:A:856:SER:HA    | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1444:GLY:CA   | 1:A:1487:MET:HG2  | 2.51                     | 0.40              |
| 1:A:3030:VAL:HG12 | 1:A:3034:HIS:CD2  | 2.57                     | 0.40              |
| 1:A:3986:LEU:HG   | 1:A:3999:MET:HE1  | 2.03                     | 0.40              |
| 1:A:4160:TRP:HB2  | 1:A:4200:MET:HE3  | 2.03                     | 0.40              |
| 1:B:810:GLU:OE1   | 1:B:1614:ARG:HA   | 2.21                     | 0.40              |
| 1:B:1086:ARG:NH2  | 1:B:1251:LEU:HD13 | 2.37                     | 0.40              |
| 1:B:1125:ASP:OD1  | 1:B:1126:GLN:N    | 2.55                     | 0.40              |
| 1:B:1154:ARG:H    | 1:B:1182:LEU:HD22 | 1.85                     | 0.40              |
| 1:B:1538:LYS:NZ   | 1:B:1636:ASN:OD1  | 2.52                     | 0.40              |
| 1:B:2347:MET:O    | 1:B:2351:ILE:HG12 | 2.22                     | 0.40              |
| 1:B:2972:ASP:HA   | 1:B:3035:ILE:HD11 | 2.03                     | 0.40              |
| 1:B:2998:ASN:OD1  | 1:B:2999:LYS:N    | 2.55                     | 0.40              |
| 1:B:3906:PHE:HB3  | 1:B:3967:LEU:HD11 | 2.04                     | 0.40              |
| 1:B:4167:GLU:OE2  | 1:B:4170:ARG:NH1  | 2.54                     | 0.40              |
| 1:B:4520:TYR:CE2  | 1:B:4559:TYR:HB3  | 2.57                     | 0.40              |
| 1:B:4622:SER:C    | 1:B:4624:ASP:H    | 2.29                     | 0.40              |
| 1:C:643:LEU:HD13  | 1:C:1657:THR:HG23 | 2.02                     | 0.40              |
| 1:C:732:LEU:HD23  | 1:C:732:LEU:HA    | 1.90                     | 0.40              |
| 1:C:1086:ARG:NH2  | 1:C:1251:LEU:HD13 | 2.37                     | 0.40              |
| 1:C:2715:GLU:HA   | 1:C:2718:GLU:HG3  | 2.03                     | 0.40              |
| 1:C:3007:LEU:O    | 1:C:3011:LEU:HD23 | 2.20                     | 0.40              |
| 1:C:3109:PHE:HD2  | 1:C:3109:PHE:N    | 2.20                     | 0.40              |
| 1:C:3109:PHE:N    | 1:C:3109:PHE:CD2  | 2.88                     | 0.40              |
| 1:C:3926:GLY:O    | 1:C:3927:PRO:C    | 2.63                     | 0.40              |
| 1:C:4617:ILE:HG13 | 1:C:4665:ARG:HH12 | 1.85                     | 0.40              |
| 1:D:992:GLN:OE1   | 1:D:992:GLN:N     | 2.54                     | 0.40              |
| 1:D:1686:LEU:HD22 | 1:D:1790:LYS:HE2  | 2.03                     | 0.40              |
| 1:D:2769:GLU:C    | 1:D:2771:TYR:N    | 2.79                     | 0.40              |
| 1:D:3109:PHE:N    | 1:D:3109:PHE:CD2  | 2.88                     | 0.40              |
| 1:D:4186:MET:HE3  | 1:D:4952:PHE:CG   | 2.57                     | 0.40              |
| 1:A:928:GLU:HA    | 1:A:931:TYR:CD2   | 2.57                     | 0.40              |
| 1:A:1086:ARG:NH2  | 1:A:1251:LEU:HD13 | 2.37                     | 0.40              |
| 1:A:1111:GLY:O    | 1:A:1140:PHE:HB2  | 2.22                     | 0.40              |
| 1:A:1939:ASN:OD1  | 1:A:1939:ASN:C    | 2.65                     | 0.40              |
| 1:A:2649:PHE:CE2  | 1:A:2962:PHE:HZ   | 2.38                     | 0.40              |
| 1:A:2759:PRO:HD2  | 1:A:2762:LEU:HD22 | 2.04                     | 0.40              |
| 1:A:2791:ARG:HD2  | 1:A:2901:TYR:CZ   | 2.56                     | 0.40              |
| 1:A:2860:LEU:HA   | 1:A:2863:LYS:HG2  | 2.03                     | 0.40              |
| 1:A:2888:LYS:HA   | 1:A:2891:ASP:OD2  | 2.21                     | 0.40              |
| 1:A:3699:CYS:O    | 1:A:3727:GLN:NE2  | 2.55                     | 0.40              |
| 1:A:4186:MET:HE3  | 1:A:4952:PHE:CG   | 2.57                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:58:LYS:O      | 2:G:62:GLU:OE1    | 2.40                     | 0.40              |
| 2:H:58:LYS:O      | 2:H:62:GLU:OE1    | 2.40                     | 0.40              |
| 1:B:227:TYR:HA    | 1:B:355:LYS:HA    | 2.03                     | 0.40              |
| 1:B:670:TYR:HE2   | 1:B:672:LYS:HB2   | 1.86                     | 0.40              |
| 1:B:999:LEU:CB    | 1:B:1050:LEU:HD21 | 2.51                     | 0.40              |
| 1:B:1444:GLY:CA   | 1:B:1487:MET:HG2  | 2.51                     | 0.40              |
| 1:B:1757:LEU:HD21 | 1:B:2113:VAL:HG13 | 2.03                     | 0.40              |
| 1:B:4160:TRP:HB2  | 1:B:4200:MET:HE3  | 2.03                     | 0.40              |
| 1:B:4484:ILE:HG13 | 1:B:4485:ILE:N    | 2.37                     | 0.40              |
| 1:C:794:PHE:HB2   | 1:C:798:ILE:HG13  | 2.04                     | 0.40              |
| 1:C:928:GLU:HA    | 1:C:931:TYR:CD2   | 2.57                     | 0.40              |
| 1:C:1054:VAL:O    | 1:C:1057:LEU:HB3  | 2.22                     | 0.40              |
| 1:C:1080:GLY:O    | 1:C:1081:THR:OG1  | 2.35                     | 0.40              |
| 1:C:2456:MET:CE   | 1:C:2462:PRO:HD3  | 2.46                     | 0.40              |
| 1:C:3699:CYS:O    | 1:C:3727:GLN:NE2  | 2.55                     | 0.40              |
| 1:D:270:HIS:CE1   | 1:D:491:GLU:HG3   | 2.56                     | 0.40              |
| 1:D:272:ARG:C     | 1:D:299:HIS:HE2   | 2.28                     | 0.40              |
| 1:D:365:HIS:CE1   | 1:D:368:THR:HG23  | 2.57                     | 0.40              |
| 1:D:456:LEU:O     | 1:D:460:ILE:HG12  | 2.21                     | 0.40              |
| 1:D:655:MET:HE1   | 1:D:836:HIS:ND1   | 2.37                     | 0.40              |
| 1:D:2486:HIS:O    | 1:D:2490:VAL:HG22 | 2.21                     | 0.40              |
| 1:D:2585:MET:HE3  | 1:D:2616:ARG:NH2  | 2.21                     | 0.40              |
| 1:D:2650:ASP:O    | 1:D:2653:SER:N    | 2.55                     | 0.40              |
| 1:D:3172:GLU:OE2  | 1:D:3174:HIS:NE2  | 2.55                     | 0.40              |
| 1:D:3714:PHE:HA   | 1:D:3717:LYS:HE2  | 2.03                     | 0.40              |
| 1:A:270:HIS:CE1   | 1:A:491:GLU:HG3   | 2.56                     | 0.40              |
| 1:A:365:HIS:HE1   | 1:A:367:ASP:HB2   | 1.86                     | 0.40              |
| 1:A:670:TYR:HE2   | 1:A:672:LYS:HB2   | 1.86                     | 0.40              |
| 1:A:1105:PHE:HB3  | 1:A:1162:VAL:HG13 | 2.02                     | 0.40              |
| 1:A:1828:LEU:HD23 | 1:A:1828:LEU:HA   | 1.95                     | 0.40              |
| 1:A:2722:ASN:C    | 1:A:2724:TYR:H    | 2.29                     | 0.40              |
| 1:A:3138:TYR:OH   | 1:A:3209:PRO:HD3  | 2.22                     | 0.40              |
| 1:A:3714:PHE:HA   | 1:A:3717:LYS:HE2  | 2.03                     | 0.40              |
| 1:A:4052:MET:HE1  | 1:A:4063:THR:HA   | 2.03                     | 0.40              |
| 1:A:4587:ILE:HG13 | 1:A:4726:MET:HE2  | 2.02                     | 0.40              |
| 1:A:4625:ASP:OD2  | 1:A:4628:GLY:HA3  | 2.22                     | 0.40              |
| 2:F:58:LYS:O      | 2:F:62:GLU:OE1    | 2.40                     | 0.40              |
| 1:B:928:GLU:HA    | 1:B:931:TYR:CD2   | 2.57                     | 0.40              |
| 1:B:964:MET:SD    | 1:B:979:ALA:HB3   | 2.61                     | 0.40              |
| 1:B:1929:SER:OG   | 1:B:3617:VAL:HG13 | 2.22                     | 0.40              |
| 1:B:4702:ASP:O    | 1:B:4706:GLN:HG2  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:14:LEU:HG     | 1:C:177:VAL:HG12  | 2.04                     | 0.40              |
| 1:C:655:MET:HE1   | 1:C:836:HIS:ND1   | 2.37                     | 0.40              |
| 1:C:670:TYR:HE2   | 1:C:672:LYS:HB2   | 1.86                     | 0.40              |
| 1:C:1979:PHE:CZ   | 1:C:1996:LEU:HD23 | 2.56                     | 0.40              |
| 1:C:2178:VAL:HG21 | 1:C:2192:MET:CE   | 2.45                     | 0.40              |
| 1:C:2856:LYS:HD3  | 1:C:2868:HIS:CE1  | 2.56                     | 0.40              |
| 1:C:3030:VAL:HG12 | 1:C:3034:HIS:CD2  | 2.57                     | 0.40              |
| 1:C:3129:SER:O    | 1:C:3133:ILE:HG13 | 2.20                     | 0.40              |
| 1:C:3197:LEU:O    | 1:C:3199:THR:HG23 | 2.22                     | 0.40              |
| 1:C:4167:GLU:OE2  | 1:C:4170:ARG:NH1  | 2.54                     | 0.40              |
| 1:D:14:LEU:HG     | 1:D:177:VAL:HG12  | 2.04                     | 0.40              |
| 1:D:704:SER:HA    | 1:D:856:SER:HA    | 2.03                     | 0.40              |
| 1:D:875:PRO:HD2   | 1:D:878:LEU:CD1   | 2.52                     | 0.40              |
| 1:D:891:GLU:O     | 1:D:895:MET:HE2   | 2.22                     | 0.40              |
| 1:D:928:GLU:HA    | 1:D:931:TYR:CD2   | 2.57                     | 0.40              |
| 1:D:1125:ASP:OD1  | 1:D:1126:GLN:N    | 2.55                     | 0.40              |
| 1:D:1757:LEU:HD21 | 1:D:2113:VAL:HG13 | 2.03                     | 0.40              |
| 1:D:1847:GLU:OE2  | 1:D:1849:SER:OG   | 2.32                     | 0.40              |
| 1:D:2953:HIS:O    | 1:D:2953:HIS:ND1  | 2.54                     | 0.40              |
| 1:D:3678:GLU:C    | 1:D:3679:LYS:HD3  | 2.47                     | 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     | 4198/4967 (84%) | 4054 (97%) | 140 (3%) | 4 (0%)   | 48          | 78 |
| 1   | B     | 4198/4967 (84%) | 4055 (97%) | 139 (3%) | 4 (0%)   | 48          | 78 |
| 1   | C     | 4198/4967 (84%) | 4053 (96%) | 141 (3%) | 4 (0%)   | 48          | 78 |
| 1   | D     | 4198/4967 (84%) | 4053 (96%) | 141 (3%) | 4 (0%)   | 48          | 78 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 2   | E     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 2   | F     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 2   | G     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 2   | H     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| All | All   | 17212/20300 (85%) | 16623 (97%) | 573 (3%) | 16 (0%)  | 49          | 78  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3927 | PRO  |
| 1   | A     | 4641 | PRO  |
| 1   | B     | 3927 | PRO  |
| 1   | B     | 4641 | PRO  |
| 1   | C     | 3927 | PRO  |
| 1   | C     | 4641 | PRO  |
| 1   | D     | 3927 | PRO  |
| 1   | D     | 4641 | PRO  |
| 1   | A     | 3291 | ASP  |
| 1   | B     | 3291 | ASP  |
| 1   | C     | 3291 | ASP  |
| 1   | D     | 3291 | ASP  |
| 1   | A     | 2770 | ILE  |
| 1   | B     | 2770 | ILE  |
| 1   | C     | 2770 | ILE  |
| 1   | D     | 2770 | ILE  |

### 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     | 3708/4358 (85%) | 3699 (100%) | 9 (0%)   | 87          | 84 |
| 1   | B     | 3708/4358 (85%) | 3699 (100%) | 9 (0%)   | 87          | 84 |
| 1   | C     | 3708/4358 (85%) | 3699 (100%) | 9 (0%)   | 87          | 84 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 1   | D     | 3708/4358 (85%)   | 3699 (100%)  | 9 (0%)   | 87          | 84  |
| 2   | E     | 88/89 (99%)       | 88 (100%)    | 0        | 100         | 100 |
| 2   | F     | 88/89 (99%)       | 88 (100%)    | 0        | 100         | 100 |
| 2   | G     | 88/89 (99%)       | 87 (99%)     | 1 (1%)   | 65          | 71  |
| 2   | H     | 88/89 (99%)       | 88 (100%)    | 0        | 100         | 100 |
| All | All   | 15184/17788 (85%) | 15147 (100%) | 37 (0%)  | 85          | 84  |

All (37) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 317  | MET  |
| 1   | A     | 2779 | LEU  |
| 1   | A     | 3246 | MET  |
| 1   | A     | 3319 | PHE  |
| 1   | A     | 3689 | MET  |
| 1   | A     | 4274 | MET  |
| 1   | A     | 4292 | MET  |
| 1   | A     | 4504 | MET  |
| 1   | A     | 4814 | MET  |
| 2   | G     | 26   | HIS  |
| 1   | B     | 317  | MET  |
| 1   | B     | 2779 | LEU  |
| 1   | B     | 3246 | MET  |
| 1   | B     | 3319 | PHE  |
| 1   | B     | 3689 | MET  |
| 1   | B     | 4274 | MET  |
| 1   | B     | 4292 | MET  |
| 1   | B     | 4504 | MET  |
| 1   | B     | 4814 | MET  |
| 1   | C     | 317  | MET  |
| 1   | C     | 2779 | LEU  |
| 1   | C     | 3246 | MET  |
| 1   | C     | 3319 | PHE  |
| 1   | C     | 3689 | MET  |
| 1   | C     | 4274 | MET  |
| 1   | C     | 4292 | MET  |
| 1   | C     | 4504 | MET  |
| 1   | C     | 4814 | MET  |
| 1   | D     | 317  | MET  |
| 1   | D     | 2779 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 3246 | MET  |
| 1   | D     | 3319 | PHE  |
| 1   | D     | 3689 | MET  |
| 1   | D     | 4274 | MET  |
| 1   | D     | 4292 | MET  |
| 1   | D     | 4504 | MET  |
| 1   | D     | 4814 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 29   | HIS  |
| 1   | A     | 57   | ASN  |
| 1   | A     | 71   | GLN  |
| 1   | A     | 261  | HIS  |
| 1   | A     | 477  | ASN  |
| 1   | A     | 506  | HIS  |
| 1   | A     | 934  | GLN  |
| 1   | A     | 1004 | HIS  |
| 1   | A     | 1005 | ASN  |
| 1   | A     | 1021 | GLN  |
| 1   | A     | 1022 | GLN  |
| 1   | A     | 1046 | ASN  |
| 1   | A     | 1151 | HIS  |
| 1   | A     | 1451 | HIS  |
| 1   | A     | 1477 | HIS  |
| 1   | A     | 1577 | ASN  |
| 1   | A     | 1670 | HIS  |
| 1   | A     | 1691 | ASN  |
| 1   | A     | 2089 | HIS  |
| 1   | A     | 2217 | HIS  |
| 1   | A     | 2250 | ASN  |
| 1   | A     | 2386 | ASN  |
| 1   | A     | 2613 | HIS  |
| 1   | A     | 2802 | ASN  |
| 1   | A     | 2849 | HIS  |
| 1   | A     | 2868 | HIS  |
| 1   | A     | 2890 | GLN  |
| 1   | A     | 2973 | GLN  |
| 1   | A     | 2978 | HIS  |
| 1   | A     | 3111 | HIS  |
| 1   | A     | 3179 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3279 | ASN  |
| 1   | A     | 3286 | ASN  |
| 1   | A     | 3775 | GLN  |
| 1   | A     | 3806 | ASN  |
| 1   | A     | 3831 | GLN  |
| 1   | A     | 3865 | ASN  |
| 1   | A     | 3869 | ASN  |
| 1   | A     | 3953 | HIS  |
| 1   | A     | 4159 | GLN  |
| 1   | A     | 4489 | GLN  |
| 1   | A     | 4638 | GLN  |
| 1   | A     | 4863 | GLN  |
| 1   | A     | 4879 | GLN  |
| 2   | E     | 26   | HIS  |
| 2   | F     | 26   | HIS  |
| 2   | G     | 26   | HIS  |
| 2   | H     | 26   | HIS  |
| 1   | B     | 23   | GLN  |
| 1   | B     | 29   | HIS  |
| 1   | B     | 57   | ASN  |
| 1   | B     | 71   | GLN  |
| 1   | B     | 261  | HIS  |
| 1   | B     | 477  | ASN  |
| 1   | B     | 506  | HIS  |
| 1   | B     | 934  | GLN  |
| 1   | B     | 1005 | ASN  |
| 1   | B     | 1022 | GLN  |
| 1   | B     | 1046 | ASN  |
| 1   | B     | 1151 | HIS  |
| 1   | B     | 1451 | HIS  |
| 1   | B     | 1477 | HIS  |
| 1   | B     | 1577 | ASN  |
| 1   | B     | 1654 | HIS  |
| 1   | B     | 1670 | HIS  |
| 1   | B     | 1691 | ASN  |
| 1   | B     | 2089 | HIS  |
| 1   | B     | 2217 | HIS  |
| 1   | B     | 2250 | ASN  |
| 1   | B     | 2386 | ASN  |
| 1   | B     | 2802 | ASN  |
| 1   | B     | 2849 | HIS  |
| 1   | B     | 2868 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 2890 | GLN  |
| 1   | B     | 2937 | HIS  |
| 1   | B     | 2973 | GLN  |
| 1   | B     | 2978 | HIS  |
| 1   | B     | 3179 | ASN  |
| 1   | B     | 3279 | ASN  |
| 1   | B     | 3286 | ASN  |
| 1   | B     | 3622 | GLN  |
| 1   | B     | 3775 | GLN  |
| 1   | B     | 3806 | ASN  |
| 1   | B     | 3831 | GLN  |
| 1   | B     | 3865 | ASN  |
| 1   | B     | 3869 | ASN  |
| 1   | B     | 3949 | HIS  |
| 1   | B     | 4009 | ASN  |
| 1   | B     | 4159 | GLN  |
| 1   | B     | 4489 | GLN  |
| 1   | B     | 4638 | GLN  |
| 1   | B     | 4766 | GLN  |
| 1   | C     | 23   | GLN  |
| 1   | C     | 29   | HIS  |
| 1   | C     | 57   | ASN  |
| 1   | C     | 71   | GLN  |
| 1   | C     | 261  | HIS  |
| 1   | C     | 477  | ASN  |
| 1   | C     | 506  | HIS  |
| 1   | C     | 934  | GLN  |
| 1   | C     | 1005 | ASN  |
| 1   | C     | 1022 | GLN  |
| 1   | C     | 1046 | ASN  |
| 1   | C     | 1151 | HIS  |
| 1   | C     | 1451 | HIS  |
| 1   | C     | 1477 | HIS  |
| 1   | C     | 1577 | ASN  |
| 1   | C     | 1670 | HIS  |
| 1   | C     | 1691 | ASN  |
| 1   | C     | 2089 | HIS  |
| 1   | C     | 2217 | HIS  |
| 1   | C     | 2250 | ASN  |
| 1   | C     | 2386 | ASN  |
| 1   | C     | 2802 | ASN  |
| 1   | C     | 2849 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 2868 | HIS  |
| 1   | C     | 2890 | GLN  |
| 1   | C     | 2937 | HIS  |
| 1   | C     | 2958 | GLN  |
| 1   | C     | 2973 | GLN  |
| 1   | C     | 3179 | ASN  |
| 1   | C     | 3279 | ASN  |
| 1   | C     | 3286 | ASN  |
| 1   | C     | 3775 | GLN  |
| 1   | C     | 3806 | ASN  |
| 1   | C     | 3865 | ASN  |
| 1   | C     | 3869 | ASN  |
| 1   | C     | 3953 | HIS  |
| 1   | C     | 4009 | ASN  |
| 1   | C     | 4159 | GLN  |
| 1   | C     | 4489 | GLN  |
| 1   | C     | 4638 | GLN  |
| 1   | C     | 4766 | GLN  |
| 1   | D     | 23   | GLN  |
| 1   | D     | 29   | HIS  |
| 1   | D     | 57   | ASN  |
| 1   | D     | 71   | GLN  |
| 1   | D     | 261  | HIS  |
| 1   | D     | 477  | ASN  |
| 1   | D     | 506  | HIS  |
| 1   | D     | 934  | GLN  |
| 1   | D     | 1005 | ASN  |
| 1   | D     | 1022 | GLN  |
| 1   | D     | 1046 | ASN  |
| 1   | D     | 1151 | HIS  |
| 1   | D     | 1451 | HIS  |
| 1   | D     | 1477 | HIS  |
| 1   | D     | 1577 | ASN  |
| 1   | D     | 1654 | HIS  |
| 1   | D     | 1670 | HIS  |
| 1   | D     | 1691 | ASN  |
| 1   | D     | 2089 | HIS  |
| 1   | D     | 2217 | HIS  |
| 1   | D     | 2250 | ASN  |
| 1   | D     | 2318 | ASN  |
| 1   | D     | 2386 | ASN  |
| 1   | D     | 2802 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 2849 | HIS  |
| 1   | D     | 2868 | HIS  |
| 1   | D     | 2890 | GLN  |
| 1   | D     | 2937 | HIS  |
| 1   | D     | 2973 | GLN  |
| 1   | D     | 2978 | HIS  |
| 1   | D     | 3179 | ASN  |
| 1   | D     | 3279 | ASN  |
| 1   | D     | 3286 | ASN  |
| 1   | D     | 3775 | GLN  |
| 1   | D     | 3806 | ASN  |
| 1   | D     | 3831 | GLN  |
| 1   | D     | 3865 | ASN  |
| 1   | D     | 3869 | ASN  |
| 1   | D     | 3953 | HIS  |
| 1   | D     | 4159 | GLN  |
| 1   | D     | 4489 | GLN  |
| 1   | D     | 4638 | GLN  |
| 1   | D     | 4766 | GLN  |
| 1   | D     | 4879 | 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 | $\# Z  > 2$ |
| 4   | ATP  | C     | 5002 | -    | 32,33,33     | 0.31 | 0           | 48,52,52    | 0.34 | 0           |
| 4   | ATP  | A     | 5003 | -    | 32,33,33     | 0.26 | 0           | 48,52,52    | 0.27 | 0           |
| 4   | ATP  | D     | 5002 | -    | 32,33,33     | 0.31 | 0           | 48,52,52    | 0.34 | 0           |
| 4   | ATP  | D     | 5003 | -    | 32,33,33     | 0.26 | 0           | 48,52,52    | 0.27 | 0           |
| 4   | ATP  | A     | 5002 | -    | 32,33,33     | 0.31 | 0           | 48,52,52    | 0.34 | 0           |
| 4   | ATP  | C     | 5003 | -    | 32,33,33     | 0.25 | 0           | 48,52,52    | 0.27 | 0           |
| 4   | ATP  | B     | 5002 | -    | 32,33,33     | 0.31 | 0           | 48,52,52    | 0.34 | 0           |
| 4   | ATP  | B     | 5003 | -    | 32,33,33     | 0.25 | 0           | 48,52,52    | 0.27 | 0           |

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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 4   | ATP  | C     | 5002 | -    | -       | 10/22/38/38 | 0/3/3/3 |
| 4   | ATP  | A     | 5003 | -    | -       | 5/22/38/38  | 0/3/3/3 |
| 4   | ATP  | D     | 5002 | -    | -       | 10/22/38/38 | 0/3/3/3 |
| 4   | ATP  | D     | 5003 | -    | -       | 5/22/38/38  | 0/3/3/3 |
| 4   | ATP  | A     | 5002 | -    | -       | 10/22/38/38 | 0/3/3/3 |
| 4   | ATP  | C     | 5003 | -    | -       | 5/22/38/38  | 0/3/3/3 |
| 4   | ATP  | B     | 5002 | -    | -       | 10/22/38/38 | 0/3/3/3 |
| 4   | ATP  | B     | 5003 | -    | -       | 5/22/38/38  | 0/3/3/3 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (60) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 4   | A     | 5002 | ATP  | PB-O3B-PG-O3G  |
| 4   | A     | 5002 | ATP  | C5'-O5'-PA-O1A |
| 4   | A     | 5002 | ATP  | C5'-O5'-PA-O2A |
| 4   | B     | 5002 | ATP  | PB-O3B-PG-O3G  |
| 4   | B     | 5002 | ATP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | B     | 5002 | ATP  | C5'-O5'-PA-O2A  |
| 4   | C     | 5002 | ATP  | PB-O3B-PG-O3G   |
| 4   | C     | 5002 | ATP  | C5'-O5'-PA-O1A  |
| 4   | C     | 5002 | ATP  | C5'-O5'-PA-O2A  |
| 4   | D     | 5002 | ATP  | PB-O3B-PG-O3G   |
| 4   | D     | 5002 | ATP  | C5'-O5'-PA-O1A  |
| 4   | D     | 5002 | ATP  | C5'-O5'-PA-O2A  |
| 4   | A     | 5003 | ATP  | C2'-C1'-N9-C8   |
| 4   | B     | 5003 | ATP  | C2'-C1'-N9-C8   |
| 4   | C     | 5003 | ATP  | C2'-C1'-N9-C8   |
| 4   | D     | 5003 | ATP  | C2'-C1'-N9-C8   |
| 4   | A     | 5003 | ATP  | C2'-C1'-N9-C4   |
| 4   | B     | 5003 | ATP  | C2'-C1'-N9-C4   |
| 4   | C     | 5003 | ATP  | C2'-C1'-N9-C4   |
| 4   | D     | 5003 | ATP  | C2'-C1'-N9-C4   |
| 4   | A     | 5003 | ATP  | PG-O3B-PB-O3A   |
| 4   | B     | 5003 | ATP  | PG-O3B-PB-O3A   |
| 4   | C     | 5003 | ATP  | PG-O3B-PB-O3A   |
| 4   | D     | 5003 | ATP  | PG-O3B-PB-O3A   |
| 4   | A     | 5002 | ATP  | C5'-O5'-PA-O3A  |
| 4   | B     | 5002 | ATP  | C5'-O5'-PA-O3A  |
| 4   | C     | 5002 | ATP  | C5'-O5'-PA-O3A  |
| 4   | D     | 5002 | ATP  | C5'-O5'-PA-O3A  |
| 4   | A     | 5002 | ATP  | C3'-C4'-C5'-O5' |
| 4   | B     | 5002 | ATP  | C3'-C4'-C5'-O5' |
| 4   | C     | 5002 | ATP  | C3'-C4'-C5'-O5' |
| 4   | D     | 5002 | ATP  | C3'-C4'-C5'-O5' |
| 4   | A     | 5002 | ATP  | PA-O3A-PB-O3B   |
| 4   | B     | 5002 | ATP  | PA-O3A-PB-O3B   |
| 4   | C     | 5002 | ATP  | PA-O3A-PB-O3B   |
| 4   | D     | 5002 | ATP  | PA-O3A-PB-O3B   |
| 4   | A     | 5002 | ATP  | PG-O3B-PB-O1B   |
| 4   | A     | 5002 | ATP  | PG-O3B-PB-O2B   |
| 4   | A     | 5002 | ATP  | PA-O3A-PB-O1B   |
| 4   | A     | 5003 | ATP  | PG-O3B-PB-O2B   |
| 4   | B     | 5002 | ATP  | PG-O3B-PB-O1B   |
| 4   | B     | 5002 | ATP  | PG-O3B-PB-O2B   |
| 4   | B     | 5002 | ATP  | PA-O3A-PB-O1B   |
| 4   | B     | 5003 | ATP  | PG-O3B-PB-O2B   |
| 4   | C     | 5002 | ATP  | PG-O3B-PB-O1B   |
| 4   | C     | 5002 | ATP  | PG-O3B-PB-O2B   |
| 4   | C     | 5003 | ATP  | PG-O3B-PB-O2B   |

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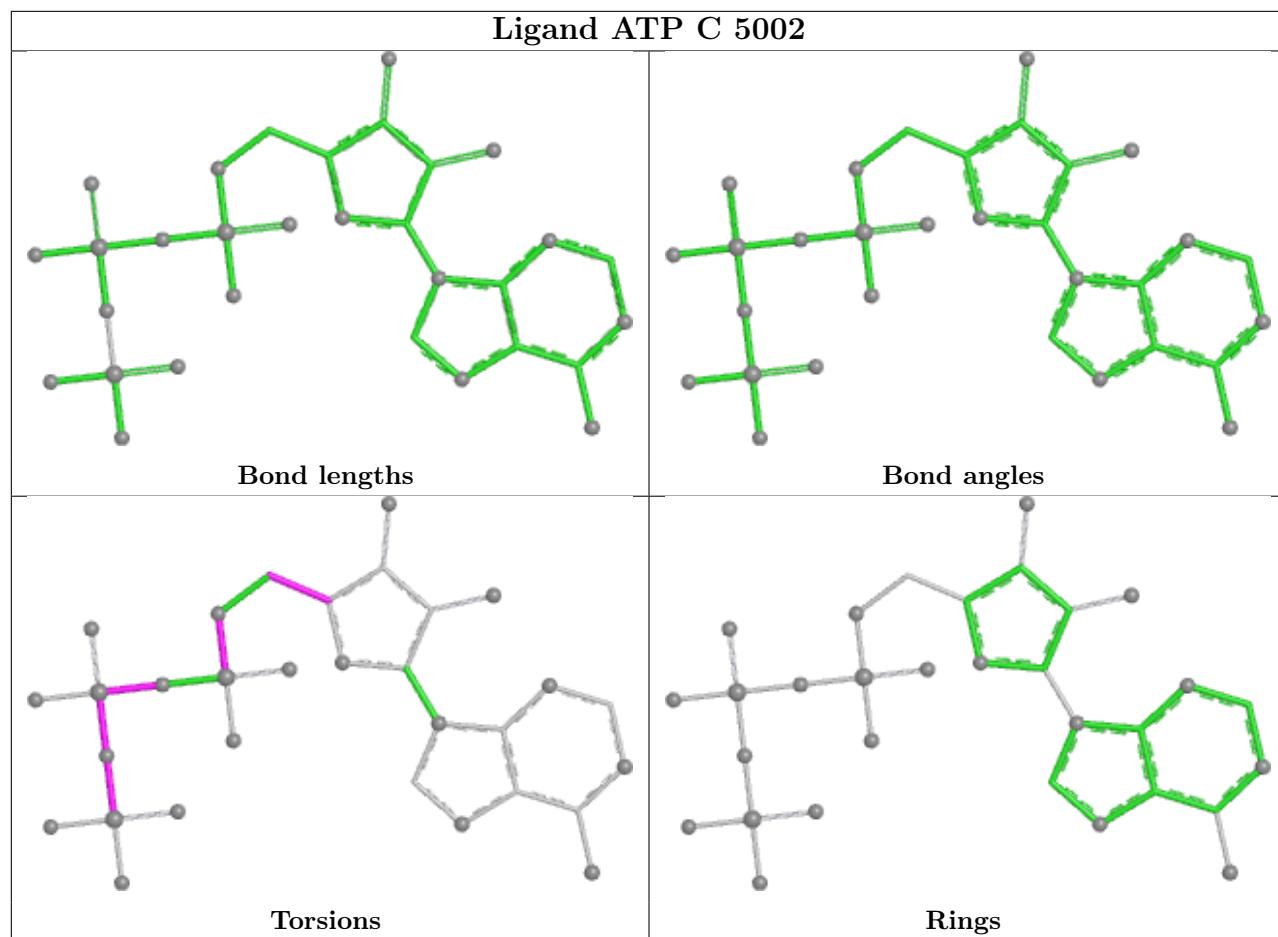
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | D     | 5002 | ATP  | PG-O3B-PB-O1B   |
| 4   | D     | 5002 | ATP  | PG-O3B-PB-O2B   |
| 4   | D     | 5002 | ATP  | PA-O3A-PB-O1B   |
| 4   | D     | 5003 | ATP  | PG-O3B-PB-O2B   |
| 4   | A     | 5002 | ATP  | O4'-C4'-C5'-O5' |
| 4   | B     | 5002 | ATP  | O4'-C4'-C5'-O5' |
| 4   | C     | 5002 | ATP  | O4'-C4'-C5'-O5' |
| 4   | D     | 5002 | ATP  | O4'-C4'-C5'-O5' |
| 4   | A     | 5003 | ATP  | PG-O3B-PB-O1B   |
| 4   | B     | 5003 | ATP  | PG-O3B-PB-O1B   |
| 4   | C     | 5002 | ATP  | PA-O3A-PB-O1B   |
| 4   | C     | 5003 | ATP  | PG-O3B-PB-O1B   |
| 4   | D     | 5003 | ATP  | PG-O3B-PB-O1B   |

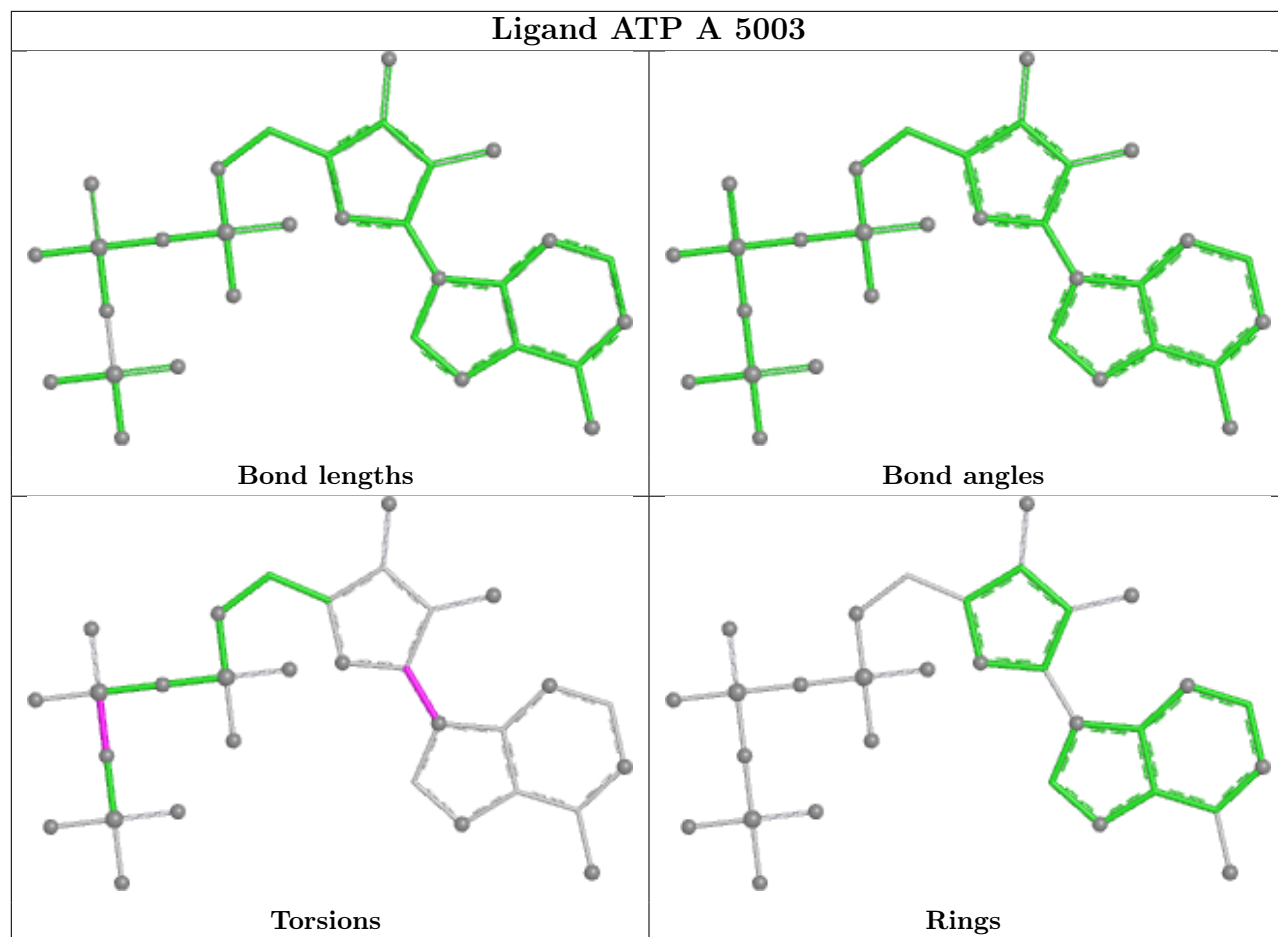
There are no ring outliers.

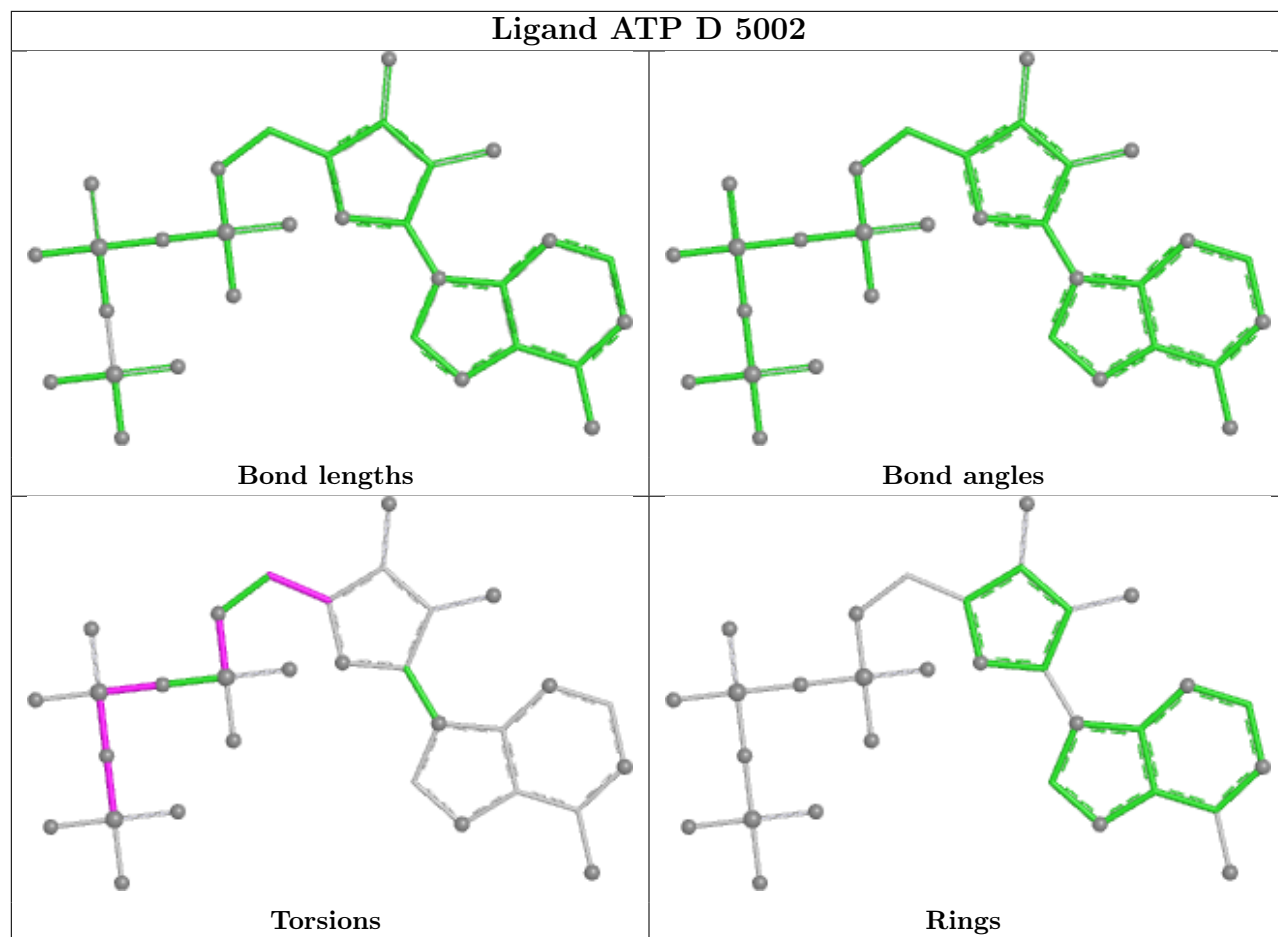
8 monomers are involved in 16 short contacts:

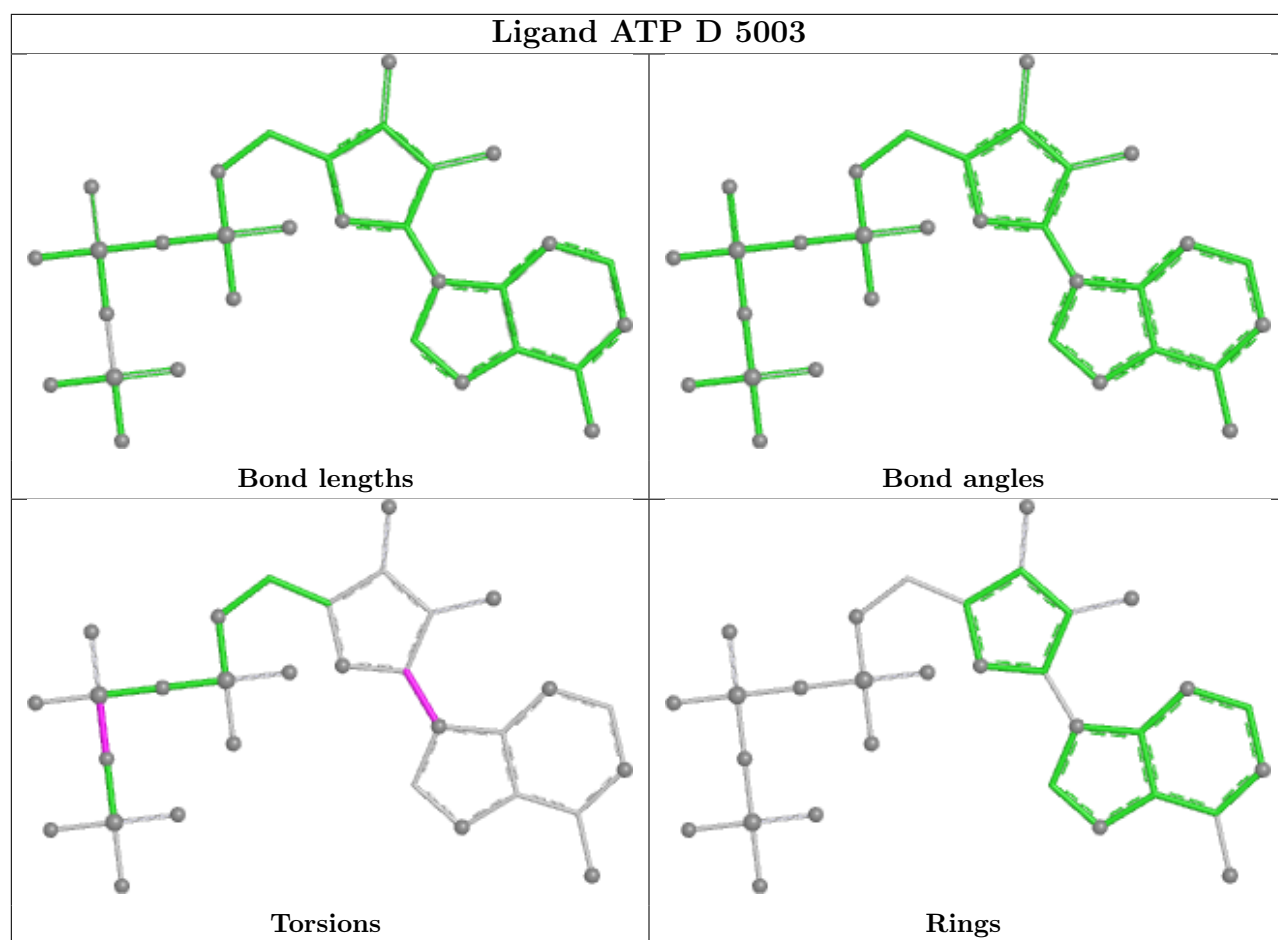
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | C     | 5002 | ATP  | 1       | 0            |
| 4   | A     | 5003 | ATP  | 3       | 0            |
| 4   | D     | 5002 | ATP  | 1       | 0            |
| 4   | D     | 5003 | ATP  | 3       | 0            |
| 4   | A     | 5002 | ATP  | 1       | 0            |
| 4   | C     | 5003 | ATP  | 3       | 0            |
| 4   | B     | 5002 | ATP  | 1       | 0            |
| 4   | B     | 5003 | ATP  | 3       | 0            |

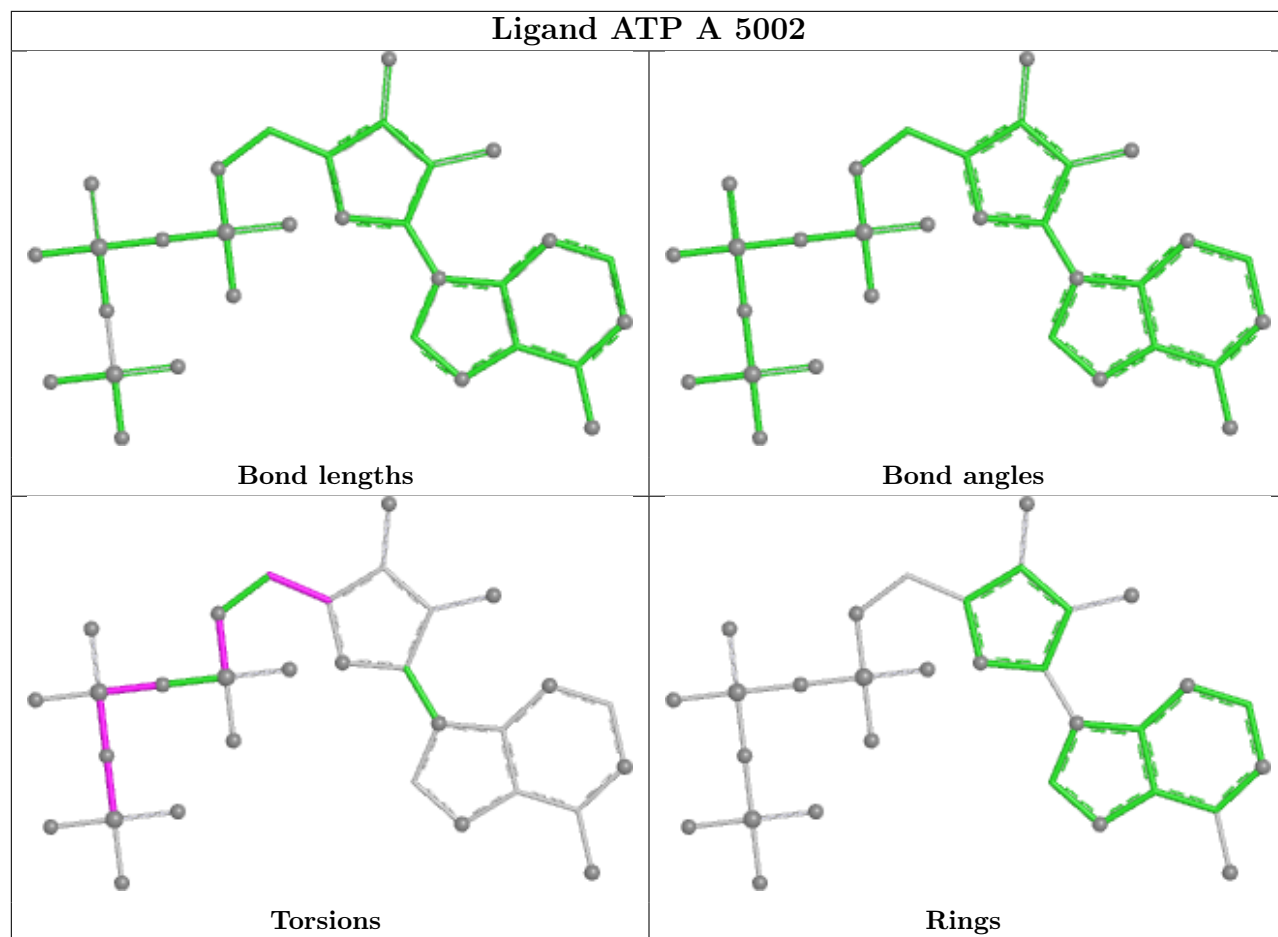
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

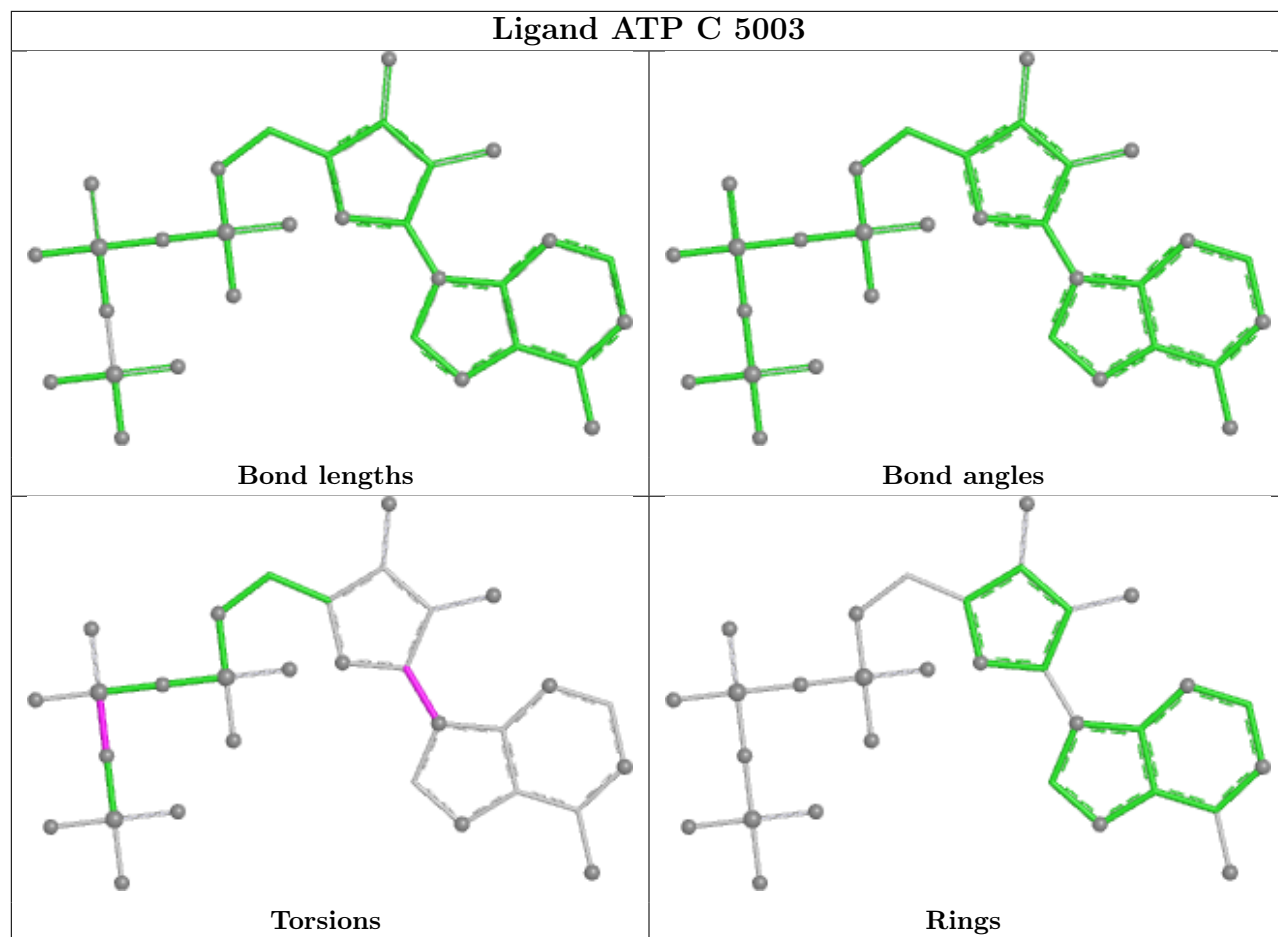


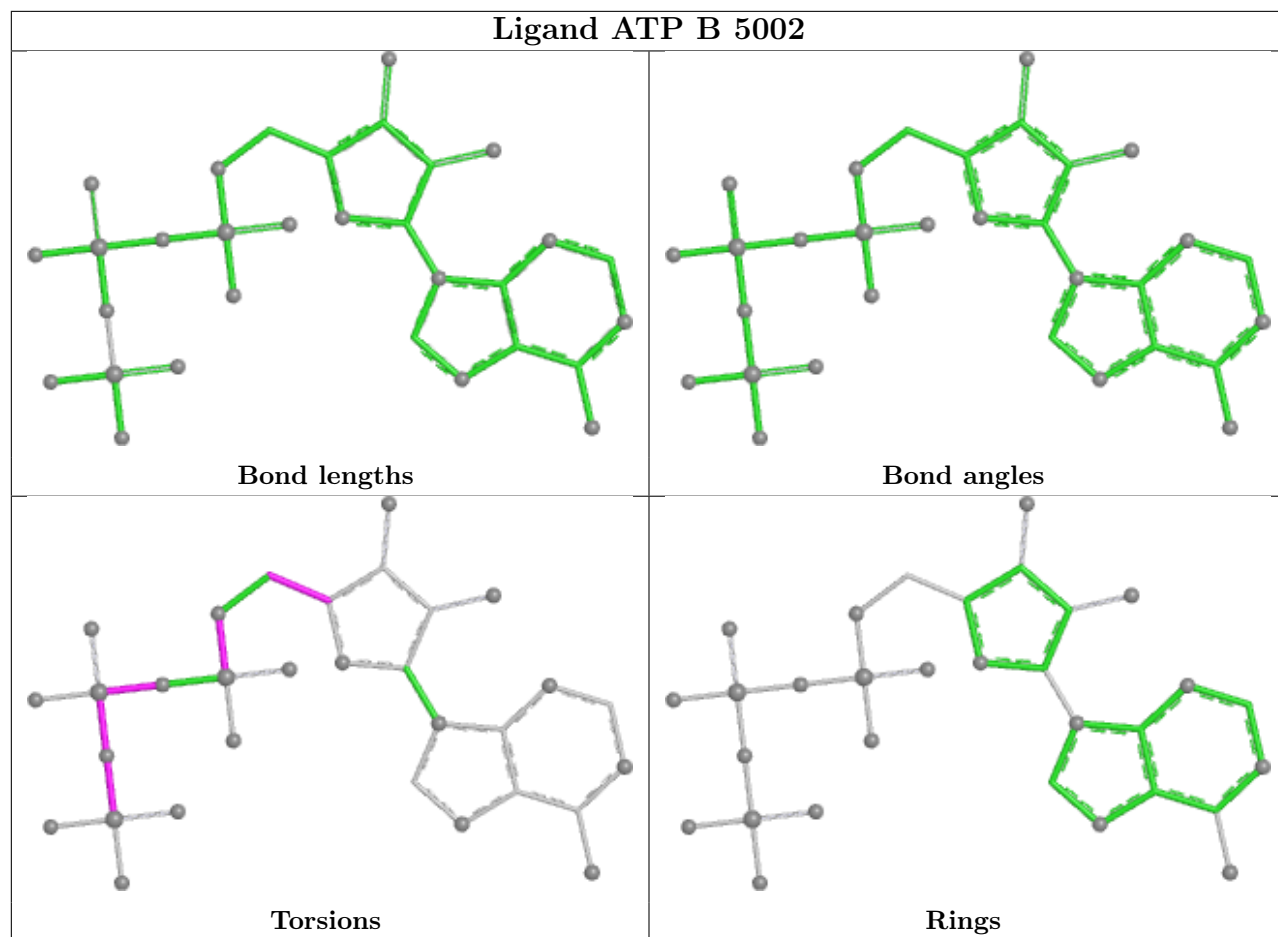


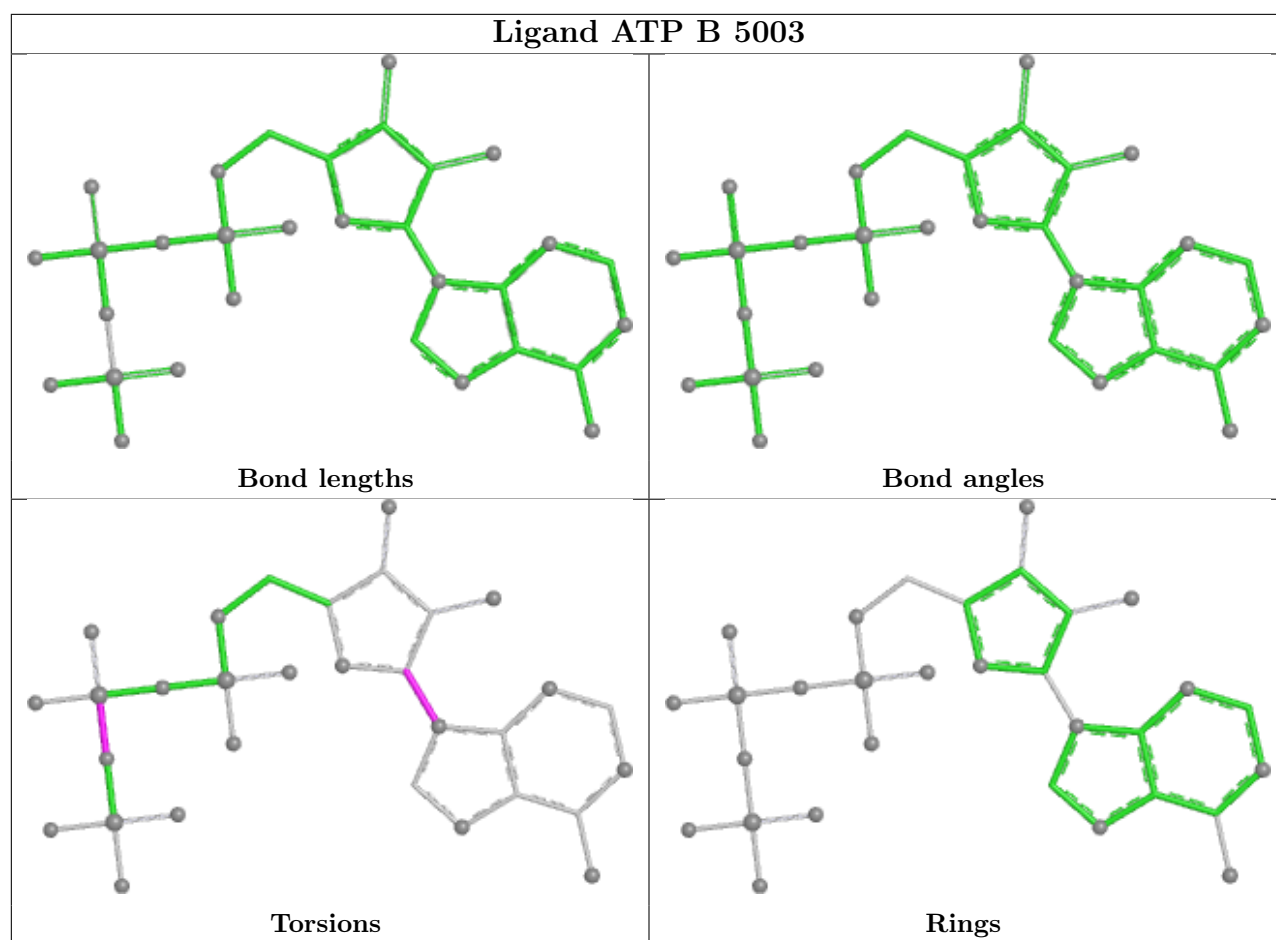












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

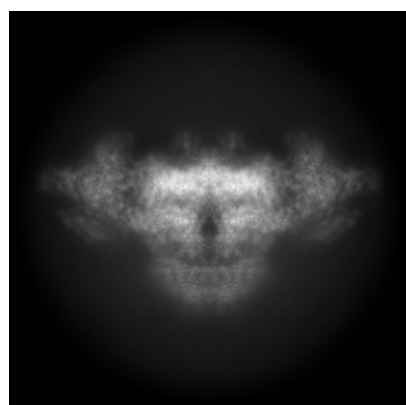
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42460. These allow visual inspection of the internal detail of the map and identification of artifacts.

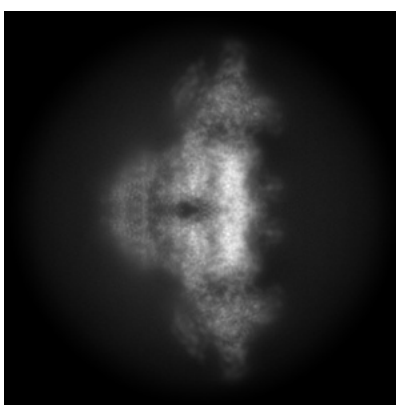
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

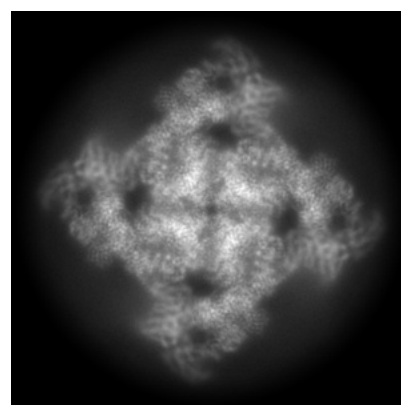
#### 6.1.1 Primary map



X



Y

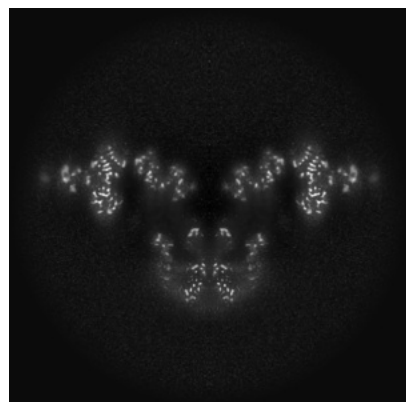


Z

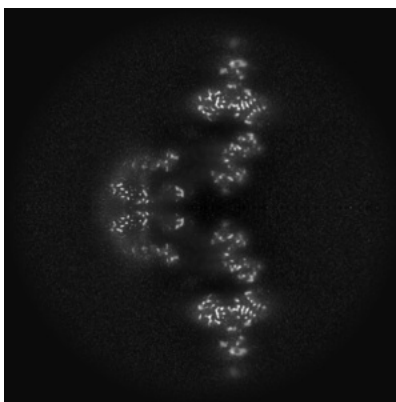
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

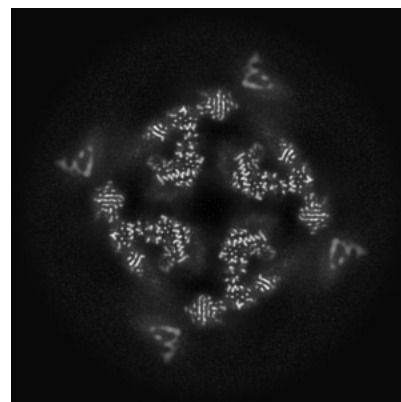
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

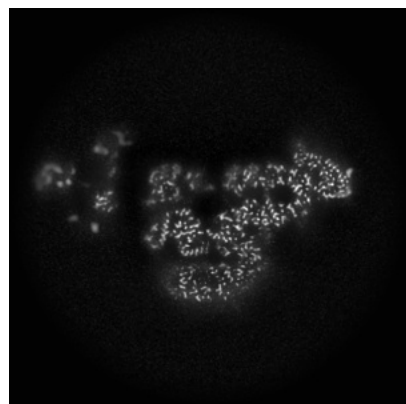


Z Index: 256

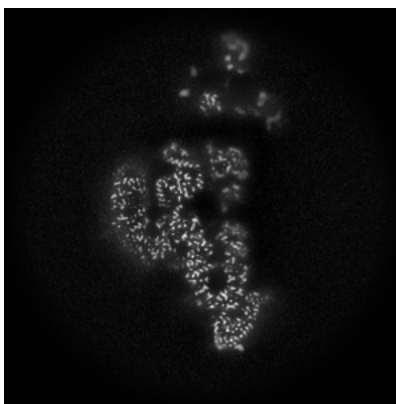
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

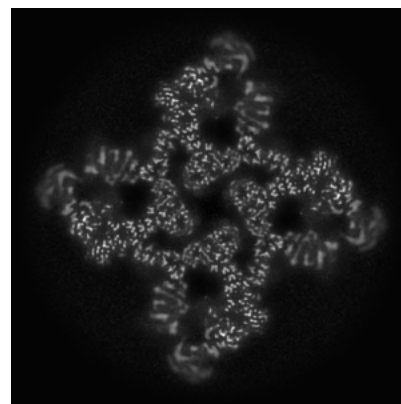
### 6.3.1 Primary map



X Index: 233



Y Index: 233

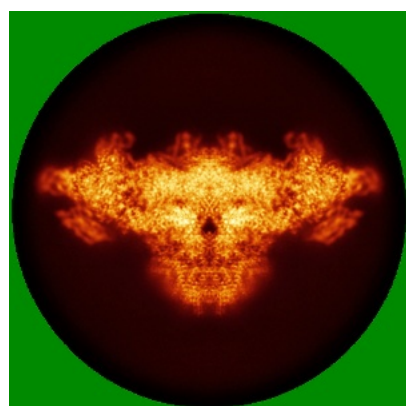


Z Index: 290

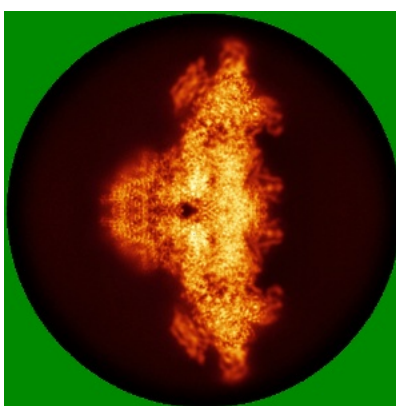
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

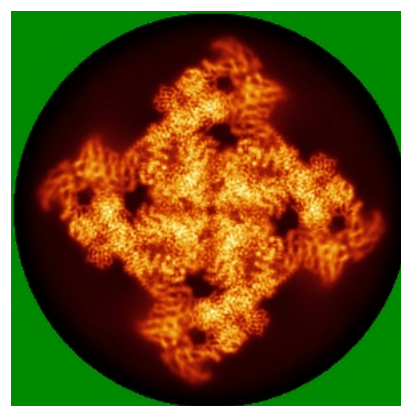
### 6.4.1 Primary map



X



Y

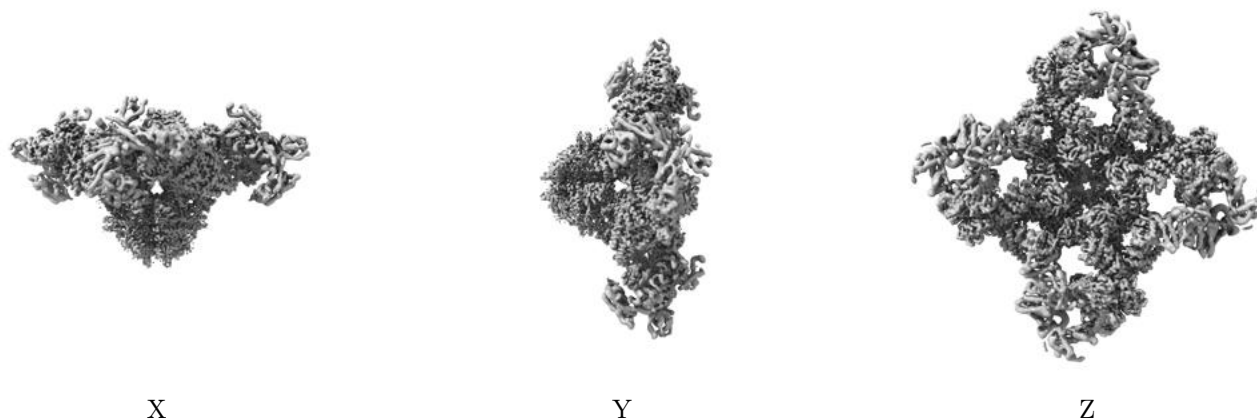


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

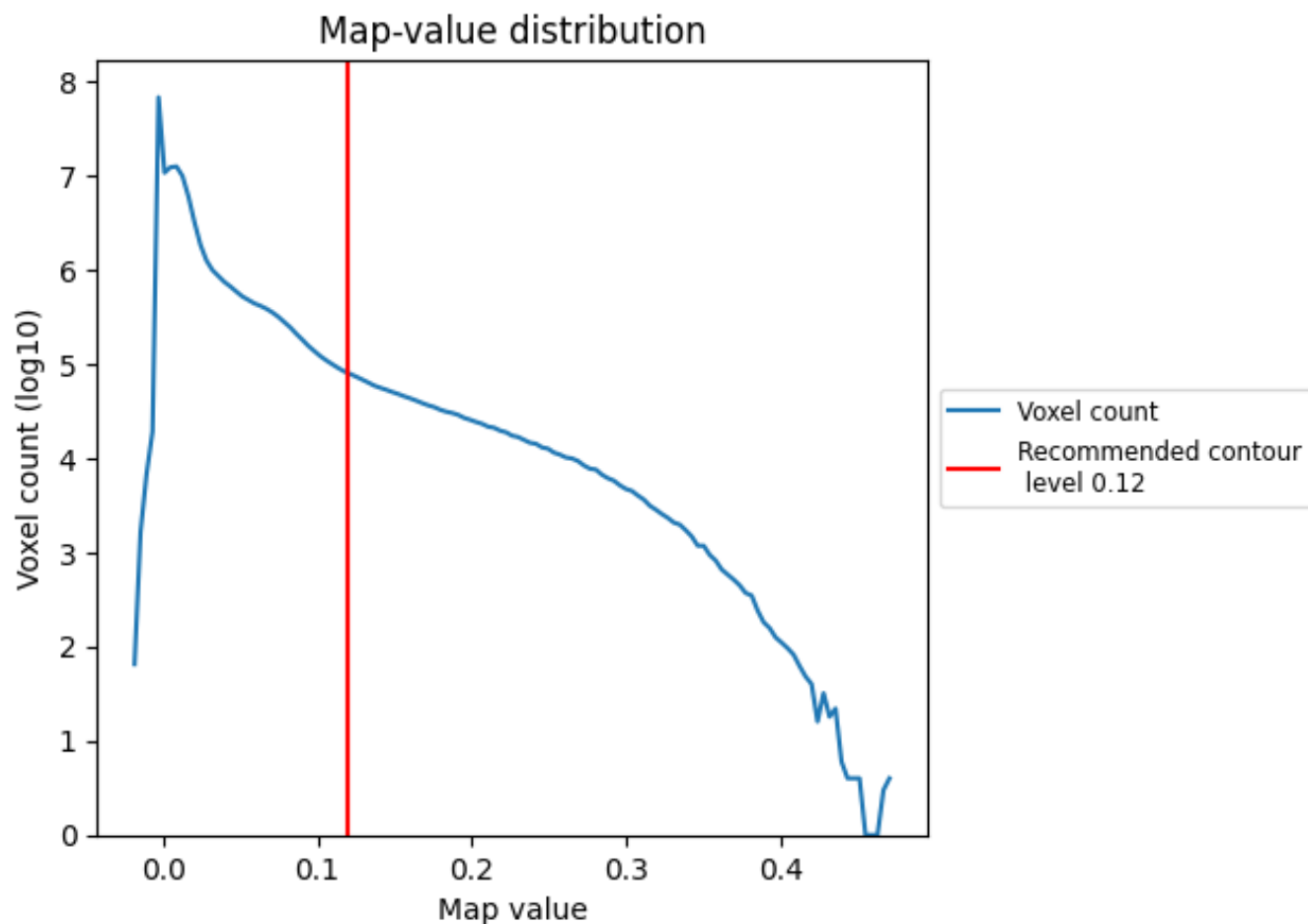
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

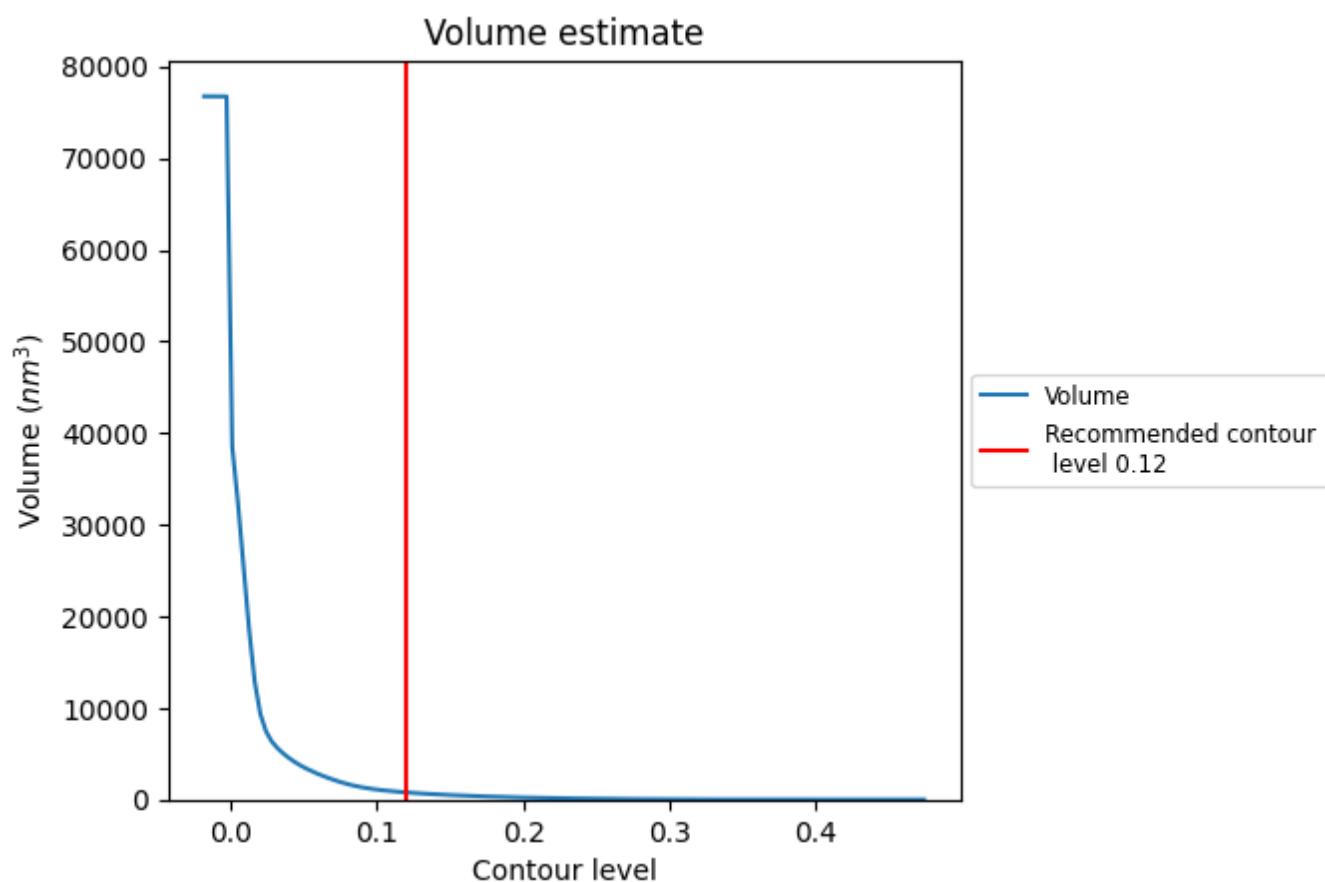
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

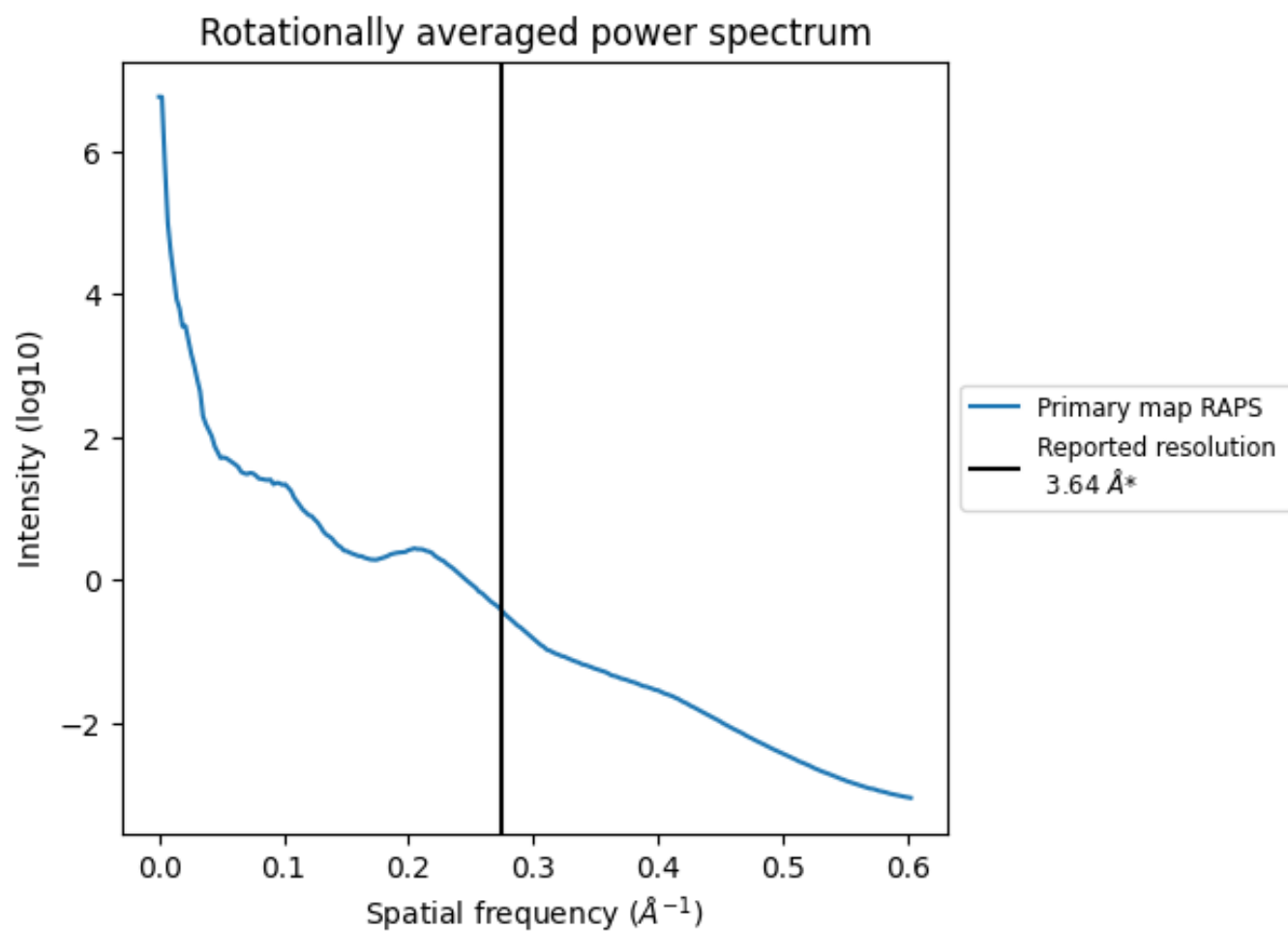
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 778 nm<sup>3</sup>; this corresponds to an approximate mass of 703 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.275 Å<sup>-1</sup>

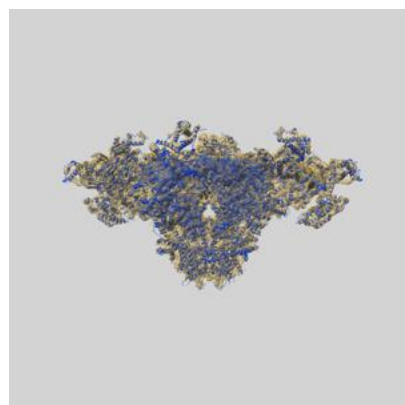
## 8 Fourier-Shell correlation ⓘ

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

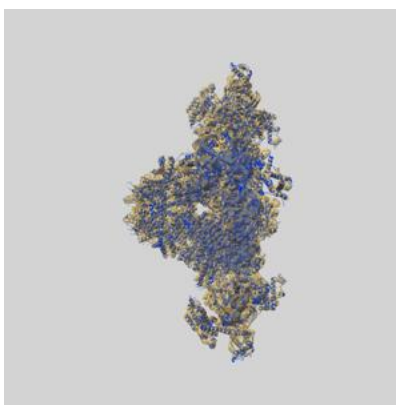
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42460 and PDB model 8UQ4. Per-residue inclusion information can be found in section 3 on page 7.

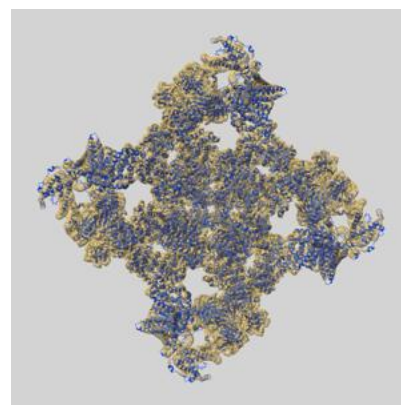
### 9.1 Map-model overlay [i](#)



X



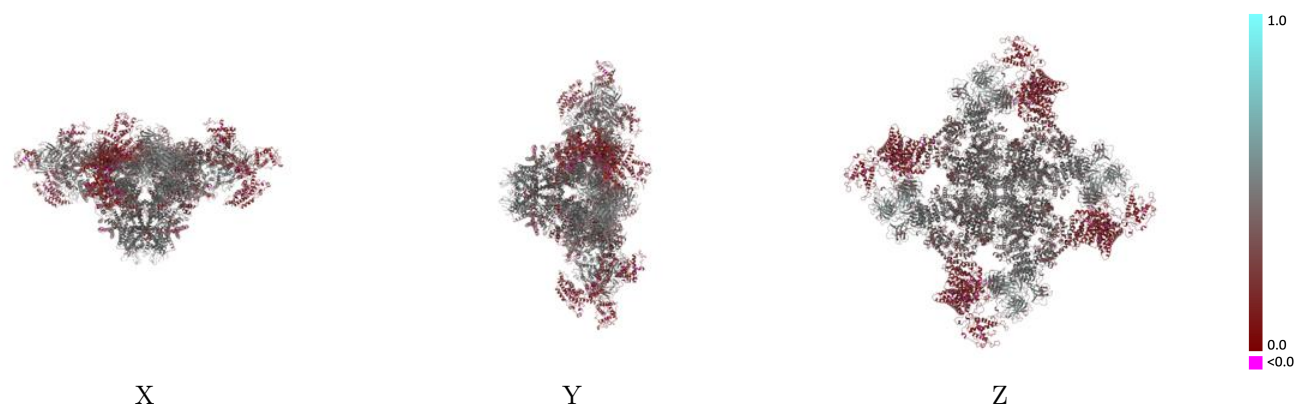
Y



Z

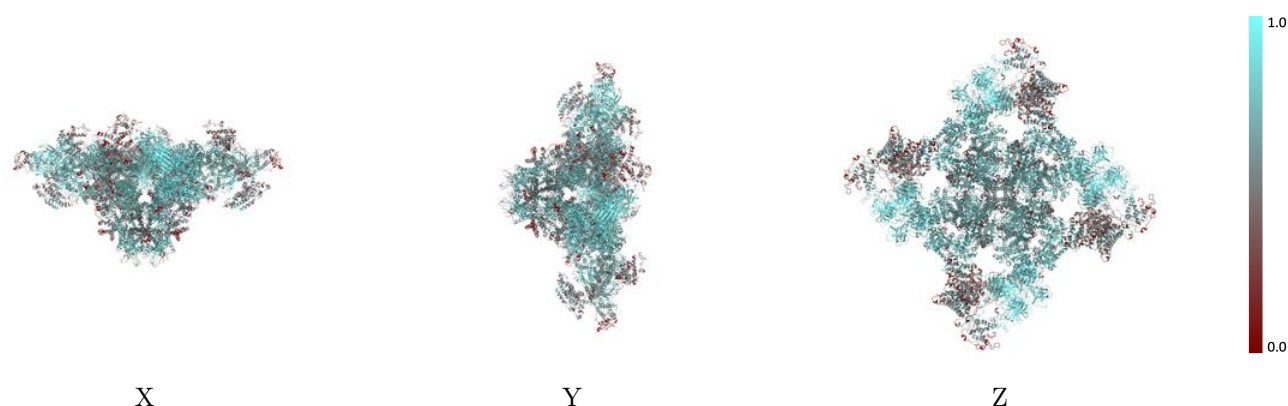
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



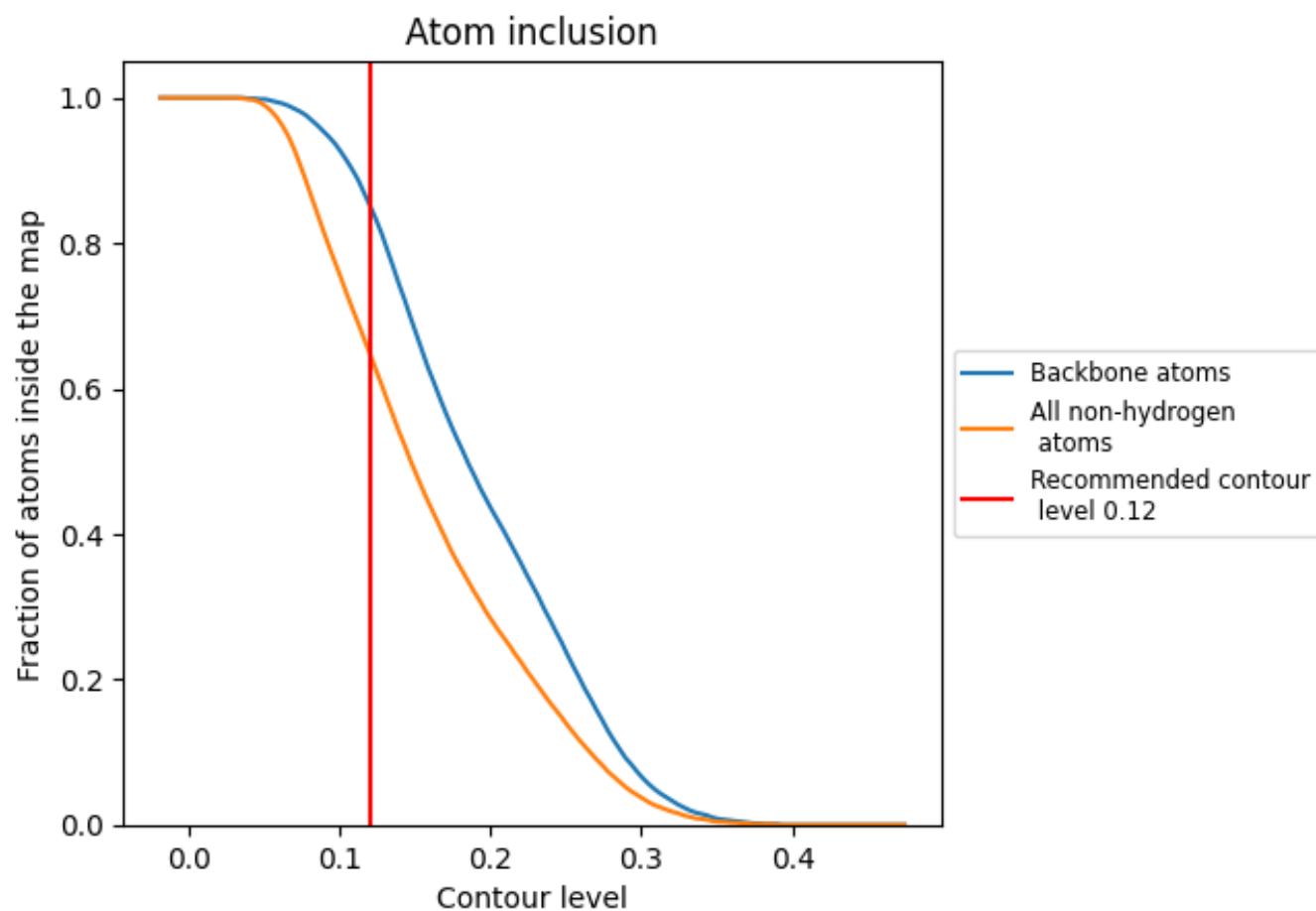
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.12).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 65% 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 (0.12) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6480 | <div></div> 0.3650 |
| A     | <div></div> 0.6440 | <div></div> 0.3620 |
| B     | <div></div> 0.6450 | <div></div> 0.3630 |
| C     | <div></div> 0.6450 | <div></div> 0.3630 |
| D     | <div></div> 0.6450 | <div></div> 0.3630 |
| E     | <div></div> 0.7900 | <div></div> 0.4640 |
| F     | <div></div> 0.7960 | <div></div> 0.4670 |
| G     | <div></div> 0.7990 | <div></div> 0.4680 |
| H     | <div></div> 0.7930 | <div></div> 0.4670 |

