



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:06 PM UTC

PDB ID : 9E1G / pdb\_00009e1g  
EMDB ID : EMD-47393  
Title : Structure of RyR1 in the primed state in the presence of oxypurinol  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2024-10-21  
Resolution : 3.17 Å(reported)  
Based on initial model : 7TZC

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:

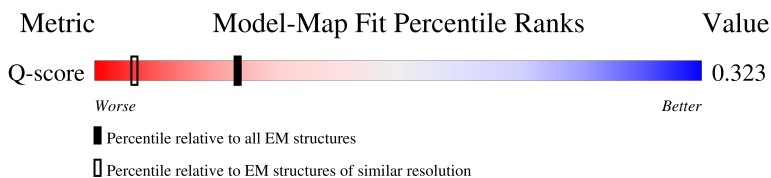
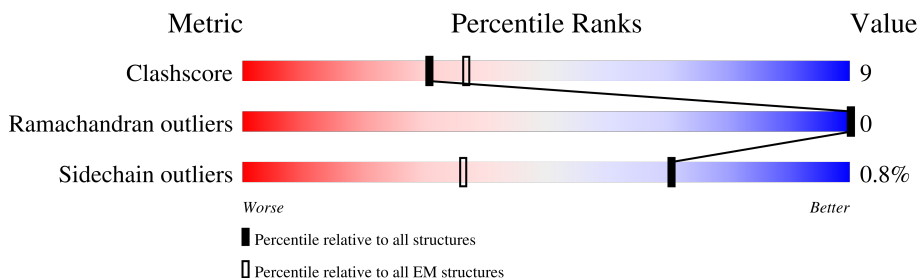
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.17 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                       | 14465 ( 2.67 - 3.67 )                                    |

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     | 5037   | <div> <div>40%</div> <div>70%</div> <div>17%</div> <div>13%</div> </div> |
| 1   | B     | 5037   | <div> <div>40%</div> <div>70%</div> <div>17%</div> <div>13%</div> </div> |
| 1   | C     | 5037   | <div> <div>40%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div> |
| 1   | D     | 5037   | <div> <div>40%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                                                                            |
|-----|-------|--------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 2   | E     | 108    | <div><div><div>66%</div><div></div><div></div></div><div><div></div><div>69%</div><div>29%</div></div><div><div></div><div></div><div>..</div></div></div>  |
| 2   | F     | 108    | <div><div><div>66%</div><div></div><div></div></div><div><div></div><div>77%</div><div>21%</div></div><div><div></div><div></div><div>..</div></div></div>  |
| 2   | G     | 108    | <div><div><div>65%</div><div></div><div></div></div><div><div></div><div>71%</div><div>27%</div></div><div><div></div><div></div><div>..</div></div></div>  |
| 2   | H     | 108    | <div><div><div>65%</div><div></div><div></div></div><div><div></div><div>74%</div><div>22%</div></div><div><div></div><div></div><div>. .</div></div></div> |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

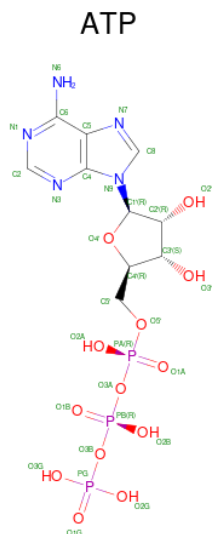
- Molecule 1 is a protein called Ryanodine receptor 1.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 1   | A     | 4404     | Total | C     | N    | O    | S   | 9       | 0     |
|     |       |          | 35150 | 22365 | 6063 | 6485 | 237 |         |       |
| 1   | B     | 4404     | Total | C     | N    | O    | S   | 9       | 0     |
|     |       |          | 35150 | 22365 | 6063 | 6485 | 237 |         |       |
| 1   | D     | 4404     | Total | C     | N    | O    | S   | 9       | 0     |
|     |       |          | 35150 | 22365 | 6063 | 6485 | 237 |         |       |
| 1   | C     | 4404     | Total | C     | N    | O    | S   | 9       | 0     |
|     |       |          | 35150 | 22365 | 6063 | 6485 | 237 |         |       |

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | E     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 831   | 527 | 146 | 154 | 4 |         |       |
| 2   | H     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 831   | 527 | 146 | 154 | 4 |         |       |
| 2   | G     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 831   | 527 | 146 | 154 | 4 |         |       |
| 2   | F     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 831   | 527 | 146 | 154 | 4 |         |       |

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 3   | A     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 3   | B     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 3   | D     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 3   | C     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       |

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4   | A     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | B     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | D     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | C     | 1        | Total<br>1 | Ca<br>1 | 0       |

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

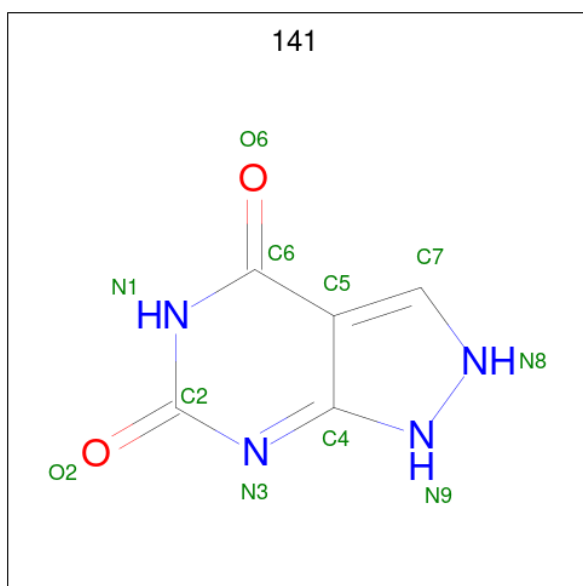
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 5   | A     | 1        | Total Zn<br>1 1 | 0       |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 5   | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 5   | D     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 5   | C     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 6 is Oxypurinol (CCD ID: 141) (formula:  $C_5H_4N_4O_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 6   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 11    | 5 | 4 | 2 |         |
| 6   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 11    | 5 | 4 | 2 |         |
| 6   | D     | 1        | Total | C | N | O | 0       |
|     |       |          | 11    | 5 | 4 | 2 |         |
| 6   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 11    | 5 | 4 | 2 |         |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 7   | A     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 7   | B     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

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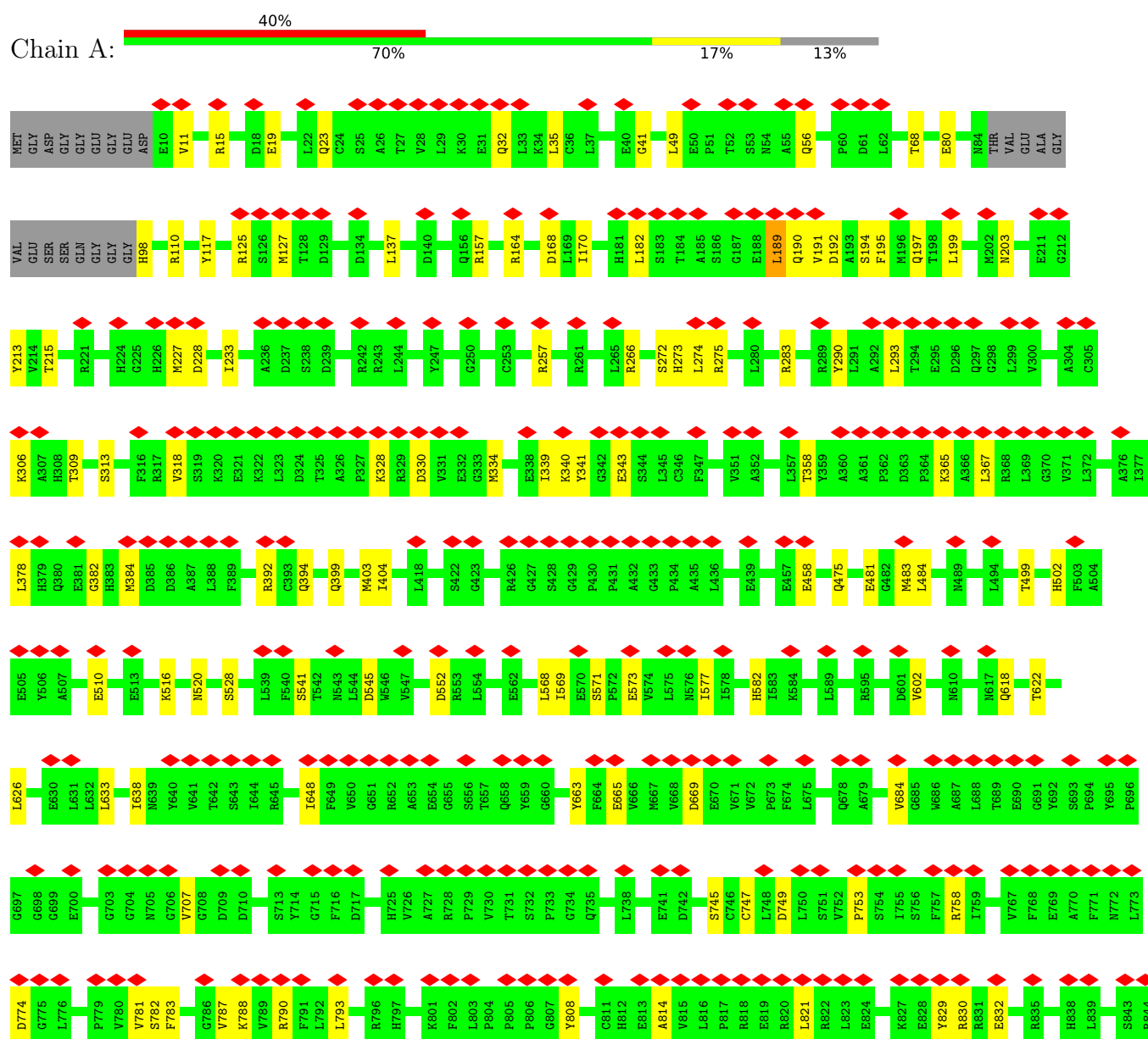
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| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 7   | D     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |
| 7   | C     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Ryanodine receptor 1



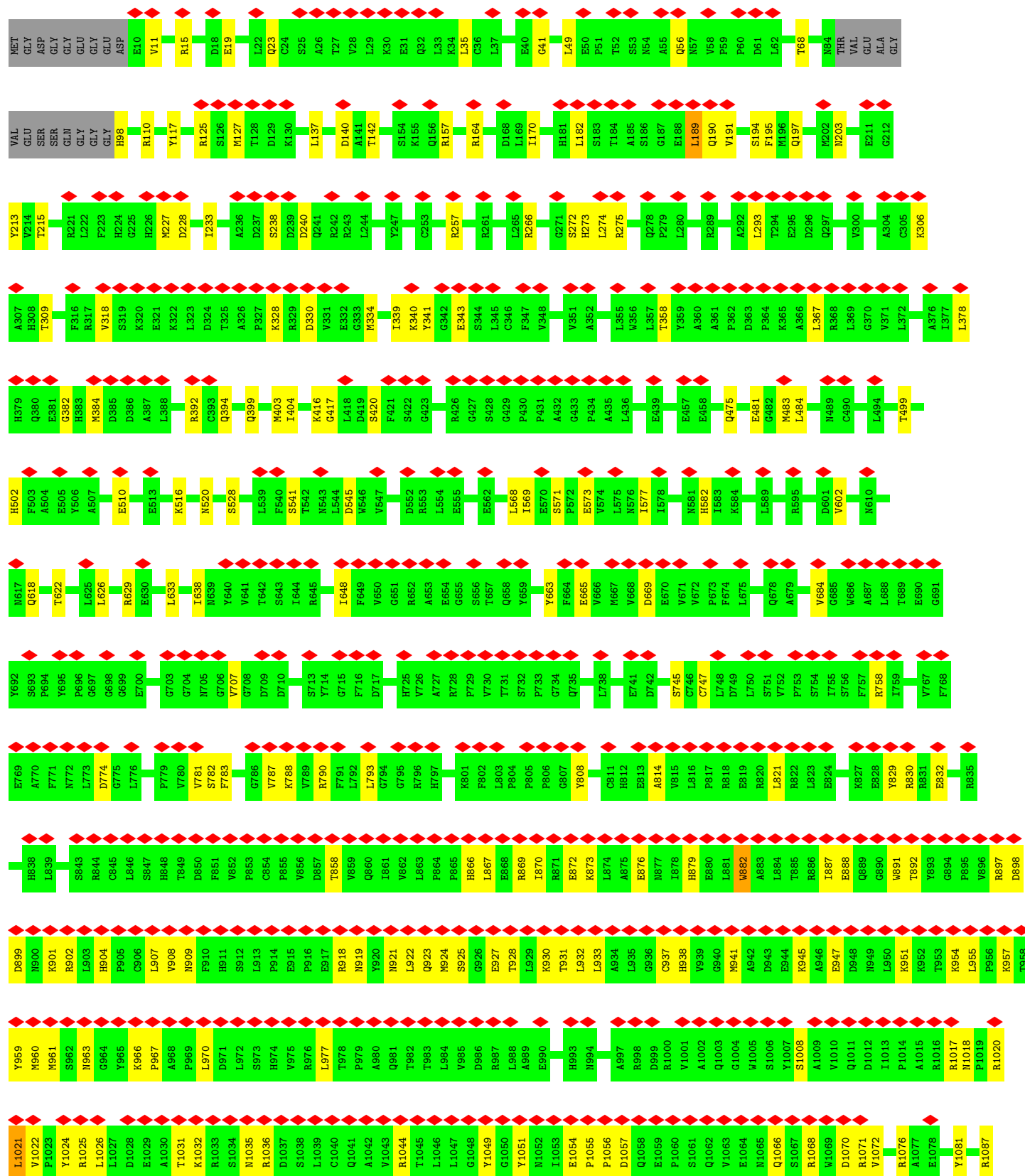










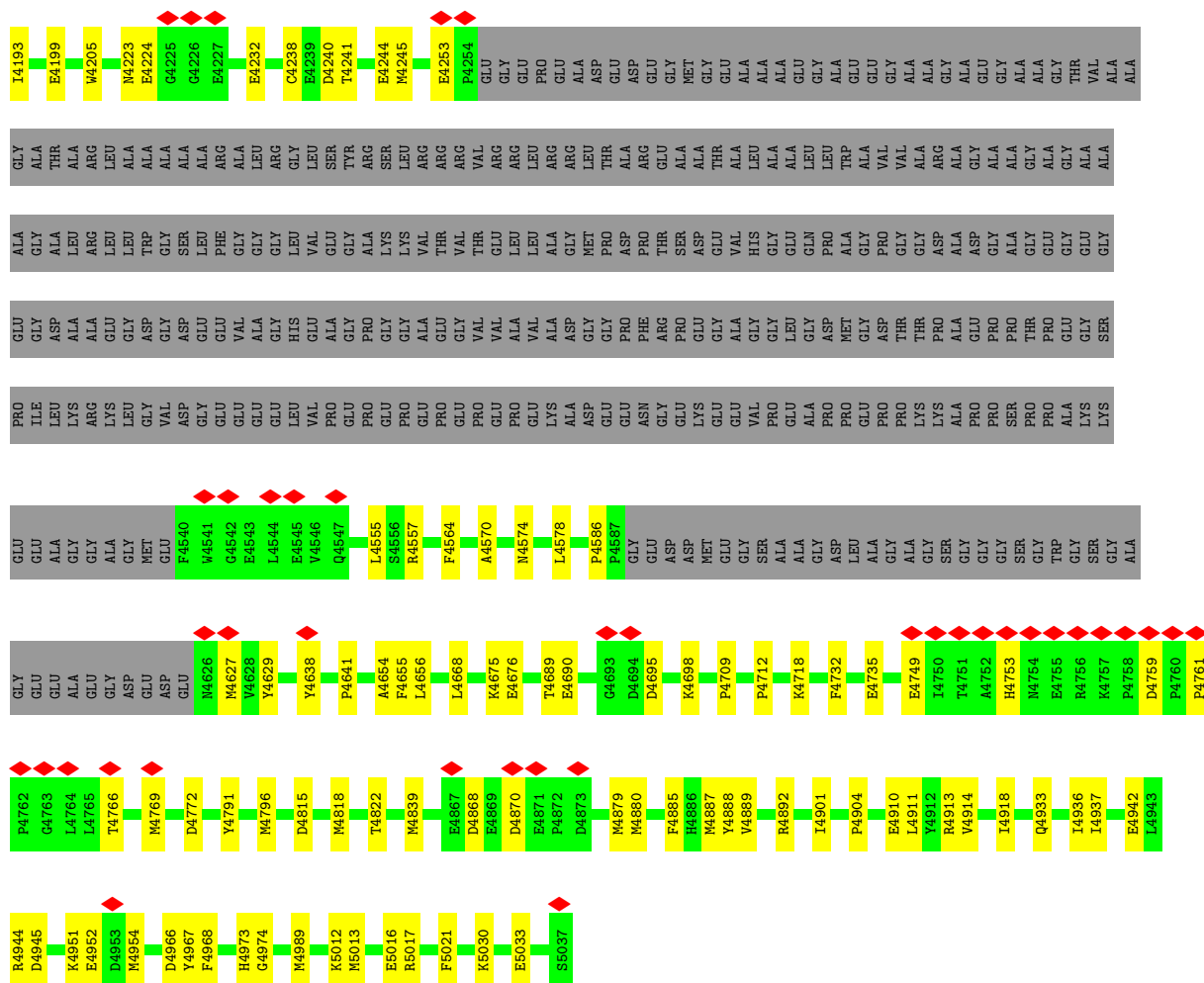




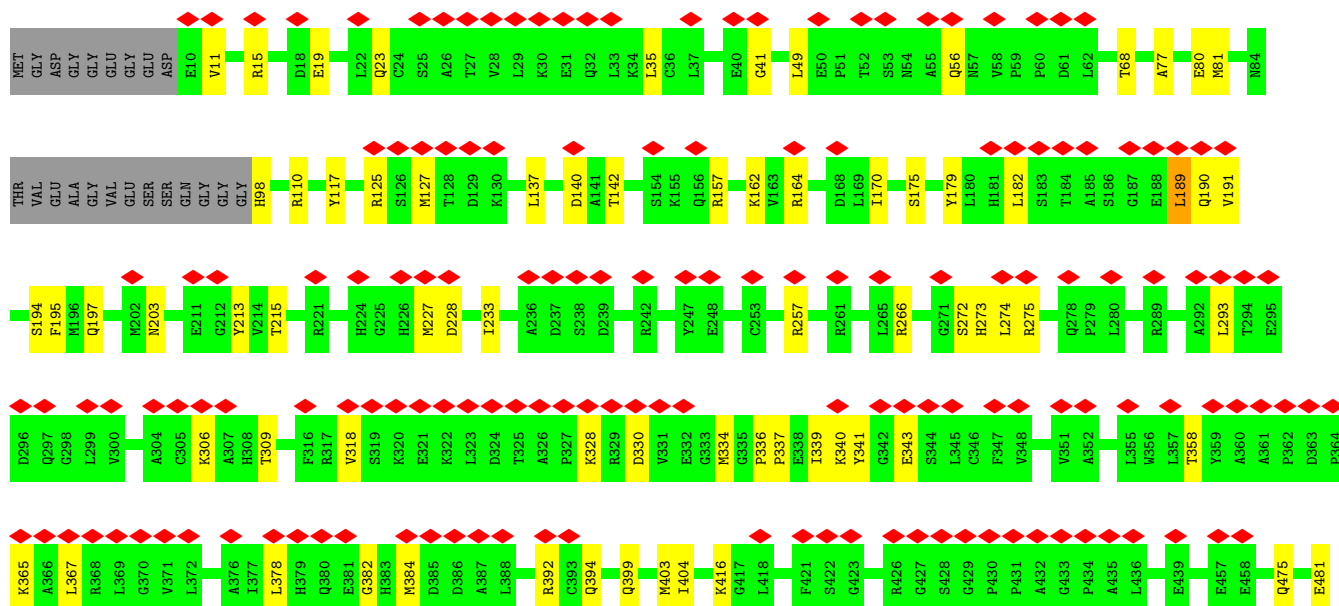
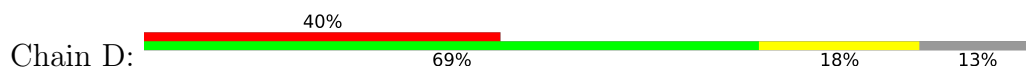
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G3029 | I2969 | D2909 | T2789 | TYR   | P2789 | VAL   | E2669 | L2607 | S2535 | D2464 | L2377 | M2267 | E2175 |
| H3030 | S2970 | T2910 | M2790 | ASP   | M2790 | ASP   | E2670 | M2608 | L2536 | D2465 | I2380 | T2271 | M2176 |
| A3031 | Q2971 | L2911 | L2791 | PRO   | L2791 | ALA   | E2671 | A2609 | D2537 | L2466 | E2381 | D2282 | M2177 |
| S3032 | E2972 | T2912 | R2792 | ARG   | R2792 | GLY   | L2672 | L2610 | T2538 | L2467 | E2382 | Q2293 | M2178 |
| K3033 | F2973 | A2913 | F2793 | GLY   | F2793 | M2734 | H2673 | C2611 | F2541 | I2469 | E2383 | I2182 | I2182 |
| E3035 | A2975 | E2915 | K2795 | M2856 | K2795 | D2735 | L2674 | R2612 | S2542 | I2470 | A2383 | I2185 | I2185 |
| K3036 | H2976 | K2916 | T2796 | P2857 | T2796 | D2736 | T2675 | Y2613 | E2545 | S2471 | R2384 | M2186 | M2186 |
| E3037 | L2977 | A2917 | F2797 | Q2858 | F2797 | R2737 | R2676 | L2614 | E2546 | L2472 | R2385 | E2296 | E2296 |
| K3038 | E2978 | R2918 | S2797 | P2859 | S2797 | R2738 | K2677 | R2616 | R2546 | P2473 | I2386 | Y2301 | F2191 |
| I3039 | A2979 | D2919 | E2799 | P2860 | E2799 | P2739 | L2678 | P2617 | R2552 | Q2475 | E2387 | L2302 | M2198 |
| T3040 | V2980 | R2920 | K2800 | D2861 | K2800 | V2740 | F2679 | M2618 | R2556 | I2476 | E2388 | A2303 | M2198 |
| S3041 | V2981 | R2921 | D2801 | L2862 | D2801 | E2741 | Q2680 | Q2617 | L2556 | P2477 | P2390 | G2304 | M2203 |
| F3042 | S2982 | K2922 | K2802 | L2743 | K2802 | T2742 | Q2681 | L2619 | A2557 | P2478 | A2391 | L2307 | M2208 |
| F3043 | S2983 | E2923 | E2803 | L2744 | E2803 | H2744 | F2683 | Q2620 | V2558 | T2478 | R2392 | Q2308 | E2209 |
| C3044 | Q2984 | A2924 | I2804 | V2745 | I2804 | V2745 | D2684 | L2622 | L2562 | L2479 | R2393 | S2309 | E2210 |
| K3045 | R2985 | E2925 | T2805 | L2746 | T2805 | L2746 | D2685 | L2623 | K2564 | Q2481 | G2394 | C2310 | M2211 |
| V2986 | L2986 | L2926 | R2806 | L2747 | R2806 | L2747 | L2686 | R2624 | K2565 | D2482 | G2395 | M2312 | M2212 |
| E2987 | S2987 | L2927 | W2807 | P2748 | W2807 | P2748 | A2687 | R2625 | C2566 | G2483 | V2397 | M2313 | W2213 |
| K2988 | K2988 | F2928 | P2808 | E2749 | P2808 | E2749 | H2688 | Y2627 | A2566 | A2484 | ARG   | L2314 | V2214 |
| S2989 | S2989 | F2929 | I2809 | K2750 | I2809 | K2750 | K2689 | F2628 | P2567 | A2485 | ASP   | L2315 | L2215 |
| V3050 | P2990 | L2930 | K2810 | L2751 | K2810 | L2751 | K2690 | D2629 | P2567 | L2485 | ASP   | A2315 | G2216 |
| R3051 | H2991 | Q2931 | E2811 | D2752 | E2811 | D2752 | Y2691 | V2630 | F2569 | V2486 | ARG   | G2217 | G2217 |
| K3052 | E2992 | M2932 | S2812 | S2753 | S2812 | S2753 | D2692 | P2631 | P2570 | Q2487 | ARG   | G2218 | G2218 |
| Q2993 | Q2993 | M2933 | L2813 | F2754 | L2813 | F2754 | Q2693 | T2632 | Q2571 | P2488 | GLU   | Y2318 | T2219 |
| E2994 | E2994 | K2934 | K2814 | L2755 | K2814 | L2755 | E2694 | L2633 | T2572 | K2489 | HIS   | P2319 | T2220 |
| I2995 | I2995 | Y2935 | A2815 | M2756 | A2815 | M2756 | L2695 | W2634 | E2573 | S2493 | PHE   | K2221 | K2221 |
| K2996 | K2996 | A2936 | M2816 | K2757 | M2816 | K2757 | L2696 | E2635 | H2574 | F2494 | GLY   | E2222 | E2222 |
| F2997 | F2997 | T2937 | I2817 | F2758 | I2817 | F2758 | Y2696 | A2637 | R2575 | P2410 | GLU   | R2224 | R2224 |
| G3058 | G2979 | T2938 | W2818 | A2759 | W2818 | A2759 | M2698 | K2638 | I2577 | D2497 | P2411 | R2330 | F2225 |
| T3059 | A2999 | R2939 | W2819 | E2760 | W2819 | E2760 | M2699 | A2637 | M2578 | H2498 | E2412 | R2331 | K2228 |
| D3060 | K3000 | GLY   | E2820 | Y2761 | E2820 | Y2761 | M2700 | W2639 | I2579 | K2499 | E2413 | R2336 | M2228 |
| A3061 | I3001 | L3001 | W2821 | T2762 | W2821 | T2762 | P2701 | P2640 | M2581 | M2502 | N2414 | V2341 | T2230 |
| A3063 | L3002 | L3002 | K2822 | H2763 | K2822 | H2763 | C2702 | L2641 | S2582 | V2509 | R2415 | E2347 | F2235 |
| V3064 | L3003 | ASP   | I2823 | E2764 | I2823 | E2764 | C2704 | K2642 | L2583 | V2416 | H2417 | R2355 | Y2238 |
| V3065 | P3004 | GLY   | E2824 | K2765 | E2824 | K2765 | A2705 | L2643 | L2584 | L2418 | L2418 | I2368 | M2244 |
| N3066 | L3005 | L2946 | K2825 | W2766 | K2825 | W2766 | L2706 | T2644 | T2585 | E2512 | G2419 | R2359 | Q2245 |
| C3067 | I3006 | D2947 | A2826 | A2767 | A2826 | A2767 | A2707 | W2645 | Y2586 | N2514 | H2420 | E2362 | M2250 |
| L3068 | N3007 | T2948 | R2827 | F2768 | R2827 | F2768 | G2708 | H2647 | I2587 | Q2515 | M2423 | C2363 | H2253 |
| H3069 | Q3008 | S2949 | E2828 | D2769 | E2828 | D2769 | G2709 | Y2648 | R2588 | D2516 | E2364 | F2364 | Y2256 |
| F3070 | S3009 | S2950 | G2829 | K2770 | G2829 | K2770 | L2710 | E2649 | L2589 | F2517 | G2365 | P2366 | E2269 |
| I3071 | F3010 | I2951 | E2830 | I2771 | E2830 | I2771 | P2711 | C2651 | S2590 | L2519 | P2367 | A2367 | Q2262 |
| T3072 | T3011 | E2952 | GLY   | Q2772 | GLY   | Q2772 | P2712 | Q2655 | R2591 | H2520 | R2435 | G2369 | I2263 |
| A3073 | H3012 | K2953 | ARG   | L2773 | ARG   | L2773 | D2713 | T2655 | G2592 | Y2521 | R2436 | G2370 | I2264 |
| S3074 | H3013 | L2894 | THR   | M2774 | THR   | M2774 | Y2714 | C2656 | R2593 | L2522 | P2437 | E2371 | L2265 |
| L3075 | C3014 | F2955 | GLY   | W2775 | GLY   | W2775 | V2715 | L2657 | S2594 | D2523 | E2438 | G2372 | G2266 |
| I3076 | L3015 | A2956 | LYS   | S2776 | LYS   | S2776 | V2716 | P2658 | L2595 | Y2524 | E2439 | G2373 | G2266 |
| F3077 | F3016 | F2957 | LYS   | Y2777 | LYS   | Y2777 | A2717 | T2659 | A2598 | F2526 | M2440 | G2374 | G2266 |
| L3078 | L3018 | G2958 | THR   | Q2778 | THR   | Q2778 | S2718 | Q2660 | Q2599 | L2442 | L2432 | G2375 | G2266 |
| T3079 | S3019 | F2959 | ARG   | E2779 | ARG   | E2779 | S2719 | W2661 | R2600 | E2449 | E2449 | G2376 | G2266 |
| V3080 | T3020 | Q2961 | LYS   | W2780 | LYS   | W2780 | Y2719 | A2662 | L2603 | L2460 | L2460 | L2376 | G2266 |
| M3081 | P3021 | Q2962 | ILE   | V2781 | ILE   | V2781 | S2720 | K2663 | E2604 |       |       |       |       |
| K3082 | A3022 | L2963 | GLN   | D2782 | GLN   | D2782 | K2721 | F2664 | D2605 |       |       |       |       |
| G3083 | K3023 | L2964 | THR   | E2783 | THR   | E2783 | A2723 | G2665 | G2606 |       |       |       |       |
| F3084 | G3024 | R2965 | ALA   | E2784 | ALA   | E2784 | G2724 | V2666 |       |       |       |       |       |
| F3085 | L3025 | W2966 | L2785 | L2785 | L2785 | L2785 | K2725 | T2667 |       |       |       |       |       |
| E3086 | G3026 | M2967 | K2786 | K2786 | K2786 | K2786 | LYS   | S2668 |       |       |       |       |       |
| I3087 | S3027 | D2968 | T2787 | T2787 | T2787 | T2787 | ALA   |       |       |       |       |       |       |
| V3088 | G3028 |       | THR   | H2788 | THR   | H2788 | THR   |       |       |       |       |       |       |

|       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| D4018 | L3866 | L3735 | E3630 | L3569 | L3509 | H3449 | E3389 | I3329 | V3289 | Q3209 | Q3149 | K3089 |
| L4019 | N3867 | E3736 | A3631 | R3570 | I3510 | N3450 | G3390 | D3330 | I3270 | L3210 | H3150 | A3090 |
| K4020 | R3868 | GLU   | V3632 | N3571 | V3511 | F3451 | E3391 | E3331 | E3271 | N3211 | Q3151 | G3091 |
| D4022 | Q3869 | GLY   | V3633 | N3573 | A3512 | K3452 | L3392 | A3332 | I3272 | E3212 | F3152 | L3092 |
| M4039 | N3870 | GLU   | A3634 | A3574 | T3513 | R3453 | L3393 | I3333 | T3273 | N3213 | G3153 | R3093 |
| I4040 | K3871 | ASN   | C3635 | L3575 | L3514 | E3454 | V3394 | M3334 | L3274 | N3214 | D3154 | S3094 |
|       | E3872 | GLY   | F3636 | T3576 | K3515 | Q3455 | R3395 | M3335 | F3275 | A3215 | D3155 | F3095 |
| M4044 | K3873 | GLU   | R3637 | R3577 | K3516 | N3457 | D3396 | K3336 | N3276 | C3216 | V3156 | F3096 |
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| R3949 | Q3766 | G3681 | G3682 | V3596 | A3536 | K3475 | Y3416 | S3356 | L3296 | V3236 | G3176 | V3116 |
| N3950 | Q3767 | Q3682 | Q3683 | E3598 | K3537 | K3477 | V3417 | H3357 | P3297 | E3237 | T3177 | ALA   |
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|       |       |       | E3718 | V3618 | L3557 | D3501 | N3437 | L3256 | R3196 | L3137 |       |       |
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|       |       |       |       | S3625 | V3563 | T3507 | T3443 | R3262 | V3203 | L3143 |       |       |
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● Molecule 1: Ryanodine receptor 1

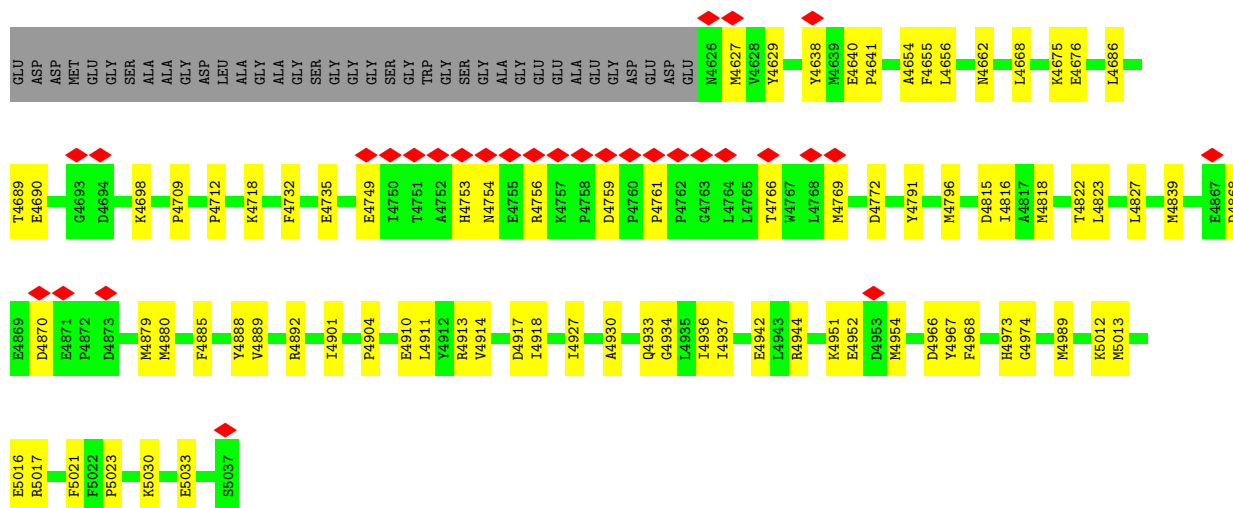




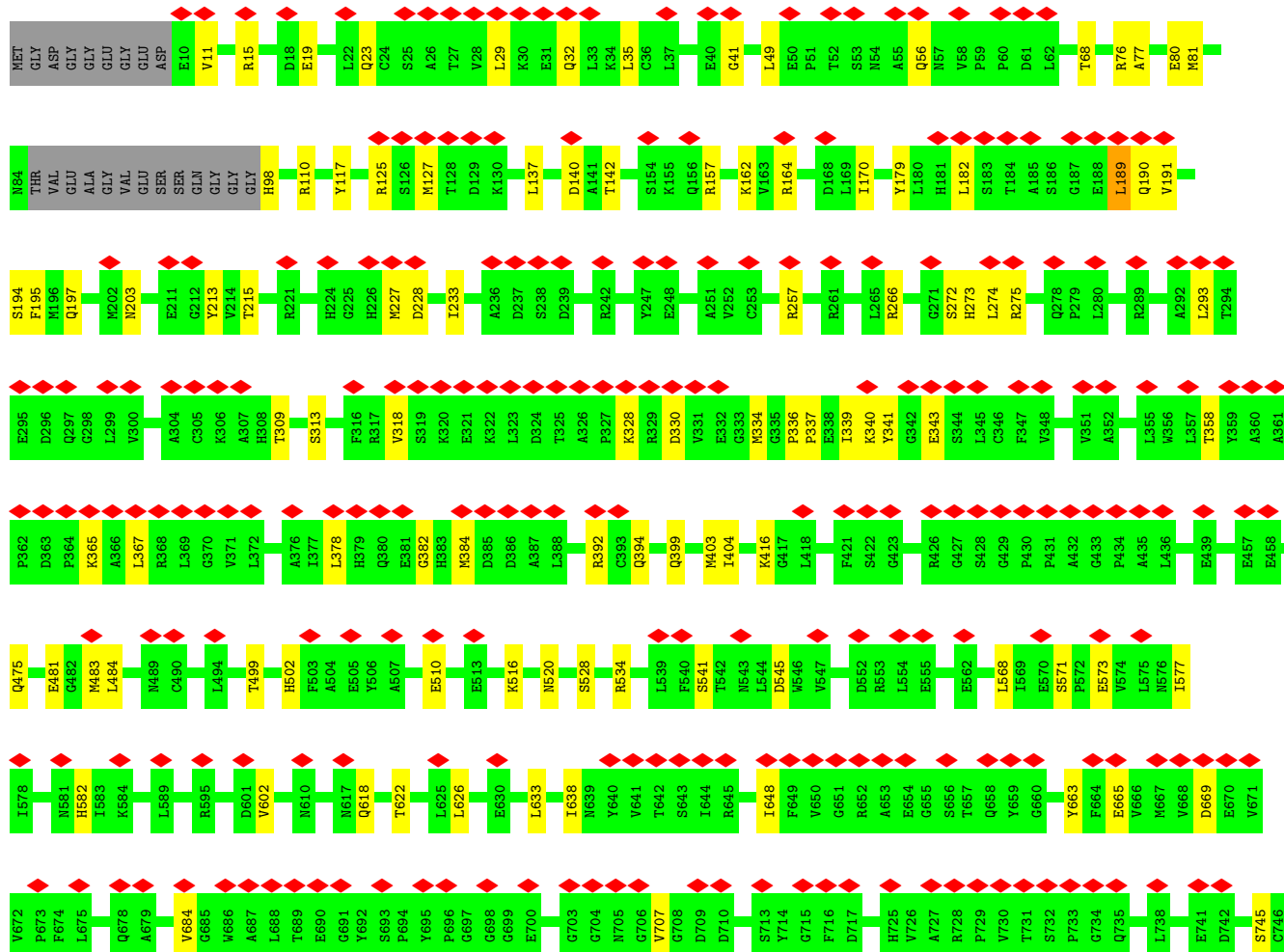
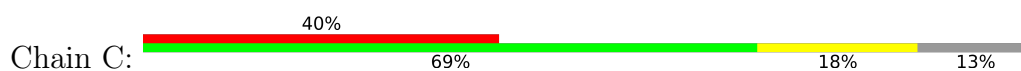
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| Q2515 | G2419 | R2359 | R2126 | GLU   | V1783 | D1649 | Q1569 | G1504 | F1440 |
| D2516 | H2420 | R2362 | Q2127 | GLU   | A1784 | I1650 | K1570 | Q1505 | A1441 |
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| V2521 | L2436 | F2364 | R2136 | GLU   | L1786 | E1655 | P1574 | G1508 | Q1443 |
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| D2529 | H2441 | E2370 | M2153 | SER   | E1793 | R1668 | E1583 | V1515 | Y1457 |
| H2530 | L2442 | G2371 | L2165 | ARG   | A1794 | R1671 | R1584 | L1516 | H1458 |
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| N3312 | D3252 | E3192 | T3132 | A3072 | N3012 | E2952 | Q2892 | ARG   | Q2772 | P2712 | R2650 | L2589 |
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| P3297 | E3237 | ALA   | T3178 | ALA   | F3057 | F2997 | A2937 | Y2882 | M2816 | R2758 | R2697 | F2636 |
| L3298 | E3238 | ARG   | K3179 | ARG   | G3058 | F2998 | T2937 | H2883 | L2817 | A2759 | M2698 | A2637 |
| G3299 | M3239 | THR   | N3180 | THR   | T3059 | A2999 | T2938 | H2884 | A2818 | E2760 | K2638 | K2638 |
| A3300 | C3240 | GLN   | T3181 | GLN   | D3060 | K3000 | R2939 | T2885 | W2819 | E2761 | M2700 | M2639 |
| P3301 | P3241 | VAL   | F3182 | VAL   | A3061 | I3001 | GLY   | W2886 | E2820 | T2762 | C2702 | L2641 |
| L3302 | D3242 | K3123 | Y3183 | K3123 | P3062 | L3002 | LYS   | G2887 | W2821 | H2763 | L2703 | K2642 |
| C3303 | I3243 | G3124 | V3183 | G3124 | A3063 | L3003 | ASP   | G2887 | T2822 | E2764 | C2704 | L2643 |
| C3304 | P3244 | V3125 | V3064 | V3125 | V3064 | L3004 | WET   | R2888 | I2823 | K2765 | A2705 | L2644 |
| L3305 | V3245 | G3126 | V3065 | G3126 | V3065 | L3005 | GLU   |       | E2824 | W2766 | L2706 | T2645 |
| A3306 | L3246 | Q3127 | N3066 | Q3127 | N3066 | I3006 |       |       | K2825 | A2767 | A2707 | H2646 |
| L3307 | D3247 | N3128 | C3067 | N3128 | C3067 | N3007 |       |       | A2826 | F2768 | G2708 |       |
| R3308 | P3188 | P3188 | L3068 |       | L3068 | Q3008 |       |       | E2827 |       |       |       |





• Molecule 1: Ryanodine receptor 1



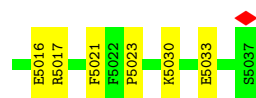




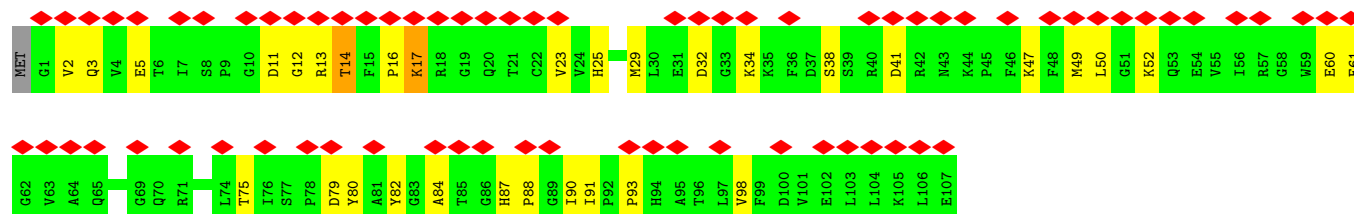




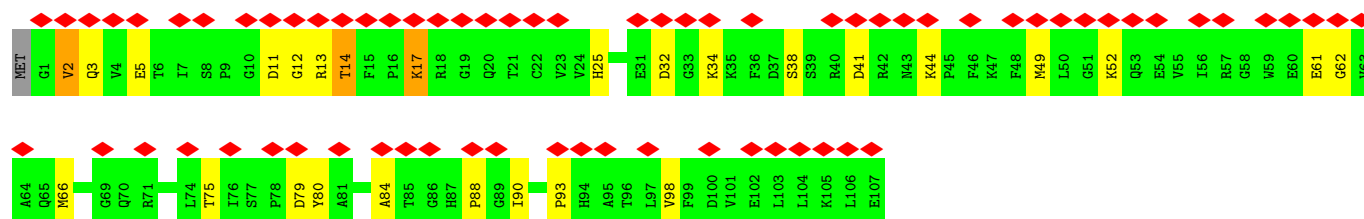
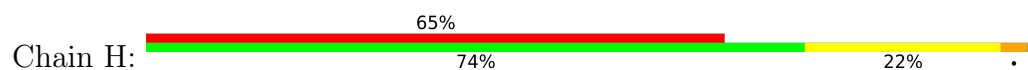




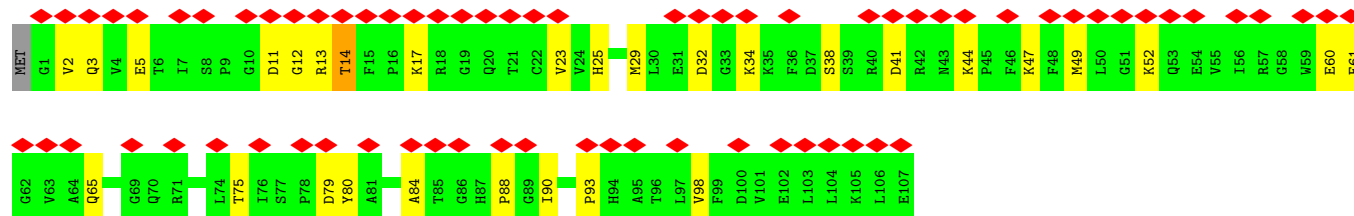
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



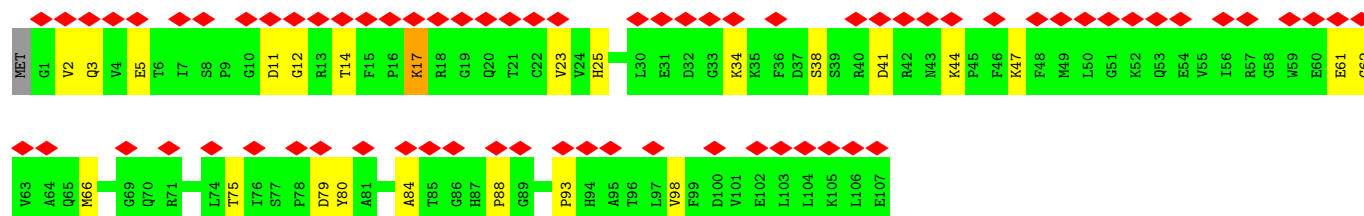
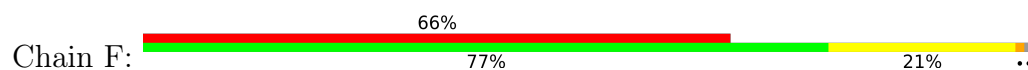
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 17393                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 58                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.436                                   | Depositor |
| Minimum map value                    | -0.223                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.018                                   | Depositor |
| Recommended contour level            | 0.1                                     | Depositor |
| Map size (Å)                         | 428.288, 428.288, 428.288               | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.8365, 0.8365, 0.8365                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, CA, 141, ZN

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.29         | 0/35977     | 0.38        | 1/48726 (0.0%)  |
| 1   | B     | 0.29         | 0/35977     | 0.38        | 1/48726 (0.0%)  |
| 1   | C     | 0.29         | 0/35977     | 0.38        | 1/48726 (0.0%)  |
| 1   | D     | 0.29         | 0/35977     | 0.38        | 1/48726 (0.0%)  |
| 2   | E     | 0.30         | 0/850       | 0.43        | 0/1146          |
| 2   | F     | 0.27         | 0/850       | 0.40        | 0/1146          |
| 2   | G     | 0.28         | 0/850       | 0.40        | 0/1146          |
| 2   | H     | 0.29         | 0/850       | 0.41        | 0/1146          |
| All | All   | 0.29         | 0/147308    | 0.38        | 4/199488 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1   | D     | 3239 | MET  | CB-CG-SD | 7.01 | 133.72      | 112.70   |
| 1   | A     | 3239 | MET  | CB-CG-SD | 7.00 | 133.71      | 112.70   |
| 1   | C     | 3239 | MET  | CB-CG-SD | 7.00 | 133.69      | 112.70   |
| 1   | B     | 3239 | MET  | CB-CG-SD | 6.99 | 133.67      | 112.70   |

There are no chirality outliers.

There are no planarity outliers.

### 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     | 35150  | 0        | 34797    | 630     | 0            |
| 1   | B     | 35150  | 0        | 34797    | 622     | 0            |
| 1   | C     | 35150  | 0        | 34797    | 648     | 0            |
| 1   | D     | 35150  | 0        | 34797    | 650     | 0            |
| 2   | E     | 831    | 0        | 831      | 25      | 0            |
| 2   | F     | 831    | 0        | 831      | 18      | 0            |
| 2   | G     | 831    | 0        | 831      | 23      | 0            |
| 2   | H     | 831    | 0        | 831      | 21      | 0            |
| 3   | A     | 31     | 0        | 12       | 0       | 0            |
| 3   | B     | 31     | 0        | 12       | 0       | 0            |
| 3   | C     | 31     | 0        | 12       | 0       | 0            |
| 3   | D     | 31     | 0        | 12       | 0       | 0            |
| 4   | A     | 1      | 0        | 0        | 0       | 0            |
| 4   | B     | 1      | 0        | 0        | 0       | 0            |
| 4   | C     | 1      | 0        | 0        | 0       | 0            |
| 4   | D     | 1      | 0        | 0        | 0       | 0            |
| 5   | A     | 1      | 0        | 0        | 0       | 0            |
| 5   | B     | 1      | 0        | 0        | 0       | 0            |
| 5   | C     | 1      | 0        | 0        | 0       | 0            |
| 5   | D     | 1      | 0        | 0        | 0       | 0            |
| 6   | A     | 11     | 0        | 4        | 0       | 0            |
| 6   | B     | 11     | 0        | 4        | 0       | 0            |
| 6   | C     | 11     | 0        | 4        | 0       | 0            |
| 6   | D     | 11     | 0        | 4        | 0       | 0            |
| 7   | A     | 1      | 0        | 0        | 0       | 0            |
| 7   | B     | 1      | 0        | 0        | 0       | 0            |
| 7   | C     | 1      | 0        | 0        | 0       | 0            |
| 7   | D     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 144104 | 0        | 142576   | 2538    | 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 9.

All (2538) 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:C:1573:MET:HE3 | 1:C:1574:PRO:HD2 | 1.37                     | 1.05              |
| 1:A:1573:MET:HE3 | 1:A:1574:PRO:HD2 | 1.37                     | 1.03              |
| 1:D:1573:MET:HE3 | 1:D:1574:PRO:HD2 | 1.37                     | 1.02              |
| 1:B:1573:MET:HE3 | 1:B:1574:PRO:HD2 | 1.37                     | 1.02              |
| 1:B:3467:MET:HE1 | 1:C:1174:GLY:CA  | 1.99                     | 0.93              |
| 1:A:4942:GLU:OE1 | 1:D:4944:ARG:NH1 | 2.00                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1174:GLY:CA   | 1:C:3467:MET:HE1  | 2.00                     | 0.90              |
| 1:A:1174:GLY:CA   | 1:D:3467:MET:HE1  | 2.02                     | 0.90              |
| 1:A:1066:GLN:HB2  | 1:A:1071:ARG:HH22 | 1.39                     | 0.88              |
| 1:D:1066:GLN:HB2  | 1:D:1071:ARG:HH22 | 1.39                     | 0.88              |
| 1:C:1066:GLN:HB2  | 1:C:1071:ARG:HH22 | 1.39                     | 0.88              |
| 1:B:1066:GLN:HB2  | 1:B:1071:ARG:HH22 | 1.39                     | 0.86              |
| 1:A:4578:LEU:O    | 1:B:4879:MET:HB3  | 1.76                     | 0.85              |
| 1:A:2420:HIS:HA   | 1:A:2423:MET:HE2  | 1.60                     | 0.84              |
| 1:D:2420:HIS:HA   | 1:D:2423:MET:HE2  | 1.60                     | 0.83              |
| 1:A:4892:ARG:HD3  | 1:B:4918:ILE:HD13 | 1.60                     | 0.83              |
| 1:B:2420:HIS:HA   | 1:B:2423:MET:HE2  | 1.60                     | 0.83              |
| 1:C:2420:HIS:HA   | 1:C:2423:MET:HE2  | 1.60                     | 0.82              |
| 1:B:4892:ARG:HD3  | 1:C:4918:ILE:HD13 | 1.60                     | 0.81              |
| 1:A:1773:PRO:HA   | 1:A:2153:MET:HE1  | 1.63                     | 0.80              |
| 1:B:4944:ARG:NH1  | 1:C:4942:GLU:OE1  | 2.15                     | 0.80              |
| 1:D:1773:PRO:HA   | 1:D:2153:MET:HE1  | 1.63                     | 0.80              |
| 1:A:1527:MET:HE2  | 1:A:1540:PHE:HB2  | 1.64                     | 0.80              |
| 1:C:1527:MET:HE2  | 1:C:1540:PHE:HB2  | 1.64                     | 0.80              |
| 1:A:4892:ARG:HD3  | 1:B:4918:ILE:CD1  | 2.12                     | 0.80              |
| 1:D:4942:GLU:OE1  | 1:C:4944:ARG:NH1  | 2.14                     | 0.80              |
| 1:B:1527:MET:HE2  | 1:B:1540:PHE:HB2  | 1.64                     | 0.79              |
| 1:B:1773:PRO:HA   | 1:B:2153:MET:HE1  | 1.63                     | 0.79              |
| 1:D:4918:ILE:HD13 | 1:C:4892:ARG:HD3  | 1.62                     | 0.79              |
| 1:A:1174:GLY:HA2  | 1:D:3467:MET:HE1  | 1.64                     | 0.79              |
| 1:C:1773:PRO:HA   | 1:C:2153:MET:HE1  | 1.63                     | 0.78              |
| 1:D:1527:MET:HE2  | 1:D:1540:PHE:HB2  | 1.64                     | 0.78              |
| 1:D:858:THR:HB    | 1:D:930:LYS:HD2   | 1.66                     | 0.78              |
| 1:B:858:THR:HB    | 1:B:930:LYS:HD2   | 1.66                     | 0.78              |
| 1:D:1025:ARG:H    | 1:D:1025:ARG:HD3  | 1.49                     | 0.78              |
| 1:A:858:THR:HB    | 1:A:930:LYS:HD2   | 1.66                     | 0.77              |
| 1:A:1025:ARG:HD3  | 1:A:1025:ARG:H    | 1.49                     | 0.77              |
| 1:C:858:THR:HB    | 1:C:930:LYS:HD2   | 1.66                     | 0.77              |
| 1:D:2747:ILE:HD13 | 1:D:2814:LYS:HG2  | 1.67                     | 0.77              |
| 1:B:23:GLN:NE2    | 1:B:203:ASN:OD1   | 2.18                     | 0.77              |
| 1:C:1025:ARG:HD3  | 1:C:1025:ARG:H    | 1.49                     | 0.77              |
| 1:C:2747:ILE:HD13 | 1:C:2814:LYS:HG2  | 1.67                     | 0.76              |
| 1:B:2747:ILE:HD13 | 1:B:2814:LYS:HG2  | 1.67                     | 0.76              |
| 1:C:23:GLN:NE2    | 1:C:203:ASN:OD1   | 2.18                     | 0.76              |
| 2:G:61:GLU:OE1    | 2:G:61:GLU:N      | 2.17                     | 0.76              |
| 1:B:2765:LYS:HZ3  | 1:B:2857:PRO:HB2  | 1.50                     | 0.76              |
| 1:B:1025:ARG:H    | 1:B:1025:ARG:HD3  | 1.49                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:23:GLN:NE2    | 1:A:203:ASN:OD1   | 2.18                     | 0.76              |
| 2:E:61:GLU:OE1    | 2:E:61:GLU:N      | 2.18                     | 0.75              |
| 1:A:2747:ILE:HD13 | 1:A:2814:LYS:HG2  | 1.67                     | 0.75              |
| 1:D:23:GLN:NE2    | 1:D:203:ASN:OD1   | 2.18                     | 0.75              |
| 1:D:182:LEU:HD11  | 1:D:189:LEU:HD12  | 1.70                     | 0.74              |
| 1:D:977:LEU:HG    | 1:D:1044:ARG:HH12 | 1.51                     | 0.74              |
| 1:D:4954:MET:HE2  | 1:D:4954:MET:HA   | 1.69                     | 0.74              |
| 1:C:4954:MET:HE2  | 1:C:4954:MET:HA   | 1.69                     | 0.74              |
| 1:B:977:LEU:HG    | 1:B:1044:ARG:HH12 | 1.51                     | 0.74              |
| 1:C:977:LEU:HG    | 1:C:1044:ARG:HH12 | 1.51                     | 0.74              |
| 1:A:4954:MET:HA   | 1:A:4954:MET:HE2  | 1.69                     | 0.73              |
| 1:B:2970:SER:HA   | 1:B:2973:PHE:CE1  | 2.23                     | 0.73              |
| 1:C:182:LEU:HD11  | 1:C:189:LEU:HD12  | 1.70                     | 0.73              |
| 1:A:182:LEU:HD11  | 1:A:189:LEU:HD12  | 1.70                     | 0.73              |
| 1:C:2970:SER:HA   | 1:C:2973:PHE:CE1  | 2.24                     | 0.73              |
| 1:C:3946:GLN:OE1  | 1:C:3949:ARG:NH1  | 2.17                     | 0.73              |
| 2:E:90:ILE:HG22   | 2:E:91:ILE:HG13   | 1.70                     | 0.73              |
| 1:A:977:LEU:HG    | 1:A:1044:ARG:HH12 | 1.52                     | 0.73              |
| 1:D:2970:SER:HA   | 1:D:2973:PHE:CE1  | 2.24                     | 0.73              |
| 1:A:2970:SER:HA   | 1:A:2973:PHE:CE1  | 2.24                     | 0.73              |
| 1:A:4578:LEU:HD23 | 1:B:4879:MET:HG3  | 1.71                     | 0.73              |
| 1:B:876:GLU:HG2   | 1:B:918:ARG:HD3   | 1.70                     | 0.72              |
| 1:B:2867:LEU:HB2  | 1:B:2928:LYS:HZ3  | 1.54                     | 0.72              |
| 1:B:4954:MET:HE2  | 1:B:4954:MET:HA   | 1.69                     | 0.72              |
| 1:A:2867:LEU:HB2  | 1:A:2928:LYS:HZ3  | 1.54                     | 0.72              |
| 1:B:182:LEU:HD11  | 1:B:189:LEU:HD12  | 1.70                     | 0.72              |
| 1:B:3467:MET:HE1  | 1:C:1174:GLY:HA2  | 1.71                     | 0.72              |
| 1:D:876:GLU:HG2   | 1:D:918:ARG:HD3   | 1.71                     | 0.72              |
| 1:C:3366:ARG:NH1  | 1:C:3440:GLU:OE1  | 2.22                     | 0.72              |
| 1:C:2867:LEU:HB2  | 1:C:2928:LYS:HZ3  | 1.55                     | 0.72              |
| 1:D:125:ARG:NH1   | 1:D:190:GLN:OE1   | 2.23                     | 0.72              |
| 1:C:125:ARG:NH1   | 1:C:190:GLN:OE1   | 2.23                     | 0.72              |
| 1:C:876:GLU:HG2   | 1:C:918:ARG:HD3   | 1.71                     | 0.72              |
| 1:A:125:ARG:NH1   | 1:A:190:GLN:OE1   | 2.23                     | 0.71              |
| 1:D:2867:LEU:HB2  | 1:D:2928:LYS:HZ3  | 1.54                     | 0.71              |
| 1:A:876:GLU:HG2   | 1:A:918:ARG:HD3   | 1.71                     | 0.71              |
| 2:F:88:PRO:HB2    | 1:B:1680:ARG:HH12 | 1.55                     | 0.71              |
| 1:B:125:ARG:NH1   | 1:B:190:GLN:OE1   | 2.23                     | 0.71              |
| 1:B:3366:ARG:NH1  | 1:B:3440:GLU:OE1  | 2.22                     | 0.71              |
| 1:C:961:MET:HE2   | 1:C:963:ASN:HB3   | 1.73                     | 0.71              |
| 1:D:961:MET:HE2   | 1:D:963:ASN:HB3   | 1.73                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3250:MET:HE2  | 1:D:3277:LEU:HD13 | 1.73                     | 0.71              |
| 1:D:3946:GLN:OE1  | 1:D:3949:ARG:NH1  | 2.17                     | 0.71              |
| 1:C:4091:LYS:HZ1  | 1:C:4095:LYS:HB3  | 1.56                     | 0.71              |
| 1:A:2577:ILE:HD12 | 1:A:2578:MET:H    | 1.56                     | 0.70              |
| 1:A:3250:MET:HE2  | 1:A:3277:LEU:HD13 | 1.73                     | 0.70              |
| 2:H:61:GLU:OE1    | 2:H:61:GLU:N      | 2.19                     | 0.70              |
| 1:B:3946:GLN:OE1  | 1:B:3949:ARG:NH1  | 2.17                     | 0.70              |
| 1:A:4091:LYS:HZ1  | 1:A:4095:LYS:HB3  | 1.56                     | 0.70              |
| 1:D:2170:MET:HE2  | 1:D:2228:MET:HE2  | 1.74                     | 0.70              |
| 1:A:1684:ALA:HA   | 2:E:90:ILE:HD11   | 1.73                     | 0.70              |
| 1:A:2170:MET:HE2  | 1:A:2228:MET:HE2  | 1.74                     | 0.70              |
| 1:A:961:MET:HE2   | 1:A:963:ASN:HB3   | 1.73                     | 0.70              |
| 1:A:3946:GLN:OE1  | 1:A:3949:ARG:NH1  | 2.17                     | 0.70              |
| 2:G:88:PRO:HB2    | 1:C:1680:ARG:HH12 | 1.57                     | 0.70              |
| 1:B:2170:MET:HE2  | 1:B:2228:MET:HE2  | 1.74                     | 0.70              |
| 1:D:4091:LYS:HZ1  | 1:D:4095:LYS:HB3  | 1.56                     | 0.70              |
| 1:C:2577:ILE:HD12 | 1:C:2578:MET:H    | 1.56                     | 0.70              |
| 1:B:2577:ILE:HD12 | 1:B:2578:MET:H    | 1.56                     | 0.70              |
| 1:B:2902:HIS:HB3  | 1:B:2905:LEU:HG   | 1.74                     | 0.70              |
| 1:D:2902:HIS:HB3  | 1:D:2905:LEU:HG   | 1.74                     | 0.70              |
| 1:B:961:MET:HE2   | 1:B:963:ASN:HB3   | 1.73                     | 0.70              |
| 1:D:1174:GLY:HA2  | 1:C:3467:MET:HE1  | 1.72                     | 0.70              |
| 1:C:2170:MET:HE2  | 1:C:2228:MET:HE2  | 1.74                     | 0.70              |
| 1:C:3250:MET:HE2  | 1:C:3277:LEU:HD13 | 1.73                     | 0.69              |
| 1:C:227:MET:HA    | 1:C:227:MET:HE3   | 1.75                     | 0.69              |
| 1:C:2902:HIS:HB3  | 1:C:2905:LEU:HG   | 1.74                     | 0.69              |
| 1:A:2902:HIS:HB3  | 1:A:2905:LEU:HG   | 1.74                     | 0.69              |
| 1:A:3366:ARG:NH1  | 1:A:3440:GLU:OE1  | 2.22                     | 0.69              |
| 1:D:1996:ARG:HH21 | 1:D:1999:ARG:HG3  | 1.58                     | 0.69              |
| 2:H:88:PRO:HB2    | 1:D:1680:ARG:HH12 | 1.57                     | 0.69              |
| 1:D:227:MET:HA    | 1:D:227:MET:HE3   | 1.75                     | 0.69              |
| 1:A:1996:ARG:HH21 | 1:A:1999:ARG:HG3  | 1.58                     | 0.69              |
| 1:B:3250:MET:HE2  | 1:B:3277:LEU:HD13 | 1.73                     | 0.69              |
| 1:D:4966:ASP:OD2  | 1:D:4967:TYR:N    | 2.26                     | 0.69              |
| 1:C:1996:ARG:HH21 | 1:C:1999:ARG:HG3  | 1.58                     | 0.69              |
| 1:A:227:MET:HA    | 1:A:227:MET:HE3   | 1.75                     | 0.69              |
| 1:A:4966:ASP:OD2  | 1:A:4967:TYR:N    | 2.26                     | 0.69              |
| 1:B:227:MET:HA    | 1:B:227:MET:HE3   | 1.75                     | 0.69              |
| 1:D:3324:VAL:HG11 | 1:D:3361:THR:HG22 | 1.75                     | 0.69              |
| 1:D:2577:ILE:HD12 | 1:D:2578:MET:H    | 1.56                     | 0.69              |
| 1:D:4818:MET:N    | 1:D:4818:MET:SD   | 2.66                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1987:SER:HB2  | 1:D:1994:ARG:HH22 | 1.59                     | 0.68              |
| 1:C:4966:ASP:OD2  | 1:C:4967:TYR:N    | 2.26                     | 0.68              |
| 2:F:61:GLU:OE1    | 2:F:61:GLU:N      | 2.20                     | 0.68              |
| 1:B:4818:MET:N    | 1:B:4818:MET:SD   | 2.66                     | 0.68              |
| 1:C:891:TRP:HA    | 1:C:902:ARG:HB3   | 1.75                     | 0.68              |
| 1:B:4091:LYS:HZ1  | 1:B:4095:LYS:HB3  | 1.56                     | 0.68              |
| 1:C:4818:MET:SD   | 1:C:4818:MET:N    | 2.67                     | 0.68              |
| 1:B:3324:VAL:HG11 | 1:B:3361:THR:HG22 | 1.75                     | 0.68              |
| 1:D:4904:PRO:HB3  | 1:D:4913:ARG:HG2  | 1.76                     | 0.68              |
| 1:B:4966:ASP:OD2  | 1:B:4967:TYR:N    | 2.26                     | 0.68              |
| 1:D:955:LEU:O     | 1:D:966:LYS:NZ    | 2.27                     | 0.68              |
| 1:A:1099:GLU:OE1  | 1:A:1128:ARG:NH2  | 2.27                     | 0.68              |
| 1:C:4904:PRO:HB3  | 1:C:4913:ARG:HG2  | 1.76                     | 0.68              |
| 1:A:4818:MET:N    | 1:A:4818:MET:SD   | 2.66                     | 0.68              |
| 1:D:3114:LYS:HD3  | 1:D:3116:SER:H    | 1.59                     | 0.68              |
| 1:D:3366:ARG:NH1  | 1:D:3440:GLU:OE1  | 2.22                     | 0.68              |
| 1:B:1996:ARG:HH21 | 1:B:1999:ARG:HG3  | 1.58                     | 0.68              |
| 1:C:1099:GLU:OE1  | 1:C:1128:ARG:NH2  | 2.27                     | 0.68              |
| 1:C:3114:LYS:HD3  | 1:C:3116:SER:H    | 1.59                     | 0.67              |
| 1:A:891:TRP:HA    | 1:A:902:ARG:HB3   | 1.75                     | 0.67              |
| 1:A:3324:VAL:HG11 | 1:A:3361:THR:HG22 | 1.75                     | 0.67              |
| 1:B:928:THR:O     | 1:B:931:THR:OG1   | 2.12                     | 0.67              |
| 1:D:891:TRP:HA    | 1:D:902:ARG:HB3   | 1.75                     | 0.67              |
| 1:D:3645:PRO:HG2  | 1:D:3648:ARG:HH21 | 1.60                     | 0.67              |
| 1:A:4654:ALA:C    | 1:A:4796:MET:HE1  | 2.20                     | 0.67              |
| 1:A:4839:MET:HA   | 1:A:4839:MET:HE3  | 1.76                     | 0.67              |
| 1:B:955:LEU:O     | 1:B:966:LYS:NZ    | 2.27                     | 0.67              |
| 1:B:1099:GLU:OE1  | 1:B:1128:ARG:NH2  | 2.27                     | 0.67              |
| 1:C:3324:VAL:HG11 | 1:C:3361:THR:HG22 | 1.75                     | 0.67              |
| 1:C:3645:PRO:HG2  | 1:C:3648:ARG:HH21 | 1.60                     | 0.67              |
| 1:A:1987:SER:HB2  | 1:A:1994:ARG:HH22 | 1.59                     | 0.67              |
| 1:A:2765:LYS:HZ3  | 1:A:2857:PRO:HB2  | 1.60                     | 0.67              |
| 1:C:3329:ILE:HD11 | 1:C:3332:ALA:HB2  | 1.76                     | 0.67              |
| 1:D:4839:MET:HA   | 1:D:4839:MET:HE3  | 1.76                     | 0.67              |
| 1:C:1987:SER:HB2  | 1:C:1994:ARG:HH22 | 1.59                     | 0.67              |
| 1:A:1985:THR:OG1  | 1:A:1986:MET:SD   | 2.53                     | 0.67              |
| 1:A:3329:ILE:HD11 | 1:A:3332:ALA:HB2  | 1.76                     | 0.67              |
| 1:B:891:TRP:HA    | 1:B:902:ARG:HB3   | 1.75                     | 0.67              |
| 1:B:1987:SER:HB2  | 1:B:1994:ARG:HH22 | 1.59                     | 0.67              |
| 1:A:955:LEU:O     | 1:A:966:LYS:NZ    | 2.27                     | 0.67              |
| 1:A:2519:LEU:HD13 | 1:A:2575:ARG:HG3  | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4904:PRO:HB3  | 1:A:4913:ARG:HG2  | 1.75                     | 0.67              |
| 1:B:3020:THR:HG23 | 1:B:3023:LYS:H    | 1.59                     | 0.67              |
| 1:D:2519:LEU:HD13 | 1:D:2575:ARG:HG3  | 1.77                     | 0.67              |
| 1:A:3114:LYS:HD3  | 1:A:3116:SER:H    | 1.59                     | 0.66              |
| 1:B:3329:ILE:HD11 | 1:B:3332:ALA:HB2  | 1.76                     | 0.66              |
| 1:D:4654:ALA:C    | 1:D:4796:MET:HE1  | 2.20                     | 0.66              |
| 1:B:3114:LYS:HD3  | 1:B:3116:SER:H    | 1.59                     | 0.66              |
| 1:B:4888:TYR:OH   | 1:C:4917:ASP:OD2  | 2.08                     | 0.66              |
| 1:C:4654:ALA:C    | 1:C:4796:MET:HE1  | 2.20                     | 0.66              |
| 1:A:3523:ASN:O    | 1:A:3582:ARG:NH2  | 2.29                     | 0.66              |
| 1:A:3645:PRO:HG2  | 1:A:3648:ARG:HH21 | 1.60                     | 0.66              |
| 1:B:3291:ALA:O    | 1:B:3293:PRO:HD3  | 1.96                     | 0.66              |
| 1:C:4839:MET:HE3  | 1:C:4839:MET:HA   | 1.76                     | 0.66              |
| 1:B:2018:GLU:OE1  | 1:B:2028:ARG:NH1  | 2.29                     | 0.66              |
| 1:B:3523:ASN:O    | 1:B:3582:ARG:NH2  | 2.29                     | 0.66              |
| 1:B:3645:PRO:HG2  | 1:B:3648:ARG:HH21 | 1.60                     | 0.66              |
| 1:B:4904:PRO:HB3  | 1:B:4913:ARG:HG2  | 1.75                     | 0.66              |
| 1:D:1099:GLU:OE1  | 1:D:1128:ARG:NH2  | 2.27                     | 0.66              |
| 1:D:2018:GLU:OE1  | 1:D:2028:ARG:NH1  | 2.29                     | 0.66              |
| 1:D:3523:ASN:O    | 1:D:3582:ARG:NH2  | 2.29                     | 0.66              |
| 1:C:955:LEU:O     | 1:C:966:LYS:NZ    | 2.27                     | 0.66              |
| 1:C:3523:ASN:O    | 1:C:3582:ARG:NH2  | 2.29                     | 0.66              |
| 1:A:2018:GLU:OE1  | 1:A:2028:ARG:NH1  | 2.29                     | 0.66              |
| 1:B:2644:LEU:HD13 | 1:B:2678:LEU:HD21 | 1.78                     | 0.66              |
| 1:B:4839:MET:HA   | 1:B:4839:MET:HE3  | 1.76                     | 0.66              |
| 1:D:928:THR:O     | 1:D:931:THR:OG1   | 2.12                     | 0.66              |
| 1:C:928:THR:O     | 1:C:931:THR:OG1   | 2.12                     | 0.66              |
| 1:A:3020:THR:HG23 | 1:A:3023:LYS:H    | 1.59                     | 0.66              |
| 1:B:3540:TYR:HB3  | 1:B:3604:TYR:CD1  | 2.31                     | 0.66              |
| 1:D:2644:LEU:HD13 | 1:D:2678:LEU:HD21 | 1.78                     | 0.66              |
| 1:A:4839:MET:HE2  | 1:D:4823:LEU:HD21 | 1.77                     | 0.66              |
| 1:D:3291:ALA:O    | 1:D:3293:PRO:HD3  | 1.96                     | 0.66              |
| 1:D:3329:ILE:HD11 | 1:D:3332:ALA:HB2  | 1.76                     | 0.66              |
| 1:B:4654:ALA:C    | 1:B:4796:MET:HE1  | 2.20                     | 0.66              |
| 1:C:2018:GLU:OE1  | 1:C:2028:ARG:NH1  | 2.29                     | 0.66              |
| 1:C:2644:LEU:HD13 | 1:C:2678:LEU:HD21 | 1.78                     | 0.66              |
| 1:A:2781:VAL:HA   | 1:A:2789:PRO:HB2  | 1.78                     | 0.65              |
| 1:A:2644:LEU:HD13 | 1:A:2678:LEU:HD21 | 1.78                     | 0.65              |
| 1:D:3020:THR:HG23 | 1:D:3023:LYS:H    | 1.59                     | 0.65              |
| 1:B:1066:GLN:HB2  | 1:B:1071:ARG:NH2  | 2.11                     | 0.65              |
| 1:B:2519:LEU:HD13 | 1:B:2575:ARG:HG3  | 1.77                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3540:TYR:HB3  | 1:D:3604:TYR:CD1  | 2.31                     | 0.65              |
| 1:A:3540:TYR:HB3  | 1:A:3604:TYR:CD1  | 2.31                     | 0.65              |
| 1:A:4944:ARG:NH1  | 1:B:4942:GLU:OE1  | 2.29                     | 0.65              |
| 1:C:3291:ALA:O    | 1:C:3293:PRO:HD3  | 1.96                     | 0.65              |
| 1:A:928:THR:O     | 1:A:931:THR:OG1   | 2.12                     | 0.65              |
| 1:A:3291:ALA:O    | 1:A:3293:PRO:HD3  | 1.96                     | 0.65              |
| 1:B:2781:VAL:HA   | 1:B:2789:PRO:HB2  | 1.78                     | 0.65              |
| 1:B:2182:ILE:O    | 1:B:2186:MET:HG2  | 1.97                     | 0.65              |
| 1:C:1066:GLN:HB2  | 1:C:1071:ARG:NH2  | 2.11                     | 0.65              |
| 1:B:3434:LEU:HB3  | 1:B:3517:MET:HE1  | 1.79                     | 0.65              |
| 1:C:3434:LEU:HB3  | 1:C:3517:MET:HE1  | 1.79                     | 0.65              |
| 1:D:2466:LEU:HD23 | 1:D:2502:MET:HE3  | 1.79                     | 0.65              |
| 1:D:2781:VAL:HA   | 1:D:2789:PRO:HB2  | 1.78                     | 0.65              |
| 1:C:3020:THR:HG23 | 1:C:3023:LYS:H    | 1.59                     | 0.65              |
| 1:D:1232:ARG:NH2  | 1:D:1828:ASP:O    | 2.30                     | 0.65              |
| 1:D:2182:ILE:O    | 1:D:2186:MET:HG2  | 1.97                     | 0.65              |
| 1:D:2978:GLU:OE2  | 1:D:3053:ARG:NH1  | 2.30                     | 0.65              |
| 1:C:2978:GLU:OE2  | 1:C:3053:ARG:NH1  | 2.30                     | 0.64              |
| 1:A:2466:LEU:HD23 | 1:A:2502:MET:HE3  | 1.79                     | 0.64              |
| 1:B:1127:HIS:HB3  | 1:B:1128:ARG:HH21 | 1.63                     | 0.64              |
| 1:B:1985:THR:OG1  | 1:B:1986:MET:SD   | 2.53                     | 0.64              |
| 1:B:3017:PHE:O    | 1:B:3036:LYS:NZ   | 2.31                     | 0.64              |
| 1:D:2765:LYS:HZ3  | 1:D:2857:PRO:HB2  | 1.62                     | 0.64              |
| 1:C:2519:LEU:HD13 | 1:C:2575:ARG:HG3  | 1.77                     | 0.64              |
| 1:A:2794:TYR:H    | 1:A:2855:TYR:HB2  | 1.63                     | 0.64              |
| 1:A:2978:GLU:OE2  | 1:A:3053:ARG:NH1  | 2.30                     | 0.64              |
| 2:E:11:ASP:OD1    | 2:E:12:GLY:N      | 2.31                     | 0.64              |
| 1:B:367:LEU:HD23  | 1:B:367:LEU:H     | 1.62                     | 0.64              |
| 1:C:367:LEU:HD23  | 1:C:367:LEU:H     | 1.62                     | 0.64              |
| 1:C:1127:HIS:HB3  | 1:C:1128:ARG:HH21 | 1.63                     | 0.64              |
| 1:C:3540:TYR:HB3  | 1:C:3604:TYR:CD1  | 2.31                     | 0.64              |
| 1:A:2182:ILE:O    | 1:A:2186:MET:HG2  | 1.97                     | 0.64              |
| 1:B:2978:GLU:OE2  | 1:B:3053:ARG:NH1  | 2.30                     | 0.64              |
| 1:A:1127:HIS:HB3  | 1:A:1128:ARG:HH21 | 1.63                     | 0.64              |
| 1:B:2794:TYR:H    | 1:B:2855:TYR:HB2  | 1.63                     | 0.64              |
| 1:D:2794:TYR:H    | 1:D:2855:TYR:HB2  | 1.63                     | 0.64              |
| 2:G:11:ASP:OD1    | 2:G:12:GLY:N      | 2.31                     | 0.64              |
| 1:B:19:GLU:HG2    | 1:B:68:THR:HG22   | 1.79                     | 0.64              |
| 1:B:56:GLN:O      | 1:B:309:THR:OG1   | 2.16                     | 0.64              |
| 1:C:56:GLN:O      | 1:C:309:THR:OG1   | 2.16                     | 0.64              |
| 1:C:2182:ILE:O    | 1:C:2186:MET:HG2  | 1.97                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3434:LEU:HB3  | 1:A:3517:MET:HE1  | 1.79                     | 0.64              |
| 1:C:3017:PHE:O    | 1:C:3036:LYS:NZ   | 2.31                     | 0.64              |
| 1:C:19:GLU:HG2    | 1:C:68:THR:HG22   | 1.79                     | 0.64              |
| 1:C:1252:HIS:O    | 1:C:1275:ARG:NH1  | 2.31                     | 0.64              |
| 1:A:3017:PHE:O    | 1:A:3036:LYS:NZ   | 2.31                     | 0.64              |
| 1:B:1232:ARG:NH2  | 1:B:1828:ASP:O    | 2.30                     | 0.64              |
| 1:D:56:GLN:O      | 1:D:309:THR:OG1   | 2.16                     | 0.64              |
| 1:D:3434:LEU:HB3  | 1:D:3517:MET:HE1  | 1.79                     | 0.64              |
| 1:C:2466:LEU:HD23 | 1:C:2502:MET:HE3  | 1.79                     | 0.64              |
| 1:A:1066:GLN:HB2  | 1:A:1071:ARG:NH2  | 2.11                     | 0.63              |
| 2:H:11:ASP:OD1    | 2:H:12:GLY:N      | 2.31                     | 0.63              |
| 1:B:1252:HIS:O    | 1:B:1275:ARG:NH1  | 2.31                     | 0.63              |
| 1:D:2128:TYR:OH   | 1:D:3676:ASP:OD2  | 2.16                     | 0.63              |
| 1:D:3017:PHE:O    | 1:D:3036:LYS:NZ   | 2.31                     | 0.63              |
| 1:C:1985:THR:OG1  | 1:C:1986:MET:SD   | 2.53                     | 0.63              |
| 1:C:2781:VAL:HA   | 1:C:2789:PRO:HB2  | 1.78                     | 0.63              |
| 1:A:1252:HIS:O    | 1:A:1275:ARG:NH1  | 2.31                     | 0.63              |
| 1:D:367:LEU:H     | 1:D:367:LEU:HD23  | 1.62                     | 0.63              |
| 1:C:1232:ARG:NH2  | 1:C:1828:ASP:O    | 2.30                     | 0.63              |
| 1:D:1127:HIS:HB3  | 1:D:1128:ARG:HH21 | 1.63                     | 0.63              |
| 1:D:1252:HIS:O    | 1:D:1275:ARG:NH1  | 2.31                     | 0.63              |
| 1:A:19:GLU:HG2    | 1:A:68:THR:HG22   | 1.79                     | 0.63              |
| 2:F:11:ASP:OD1    | 2:F:12:GLY:N      | 2.32                     | 0.63              |
| 1:C:2777:TYR:HB3  | 1:C:2791:LEU:HD23 | 1.80                     | 0.63              |
| 1:A:367:LEU:HD23  | 1:A:367:LEU:H     | 1.62                     | 0.63              |
| 1:B:2128:TYR:OH   | 1:B:3676:ASP:OD2  | 2.17                     | 0.63              |
| 1:B:4892:ARG:HD3  | 1:C:4918:ILE:CD1  | 2.27                     | 0.63              |
| 1:D:2777:TYR:HB3  | 1:D:2791:LEU:HD23 | 1.80                     | 0.63              |
| 1:C:4232:GLU:OE1  | 1:C:5017:ARG:NH2  | 2.32                     | 0.63              |
| 1:A:2128:TYR:OH   | 1:A:3676:ASP:OD2  | 2.17                     | 0.63              |
| 1:A:3034:LYS:O    | 1:A:3038:MET:HG3  | 1.99                     | 0.63              |
| 1:B:2777:TYR:HB3  | 1:B:2791:LEU:HD23 | 1.80                     | 0.63              |
| 1:B:4157:ASP:N    | 1:B:4161:ARG:HH21 | 1.97                     | 0.63              |
| 1:D:1990:GLU:OE1  | 1:D:1994:ARG:NH2  | 2.32                     | 0.63              |
| 1:D:3034:LYS:O    | 1:D:3038:MET:HG3  | 1.99                     | 0.63              |
| 1:C:4157:ASP:N    | 1:C:4161:ARG:HH21 | 1.97                     | 0.63              |
| 1:D:1066:GLN:HB2  | 1:D:1071:ARG:NH2  | 2.11                     | 0.63              |
| 1:A:3377:GLU:HA   | 1:A:3380:ARG:HG2  | 1.81                     | 0.63              |
| 1:C:2128:TYR:OH   | 1:C:3676:ASP:OD2  | 2.16                     | 0.63              |
| 1:B:2466:LEU:HD23 | 1:B:2502:MET:HE3  | 1.79                     | 0.62              |
| 1:D:1985:THR:OG1  | 1:D:1986:MET:SD   | 2.53                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:56:GLN:O      | 1:A:309:THR:OG1   | 2.16                     | 0.62              |
| 1:B:1990:GLU:OE1  | 1:B:1994:ARG:NH2  | 2.32                     | 0.62              |
| 1:B:4232:GLU:OE1  | 1:B:5017:ARG:NH2  | 2.32                     | 0.62              |
| 1:A:1232:ARG:NH2  | 1:A:1828:ASP:O    | 2.30                     | 0.62              |
| 1:A:4232:GLU:OE1  | 1:A:5017:ARG:NH2  | 2.32                     | 0.62              |
| 1:C:2794:TYR:H    | 1:C:2855:TYR:HB2  | 1.63                     | 0.62              |
| 1:A:4157:ASP:N    | 1:A:4161:ARG:HH21 | 1.96                     | 0.62              |
| 1:D:4232:GLU:OE1  | 1:D:5017:ARG:NH2  | 2.32                     | 0.62              |
| 1:C:2970:SER:HA   | 1:C:2973:PHE:HE1  | 1.64                     | 0.62              |
| 1:A:2777:TYR:HB3  | 1:A:2791:LEU:HD23 | 1.80                     | 0.62              |
| 1:B:1448:VAL:HG22 | 1:B:1554:VAL:HG23 | 1.82                     | 0.62              |
| 1:D:4157:ASP:N    | 1:D:4161:ARG:HH21 | 1.96                     | 0.62              |
| 1:C:2779:GLU:HG3  | 1:C:2792:ARG:HG2  | 1.82                     | 0.62              |
| 1:A:1448:VAL:HG22 | 1:A:1554:VAL:HG23 | 1.82                     | 0.62              |
| 1:B:516:LYS:O     | 1:B:520:ASN:ND2   | 2.30                     | 0.62              |
| 1:B:2779:GLU:HG3  | 1:B:2792:ARG:HG2  | 1.82                     | 0.62              |
| 1:B:3377:GLU:HA   | 1:B:3380:ARG:HG2  | 1.81                     | 0.62              |
| 1:D:19:GLU:HG2    | 1:D:68:THR:HG22   | 1.79                     | 0.62              |
| 1:C:1990:GLU:OE1  | 1:C:1994:ARG:NH2  | 2.32                     | 0.62              |
| 1:A:1990:GLU:OE1  | 1:A:1994:ARG:NH2  | 2.32                     | 0.62              |
| 1:A:2875:ALA:HB2  | 1:A:2927:LEU:HD22 | 1.82                     | 0.62              |
| 1:B:2582:MET:HE3  | 1:B:2610:LEU:HD13 | 1.82                     | 0.62              |
| 1:D:897:ARG:NH2   | 1:D:899:ASP:OD1   | 2.33                     | 0.62              |
| 1:A:127:MET:SD    | 1:A:127:MET:N     | 2.73                     | 0.61              |
| 1:A:2779:GLU:HG3  | 1:A:2792:ARG:HG2  | 1.82                     | 0.61              |
| 1:D:2779:GLU:HG3  | 1:D:2792:ARG:HG2  | 1.82                     | 0.61              |
| 1:D:2827:ARG:NH2  | 1:D:2935:TYR:OH   | 2.33                     | 0.61              |
| 1:D:3377:GLU:HA   | 1:D:3380:ARG:HG2  | 1.81                     | 0.61              |
| 1:B:2875:ALA:HB2  | 1:B:2927:LEU:HD22 | 1.82                     | 0.61              |
| 1:D:2875:ALA:HB2  | 1:D:2927:LEU:HD22 | 1.82                     | 0.61              |
| 1:D:3235:SER:OG   | 1:D:3237:GLU:OE1  | 2.18                     | 0.61              |
| 1:B:897:ARG:NH2   | 1:B:899:ASP:OD1   | 2.33                     | 0.61              |
| 1:B:3850:GLN:NE2  | 1:B:3872:GLU:OE1  | 2.33                     | 0.61              |
| 1:D:4917:ASP:OD2  | 1:C:4888:TYR:OH   | 2.09                     | 0.61              |
| 1:A:4689:THR:OG1  | 1:A:4690:GLU:OE1  | 2.18                     | 0.61              |
| 1:B:3034:LYS:O    | 1:B:3038:MET:HG3  | 1.99                     | 0.61              |
| 1:D:2582:MET:HE3  | 1:D:2610:LEU:HD13 | 1.82                     | 0.61              |
| 1:C:3235:SER:OG   | 1:C:3237:GLU:OE1  | 2.18                     | 0.61              |
| 1:A:2970:SER:HA   | 1:A:2973:PHE:HE1  | 1.64                     | 0.61              |
| 1:A:2827:ARG:NH2  | 1:A:2935:TYR:OH   | 2.33                     | 0.61              |
| 1:A:3850:GLN:NE2  | 1:A:3872:GLU:OE1  | 2.33                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:38:SER:OG     | 2:F:41:ASP:OD1    | 2.15                     | 0.61              |
| 1:B:951:LYS:H     | 1:B:951:LYS:HD2   | 1.66                     | 0.61              |
| 1:B:3235:SER:OG   | 1:B:3237:GLU:OE1  | 2.18                     | 0.61              |
| 1:D:4918:ILE:CD1  | 1:C:4892:ARG:HD3  | 2.28                     | 0.61              |
| 1:C:3034:LYS:O    | 1:C:3038:MET:HG3  | 1.99                     | 0.61              |
| 1:C:3377:GLU:HA   | 1:C:3380:ARG:HG2  | 1.81                     | 0.61              |
| 1:C:3850:GLN:NE2  | 1:C:3872:GLU:OE1  | 2.33                     | 0.61              |
| 1:B:4689:THR:OG1  | 1:B:4690:GLU:OE1  | 2.18                     | 0.61              |
| 1:A:2582:MET:HE3  | 1:A:2610:LEU:HD13 | 1.82                     | 0.61              |
| 1:B:2827:ARG:NH2  | 1:B:2935:TYR:OH   | 2.34                     | 0.61              |
| 1:C:897:ARG:NH2   | 1:C:899:ASP:OD1   | 2.33                     | 0.61              |
| 1:B:2765:LYS:NZ   | 1:B:2859:PRO:O    | 2.34                     | 0.60              |
| 1:D:2765:LYS:NZ   | 1:D:2859:PRO:O    | 2.34                     | 0.60              |
| 1:A:897:ARG:NH2   | 1:A:899:ASP:OD1   | 2.33                     | 0.60              |
| 1:B:4769:MET:SD   | 1:B:4769:MET:N    | 2.70                     | 0.60              |
| 1:D:2970:SER:HA   | 1:D:2973:PHE:HE1  | 1.64                     | 0.60              |
| 1:B:1730:MET:HE3  | 1:B:1773:PRO:HG3  | 1.83                     | 0.60              |
| 1:B:4888:TYR:HE1  | 1:C:4917:ASP:HB2  | 1.65                     | 0.60              |
| 1:C:2765:LYS:NZ   | 1:C:2859:PRO:O    | 2.34                     | 0.60              |
| 1:B:2970:SER:HA   | 1:B:2973:PHE:HE1  | 1.64                     | 0.60              |
| 1:C:2875:ALA:HB2  | 1:C:2927:LEU:HD22 | 1.82                     | 0.60              |
| 1:A:951:LYS:H     | 1:A:951:LYS:HD2   | 1.66                     | 0.60              |
| 1:A:1066:GLN:CB   | 1:A:1071:ARG:HH22 | 2.13                     | 0.60              |
| 1:B:4791:TYR:OH   | 1:B:4815:ASP:OD1  | 2.13                     | 0.60              |
| 1:D:3850:GLN:NE2  | 1:D:3872:GLU:OE1  | 2.33                     | 0.60              |
| 1:C:1448:VAL:HG22 | 1:C:1554:VAL:HG23 | 1.82                     | 0.60              |
| 1:D:1448:VAL:HG22 | 1:D:1554:VAL:HG23 | 1.82                     | 0.60              |
| 1:A:516:LYS:O     | 1:A:520:ASN:ND2   | 2.30                     | 0.60              |
| 1:A:3235:SER:OG   | 1:A:3237:GLU:OE1  | 2.18                     | 0.60              |
| 2:E:38:SER:OG     | 2:E:41:ASP:OD1    | 2.16                     | 0.60              |
| 1:D:1730:MET:HE3  | 1:D:1773:PRO:HG3  | 1.83                     | 0.60              |
| 1:C:2582:MET:HE3  | 1:C:2610:LEU:HD13 | 1.82                     | 0.60              |
| 1:C:2827:ARG:NH2  | 1:C:2935:TYR:OH   | 2.33                     | 0.60              |
| 1:A:3371:LYS:NZ   | 1:A:3375:GLU:OE2  | 2.34                     | 0.60              |
| 1:B:3995:VAL:O    | 1:B:3999:MET:HB2  | 2.02                     | 0.60              |
| 1:C:951:LYS:H     | 1:C:951:LYS:HD2   | 1.66                     | 0.60              |
| 1:C:4241:THR:HG22 | 1:C:4245:MET:HE3  | 1.84                     | 0.60              |
| 1:D:951:LYS:H     | 1:D:951:LYS:HD2   | 1.66                     | 0.59              |
| 1:D:3995:VAL:O    | 1:D:3999:MET:HB2  | 2.02                     | 0.59              |
| 1:D:4917:ASP:HB2  | 1:C:4888:TYR:HE1  | 1.66                     | 0.59              |
| 1:C:3995:VAL:O    | 1:C:3999:MET:HB2  | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4689:THR:OG1  | 1:C:4690:GLU:OE1  | 2.18                     | 0.59              |
| 1:C:3391:GLU:O    | 1:C:3395:ARG:HG2  | 2.02                     | 0.59              |
| 1:A:3445:TRP:NE1  | 1:A:3455:GLU:OE1  | 2.32                     | 0.59              |
| 1:B:3391:GLU:O    | 1:B:3395:ARG:HG2  | 2.02                     | 0.59              |
| 1:C:384:MET:SD    | 1:C:384:MET:N     | 2.72                     | 0.59              |
| 1:A:4769:MET:SD   | 1:A:4769:MET:N    | 2.71                     | 0.59              |
| 1:B:3445:TRP:NE1  | 1:B:3455:GLU:OE1  | 2.32                     | 0.59              |
| 1:B:3769:ARG:O    | 1:B:3773:ARG:NH1  | 2.35                     | 0.59              |
| 1:B:925:SER:O     | 1:B:928:THR:OG1   | 2.19                     | 0.59              |
| 1:B:2208:MET:HE1  | 1:B:2253:HIS:CD2  | 2.38                     | 0.59              |
| 1:A:2986:VAL:HG22 | 1:A:2988:LYS:H    | 1.68                     | 0.59              |
| 1:A:5012:LYS:NZ   | 1:A:5016:GLU:OE2  | 2.35                     | 0.59              |
| 1:D:127:MET:SD    | 1:D:127:MET:N     | 2.73                     | 0.59              |
| 1:C:5013:MET:HE2  | 1:C:5021:PHE:HD1  | 1.67                     | 0.59              |
| 1:B:1864:LYS:HE3  | 1:B:1872:THR:HA   | 1.84                     | 0.59              |
| 1:B:3087:ILE:HD12 | 1:B:3087:ILE:H    | 1.68                     | 0.59              |
| 1:D:1864:LYS:HE3  | 1:D:1872:THR:HA   | 1.84                     | 0.59              |
| 1:C:4769:MET:SD   | 1:C:4769:MET:N    | 2.70                     | 0.59              |
| 1:A:3995:VAL:O    | 1:A:3999:MET:HB2  | 2.02                     | 0.59              |
| 1:B:1808:ARG:HD3  | 1:B:1853:ILE:HG22 | 1.85                     | 0.59              |
| 1:B:3371:LYS:NZ   | 1:B:3375:GLU:OE2  | 2.34                     | 0.59              |
| 1:B:5013:MET:HE2  | 1:B:5021:PHE:HD1  | 1.67                     | 0.59              |
| 1:D:4791:TYR:OH   | 1:D:4815:ASP:OD1  | 2.13                     | 0.59              |
| 1:C:1108:GLU:OE2  | 1:C:1108:GLU:N    | 2.28                     | 0.59              |
| 1:C:1730:MET:HE3  | 1:C:1773:PRO:HG3  | 1.83                     | 0.59              |
| 1:A:1730:MET:HE3  | 1:A:1773:PRO:HG3  | 1.83                     | 0.59              |
| 1:A:2208:MET:HE1  | 1:A:2253:HIS:CD2  | 2.38                     | 0.59              |
| 1:A:2765:LYS:NZ   | 1:A:2859:PRO:O    | 2.34                     | 0.59              |
| 1:A:4934:GLY:HA3  | 1:D:4937:ILE:HG12 | 1.85                     | 0.59              |
| 1:B:2986:VAL:HG22 | 1:B:2988:LYS:H    | 1.68                     | 0.59              |
| 1:C:3169:LEU:HD12 | 1:C:3194:LEU:HD11 | 1.85                     | 0.59              |
| 1:A:4241:THR:HG22 | 1:A:4245:MET:HE3  | 1.84                     | 0.59              |
| 2:G:49:MET:HB3    | 2:G:52:LYS:HD3    | 1.83                     | 0.59              |
| 1:B:3169:LEU:HD12 | 1:B:3194:LEU:HD11 | 1.85                     | 0.59              |
| 1:D:3535:LEU:O    | 1:D:3538:THR:OG1  | 2.20                     | 0.59              |
| 1:D:4689:THR:OG1  | 1:D:4690:GLU:OE1  | 2.18                     | 0.59              |
| 1:D:5012:LYS:NZ   | 1:D:5016:GLU:OE2  | 2.35                     | 0.59              |
| 1:C:516:LYS:O     | 1:C:520:ASN:ND2   | 2.30                     | 0.59              |
| 1:C:3836:MET:HG3  | 1:C:3884:LEU:HD21 | 1.84                     | 0.59              |
| 1:A:3391:GLU:O    | 1:A:3395:ARG:HG2  | 2.02                     | 0.58              |
| 2:G:38:SER:OG     | 2:G:41:ASP:OD1    | 2.14                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3391:GLU:O    | 1:D:3395:ARG:HG2  | 2.02                     | 0.58              |
| 1:C:1864:LYS:HE3  | 1:C:1872:THR:HA   | 1.84                     | 0.58              |
| 1:A:1748:PHE:HB2  | 1:A:1758:ARG:HH21 | 1.68                     | 0.58              |
| 1:A:1864:LYS:HE3  | 1:A:1872:THR:HA   | 1.84                     | 0.58              |
| 1:A:2477:PRO:HD3  | 1:A:2546:MET:HG2  | 1.86                     | 0.58              |
| 1:D:4241:THR:HG22 | 1:D:4245:MET:HE3  | 1.84                     | 0.58              |
| 1:C:1808:ARG:HD3  | 1:C:1853:ILE:HG22 | 1.85                     | 0.58              |
| 1:B:2737:PRO:HD2  | 1:B:2891:LYS:HD3  | 1.86                     | 0.58              |
| 1:D:1066:GLN:CB   | 1:D:1071:ARG:HH22 | 2.13                     | 0.58              |
| 1:D:2208:MET:HE1  | 1:D:2253:HIS:CD2  | 2.38                     | 0.58              |
| 1:D:2737:PRO:HD2  | 1:D:2891:LYS:HD3  | 1.86                     | 0.58              |
| 1:D:5013:MET:HE2  | 1:D:5021:PHE:HD1  | 1.67                     | 0.58              |
| 1:A:1228:ILE:HG12 | 1:D:3571:TRP:CE2  | 2.39                     | 0.58              |
| 1:B:633:LEU:HD13  | 1:B:1639:LEU:HD21 | 1.85                     | 0.58              |
| 1:B:3535:LEU:O    | 1:B:3538:THR:OG1  | 2.20                     | 0.58              |
| 1:D:908:VAL:HA    | 1:D:961:MET:HE3   | 1.86                     | 0.58              |
| 1:D:2271:THR:OG1  | 1:D:2330:ARG:NH2  | 2.36                     | 0.58              |
| 1:D:3836:MET:HG3  | 1:D:3884:LEU:HD21 | 1.84                     | 0.58              |
| 1:C:2208:MET:HE1  | 1:C:2253:HIS:CD2  | 2.38                     | 0.58              |
| 1:C:2973:PHE:CE2  | 1:C:2995:ILE:HG12 | 2.39                     | 0.58              |
| 1:C:3769:ARG:O    | 1:C:3773:ARG:NH1  | 2.35                     | 0.58              |
| 1:A:2419:GLY:O    | 1:A:2423:MET:HG3  | 2.04                     | 0.58              |
| 1:A:3836:MET:HG3  | 1:A:3884:LEU:HD21 | 1.84                     | 0.58              |
| 1:A:4676:GLU:OE2  | 1:A:4698:LYS:NZ   | 2.37                     | 0.58              |
| 1:B:127:MET:N     | 1:B:127:MET:SD    | 2.73                     | 0.58              |
| 1:D:3371:LYS:NZ   | 1:D:3375:GLU:OE2  | 2.34                     | 0.58              |
| 1:C:908:VAL:HA    | 1:C:961:MET:HE3   | 1.86                     | 0.58              |
| 1:C:1066:GLN:CB   | 1:C:1071:ARG:HH22 | 2.13                     | 0.58              |
| 1:A:3400:VAL:HG23 | 1:A:3403:ARG:HH21 | 1.68                     | 0.58              |
| 1:B:4241:THR:HG22 | 1:B:4245:MET:HE3  | 1.84                     | 0.58              |
| 1:D:2986:VAL:HG22 | 1:D:2988:LYS:H    | 1.68                     | 0.58              |
| 1:C:2660:GLY:HA3  | 1:C:2666:VAL:HG22 | 1.85                     | 0.58              |
| 1:C:2737:PRO:HD2  | 1:C:2891:LYS:HD3  | 1.86                     | 0.58              |
| 1:C:3734:HIS:CD2  | 1:C:3736:GLU:H    | 2.21                     | 0.58              |
| 1:A:947:GLU:OE1   | 1:A:1051:TYR:OH   | 2.22                     | 0.58              |
| 1:A:1808:ARG:HD3  | 1:A:1853:ILE:HG22 | 1.85                     | 0.58              |
| 2:E:49:MET:HB3    | 2:E:52:LYS:HD3    | 1.86                     | 0.58              |
| 1:B:2419:GLY:O    | 1:B:2423:MET:HG3  | 2.04                     | 0.58              |
| 1:B:3734:HIS:CD2  | 1:B:3736:GLU:H    | 2.21                     | 0.58              |
| 1:B:4676:GLU:OE2  | 1:B:4698:LYS:NZ   | 2.37                     | 0.58              |
| 1:D:3169:LEU:HD12 | 1:D:3194:LEU:HD11 | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2477:PRO:HD3  | 1:C:2546:MET:HG2  | 1.86                     | 0.58              |
| 1:A:618:GLN:OE1   | 1:A:1678:ASN:ND2  | 2.35                     | 0.58              |
| 1:A:2737:PRO:HD2  | 1:A:2891:LYS:HD3  | 1.86                     | 0.58              |
| 1:A:3467:MET:HE1  | 1:B:1174:GLY:CA   | 2.34                     | 0.58              |
| 1:A:4578:LEU:HA   | 1:B:4879:MET:CG   | 2.34                     | 0.58              |
| 1:A:5013:MET:HE2  | 1:A:5021:PHE:HD1  | 1.67                     | 0.58              |
| 1:B:2477:PRO:HD3  | 1:B:2546:MET:HG2  | 1.85                     | 0.58              |
| 1:B:3400:VAL:HG23 | 1:B:3403:ARG:HH21 | 1.69                     | 0.58              |
| 1:D:1748:PHE:HB2  | 1:D:1758:ARG:HH21 | 1.68                     | 0.58              |
| 1:D:2410:PRO:HB3  | 1:D:2415:ARG:HB3  | 1.86                     | 0.58              |
| 1:D:3162:GLN:NE2  | 1:D:3216:CYS:O    | 2.37                     | 0.58              |
| 1:D:3400:VAL:HG23 | 1:D:3403:ARG:HH21 | 1.69                     | 0.58              |
| 1:D:3769:ARG:O    | 1:D:3773:ARG:NH1  | 2.35                     | 0.58              |
| 1:C:2419:GLY:O    | 1:C:2423:MET:HG3  | 2.04                     | 0.58              |
| 1:A:3162:GLN:NE2  | 1:A:3216:CYS:O    | 2.37                     | 0.58              |
| 1:D:618:GLN:OE1   | 1:D:1678:ASN:ND2  | 2.35                     | 0.58              |
| 1:D:1653:LEU:O    | 1:D:1660:GLN:NE2  | 2.37                     | 0.58              |
| 1:A:2973:PHE:CE2  | 1:A:2995:ILE:HG12 | 2.39                     | 0.58              |
| 1:B:2660:GLY:HA3  | 1:B:2666:VAL:HG22 | 1.85                     | 0.58              |
| 1:D:1808:ARG:HD3  | 1:D:1853:ILE:HG22 | 1.85                     | 0.58              |
| 1:C:925:SER:O     | 1:C:928:THR:OG1   | 2.19                     | 0.58              |
| 1:A:1653:LEU:O    | 1:A:1660:GLN:NE2  | 2.37                     | 0.57              |
| 1:A:3087:ILE:H    | 1:A:3087:ILE:HD12 | 1.68                     | 0.57              |
| 1:B:4901:ILE:HG13 | 1:B:4913:ARG:NH2  | 2.19                     | 0.57              |
| 1:D:3087:ILE:H    | 1:D:3087:ILE:HD12 | 1.68                     | 0.57              |
| 1:C:867:LEU:HD12  | 1:C:941:MET:HE1   | 1.85                     | 0.57              |
| 1:C:2410:PRO:HB3  | 1:C:2415:ARG:HB3  | 1.86                     | 0.57              |
| 1:C:4676:GLU:OE2  | 1:C:4698:LYS:NZ   | 2.37                     | 0.57              |
| 1:A:2660:GLY:HA3  | 1:A:2666:VAL:HG22 | 1.85                     | 0.57              |
| 1:A:3169:LEU:HD12 | 1:A:3194:LEU:HD11 | 1.85                     | 0.57              |
| 1:B:2208:MET:HA   | 1:B:2211:MET:HE3  | 1.87                     | 0.57              |
| 1:D:2973:PHE:CE2  | 1:D:2995:ILE:HG12 | 2.39                     | 0.57              |
| 1:C:2208:MET:HA   | 1:C:2211:MET:HE3  | 1.87                     | 0.57              |
| 1:A:867:LEU:HD12  | 1:A:941:MET:HE1   | 1.85                     | 0.57              |
| 1:A:4039:MET:SD   | 1:A:4040:ILE:HG13 | 2.44                     | 0.57              |
| 1:D:3734:HIS:CD2  | 1:D:3736:GLU:H    | 2.21                     | 0.57              |
| 1:C:127:MET:SD    | 1:C:127:MET:N     | 2.73                     | 0.57              |
| 1:C:3752:SER:N    | 1:C:3755:GLU:OE2  | 2.32                     | 0.57              |
| 1:A:2967:MET:O    | 1:A:2970:SER:OG   | 2.17                     | 0.57              |
| 1:B:3162:GLN:NE2  | 1:B:3216:CYS:O    | 2.37                     | 0.57              |
| 1:B:3836:MET:HG3  | 1:B:3884:LEU:HD21 | 1.84                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:867:LEU:HD12  | 1:D:941:MET:HE1   | 1.85                     | 0.57              |
| 1:C:4901:ILE:HG13 | 1:C:4913:ARG:NH2  | 2.19                     | 0.57              |
| 1:A:3535:LEU:O    | 1:A:3538:THR:OG1  | 2.20                     | 0.57              |
| 1:A:3545:THR:HG22 | 1:A:3548:GLU:HG3  | 1.86                     | 0.57              |
| 1:A:3734:HIS:CD2  | 1:A:3736:GLU:H    | 2.21                     | 0.57              |
| 1:B:5012:LYS:NZ   | 1:B:5016:GLU:OE2  | 2.35                     | 0.57              |
| 1:D:3545:THR:HG22 | 1:D:3548:GLU:HG3  | 1.86                     | 0.57              |
| 1:D:4769:MET:SD   | 1:D:4769:MET:N    | 2.71                     | 0.57              |
| 1:C:618:GLN:OE1   | 1:C:1678:ASN:ND2  | 2.35                     | 0.57              |
| 1:C:4570:ALA:O    | 1:C:4574:ASN:ND2  | 2.36                     | 0.57              |
| 1:D:2419:GLY:O    | 1:D:2423:MET:HG3  | 2.04                     | 0.57              |
| 1:D:4039:MET:SD   | 1:D:4040:ILE:HG13 | 2.44                     | 0.57              |
| 1:D:4676:GLU:OE2  | 1:D:4698:LYS:NZ   | 2.37                     | 0.57              |
| 1:C:1024:TYR:CZ   | 1:C:1032:LYS:HG3  | 2.40                     | 0.57              |
| 1:C:2986:VAL:HG22 | 1:C:2988:LYS:H    | 1.68                     | 0.57              |
| 1:C:3400:VAL:HG23 | 1:C:3403:ARG:HH21 | 1.68                     | 0.57              |
| 1:A:2410:PRO:HB3  | 1:A:2415:ARG:HB3  | 1.86                     | 0.57              |
| 1:B:4039:MET:SD   | 1:B:4040:ILE:HG13 | 2.44                     | 0.57              |
| 1:D:516:LYS:O     | 1:D:520:ASN:ND2   | 2.30                     | 0.57              |
| 1:D:2660:GLY:HA3  | 1:D:2666:VAL:HG22 | 1.86                     | 0.57              |
| 1:C:947:GLU:OE1   | 1:C:1051:TYR:OH   | 2.22                     | 0.57              |
| 1:C:2765:LYS:HZ3  | 1:C:2857:PRO:HB2  | 1.69                     | 0.57              |
| 1:A:908:VAL:HA    | 1:A:961:MET:HE3   | 1.86                     | 0.57              |
| 1:A:3769:ARG:O    | 1:A:3773:ARG:NH1  | 2.35                     | 0.57              |
| 1:D:633:LEU:HD13  | 1:D:1639:LEU:HD21 | 1.86                     | 0.57              |
| 1:C:3087:ILE:H    | 1:C:3087:ILE:HD12 | 1.68                     | 0.57              |
| 1:C:3545:THR:HG22 | 1:C:3548:GLU:HG3  | 1.86                     | 0.57              |
| 1:C:4039:MET:SD   | 1:C:4040:ILE:HG13 | 2.44                     | 0.57              |
| 1:A:925:SER:O     | 1:A:928:THR:OG1   | 2.19                     | 0.57              |
| 1:B:1653:LEU:O    | 1:B:1660:GLN:NE2  | 2.37                     | 0.57              |
| 1:B:2973:PHE:CE2  | 1:B:2995:ILE:HG12 | 2.39                     | 0.57              |
| 1:D:2477:PRO:HD3  | 1:D:2546:MET:HG2  | 1.85                     | 0.57              |
| 1:D:3445:TRP:NE1  | 1:D:3455:GLU:OE1  | 2.32                     | 0.57              |
| 1:C:3371:LYS:NZ   | 1:C:3375:GLU:OE2  | 2.34                     | 0.57              |
| 1:C:3535:LEU:O    | 1:C:3538:THR:OG1  | 2.20                     | 0.57              |
| 1:A:633:LEU:HD13  | 1:A:1639:LEU:HD21 | 1.85                     | 0.57              |
| 2:E:11:ASP:OD2    | 2:E:14:THR:OG1    | 2.23                     | 0.57              |
| 1:B:867:LEU:HD12  | 1:B:941:MET:HE1   | 1.85                     | 0.57              |
| 1:B:908:VAL:HA    | 1:B:961:MET:HE3   | 1.86                     | 0.57              |
| 1:B:1299:GLN:NE2  | 1:B:1545:ASN:OD1  | 2.38                     | 0.57              |
| 1:D:1299:GLN:NE2  | 1:D:1545:ASN:OD1  | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1753:LYS:HB3  | 1:D:1758:ARG:HA   | 1.87                     | 0.57              |
| 1:C:1748:PHE:HB2  | 1:C:1758:ARG:HH21 | 1.68                     | 0.57              |
| 1:C:5012:LYS:NZ   | 1:C:5016:GLU:OE2  | 2.35                     | 0.57              |
| 1:A:1299:GLN:NE2  | 1:A:1545:ASN:OD1  | 2.38                     | 0.56              |
| 1:A:2208:MET:HA   | 1:A:2211:MET:HE3  | 1.86                     | 0.56              |
| 1:A:4901:ILE:HG13 | 1:A:4913:ARG:NH2  | 2.19                     | 0.56              |
| 1:A:4910:GLU:O    | 1:A:4914:VAL:HG13 | 2.05                     | 0.56              |
| 1:B:571:SER:OG    | 1:B:573:GLU:OE1   | 2.21                     | 0.56              |
| 1:B:1748:PHE:HB2  | 1:B:1758:ARG:HH21 | 1.68                     | 0.56              |
| 1:C:633:LEU:HD13  | 1:C:1639:LEU:HD21 | 1.85                     | 0.56              |
| 1:A:293:LEU:HD13  | 1:A:378:LEU:HD12  | 1.87                     | 0.56              |
| 1:A:2679:PHE:HB2  | 1:A:2706:ILE:HG21 | 1.87                     | 0.56              |
| 1:B:2410:PRO:HB3  | 1:B:2415:ARG:HB3  | 1.86                     | 0.56              |
| 1:B:2967:MET:O    | 1:B:2970:SER:OG   | 2.17                     | 0.56              |
| 1:B:3545:THR:HG22 | 1:B:3548:GLU:HG3  | 1.86                     | 0.56              |
| 1:D:1087:ARG:HB3  | 1:D:1223:PHE:CD2  | 2.41                     | 0.56              |
| 1:C:1619:ARG:NH2  | 1:C:1622:GLU:OE1  | 2.39                     | 0.56              |
| 1:C:1653:LEU:O    | 1:C:1660:GLN:NE2  | 2.37                     | 0.56              |
| 1:C:1753:LYS:HB3  | 1:C:1758:ARG:HA   | 1.87                     | 0.56              |
| 1:A:1024:TYR:CZ   | 1:A:1032:LYS:HG3  | 2.40                     | 0.56              |
| 1:A:1087:ARG:HB3  | 1:A:1223:PHE:CD2  | 2.40                     | 0.56              |
| 1:B:618:GLN:OE1   | 1:B:1678:ASN:ND2  | 2.35                     | 0.56              |
| 1:B:1024:TYR:CZ   | 1:B:1032:LYS:HG3  | 2.40                     | 0.56              |
| 1:B:2679:PHE:HB2  | 1:B:2706:ILE:HG21 | 1.87                     | 0.56              |
| 1:B:4910:GLU:O    | 1:B:4914:VAL:HG13 | 2.05                     | 0.56              |
| 1:D:1619:ARG:NH2  | 1:D:1622:GLU:OE1  | 2.39                     | 0.56              |
| 1:C:1087:ARG:HB3  | 1:C:1223:PHE:CD2  | 2.40                     | 0.56              |
| 1:C:3445:TRP:NE1  | 1:C:3455:GLU:OE1  | 2.32                     | 0.56              |
| 1:A:1619:ARG:NH2  | 1:A:1622:GLU:OE1  | 2.39                     | 0.56              |
| 1:D:4910:GLU:O    | 1:D:4914:VAL:HG13 | 2.05                     | 0.56              |
| 1:C:1299:GLN:NE2  | 1:C:1545:ASN:OD1  | 2.38                     | 0.56              |
| 1:A:1753:LYS:HB3  | 1:A:1758:ARG:HA   | 1.87                     | 0.56              |
| 1:A:2214:VAL:HG11 | 1:A:2228:MET:HE1  | 1.87                     | 0.56              |
| 1:B:2214:VAL:HG11 | 1:B:2228:MET:HE1  | 1.87                     | 0.56              |
| 1:B:3752:SER:N    | 1:B:3755:GLU:OE2  | 2.32                     | 0.56              |
| 1:D:1024:TYR:CZ   | 1:D:1032:LYS:HG3  | 2.40                     | 0.56              |
| 1:A:394:GLN:OE1   | 1:A:394:GLN:N     | 2.35                     | 0.56              |
| 2:G:11:ASP:OD2    | 2:G:14:THR:OG1    | 2.24                     | 0.56              |
| 1:B:1619:ARG:NH2  | 1:B:1622:GLU:OE1  | 2.39                     | 0.56              |
| 1:B:1753:LYS:HB3  | 1:B:1758:ARG:HA   | 1.87                     | 0.56              |
| 1:D:1289:LEU:HD12 | 1:D:1562:ILE:HD11 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2967:MET:O    | 1:C:2970:SER:OG   | 2.17                     | 0.56              |
| 1:C:4006:ASP:N    | 1:C:4006:ASP:OD1  | 2.38                     | 0.56              |
| 1:A:4839:MET:HG3  | 1:D:4822:THR:HG21 | 1.88                     | 0.56              |
| 2:H:38:SER:OG     | 2:H:41:ASP:OD2    | 2.17                     | 0.56              |
| 1:B:394:GLN:OE1   | 1:B:394:GLN:N     | 2.35                     | 0.56              |
| 1:D:947:GLU:OE1   | 1:D:1051:TYR:OH   | 2.22                     | 0.56              |
| 1:D:1992:ALA:HB1  | 1:D:1996:ARG:HH12 | 1.70                     | 0.56              |
| 1:D:2116:LEU:O    | 1:D:2120:MET:HG2  | 2.06                     | 0.56              |
| 1:D:2208:MET:HA   | 1:D:2211:MET:HE3  | 1.87                     | 0.56              |
| 1:D:4006:ASP:N    | 1:D:4006:ASP:OD1  | 2.38                     | 0.56              |
| 1:C:293:LEU:HD13  | 1:C:378:LEU:HD12  | 1.87                     | 0.56              |
| 1:A:1289:LEU:HD12 | 1:A:1562:ILE:HD11 | 1.87                     | 0.56              |
| 1:B:1066:GLN:CB   | 1:B:1071:ARG:HH22 | 2.13                     | 0.56              |
| 1:D:4901:ILE:HG13 | 1:D:4913:ARG:NH2  | 2.19                     | 0.56              |
| 1:C:394:GLN:OE1   | 1:C:394:GLN:N     | 2.35                     | 0.56              |
| 1:A:2700:MET:HE3  | 1:A:2701:PRO:HD3  | 1.88                     | 0.56              |
| 1:B:947:GLU:OE1   | 1:B:1051:TYR:OH   | 2.22                     | 0.56              |
| 1:B:2970:SER:HA   | 1:B:2973:PHE:CD1  | 2.41                     | 0.56              |
| 1:D:1108:GLU:OE2  | 1:D:1108:GLU:N    | 2.28                     | 0.56              |
| 1:A:2970:SER:HA   | 1:A:2973:PHE:CD1  | 2.41                     | 0.56              |
| 1:B:2271:THR:OG1  | 1:B:2330:ARG:NH2  | 2.36                     | 0.56              |
| 1:B:2309:SER:OG   | 1:B:2320:ASP:OD1  | 2.24                     | 0.56              |
| 1:B:3539:ARG:NH1  | 1:B:3544:ASP:OD2  | 2.39                     | 0.56              |
| 1:D:4570:ALA:O    | 1:D:4574:ASN:ND2  | 2.36                     | 0.56              |
| 1:C:2970:SER:HA   | 1:C:2973:PHE:CD1  | 2.41                     | 0.56              |
| 1:C:4555:LEU:HD21 | 1:C:4656:LEU:HD22 | 1.87                     | 0.56              |
| 1:B:1992:ALA:HB1  | 1:B:1996:ARG:HH12 | 1.70                     | 0.55              |
| 1:B:3571:TRP:CE2  | 1:C:1228:ILE:HG12 | 2.41                     | 0.55              |
| 1:D:293:LEU:HD13  | 1:D:378:LEU:HD12  | 1.87                     | 0.55              |
| 1:D:2700:MET:HE3  | 1:D:2701:PRO:HD3  | 1.88                     | 0.55              |
| 1:C:3648:ARG:O    | 1:C:3652:MET:HG3  | 2.07                     | 0.55              |
| 1:A:3539:ARG:NH1  | 1:A:3544:ASP:OD2  | 2.39                     | 0.55              |
| 1:A:3840:SER:OG   | 1:A:3877:ASP:OD1  | 2.24                     | 0.55              |
| 1:B:4006:ASP:OD1  | 1:B:4006:ASP:N    | 2.38                     | 0.55              |
| 1:C:545:ASP:OD1   | 1:C:582:HIS:NE2   | 2.32                     | 0.55              |
| 1:C:3539:ARG:NH1  | 1:C:3544:ASP:OD2  | 2.39                     | 0.55              |
| 1:A:2765:LYS:NZ   | 1:A:2857:PRO:HB2  | 2.22                     | 0.55              |
| 1:A:3648:ARG:O    | 1:A:3652:MET:HG3  | 2.07                     | 0.55              |
| 1:C:2116:LEU:O    | 1:C:2120:MET:HG2  | 2.06                     | 0.55              |
| 1:C:2881:ASN:HA   | 1:C:2884:ASN:ND2  | 2.22                     | 0.55              |
| 1:A:2309:SER:OG   | 1:A:2321:ILE:O    | 2.22                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:293:LEU:HD13  | 1:B:378:LEU:HD12  | 1.87                     | 0.55              |
| 1:B:2700:MET:HE3  | 1:B:2701:PRO:HD3  | 1.88                     | 0.55              |
| 1:B:2881:ASN:HA   | 1:B:2884:ASN:ND2  | 2.22                     | 0.55              |
| 1:B:3467:MET:CE   | 1:C:1174:GLY:N    | 2.69                     | 0.55              |
| 1:D:648:ILE:HG23  | 1:D:814:ALA:HB3   | 1.89                     | 0.55              |
| 1:D:3564:GLU:HA   | 1:D:3570:ARG:HH22 | 1.72                     | 0.55              |
| 1:C:3162:GLN:NE2  | 1:C:3216:CYS:O    | 2.37                     | 0.55              |
| 1:C:4910:GLU:O    | 1:C:4914:VAL:HG13 | 2.05                     | 0.55              |
| 1:A:648:ILE:HG23  | 1:A:814:ALA:HB3   | 1.89                     | 0.55              |
| 1:A:4712:PRO:O    | 1:A:4718:LYS:NZ   | 2.32                     | 0.55              |
| 2:G:79:ASP:OD2    | 2:G:80:TYR:HD2    | 1.89                     | 0.55              |
| 1:B:1087:ARG:HB3  | 1:B:1223:PHE:CD2  | 2.40                     | 0.55              |
| 1:B:3648:ARG:O    | 1:B:3652:MET:HG3  | 2.07                     | 0.55              |
| 1:D:925:SER:O     | 1:D:928:THR:OG1   | 2.19                     | 0.55              |
| 1:D:2679:PHE:HB2  | 1:D:2706:ILE:HG21 | 1.87                     | 0.55              |
| 1:D:3648:ARG:O    | 1:D:3652:MET:HG3  | 2.07                     | 0.55              |
| 1:A:1031:THR:O    | 1:A:1035:ASN:ND2  | 2.37                     | 0.55              |
| 1:A:2116:LEU:O    | 1:A:2120:MET:HG2  | 2.06                     | 0.55              |
| 1:B:404:ILE:HD13  | 1:B:481:GLU:HG3   | 1.89                     | 0.55              |
| 1:D:571:SER:OG    | 1:D:573:GLU:OE1   | 2.21                     | 0.55              |
| 1:C:275:ARG:HH12  | 1:C:330:ASP:HA    | 1.72                     | 0.55              |
| 1:C:2309:SER:OG   | 1:C:2320:ASP:OD1  | 2.24                     | 0.55              |
| 1:B:275:ARG:HH12  | 1:B:330:ASP:HA    | 1.72                     | 0.55              |
| 1:D:2214:VAL:HG11 | 1:D:2228:MET:HE1  | 1.87                     | 0.55              |
| 1:D:4555:LEU:HD21 | 1:D:4656:LEU:HD22 | 1.88                     | 0.55              |
| 1:C:1289:LEU:HD12 | 1:C:1562:ILE:HD11 | 1.87                     | 0.55              |
| 1:A:2881:ASN:HA   | 1:A:2884:ASN:ND2  | 2.22                     | 0.55              |
| 1:A:3442:PHE:HE1  | 1:A:3511:VAL:HG12 | 1.72                     | 0.55              |
| 1:D:1867:GLU:OE2  | 1:D:1928:GLN:NE2  | 2.40                     | 0.55              |
| 1:D:2970:SER:HA   | 1:D:2973:PHE:CD1  | 2.41                     | 0.55              |
| 1:D:3442:PHE:HE1  | 1:D:3511:VAL:HG12 | 1.72                     | 0.55              |
| 1:C:2214:VAL:HG11 | 1:C:2228:MET:HE1  | 1.87                     | 0.55              |
| 1:C:2679:PHE:HB2  | 1:C:2706:ILE:HG21 | 1.87                     | 0.55              |
| 1:A:3564:GLU:HA   | 1:A:3570:ARG:HH22 | 1.72                     | 0.55              |
| 2:F:79:ASP:OD2    | 2:F:80:TYR:N      | 2.40                     | 0.55              |
| 1:B:2661:TRP:HB3  | 1:B:2664:PHE:HB2  | 1.89                     | 0.55              |
| 1:B:4555:LEU:HD21 | 1:B:4656:LEU:HD22 | 1.88                     | 0.55              |
| 1:D:919:ASN:HA    | 1:D:922:LEU:HD23  | 1.89                     | 0.55              |
| 1:D:1561:VAL:HG12 | 1:D:1562:ILE:HG23 | 1.89                     | 0.55              |
| 1:C:404:ILE:HD13  | 1:C:481:GLU:HG3   | 1.89                     | 0.55              |
| 1:C:1031:THR:O    | 1:C:1035:ASN:ND2  | 2.37                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1992:ALA:HB1  | 1:C:1996:ARG:HH12 | 1.70                     | 0.55              |
| 1:C:3442:PHE:HE1  | 1:C:3511:VAL:HG12 | 1.72                     | 0.55              |
| 1:A:275:ARG:HH12  | 1:A:330:ASP:HA    | 1.72                     | 0.55              |
| 1:A:1992:ALA:HB1  | 1:A:1996:ARG:HH12 | 1.70                     | 0.55              |
| 2:F:79:ASP:OD2    | 2:F:80:TYR:HD1    | 1.90                     | 0.55              |
| 1:D:266:ARG:NH2   | 1:D:272:SER:OG    | 2.40                     | 0.55              |
| 1:D:404:ILE:HD13  | 1:D:481:GLU:HG3   | 1.89                     | 0.55              |
| 1:D:2309:SER:OG   | 1:D:2320:ASP:OD1  | 2.25                     | 0.55              |
| 1:D:3840:SER:OG   | 1:D:3877:ASP:OD1  | 2.24                     | 0.55              |
| 1:C:648:ILE:HG23  | 1:C:814:ALA:HB3   | 1.89                     | 0.55              |
| 1:C:2700:MET:HE3  | 1:C:2701:PRO:HD3  | 1.88                     | 0.55              |
| 1:A:3752:SER:N    | 1:A:3755:GLU:OE2  | 2.32                     | 0.54              |
| 1:A:4555:LEU:HD21 | 1:A:4656:LEU:HD22 | 1.88                     | 0.54              |
| 2:H:79:ASP:OD2    | 2:H:80:TYR:N      | 2.40                     | 0.54              |
| 1:B:866:HIS:CD2   | 1:B:941:MET:HE3   | 2.43                     | 0.54              |
| 1:B:1561:VAL:HG12 | 1:B:1562:ILE:HG23 | 1.89                     | 0.54              |
| 1:D:2108:GLU:O    | 1:D:3694:LYS:NZ   | 2.40                     | 0.54              |
| 1:D:2765:LYS:NZ   | 1:D:2857:PRO:HB2  | 2.22                     | 0.54              |
| 1:C:1867:GLU:OE2  | 1:C:1928:GLN:NE2  | 2.40                     | 0.54              |
| 1:A:1867:GLU:OE2  | 1:A:1928:GLN:NE2  | 2.40                     | 0.54              |
| 1:A:4570:ALA:O    | 1:A:4574:ASN:ND2  | 2.36                     | 0.54              |
| 1:B:266:ARG:NH2   | 1:B:272:SER:OG    | 2.40                     | 0.54              |
| 1:B:1867:GLU:OE2  | 1:B:1928:GLN:NE2  | 2.40                     | 0.54              |
| 1:B:3564:GLU:HA   | 1:B:3570:ARG:HH22 | 1.72                     | 0.54              |
| 1:D:3539:ARG:NH1  | 1:D:3544:ASP:OD2  | 2.39                     | 0.54              |
| 1:C:919:ASN:HA    | 1:C:922:LEU:HD23  | 1.88                     | 0.54              |
| 1:A:11:VAL:HG11   | 1:A:164:ARG:HH11  | 1.73                     | 0.54              |
| 1:A:2108:GLU:O    | 1:A:3694:LYS:NZ   | 2.40                     | 0.54              |
| 1:A:2309:SER:OG   | 1:A:2320:ASP:OD1  | 2.24                     | 0.54              |
| 1:B:1289:LEU:HD12 | 1:B:1562:ILE:HD11 | 1.87                     | 0.54              |
| 1:B:2116:LEU:O    | 1:B:2120:MET:HG2  | 2.06                     | 0.54              |
| 1:D:1228:ILE:HG12 | 1:C:3571:TRP:CE2  | 2.42                     | 0.54              |
| 1:D:2881:ASN:HA   | 1:D:2884:ASN:ND2  | 2.22                     | 0.54              |
| 1:D:3604:TYR:O    | 1:D:3607:GLU:HG3  | 2.08                     | 0.54              |
| 1:D:3959:LYS:NZ   | 1:D:4022:ASP:OD2  | 2.40                     | 0.54              |
| 1:C:266:ARG:NH2   | 1:C:272:SER:OG    | 2.40                     | 0.54              |
| 1:C:3564:GLU:HA   | 1:C:3570:ARG:HH22 | 1.72                     | 0.54              |
| 1:A:1131:ARG:NH1  | 1:A:1178:ALA:O    | 2.40                     | 0.54              |
| 1:B:648:ILE:HG23  | 1:B:814:ALA:HB3   | 1.89                     | 0.54              |
| 1:B:3465:ASN:ND2  | 1:B:3468:SER:OG   | 2.41                     | 0.54              |
| 1:D:275:ARG:HH12  | 1:D:330:ASP:HA    | 1.72                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1174:GLY:N    | 1:C:3467:MET:CE   | 2.71                     | 0.54              |
| 1:C:4712:PRO:O    | 1:C:4718:LYS:NZ   | 2.32                     | 0.54              |
| 1:A:919:ASN:HA    | 1:A:922:LEU:HD23  | 1.89                     | 0.54              |
| 1:A:4791:TYR:OH   | 1:A:4815:ASP:OD1  | 2.13                     | 0.54              |
| 1:B:3442:PHE:HE1  | 1:B:3511:VAL:HG12 | 1.72                     | 0.54              |
| 1:D:1071:ARG:NE   | 1:D:1071:ARG:HA   | 2.23                     | 0.54              |
| 1:D:4000:MET:SD   | 1:D:4020:GLN:NE2  | 2.79                     | 0.54              |
| 1:D:4759:ASP:O    | 1:D:4761:PRO:HD3  | 2.08                     | 0.54              |
| 1:D:4967:TYR:OH   | 1:D:5033:GLU:OE2  | 2.24                     | 0.54              |
| 1:A:266:ARG:NH2   | 1:A:272:SER:OG    | 2.40                     | 0.54              |
| 1:A:404:ILE:HD13  | 1:A:481:GLU:HG3   | 1.89                     | 0.54              |
| 1:A:1174:GLY:CA   | 1:D:3467:MET:CE   | 2.82                     | 0.54              |
| 1:A:3604:TYR:O    | 1:A:3607:GLU:HG3  | 2.08                     | 0.54              |
| 1:A:4006:ASP:N    | 1:A:4006:ASP:OD1  | 2.38                     | 0.54              |
| 1:B:11:VAL:HG11   | 1:B:164:ARG:HH11  | 1.73                     | 0.54              |
| 1:B:1108:GLU:OE2  | 1:B:1108:GLU:N    | 2.28                     | 0.54              |
| 1:B:3604:TYR:O    | 1:B:3607:GLU:HG3  | 2.08                     | 0.54              |
| 1:D:394:GLN:OE1   | 1:D:394:GLN:N     | 2.35                     | 0.54              |
| 1:D:2967:MET:O    | 1:D:2970:SER:OG   | 2.17                     | 0.54              |
| 1:C:1931:LEU:HB3  | 1:C:1935:VAL:HB   | 1.90                     | 0.54              |
| 1:C:2108:GLU:O    | 1:C:3694:LYS:NZ   | 2.40                     | 0.54              |
| 1:C:3840:SER:OG   | 1:C:3877:ASP:OD1  | 2.24                     | 0.54              |
| 1:A:866:HIS:CD2   | 1:A:941:MET:HE3   | 2.43                     | 0.54              |
| 1:A:2198:MET:HG3  | 1:A:2203:MET:SD   | 2.48                     | 0.54              |
| 1:A:2661:TRP:HB3  | 1:A:2664:PHE:HB2  | 1.89                     | 0.54              |
| 1:A:4223:ASN:ND2  | 1:A:4224:GLU:OE1  | 2.41                     | 0.54              |
| 1:D:1174:GLY:HA3  | 1:C:3467:MET:HE1  | 1.88                     | 0.54              |
| 1:D:2661:TRP:HB3  | 1:D:2664:PHE:HB2  | 1.89                     | 0.54              |
| 1:D:4223:ASN:ND2  | 1:D:4224:GLU:OE1  | 2.41                     | 0.54              |
| 1:C:866:HIS:CD2   | 1:C:941:MET:HE3   | 2.42                     | 0.54              |
| 1:C:1131:ARG:NH1  | 1:C:1178:ALA:O    | 2.40                     | 0.54              |
| 1:C:2765:LYS:NZ   | 1:C:2857:PRO:HB2  | 2.22                     | 0.54              |
| 1:B:4759:ASP:O    | 1:B:4761:PRO:HD3  | 2.08                     | 0.54              |
| 1:D:1131:ARG:NH1  | 1:D:1178:ALA:O    | 2.40                     | 0.54              |
| 1:D:3465:ASN:ND2  | 1:D:3468:SER:OG   | 2.41                     | 0.54              |
| 1:C:2587:TYR:O    | 1:C:2590:SER:OG   | 2.20                     | 0.54              |
| 1:B:919:ASN:HA    | 1:B:922:LEU:HD23  | 1.89                     | 0.54              |
| 1:D:669:ASP:OD2   | 1:D:790:ARG:NE    | 2.41                     | 0.54              |
| 1:D:2307:LEU:HD11 | 1:D:2362:GLU:HG3  | 1.90                     | 0.54              |
| 1:C:951:LYS:HD2   | 1:C:951:LYS:N     | 2.23                     | 0.54              |
| 1:C:4766:THR:HA   | 1:C:4769:MET:HE1  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:951:LYS:HD2   | 1:A:951:LYS:N     | 2.23                     | 0.54              |
| 1:A:4205:TRP:CZ3  | 1:A:4989:MET:HE3  | 2.44                     | 0.54              |
| 1:D:1996:ARG:NE   | 1:D:1996:ARG:HA   | 2.23                     | 0.54              |
| 1:D:2439:GLU:HB2  | 1:D:2442:LEU:HD23 | 1.89                     | 0.54              |
| 1:C:11:VAL:HG11   | 1:C:164:ARG:HH11  | 1.73                     | 0.54              |
| 1:A:2293:GLN:OE1  | 1:A:2293:GLN:N    | 2.41                     | 0.53              |
| 1:B:4223:ASN:ND2  | 1:B:4224:GLU:OE1  | 2.41                     | 0.53              |
| 1:B:4627:MET:HE1  | 1:B:4629:TYR:HE2  | 1.73                     | 0.53              |
| 1:D:2198:MET:HG3  | 1:D:2203:MET:SD   | 2.48                     | 0.53              |
| 1:D:4205:TRP:CZ3  | 1:D:4989:MET:HE3  | 2.43                     | 0.53              |
| 1:C:2293:GLN:OE1  | 1:C:2293:GLN:N    | 2.41                     | 0.53              |
| 1:A:872:GLU:HG2   | 1:A:922:LEU:HD11  | 1.90                     | 0.53              |
| 1:A:2307:LEU:HD11 | 1:A:2362:GLU:HG3  | 1.90                     | 0.53              |
| 2:G:79:ASP:OD2    | 2:G:80:TYR:N      | 2.41                     | 0.53              |
| 1:B:1996:ARG:HA   | 1:B:1996:ARG:NE   | 2.23                     | 0.53              |
| 1:B:2307:LEU:HD11 | 1:B:2362:GLU:HG3  | 1.90                     | 0.53              |
| 1:B:3725:TYR:O    | 1:B:3729:MET:HG3  | 2.08                     | 0.53              |
| 1:B:4205:TRP:CZ3  | 1:B:4989:MET:HE3  | 2.43                     | 0.53              |
| 1:D:11:VAL:HG11   | 1:D:164:ARG:HH11  | 1.73                     | 0.53              |
| 1:D:872:GLU:HG2   | 1:D:922:LEU:HD11  | 1.90                     | 0.53              |
| 1:C:3465:ASN:ND2  | 1:C:3468:SER:OG   | 2.41                     | 0.53              |
| 1:C:3725:TYR:O    | 1:C:3729:MET:HG3  | 2.08                     | 0.53              |
| 1:C:4205:TRP:CZ3  | 1:C:4989:MET:HE3  | 2.43                     | 0.53              |
| 1:A:1049:TYR:HB3  | 1:A:1051:TYR:CZ   | 2.43                     | 0.53              |
| 1:A:1108:GLU:OE2  | 1:A:1108:GLU:N    | 2.28                     | 0.53              |
| 1:A:1996:ARG:NE   | 1:A:1996:ARG:HA   | 2.23                     | 0.53              |
| 1:B:545:ASP:OD1   | 1:B:582:HIS:NE2   | 2.32                     | 0.53              |
| 1:B:1071:ARG:NE   | 1:B:1071:ARG:HA   | 2.23                     | 0.53              |
| 1:B:1931:LEU:HB3  | 1:B:1935:VAL:HB   | 1.90                     | 0.53              |
| 1:B:2293:GLN:OE1  | 1:B:2293:GLN:N    | 2.42                     | 0.53              |
| 1:D:2293:GLN:OE1  | 1:D:2293:GLN:N    | 2.41                     | 0.53              |
| 1:C:3412:LEU:HD11 | 1:C:3434:LEU:HD21 | 1.90                     | 0.53              |
| 1:C:3604:TYR:O    | 1:C:3607:GLU:HG3  | 2.08                     | 0.53              |
| 1:C:4000:MET:SD   | 1:C:4020:GLN:NE2  | 2.79                     | 0.53              |
| 1:A:571:SER:OG    | 1:A:573:GLU:OE1   | 2.21                     | 0.53              |
| 1:A:938:HIS:HB3   | 1:A:1054:GLU:HB3  | 1.90                     | 0.53              |
| 1:A:3465:ASN:ND2  | 1:A:3468:SER:OG   | 2.41                     | 0.53              |
| 1:D:866:HIS:O     | 1:D:869:ARG:HG3   | 2.09                     | 0.53              |
| 1:D:3725:TYR:O    | 1:D:3729:MET:HG3  | 2.08                     | 0.53              |
| 1:D:4205:TRP:HZ3  | 1:D:4989:MET:HE3  | 1.74                     | 0.53              |
| 1:D:4879:MET:HG3  | 1:C:4578:LEU:HD23 | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1561:VAL:HG12 | 1:C:1562:ILE:HG23 | 1.89                     | 0.53              |
| 1:C:1748:PHE:HB2  | 1:C:1758:ARG:NH2  | 2.24                     | 0.53              |
| 1:C:1996:ARG:NE   | 1:C:1996:ARG:HA   | 2.23                     | 0.53              |
| 1:C:4223:ASN:ND2  | 1:C:4224:GLU:OE1  | 2.41                     | 0.53              |
| 1:A:4759:ASP:O    | 1:A:4761:PRO:HD3  | 2.08                     | 0.53              |
| 2:H:11:ASP:OD2    | 2:H:14:THR:OG1    | 2.24                     | 0.53              |
| 1:B:1031:THR:O    | 1:B:1035:ASN:ND2  | 2.37                     | 0.53              |
| 1:B:2108:GLU:O    | 1:B:3694:LYS:NZ   | 2.40                     | 0.53              |
| 1:B:2198:MET:HG3  | 1:B:2203:MET:SD   | 2.48                     | 0.53              |
| 1:D:4627:MET:HE1  | 1:D:4629:TYR:HE2  | 1.73                     | 0.53              |
| 1:A:2439:GLU:HB2  | 1:A:2442:LEU:HD23 | 1.89                     | 0.53              |
| 1:A:3412:LEU:HD11 | 1:A:3434:LEU:HD21 | 1.90                     | 0.53              |
| 2:E:79:ASP:OD2    | 2:E:80:TYR:N      | 2.42                     | 0.53              |
| 1:B:866:HIS:O     | 1:B:869:ARG:HG3   | 2.09                     | 0.53              |
| 1:B:3412:LEU:HD11 | 1:B:3434:LEU:HD21 | 1.90                     | 0.53              |
| 1:B:4112:LEU:O    | 1:B:4115:SER:OG   | 2.27                     | 0.53              |
| 1:B:4578:LEU:HD23 | 1:C:4879:MET:HG3  | 1.90                     | 0.53              |
| 1:D:866:HIS:CD2   | 1:D:941:MET:HE3   | 2.42                     | 0.53              |
| 1:D:1931:LEU:HB3  | 1:D:1935:VAL:HB   | 1.90                     | 0.53              |
| 1:C:938:HIS:HB3   | 1:C:1054:GLU:HB3  | 1.90                     | 0.53              |
| 1:C:2439:GLU:HB2  | 1:C:2442:LEU:HD23 | 1.89                     | 0.53              |
| 1:C:4205:TRP:HZ3  | 1:C:4989:MET:HE3  | 1.74                     | 0.53              |
| 1:A:1071:ARG:NE   | 1:A:1071:ARG:HA   | 2.23                     | 0.53              |
| 1:A:1561:VAL:HG12 | 1:A:1562:ILE:HG23 | 1.89                     | 0.53              |
| 1:A:2271:THR:OG1  | 1:A:2330:ARG:NH2  | 2.36                     | 0.53              |
| 1:B:3768:SER:HA   | 1:B:3771:HIS:CD2  | 2.44                     | 0.53              |
| 1:B:4766:THR:HA   | 1:B:4769:MET:HE1  | 1.90                     | 0.53              |
| 1:C:2765:LYS:HZ1  | 1:C:2860:PRO:HA   | 1.73                     | 0.53              |
| 1:A:2924:GLN:O    | 1:A:2928:LYS:HG2  | 2.08                     | 0.53              |
| 1:A:4000:MET:SD   | 1:A:4020:GLN:NE2  | 2.79                     | 0.53              |
| 1:A:4205:TRP:HZ3  | 1:A:4989:MET:HE3  | 1.74                     | 0.53              |
| 1:B:938:HIS:HB3   | 1:B:1054:GLU:HB3  | 1.90                     | 0.53              |
| 1:B:1049:TYR:HB3  | 1:B:1051:TYR:CZ   | 2.44                     | 0.53              |
| 1:B:4570:ALA:O    | 1:B:4574:ASN:ND2  | 2.36                     | 0.53              |
| 1:D:2924:GLN:O    | 1:D:2928:LYS:HG2  | 2.08                     | 0.53              |
| 1:D:3768:SER:HA   | 1:D:3771:HIS:CD2  | 2.44                     | 0.53              |
| 1:C:4759:ASP:O    | 1:C:4761:PRO:HD3  | 2.08                     | 0.53              |
| 1:A:4627:MET:HE1  | 1:A:4629:TYR:HE2  | 1.73                     | 0.53              |
| 1:B:2924:GLN:O    | 1:B:2928:LYS:HG2  | 2.08                     | 0.53              |
| 1:D:830:ARG:NH2   | 1:D:832:GLU:OE2   | 2.42                     | 0.53              |
| 1:D:951:LYS:HD2   | 1:D:951:LYS:N     | 2.23                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1049:TYR:HB3  | 1:D:1051:TYR:CZ   | 2.44                     | 0.53              |
| 1:D:3412:LEU:HD11 | 1:D:3434:LEU:HD21 | 1.90                     | 0.53              |
| 1:D:4069:LYS:NZ   | 1:D:4133:GLN:OE1  | 2.41                     | 0.53              |
| 1:D:4766:THR:HA   | 1:D:4769:MET:HE1  | 1.90                     | 0.53              |
| 1:C:866:HIS:O     | 1:C:869:ARG:HG3   | 2.09                     | 0.53              |
| 1:C:2307:LEU:HD11 | 1:C:2362:GLU:HG3  | 1.90                     | 0.53              |
| 1:A:866:HIS:O     | 1:A:869:ARG:HG3   | 2.09                     | 0.53              |
| 1:A:1748:PHE:HB2  | 1:A:1758:ARG:NH2  | 2.24                     | 0.53              |
| 1:A:3768:SER:HA   | 1:A:3771:HIS:CD2  | 2.44                     | 0.53              |
| 1:A:4069:LYS:NZ   | 1:A:4133:GLN:OE1  | 2.41                     | 0.53              |
| 1:B:1131:ARG:NH1  | 1:B:1178:ALA:O    | 2.40                     | 0.53              |
| 1:D:1116:GLY:HA3  | 1:D:1132:TRP:HB3  | 1.90                     | 0.53              |
| 1:C:1808:ARG:NH1  | 1:C:1853:ILE:O    | 2.42                     | 0.53              |
| 1:C:3185:LYS:HD2  | 1:C:3186:LEU:HG   | 1.91                     | 0.53              |
| 1:C:4069:LYS:NZ   | 1:C:4133:GLN:OE1  | 2.41                     | 0.53              |
| 1:A:1116:GLY:HA3  | 1:A:1132:TRP:HB3  | 1.90                     | 0.52              |
| 1:A:3335:MET:SD   | 1:A:3403:ARG:NH1  | 2.82                     | 0.52              |
| 1:B:830:ARG:NH2   | 1:B:832:GLU:OE2   | 2.42                     | 0.52              |
| 1:B:3467:MET:HE1  | 1:C:1174:GLY:N    | 2.23                     | 0.52              |
| 1:B:3935:TRP:O    | 1:C:80:GLU:HG3    | 2.10                     | 0.52              |
| 1:D:1748:PHE:HB2  | 1:D:1758:ARG:NH2  | 2.24                     | 0.52              |
| 1:C:1049:TYR:HB3  | 1:C:1051:TYR:CZ   | 2.44                     | 0.52              |
| 1:C:1071:ARG:HA   | 1:C:1071:ARG:NE   | 2.23                     | 0.52              |
| 1:C:1474:VAL:HG12 | 1:C:1476:MET:HE2  | 1.91                     | 0.52              |
| 1:C:2198:MET:HG3  | 1:C:2203:MET:SD   | 2.48                     | 0.52              |
| 1:C:2271:THR:OG1  | 1:C:2330:ARG:NH2  | 2.36                     | 0.52              |
| 1:C:4627:MET:HE1  | 1:C:4629:TYR:HE2  | 1.73                     | 0.52              |
| 1:A:334:MET:HE2   | 1:A:334:MET:HA    | 1.91                     | 0.52              |
| 1:B:872:GLU:HG2   | 1:B:922:LEU:HD11  | 1.90                     | 0.52              |
| 1:B:3959:LYS:NZ   | 1:B:4022:ASP:OD2  | 2.40                     | 0.52              |
| 1:D:876:GLU:OE2   | 1:D:918:ARG:NH1   | 2.43                     | 0.52              |
| 1:D:4712:PRO:O    | 1:D:4718:LYS:NZ   | 2.32                     | 0.52              |
| 1:C:2185:ILE:HG21 | 1:C:2203:MET:HE1  | 1.91                     | 0.52              |
| 1:C:2661:TRP:HB3  | 1:C:2664:PHE:HB2  | 1.89                     | 0.52              |
| 2:H:79:ASP:OD2    | 2:H:80:TYR:HD1    | 1.91                     | 0.52              |
| 1:B:1808:ARG:NH1  | 1:B:1853:ILE:O    | 2.42                     | 0.52              |
| 1:B:3335:MET:SD   | 1:B:3403:ARG:NH1  | 2.82                     | 0.52              |
| 1:B:4000:MET:SD   | 1:B:4020:GLN:NE2  | 2.79                     | 0.52              |
| 1:B:4069:LYS:NZ   | 1:B:4133:GLN:OE1  | 2.41                     | 0.52              |
| 1:A:622:THR:HG23  | 1:A:626:LEU:HD12  | 1.92                     | 0.52              |
| 1:A:830:ARG:NH2   | 1:A:832:GLU:OE2   | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4766:THR:HA   | 1:A:4769:MET:HE1  | 1.90                     | 0.52              |
| 1:B:417:GLY:O     | 1:B:420:SER:OG    | 2.26                     | 0.52              |
| 1:B:1116:GLY:HA3  | 1:B:1132:TRP:HB3  | 1.90                     | 0.52              |
| 1:B:3185:LYS:HD2  | 1:B:3186:LEU:HG   | 1.91                     | 0.52              |
| 1:D:622:THR:HG23  | 1:D:626:LEU:HD12  | 1.92                     | 0.52              |
| 1:C:830:ARG:NH2   | 1:C:832:GLU:OE2   | 2.42                     | 0.52              |
| 1:C:2924:GLN:O    | 1:C:2928:LYS:HG2  | 2.08                     | 0.52              |
| 1:A:1931:LEU:HB3  | 1:A:1935:VAL:HB   | 1.90                     | 0.52              |
| 1:B:951:LYS:HD2   | 1:B:951:LYS:N     | 2.23                     | 0.52              |
| 1:B:2439:GLU:HB2  | 1:B:2442:LEU:HD23 | 1.89                     | 0.52              |
| 1:D:334:MET:HE2   | 1:D:334:MET:HA    | 1.91                     | 0.52              |
| 1:D:3465:ASN:OD1  | 1:D:3468:SER:N    | 2.42                     | 0.52              |
| 1:C:3538:THR:O    | 1:C:3542:LEU:HD12 | 2.10                     | 0.52              |
| 1:C:3768:SER:HA   | 1:C:3771:HIS:CD2  | 2.44                     | 0.52              |
| 1:A:3420:ARG:HG3  | 1:A:3520:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:3725:TYR:O    | 1:A:3729:MET:HG3  | 2.08                     | 0.52              |
| 1:D:2185:ILE:HG21 | 1:D:2203:MET:HE1  | 1.91                     | 0.52              |
| 1:D:3335:MET:SD   | 1:D:3403:ARG:NH1  | 2.82                     | 0.52              |
| 1:A:669:ASP:OD2   | 1:A:790:ARG:NE    | 2.41                     | 0.52              |
| 1:A:3465:ASN:OD1  | 1:A:3468:SER:N    | 2.42                     | 0.52              |
| 1:B:3420:ARG:HG3  | 1:B:3520:ILE:HD11 | 1.92                     | 0.52              |
| 1:B:4205:TRP:HZ3  | 1:B:4989:MET:HE3  | 1.74                     | 0.52              |
| 1:C:872:GLU:HG2   | 1:C:922:LEU:HD11  | 1.90                     | 0.52              |
| 1:C:4791:TYR:OH   | 1:C:4815:ASP:OD1  | 2.13                     | 0.52              |
| 1:A:882:TRP:HE1   | 1:A:904:HIS:HE2   | 1.58                     | 0.52              |
| 1:A:4839:MET:HG3  | 1:D:4822:THR:CG2  | 2.40                     | 0.52              |
| 1:C:669:ASP:OD2   | 1:C:790:ARG:NE    | 2.41                     | 0.52              |
| 1:A:977:LEU:HG    | 1:A:1044:ARG:NH1  | 2.24                     | 0.52              |
| 1:B:876:GLU:OE2   | 1:B:918:ARG:NH1   | 2.43                     | 0.52              |
| 1:D:3185:LYS:HD2  | 1:D:3186:LEU:HG   | 1.91                     | 0.52              |
| 1:C:876:GLU:OE2   | 1:C:918:ARG:NH1   | 2.43                     | 0.52              |
| 1:C:1116:GLY:HA3  | 1:C:1132:TRP:HB3  | 1.90                     | 0.52              |
| 1:A:1547:LYS:NZ   | 1:A:1642:PRO:O    | 2.43                     | 0.52              |
| 1:B:1272:LEU:HD22 | 1:B:1289:LEU:HD11 | 1.91                     | 0.52              |
| 1:B:1981:MET:HE2  | 1:B:1981:MET:HA   | 1.92                     | 0.52              |
| 1:B:3467:MET:HE1  | 1:C:1174:GLY:HA3  | 1.88                     | 0.52              |
| 1:D:1174:GLY:N    | 1:C:3467:MET:HE1  | 2.25                     | 0.52              |
| 1:C:3335:MET:SD   | 1:C:3403:ARG:NH1  | 2.83                     | 0.52              |
| 1:C:3420:ARG:HG3  | 1:C:3520:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:876:GLU:OE2   | 1:A:918:ARG:NH1   | 2.43                     | 0.51              |
| 1:A:1474:VAL:HG12 | 1:A:1476:MET:HE2  | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1981:MET:HA   | 1:A:1981:MET:HE2  | 1.92                     | 0.51              |
| 1:D:938:HIS:HB3   | 1:D:1054:GLU:HB3  | 1.90                     | 0.51              |
| 1:D:1547:LYS:NZ   | 1:D:1642:PRO:O    | 2.43                     | 0.51              |
| 1:B:1748:PHE:HB2  | 1:B:1758:ARG:NH2  | 2.24                     | 0.51              |
| 1:C:4185:GLY:O    | 1:C:4188:ARG:NH1  | 2.44                     | 0.51              |
| 1:A:4930:ALA:HB2  | 1:D:4933:GLN:HG2  | 1.91                     | 0.51              |
| 1:B:882:TRP:HE1   | 1:B:904:HIS:HE2   | 1.58                     | 0.51              |
| 1:B:1093:GLU:HB3  | 1:B:1201:HIS:HB3  | 1.93                     | 0.51              |
| 1:B:1547:LYS:NZ   | 1:B:1642:PRO:O    | 2.43                     | 0.51              |
| 1:D:1474:VAL:HG12 | 1:D:1476:MET:HE2  | 1.91                     | 0.51              |
| 1:D:3420:ARG:HG3  | 1:D:3520:ILE:HD11 | 1.92                     | 0.51              |
| 1:D:3538:THR:O    | 1:D:3542:LEU:HD12 | 2.10                     | 0.51              |
| 1:D:4185:GLY:O    | 1:D:4188:ARG:NH1  | 2.44                     | 0.51              |
| 1:A:1272:LEU:HD22 | 1:A:1289:LEU:HD11 | 1.91                     | 0.51              |
| 1:A:2751:LEU:O    | 1:A:2755:ILE:HG12 | 2.11                     | 0.51              |
| 1:B:334:MET:HA    | 1:B:334:MET:HE2   | 1.91                     | 0.51              |
| 1:B:1474:VAL:HG12 | 1:B:1476:MET:HE2  | 1.91                     | 0.51              |
| 1:B:3538:THR:O    | 1:B:3542:LEU:HD12 | 2.10                     | 0.51              |
| 1:B:4185:GLY:O    | 1:B:4188:ARG:NH1  | 2.44                     | 0.51              |
| 1:D:80:GLU:HG3    | 1:C:3935:TRP:O    | 2.10                     | 0.51              |
| 1:D:1808:ARG:NH1  | 1:D:1853:ILE:O    | 2.42                     | 0.51              |
| 1:C:215:THR:HG22  | 1:C:273:HIS:HA    | 1.93                     | 0.51              |
| 1:A:1068:ARG:HH21 | 1:A:1071:ARG:HG3  | 1.76                     | 0.51              |
| 1:A:1093:GLU:HB3  | 1:A:1201:HIS:HB3  | 1.93                     | 0.51              |
| 1:A:1808:ARG:NH1  | 1:A:1853:ILE:O    | 2.42                     | 0.51              |
| 1:A:2185:ILE:HG21 | 1:A:2203:MET:HE1  | 1.91                     | 0.51              |
| 1:A:3538:THR:O    | 1:A:3542:LEU:HD12 | 2.10                     | 0.51              |
| 1:B:1068:ARG:HH21 | 1:B:1071:ARG:HG3  | 1.76                     | 0.51              |
| 1:B:2185:ILE:HG21 | 1:B:2203:MET:HE1  | 1.91                     | 0.51              |
| 1:B:2309:SER:OG   | 1:B:2321:ILE:O    | 2.22                     | 0.51              |
| 1:D:2751:LEU:O    | 1:D:2755:ILE:HG12 | 2.11                     | 0.51              |
| 1:D:3357:HIS:O    | 1:D:3361:THR:HG23 | 2.10                     | 0.51              |
| 1:D:4056:GLU:HG2  | 1:D:4166:LEU:HD13 | 1.93                     | 0.51              |
| 1:C:309:THR:O     | 1:C:313:SER:OG    | 2.22                     | 0.51              |
| 1:C:932:LEU:HD23  | 1:C:932:LEU:H     | 1.76                     | 0.51              |
| 1:C:1068:ARG:HH21 | 1:C:1071:ARG:HG3  | 1.76                     | 0.51              |
| 1:C:1093:GLU:HB3  | 1:C:1201:HIS:HB3  | 1.93                     | 0.51              |
| 1:C:2626:LEU:HD22 | 1:C:2640:PRO:HB3  | 1.92                     | 0.51              |
| 1:A:4112:LEU:O    | 1:A:4115:SER:OG   | 2.27                     | 0.51              |
| 1:D:215:THR:HG22  | 1:D:273:HIS:HA    | 1.93                     | 0.51              |
| 1:D:1093:GLU:HB3  | 1:D:1201:HIS:HB3  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3570:ARG:CZ   | 1:C:3570:ARG:HB2  | 2.41                     | 0.51              |
| 1:C:3695:PRO:HB3  | 1:C:3699:HIS:HB3  | 1.93                     | 0.51              |
| 1:A:1680:ARG:HH12 | 2:E:88:PRO:HB2    | 1.75                     | 0.51              |
| 1:A:3185:LYS:HD2  | 1:A:3186:LEU:HG   | 1.91                     | 0.51              |
| 1:A:4917:ASP:HB2  | 1:D:4888:TYR:HE1  | 1.76                     | 0.51              |
| 1:B:622:THR:HG23  | 1:B:626:LEU:HD12  | 1.92                     | 0.51              |
| 1:B:2792:ARG:NH2  | 1:B:2798:SER:OG   | 2.44                     | 0.51              |
| 1:D:1068:ARG:HH21 | 1:D:1071:ARG:HG3  | 1.76                     | 0.51              |
| 1:C:334:MET:HE2   | 1:C:334:MET:HA    | 1.91                     | 0.51              |
| 1:C:3959:LYS:NZ   | 1:C:4022:ASP:OD2  | 2.40                     | 0.51              |
| 1:A:215:THR:HG22  | 1:A:273:HIS:HA    | 1.93                     | 0.51              |
| 1:A:3357:HIS:O    | 1:A:3361:THR:HG23 | 2.10                     | 0.51              |
| 1:B:932:LEU:HD23  | 1:B:932:LEU:H     | 1.76                     | 0.51              |
| 1:D:977:LEU:HG    | 1:D:1044:ARG:NH1  | 2.24                     | 0.51              |
| 1:D:3695:PRO:HB3  | 1:D:3699:HIS:HB3  | 1.93                     | 0.51              |
| 1:C:510:GLU:OE2   | 1:C:510:GLU:N     | 2.44                     | 0.51              |
| 1:C:1547:LYS:NZ   | 1:C:1642:PRO:O    | 2.43                     | 0.51              |
| 1:A:545:ASP:OD1   | 1:A:582:HIS:NE2   | 2.32                     | 0.51              |
| 1:B:2090:LYS:HZ2  | 1:B:2092:GLN:HG3  | 1.76                     | 0.51              |
| 1:B:2587:TYR:O    | 1:B:2590:SER:OG   | 2.20                     | 0.51              |
| 1:B:2751:LEU:O    | 1:B:2755:ILE:HG12 | 2.11                     | 0.51              |
| 1:D:1981:MET:HA   | 1:D:1981:MET:HE2  | 1.92                     | 0.51              |
| 1:D:2792:ARG:NH2  | 1:D:2798:SER:OG   | 2.44                     | 0.51              |
| 1:A:2792:ARG:NH2  | 1:A:2798:SER:OG   | 2.44                     | 0.50              |
| 1:A:3940:LYS:O    | 1:A:4002:LYS:NZ   | 2.36                     | 0.50              |
| 1:A:4056:GLU:HG2  | 1:A:4166:LEU:HD13 | 1.93                     | 0.50              |
| 2:F:11:ASP:OD2    | 2:F:14:THR:OG1    | 2.27                     | 0.50              |
| 1:B:215:THR:HG22  | 1:B:273:HIS:HA    | 1.93                     | 0.50              |
| 1:B:510:GLU:N     | 1:B:510:GLU:OE2   | 2.44                     | 0.50              |
| 1:D:3226:GLU:C    | 1:D:3228:ALA:H    | 2.19                     | 0.50              |
| 1:C:622:THR:HG23  | 1:C:626:LEU:HD12  | 1.92                     | 0.50              |
| 1:C:1272:LEU:HD22 | 1:C:1289:LEU:HD11 | 1.91                     | 0.50              |
| 1:A:3570:ARG:CZ   | 1:A:3570:ARG:HB2  | 2.41                     | 0.50              |
| 1:A:4917:ASP:OD2  | 1:D:4888:TYR:OH   | 2.13                     | 0.50              |
| 1:B:3695:PRO:HB3  | 1:B:3699:HIS:HB3  | 1.93                     | 0.50              |
| 1:D:684:VAL:HG22  | 1:D:781:VAL:HG12  | 1.94                     | 0.50              |
| 1:C:882:TRP:HE1   | 1:C:904:HIS:HE2   | 1.58                     | 0.50              |
| 1:A:2626:LEU:HD22 | 1:A:2640:PRO:HB3  | 1.93                     | 0.50              |
| 1:A:3695:PRO:HB3  | 1:A:3699:HIS:HB3  | 1.93                     | 0.50              |
| 1:A:4185:GLY:O    | 1:A:4188:ARG:NH1  | 2.44                     | 0.50              |
| 1:B:2626:LEU:HD22 | 1:B:2640:PRO:HB3  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3465:ASN:OD1  | 1:B:3468:SER:N    | 2.42                     | 0.50              |
| 1:D:882:TRP:HE1   | 1:D:904:HIS:HE2   | 1.58                     | 0.50              |
| 1:D:3570:ARG:CZ   | 1:D:3570:ARG:HB2  | 2.41                     | 0.50              |
| 1:A:3686:GLU:HB2  | 1:A:3688:GLU:OE1  | 2.11                     | 0.50              |
| 1:A:4067:LYS:NZ   | 1:A:4102:GLN:O    | 2.44                     | 0.50              |
| 2:F:88:PRO:HB2    | 1:B:1680:ARG:NH1  | 2.24                     | 0.50              |
| 1:B:3357:HIS:O    | 1:B:3361:THR:HG23 | 2.10                     | 0.50              |
| 1:B:3840:SER:OG   | 1:B:3877:ASP:OD1  | 2.24                     | 0.50              |
| 1:D:2736:ASP:OD1  | 1:D:2736:ASP:N    | 2.44                     | 0.50              |
| 1:C:684:VAL:HG22  | 1:C:781:VAL:HG12  | 1.94                     | 0.50              |
| 1:C:2751:LEU:O    | 1:C:2755:ILE:HG12 | 2.11                     | 0.50              |
| 1:B:3570:ARG:HB2  | 1:B:3570:ARG:CZ   | 2.41                     | 0.50              |
| 1:D:2021:CYS:O    | 1:D:2028:ARG:NH2  | 2.45                     | 0.50              |
| 1:C:3357:HIS:O    | 1:C:3361:THR:HG23 | 2.10                     | 0.50              |
| 1:C:4056:GLU:HG2  | 1:C:4166:LEU:HD13 | 1.93                     | 0.50              |
| 1:A:3105:LYS:O    | 1:A:3108:GLU:HG3  | 2.12                     | 0.50              |
| 1:A:3527:PRO:HD2  | 1:A:3573:MET:SD   | 2.52                     | 0.50              |
| 1:B:3686:GLU:HB2  | 1:B:3688:GLU:OE1  | 2.11                     | 0.50              |
| 1:D:932:LEU:HD23  | 1:D:932:LEU:H     | 1.76                     | 0.50              |
| 1:D:3527:PRO:HD2  | 1:D:3573:MET:SD   | 2.52                     | 0.50              |
| 1:D:3686:GLU:HB2  | 1:D:3688:GLU:OE1  | 2.11                     | 0.50              |
| 1:D:4112:LEU:O    | 1:D:4115:SER:OG   | 2.27                     | 0.50              |
| 1:C:1981:MET:HE2  | 1:C:1981:MET:HA   | 1.92                     | 0.50              |
| 1:C:2175:GLU:HG3  | 1:C:2228:MET:HB2  | 1.94                     | 0.50              |
| 1:B:2175:GLU:HG3  | 1:B:2228:MET:HB2  | 1.94                     | 0.50              |
| 1:D:2441:HIS:CE1  | 1:D:2442:LEU:HD22 | 2.47                     | 0.50              |
| 1:D:2587:TYR:O    | 1:D:2590:SER:OG   | 2.20                     | 0.50              |
| 1:D:2626:LEU:HD22 | 1:D:2640:PRO:HB3  | 1.92                     | 0.50              |
| 1:D:3105:LYS:O    | 1:D:3108:GLU:HG3  | 2.12                     | 0.50              |
| 1:C:2441:HIS:CE1  | 1:C:2442:LEU:HD22 | 2.47                     | 0.50              |
| 1:C:3527:PRO:HD2  | 1:C:3573:MET:SD   | 2.52                     | 0.50              |
| 1:A:510:GLU:N     | 1:A:510:GLU:OE2   | 2.44                     | 0.50              |
| 1:A:2858:GLN:HB2  | 1:A:2859:PRO:HD3  | 1.94                     | 0.50              |
| 1:A:3862:ASP:OD1  | 1:A:3862:ASP:N    | 2.45                     | 0.50              |
| 1:B:684:VAL:HG22  | 1:B:781:VAL:HG12  | 1.94                     | 0.50              |
| 1:B:3465:ASN:OD1  | 1:B:3467:MET:N    | 2.34                     | 0.50              |
| 1:D:1272:LEU:HD22 | 1:D:1289:LEU:HD11 | 1.91                     | 0.50              |
| 1:D:2858:GLN:HB2  | 1:D:2859:PRO:HD3  | 1.94                     | 0.50              |
| 1:C:3226:GLU:C    | 1:C:3228:ALA:H    | 2.19                     | 0.50              |
| 1:A:663:TYR:OH    | 1:A:665:GLU:OE2   | 2.24                     | 0.50              |
| 1:A:684:VAL:HG22  | 1:A:781:VAL:HG12  | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2021:CYS:O    | 1:A:2028:ARG:NH2  | 2.45                     | 0.50              |
| 1:B:2021:CYS:O    | 1:B:2028:ARG:NH2  | 2.45                     | 0.50              |
| 1:D:1031:THR:O    | 1:D:1035:ASN:ND2  | 2.37                     | 0.50              |
| 1:C:2021:CYS:O    | 1:C:2028:ARG:NH2  | 2.45                     | 0.50              |
| 1:C:2792:ARG:NH2  | 1:C:2798:SER:OG   | 2.44                     | 0.50              |
| 1:A:2700:MET:HE3  | 1:A:2701:PRO:CD   | 2.42                     | 0.49              |
| 1:B:1838:PHE:CZ   | 1:B:1929:MET:HE1  | 2.47                     | 0.49              |
| 1:B:4056:GLU:HG2  | 1:B:4166:LEU:HD13 | 1.93                     | 0.49              |
| 1:D:3535:LEU:O    | 1:D:3539:ARG:HG2  | 2.12                     | 0.49              |
| 1:C:2858:GLN:HB2  | 1:C:2859:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:1838:PHE:CZ   | 1:A:1929:MET:HE1  | 2.47                     | 0.49              |
| 1:B:4063:ASP:OD1  | 1:B:4064:MET:N    | 2.45                     | 0.49              |
| 1:B:4822:THR:HG21 | 1:C:4839:MET:HG3  | 1.94                     | 0.49              |
| 1:D:510:GLU:N     | 1:D:510:GLU:OE2   | 2.44                     | 0.49              |
| 1:D:4839:MET:HG3  | 1:C:4822:THR:HG21 | 1.93                     | 0.49              |
| 1:C:1676:LEU:HD22 | 1:C:2167:ILE:HD12 | 1.94                     | 0.49              |
| 1:C:3686:GLU:HB2  | 1:C:3688:GLU:OE1  | 2.11                     | 0.49              |
| 1:C:3734:HIS:CG   | 1:C:3735:LEU:N    | 2.80                     | 0.49              |
| 1:A:2441:HIS:CE1  | 1:A:2442:LEU:HD22 | 2.47                     | 0.49              |
| 1:A:3535:LEU:O    | 1:A:3539:ARG:HG2  | 2.12                     | 0.49              |
| 1:B:2441:HIS:CE1  | 1:B:2442:LEU:HD22 | 2.47                     | 0.49              |
| 1:B:2700:MET:HE3  | 1:B:2701:PRO:CD   | 2.42                     | 0.49              |
| 1:B:3226:GLU:C    | 1:B:3228:ALA:H    | 2.19                     | 0.49              |
| 1:B:3376:GLU:OE1  | 1:B:3448:SER:OG   | 2.28                     | 0.49              |
| 1:D:384:MET:SD    | 1:D:384:MET:N     | 2.72                     | 0.49              |
| 1:D:3465:ASN:OD1  | 1:D:3467:MET:N    | 2.34                     | 0.49              |
| 1:C:2615:ARG:HG2  | 1:C:2664:PHE:HE1  | 1.78                     | 0.49              |
| 1:C:2700:MET:HE3  | 1:C:2701:PRO:CD   | 2.42                     | 0.49              |
| 1:C:3535:LEU:O    | 1:C:3539:ARG:HG2  | 2.12                     | 0.49              |
| 1:A:3226:GLU:C    | 1:A:3228:ALA:H    | 2.19                     | 0.49              |
| 1:A:3872:GLU:HG3  | 1:A:3874:VAL:H    | 1.77                     | 0.49              |
| 1:A:4063:ASP:OD1  | 1:A:4064:MET:N    | 2.45                     | 0.49              |
| 1:A:3734:HIS:CG   | 1:A:3735:LEU:N    | 2.80                     | 0.49              |
| 1:A:4918:ILE:HD11 | 1:D:4888:TYR:HA   | 1.93                     | 0.49              |
| 1:B:384:MET:SD    | 1:B:384:MET:N     | 2.72                     | 0.49              |
| 1:B:2765:LYS:NZ   | 1:B:2857:PRO:HB2  | 2.22                     | 0.49              |
| 1:B:3880:PHE:HA   | 1:B:3883:ASP:OD2  | 2.13                     | 0.49              |
| 1:D:1172:ASP:OD1  | 1:D:1172:ASP:N    | 2.37                     | 0.49              |
| 1:D:1838:PHE:CZ   | 1:D:1929:MET:HE1  | 2.47                     | 0.49              |
| 1:D:3734:HIS:CG   | 1:D:3735:LEU:N    | 2.80                     | 0.49              |
| 1:D:3880:PHE:HA   | 1:D:3883:ASP:OD2  | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:4063:ASP:OD1  | 1:D:4064:MET:N    | 2.45                     | 0.49              |
| 1:C:1838:PHE:CZ   | 1:C:1929:MET:HE1  | 2.47                     | 0.49              |
| 1:C:2198:MET:N    | 1:C:2198:MET:HE2  | 2.27                     | 0.49              |
| 1:C:3105:LYS:O    | 1:C:3108:GLU:HG3  | 2.12                     | 0.49              |
| 1:C:3114:LYS:HE3  | 1:C:3123:LYS:HD2  | 1.95                     | 0.49              |
| 1:A:2929:PHE:HA   | 1:A:2932:MET:SD   | 2.52                     | 0.49              |
| 1:C:3624:LEU:HD13 | 1:C:3628:ARG:HB3  | 1.94                     | 0.49              |
| 1:A:3629:ARG:HA   | 1:A:3632:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:4627:MET:HE1  | 1:A:4629:TYR:CE2  | 2.48                     | 0.49              |
| 1:B:3535:LEU:O    | 1:B:3539:ARG:HG2  | 2.12                     | 0.49              |
| 1:B:3862:ASP:N    | 1:B:3862:ASP:OD1  | 2.45                     | 0.49              |
| 1:D:2615:ARG:HG2  | 1:D:2664:PHE:HE1  | 1.78                     | 0.49              |
| 1:D:3629:ARG:HA   | 1:D:3632:VAL:HG22 | 1.95                     | 0.49              |
| 1:D:4627:MET:HE1  | 1:D:4629:TYR:CE2  | 2.48                     | 0.49              |
| 1:A:384:MET:SD    | 1:A:384:MET:N     | 2.72                     | 0.49              |
| 1:A:2175:GLU:HG3  | 1:A:2228:MET:HB2  | 1.94                     | 0.49              |
| 2:H:75:THR:HG23   | 2:H:98:VAL:HG22   | 1.95                     | 0.49              |
| 1:B:1072:VAL:HG23 | 1:B:1193:SER:HB2  | 1.95                     | 0.49              |
| 1:B:2929:PHE:HA   | 1:B:2932:MET:SD   | 2.52                     | 0.49              |
| 1:B:3105:LYS:O    | 1:B:3108:GLU:HG3  | 2.12                     | 0.49              |
| 1:D:1128:ARG:H    | 1:D:1128:ARG:HE   | 1.61                     | 0.49              |
| 1:D:1976:ARG:HH22 | 1:D:1997:GLU:CD   | 2.20                     | 0.49              |
| 1:C:4063:ASP:OD1  | 1:C:4064:MET:N    | 2.45                     | 0.49              |
| 1:D:2765:LYS:HZ1  | 1:D:2860:PRO:HA   | 1.78                     | 0.49              |
| 1:D:3261:ALA:HB1  | 1:D:3265:GLU:HG3  | 1.95                     | 0.49              |
| 1:D:3540:TYR:HB3  | 1:D:3604:TYR:HD1  | 1.77                     | 0.49              |
| 1:C:1792:ALA:O    | 1:C:2176:ASN:ND2  | 2.46                     | 0.49              |
| 1:C:3629:ARG:HA   | 1:C:3632:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:1128:ARG:H    | 1:A:1128:ARG:HE   | 1.61                     | 0.49              |
| 1:A:3261:ALA:HB1  | 1:A:3265:GLU:HG3  | 1.95                     | 0.49              |
| 2:G:49:MET:SD     | 2:G:52:LYS:HE2    | 2.53                     | 0.49              |
| 1:B:4627:MET:HE1  | 1:B:4629:TYR:CE2  | 2.48                     | 0.49              |
| 1:D:2282:ASP:HA   | 1:D:2341:VAL:HG13 | 1.94                     | 0.49              |
| 1:C:707:VAL:HG23  | 1:C:782:SER:HB3   | 1.95                     | 0.49              |
| 1:C:3862:ASP:N    | 1:C:3862:ASP:OD1  | 2.45                     | 0.49              |
| 1:A:2090:LYS:HZ2  | 1:A:2092:GLN:HG3  | 1.77                     | 0.48              |
| 1:A:2615:ARG:HG2  | 1:A:2664:PHE:HE1  | 1.78                     | 0.48              |
| 2:E:60:GLU:HA     | 2:E:60:GLU:OE2    | 2.13                     | 0.48              |
| 1:B:669:ASP:OD2   | 1:B:790:ARG:NE    | 2.41                     | 0.48              |
| 1:B:707:VAL:HG23  | 1:B:782:SER:HB3   | 1.95                     | 0.48              |
| 1:B:1676:LEU:HD22 | 1:B:2167:ILE:HD12 | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1792:ALA:O    | 1:B:2176:ASN:ND2  | 2.46                     | 0.48              |
| 1:B:3261:ALA:HB1  | 1:B:3265:GLU:HG3  | 1.95                     | 0.48              |
| 1:B:3527:PRO:HD2  | 1:B:3573:MET:SD   | 2.52                     | 0.48              |
| 1:B:4712:PRO:O    | 1:B:4718:LYS:NZ   | 2.32                     | 0.48              |
| 1:D:2700:MET:HE3  | 1:D:2701:PRO:CD   | 2.42                     | 0.48              |
| 1:D:3872:GLU:HG3  | 1:D:3874:VAL:H    | 1.77                     | 0.48              |
| 1:A:932:LEU:H     | 1:A:932:LEU:HD23  | 1.76                     | 0.48              |
| 1:A:3717:ASP:OD1  | 1:A:3717:ASP:N    | 2.46                     | 0.48              |
| 1:B:2282:ASP:HA   | 1:B:2341:VAL:HG13 | 1.94                     | 0.48              |
| 1:B:2858:GLN:HB2  | 1:B:2859:PRO:HD3  | 1.94                     | 0.48              |
| 1:D:2198:MET:HE2  | 1:D:2198:MET:N    | 2.27                     | 0.48              |
| 1:C:887:ILE:HD12  | 1:C:888:GLU:N     | 2.28                     | 0.48              |
| 1:C:3261:ALA:HB1  | 1:C:3265:GLU:HG3  | 1.95                     | 0.48              |
| 1:C:3376:GLU:OE1  | 1:C:3448:SER:OG   | 2.28                     | 0.48              |
| 1:A:3880:PHE:HA   | 1:A:3883:ASP:OD2  | 2.13                     | 0.48              |
| 1:B:2393:ASP:OD1  | 1:B:2418:LEU:N    | 2.46                     | 0.48              |
| 1:B:3624:LEU:HD13 | 1:B:3628:ARG:HB3  | 1.94                     | 0.48              |
| 1:B:3734:HIS:CG   | 1:B:3735:LEU:N    | 2.80                     | 0.48              |
| 1:B:3872:GLU:HG3  | 1:B:3874:VAL:H    | 1.77                     | 0.48              |
| 1:D:1676:LEU:HD22 | 1:D:2167:ILE:HD12 | 1.94                     | 0.48              |
| 1:C:3540:TYR:HB3  | 1:C:3604:TYR:HD1  | 1.77                     | 0.48              |
| 1:C:3880:PHE:HA   | 1:C:3883:ASP:OD2  | 2.13                     | 0.48              |
| 1:C:4627:MET:HE1  | 1:C:4629:TYR:CE2  | 2.48                     | 0.48              |
| 1:C:4709:PRO:HD2  | 1:C:4772:ASP:OD2  | 2.13                     | 0.48              |
| 1:A:707:VAL:HG23  | 1:A:782:SER:HB3   | 1.95                     | 0.48              |
| 1:A:954:LYS:HB3   | 1:A:966:LYS:HE3   | 1.95                     | 0.48              |
| 1:A:2191:PHE:HD1  | 1:A:2198:MET:HG2  | 1.79                     | 0.48              |
| 1:A:3624:LEU:HD13 | 1:A:3628:ARG:HB3  | 1.94                     | 0.48              |
| 1:A:4843:LEU:HD21 | 1:D:4827:LEU:HD21 | 1.94                     | 0.48              |
| 1:B:954:LYS:HB3   | 1:B:966:LYS:HE3   | 1.96                     | 0.48              |
| 1:B:2198:MET:HE2  | 1:B:2198:MET:N    | 2.28                     | 0.48              |
| 1:D:2514:ASN:N    | 1:D:2514:ASN:OD1  | 2.47                     | 0.48              |
| 1:D:2929:PHE:HA   | 1:D:2932:MET:SD   | 2.52                     | 0.48              |
| 1:D:3114:LYS:HE3  | 1:D:3123:LYS:HD2  | 1.95                     | 0.48              |
| 1:D:4709:PRO:HD2  | 1:D:4772:ASP:OD2  | 2.14                     | 0.48              |
| 1:C:904:HIS:HB3   | 1:C:907:LEU:HG    | 1.94                     | 0.48              |
| 1:C:954:LYS:HB3   | 1:C:966:LYS:HE3   | 1.95                     | 0.48              |
| 1:B:1668:ARG:HG3  | 1:B:1671:ARG:NH2  | 2.29                     | 0.48              |
| 1:B:4709:PRO:HD2  | 1:B:4772:ASP:OD2  | 2.13                     | 0.48              |
| 1:D:2175:GLU:HG3  | 1:D:2228:MET:HB2  | 1.94                     | 0.48              |
| 1:C:2191:PHE:HD1  | 1:C:2198:MET:HG2  | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2514:ASN:N    | 1:C:2514:ASN:OD1  | 2.47                     | 0.48              |
| 1:C:4868:ASP:OD1  | 1:C:4870:ASP:N    | 2.47                     | 0.48              |
| 1:A:1676:LEU:HD22 | 1:A:2167:ILE:HD12 | 1.94                     | 0.48              |
| 1:A:2198:MET:HE2  | 1:A:2198:MET:N    | 2.27                     | 0.48              |
| 1:A:2736:ASP:OD1  | 1:A:2736:ASP:N    | 2.44                     | 0.48              |
| 1:D:545:ASP:OD1   | 1:D:582:HIS:NE2   | 2.32                     | 0.48              |
| 1:D:887:ILE:HD12  | 1:D:888:GLU:N     | 2.28                     | 0.48              |
| 1:C:110:ARG:NH2   | 1:C:117:TYR:OH    | 2.47                     | 0.48              |
| 1:C:1573:MET:HE2  | 1:C:1577:ALA:HB2  | 1.95                     | 0.48              |
| 1:A:1792:ALA:O    | 1:A:2176:ASN:ND2  | 2.46                     | 0.48              |
| 1:A:2282:ASP:HA   | 1:A:2341:VAL:HG13 | 1.94                     | 0.48              |
| 1:A:2393:ASP:OD1  | 1:A:2418:LEU:N    | 2.46                     | 0.48              |
| 1:A:3842:LEU:HB2  | 1:A:3929:SER:HB2  | 1.96                     | 0.48              |
| 1:A:4709:PRO:HD2  | 1:A:4772:ASP:OD2  | 2.13                     | 0.48              |
| 2:F:62:GLY:O      | 2:F:66:MET:HG3    | 2.14                     | 0.48              |
| 2:F:75:THR:HG23   | 2:F:98:VAL:HG22   | 1.96                     | 0.48              |
| 1:B:3629:ARG:HA   | 1:B:3632:VAL:HG22 | 1.95                     | 0.48              |
| 1:B:4091:LYS:HA   | 1:B:4091:LYS:HD2  | 1.70                     | 0.48              |
| 1:D:1792:ALA:O    | 1:D:2176:ASN:ND2  | 2.46                     | 0.48              |
| 1:D:2871:LEU:HG   | 1:D:2927:LEU:HD21 | 1.96                     | 0.48              |
| 1:D:4006:ASP:OD1  | 1:D:4009:GLN:NE2  | 2.47                     | 0.48              |
| 1:C:1668:ARG:HG3  | 1:C:1671:ARG:NH2  | 2.29                     | 0.48              |
| 1:C:2929:PHE:HA   | 1:C:2932:MET:SD   | 2.53                     | 0.48              |
| 1:A:904:HIS:HB3   | 1:A:907:LEU:HG    | 1.95                     | 0.48              |
| 1:A:1668:ARG:HG3  | 1:A:1671:ARG:NH2  | 2.29                     | 0.48              |
| 1:A:1983:ALA:O    | 1:A:1987:SER:OG   | 2.25                     | 0.48              |
| 1:A:2514:ASN:OD1  | 1:A:2514:ASN:N    | 2.47                     | 0.48              |
| 1:A:2587:TYR:O    | 1:A:2590:SER:OG   | 2.20                     | 0.48              |
| 1:B:2384:ILE:O    | 1:B:2387:SER:OG   | 2.26                     | 0.48              |
| 1:D:2974:ILE:HG13 | 1:D:2975:ALA:N    | 2.29                     | 0.48              |
| 1:D:3624:LEU:HD13 | 1:D:3628:ARG:HB3  | 1.94                     | 0.48              |
| 1:C:977:LEU:HG    | 1:C:1044:ARG:NH1  | 2.24                     | 0.48              |
| 2:E:75:THR:HG23   | 2:E:98:VAL:HG22   | 1.96                     | 0.48              |
| 1:B:2514:ASN:OD1  | 1:B:2514:ASN:N    | 2.47                     | 0.48              |
| 1:B:3842:LEU:HB2  | 1:B:3929:SER:HB2  | 1.96                     | 0.48              |
| 1:D:1072:VAL:HG23 | 1:D:1193:SER:HB2  | 1.95                     | 0.48              |
| 1:D:2309:SER:OG   | 1:D:2321:ILE:O    | 2.22                     | 0.48              |
| 1:D:2393:ASP:OD1  | 1:D:2418:LEU:N    | 2.46                     | 0.48              |
| 1:C:2309:SER:OG   | 1:C:2321:ILE:O    | 2.22                     | 0.48              |
| 1:C:2871:LEU:HG   | 1:C:2927:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:1072:VAL:HG23 | 1:A:1193:SER:HB2  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1248:VAL:HG22 | 1:A:1599:MET:HE3  | 1.96                     | 0.48              |
| 2:G:75:THR:HG23   | 2:G:98:VAL:HG22   | 1.96                     | 0.48              |
| 1:B:110:ARG:NH2   | 1:B:117:TYR:OH    | 2.47                     | 0.48              |
| 1:B:2538:THR:O    | 1:B:2542:SER:HB2  | 2.14                     | 0.48              |
| 1:D:707:VAL:HG23  | 1:D:782:SER:HB3   | 1.95                     | 0.48              |
| 1:D:3752:SER:N    | 1:D:3755:GLU:OE2  | 2.32                     | 0.48              |
| 1:C:2440:MET:HA   | 1:C:2440:MET:HE2  | 1.96                     | 0.48              |
| 1:C:2538:THR:O    | 1:C:2542:SER:HB2  | 2.14                     | 0.48              |
| 1:A:2303:ALA:O    | 1:A:2307:LEU:HD12 | 2.14                     | 0.47              |
| 1:A:3114:LYS:HE3  | 1:A:3123:LYS:HD2  | 1.95                     | 0.47              |
| 1:B:2973:PHE:HE2  | 1:B:2995:ILE:HG12 | 1.79                     | 0.47              |
| 1:D:1248:VAL:HG22 | 1:D:1599:MET:HE3  | 1.96                     | 0.47              |
| 1:D:2538:THR:O    | 1:D:2542:SER:HB2  | 2.14                     | 0.47              |
| 1:C:924:MET:O     | 1:C:928:THR:HG23  | 2.14                     | 0.47              |
| 1:C:1072:VAL:HG23 | 1:C:1193:SER:HB2  | 1.95                     | 0.47              |
| 1:C:2282:ASP:HA   | 1:C:2341:VAL:HG13 | 1.94                     | 0.47              |
| 1:C:2523:ASP:HB3  | 1:C:2578:MET:HE2  | 1.96                     | 0.47              |
| 1:C:2736:ASP:OD1  | 1:C:2736:ASP:N    | 2.44                     | 0.47              |
| 1:B:924:MET:O     | 1:B:928:THR:HG23  | 2.14                     | 0.47              |
| 1:B:2245:GLN:NE2  | 1:B:3860:ASN:HB2  | 2.29                     | 0.47              |
| 1:B:2523:ASP:HB3  | 1:B:2578:MET:HE2  | 1.96                     | 0.47              |
| 1:D:904:HIS:HB3   | 1:D:907:LEU:HG    | 1.94                     | 0.47              |
| 1:D:2303:ALA:O    | 1:D:2307:LEU:HD12 | 2.14                     | 0.47              |
| 1:D:4868:ASP:OD1  | 1:D:4870:ASP:N    | 2.47                     | 0.47              |
| 1:C:3872:GLU:HG3  | 1:C:3874:VAL:H    | 1.78                     | 0.47              |
| 1:C:4967:TYR:OH   | 1:C:5033:GLU:OE2  | 2.24                     | 0.47              |
| 1:A:2637:ALA:C    | 1:A:2640:PRO:HD2  | 2.40                     | 0.47              |
| 1:A:3628:ARG:HG3  | 1:A:3631:ALA:HB3  | 1.96                     | 0.47              |
| 1:B:157:ARG:HE    | 1:B:164:ARG:HD2   | 1.79                     | 0.47              |
| 1:B:1976:ARG:HH22 | 1:B:1997:GLU:CD   | 2.20                     | 0.47              |
| 1:B:3628:ARG:HG3  | 1:B:3631:ALA:HB3  | 1.96                     | 0.47              |
| 1:D:157:ARG:HE    | 1:D:164:ARG:HD2   | 1.79                     | 0.47              |
| 1:D:2191:PHE:HD1  | 1:D:2198:MET:HG2  | 1.79                     | 0.47              |
| 1:C:157:ARG:HE    | 1:C:164:ARG:HD2   | 1.79                     | 0.47              |
| 1:C:2393:ASP:OD1  | 1:C:2418:LEU:N    | 2.46                     | 0.47              |
| 1:C:2637:ALA:C    | 1:C:2640:PRO:HD2  | 2.40                     | 0.47              |
| 1:C:3465:ASN:OD1  | 1:C:3468:SER:N    | 2.42                     | 0.47              |
| 1:A:1174:GLY:HA3  | 1:D:3467:MET:HE1  | 1.91                     | 0.47              |
| 1:A:2538:THR:O    | 1:A:2542:SER:HB2  | 2.14                     | 0.47              |
| 1:A:4006:ASP:OD1  | 1:A:4009:GLN:NE2  | 2.47                     | 0.47              |
| 1:B:904:HIS:HB3   | 1:B:907:LEU:HG    | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2191:PHE:HD1  | 1:B:2198:MET:HG2  | 1.79                     | 0.47              |
| 1:B:2303:ALA:O    | 1:B:2307:LEU:HD12 | 2.14                     | 0.47              |
| 1:B:2871:LEU:HG   | 1:B:2927:LEU:HD21 | 1.96                     | 0.47              |
| 1:D:1174:GLY:CA   | 1:C:3467:MET:CE   | 2.86                     | 0.47              |
| 1:C:1025:ARG:H    | 1:C:1025:ARG:CD   | 2.25                     | 0.47              |
| 1:A:2973:PHE:HE2  | 1:A:2995:ILE:HG12 | 1.79                     | 0.47              |
| 1:A:4868:ASP:OD1  | 1:A:4870:ASP:N    | 2.47                     | 0.47              |
| 1:B:887:ILE:HD12  | 1:B:888:GLU:N     | 2.28                     | 0.47              |
| 1:B:2637:ALA:C    | 1:B:2640:PRO:HD2  | 2.40                     | 0.47              |
| 1:D:110:ARG:NH2   | 1:D:117:TYR:OH    | 2.47                     | 0.47              |
| 1:D:954:LYS:HB3   | 1:D:966:LYS:HE3   | 1.95                     | 0.47              |
| 1:D:1996:ARG:HA   | 1:D:1996:ARG:HE   | 1.80                     | 0.47              |
| 1:D:2090:LYS:HZ2  | 1:D:2092:GLN:HG3  | 1.79                     | 0.47              |
| 1:D:4968:PHE:O    | 1:D:4974:GLY:HA3  | 2.15                     | 0.47              |
| 1:C:1128:ARG:HE   | 1:C:1128:ARG:H    | 1.61                     | 0.47              |
| 1:C:1996:ARG:HA   | 1:C:1996:ARG:HE   | 1.80                     | 0.47              |
| 1:C:2245:GLN:NE2  | 1:C:3860:ASN:HB2  | 2.30                     | 0.47              |
| 1:C:3842:LEU:HB2  | 1:C:3929:SER:HB2  | 1.96                     | 0.47              |
| 1:C:4006:ASP:OD1  | 1:C:4009:GLN:NE2  | 2.47                     | 0.47              |
| 2:E:3:GLN:NE2     | 2:E:5:GLU:HG2     | 2.30                     | 0.47              |
| 1:B:866:HIS:HB2   | 1:B:941:MET:HE3   | 1.96                     | 0.47              |
| 1:B:1248:VAL:HG22 | 1:B:1599:MET:HE3  | 1.96                     | 0.47              |
| 1:B:2440:MET:HE2  | 1:B:2440:MET:HA   | 1.96                     | 0.47              |
| 1:D:866:HIS:HB2   | 1:D:941:MET:HE3   | 1.96                     | 0.47              |
| 1:D:1573:MET:HE2  | 1:D:1577:ALA:HB2  | 1.95                     | 0.47              |
| 1:C:1248:VAL:HG22 | 1:C:1599:MET:HE3  | 1.96                     | 0.47              |
| 1:C:1976:ARG:HH22 | 1:C:1997:GLU:CD   | 2.20                     | 0.47              |
| 1:C:4968:PHE:O    | 1:C:4974:GLY:HA3  | 2.15                     | 0.47              |
| 1:A:157:ARG:HE    | 1:A:164:ARG:HD2   | 1.79                     | 0.47              |
| 1:A:887:ILE:HD12  | 1:A:888:GLU:N     | 2.28                     | 0.47              |
| 1:A:924:MET:O     | 1:A:928:THR:HG23  | 2.14                     | 0.47              |
| 1:A:930:LYS:HA    | 1:A:933:LEU:HD12  | 1.97                     | 0.47              |
| 1:A:1025:ARG:H    | 1:A:1025:ARG:CD   | 2.25                     | 0.47              |
| 1:A:1573:MET:HE2  | 1:A:1577:ALA:HB2  | 1.95                     | 0.47              |
| 1:A:4927:ILE:HG23 | 1:D:4936:ILE:CD1  | 2.44                     | 0.47              |
| 1:B:1128:ARG:HE   | 1:B:1128:ARG:H    | 1.61                     | 0.47              |
| 1:B:2224:ARG:HG2  | 1:B:2225:PHE:CD2  | 2.50                     | 0.47              |
| 1:B:2615:ARG:HG2  | 1:B:2664:PHE:HE1  | 1.78                     | 0.47              |
| 1:B:3114:LYS:HE3  | 1:B:3123:LYS:HD2  | 1.95                     | 0.47              |
| 1:B:3477:LYS:HB3  | 1:C:1141:ARG:HD3  | 1.97                     | 0.47              |
| 1:B:4006:ASP:OD1  | 1:B:4009:GLN:NE2  | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:228:ASP:OD1   | 1:D:228:ASP:N     | 2.48                     | 0.47              |
| 1:D:1668:ARG:HG3  | 1:D:1671:ARG:NH2  | 2.29                     | 0.47              |
| 1:D:3717:ASP:OD1  | 1:D:3717:ASP:N    | 2.46                     | 0.47              |
| 1:D:3842:LEU:HB2  | 1:D:3929:SER:HB2  | 1.96                     | 0.47              |
| 1:D:4749:GLU:O    | 1:D:4753:HIS:ND1  | 2.48                     | 0.47              |
| 1:C:228:ASP:N     | 1:C:228:ASP:OD1   | 2.48                     | 0.47              |
| 1:C:3628:ARG:HG3  | 1:C:3631:ALA:HB3  | 1.97                     | 0.47              |
| 1:A:110:ARG:NH2   | 1:A:117:TYR:OH    | 2.47                     | 0.47              |
| 1:A:866:HIS:HB2   | 1:A:941:MET:HE3   | 1.96                     | 0.47              |
| 1:A:2871:LEU:HG   | 1:A:2927:LEU:HD21 | 1.95                     | 0.47              |
| 1:B:1868:PRO:O    | 1:B:1872:THR:OG1  | 2.33                     | 0.47              |
| 1:B:2974:ILE:HG13 | 1:B:2975:ALA:N    | 2.29                     | 0.47              |
| 1:B:4749:GLU:O    | 1:B:4753:HIS:ND1  | 2.48                     | 0.47              |
| 1:D:924:MET:O     | 1:D:928:THR:HG23  | 2.14                     | 0.47              |
| 1:D:1465:ASP:OD1  | 1:D:1468:LYS:HG2  | 2.15                     | 0.47              |
| 1:D:2440:MET:HE2  | 1:D:2440:MET:HA   | 1.96                     | 0.47              |
| 1:D:2973:PHE:HE2  | 1:D:2995:ILE:HG12 | 1.79                     | 0.47              |
| 1:A:2765:LYS:HZ1  | 1:A:2860:PRO:HA   | 1.80                     | 0.47              |
| 1:A:4044:MET:HE3  | 1:A:4044:MET:HB2  | 1.79                     | 0.47              |
| 1:B:1996:ARG:HA   | 1:B:1996:ARG:HE   | 1.80                     | 0.47              |
| 1:B:3940:LYS:O    | 1:B:4002:LYS:NZ   | 2.36                     | 0.47              |
| 1:D:1983:ALA:O    | 1:D:1987:SER:OG   | 2.25                     | 0.47              |
| 1:D:2637:ALA:C    | 1:D:2640:PRO:HD2  | 2.40                     | 0.47              |
| 1:D:3199:ALA:HB2  | 1:D:3279:SER:OG   | 2.15                     | 0.47              |
| 1:C:2186:MET:SD   | 1:C:2235:PHE:HD1  | 2.37                     | 0.47              |
| 1:C:2224:ARG:HG2  | 1:C:2225:PHE:CD2  | 2.50                     | 0.47              |
| 1:C:3199:ALA:HB2  | 1:C:3279:SER:OG   | 2.15                     | 0.47              |
| 1:A:228:ASP:OD1   | 1:A:228:ASP:N     | 2.48                     | 0.47              |
| 1:A:1976:ARG:HH22 | 1:A:1997:GLU:CD   | 2.20                     | 0.47              |
| 1:A:2224:ARG:HG2  | 1:A:2225:PHE:CD2  | 2.50                     | 0.47              |
| 1:A:2523:ASP:HB3  | 1:A:2578:MET:HE2  | 1.96                     | 0.47              |
| 1:B:3171:SER:O    | 1:B:3174:SER:OG   | 2.33                     | 0.47              |
| 1:B:4936:ILE:CD1  | 1:C:4927:ILE:HG23 | 2.45                     | 0.47              |
| 1:D:1127:HIS:HB3  | 1:D:1128:ARG:NH2  | 2.29                     | 0.47              |
| 1:D:1868:PRO:O    | 1:D:1872:THR:OG1  | 2.33                     | 0.47              |
| 1:D:3540:TYR:CZ   | 1:D:3549:VAL:HG21 | 2.50                     | 0.47              |
| 1:C:1465:ASP:OD1  | 1:C:1468:LYS:HG2  | 2.15                     | 0.47              |
| 1:C:4749:GLU:O    | 1:C:4753:HIS:ND1  | 2.48                     | 0.47              |
| 1:A:1465:ASP:OD1  | 1:A:1468:LYS:HG2  | 2.15                     | 0.46              |
| 1:A:2245:GLN:NE2  | 1:A:3860:ASN:HB2  | 2.30                     | 0.46              |
| 1:A:3540:TYR:CZ   | 1:A:3549:VAL:HG21 | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1057:ASP:OD1  | 1:B:1057:ASP:N    | 2.48                     | 0.46              |
| 1:B:1076:ARG:HB3  | 1:B:1191:VAL:HG23 | 1.97                     | 0.46              |
| 1:D:2224:ARG:HG2  | 1:D:2225:PHE:CD2  | 2.50                     | 0.46              |
| 1:D:4927:ILE:HG23 | 1:C:4936:ILE:CD1  | 2.45                     | 0.46              |
| 1:C:1172:ASP:OD1  | 1:C:1172:ASP:N    | 2.37                     | 0.46              |
| 1:C:1868:PRO:O    | 1:C:1872:THR:OG1  | 2.33                     | 0.46              |
| 1:C:2303:ALA:O    | 1:C:2307:LEU:HD12 | 2.14                     | 0.46              |
| 1:C:2974:ILE:HG13 | 1:C:2975:ALA:N    | 2.29                     | 0.46              |
| 1:C:4015:GLU:HA   | 1:C:4018:ASP:OD2  | 2.16                     | 0.46              |
| 1:A:1868:PRO:O    | 1:A:1872:THR:OG1  | 2.33                     | 0.46              |
| 1:A:2440:MET:HE2  | 1:A:2440:MET:HA   | 1.96                     | 0.46              |
| 1:A:4749:GLU:O    | 1:A:4753:HIS:ND1  | 2.48                     | 0.46              |
| 2:E:17:LYS:HB3    | 2:E:17:LYS:HE3    | 1.80                     | 0.46              |
| 1:B:930:LYS:HA    | 1:B:933:LEU:HD12  | 1.97                     | 0.46              |
| 1:B:1573:MET:HE2  | 1:B:1577:ALA:HB2  | 1.95                     | 0.46              |
| 1:B:2029:GLN:NE2  | 1:B:2033:ASP:OD1  | 2.49                     | 0.46              |
| 1:B:4067:LYS:NZ   | 1:B:4102:GLN:O    | 2.44                     | 0.46              |
| 1:B:4868:ASP:OD1  | 1:B:4870:ASP:N    | 2.47                     | 0.46              |
| 1:B:4888:TYR:HA   | 1:C:4918:ILE:HD11 | 1.97                     | 0.46              |
| 1:D:930:LYS:HA    | 1:D:933:LEU:HD12  | 1.97                     | 0.46              |
| 1:D:1025:ARG:HG2  | 1:D:1026:LEU:HD12 | 1.97                     | 0.46              |
| 1:D:2523:ASP:HB3  | 1:D:2578:MET:HE2  | 1.96                     | 0.46              |
| 1:C:1025:ARG:HG2  | 1:C:1026:LEU:HD12 | 1.97                     | 0.46              |
| 1:C:1076:ARG:HB3  | 1:C:1191:VAL:HG23 | 1.97                     | 0.46              |
| 1:A:638:ILE:HD11  | 1:A:1636:MET:HE2  | 1.97                     | 0.46              |
| 1:A:3171:SER:O    | 1:A:3174:SER:OG   | 2.33                     | 0.46              |
| 1:A:3442:PHE:CE1  | 1:A:3511:VAL:HG12 | 2.51                     | 0.46              |
| 2:E:16:PRO:HB2    | 2:E:50:LEU:HD11   | 1.97                     | 0.46              |
| 1:B:1569:GLN:HB2  | 1:B:1572:ILE:HD12 | 1.97                     | 0.46              |
| 1:B:2736:ASP:OD1  | 1:B:2736:ASP:N    | 2.44                     | 0.46              |
| 1:B:3540:TYR:CZ   | 1:B:3549:VAL:HG21 | 2.50                     | 0.46              |
| 1:D:829:TYR:CE1   | 1:D:1608:MET:HE3  | 2.50                     | 0.46              |
| 1:D:3628:ARG:HG3  | 1:D:3631:ALA:HB3  | 1.96                     | 0.46              |
| 1:D:4015:GLU:HA   | 1:D:4018:ASP:OD2  | 2.15                     | 0.46              |
| 1:C:2029:GLN:NE2  | 1:C:2033:ASP:OD1  | 2.48                     | 0.46              |
| 1:A:213:TYR:CE1   | 1:A:340:LYS:HG2   | 2.51                     | 0.46              |
| 1:B:228:ASP:OD1   | 1:B:228:ASP:N     | 2.48                     | 0.46              |
| 1:B:774:ASP:OD2   | 1:B:1470:ARG:NH2  | 2.35                     | 0.46              |
| 1:B:3316:LEU:HD21 | 1:B:3346:VAL:HG23 | 1.97                     | 0.46              |
| 1:D:3263:TYR:HD1  | 1:D:3270:ILE:HD12 | 1.80                     | 0.46              |
| 1:C:930:LYS:HA    | 1:C:933:LEU:HD12  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2029:GLN:NE2  | 1:A:2033:ASP:OD1  | 2.48                     | 0.46              |
| 1:A:2974:ILE:HG13 | 1:A:2975:ALA:N    | 2.29                     | 0.46              |
| 1:B:2186:MET:SD   | 1:B:2235:PHE:HD1  | 2.38                     | 0.46              |
| 1:B:4967:TYR:OH   | 1:B:5033:GLU:OE2  | 2.24                     | 0.46              |
| 1:D:2029:GLN:NE2  | 1:D:2033:ASP:OD1  | 2.48                     | 0.46              |
| 1:C:4887:MET:HE3  | 1:C:4887:MET:HB3  | 1.78                     | 0.46              |
| 1:A:4578:LEU:HA   | 1:B:4879:MET:HG3  | 1.98                     | 0.46              |
| 1:A:4968:PHE:O    | 1:A:4974:GLY:HA3  | 2.15                     | 0.46              |
| 1:B:829:TYR:CE1   | 1:B:1608:MET:HE3  | 2.51                     | 0.46              |
| 1:B:4968:PHE:O    | 1:B:4974:GLY:HA3  | 2.15                     | 0.46              |
| 1:D:399:GLN:O     | 1:D:403:MET:HG3   | 2.16                     | 0.46              |
| 1:D:1573:MET:HE1  | 1:D:1587:PRO:HA   | 1.98                     | 0.46              |
| 1:D:4044:MET:HE3  | 1:D:4044:MET:HB2  | 1.79                     | 0.46              |
| 1:C:571:SER:OG    | 1:C:573:GLU:OE1   | 2.21                     | 0.46              |
| 1:C:866:HIS:HB2   | 1:C:941:MET:HE3   | 1.96                     | 0.46              |
| 1:A:399:GLN:O     | 1:A:403:MET:HG3   | 2.16                     | 0.46              |
| 1:A:955:LEU:HD12  | 1:A:967:PRO:HD2   | 1.98                     | 0.46              |
| 1:B:213:TYR:CE1   | 1:B:340:LYS:HG2   | 2.51                     | 0.46              |
| 1:B:328:LYS:HE3   | 1:B:328:LYS:HB3   | 1.74                     | 0.46              |
| 1:B:4039:MET:SD   | 1:B:4040:ILE:N    | 2.89                     | 0.46              |
| 1:D:638:ILE:HD11  | 1:D:1636:MET:HE2  | 1.97                     | 0.46              |
| 1:D:1076:ARG:HB3  | 1:D:1191:VAL:HG23 | 1.97                     | 0.46              |
| 1:D:3316:LEU:HD21 | 1:D:3346:VAL:HG23 | 1.97                     | 0.46              |
| 1:D:3696:ASP:OD2  | 1:D:3773:ARG:NE   | 2.47                     | 0.46              |
| 1:D:4091:LYS:HA   | 1:D:4091:LYS:HD2  | 1.70                     | 0.46              |
| 1:C:1573:MET:HE1  | 1:C:1587:PRO:HA   | 1.98                     | 0.46              |
| 1:C:3262:ARG:O    | 1:C:3266:MET:HG2  | 2.16                     | 0.46              |
| 1:C:3717:ASP:N    | 1:C:3717:ASP:OD1  | 2.46                     | 0.46              |
| 1:C:4039:MET:SD   | 1:C:4040:ILE:N    | 2.89                     | 0.46              |
| 1:A:3540:TYR:HB3  | 1:A:3604:TYR:HD1  | 1.77                     | 0.46              |
| 1:A:4578:LEU:HA   | 1:B:4879:MET:HG2  | 1.98                     | 0.46              |
| 2:H:62:GLY:O      | 2:H:66:MET:HG3    | 2.15                     | 0.46              |
| 1:B:955:LEU:HD12  | 1:B:967:PRO:HD2   | 1.98                     | 0.46              |
| 1:B:1465:ASP:OD1  | 1:B:1468:LYS:HG2  | 2.15                     | 0.46              |
| 1:B:3199:ALA:HB2  | 1:B:3279:SER:OG   | 2.15                     | 0.46              |
| 1:B:3467:MET:CE   | 1:C:1174:GLY:CA   | 2.85                     | 0.46              |
| 1:D:213:TYR:CE1   | 1:D:340:LYS:HG2   | 2.51                     | 0.46              |
| 1:D:2186:MET:SD   | 1:D:2235:PHE:HD1  | 2.38                     | 0.46              |
| 1:D:2245:GLN:NE2  | 1:D:3860:ASN:HB2  | 2.30                     | 0.46              |
| 1:D:3262:ARG:O    | 1:D:3266:MET:HG2  | 2.16                     | 0.46              |
| 1:C:213:TYR:CE1   | 1:C:340:LYS:HG2   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:3263:TYR:HD1  | 1:C:3270:ILE:HD12 | 1.80                     | 0.46              |
| 1:C:4112:LEU:O    | 1:C:4115:SER:OG   | 2.27                     | 0.46              |
| 1:A:2390:PRO:C    | 1:A:2392:ARG:H    | 2.24                     | 0.46              |
| 1:A:3263:TYR:HD1  | 1:A:3270:ILE:HD12 | 1.80                     | 0.46              |
| 1:A:4091:LYS:HA   | 1:A:4091:LYS:HD2  | 1.70                     | 0.46              |
| 1:B:3206:LEU:HD11 | 1:B:3276:MET:HE3  | 1.98                     | 0.46              |
| 1:B:4015:GLU:HA   | 1:B:4018:ASP:OD2  | 2.15                     | 0.46              |
| 1:D:955:LEU:HD12  | 1:D:967:PRO:HD2   | 1.98                     | 0.46              |
| 1:D:2355:ARG:NH2  | 1:D:2449:GLU:OE2  | 2.47                     | 0.46              |
| 1:D:5030:LYS:HA   | 1:D:5033:GLU:HG2  | 1.98                     | 0.46              |
| 1:C:1648:MET:HE2  | 1:C:1648:MET:HB3  | 1.88                     | 0.46              |
| 1:C:3206:LEU:HD11 | 1:C:3276:MET:HE3  | 1.98                     | 0.46              |
| 1:A:365:LYS:HE3   | 1:A:365:LYS:HB3   | 1.81                     | 0.46              |
| 1:A:774:ASP:OD2   | 1:A:1470:ARG:NH2  | 2.35                     | 0.46              |
| 1:A:829:TYR:CE1   | 1:A:1608:MET:HE3  | 2.50                     | 0.46              |
| 1:A:2186:MET:SD   | 1:A:2235:PHE:HD1  | 2.37                     | 0.46              |
| 1:A:3199:ALA:HB2  | 1:A:3279:SER:OG   | 2.15                     | 0.46              |
| 1:A:4015:GLU:HA   | 1:A:4018:ASP:OD2  | 2.15                     | 0.46              |
| 1:B:879:HIS:NE2   | 1:B:921:ASN:HB2   | 2.31                     | 0.46              |
| 1:D:1569:GLN:HB2  | 1:D:1572:ILE:HD12 | 1.98                     | 0.46              |
| 1:D:4039:MET:SD   | 1:D:4040:ILE:N    | 2.89                     | 0.46              |
| 1:D:4918:ILE:HD11 | 1:C:4888:TYR:HA   | 1.98                     | 0.46              |
| 1:C:638:ILE:HD11  | 1:C:1636:MET:HE2  | 1.97                     | 0.46              |
| 1:C:3316:LEU:HD21 | 1:C:3346:VAL:HG23 | 1.97                     | 0.46              |
| 1:A:1573:MET:HE1  | 1:A:1587:PRO:HA   | 1.98                     | 0.45              |
| 1:A:1996:ARG:HA   | 1:A:1996:ARG:HE   | 1.80                     | 0.45              |
| 1:A:4039:MET:SD   | 1:A:4040:ILE:N    | 2.89                     | 0.45              |
| 2:E:79:ASP:OD2    | 2:E:80:TYR:HD1    | 1.99                     | 0.45              |
| 1:B:399:GLN:O     | 1:B:403:MET:HG3   | 2.16                     | 0.45              |
| 1:B:638:ILE:HD11  | 1:B:1636:MET:HE2  | 1.97                     | 0.45              |
| 1:B:2390:PRO:C    | 1:B:2392:ARG:H    | 2.24                     | 0.45              |
| 1:B:3540:TYR:HB3  | 1:B:3604:TYR:HD1  | 1.77                     | 0.45              |
| 1:D:3638:MET:O    | 1:D:3638:MET:HE3  | 2.17                     | 0.45              |
| 1:C:829:TYR:CE1   | 1:C:1608:MET:HE3  | 2.50                     | 0.45              |
| 1:C:3442:PHE:CE1  | 1:C:3511:VAL:HG12 | 2.51                     | 0.45              |
| 1:C:3540:TYR:CZ   | 1:C:3549:VAL:HG21 | 2.50                     | 0.45              |
| 1:A:1569:GLN:HB2  | 1:A:1572:ILE:HD12 | 1.97                     | 0.45              |
| 1:A:3263:TYR:N    | 1:A:3326:ASN:OD1  | 2.50                     | 0.45              |
| 1:B:1025:ARG:HG2  | 1:B:1026:LEU:HD12 | 1.97                     | 0.45              |
| 1:B:1573:MET:HE1  | 1:B:1587:PRO:HA   | 1.98                     | 0.45              |
| 1:B:2358:ILE:HB   | 1:C:195:PHE:CE1   | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3263:TYR:HD1  | 1:B:3270:ILE:HD12 | 1.80                     | 0.45              |
| 1:D:475:GLN:NE2   | 1:D:528:SER:O     | 2.49                     | 0.45              |
| 1:D:2677:LYS:HE2  | 1:D:2677:LYS:HB3  | 1.79                     | 0.45              |
| 1:D:4067:LYS:NZ   | 1:D:4102:GLN:O    | 2.44                     | 0.45              |
| 1:C:663:TYR:OH    | 1:C:665:GLU:OE2   | 2.24                     | 0.45              |
| 1:C:955:LEU:HD12  | 1:C:967:PRO:HD2   | 1.98                     | 0.45              |
| 1:C:1229:ASN:C    | 1:C:1230:MET:HG2  | 2.41                     | 0.45              |
| 1:C:3579:LEU:HB2  | 1:C:3582:ARG:HG2  | 1.98                     | 0.45              |
| 1:A:1823:GLY:O    | 1:A:1825:HIS:ND1  | 2.48                     | 0.45              |
| 1:B:3262:ARG:O    | 1:B:3266:MET:HG2  | 2.16                     | 0.45              |
| 1:B:3717:ASP:N    | 1:B:3717:ASP:OD1  | 2.46                     | 0.45              |
| 1:D:3159:ASP:OD1  | 1:D:3159:ASP:N    | 2.48                     | 0.45              |
| 1:D:3171:SER:O    | 1:D:3174:SER:OG   | 2.33                     | 0.45              |
| 1:D:4879:MET:HB3  | 1:C:4578:LEU:O    | 2.17                     | 0.45              |
| 1:C:1127:HIS:HB3  | 1:C:1128:ARG:NH2  | 2.29                     | 0.45              |
| 1:C:3263:TYR:N    | 1:C:3326:ASN:OD1  | 2.50                     | 0.45              |
| 1:A:1469:VAL:HG13 | 1:A:1492:CYS:HB3  | 1.99                     | 0.45              |
| 2:G:90:ILE:HD13   | 1:C:1782:PHE:CD1  | 2.51                     | 0.45              |
| 2:F:17:LYS:HE3    | 2:F:17:LYS:HB3    | 1.78                     | 0.45              |
| 1:D:4904:PRO:CB   | 1:D:4913:ARG:HG2  | 2.45                     | 0.45              |
| 1:C:399:GLN:O     | 1:C:403:MET:HG3   | 2.16                     | 0.45              |
| 1:C:2768:PHE:O    | 1:C:2771:ILE:HG22 | 2.17                     | 0.45              |
| 1:A:1127:HIS:HB3  | 1:A:1128:ARG:NH2  | 2.29                     | 0.45              |
| 1:A:1172:ASP:OD1  | 1:A:1172:ASP:N    | 2.37                     | 0.45              |
| 1:A:3262:ARG:O    | 1:A:3266:MET:HG2  | 2.16                     | 0.45              |
| 1:A:3638:MET:O    | 1:A:3638:MET:HE3  | 2.17                     | 0.45              |
| 1:A:4689:THR:HG22 | 1:A:4732:PHE:CZ   | 2.52                     | 0.45              |
| 1:B:1068:ARG:NH2  | 1:B:1071:ARG:HG3  | 2.32                     | 0.45              |
| 1:B:1229:ASN:C    | 1:B:1230:MET:HG2  | 2.41                     | 0.45              |
| 1:B:2574:HIS:CD2  | 1:B:2574:HIS:H    | 2.35                     | 0.45              |
| 1:B:2627:VAL:HA   | 1:B:2678:LEU:HD13 | 1.99                     | 0.45              |
| 1:B:3638:MET:O    | 1:B:3638:MET:HE3  | 2.17                     | 0.45              |
| 1:D:879:HIS:NE2   | 1:D:921:ASN:HB2   | 2.31                     | 0.45              |
| 1:C:4067:LYS:NZ   | 1:C:4102:GLN:O    | 2.44                     | 0.45              |
| 1:A:879:HIS:NE2   | 1:A:921:ASN:HB2   | 2.31                     | 0.45              |
| 1:A:2531:ARG:HG2  | 1:A:2585:THR:HG21 | 1.98                     | 0.45              |
| 1:A:3206:LEU:HD11 | 1:A:3276:MET:HE3  | 1.98                     | 0.45              |
| 1:A:5030:LYS:HA   | 1:A:5033:GLU:HG2  | 1.98                     | 0.45              |
| 1:B:1020:ARG:O    | 1:B:1022:VAL:N    | 2.49                     | 0.45              |
| 1:B:1127:HIS:HB3  | 1:B:1128:ARG:NH2  | 2.29                     | 0.45              |
| 1:D:1141:ARG:HD3  | 1:C:3477:LYS:HB3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1469:VAL:HG13 | 1:D:1492:CYS:HB3  | 1.99                     | 0.45              |
| 1:D:3263:TYR:N    | 1:D:3326:ASN:OD1  | 2.50                     | 0.45              |
| 1:D:3771:HIS:O    | 1:D:3815:LYS:NZ   | 2.49                     | 0.45              |
| 1:C:140:ASP:OD1   | 1:C:142:THR:OG1   | 2.29                     | 0.45              |
| 1:C:3171:SER:O    | 1:C:3174:SER:OG   | 2.33                     | 0.45              |
| 1:A:3823:LYS:HD3  | 1:A:3823:LYS:HA   | 1.76                     | 0.45              |
| 1:B:233:ILE:O     | 1:B:257:ARG:NH1   | 2.49                     | 0.45              |
| 1:B:977:LEU:HG    | 1:B:1044:ARG:NH1  | 2.24                     | 0.45              |
| 1:B:2355:ARG:NH2  | 1:B:2449:GLU:OE2  | 2.47                     | 0.45              |
| 1:D:923:GLN:O     | 1:D:927:GLU:HG2   | 2.17                     | 0.45              |
| 1:D:2768:PHE:O    | 1:D:2771:ILE:HG22 | 2.17                     | 0.45              |
| 1:D:3442:PHE:CE1  | 1:D:3511:VAL:HG12 | 2.51                     | 0.45              |
| 1:D:4689:THR:HG22 | 1:D:4732:PHE:CZ   | 2.52                     | 0.45              |
| 1:C:1469:VAL:HG13 | 1:C:1492:CYS:HB3  | 1.99                     | 0.45              |
| 1:A:923:GLN:O     | 1:A:927:GLU:HG2   | 2.17                     | 0.45              |
| 1:A:1174:GLY:N    | 1:D:3467:MET:CE   | 2.80                     | 0.45              |
| 2:F:34:LYS:HD2    | 1:B:629:ARG:HD2   | 1.99                     | 0.45              |
| 1:B:908:VAL:HG23  | 1:B:909:ASN:H     | 1.82                     | 0.45              |
| 1:B:3735:LEU:HD12 | 1:B:3766:GLN:NE2  | 2.32                     | 0.45              |
| 1:B:4044:MET:HE3  | 1:B:4044:MET:HB2  | 1.79                     | 0.45              |
| 1:D:328:LYS:HE3   | 1:D:328:LYS:HB3   | 1.73                     | 0.45              |
| 1:D:2390:PRO:C    | 1:D:2392:ARG:H    | 2.24                     | 0.45              |
| 1:D:2765:LYS:HD3  | 1:D:2765:LYS:HA   | 1.80                     | 0.45              |
| 1:D:3579:LEU:HB2  | 1:D:3582:ARG:HG2  | 1.98                     | 0.45              |
| 1:D:3989:VAL:HG11 | 1:D:4047:MET:HE2  | 1.98                     | 0.45              |
| 1:D:4638:TYR:C    | 1:D:4641:PRO:HD2  | 2.42                     | 0.45              |
| 1:C:1031:THR:HG22 | 1:C:1035:ASN:HD21 | 1.82                     | 0.45              |
| 1:C:1569:GLN:HB2  | 1:C:1572:ILE:HD12 | 1.97                     | 0.45              |
| 1:A:1076:ARG:HB3  | 1:A:1191:VAL:HG23 | 1.97                     | 0.45              |
| 1:A:1492:CYS:SG   | 1:A:1494:MET:HG3  | 2.57                     | 0.45              |
| 1:A:3316:LEU:HD21 | 1:A:3346:VAL:HG23 | 1.97                     | 0.45              |
| 1:B:774:ASP:OD1   | 1:B:774:ASP:N     | 2.45                     | 0.45              |
| 1:B:1575:LEU:HD23 | 1:B:1575:LEU:HA   | 1.81                     | 0.45              |
| 1:D:870:ILE:HG12  | 1:D:1051:TYR:HE2  | 1.82                     | 0.45              |
| 1:D:2650:ARG:NH1  | 1:D:2651:CYS:SG   | 2.90                     | 0.45              |
| 1:C:41:GLY:HA2    | 1:C:137:LEU:HD12  | 1.99                     | 0.45              |
| 1:C:879:HIS:NE2   | 1:C:921:ASN:HB2   | 2.31                     | 0.45              |
| 1:C:2627:VAL:HA   | 1:C:2678:LEU:HD13 | 1.99                     | 0.45              |
| 1:C:3194:LEU:HD12 | 1:C:3194:LEU:HA   | 1.76                     | 0.45              |
| 1:A:1025:ARG:HG2  | 1:A:1026:LEU:HD12 | 1.97                     | 0.45              |
| 1:A:1057:ASP:N    | 1:A:1057:ASP:OD1  | 2.48                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1229:ASN:C    | 1:A:1230:MET:HG2  | 2.41                     | 0.45              |
| 1:A:2768:PHE:O    | 1:A:2771:ILE:HG22 | 2.17                     | 0.45              |
| 1:A:3159:ASP:OD1  | 1:A:3159:ASP:N    | 2.48                     | 0.45              |
| 1:A:3735:LEU:HD12 | 1:A:3766:GLN:NE2  | 2.32                     | 0.45              |
| 1:A:3933:PHE:HD2  | 1:A:3951:PHE:CE2  | 2.35                     | 0.45              |
| 1:A:4735:GLU:H    | 1:A:4735:GLU:CD   | 2.25                     | 0.45              |
| 1:A:4918:ILE:HD13 | 1:D:4892:ARG:HD3  | 1.99                     | 0.45              |
| 1:B:1492:CYS:SG   | 1:B:1494:MET:HG3  | 2.57                     | 0.45              |
| 1:D:340:LYS:HE3   | 1:D:343:GLU:OE1   | 2.17                     | 0.45              |
| 1:D:1648:MET:HE2  | 1:D:1648:MET:HB3  | 1.88                     | 0.45              |
| 1:D:3933:PHE:HD2  | 1:D:3951:PHE:CE2  | 2.35                     | 0.45              |
| 1:C:1057:ASP:OD1  | 1:C:1057:ASP:N    | 2.48                     | 0.45              |
| 1:C:1068:ARG:NH2  | 1:C:1071:ARG:HG3  | 2.32                     | 0.45              |
| 1:C:2390:PRO:C    | 1:C:2392:ARG:H    | 2.24                     | 0.45              |
| 1:C:2782:ASP:OD1  | 1:C:2782:ASP:N    | 2.50                     | 0.45              |
| 1:C:2973:PHE:HE2  | 1:C:2995:ILE:HG12 | 1.79                     | 0.45              |
| 1:C:3227:ARG:HB3  | 1:C:3232:LEU:HD12 | 1.99                     | 0.45              |
| 1:C:3989:VAL:HG11 | 1:C:4047:MET:HE2  | 1.98                     | 0.45              |
| 1:A:194:SER:OG    | 1:A:195:PHE:N     | 2.50                     | 0.44              |
| 1:A:2574:HIS:CD2  | 1:A:2574:HIS:H    | 2.35                     | 0.44              |
| 1:A:3227:ARG:HB3  | 1:A:3232:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:4638:TYR:C    | 1:A:4641:PRO:HD2  | 2.42                     | 0.44              |
| 1:B:1469:VAL:HG13 | 1:B:1492:CYS:HB3  | 1.99                     | 0.44              |
| 1:B:3227:ARG:HB3  | 1:B:3232:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:3442:PHE:CE1  | 1:B:3511:VAL:HG12 | 2.51                     | 0.44              |
| 1:B:3579:LEU:HB2  | 1:B:3582:ARG:HG2  | 1.98                     | 0.44              |
| 1:B:3933:PHE:HD2  | 1:B:3951:PHE:CE2  | 2.35                     | 0.44              |
| 1:B:4689:THR:HG22 | 1:B:4732:PHE:CZ   | 2.52                     | 0.44              |
| 1:D:195:PHE:CE1   | 1:C:2358:ILE:HB   | 2.53                     | 0.44              |
| 1:D:1492:CYS:SG   | 1:D:1494:MET:HG3  | 2.57                     | 0.44              |
| 1:D:3227:ARG:HB3  | 1:D:3232:LEU:HD12 | 1.99                     | 0.44              |
| 1:C:2574:HIS:CD2  | 1:C:2574:HIS:H    | 2.35                     | 0.44              |
| 1:C:2650:ARG:NH1  | 1:C:2651:CYS:SG   | 2.90                     | 0.44              |
| 1:C:3933:PHE:HD2  | 1:C:3951:PHE:CE2  | 2.35                     | 0.44              |
| 1:C:4904:PRO:CB   | 1:C:4913:ARG:HG2  | 2.45                     | 0.44              |
| 1:C:5030:LYS:HA   | 1:C:5033:GLU:HG2  | 1.98                     | 0.44              |
| 1:A:2782:ASP:N    | 1:A:2782:ASP:OD1  | 2.50                     | 0.44              |
| 1:A:3633:VAL:HG13 | 1:A:3637:ARG:HH21 | 1.83                     | 0.44              |
| 1:A:3989:VAL:HG11 | 1:A:4047:MET:HE2  | 1.98                     | 0.44              |
| 2:H:17:LYS:HE3    | 2:H:17:LYS:HB3    | 1.79                     | 0.44              |
| 2:H:90:ILE:HD13   | 1:D:1782:PHE:CD1  | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1253:PRO:HG2  | 1:B:1254:HIS:CD2  | 2.53                     | 0.44              |
| 1:C:870:ILE:HG12  | 1:C:1051:TYR:HE2  | 1.82                     | 0.44              |
| 1:C:2355:ARG:NH2  | 1:C:2449:GLU:OE2  | 2.47                     | 0.44              |
| 1:A:340:LYS:HE3   | 1:A:343:GLU:OE1   | 2.17                     | 0.44              |
| 1:A:341:TYR:CZ    | 1:A:392:ARG:HD3   | 2.53                     | 0.44              |
| 1:A:870:ILE:HG12  | 1:A:1051:TYR:HE2  | 1.82                     | 0.44              |
| 1:A:1168:VAL:HG11 | 1:A:1176:GLU:HG2  | 1.99                     | 0.44              |
| 1:B:340:LYS:HE3   | 1:B:343:GLU:OE1   | 2.17                     | 0.44              |
| 1:B:2615:ARG:HG2  | 1:B:2664:PHE:CE1  | 2.53                     | 0.44              |
| 1:B:4735:GLU:H    | 1:B:4735:GLU:CD   | 2.25                     | 0.44              |
| 1:D:41:GLY:HA2    | 1:D:137:LEU:HD12  | 1.99                     | 0.44              |
| 1:D:3633:VAL:HG13 | 1:D:3637:ARG:HH21 | 1.83                     | 0.44              |
| 1:D:4253:GLU:HG3  | 1:D:4557:ARG:NH2  | 2.33                     | 0.44              |
| 1:C:340:LYS:HE3   | 1:C:343:GLU:OE1   | 2.17                     | 0.44              |
| 1:C:908:VAL:HG23  | 1:C:909:ASN:H     | 1.82                     | 0.44              |
| 1:C:1255:TYR:O    | 1:C:1275:ARG:NH1  | 2.51                     | 0.44              |
| 1:C:2615:ARG:HG2  | 1:C:2664:PHE:CE1  | 2.53                     | 0.44              |
| 1:C:3633:VAL:HG13 | 1:C:3637:ARG:HH21 | 1.83                     | 0.44              |
| 1:C:4638:TYR:C    | 1:C:4641:PRO:HD2  | 2.42                     | 0.44              |
| 1:A:2627:VAL:HA   | 1:A:2678:LEU:HD13 | 1.99                     | 0.44              |
| 1:A:2650:ARG:NH1  | 1:A:2651:CYS:SG   | 2.90                     | 0.44              |
| 1:A:4904:PRO:CB   | 1:A:4913:ARG:HG2  | 2.45                     | 0.44              |
| 1:B:901:LYS:HA    | 1:B:901:LYS:HD2   | 1.84                     | 0.44              |
| 1:B:1031:THR:HG22 | 1:B:1035:ASN:HD21 | 1.82                     | 0.44              |
| 1:B:1168:VAL:HG11 | 1:B:1176:GLU:HG2  | 1.99                     | 0.44              |
| 1:B:1668:ARG:HG3  | 1:B:1671:ARG:HH21 | 1.82                     | 0.44              |
| 1:D:1068:ARG:NH2  | 1:D:1071:ARG:HG3  | 2.32                     | 0.44              |
| 1:D:1255:TYR:O    | 1:D:1275:ARG:NH1  | 2.51                     | 0.44              |
| 1:D:1475:THR:HG23 | 1:D:1483:VAL:HG13 | 2.00                     | 0.44              |
| 1:D:2531:ARG:HG2  | 1:D:2585:THR:HG21 | 1.98                     | 0.44              |
| 1:D:3036:LYS:O    | 1:D:3039:ILE:HG22 | 2.18                     | 0.44              |
| 1:D:3206:LEU:HD11 | 1:D:3276:MET:HE3  | 1.98                     | 0.44              |
| 1:D:4586:PRO:HA   | 1:D:4629:TYR:CD1  | 2.52                     | 0.44              |
| 1:C:1071:ARG:HA   | 1:C:1071:ARG:HE   | 1.82                     | 0.44              |
| 1:C:1253:PRO:HG2  | 1:C:1254:HIS:CD2  | 2.53                     | 0.44              |
| 1:C:1270:LEU:HB2  | 1:C:1564:PHE:HB2  | 2.00                     | 0.44              |
| 1:A:483:MET:HE2   | 1:A:483:MET:N     | 2.32                     | 0.44              |
| 1:A:908:VAL:HG23  | 1:A:909:ASN:H     | 1.82                     | 0.44              |
| 1:A:1071:ARG:HA   | 1:A:1071:ARG:HE   | 1.82                     | 0.44              |
| 1:A:2208:MET:SD   | 1:A:2250:MET:HE1  | 2.57                     | 0.44              |
| 1:A:3132:THR:HG23 | 1:A:3136:LEU:HD23 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3579:LEU:HB2  | 1:A:3582:ARG:HG2  | 1.98                     | 0.44              |
| 1:A:4586:PRO:HA   | 1:A:4629:TYR:CD1  | 2.52                     | 0.44              |
| 2:F:3:GLN:HB3     | 2:F:5:GLU:OE2     | 2.17                     | 0.44              |
| 1:B:1475:THR:HG23 | 1:B:1483:VAL:HG13 | 2.00                     | 0.44              |
| 1:B:1823:GLY:O    | 1:B:1825:HIS:ND1  | 2.48                     | 0.44              |
| 1:B:2668:SER:C    | 1:B:2670:GLU:H    | 2.26                     | 0.44              |
| 1:B:2768:PHE:O    | 1:B:2771:ILE:HG22 | 2.17                     | 0.44              |
| 1:B:3003:LEU:HB2  | 1:B:3004:PRO:HD3  | 2.00                     | 0.44              |
| 1:B:3036:LYS:O    | 1:B:3039:ILE:HG22 | 2.18                     | 0.44              |
| 1:B:3455:GLU:OE2  | 1:B:3508:SER:OG   | 2.36                     | 0.44              |
| 1:B:3987:ASP:OD2  | 1:C:162:LYS:HE3   | 2.17                     | 0.44              |
| 1:D:483:MET:HE2   | 1:D:483:MET:N     | 2.32                     | 0.44              |
| 1:D:3003:LEU:HB2  | 1:D:3004:PRO:HD3  | 2.00                     | 0.44              |
| 1:D:3260:GLY:HA2  | 1:D:3325:ASN:ND2  | 2.33                     | 0.44              |
| 1:C:341:TYR:CZ    | 1:C:392:ARG:HD3   | 2.53                     | 0.44              |
| 1:C:475:GLN:NE2   | 1:C:528:SER:O     | 2.49                     | 0.44              |
| 1:C:1668:ARG:HG3  | 1:C:1671:ARG:HH21 | 1.82                     | 0.44              |
| 1:C:3003:LEU:HB2  | 1:C:3004:PRO:HD3  | 2.00                     | 0.44              |
| 1:C:3638:MET:O    | 1:C:3638:MET:HE3  | 2.17                     | 0.44              |
| 1:C:4044:MET:HE3  | 1:C:4044:MET:HB2  | 1.79                     | 0.44              |
| 1:A:957:LYS:HA    | 1:A:960:MET:HE2   | 2.00                     | 0.44              |
| 1:A:1451:GLY:HA3  | 1:A:1494:MET:HA   | 1.99                     | 0.44              |
| 1:A:1668:ARG:HG3  | 1:A:1671:ARG:HH21 | 1.82                     | 0.44              |
| 1:A:3765:TYR:CD2  | 1:A:4753:HIS:HA   | 2.53                     | 0.44              |
| 1:B:1071:ARG:HA   | 1:B:1071:ARG:HE   | 1.81                     | 0.44              |
| 1:B:1270:LEU:HB2  | 1:B:1564:PHE:HB2  | 2.00                     | 0.44              |
| 1:B:3263:TYR:N    | 1:B:3326:ASN:OD1  | 2.50                     | 0.44              |
| 1:D:2224:ARG:HG2  | 1:D:2225:PHE:CE2  | 2.53                     | 0.44              |
| 1:D:3751:VAL:O    | 1:D:3756:LYS:NZ   | 2.51                     | 0.44              |
| 1:D:3862:ASP:OD1  | 1:D:3862:ASP:N    | 2.45                     | 0.44              |
| 1:C:923:GLN:O     | 1:C:927:GLU:HG2   | 2.17                     | 0.44              |
| 1:C:3751:VAL:O    | 1:C:3756:LYS:NZ   | 2.51                     | 0.44              |
| 1:A:3003:LEU:HB2  | 1:A:3004:PRO:HD3  | 2.00                     | 0.44              |
| 1:A:3734:HIS:O    | 1:A:3736:GLU:HG3  | 2.17                     | 0.44              |
| 1:A:4253:GLU:HG3  | 1:A:4557:ARG:NH2  | 2.32                     | 0.44              |
| 1:B:1808:ARG:HB2  | 1:B:1854:PHE:CE1  | 2.53                     | 0.44              |
| 1:B:2650:ARG:NH1  | 1:B:2651:CYS:SG   | 2.90                     | 0.44              |
| 1:B:3823:LYS:HD3  | 1:B:3823:LYS:HA   | 1.76                     | 0.44              |
| 1:B:4238:CYS:HA   | 1:B:4989:MET:HE1  | 1.99                     | 0.44              |
| 1:B:4638:TYR:C    | 1:B:4641:PRO:HD2  | 2.42                     | 0.44              |
| 1:D:1943:LEU:HD13 | 1:D:2098:VAL:HG22 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3132:THR:HG23 | 1:D:3136:LEU:HD23 | 2.00                     | 0.44              |
| 1:C:534:ARG:HE    | 1:C:534:ARG:HB3   | 1.66                     | 0.44              |
| 1:C:1032:LYS:HG2  | 1:C:1036:ARG:NH1  | 2.33                     | 0.44              |
| 1:C:1808:ARG:HB2  | 1:C:1854:PHE:CE1  | 2.53                     | 0.44              |
| 1:C:2208:MET:SD   | 1:C:2250:MET:HE1  | 2.57                     | 0.44              |
| 1:C:2668:SER:C    | 1:C:2670:GLU:H    | 2.26                     | 0.44              |
| 1:C:2862:LEU:HD11 | 1:C:2865:VAL:HG13 | 2.00                     | 0.44              |
| 1:C:3980:LEU:HD13 | 1:C:3985:LEU:HD22 | 2.00                     | 0.44              |
| 1:A:1068:ARG:NH2  | 1:A:1071:ARG:HG3  | 2.32                     | 0.44              |
| 1:A:3036:LYS:O    | 1:A:3039:ILE:HG22 | 2.18                     | 0.44              |
| 2:G:23:VAL:HG22   | 2:G:47:LYS:HD3    | 1.99                     | 0.44              |
| 1:B:41:GLY:HA2    | 1:B:137:LEU:HD12  | 1.99                     | 0.44              |
| 1:B:870:ILE:HG12  | 1:B:1051:TYR:HE2  | 1.82                     | 0.44              |
| 1:B:957:LYS:HA    | 1:B:960:MET:HE2   | 2.00                     | 0.44              |
| 1:B:1451:GLY:HA3  | 1:B:1494:MET:HA   | 1.99                     | 0.44              |
| 1:B:1805:GLU:H    | 1:B:1805:GLU:CD   | 2.26                     | 0.44              |
| 1:B:2531:ARG:HG2  | 1:B:2585:THR:HG21 | 1.98                     | 0.44              |
| 1:B:2736:ASP:O    | 1:B:2738:ARG:NH1  | 2.51                     | 0.44              |
| 1:B:2782:ASP:N    | 1:B:2782:ASP:OD1  | 2.50                     | 0.44              |
| 1:B:3260:GLY:HA2  | 1:B:3325:ASN:ND2  | 2.33                     | 0.44              |
| 1:B:3367:LYS:HB2  | 1:B:3367:LYS:HE3  | 1.85                     | 0.44              |
| 1:B:3734:HIS:O    | 1:B:3736:GLU:HG3  | 2.17                     | 0.44              |
| 1:B:3989:VAL:HG11 | 1:B:4047:MET:HE2  | 1.98                     | 0.44              |
| 1:B:4253:GLU:HG3  | 1:B:4557:ARG:NH2  | 2.33                     | 0.44              |
| 1:B:5030:LYS:HA   | 1:B:5033:GLU:HG2  | 1.98                     | 0.44              |
| 1:D:336:PRO:HA    | 1:D:337:PRO:HD3   | 1.85                     | 0.44              |
| 1:D:1031:THR:HG22 | 1:D:1035:ASN:HD21 | 1.82                     | 0.44              |
| 1:D:1057:ASP:N    | 1:D:1057:ASP:OD1  | 2.48                     | 0.44              |
| 1:D:1270:LEU:HB2  | 1:D:1564:PHE:HB2  | 2.00                     | 0.44              |
| 1:D:2208:MET:SD   | 1:D:2250:MET:HE1  | 2.58                     | 0.44              |
| 1:D:2627:VAL:HA   | 1:D:2678:LEU:HD13 | 1.99                     | 0.44              |
| 1:D:3137:LEU:HD23 | 1:D:3137:LEU:HA   | 1.84                     | 0.44              |
| 1:D:3765:TYR:CD2  | 1:D:4753:HIS:HA   | 2.53                     | 0.44              |
| 1:D:3940:LYS:O    | 1:D:4002:LYS:NZ   | 2.36                     | 0.44              |
| 1:D:4735:GLU:H    | 1:D:4735:GLU:CD   | 2.25                     | 0.44              |
| 1:C:3734:HIS:O    | 1:C:3736:GLU:HG3  | 2.17                     | 0.44              |
| 1:C:4238:CYS:HA   | 1:C:4989:MET:HE1  | 1.99                     | 0.44              |
| 1:C:4240:ASP:OD1  | 1:C:4675:LYS:NZ   | 2.50                     | 0.44              |
| 1:A:1255:TYR:O    | 1:A:1275:ARG:NH1  | 2.51                     | 0.44              |
| 1:A:1808:ARG:HB2  | 1:A:1854:PHE:CE1  | 2.53                     | 0.44              |
| 1:B:341:TYR:CZ    | 1:B:392:ARG:HD3   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:475:GLN:NE2   | 1:B:528:SER:O     | 2.49                     | 0.44              |
| 1:B:866:HIS:HD2   | 1:B:941:MET:HE3   | 1.83                     | 0.44              |
| 1:B:1032:LYS:HG2  | 1:B:1036:ARG:NH1  | 2.33                     | 0.44              |
| 1:B:1255:TYR:O    | 1:B:1275:ARG:NH1  | 2.51                     | 0.44              |
| 1:B:4578:LEU:O    | 1:C:4879:MET:HB3  | 2.17                     | 0.44              |
| 1:D:341:TYR:CZ    | 1:D:392:ARG:HD3   | 2.53                     | 0.44              |
| 1:D:908:VAL:HG23  | 1:D:909:ASN:H     | 1.82                     | 0.44              |
| 1:D:1183:GLU:CD   | 1:D:1183:GLU:H    | 2.26                     | 0.44              |
| 1:D:3733:CYS:HB2  | 1:D:3803:SER:OG   | 2.18                     | 0.44              |
| 1:D:3735:LEU:HD12 | 1:D:3766:GLN:NE2  | 2.32                     | 0.44              |
| 1:C:1454:THR:OG1  | 1:C:1456:ASP:OD1  | 2.31                     | 0.44              |
| 1:C:1475:THR:HG23 | 1:C:1483:VAL:HG13 | 2.00                     | 0.44              |
| 1:C:4253:GLU:HG3  | 1:C:4557:ARG:NH2  | 2.33                     | 0.44              |
| 1:C:4586:PRO:HA   | 1:C:4629:TYR:CD1  | 2.53                     | 0.44              |
| 1:C:4689:THR:HG22 | 1:C:4732:PHE:CZ   | 2.52                     | 0.44              |
| 1:A:783:PHE:HB2   | 1:A:787:VAL:HG21  | 2.01                     | 0.43              |
| 1:A:1475:THR:HG23 | 1:A:1483:VAL:HG13 | 2.00                     | 0.43              |
| 1:A:3260:GLY:HA2  | 1:A:3325:ASN:ND2  | 2.33                     | 0.43              |
| 1:A:3733:CYS:HB2  | 1:A:3803:SER:OG   | 2.18                     | 0.43              |
| 1:A:3751:VAL:O    | 1:A:3756:LYS:NZ   | 2.51                     | 0.43              |
| 2:H:3:GLN:HB3     | 2:H:5:GLU:OE2     | 2.17                     | 0.43              |
| 1:B:747:CYS:HB3   | 1:B:808:TYR:CE2   | 2.53                     | 0.43              |
| 1:B:923:GLN:O     | 1:B:927:GLU:HG2   | 2.17                     | 0.43              |
| 1:B:3980:LEU:HD13 | 1:B:3985:LEU:HD22 | 2.00                     | 0.43              |
| 1:B:4586:PRO:HA   | 1:B:4629:TYR:CD1  | 2.53                     | 0.43              |
| 1:D:15:ARG:HD2    | 1:D:98:HIS:HB3    | 2.00                     | 0.43              |
| 1:D:1808:ARG:HB2  | 1:D:1854:PHE:CE1  | 2.53                     | 0.43              |
| 1:D:2615:ARG:HG2  | 1:D:2664:PHE:CE1  | 2.53                     | 0.43              |
| 1:D:3734:HIS:O    | 1:D:3736:GLU:HG3  | 2.17                     | 0.43              |
| 1:C:941:MET:SD    | 1:C:1051:TYR:CE1  | 3.11                     | 0.43              |
| 1:C:1008:SER:HB3  | 1:C:1017:ARG:HB3  | 2.00                     | 0.43              |
| 1:C:1018:ASN:HB3  | 1:C:1021:LEU:HB2  | 2.00                     | 0.43              |
| 1:C:1128:ARG:H    | 1:C:1128:ARG:NE   | 2.16                     | 0.43              |
| 1:C:1183:GLU:H    | 1:C:1183:GLU:CD   | 2.26                     | 0.43              |
| 1:C:1492:CYS:SG   | 1:C:1494:MET:HG3  | 2.57                     | 0.43              |
| 1:C:3733:CYS:HB2  | 1:C:3803:SER:OG   | 2.18                     | 0.43              |
| 1:C:3765:TYR:CD2  | 1:C:4753:HIS:HA   | 2.53                     | 0.43              |
| 1:A:747:CYS:HB3   | 1:A:808:TYR:CE2   | 2.53                     | 0.43              |
| 1:A:2862:LEU:HD11 | 1:A:2865:VAL:HG13 | 2.00                     | 0.43              |
| 1:B:140:ASP:OD1   | 1:B:142:THR:OG1   | 2.30                     | 0.43              |
| 1:B:483:MET:HE2   | 1:B:483:MET:N     | 2.32                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1943:LEU:HD13 | 1:B:2098:VAL:HG22 | 2.00                     | 0.43              |
| 1:B:4655:PHE:N    | 1:B:4796:MET:HE1  | 2.33                     | 0.43              |
| 1:D:162:LYS:HE3   | 1:C:3987:ASP:OD2  | 2.18                     | 0.43              |
| 1:D:745:SER:HB2   | 1:D:758:ARG:HB2   | 2.00                     | 0.43              |
| 1:D:957:LYS:HA    | 1:D:960:MET:HE2   | 2.00                     | 0.43              |
| 1:D:1018:ASN:HB3  | 1:D:1021:LEU:HB2  | 2.00                     | 0.43              |
| 1:D:2502:MET:H    | 1:D:2502:MET:HG2  | 1.57                     | 0.43              |
| 1:D:2736:ASP:O    | 1:D:2738:ARG:NH1  | 2.51                     | 0.43              |
| 1:D:3194:LEU:HD12 | 1:D:3194:LEU:HA   | 1.76                     | 0.43              |
| 1:C:15:ARG:HD2    | 1:C:98:HIS:HB3    | 2.00                     | 0.43              |
| 1:C:1451:GLY:HA3  | 1:C:1494:MET:HA   | 1.99                     | 0.43              |
| 1:C:2531:ARG:HG2  | 1:C:2585:THR:HG21 | 1.98                     | 0.43              |
| 1:C:2758:PHE:O    | 1:C:2762:THR:HG23 | 2.18                     | 0.43              |
| 1:C:3266:MET:HE3  | 1:C:3266:MET:HB2  | 1.92                     | 0.43              |
| 1:C:3765:TYR:CE2  | 1:C:4753:HIS:HA   | 2.54                     | 0.43              |
| 1:A:41:GLY:HA2    | 1:A:137:LEU:HD12  | 1.99                     | 0.43              |
| 1:A:1018:ASN:HB3  | 1:A:1021:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:1690:ASP:OD2  | 1:A:1693:GLN:NE2  | 2.52                     | 0.43              |
| 1:A:4138:ASP:OD1  | 1:A:4138:ASP:N    | 2.51                     | 0.43              |
| 1:A:4655:PHE:N    | 1:A:4796:MET:HE1  | 2.33                     | 0.43              |
| 2:E:3:GLN:HE21    | 2:E:5:GLU:HG2     | 1.82                     | 0.43              |
| 2:E:49:MET:SD     | 2:E:52:LYS:HE2    | 2.59                     | 0.43              |
| 1:B:306:LYS:HB2   | 1:B:306:LYS:HE3   | 1.83                     | 0.43              |
| 1:B:569:ILE:HD13  | 1:B:569:ILE:HA    | 1.89                     | 0.43              |
| 1:B:783:PHE:HB2   | 1:B:787:VAL:HG21  | 2.00                     | 0.43              |
| 1:B:1128:ARG:H    | 1:B:1128:ARG:NE   | 2.16                     | 0.43              |
| 1:B:2862:LEU:HD11 | 1:B:2865:VAL:HG13 | 2.00                     | 0.43              |
| 1:B:3633:VAL:HG13 | 1:B:3637:ARG:HH21 | 1.83                     | 0.43              |
| 1:B:3765:TYR:CD2  | 1:B:4753:HIS:HA   | 2.53                     | 0.43              |
| 1:D:941:MET:SD    | 1:D:1051:TYR:CE1  | 3.11                     | 0.43              |
| 1:D:1032:LYS:HG2  | 1:D:1036:ARG:NH1  | 2.33                     | 0.43              |
| 1:D:3266:MET:HE3  | 1:D:3266:MET:HB2  | 1.92                     | 0.43              |
| 1:D:4238:CYS:HA   | 1:D:4989:MET:HE1  | 1.99                     | 0.43              |
| 1:C:274:LEU:HB3   | 1:C:339:ILE:HD12  | 1.99                     | 0.43              |
| 1:C:483:MET:N     | 1:C:483:MET:HE2   | 2.32                     | 0.43              |
| 1:C:745:SER:HB2   | 1:C:758:ARG:HB2   | 2.00                     | 0.43              |
| 1:C:957:LYS:HA    | 1:C:960:MET:HE2   | 2.00                     | 0.43              |
| 1:C:4735:GLU:CD   | 1:C:4735:GLU:H    | 2.25                     | 0.43              |
| 1:A:384:MET:H     | 1:A:384:MET:CE    | 2.32                     | 0.43              |
| 1:A:1031:THR:HG22 | 1:A:1035:ASN:HD21 | 1.82                     | 0.43              |
| 1:A:1998:PHE:C    | 1:A:1999:ARG:HD2  | 2.44                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2101:MET:HE2  | 1:A:2102:VAL:HG23 | 2.00                     | 0.43              |
| 1:A:4238:CYS:HA   | 1:A:4989:MET:HE1  | 1.99                     | 0.43              |
| 1:B:194:SER:OG    | 1:B:195:PHE:N     | 2.50                     | 0.43              |
| 1:B:384:MET:H     | 1:B:384:MET:CE    | 2.32                     | 0.43              |
| 1:B:663:TYR:OH    | 1:B:665:GLU:OE2   | 2.24                     | 0.43              |
| 1:B:1018:ASN:HB3  | 1:B:1021:LEU:HB2  | 2.00                     | 0.43              |
| 1:B:1070:ASP:O    | 1:B:1071:ARG:NH2  | 2.52                     | 0.43              |
| 1:B:1183:GLU:H    | 1:B:1183:GLU:CD   | 2.26                     | 0.43              |
| 1:B:2905:LEU:HD23 | 1:B:2905:LEU:HA   | 1.88                     | 0.43              |
| 1:B:3751:VAL:O    | 1:B:3756:LYS:NZ   | 2.51                     | 0.43              |
| 1:D:1229:ASN:C    | 1:D:1230:MET:HG2  | 2.41                     | 0.43              |
| 1:D:1253:PRO:HG2  | 1:D:1254:HIS:CD2  | 2.53                     | 0.43              |
| 1:D:2101:MET:HE2  | 1:D:2102:VAL:HG23 | 2.00                     | 0.43              |
| 1:D:2186:MET:HG2  | 1:D:2186:MET:H    | 1.70                     | 0.43              |
| 1:D:2574:HIS:CD2  | 1:D:2574:HIS:H    | 2.35                     | 0.43              |
| 1:C:233:ILE:O     | 1:C:257:ARG:NH1   | 2.49                     | 0.43              |
| 1:C:1823:GLY:O    | 1:C:1825:HIS:ND1  | 2.48                     | 0.43              |
| 1:C:2736:ASP:O    | 1:C:2738:ARG:NH1  | 2.51                     | 0.43              |
| 1:C:2821:TRP:HD1  | 1:C:2939:ARG:HA   | 1.84                     | 0.43              |
| 1:C:3260:GLY:HA2  | 1:C:3325:ASN:ND2  | 2.33                     | 0.43              |
| 1:A:80:GLU:HG3    | 1:D:3935:TRP:O    | 2.19                     | 0.43              |
| 1:A:484:LEU:HD12  | 1:A:484:LEU:HA    | 1.79                     | 0.43              |
| 1:A:1253:PRO:HG2  | 1:A:1254:HIS:CD2  | 2.53                     | 0.43              |
| 1:A:1270:LEU:HB2  | 1:A:1564:PHE:HB2  | 2.00                     | 0.43              |
| 1:A:1805:GLU:CD   | 1:A:1805:GLU:H    | 2.26                     | 0.43              |
| 1:A:2336:ARG:HG2  | 1:A:2435:ARG:HD2  | 2.00                     | 0.43              |
| 1:A:2355:ARG:NH2  | 1:A:2449:GLU:OE2  | 2.47                     | 0.43              |
| 1:A:3367:LYS:HE3  | 1:A:3367:LYS:HB2  | 1.85                     | 0.43              |
| 1:A:3765:TYR:CE2  | 1:A:4753:HIS:HA   | 2.54                     | 0.43              |
| 1:A:4822:THR:HG21 | 1:B:4839:MET:HG3  | 2.00                     | 0.43              |
| 2:E:84:ALA:O      | 2:E:93:PRO:HB3    | 2.19                     | 0.43              |
| 2:H:79:ASP:OD2    | 2:H:79:ASP:C      | 2.61                     | 0.43              |
| 2:H:84:ALA:O      | 2:H:93:PRO:HB3    | 2.19                     | 0.43              |
| 2:G:3:GLN:HB3     | 2:G:5:GLU:OE2     | 2.18                     | 0.43              |
| 1:B:1008:SER:HB3  | 1:B:1017:ARG:HB3  | 2.00                     | 0.43              |
| 1:B:2758:PHE:O    | 1:B:2762:THR:HG23 | 2.18                     | 0.43              |
| 1:D:233:ILE:O     | 1:D:257:ARG:NH1   | 2.49                     | 0.43              |
| 1:D:747:CYS:HB3   | 1:D:808:TYR:CE2   | 2.53                     | 0.43              |
| 1:D:1071:ARG:HA   | 1:D:1071:ARG:HE   | 1.82                     | 0.43              |
| 1:D:1451:GLY:HA3  | 1:D:1494:MET:HA   | 1.99                     | 0.43              |
| 1:D:1998:PHE:C    | 1:D:1999:ARG:HD2  | 2.44                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2821:TRP:HD1  | 1:D:2939:ARG:HA   | 1.84                     | 0.43              |
| 1:D:3453:ARG:NH2  | 1:D:3456:GLN:HB3  | 2.34                     | 0.43              |
| 1:D:3604:TYR:O    | 1:D:3608:GLN:HG2  | 2.19                     | 0.43              |
| 1:D:4138:ASP:OD1  | 1:D:4138:ASP:N    | 2.51                     | 0.43              |
| 1:C:747:CYS:HB3   | 1:C:808:TYR:CE2   | 2.53                     | 0.43              |
| 1:C:783:PHE:HB2   | 1:C:787:VAL:HG21  | 2.00                     | 0.43              |
| 1:C:866:HIS:HD2   | 1:C:941:MET:HE3   | 1.83                     | 0.43              |
| 1:C:3036:LYS:O    | 1:C:3039:ILE:HG22 | 2.18                     | 0.43              |
| 1:C:3696:ASP:OD2  | 1:C:3773:ARG:NE   | 2.47                     | 0.43              |
| 1:C:3735:LEU:HD12 | 1:C:3766:GLN:NE2  | 2.32                     | 0.43              |
| 1:A:2641:LEU:HD23 | 1:A:2641:LEU:HA   | 1.88                     | 0.43              |
| 1:A:3959:LYS:NZ   | 1:A:4022:ASP:OD2  | 2.40                     | 0.43              |
| 1:A:3996:PHE:CD2  | 1:A:4020:GLN:HG2  | 2.53                     | 0.43              |
| 2:G:84:ALA:O      | 2:G:93:PRO:HB3    | 2.19                     | 0.43              |
| 1:B:941:MET:SD    | 1:B:1051:TYR:CE1  | 3.11                     | 0.43              |
| 1:B:1297:PHE:CE2  | 1:B:1525:GLY:HA2  | 2.54                     | 0.43              |
| 1:B:2208:MET:SD   | 1:B:2250:MET:HE1  | 2.57                     | 0.43              |
| 1:B:2224:ARG:HG2  | 1:B:2225:PHE:CE2  | 2.53                     | 0.43              |
| 1:B:2785:LEU:C    | 1:B:2786:LYS:HG3  | 2.44                     | 0.43              |
| 1:B:3132:THR:HG23 | 1:B:3136:LEU:HD23 | 2.00                     | 0.43              |
| 1:B:3288:GLY:HA2  | 1:B:3303:PRO:HB3  | 2.01                     | 0.43              |
| 1:D:274:LEU:HB3   | 1:D:339:ILE:HD12  | 1.99                     | 0.43              |
| 1:D:1147:ASP:HB3  | 1:D:1164:LEU:HD11 | 2.00                     | 0.43              |
| 1:D:3823:LYS:HD3  | 1:D:3823:LYS:HA   | 1.76                     | 0.43              |
| 1:C:1070:ASP:O    | 1:C:1071:ARG:NH2  | 2.52                     | 0.43              |
| 1:C:1168:VAL:HG11 | 1:C:1176:GLU:HG2  | 1.99                     | 0.43              |
| 1:C:1447:CYS:HB3  | 1:C:1555:LEU:HB3  | 2.00                     | 0.43              |
| 1:C:2122:SER:O    | 1:C:2126:ARG:HG3  | 2.18                     | 0.43              |
| 1:C:3570:ARG:HB2  | 1:C:3570:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:15:ARG:HD2    | 1:A:98:HIS:HB3    | 2.01                     | 0.43              |
| 1:A:274:LEU:HB3   | 1:A:339:ILE:HD12  | 1.99                     | 0.43              |
| 1:A:1032:LYS:HG2  | 1:A:1036:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:1183:GLU:CD   | 1:A:1183:GLU:H    | 2.26                     | 0.43              |
| 1:A:1447:CYS:HB3  | 1:A:1555:LEU:HB3  | 2.00                     | 0.43              |
| 1:A:2224:ARG:HG2  | 1:A:2225:PHE:CE2  | 2.53                     | 0.43              |
| 1:A:2668:SER:C    | 1:A:2670:GLU:H    | 2.26                     | 0.43              |
| 1:A:3395:ARG:HD2  | 1:A:3454:GLU:OE2  | 2.19                     | 0.43              |
| 2:F:79:ASP:OD2    | 2:F:79:ASP:C      | 2.61                     | 0.43              |
| 1:B:3733:CYS:HB2  | 1:B:3803:SER:OG   | 2.18                     | 0.43              |
| 1:B:4240:ASP:OD1  | 1:B:4675:LYS:NZ   | 2.50                     | 0.43              |
| 1:D:2336:ARG:HG2  | 1:D:2435:ARG:HD2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3765:TYR:CE2  | 1:D:4753:HIS:HA   | 2.54                     | 0.43              |
| 1:D:3996:PHE:CD2  | 1:D:4020:GLN:HG2  | 2.53                     | 0.43              |
| 1:D:4026:MET:HE2  | 1:D:4026:MET:HB3  | 1.80                     | 0.43              |
| 1:C:365:LYS:HE3   | 1:C:365:LYS:HB3   | 1.81                     | 0.43              |
| 1:C:1690:ASP:OD2  | 1:C:1693:GLN:NE2  | 2.52                     | 0.43              |
| 1:C:2224:ARG:HG2  | 1:C:2225:PHE:CE2  | 2.53                     | 0.43              |
| 1:C:2881:ASN:HA   | 1:C:2884:ASN:HD21 | 1.84                     | 0.43              |
| 1:C:3996:PHE:CD2  | 1:C:4020:GLN:HG2  | 2.53                     | 0.43              |
| 1:A:1943:LEU:HD13 | 1:A:2098:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:2736:ASP:O    | 1:A:2738:ARG:NH1  | 2.51                     | 0.43              |
| 2:E:23:VAL:HG22   | 2:E:47:LYS:HD3    | 2.00                     | 0.43              |
| 2:G:44:LYS:HB3    | 2:G:44:LYS:HE3    | 1.78                     | 0.43              |
| 2:G:88:PRO:HB2    | 1:C:1680:ARG:NH1  | 2.31                     | 0.43              |
| 1:B:3230:LEU:HD23 | 1:B:3230:LEU:H    | 1.84                     | 0.43              |
| 1:B:3765:TYR:CE2  | 1:B:4753:HIS:HA   | 2.54                     | 0.43              |
| 1:B:3935:TRP:CE2  | 1:C:77:ALA:HB2    | 2.53                     | 0.43              |
| 1:D:11:VAL:HG11   | 1:D:164:ARG:NH1   | 2.33                     | 0.43              |
| 1:D:1070:ASP:O    | 1:D:1071:ARG:NH2  | 2.52                     | 0.43              |
| 1:D:1128:ARG:H    | 1:D:1128:ARG:NE   | 2.16                     | 0.43              |
| 1:D:1168:VAL:HG11 | 1:D:1176:GLU:HG2  | 1.99                     | 0.43              |
| 1:D:1668:ARG:HG3  | 1:D:1671:ARG:HH21 | 1.82                     | 0.43              |
| 1:D:1748:PHE:HB2  | 1:D:1758:ARG:HE   | 1.84                     | 0.43              |
| 1:D:1864:LYS:NZ   | 1:D:1871:PHE:O    | 2.49                     | 0.43              |
| 1:D:2751:LEU:HD13 | 1:D:2823:ILE:HD13 | 2.01                     | 0.43              |
| 1:D:4966:ASP:OD2  | 1:D:4966:ASP:C    | 2.62                     | 0.43              |
| 1:A:458:GLU:H     | 1:A:458:GLU:HG3   | 1.69                     | 0.43              |
| 1:A:745:SER:HB2   | 1:A:758:ARG:HB2   | 2.00                     | 0.43              |
| 1:A:1020:ARG:O    | 1:A:1022:VAL:N    | 2.49                     | 0.43              |
| 1:A:1070:ASP:O    | 1:A:1071:ARG:NH2  | 2.52                     | 0.43              |
| 1:A:1128:ARG:H    | 1:A:1128:ARG:NE   | 2.16                     | 0.43              |
| 1:A:1748:PHE:HB2  | 1:A:1758:ARG:HE   | 1.84                     | 0.43              |
| 1:A:2318:TYR:CZ   | 1:A:2395:PRO:HD3  | 2.54                     | 0.43              |
| 1:A:2758:PHE:O    | 1:A:2762:THR:HG23 | 2.18                     | 0.43              |
| 1:A:2785:LEU:C    | 1:A:2786:LYS:HG3  | 2.44                     | 0.43              |
| 1:A:3453:ARG:NH2  | 1:A:3456:GLN:HB3  | 2.34                     | 0.43              |
| 1:A:3455:GLU:OE2  | 1:A:3508:SER:OG   | 2.36                     | 0.43              |
| 1:A:3604:TYR:O    | 1:A:3608:GLN:HG2  | 2.19                     | 0.43              |
| 1:A:3980:LEU:HD13 | 1:A:3985:LEU:HD22 | 2.00                     | 0.43              |
| 2:F:11:ASP:OD1    | 2:F:11:ASP:C      | 2.61                     | 0.43              |
| 1:B:274:LEU:HB3   | 1:B:339:ILE:HD12  | 1.99                     | 0.43              |
| 1:B:927:GLU:O     | 1:B:931:THR:HG23  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2318:TYR:CZ   | 1:B:2395:PRO:HD3  | 2.54                     | 0.43              |
| 1:D:384:MET:H     | 1:D:384:MET:CE    | 2.32                     | 0.43              |
| 1:D:2437:ALA:HB2  | 1:D:2509:VAL:HG22 | 2.01                     | 0.43              |
| 1:D:3230:LEU:H    | 1:D:3230:LEU:HD23 | 1.84                     | 0.43              |
| 1:D:3395:ARG:HD2  | 1:D:3454:GLU:OE2  | 2.19                     | 0.43              |
| 1:C:1147:ASP:HB3  | 1:C:1164:LEU:HD11 | 2.00                     | 0.43              |
| 1:C:1805:GLU:CD   | 1:C:1805:GLU:H    | 2.26                     | 0.43              |
| 1:C:3288:GLY:HA2  | 1:C:3303:PRO:HB3  | 2.01                     | 0.43              |
| 1:A:306:LYS:HB2   | 1:A:306:LYS:HE3   | 1.83                     | 0.43              |
| 1:A:941:MET:SD    | 1:A:1051:TYR:CE1  | 3.11                     | 0.43              |
| 1:A:1297:PHE:CE2  | 1:A:1525:GLY:HA2  | 2.54                     | 0.43              |
| 1:A:1992:ALA:HB1  | 1:A:1996:ARG:NH1  | 2.34                     | 0.43              |
| 1:A:2178:MET:HE2  | 1:A:2178:MET:HB2  | 1.85                     | 0.43              |
| 1:A:2437:ALA:HB2  | 1:A:2509:VAL:HG22 | 2.01                     | 0.43              |
| 1:A:2615:ARG:HG2  | 1:A:2664:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:2754:PHE:HE2  | 1:A:2813:LEU:HD11 | 1.84                     | 0.43              |
| 1:A:3570:ARG:HB2  | 1:A:3570:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:3696:ASP:OD2  | 1:A:3773:ARG:NE   | 2.47                     | 0.43              |
| 1:A:4183:ILE:HG12 | 1:A:4193:ILE:HD13 | 2.00                     | 0.43              |
| 1:B:15:ARG:HD2    | 1:B:98:HIS:HB3    | 2.01                     | 0.43              |
| 1:B:2821:TRP:HD1  | 1:B:2939:ARG:HA   | 1.84                     | 0.43              |
| 1:B:3570:ARG:HB2  | 1:B:3570:ARG:NH1  | 2.34                     | 0.43              |
| 1:B:4138:ASP:OD1  | 1:B:4138:ASP:N    | 2.51                     | 0.43              |
| 1:B:4966:ASP:OD2  | 1:B:4966:ASP:C    | 2.62                     | 0.43              |
| 1:D:1008:SER:HB3  | 1:D:1017:ARG:HB3  | 2.00                     | 0.43              |
| 1:D:2122:SER:O    | 1:D:2126:ARG:HG3  | 2.18                     | 0.43              |
| 1:D:2668:SER:C    | 1:D:2670:GLU:H    | 2.26                     | 0.43              |
| 1:D:4240:ASP:OD1  | 1:D:4675:LYS:NZ   | 2.50                     | 0.43              |
| 1:C:2090:LYS:HZ2  | 1:C:2092:GLN:HG3  | 1.83                     | 0.43              |
| 1:C:2754:PHE:HE2  | 1:C:2813:LEU:HD11 | 1.84                     | 0.43              |
| 1:C:3940:LYS:O    | 1:C:4002:LYS:NZ   | 2.36                     | 0.43              |
| 1:A:2464:ASP:OD1  | 1:A:2465:ASP:N    | 2.52                     | 0.42              |
| 1:A:2821:TRP:HD1  | 1:A:2939:ARG:HA   | 1.84                     | 0.42              |
| 1:A:3230:LEU:HD23 | 1:A:3230:LEU:H    | 1.84                     | 0.42              |
| 2:H:44:LYS:HE3    | 2:H:44:LYS:HB3    | 1.78                     | 0.42              |
| 1:B:1447:CYS:HB3  | 1:B:1555:LEU:HB3  | 2.00                     | 0.42              |
| 1:B:2751:LEU:HD13 | 1:B:2823:ILE:HD13 | 2.01                     | 0.42              |
| 1:B:2754:PHE:HE2  | 1:B:2813:LEU:HD11 | 1.84                     | 0.42              |
| 1:B:4183:ILE:HG12 | 1:B:4193:ILE:HD13 | 2.00                     | 0.42              |
| 1:D:194:SER:OG    | 1:D:195:PHE:N     | 2.50                     | 0.42              |
| 1:D:1992:ALA:HB1  | 1:D:1996:ARG:NH1  | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3570:ARG:HB2  | 1:D:3570:ARG:NH1  | 2.33                     | 0.42              |
| 1:D:4934:GLY:HA3  | 1:C:4937:ILE:HG12 | 2.01                     | 0.42              |
| 1:C:11:VAL:HG11   | 1:C:164:ARG:NH1   | 2.33                     | 0.42              |
| 1:C:358:THR:HG21  | 1:C:382:GLY:HA2   | 2.02                     | 0.42              |
| 1:C:1998:PHE:C    | 1:C:1999:ARG:HD2  | 2.44                     | 0.42              |
| 1:C:2101:MET:HE2  | 1:C:2102:VAL:HG23 | 2.00                     | 0.42              |
| 1:C:2751:LEU:HD13 | 1:C:2823:ILE:HD13 | 2.01                     | 0.42              |
| 1:C:2785:LEU:C    | 1:C:2786:LYS:HG3  | 2.44                     | 0.42              |
| 1:C:3455:GLU:OE2  | 1:C:3508:SER:OG   | 2.36                     | 0.42              |
| 1:C:3666:ASP:OD2  | 1:C:3666:ASP:N    | 2.45                     | 0.42              |
| 1:A:891:TRP:CZ2   | 1:A:899:ASP:HA    | 2.55                     | 0.42              |
| 1:A:1147:ASP:HB3  | 1:A:1164:LEU:HD11 | 2.00                     | 0.42              |
| 1:A:3233:PRO:HD2  | 1:A:3239:MET:HG2  | 2.01                     | 0.42              |
| 1:A:3461:GLN:HG2  | 1:A:3462:ASN:ND2  | 2.34                     | 0.42              |
| 1:A:4026:MET:HE2  | 1:A:4026:MET:HB3  | 1.80                     | 0.42              |
| 2:E:11:ASP:OD1    | 2:E:11:ASP:C      | 2.62                     | 0.42              |
| 2:G:13:ARG:HB3    | 2:G:13:ARG:NH1    | 2.34                     | 0.42              |
| 1:B:358:THR:HG21  | 1:B:382:GLY:HA2   | 2.01                     | 0.42              |
| 1:B:1081:TYR:CD1  | 1:B:1230:MET:HE1  | 2.55                     | 0.42              |
| 1:B:1147:ASP:HB3  | 1:B:1164:LEU:HD11 | 2.00                     | 0.42              |
| 1:B:2464:ASP:OD1  | 1:B:2465:ASP:N    | 2.52                     | 0.42              |
| 1:B:2677:LYS:HE2  | 1:B:2677:LYS:HB3  | 1.79                     | 0.42              |
| 1:B:2888:ARG:O    | 1:B:2892:GLN:HG2  | 2.19                     | 0.42              |
| 1:B:3996:PHE:CD2  | 1:B:4020:GLN:HG2  | 2.53                     | 0.42              |
| 1:D:783:PHE:HB2   | 1:D:787:VAL:HG21  | 2.00                     | 0.42              |
| 1:D:1575:LEU:HA   | 1:D:1575:LEU:HD23 | 1.81                     | 0.42              |
| 1:D:2758:PHE:O    | 1:D:2762:THR:HG23 | 2.18                     | 0.42              |
| 1:D:3288:GLY:HA2  | 1:D:3303:PRO:HB3  | 2.01                     | 0.42              |
| 1:D:3554:GLN:HE21 | 1:D:3593:VAL:HG21 | 1.84                     | 0.42              |
| 1:D:3980:LEU:HD13 | 1:D:3985:LEU:HD22 | 2.00                     | 0.42              |
| 1:C:1260:MET:HE3  | 1:C:1260:MET:HB3  | 1.90                     | 0.42              |
| 1:C:3132:THR:HG23 | 1:C:3136:LEU:HD23 | 2.00                     | 0.42              |
| 1:C:3395:ARG:HD2  | 1:C:3454:GLU:OE2  | 2.19                     | 0.42              |
| 1:C:4655:PHE:N    | 1:C:4796:MET:HE1  | 2.33                     | 0.42              |
| 1:A:669:ASP:OD1   | 1:A:790:ARG:NH2   | 2.52                     | 0.42              |
| 1:A:1008:SER:HB3  | 1:A:1017:ARG:HB3  | 2.00                     | 0.42              |
| 1:A:2222:GLU:O    | 1:A:2224:ARG:NH2  | 2.32                     | 0.42              |
| 1:B:891:TRP:CZ2   | 1:B:899:ASP:HA    | 2.55                     | 0.42              |
| 1:B:1172:ASP:OD1  | 1:B:1172:ASP:N    | 2.37                     | 0.42              |
| 1:B:1998:PHE:C    | 1:B:1999:ARG:HD2  | 2.44                     | 0.42              |
| 1:B:2122:SER:O    | 1:B:2126:ARG:HG3  | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2538:THR:HG23 | 1:B:2541:PHE:H    | 1.85                     | 0.42              |
| 1:B:2582:MET:CE   | 1:B:2610:LEU:HD13 | 2.49                     | 0.42              |
| 1:B:3233:PRO:HD2  | 1:B:3239:MET:HG2  | 2.01                     | 0.42              |
| 1:B:3467:MET:HE2  | 1:C:1174:GLY:N    | 2.34                     | 0.42              |
| 1:B:4885:PHE:O    | 1:B:4889:VAL:HG22 | 2.20                     | 0.42              |
| 1:B:4937:ILE:HG12 | 1:C:4934:GLY:HA3  | 2.01                     | 0.42              |
| 1:D:365:LYS:HB3   | 1:D:365:LYS:HE3   | 1.81                     | 0.42              |
| 1:D:866:HIS:HD2   | 1:D:941:MET:HE3   | 1.83                     | 0.42              |
| 1:D:2318:TYR:CZ   | 1:D:2395:PRO:HD3  | 2.54                     | 0.42              |
| 1:D:2765:LYS:NZ   | 1:D:2860:PRO:HA   | 2.34                     | 0.42              |
| 1:D:2782:ASP:N    | 1:D:2782:ASP:OD1  | 2.50                     | 0.42              |
| 1:D:3347:SER:HA   | 1:D:3418:ASN:ND2  | 2.35                     | 0.42              |
| 1:D:3666:ASP:OD2  | 1:D:3666:ASP:N    | 2.45                     | 0.42              |
| 1:C:1152:MET:HE1  | 1:C:1163:THR:HG23 | 2.01                     | 0.42              |
| 1:C:3230:LEU:HD23 | 1:C:3230:LEU:H    | 1.84                     | 0.42              |
| 1:C:4885:PHE:O    | 1:C:4889:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:11:VAL:HG11   | 1:A:164:ARG:NH1   | 2.33                     | 0.42              |
| 1:A:475:GLN:NE2   | 1:A:528:SER:O     | 2.49                     | 0.42              |
| 1:A:901:LYS:HD2   | 1:A:901:LYS:HA    | 1.84                     | 0.42              |
| 1:A:3288:GLY:HA2  | 1:A:3303:PRO:HB3  | 2.01                     | 0.42              |
| 1:A:3941:ASP:OD1  | 1:A:3941:ASP:N    | 2.53                     | 0.42              |
| 1:A:4938:ASP:OD1  | 1:D:4944:ARG:NH2  | 2.51                     | 0.42              |
| 2:E:13:ARG:HB3    | 2:E:13:ARG:NH1    | 2.34                     | 0.42              |
| 1:B:892:THR:C     | 1:B:907:LEU:HD12  | 2.45                     | 0.42              |
| 1:B:3453:ARG:NH2  | 1:B:3456:GLN:HB3  | 2.34                     | 0.42              |
| 1:B:4244:GLU:CD   | 1:B:4668:LEU:HD22 | 2.45                     | 0.42              |
| 1:B:4904:PRO:CB   | 1:B:4913:ARG:HG2  | 2.45                     | 0.42              |
| 1:D:416:LYS:HE3   | 1:D:416:LYS:HB2   | 1.84                     | 0.42              |
| 1:D:1025:ARG:H    | 1:D:1025:ARG:CD   | 2.25                     | 0.42              |
| 1:D:3376:GLU:OE1  | 1:D:3448:SER:OG   | 2.28                     | 0.42              |
| 1:D:3461:GLN:HG2  | 1:D:3462:ASN:ND2  | 2.34                     | 0.42              |
| 1:D:4244:GLU:CD   | 1:D:4668:LEU:HD22 | 2.45                     | 0.42              |
| 1:C:194:SER:OG    | 1:C:195:PHE:N     | 2.50                     | 0.42              |
| 1:C:384:MET:H     | 1:C:384:MET:CE    | 2.32                     | 0.42              |
| 1:C:416:LYS:HE3   | 1:C:416:LYS:HB2   | 1.84                     | 0.42              |
| 1:C:2037:ASP:OD2  | 1:C:2038:LEU:N    | 2.53                     | 0.42              |
| 1:C:2384:ILE:O    | 1:C:2387:SER:OG   | 2.26                     | 0.42              |
| 1:C:2464:ASP:OD1  | 1:C:2465:ASP:N    | 2.52                     | 0.42              |
| 1:C:2538:THR:HG23 | 1:C:2541:PHE:H    | 1.85                     | 0.42              |
| 1:C:2582:MET:CE   | 1:C:2610:LEU:HD13 | 2.49                     | 0.42              |
| 1:A:273:HIS:CE1   | 1:A:334:MET:HB3   | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:358:THR:HG21  | 1:A:382:GLY:HA2   | 2.01                     | 0.42              |
| 1:A:1152:MET:HE1  | 1:A:1163:THR:HG23 | 2.01                     | 0.42              |
| 1:A:3376:GLU:OE1  | 1:A:3448:SER:OG   | 2.28                     | 0.42              |
| 1:A:3465:ASN:OD1  | 1:A:3467:MET:N    | 2.34                     | 0.42              |
| 1:A:4695:ASP:OD1  | 1:A:4695:ASP:N    | 2.35                     | 0.42              |
| 2:H:13:ARG:NH1    | 2:H:13:ARG:HB3    | 2.35                     | 0.42              |
| 2:G:11:ASP:OD1    | 2:G:11:ASP:C      | 2.62                     | 0.42              |
| 1:B:11:VAL:HG11   | 1:B:164:ARG:NH1   | 2.33                     | 0.42              |
| 1:B:745:SER:HB2   | 1:B:758:ARG:HB2   | 2.00                     | 0.42              |
| 1:B:2209:GLU:HA   | 1:B:2212:VAL:HG22 | 2.02                     | 0.42              |
| 1:B:2711:PRO:HA   | 1:B:2712:PRO:HD3  | 1.93                     | 0.42              |
| 1:B:3395:ARG:HD2  | 1:B:3454:GLU:OE2  | 2.19                     | 0.42              |
| 1:B:3554:GLN:HE21 | 1:B:3593:VAL:HG21 | 1.84                     | 0.42              |
| 1:B:3996:PHE:O    | 1:B:4000:MET:HG3  | 2.20                     | 0.42              |
| 1:B:4066:LEU:HA   | 1:B:4066:LEU:HD23 | 1.81                     | 0.42              |
| 1:D:77:ALA:HB2    | 1:C:3935:TRP:CE2  | 2.55                     | 0.42              |
| 1:D:1447:CYS:HB3  | 1:D:1555:LEU:HB3  | 2.00                     | 0.42              |
| 1:D:2785:LEU:C    | 1:D:2786:LYS:HG3  | 2.44                     | 0.42              |
| 1:D:4066:LEU:HD23 | 1:D:4066:LEU:HA   | 1.81                     | 0.42              |
| 1:C:1081:TYR:CD1  | 1:C:1230:MET:HE1  | 2.55                     | 0.42              |
| 1:C:1943:LEU:HD13 | 1:C:2098:VAL:HG22 | 2.00                     | 0.42              |
| 1:C:3347:SER:HA   | 1:C:3418:ASN:ND2  | 2.35                     | 0.42              |
| 1:C:3554:GLN:HE21 | 1:C:3593:VAL:HG21 | 1.85                     | 0.42              |
| 1:C:3604:TYR:O    | 1:C:3608:GLN:HG2  | 2.18                     | 0.42              |
| 1:A:2711:PRO:HA   | 1:A:2712:PRO:HD3  | 1.93                     | 0.42              |
| 1:A:2751:LEU:HD13 | 1:A:2823:ILE:HD13 | 2.01                     | 0.42              |
| 1:A:4244:GLU:CD   | 1:A:4668:LEU:HD22 | 2.45                     | 0.42              |
| 1:B:1152:MET:HE1  | 1:B:1163:THR:HG23 | 2.01                     | 0.42              |
| 1:B:1690:ASP:OD2  | 1:B:1693:GLN:NE2  | 2.52                     | 0.42              |
| 1:D:2754:PHE:HE2  | 1:D:2813:LEU:HD11 | 1.84                     | 0.42              |
| 1:D:4137:ARG:NH2  | 1:D:4199:GLU:OE2  | 2.53                     | 0.42              |
| 1:D:4183:ILE:HG12 | 1:D:4193:ILE:HD13 | 2.00                     | 0.42              |
| 1:C:1816:GLY:CA   | 1:C:1865:MET:HE2  | 2.49                     | 0.42              |
| 1:C:2886:TRP:HA   | 1:C:2889:LYS:HG2  | 2.02                     | 0.42              |
| 1:C:4138:ASP:N    | 1:C:4138:ASP:OD1  | 2.51                     | 0.42              |
| 1:A:793:LEU:HD12  | 1:A:821:LEU:HD21  | 2.02                     | 0.42              |
| 1:A:866:HIS:HD2   | 1:A:941:MET:HE3   | 1.83                     | 0.42              |
| 1:A:892:THR:C     | 1:A:907:LEU:HD12  | 2.45                     | 0.42              |
| 1:A:1816:GLY:CA   | 1:A:1865:MET:HE2  | 2.49                     | 0.42              |
| 1:A:4966:ASP:OD2  | 1:A:4966:ASP:C    | 2.62                     | 0.42              |
| 2:E:13:ARG:HB3    | 2:E:13:ARG:CZ     | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:79:ASP:OD2    | 2:E:79:ASP:C      | 2.62                     | 0.42              |
| 2:H:13:ARG:HB3    | 2:H:13:ARG:CZ     | 2.49                     | 0.42              |
| 2:F:23:VAL:HG22   | 2:F:47:LYS:HD3    | 2.02                     | 0.42              |
| 1:B:273:HIS:CE1   | 1:B:334:MET:HB3   | 2.55                     | 0.42              |
| 1:B:2881:ASN:HA   | 1:B:2884:ASN:HD21 | 1.84                     | 0.42              |
| 1:B:4564:PHE:CD2  | 1:B:4564:PHE:C    | 2.98                     | 0.42              |
| 1:D:273:HIS:CE1   | 1:D:334:MET:HB3   | 2.55                     | 0.42              |
| 1:D:1081:TYR:CD1  | 1:D:1230:MET:HE1  | 2.55                     | 0.42              |
| 1:D:1297:PHE:CE2  | 1:D:1525:GLY:HA2  | 2.54                     | 0.42              |
| 1:D:2464:ASP:OD1  | 1:D:2465:ASP:N    | 2.52                     | 0.42              |
| 1:D:2582:MET:CE   | 1:D:2610:LEU:HD13 | 2.49                     | 0.42              |
| 1:D:2888:ARG:O    | 1:D:2892:GLN:HG2  | 2.20                     | 0.42              |
| 1:D:4655:PHE:N    | 1:D:4796:MET:HE1  | 2.33                     | 0.42              |
| 1:C:336:PRO:HA    | 1:C:337:PRO:HD3   | 1.85                     | 0.42              |
| 1:C:891:TRP:CZ2   | 1:C:899:ASP:HA    | 2.55                     | 0.42              |
| 1:C:892:THR:C     | 1:C:907:LEU:HD12  | 2.45                     | 0.42              |
| 1:C:3822:ASP:OD1  | 1:C:3823:LYS:N    | 2.53                     | 0.42              |
| 1:A:1081:TYR:CD1  | 1:A:1230:MET:HE1  | 2.55                     | 0.42              |
| 1:A:2888:ARG:O    | 1:A:2892:GLN:HG2  | 2.19                     | 0.42              |
| 1:A:3554:GLN:HE21 | 1:A:3593:VAL:HG21 | 1.84                     | 0.42              |
| 1:A:4060:LYS:HA   | 1:A:4060:LYS:HD2  | 1.89                     | 0.42              |
| 1:A:4885:PHE:O    | 1:A:4889:VAL:HG22 | 2.20                     | 0.42              |
| 1:B:2886:TRP:HA   | 1:B:2889:LYS:HG2  | 2.02                     | 0.42              |
| 1:D:891:TRP:CZ2   | 1:D:899:ASP:HA    | 2.55                     | 0.42              |
| 1:D:892:THR:C     | 1:D:907:LEU:HD12  | 2.45                     | 0.42              |
| 1:D:1805:GLU:H    | 1:D:1805:GLU:CD   | 2.26                     | 0.42              |
| 1:D:2037:ASP:OD2  | 1:D:2038:LEU:N    | 2.52                     | 0.42              |
| 1:D:2538:THR:HG23 | 1:D:2541:PHE:H    | 1.85                     | 0.42              |
| 1:D:2862:LEU:HD11 | 1:D:2865:VAL:HG13 | 2.00                     | 0.42              |
| 1:D:3158:LEU:HD23 | 1:D:3158:LEU:HA   | 1.89                     | 0.42              |
| 1:C:2230:THR:HB   | 1:C:2267:MET:HE3  | 2.02                     | 0.42              |
| 1:C:2336:ARG:HG2  | 1:C:2435:ARG:HD2  | 2.00                     | 0.42              |
| 1:C:3453:ARG:NH2  | 1:C:3456:GLN:HB3  | 2.34                     | 0.42              |
| 1:C:4951:LYS:NZ   | 1:C:4951:LYS:HB2  | 2.35                     | 0.42              |
| 1:A:170:ILE:HD12  | 1:A:197:GLN:HB2   | 2.02                     | 0.42              |
| 1:A:927:GLU:O     | 1:A:931:THR:HG23  | 2.19                     | 0.42              |
| 1:A:2122:SER:O    | 1:A:2126:ARG:HG3  | 2.19                     | 0.42              |
| 1:A:3347:SER:HA   | 1:A:3418:ASN:ND2  | 2.35                     | 0.42              |
| 1:A:3996:PHE:O    | 1:A:4000:MET:HG3  | 2.20                     | 0.42              |
| 2:F:84:ALA:O      | 2:F:93:PRO:HB3    | 2.19                     | 0.42              |
| 1:B:2765:LYS:NZ   | 1:B:2860:PRO:HA   | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3696:ASP:OD2  | 1:B:3773:ARG:NE   | 2.47                     | 0.42              |
| 1:B:4887:MET:HE3  | 1:B:4887:MET:HB3  | 1.78                     | 0.42              |
| 1:D:793:LEU:HD12  | 1:D:821:LEU:HD21  | 2.02                     | 0.42              |
| 1:D:1690:ASP:OD2  | 1:D:1693:GLN:NE2  | 2.52                     | 0.42              |
| 1:D:2230:THR:HB   | 1:D:2267:MET:HE3  | 2.02                     | 0.42              |
| 1:D:2301:TYR:HB3  | 1:D:2331:TYR:CZ   | 2.55                     | 0.42              |
| 1:D:3455:GLU:OE2  | 1:D:3508:SER:OG   | 2.36                     | 0.42              |
| 1:C:1297:PHE:CE2  | 1:C:1525:GLY:HA2  | 2.54                     | 0.42              |
| 1:C:1634:LEU:HD23 | 1:C:1634:LEU:HA   | 1.95                     | 0.42              |
| 1:C:2209:GLU:HA   | 1:C:2212:VAL:HG22 | 2.02                     | 0.42              |
| 1:C:4137:ARG:NH2  | 1:C:4199:GLU:OE2  | 2.53                     | 0.42              |
| 1:C:4183:ILE:HG12 | 1:C:4193:ILE:HD13 | 2.00                     | 0.42              |
| 1:A:328:LYS:HB3   | 1:A:328:LYS:HE3   | 1.74                     | 0.42              |
| 1:A:1115:LEU:HD13 | 1:A:1123:VAL:HG11 | 2.02                     | 0.42              |
| 1:A:2301:TYR:HB3  | 1:A:2331:TYR:CZ   | 2.55                     | 0.42              |
| 1:A:2538:THR:HG23 | 1:A:2541:PHE:H    | 1.85                     | 0.42              |
| 1:A:2881:ASN:HA   | 1:A:2884:ASN:HD21 | 1.84                     | 0.42              |
| 1:A:3194:LEU:HA   | 1:A:3194:LEU:HD12 | 1.76                     | 0.42              |
| 1:A:4967:TYR:OH   | 1:A:5033:GLU:OE2  | 2.24                     | 0.42              |
| 2:E:32:ASP:OD2    | 2:E:34:LYS:HG3    | 2.20                     | 0.42              |
| 1:B:1115:LEU:HD13 | 1:B:1123:VAL:HG11 | 2.02                     | 0.42              |
| 1:B:1816:GLY:CA   | 1:B:1865:MET:HE2  | 2.49                     | 0.42              |
| 1:B:2336:ARG:HG2  | 1:B:2435:ARG:HD2  | 2.00                     | 0.42              |
| 1:B:3384:LYS:HD2  | 1:B:3386:GLU:HB3  | 2.02                     | 0.42              |
| 1:B:3461:GLN:HG2  | 1:B:3462:ASN:ND2  | 2.34                     | 0.42              |
| 1:B:3604:TYR:O    | 1:B:3608:GLN:HG2  | 2.19                     | 0.42              |
| 1:D:170:ILE:HD12  | 1:D:197:GLN:HB2   | 2.02                     | 0.42              |
| 1:D:358:THR:HG21  | 1:D:382:GLY:HA2   | 2.01                     | 0.42              |
| 1:D:1020:ARG:O    | 1:D:1022:VAL:N    | 2.49                     | 0.42              |
| 1:D:1152:MET:HE1  | 1:D:1163:THR:HG23 | 2.01                     | 0.42              |
| 1:D:1236:THR:OG1  | 1:D:1608:MET:SD   | 2.76                     | 0.42              |
| 1:D:1773:PRO:CA   | 1:D:2153:MET:HE1  | 2.44                     | 0.42              |
| 1:D:3128:ASN:O    | 1:D:3132:THR:OG1  | 2.30                     | 0.42              |
| 1:D:3384:LYS:HD2  | 1:D:3386:GLU:HB3  | 2.02                     | 0.42              |
| 1:C:2301:TYR:HB3  | 1:C:2331:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:2888:ARG:O    | 1:C:2892:GLN:HG2  | 2.19                     | 0.42              |
| 1:C:3384:LYS:HD2  | 1:C:3386:GLU:HB3  | 2.02                     | 0.42              |
| 1:C:3823:LYS:HA   | 1:C:3823:LYS:HD3  | 1.76                     | 0.42              |
| 1:C:4244:GLU:CD   | 1:C:4668:LEU:HD22 | 2.45                     | 0.42              |
| 1:C:4954:MET:HA   | 1:C:4954:MET:CE   | 2.46                     | 0.42              |
| 1:A:309:THR:O     | 1:A:313:SER:OG    | 2.22                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:552:ASP:OD1  | 1:A:552:ASP:N     | 2.52                     | 0.41              |
| 1:A:2209:GLU:HA  | 1:A:2212:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:2230:THR:HB  | 1:A:2267:MET:HE3  | 2.02                     | 0.41              |
| 1:A:2886:TRP:HA  | 1:A:2889:LYS:HG2  | 2.02                     | 0.41              |
| 1:A:4240:ASP:OD1 | 1:A:4675:LYS:NZ   | 2.50                     | 0.41              |
| 2:G:13:ARG:HB3   | 2:G:13:ARG:CZ     | 2.50                     | 0.41              |
| 1:B:35:LEU:HD13  | 1:B:49:LEU:HD13   | 2.02                     | 0.41              |
| 1:B:568:LEU:HD12 | 1:B:602:VAL:HG13  | 2.02                     | 0.41              |
| 1:B:1748:PHE:HB2 | 1:B:1758:ARG:HE   | 1.84                     | 0.41              |
| 1:B:1992:ALA:HB1 | 1:B:1996:ARG:NH1  | 2.34                     | 0.41              |
| 1:B:3212:GLU:HG2 | 1:B:3213:TYR:CD1  | 2.55                     | 0.41              |
| 1:B:3666:ASP:OD2 | 1:B:3666:ASP:N    | 2.45                     | 0.41              |
| 1:B:4177:TYR:CE1 | 1:B:4199:GLU:HG3  | 2.55                     | 0.41              |
| 1:B:4951:LYS:HB2 | 1:B:4951:LYS:NZ   | 2.35                     | 0.41              |
| 1:D:1816:GLY:CA  | 1:D:1865:MET:HE2  | 2.49                     | 0.41              |
| 1:D:4188:ARG:NH1 | 1:D:4188:ARG:H    | 2.18                     | 0.41              |
| 1:C:1983:ALA:O   | 1:C:1987:SER:OG   | 2.25                     | 0.41              |
| 1:C:2318:TYR:CZ  | 1:C:2395:PRO:HD3  | 2.54                     | 0.41              |
| 1:C:3569:LEU:O   | 1:C:3573:MET:HB2  | 2.20                     | 0.41              |
| 1:C:4091:LYS:HA  | 1:C:4091:LYS:HD2  | 1.70                     | 0.41              |
| 1:A:330:ASP:N    | 1:A:330:ASP:OD1   | 2.53                     | 0.41              |
| 1:A:3062:PRO:HA  | 1:A:3065:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:3226:GLU:C   | 1:A:3228:ALA:N    | 2.78                     | 0.41              |
| 1:B:669:ASP:OD1  | 1:B:790:ARG:NH2   | 2.52                     | 0.41              |
| 1:B:2101:MET:HE2 | 1:B:2102:VAL:HG23 | 2.01                     | 0.41              |
| 1:B:2359:ARG:NE  | 1:C:179:TYR:OH    | 2.53                     | 0.41              |
| 1:B:2516:ASP:OD1 | 1:B:2517:PHE:N    | 2.53                     | 0.41              |
| 1:B:2749:GLU:HG3 | 1:B:2752:ASP:HB2  | 2.02                     | 0.41              |
| 1:D:774:ASP:OD2  | 1:D:1470:ARG:NH2  | 2.35                     | 0.41              |
| 1:D:873:LYS:NZ   | 1:D:970:LEU:HD21  | 2.35                     | 0.41              |
| 1:D:1260:MET:HE3 | 1:D:1260:MET:HB3  | 1.90                     | 0.41              |
| 1:D:2765:LYS:HE3 | 1:D:2861:ASP:CG   | 2.45                     | 0.41              |
| 1:D:3233:PRO:HD2 | 1:D:3239:MET:HG2  | 2.02                     | 0.41              |
| 1:D:3822:ASP:OD1 | 1:D:3823:LYS:N    | 2.53                     | 0.41              |
| 1:C:1020:ARG:O   | 1:C:1022:VAL:N    | 2.49                     | 0.41              |
| 1:C:2008:MET:HE2 | 1:C:2008:MET:HB3  | 1.90                     | 0.41              |
| 1:C:2437:ALA:HB2 | 1:C:2509:VAL:HG22 | 2.01                     | 0.41              |
| 1:C:3062:PRO:HA  | 1:C:3065:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:4564:PHE:CD2 | 1:C:4564:PHE:C    | 2.98                     | 0.41              |
| 1:A:3822:ASP:OD1 | 1:A:3823:LYS:N    | 2.53                     | 0.41              |
| 2:H:11:ASP:OD1   | 2:H:11:ASP:C      | 2.62                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:170:ILE:HD12  | 1:B:197:GLN:HB2   | 2.02                     | 0.41              |
| 1:B:2230:THR:HB   | 1:B:2267:MET:HE3  | 2.02                     | 0.41              |
| 1:B:2362:GLU:H    | 1:B:2362:GLU:CD   | 2.29                     | 0.41              |
| 1:B:2439:GLU:HB2  | 1:B:2442:LEU:CD2  | 2.51                     | 0.41              |
| 1:B:3347:SER:HA   | 1:B:3418:ASN:ND2  | 2.35                     | 0.41              |
| 1:B:4188:ARG:NH1  | 1:B:4188:ARG:H    | 2.18                     | 0.41              |
| 1:D:179:TYR:OH    | 1:C:2359:ARG:NE   | 2.53                     | 0.41              |
| 1:D:306:LYS:HB2   | 1:D:306:LYS:HE3   | 1.83                     | 0.41              |
| 1:D:569:ILE:HD13  | 1:D:569:ILE:HA    | 1.89                     | 0.41              |
| 1:D:1658:ASP:OD1  | 1:D:1658:ASP:N    | 2.53                     | 0.41              |
| 1:D:2008:MET:HE2  | 1:D:2008:MET:HB3  | 1.90                     | 0.41              |
| 1:D:2886:TRP:HA   | 1:D:2889:LYS:HG2  | 2.02                     | 0.41              |
| 1:C:35:LEU:HD13   | 1:C:49:LEU:HD13   | 2.02                     | 0.41              |
| 1:C:873:LYS:NZ    | 1:C:970:LEU:HD21  | 2.36                     | 0.41              |
| 1:C:2412:GLU:C    | 1:C:2414:ASN:H    | 2.29                     | 0.41              |
| 1:C:2502:MET:HE3  | 1:C:2502:MET:HB3  | 1.98                     | 0.41              |
| 1:C:2765:LYS:HE3  | 1:C:2861:ASP:CG   | 2.45                     | 0.41              |
| 1:C:2907:PRO:O    | 1:C:2910:THR:OG1  | 2.37                     | 0.41              |
| 1:C:4066:LEU:HA   | 1:C:4066:LEU:HD23 | 1.81                     | 0.41              |
| 1:A:873:LYS:NZ    | 1:A:970:LEU:HD21  | 2.35                     | 0.41              |
| 1:A:3384:LYS:HD2  | 1:A:3386:GLU:HB3  | 2.02                     | 0.41              |
| 2:G:61:GLU:O      | 2:G:65:GLN:HG3    | 2.20                     | 0.41              |
| 1:B:873:LYS:NZ    | 1:B:970:LEU:HD21  | 2.36                     | 0.41              |
| 1:B:2037:ASP:OD2  | 1:B:2038:LEU:N    | 2.53                     | 0.41              |
| 1:B:2263:ILE:HD12 | 1:B:2263:ILE:HA   | 1.94                     | 0.41              |
| 1:B:3062:PRO:HA   | 1:B:3065:VAL:HG22 | 2.02                     | 0.41              |
| 1:D:541:SER:O     | 1:D:577:ILE:HD13  | 2.20                     | 0.41              |
| 1:D:884:LEU:HG    | 1:D:955:LEU:HD21  | 2.03                     | 0.41              |
| 1:D:2020:ASP:OD1  | 1:D:2020:ASP:N    | 2.45                     | 0.41              |
| 1:D:2238:TYR:C    | 1:D:2238:TYR:CD2  | 2.98                     | 0.41              |
| 1:D:3062:PRO:HA   | 1:D:3065:VAL:HG22 | 2.02                     | 0.41              |
| 1:D:3959:LYS:HG2  | 1:D:4022:ASP:OD2  | 2.21                     | 0.41              |
| 1:C:273:HIS:CE1   | 1:C:334:MET:HB3   | 2.55                     | 0.41              |
| 1:C:499:THR:HG23  | 1:C:502:HIS:H     | 1.86                     | 0.41              |
| 1:C:568:LEU:HD12  | 1:C:602:VAL:HG13  | 2.02                     | 0.41              |
| 1:C:1748:PHE:HB2  | 1:C:1758:ARG:HE   | 1.84                     | 0.41              |
| 1:C:2238:TYR:C    | 1:C:2238:TYR:CD2  | 2.98                     | 0.41              |
| 1:C:3504:SER:OG   | 1:C:3507:THR:OG1  | 2.32                     | 0.41              |
| 1:C:3836:MET:HE1  | 1:C:3918:CYS:HB3  | 2.03                     | 0.41              |
| 1:C:4911:LEU:O    | 1:C:4914:VAL:HG22 | 2.21                     | 0.41              |
| 1:C:4989:MET:HE2  | 1:C:4989:MET:HB2  | 1.94                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1286:MET:H    | 1:A:1462:MET:HE1  | 1.85                     | 0.41              |
| 1:A:2037:ASP:OD2  | 1:A:2038:LEU:N    | 2.53                     | 0.41              |
| 1:A:2478:THR:OG1  | 1:A:2479:LEU:N    | 2.54                     | 0.41              |
| 1:A:2907:PRO:O    | 1:A:2910:THR:OG1  | 2.37                     | 0.41              |
| 1:A:3212:GLU:HG2  | 1:A:3213:TYR:CD1  | 2.55                     | 0.41              |
| 1:A:3689:GLU:C    | 1:A:3691:GLU:H    | 2.28                     | 0.41              |
| 1:A:4177:TYR:CE1  | 1:A:4199:GLU:HG3  | 2.55                     | 0.41              |
| 1:A:4564:PHE:CD2  | 1:A:4564:PHE:C    | 2.98                     | 0.41              |
| 1:B:484:LEU:HD12  | 1:B:484:LEU:HA    | 1.79                     | 0.41              |
| 1:B:1658:ASP:OD1  | 1:B:1658:ASP:N    | 2.53                     | 0.41              |
| 1:B:2912:THR:HG23 | 1:B:2914:LYS:HG3  | 2.03                     | 0.41              |
| 1:B:3209:GLN:HG2  | 1:B:3210:LEU:HG   | 2.02                     | 0.41              |
| 1:B:3569:LEU:O    | 1:B:3573:MET:HB2  | 2.20                     | 0.41              |
| 1:B:3822:ASP:OD1  | 1:B:3823:LYS:N    | 2.53                     | 0.41              |
| 1:B:4137:ARG:NH2  | 1:B:4199:GLU:OE2  | 2.53                     | 0.41              |
| 1:D:140:ASP:OD1   | 1:D:142:THR:OG1   | 2.29                     | 0.41              |
| 1:C:793:LEU:HD12  | 1:C:821:LEU:HD21  | 2.02                     | 0.41              |
| 1:C:927:GLU:O     | 1:C:931:THR:HG23  | 2.19                     | 0.41              |
| 1:C:1658:ASP:N    | 1:C:1658:ASP:OD1  | 2.53                     | 0.41              |
| 1:C:2516:ASP:OD1  | 1:C:2517:PHE:N    | 2.53                     | 0.41              |
| 1:C:2749:GLU:HG3  | 1:C:2752:ASP:HB2  | 2.03                     | 0.41              |
| 1:C:3212:GLU:HG2  | 1:C:3213:TYR:CD1  | 2.55                     | 0.41              |
| 1:C:3461:GLN:HG2  | 1:C:3462:ASN:ND2  | 2.34                     | 0.41              |
| 1:A:1478:ASP:CG   | 1:A:1482:ASN:HB2  | 2.46                     | 0.41              |
| 1:A:3569:LEU:O    | 1:A:3573:MET:HB2  | 2.20                     | 0.41              |
| 1:A:3836:MET:CE   | 1:A:3918:CYS:HB3  | 2.51                     | 0.41              |
| 1:A:4188:ARG:NH1  | 1:A:4188:ARG:H    | 2.18                     | 0.41              |
| 2:H:32:ASP:OD2    | 2:H:34:LYS:HG3    | 2.21                     | 0.41              |
| 1:B:793:LEU:HD12  | 1:B:821:LEU:HD21  | 2.02                     | 0.41              |
| 1:B:1286:MET:H    | 1:B:1462:MET:HE1  | 1.85                     | 0.41              |
| 1:B:2412:GLU:C    | 1:B:2414:ASN:H    | 2.29                     | 0.41              |
| 1:B:2437:ALA:HB2  | 1:B:2509:VAL:HG22 | 2.01                     | 0.41              |
| 1:B:2478:THR:OG1  | 1:B:2479:LEU:N    | 2.54                     | 0.41              |
| 1:D:484:LEU:HD12  | 1:D:484:LEU:HA    | 1.79                     | 0.41              |
| 1:D:927:GLU:O     | 1:D:931:THR:HG23  | 2.19                     | 0.41              |
| 1:D:1286:MET:H    | 1:D:1462:MET:HE1  | 1.85                     | 0.41              |
| 1:D:2263:ILE:HD12 | 1:D:2263:ILE:HA   | 1.94                     | 0.41              |
| 1:D:4060:LYS:HA   | 1:D:4060:LYS:HD2  | 1.89                     | 0.41              |
| 1:D:4951:LYS:NZ   | 1:D:4951:LYS:HB2  | 2.35                     | 0.41              |
| 1:C:170:ILE:HD12  | 1:C:197:GLN:HB2   | 2.02                     | 0.41              |
| 1:C:328:LYS:HB3   | 1:C:328:LYS:HE3   | 1.73                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1155:LEU:HD23 | 1:C:1155:LEU:HA   | 1.92                     | 0.41              |
| 1:C:2912:THR:HG23 | 1:C:2914:LYS:HG3  | 2.03                     | 0.41              |
| 1:C:3209:GLN:HG2  | 1:C:3210:LEU:HG   | 2.02                     | 0.41              |
| 1:C:3233:PRO:HD2  | 1:C:3239:MET:HG2  | 2.02                     | 0.41              |
| 1:C:3400:VAL:HG23 | 1:C:3403:ARG:NH2  | 2.35                     | 0.41              |
| 1:C:3501:ASP:OD1  | 1:C:3501:ASP:N    | 2.54                     | 0.41              |
| 1:C:3996:PHE:O    | 1:C:4000:MET:HG3  | 2.20                     | 0.41              |
| 1:A:35:LEU:HD13   | 1:A:49:LEU:HD13   | 2.02                     | 0.41              |
| 1:A:1608:MET:HE2  | 1:A:1608:MET:HB3  | 1.91                     | 0.41              |
| 1:A:2412:GLU:C    | 1:A:2414:ASN:H    | 2.29                     | 0.41              |
| 1:A:2439:GLU:HB2  | 1:A:2442:LEU:CD2  | 2.51                     | 0.41              |
| 1:A:2765:LYS:NZ   | 1:A:2860:PRO:HA   | 2.34                     | 0.41              |
| 1:A:4952:GLU:OE1  | 1:A:4952:GLU:N    | 2.54                     | 0.41              |
| 1:B:238:SER:OG    | 1:B:240:ASP:OD1   | 2.36                     | 0.41              |
| 1:B:1478:ASP:CG   | 1:B:1482:ASN:HB2  | 2.46                     | 0.41              |
| 1:B:2309:SER:HB2  | 1:B:2314:LEU:HD11 | 2.03                     | 0.41              |
| 1:B:4695:ASP:OD1  | 1:B:4695:ASP:N    | 2.35                     | 0.41              |
| 1:B:4911:LEU:O    | 1:B:4914:VAL:HG22 | 2.21                     | 0.41              |
| 1:D:1115:LEU:HD13 | 1:D:1123:VAL:HG11 | 2.02                     | 0.41              |
| 1:D:1119:GLU:H    | 1:D:1119:GLU:CD   | 2.29                     | 0.41              |
| 1:D:2604:GLU:HG2  | 1:D:2639:MET:HG3  | 2.03                     | 0.41              |
| 1:D:2819:TRP:O    | 1:D:2820:GLU:HG3  | 2.21                     | 0.41              |
| 1:D:2881:ASN:HA   | 1:D:2884:ASN:HD21 | 1.84                     | 0.41              |
| 1:D:3226:GLU:C    | 1:D:3228:ALA:N    | 2.78                     | 0.41              |
| 1:D:3459:VAL:HG11 | 1:D:3503:TYR:HD1  | 1.86                     | 0.41              |
| 1:D:4177:TYR:CE1  | 1:D:4199:GLU:HG3  | 2.55                     | 0.41              |
| 1:D:4952:GLU:N    | 1:D:4952:GLU:OE1  | 2.54                     | 0.41              |
| 1:C:541:SER:O     | 1:C:577:ILE:HD13  | 2.20                     | 0.41              |
| 1:C:1286:MET:H    | 1:C:1462:MET:HE1  | 1.85                     | 0.41              |
| 1:C:2238:TYR:HD2  | 1:C:2238:TYR:O    | 2.03                     | 0.41              |
| 1:C:2478:THR:OG1  | 1:C:2479:LEU:N    | 2.54                     | 0.41              |
| 1:C:2996:LYS:HD3  | 1:C:2996:LYS:HA   | 1.89                     | 0.41              |
| 1:C:3465:ASN:OD1  | 1:C:3467:MET:N    | 2.34                     | 0.41              |
| 1:C:3688:GLU:C    | 1:C:3690:VAL:H    | 2.29                     | 0.41              |
| 1:C:4177:TYR:CE1  | 1:C:4199:GLU:HG3  | 2.55                     | 0.41              |
| 1:A:499:THR:HG23  | 1:A:502:HIS:H     | 1.86                     | 0.41              |
| 1:A:569:ILE:HD13  | 1:A:569:ILE:HA    | 1.89                     | 0.41              |
| 1:A:884:LEU:HG    | 1:A:955:LEU:HD21  | 2.03                     | 0.41              |
| 1:A:2209:GLU:C    | 1:A:2209:GLU:OE2  | 2.64                     | 0.41              |
| 1:A:2362:GLU:H    | 1:A:2362:GLU:CD   | 2.29                     | 0.41              |
| 1:A:2749:GLU:HG3  | 1:A:2752:ASP:HB2  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2775:TRP:CD2  | 1:A:2786:LYS:HE3  | 2.56                     | 0.41              |
| 1:A:3467:MET:HE1  | 1:B:1174:GLY:HA2  | 2.02                     | 0.41              |
| 1:A:4190:ILE:HD12 | 1:A:5023:PRO:HB3  | 2.03                     | 0.41              |
| 1:B:891:TRP:HB3   | 1:B:907:LEU:HD11  | 2.03                     | 0.41              |
| 1:B:1424:PRO:HA   | 1:B:1427:ILE:HG22 | 2.03                     | 0.41              |
| 1:B:3400:VAL:HG23 | 1:B:3403:ARG:NH2  | 2.35                     | 0.41              |
| 1:B:3941:ASP:OD1  | 1:B:3941:ASP:N    | 2.53                     | 0.41              |
| 1:B:3959:LYS:HG2  | 1:B:4022:ASP:OD2  | 2.21                     | 0.41              |
| 1:D:663:TYR:OH    | 1:D:665:GLU:OE2   | 2.24                     | 0.41              |
| 1:D:1155:LEU:HD23 | 1:D:1155:LEU:HA   | 1.92                     | 0.41              |
| 1:D:1478:ASP:CG   | 1:D:1482:ASN:HB2  | 2.46                     | 0.41              |
| 1:D:3501:ASP:OD1  | 1:D:3501:ASP:N    | 2.54                     | 0.41              |
| 1:D:3562:LYS:HE2  | 1:D:3562:LYS:HB2  | 1.91                     | 0.41              |
| 1:D:3688:GLU:C    | 1:D:3690:VAL:H    | 2.29                     | 0.41              |
| 1:D:3836:MET:CE   | 1:D:3918:CYS:HB3  | 2.51                     | 0.41              |
| 1:D:4662:ASN:OD1  | 1:D:4662:ASN:C    | 2.64                     | 0.41              |
| 1:C:1575:LEU:HA   | 1:C:1575:LEU:HD23 | 1.81                     | 0.41              |
| 1:C:4966:ASP:OD2  | 1:C:4966:ASP:C    | 2.62                     | 0.41              |
| 1:A:1119:GLU:H    | 1:A:1119:GLU:CD   | 2.29                     | 0.41              |
| 1:A:1575:LEU:HD23 | 1:A:1575:LEU:HA   | 1.81                     | 0.41              |
| 1:A:1995:THR:O    | 1:A:1999:ARG:HG2  | 2.21                     | 0.41              |
| 1:A:2238:TYR:HD2  | 1:A:2238:TYR:O    | 2.03                     | 0.41              |
| 1:A:2577:ILE:HD12 | 1:A:2578:MET:N    | 2.32                     | 0.41              |
| 1:A:2604:GLU:HG2  | 1:A:2639:MET:HG3  | 2.03                     | 0.41              |
| 1:A:2677:LYS:HB3  | 1:A:2677:LYS:HE2  | 1.79                     | 0.41              |
| 1:A:3209:GLN:HG2  | 1:A:3210:LEU:HG   | 2.02                     | 0.41              |
| 1:A:3400:VAL:HG23 | 1:A:3403:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:3688:GLU:C    | 1:A:3690:VAL:H    | 2.29                     | 0.41              |
| 1:A:4662:ASN:OD1  | 1:A:4662:ASN:C    | 2.64                     | 0.41              |
| 1:A:4887:MET:HE3  | 1:A:4887:MET:HB3  | 1.78                     | 0.41              |
| 2:H:2:VAL:HG11    | 2:H:61:GLU:HB2    | 2.03                     | 0.41              |
| 2:H:49:MET:SD     | 2:H:52:LYS:NZ     | 2.94                     | 0.41              |
| 2:G:32:ASP:OD2    | 2:G:34:LYS:HG3    | 2.21                     | 0.41              |
| 1:B:499:THR:HG23  | 1:B:502:HIS:H     | 1.86                     | 0.41              |
| 1:B:1249:PRO:HA   | 1:B:1250:PRO:HD3  | 1.96                     | 0.41              |
| 1:B:1608:MET:HE2  | 1:B:1608:MET:HB3  | 1.91                     | 0.41              |
| 1:B:1995:THR:O    | 1:B:1999:ARG:HG2  | 2.21                     | 0.41              |
| 1:B:2238:TYR:O    | 1:B:2238:TYR:HD2  | 2.03                     | 0.41              |
| 1:B:2301:TYR:HB3  | 1:B:2331:TYR:CZ   | 2.55                     | 0.41              |
| 1:B:3194:LEU:HD12 | 1:B:3194:LEU:HA   | 1.76                     | 0.41              |
| 1:B:3564:GLU:HA   | 1:B:3570:ARG:NH2  | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3621:HIS:C    | 1:B:3622:LYS:HG3  | 2.46                     | 0.41              |
| 1:B:3689:GLU:C    | 1:B:3691:GLU:H    | 2.28                     | 0.41              |
| 1:B:4942:GLU:HA   | 1:B:4945:ASP:OD2  | 2.21                     | 0.41              |
| 1:B:4952:GLU:OE1  | 1:B:4952:GLU:N    | 2.54                     | 0.41              |
| 1:D:81:MET:HE2    | 1:D:81:MET:HB3    | 1.98                     | 0.41              |
| 1:D:901:LYS:HA    | 1:D:901:LYS:HD2   | 1.84                     | 0.41              |
| 1:D:1174:GLY:N    | 1:C:3467:MET:HE2  | 2.36                     | 0.41              |
| 1:D:1929:MET:HE3  | 1:D:1929:MET:HB3  | 1.86                     | 0.41              |
| 1:D:1992:ALA:HA   | 1:D:1995:THR:HG22 | 2.02                     | 0.41              |
| 1:D:2209:GLU:HA   | 1:D:2212:VAL:HG22 | 2.02                     | 0.41              |
| 1:D:2238:TYR:HD2  | 1:D:2238:TYR:O    | 2.03                     | 0.41              |
| 1:D:2412:GLU:C    | 1:D:2414:ASN:H    | 2.29                     | 0.41              |
| 1:D:2439:GLU:HB2  | 1:D:2442:LEU:CD2  | 2.51                     | 0.41              |
| 1:D:2749:GLU:HG3  | 1:D:2752:ASP:HB2  | 2.03                     | 0.41              |
| 1:D:3569:LEU:O    | 1:D:3573:MET:HB2  | 2.20                     | 0.41              |
| 1:D:3852:LYS:HE3  | 1:D:3852:LYS:HB3  | 1.85                     | 0.41              |
| 1:D:4564:PHE:CD2  | 1:D:4564:PHE:C    | 2.98                     | 0.41              |
| 1:D:4754:ASN:HB3  | 1:D:4756:ARG:HH21 | 1.86                     | 0.41              |
| 1:C:81:MET:HE2    | 1:C:81:MET:HB3    | 1.98                     | 0.41              |
| 1:C:788:LYS:HE3   | 1:C:788:LYS:HB2   | 1.79                     | 0.41              |
| 1:C:884:LEU:HG    | 1:C:955:LEU:HD21  | 2.03                     | 0.41              |
| 1:C:1128:ARG:HD3  | 1:C:1130:GLN:CD   | 2.46                     | 0.41              |
| 1:C:1695:LEU:HB3  | 1:C:1810:LYS:NZ   | 2.36                     | 0.41              |
| 1:C:2095:GLN:HG3  | 1:C:2127:GLN:HB3  | 2.03                     | 0.41              |
| 1:C:2309:SER:HB2  | 1:C:2314:LEU:HD11 | 2.03                     | 0.41              |
| 1:C:2527:LEU:HD12 | 1:C:2527:LEU:HA   | 1.82                     | 0.41              |
| 1:C:3158:LEU:HA   | 1:C:3158:LEU:HD23 | 1.89                     | 0.41              |
| 1:C:3959:LYS:HG2  | 1:C:4022:ASP:OD2  | 2.21                     | 0.41              |
| 1:C:4017:LEU:HD23 | 1:C:4017:LEU:HA   | 1.93                     | 0.41              |
| 1:C:4662:ASN:OD1  | 1:C:4662:ASN:C    | 2.64                     | 0.41              |
| 1:A:32:GLN:OE1    | 1:A:32:GLN:HA     | 2.21                     | 0.41              |
| 1:A:2582:MET:CE   | 1:A:2610:LEU:HD13 | 2.49                     | 0.41              |
| 1:A:2764:GLU:HG3  | 1:A:2857:PRO:HB3  | 2.04                     | 0.41              |
| 1:A:2912:THR:HG23 | 1:A:2914:LYS:HG3  | 2.03                     | 0.41              |
| 1:A:3959:LYS:HG2  | 1:A:4022:ASP:OD2  | 2.21                     | 0.41              |
| 1:A:4879:MET:HG3  | 1:D:4578:LEU:HD23 | 2.03                     | 0.41              |
| 1:A:4902:GLU:O    | 1:A:4913:ARG:NH1  | 2.53                     | 0.41              |
| 1:B:2382:GLU:OE1  | 1:B:2385:ARG:NH1  | 2.49                     | 0.41              |
| 1:B:2413:GLU:OE1  | 1:B:2413:GLU:N    | 2.54                     | 0.41              |
| 1:B:2604:GLU:HG2  | 1:B:2639:MET:HG3  | 2.03                     | 0.41              |
| 1:B:3110:LEU:C    | 1:B:3112:LEU:H    | 2.29                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3693:LYS:HA   | 1:B:3693:LYS:HD2  | 1.85                     | 0.41              |
| 1:B:3836:MET:HE1  | 1:B:3918:CYS:HB3  | 2.03                     | 0.41              |
| 1:D:937:CYS:N     | 1:D:1056:PRO:HG3  | 2.36                     | 0.41              |
| 1:D:1128:ARG:HD3  | 1:D:1130:GLN:CD   | 2.46                     | 0.41              |
| 1:D:2382:GLU:OE1  | 1:D:2385:ARG:NH1  | 2.49                     | 0.41              |
| 1:D:2615:ARG:HB2  | 1:D:2618:MET:CE   | 2.51                     | 0.41              |
| 1:D:2716:ASP:OD1  | 1:D:2716:ASP:N    | 2.54                     | 0.41              |
| 1:D:3836:MET:HE1  | 1:D:3918:CYS:HB3  | 2.03                     | 0.41              |
| 1:D:4930:ALA:HB2  | 1:C:4933:GLN:HG2  | 2.03                     | 0.41              |
| 1:C:891:TRP:HB3   | 1:C:907:LEU:HD11  | 2.03                     | 0.41              |
| 1:C:1992:ALA:HB1  | 1:C:1996:ARG:NH1  | 2.34                     | 0.41              |
| 1:C:2615:ARG:HB2  | 1:C:2618:MET:CE   | 2.51                     | 0.41              |
| 1:C:2765:LYS:NZ   | 1:C:2860:PRO:HA   | 2.34                     | 0.41              |
| 1:C:2977:LEU:HA   | 1:C:2980:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:3689:GLU:C    | 1:C:3691:GLU:H    | 2.28                     | 0.41              |
| 1:C:4952:GLU:OE1  | 1:C:4952:GLU:N    | 2.54                     | 0.41              |
| 1:A:192:ASP:OD1   | 1:A:192:ASP:N     | 2.54                     | 0.40              |
| 1:A:233:ILE:O     | 1:A:257:ARG:NH1   | 2.49                     | 0.40              |
| 1:A:788:LYS:HE2   | 1:A:1629:GLN:CD   | 2.46                     | 0.40              |
| 1:A:1174:GLY:N    | 1:D:3467:MET:HE2  | 2.36                     | 0.40              |
| 1:A:1773:PRO:CA   | 1:A:2153:MET:HE1  | 2.44                     | 0.40              |
| 1:A:2615:ARG:HB2  | 1:A:2618:MET:CE   | 2.51                     | 0.40              |
| 1:A:4754:ASN:HB3  | 1:A:4756:ARG:HH21 | 1.86                     | 0.40              |
| 1:A:4813:LEU:HD23 | 1:A:4813:LEU:HA   | 1.84                     | 0.40              |
| 1:A:4895:GLY:O    | 1:D:4892:ARG:NH1  | 2.45                     | 0.40              |
| 1:B:1055:PRO:HA   | 1:B:1056:PRO:HD3  | 1.97                     | 0.40              |
| 1:B:2615:ARG:HB2  | 1:B:2618:MET:CE   | 2.51                     | 0.40              |
| 1:B:2765:LYS:HE3  | 1:B:2861:ASP:CG   | 2.45                     | 0.40              |
| 1:B:2825:LYS:HG3  | 1:B:2935:TYR:CE2  | 2.57                     | 0.40              |
| 1:B:3038:MET:HE2  | 1:B:3038:MET:HB3  | 1.92                     | 0.40              |
| 1:B:3132:THR:HA   | 1:B:3136:LEU:HB3  | 2.03                     | 0.40              |
| 1:B:3501:ASP:OD1  | 1:B:3501:ASP:N    | 2.54                     | 0.40              |
| 1:B:3508:SER:HB3  | 1:B:3511:VAL:HG22 | 2.04                     | 0.40              |
| 1:B:4091:LYS:HG3  | 1:B:4095:LYS:NZ   | 2.37                     | 0.40              |
| 1:D:35:LEU:HD13   | 1:D:49:LEU:HD13   | 2.03                     | 0.40              |
| 1:D:955:LEU:HD23  | 1:D:955:LEU:HA    | 1.91                     | 0.40              |
| 1:D:3209:GLN:HG2  | 1:D:3210:LEU:HG   | 2.02                     | 0.40              |
| 1:D:3996:PHE:O    | 1:D:4000:MET:HG3  | 2.20                     | 0.40              |
| 1:D:4885:PHE:O    | 1:D:4889:VAL:HG22 | 2.20                     | 0.40              |
| 1:D:4911:LEU:O    | 1:D:4914:VAL:HG22 | 2.21                     | 0.40              |
| 1:C:32:GLN:OE1    | 1:C:32:GLN:HA     | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1424:PRO:HA   | 1:C:1427:ILE:HG22 | 2.03                     | 0.40              |
| 1:C:2598:ALA:HA   | 1:C:2601:ASP:OD2  | 2.22                     | 0.40              |
| 1:C:3836:MET:CE   | 1:C:3918:CYS:HB3  | 2.51                     | 0.40              |
| 1:C:4188:ARG:NH1  | 1:C:4188:ARG:H    | 2.18                     | 0.40              |
| 1:A:541:SER:O     | 1:A:577:ILE:HD13  | 2.20                     | 0.40              |
| 1:A:568:LEU:HD12  | 1:A:602:VAL:HG13  | 2.02                     | 0.40              |
| 1:A:2095:GLN:HG3  | 1:A:2127:GLN:HB3  | 2.03                     | 0.40              |
| 1:A:2413:GLU:N    | 1:A:2413:GLU:OE1  | 2.54                     | 0.40              |
| 1:A:3501:ASP:N    | 1:A:3501:ASP:OD1  | 2.54                     | 0.40              |
| 1:A:3564:GLU:HA   | 1:A:3570:ARG:NH2  | 2.36                     | 0.40              |
| 1:A:3673:MET:CE   | 1:A:3728:ILE:HD13 | 2.52                     | 0.40              |
| 1:A:4137:ARG:NH2  | 1:A:4199:GLU:OE2  | 2.53                     | 0.40              |
| 1:A:4942:GLU:HA   | 1:A:4945:ASP:OD2  | 2.21                     | 0.40              |
| 2:G:60:GLU:HA     | 2:G:60:GLU:OE1    | 2.22                     | 0.40              |
| 1:B:416:LYS:HB2   | 1:B:416:LYS:HE3   | 1.84                     | 0.40              |
| 1:B:2238:TYR:C    | 1:B:2238:TYR:CD2  | 2.98                     | 0.40              |
| 1:B:3688:GLU:C    | 1:B:3690:VAL:H    | 2.29                     | 0.40              |
| 1:B:4064:MET:HE1  | 1:B:4110:PHE:CD2  | 2.57                     | 0.40              |
| 1:D:891:TRP:HB3   | 1:D:907:LEU:HD11  | 2.03                     | 0.40              |
| 1:D:1695:LEU:HB3  | 1:D:1810:LYS:NZ   | 2.36                     | 0.40              |
| 1:D:1823:GLY:O    | 1:D:1825:HIS:ND1  | 2.48                     | 0.40              |
| 1:D:2598:ALA:HA   | 1:D:2601:ASP:OD2  | 2.22                     | 0.40              |
| 1:C:1115:LEU:HD13 | 1:C:1123:VAL:HG11 | 2.02                     | 0.40              |
| 1:A:891:TRP:HB3   | 1:A:907:LEU:HD11  | 2.03                     | 0.40              |
| 1:A:1155:LEU:HD23 | 1:A:1155:LEU:HA   | 1.92                     | 0.40              |
| 1:A:1992:ALA:HA   | 1:A:1995:THR:HG22 | 2.02                     | 0.40              |
| 1:A:2238:TYR:C    | 1:A:2238:TYR:CD2  | 2.98                     | 0.40              |
| 1:A:2516:ASP:OD1  | 1:A:2517:PHE:N    | 2.53                     | 0.40              |
| 1:A:2765:LYS:HE3  | 1:A:2861:ASP:CG   | 2.45                     | 0.40              |
| 1:A:3112:LEU:HD21 | 1:A:3180:ASN:ND2  | 2.37                     | 0.40              |
| 1:A:4148:THR:HG21 | 1:A:4180:ARG:HH21 | 1.86                     | 0.40              |
| 1:A:4897:ILE:HD12 | 1:A:4897:ILE:HA   | 1.95                     | 0.40              |
| 1:A:4951:LYS:NZ   | 1:A:4951:LYS:HB2  | 2.35                     | 0.40              |
| 2:F:44:LYS:HE3    | 2:F:44:LYS:HB3    | 1.78                     | 0.40              |
| 1:B:541:SER:O     | 1:B:577:ILE:HD13  | 2.20                     | 0.40              |
| 1:B:2209:GLU:OE2  | 1:B:2209:GLU:C    | 2.64                     | 0.40              |
| 1:B:3354:LEU:HD22 | 1:B:3423:TRP:CZ2  | 2.56                     | 0.40              |
| 1:D:484:LEU:O     | 1:D:488:LEU:HG    | 2.22                     | 0.40              |
| 1:D:1995:THR:O    | 1:D:1999:ARG:HG2  | 2.21                     | 0.40              |
| 1:D:2711:PRO:HA   | 1:D:2712:PRO:HD3  | 1.93                     | 0.40              |
| 1:D:2775:TRP:CD2  | 1:D:2786:LYS:HE3  | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3955:MET:HG2  | 1:D:4019:LEU:HD22 | 2.04                     | 0.40              |
| 1:D:4816:ILE:H    | 1:D:4816:ILE:HG13 | 1.73                     | 0.40              |
| 1:C:937:CYS:N     | 1:C:1056:PRO:HG3  | 2.36                     | 0.40              |
| 1:C:970:LEU:HD11  | 1:C:1049:TYR:CZ   | 2.57                     | 0.40              |
| 1:C:1995:THR:O    | 1:C:1999:ARG:HG2  | 2.21                     | 0.40              |
| 1:C:2123:LEU:O    | 1:C:2127:GLN:HG2  | 2.22                     | 0.40              |
| 1:C:2819:TRP:O    | 1:C:2820:GLU:HG3  | 2.21                     | 0.40              |
| 1:C:2965:ARG:HA   | 1:C:2968:ASP:OD2  | 2.22                     | 0.40              |
| 1:C:3128:ASN:O    | 1:C:3132:THR:OG1  | 2.30                     | 0.40              |
| 1:C:3132:THR:HA   | 1:C:3136:LEU:HB3  | 2.03                     | 0.40              |
| 1:C:3354:LEU:HD22 | 1:C:3423:TRP:CZ2  | 2.56                     | 0.40              |
| 1:C:3459:VAL:HG11 | 1:C:3503:TYR:HD1  | 1.86                     | 0.40              |
| 1:C:3508:SER:HB3  | 1:C:3511:VAL:HG22 | 2.03                     | 0.40              |
| 1:C:3673:MET:CE   | 1:C:3728:ILE:HD13 | 2.52                     | 0.40              |
| 1:A:168:ASP:HB3   | 1:A:199:LEU:HD23  | 2.04                     | 0.40              |
| 1:A:749:ASP:O     | 1:A:753:PRO:HA    | 2.22                     | 0.40              |
| 1:A:898:ASP:OD1   | 1:A:898:ASP:N     | 2.55                     | 0.40              |
| 1:A:1617:THR:HA   | 1:A:1627:ALA:O    | 2.22                     | 0.40              |
| 1:A:2819:TRP:O    | 1:A:2820:GLU:HG3  | 2.21                     | 0.40              |
| 1:A:3459:VAL:HG11 | 1:A:3503:TYR:HD1  | 1.86                     | 0.40              |
| 1:A:4064:MET:HE1  | 1:A:4110:PHE:CD2  | 2.56                     | 0.40              |
| 1:B:788:LYS:HE2   | 1:B:1629:GLN:CD   | 2.46                     | 0.40              |
| 1:B:1699:GLU:OE2  | 1:B:1813:ARG:NH2  | 2.45                     | 0.40              |
| 1:B:2095:GLN:HG3  | 1:B:2127:GLN:HB3  | 2.03                     | 0.40              |
| 1:B:2775:TRP:CD2  | 1:B:2786:LYS:HE3  | 2.56                     | 0.40              |
| 1:B:3836:MET:CE   | 1:B:3918:CYS:HB3  | 2.51                     | 0.40              |
| 1:D:189:LEU:HD13  | 1:D:189:LEU:HA    | 1.91                     | 0.40              |
| 1:D:970:LEU:HD11  | 1:D:1049:TYR:CZ   | 2.57                     | 0.40              |
| 1:D:1205:GLY:HA3  | 1:D:1225:PRO:HB3  | 2.04                     | 0.40              |
| 1:D:2309:SER:HB2  | 1:D:2314:LEU:HD11 | 2.03                     | 0.40              |
| 1:D:2825:LYS:HG3  | 1:D:2935:TYR:CE2  | 2.57                     | 0.40              |
| 1:D:2907:PRO:O    | 1:D:2910:THR:OG1  | 2.37                     | 0.40              |
| 1:D:3693:LYS:HD2  | 1:D:3693:LYS:HA   | 1.85                     | 0.40              |
| 1:D:4686:LEU:HD12 | 1:D:4686:LEU:HA   | 1.88                     | 0.40              |
| 1:C:29:LEU:HD13   | 1:C:29:LEU:HA     | 1.93                     | 0.40              |
| 1:C:484:LEU:HA    | 1:C:484:LEU:HD12  | 1.79                     | 0.40              |
| 1:C:2209:GLU:C    | 1:C:2209:GLU:OE2  | 2.64                     | 0.40              |
| 1:C:2775:TRP:CD2  | 1:C:2786:LYS:HE3  | 2.56                     | 0.40              |
| 1:C:2825:LYS:HG3  | 1:C:2935:TYR:CE2  | 2.57                     | 0.40              |
| 1:C:4190:ILE:HD12 | 1:C:5023:PRO:HB3  | 2.03                     | 0.40              |
| 1:C:4754:ASN:HB3  | 1:C:4756:ARG:HH21 | 1.86                     | 0.40              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:A:283:ARG:HB2   | 1:A:290:TYR:CE2     | 2.57                     | 0.40              |
| 1:A:1782:PHE:O    | 2:E:82:TYR:OH       | 2.29                     | 0.40              |
| 1:A:3132:THR:HA   | 1:A:3136:LEU:HB3    | 2.03                     | 0.40              |
| 1:A:3272:ILE:C    | 1:A:3275:PRO:HD2    | 2.47                     | 0.40              |
| 1:A:4954:MET:HA   | 1:A:4954:MET:CE     | 2.46                     | 0.40              |
| 2:G:79:ASP:OD2    | 2:G:79:ASP:C        | 2.63                     | 0.40              |
| 1:B:937:CYS:N     | 1:B:1056:PRO:HG3    | 2.36                     | 0.40              |
| 1:B:1617:THR:HA   | 1:B:1627:ALA:O      | 2.22                     | 0.40              |
| 1:B:1703:LEU:HD23 | 1:B:1703:LEU:HA     | 1.94                     | 0.40              |
| 1:B:3112:LEU:HD21 | 1:B:3180:ASN:ND2    | 2.37                     | 0.40              |
| 1:B:3844:LEU:HD13 | 1:C:76:ARG:NE       | 2.37                     | 0.40              |
| 1:B:4933:GLN:HG2  | 1:C:4930:ALA:HB2    | 2.03                     | 0.40              |
| 1:D:175:SER:O     | 1:C:2452:ARG:HG3    | 2.22                     | 0.40              |
| 1:D:552:ASP:OD1   | 1:D:552:ASP:N       | 2.52                     | 0.40              |
| 1:D:568:LEU:HD12  | 1:D:602:VAL:HG13    | 2.02                     | 0.40              |
| 1:D:669:ASP:OD1   | 1:D:790:ARG:NH2     | 2.52                     | 0.40              |
| 1:D:2965:ARG:HA   | 1:D:2968:ASP:OD2    | 2.22                     | 0.40              |
| 1:D:3272:ILE:C    | 1:D:3275:PRO:HD2    | 2.47                     | 0.40              |
| 1:D:3354:LEU:HD22 | 1:D:3423:TRP:CZ2    | 2.56                     | 0.40              |
| 1:D:4092:ASP:HA   | 1:D:4095:LYS:HG2    | 2.04                     | 0.40              |
| 1:D:4190:ILE:HD12 | 1:D:5023:PRO:HB3    | 2.03                     | 0.40              |
| 1:D:4640:GLU:HB3  | 1:D:4641:PRO:HD3    | 2.04                     | 0.40              |
| 1:C:330:ASP:OD1   | 1:C:330:ASP:N       | 2.53                     | 0.40              |
| 1:C:1205:GLY:HA3  | 1:C:1225:PRO:HB3    | 2.04                     | 0.40              |
| 1:C:1231[B]:GLN:H | 1:C:1231[B]:GLN:HG3 | 1.74                     | 0.40              |
| 1:C:3272:ILE:C    | 1:C:3275:PRO:HD2    | 2.47                     | 0.40              |
| 1:C:3621:HIS:C    | 1:C:3622:LYS:HG3    | 2.46                     | 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     | 4385/5037 (87%)   | 4246 (97%)  | 139 (3%) | 0        | 100         | 100 |
| 1   | B     | 4385/5037 (87%)   | 4245 (97%)  | 140 (3%) | 0        | 100         | 100 |
| 1   | C     | 4385/5037 (87%)   | 4247 (97%)  | 138 (3%) | 0        | 100         | 100 |
| 1   | D     | 4385/5037 (87%)   | 4246 (97%)  | 139 (3%) | 0        | 100         | 100 |
| 2   | E     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 2   | F     | 105/108 (97%)     | 103 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 2   | G     | 105/108 (97%)     | 102 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 2   | H     | 105/108 (97%)     | 101 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| All | All   | 17960/20580 (87%) | 17392 (97%) | 568 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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     | 3836/4276 (90%)   | 3808 (99%)  | 28 (1%)  | 76          | 81 |
| 1   | B     | 3836/4276 (90%)   | 3808 (99%)  | 28 (1%)  | 76          | 81 |
| 1   | C     | 3836/4276 (90%)   | 3808 (99%)  | 28 (1%)  | 76          | 81 |
| 1   | D     | 3836/4276 (90%)   | 3807 (99%)  | 29 (1%)  | 73          | 80 |
| 2   | E     | 89/90 (99%)       | 83 (93%)    | 6 (7%)   | 15          | 43 |
| 2   | F     | 89/90 (99%)       | 86 (97%)    | 3 (3%)   | 32          | 61 |
| 2   | G     | 89/90 (99%)       | 84 (94%)    | 5 (6%)   | 19          | 48 |
| 2   | H     | 89/90 (99%)       | 85 (96%)    | 4 (4%)   | 24          | 55 |
| All | All   | 15700/17464 (90%) | 15569 (99%) | 131 (1%) | 70          | 80 |

All (131) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 189 | LEU  |
| 1   | A     | 191 | VAL  |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 318     | VAL  |
| 1   | A     | 882     | TRP  |
| 1   | A     | 898     | ASP  |
| 1   | A     | 945     | LYS  |
| 1   | A     | 959     | TYR  |
| 1   | A     | 1021    | LEU  |
| 1   | A     | 1230    | MET  |
| 1   | A     | 1506    | GLN  |
| 1   | A     | 1538    | THR  |
| 1   | A     | 1814    | MET  |
| 1   | A     | 1979    | LEU  |
| 1   | A     | 2178    | MET  |
| 1   | A     | 2369[A] | ARG  |
| 1   | A     | 2369[B] | ARG  |
| 1   | A     | 2577    | ILE  |
| 1   | A     | 2608    | MET  |
| 1   | A     | 2636    | PHE  |
| 1   | A     | 2742    | THR  |
| 1   | A     | 2781    | VAL  |
| 1   | A     | 2932    | MET  |
| 1   | A     | 3461    | GLN  |
| 1   | A     | 3639    | THR  |
| 1   | A     | 3751    | VAL  |
| 1   | A     | 3899    | PHE  |
| 1   | A     | 4880    | MET  |
| 1   | A     | 4973    | HIS  |
| 2   | E     | 2       | VAL  |
| 2   | E     | 14      | THR  |
| 2   | E     | 17      | LYS  |
| 2   | E     | 25      | HIS  |
| 2   | E     | 29      | MET  |
| 2   | E     | 87      | HIS  |
| 2   | H     | 2       | VAL  |
| 2   | H     | 14      | THR  |
| 2   | H     | 17      | LYS  |
| 2   | H     | 25      | HIS  |
| 2   | G     | 2       | VAL  |
| 2   | G     | 14      | THR  |
| 2   | G     | 17      | LYS  |
| 2   | G     | 25      | HIS  |
| 2   | G     | 29      | MET  |
| 2   | F     | 2       | VAL  |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 2   | F     | 17      | LYS  |
| 2   | F     | 25      | HIS  |
| 1   | B     | 189     | LEU  |
| 1   | B     | 191     | VAL  |
| 1   | B     | 318     | VAL  |
| 1   | B     | 882     | TRP  |
| 1   | B     | 898     | ASP  |
| 1   | B     | 945     | LYS  |
| 1   | B     | 959     | TYR  |
| 1   | B     | 1021    | LEU  |
| 1   | B     | 1230    | MET  |
| 1   | B     | 1506    | GLN  |
| 1   | B     | 1538    | THR  |
| 1   | B     | 1814    | MET  |
| 1   | B     | 1979    | LEU  |
| 1   | B     | 2178    | MET  |
| 1   | B     | 2369[A] | ARG  |
| 1   | B     | 2369[B] | ARG  |
| 1   | B     | 2577    | ILE  |
| 1   | B     | 2608    | MET  |
| 1   | B     | 2636    | PHE  |
| 1   | B     | 2742    | THR  |
| 1   | B     | 2781    | VAL  |
| 1   | B     | 2932    | MET  |
| 1   | B     | 3461    | GLN  |
| 1   | B     | 3639    | THR  |
| 1   | B     | 3751    | VAL  |
| 1   | B     | 3899    | PHE  |
| 1   | B     | 4880    | MET  |
| 1   | B     | 4973    | HIS  |
| 1   | D     | 189     | LEU  |
| 1   | D     | 191     | VAL  |
| 1   | D     | 318     | VAL  |
| 1   | D     | 882     | TRP  |
| 1   | D     | 898     | ASP  |
| 1   | D     | 945     | LYS  |
| 1   | D     | 959     | TYR  |
| 1   | D     | 1021    | LEU  |
| 1   | D     | 1230    | MET  |
| 1   | D     | 1506    | GLN  |
| 1   | D     | 1538    | THR  |
| 1   | D     | 1814    | MET  |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | D     | 1979    | LEU  |
| 1   | D     | 2178    | MET  |
| 1   | D     | 2186    | MET  |
| 1   | D     | 2369[A] | ARG  |
| 1   | D     | 2369[B] | ARG  |
| 1   | D     | 2577    | ILE  |
| 1   | D     | 2608    | MET  |
| 1   | D     | 2636    | PHE  |
| 1   | D     | 2742    | THR  |
| 1   | D     | 2781    | VAL  |
| 1   | D     | 2932    | MET  |
| 1   | D     | 3461    | GLN  |
| 1   | D     | 3639    | THR  |
| 1   | D     | 3751    | VAL  |
| 1   | D     | 3899    | PHE  |
| 1   | D     | 4880    | MET  |
| 1   | D     | 4973    | HIS  |
| 1   | C     | 189     | LEU  |
| 1   | C     | 191     | VAL  |
| 1   | C     | 318     | VAL  |
| 1   | C     | 882     | TRP  |
| 1   | C     | 898     | ASP  |
| 1   | C     | 945     | LYS  |
| 1   | C     | 959     | TYR  |
| 1   | C     | 1021    | LEU  |
| 1   | C     | 1230    | MET  |
| 1   | C     | 1506    | GLN  |
| 1   | C     | 1538    | THR  |
| 1   | C     | 1814    | MET  |
| 1   | C     | 1979    | LEU  |
| 1   | C     | 2178    | MET  |
| 1   | C     | 2369[A] | ARG  |
| 1   | C     | 2369[B] | ARG  |
| 1   | C     | 2577    | ILE  |
| 1   | C     | 2608    | MET  |
| 1   | C     | 2636    | PHE  |
| 1   | C     | 2742    | THR  |
| 1   | C     | 2781    | VAL  |
| 1   | C     | 2932    | MET  |
| 1   | C     | 3461    | GLN  |
| 1   | C     | 3639    | THR  |
| 1   | C     | 3751    | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 3899 | PHE  |
| 1   | C     | 4880 | MET  |
| 1   | C     | 4973 | HIS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 79   | GLN  |
| 1   | A     | 224  | HIS  |
| 1   | A     | 255  | HIS  |
| 1   | A     | 495  | ASN  |
| 1   | A     | 581  | ASN  |
| 1   | A     | 838  | HIS  |
| 1   | A     | 921  | ASN  |
| 1   | A     | 994  | ASN  |
| 1   | A     | 1220 | GLN  |
| 1   | A     | 1229 | ASN  |
| 1   | A     | 1640 | HIS  |
| 1   | A     | 1660 | GLN  |
| 1   | A     | 1776 | HIS  |
| 1   | A     | 2003 | GLN  |
| 1   | A     | 2253 | HIS  |
| 1   | A     | 2260 | ASN  |
| 1   | A     | 2487 | GLN  |
| 1   | A     | 2962 | GLN  |
| 1   | A     | 3180 | ASN  |
| 1   | A     | 3211 | ASN  |
| 1   | A     | 3355 | HIS  |
| 1   | A     | 3766 | GLN  |
| 1   | A     | 4034 | ASN  |
| 1   | A     | 4836 | GLN  |
| 1   | A     | 4864 | ASN  |
| 1   | A     | 4997 | ASN  |
| 2   | E     | 3    | GLN  |
| 2   | E     | 20   | GLN  |
| 2   | H     | 20   | GLN  |
| 2   | G     | 20   | GLN  |
| 2   | F     | 20   | GLN  |
| 1   | B     | 79   | GLN  |
| 1   | B     | 224  | HIS  |
| 1   | B     | 255  | HIS  |
| 1   | B     | 495  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 581  | ASN  |
| 1   | B     | 838  | HIS  |
| 1   | B     | 921  | ASN  |
| 1   | B     | 994  | ASN  |
| 1   | B     | 1229 | ASN  |
| 1   | B     | 1640 | HIS  |
| 1   | B     | 1660 | GLN  |
| 1   | B     | 1719 | HIS  |
| 1   | B     | 2003 | GLN  |
| 1   | B     | 2127 | GLN  |
| 1   | B     | 2253 | HIS  |
| 1   | B     | 2883 | HIS  |
| 1   | B     | 2962 | GLN  |
| 1   | B     | 3180 | ASN  |
| 1   | B     | 3211 | ASN  |
| 1   | B     | 3766 | GLN  |
| 1   | B     | 4034 | ASN  |
| 1   | B     | 4836 | GLN  |
| 1   | B     | 4864 | ASN  |
| 1   | B     | 4997 | ASN  |
| 1   | D     | 79   | GLN  |
| 1   | D     | 224  | HIS  |
| 1   | D     | 255  | HIS  |
| 1   | D     | 495  | ASN  |
| 1   | D     | 581  | ASN  |
| 1   | D     | 838  | HIS  |
| 1   | D     | 921  | ASN  |
| 1   | D     | 994  | ASN  |
| 1   | D     | 1220 | GLN  |
| 1   | D     | 1229 | ASN  |
| 1   | D     | 1640 | HIS  |
| 1   | D     | 1660 | GLN  |
| 1   | D     | 2003 | GLN  |
| 1   | D     | 2127 | GLN  |
| 1   | D     | 2253 | HIS  |
| 1   | D     | 2284 | ASN  |
| 1   | D     | 2342 | ASN  |
| 1   | D     | 2487 | GLN  |
| 1   | D     | 2962 | GLN  |
| 1   | D     | 3180 | ASN  |
| 1   | D     | 3211 | ASN  |
| 1   | D     | 3355 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 3766 | GLN  |
| 1   | D     | 4009 | GLN  |
| 1   | D     | 4034 | ASN  |
| 1   | D     | 4836 | GLN  |
| 1   | D     | 4864 | ASN  |
| 1   | D     | 4997 | ASN  |
| 1   | C     | 79   | GLN  |
| 1   | C     | 224  | HIS  |
| 1   | C     | 255  | HIS  |
| 1   | C     | 495  | ASN  |
| 1   | C     | 581  | ASN  |
| 1   | C     | 838  | HIS  |
| 1   | C     | 921  | ASN  |
| 1   | C     | 994  | ASN  |
| 1   | C     | 1220 | GLN  |
| 1   | C     | 1229 | ASN  |
| 1   | C     | 1640 | HIS  |
| 1   | C     | 1660 | GLN  |
| 1   | C     | 2003 | GLN  |
| 1   | C     | 2253 | HIS  |
| 1   | C     | 2962 | GLN  |
| 1   | C     | 3180 | ASN  |
| 1   | C     | 3211 | ASN  |
| 1   | C     | 3355 | HIS  |
| 1   | C     | 3462 | ASN  |
| 1   | C     | 3766 | GLN  |
| 1   | C     | 4034 | ASN  |
| 1   | C     | 4836 | GLN  |
| 1   | C     | 4864 | ASN  |
| 1   | C     | 4997 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 16 ligands modelled in this entry, 8 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 |
| 6   | 141  | D     | 5304 | -    | 11,12,12     | 1.77 | 3 (27%)  | 11,17,17    | 0.97 | 0        |
| 6   | 141  | A     | 5304 | -    | 11,12,12     | 1.76 | 3 (27%)  | 11,17,17    | 0.97 | 0        |
| 3   | ATP  | D     | 5301 | -    | 32,33,33     | 0.46 | 0        | 48,52,52    | 0.41 | 0        |
| 3   | ATP  | C     | 5301 | -    | 32,33,33     | 0.45 | 0        | 48,52,52    | 0.40 | 0        |
| 6   | 141  | C     | 5304 | -    | 11,12,12     | 1.76 | 3 (27%)  | 11,17,17    | 0.98 | 0        |
| 3   | ATP  | B     | 5301 | -    | 32,33,33     | 0.45 | 0        | 48,52,52    | 0.41 | 0        |
| 3   | ATP  | A     | 5301 | -    | 32,33,33     | 0.45 | 0        | 48,52,52    | 0.41 | 0        |
| 6   | 141  | B     | 5304 | -    | 11,12,12     | 1.76 | 3 (27%)  | 11,17,17    | 0.97 | 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   |
|-----|------|-------|------|------|---------|------------|---------|
| 6   | 141  | D     | 5304 | -    | -       | -          | 0/2/2/2 |
| 6   | 141  | A     | 5304 | -    | -       | -          | 0/2/2/2 |
| 3   | ATP  | D     | 5301 | -    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | ATP  | C     | 5301 | -    | -       | 6/22/38/38 | 0/3/3/3 |
| 6   | 141  | C     | 5304 | -    | -       | -          | 0/2/2/2 |
| 3   | ATP  | B     | 5301 | -    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | ATP  | A     | 5301 | -    | -       | 6/22/38/38 | 0/3/3/3 |
| 6   | 141  | B     | 5304 | -    | -       | -          | 0/2/2/2 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 6   | C     | 5304 | 141  | C5-C4 | -4.04 | 1.38        | 1.45     |
| 6   | A     | 5304 | 141  | C5-C4 | -4.01 | 1.38        | 1.45     |
| 6   | B     | 5304 | 141  | C5-C4 | -3.99 | 1.38        | 1.45     |
| 6   | D     | 5304 | 141  | C5-C4 | -3.99 | 1.38        | 1.45     |
| 6   | B     | 5304 | 141  | C7-N8 | 2.49  | 1.35        | 1.33     |
| 6   | D     | 5304 | 141  | C7-N8 | 2.49  | 1.35        | 1.33     |
| 6   | A     | 5304 | 141  | C7-N8 | 2.44  | 1.35        | 1.33     |
| 6   | C     | 5304 | 141  | C7-N8 | 2.44  | 1.35        | 1.33     |
| 6   | B     | 5304 | 141  | C2-N1 | -2.17 | 1.34        | 1.39     |
| 6   | A     | 5304 | 141  | C2-N1 | -2.16 | 1.34        | 1.39     |
| 6   | D     | 5304 | 141  | C2-N1 | -2.15 | 1.34        | 1.39     |
| 6   | C     | 5304 | 141  | C2-N1 | -2.13 | 1.34        | 1.39     |

There are no bond angle outliers.

There are no chirality outliers.

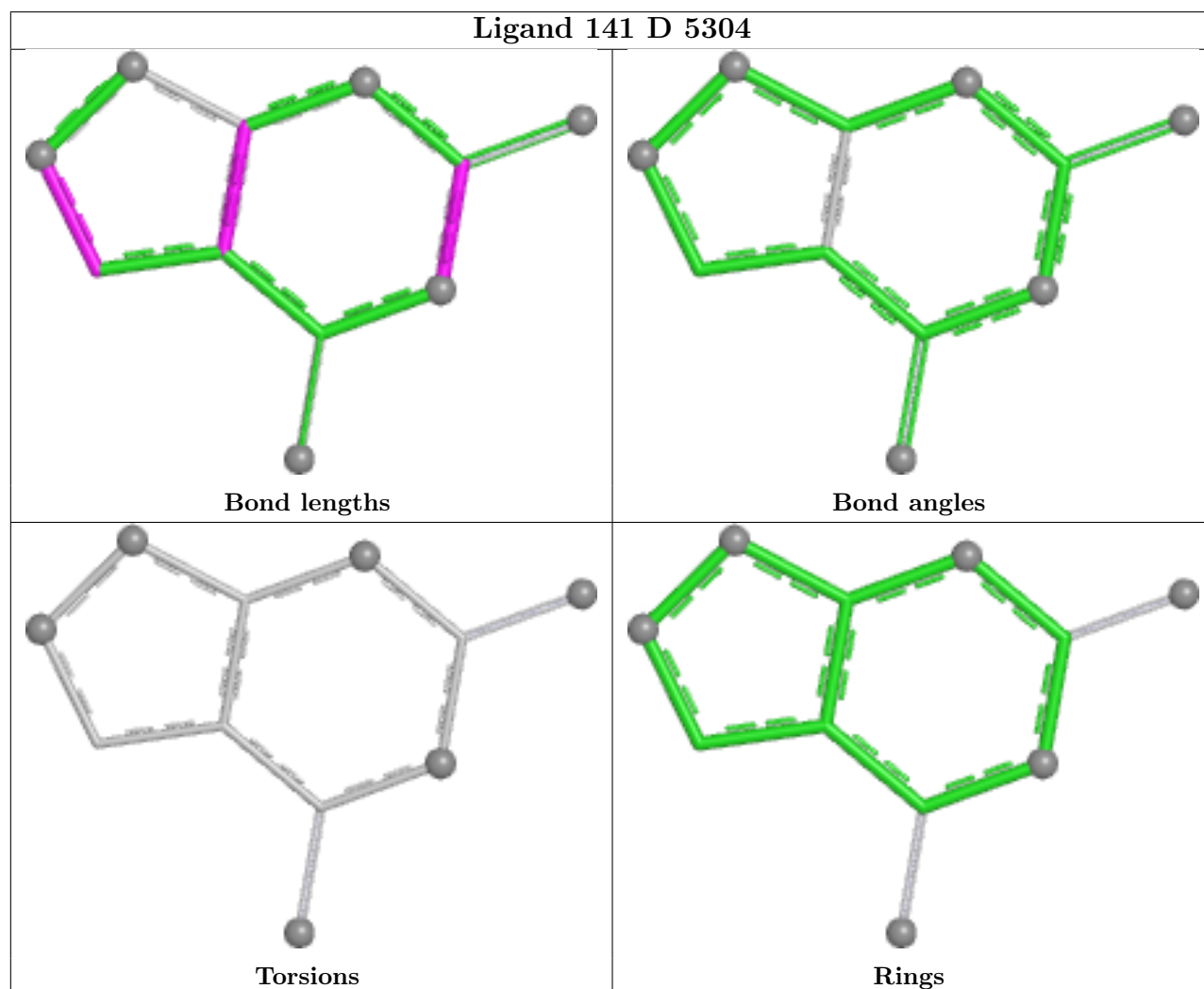
All (24) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 5301 | ATP  | PB-O3B-PG-O2G   |
| 3   | B     | 5301 | ATP  | PB-O3B-PG-O2G   |
| 3   | D     | 5301 | ATP  | PB-O3B-PG-O2G   |
| 3   | C     | 5301 | ATP  | PB-O3B-PG-O2G   |
| 3   | A     | 5301 | ATP  | O4'-C4'-C5'-O5' |
| 3   | A     | 5301 | ATP  | C3'-C4'-C5'-O5' |
| 3   | B     | 5301 | ATP  | O4'-C4'-C5'-O5' |
| 3   | B     | 5301 | ATP  | C3'-C4'-C5'-O5' |
| 3   | D     | 5301 | ATP  | O4'-C4'-C5'-O5' |
| 3   | D     | 5301 | ATP  | C3'-C4'-C5'-O5' |
| 3   | C     | 5301 | ATP  | O4'-C4'-C5'-O5' |
| 3   | C     | 5301 | ATP  | C3'-C4'-C5'-O5' |
| 3   | A     | 5301 | ATP  | PA-O3A-PB-O2B   |
| 3   | B     | 5301 | ATP  | PA-O3A-PB-O2B   |
| 3   | D     | 5301 | ATP  | PA-O3A-PB-O2B   |
| 3   | C     | 5301 | ATP  | PA-O3A-PB-O2B   |
| 3   | A     | 5301 | ATP  | PB-O3B-PG-O1G   |
| 3   | B     | 5301 | ATP  | PB-O3B-PG-O1G   |
| 3   | D     | 5301 | ATP  | PB-O3B-PG-O1G   |
| 3   | C     | 5301 | ATP  | PB-O3B-PG-O1G   |
| 3   | A     | 5301 | ATP  | PB-O3A-PA-O2A   |
| 3   | B     | 5301 | ATP  | PB-O3A-PA-O2A   |
| 3   | D     | 5301 | ATP  | PB-O3A-PA-O2A   |
| 3   | C     | 5301 | ATP  | PB-O3A-PA-O2A   |

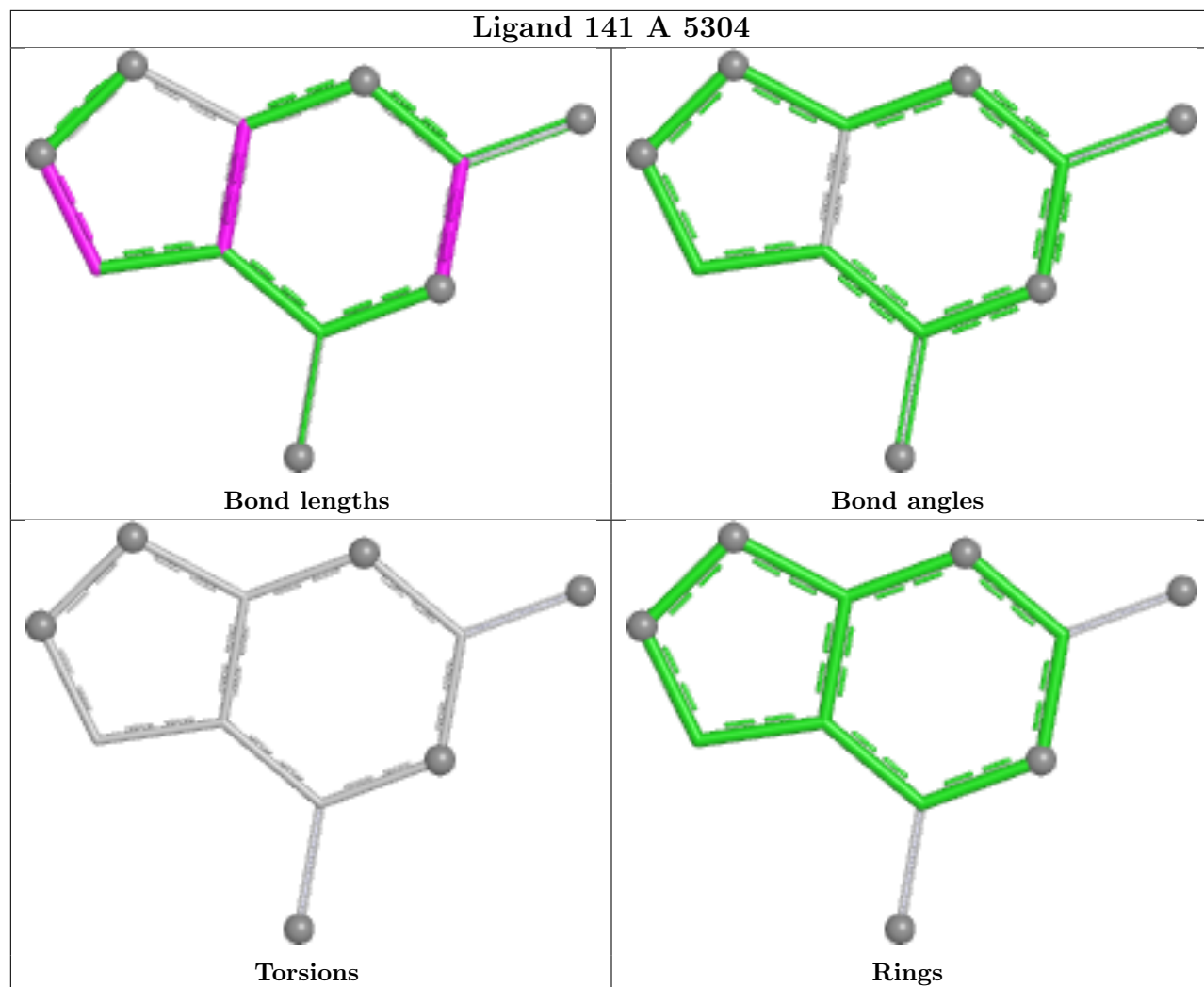
There are no ring outliers.

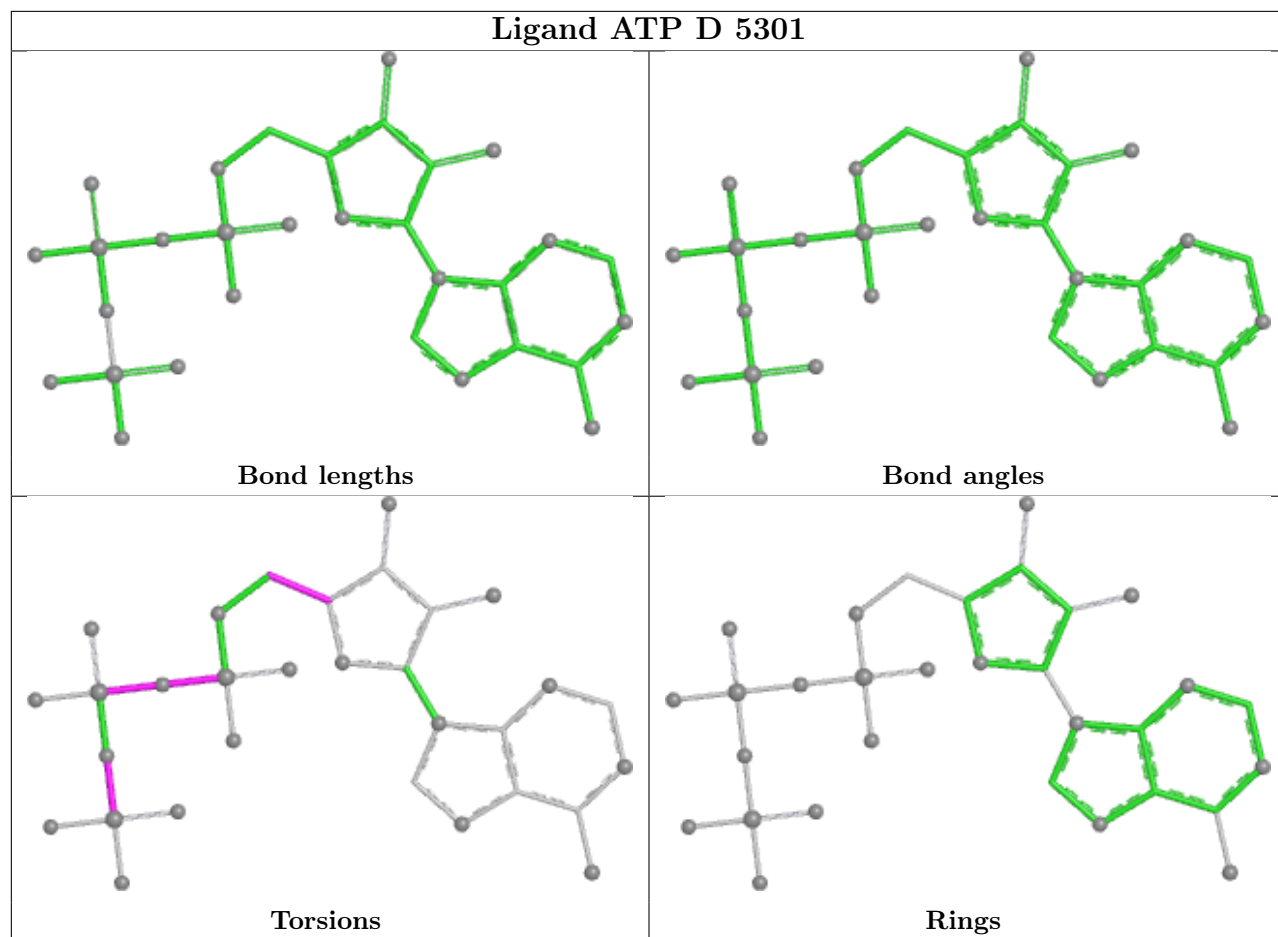
No monomer is involved in short contacts.

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

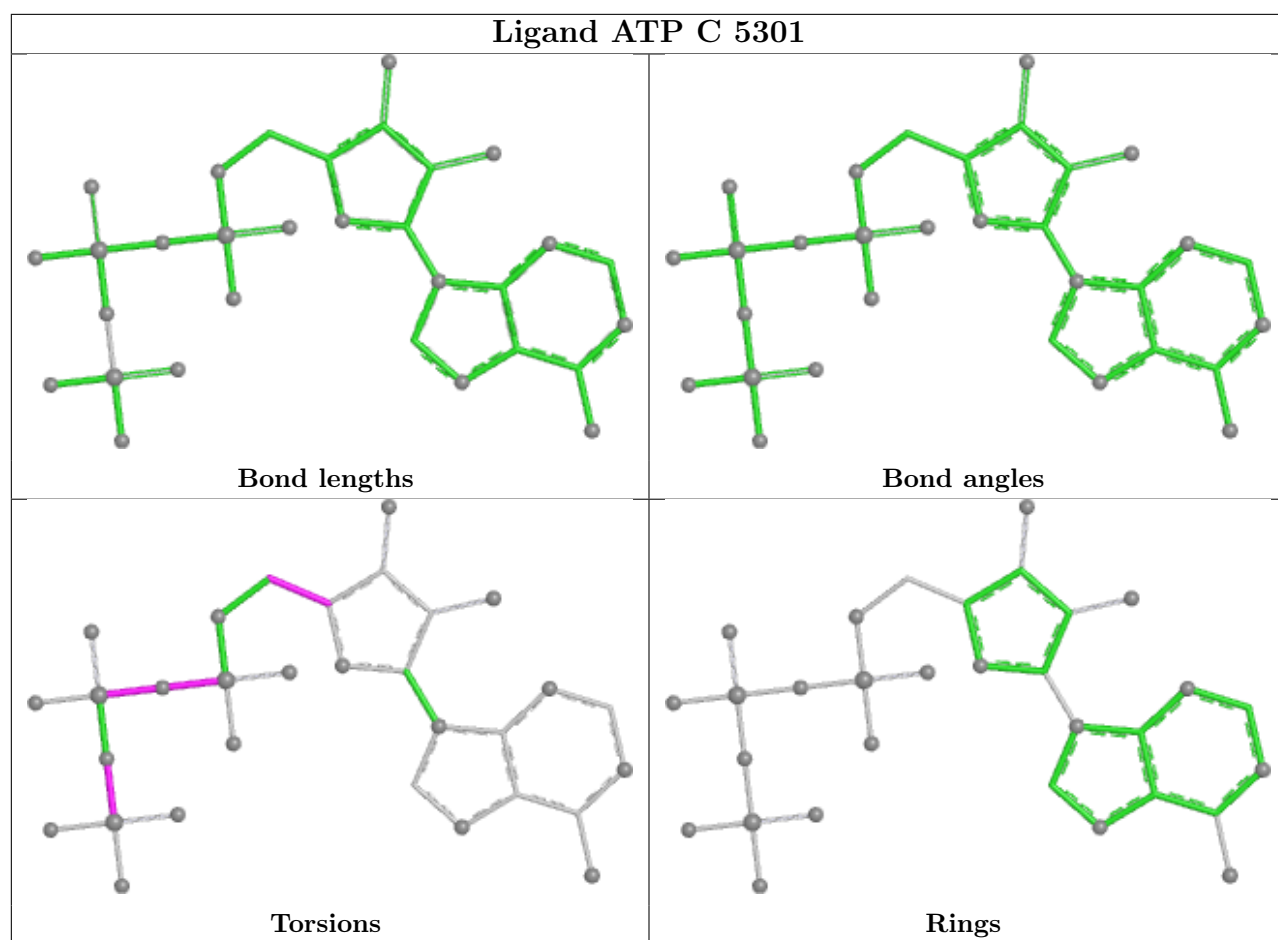


## Ligand 141 A 5304

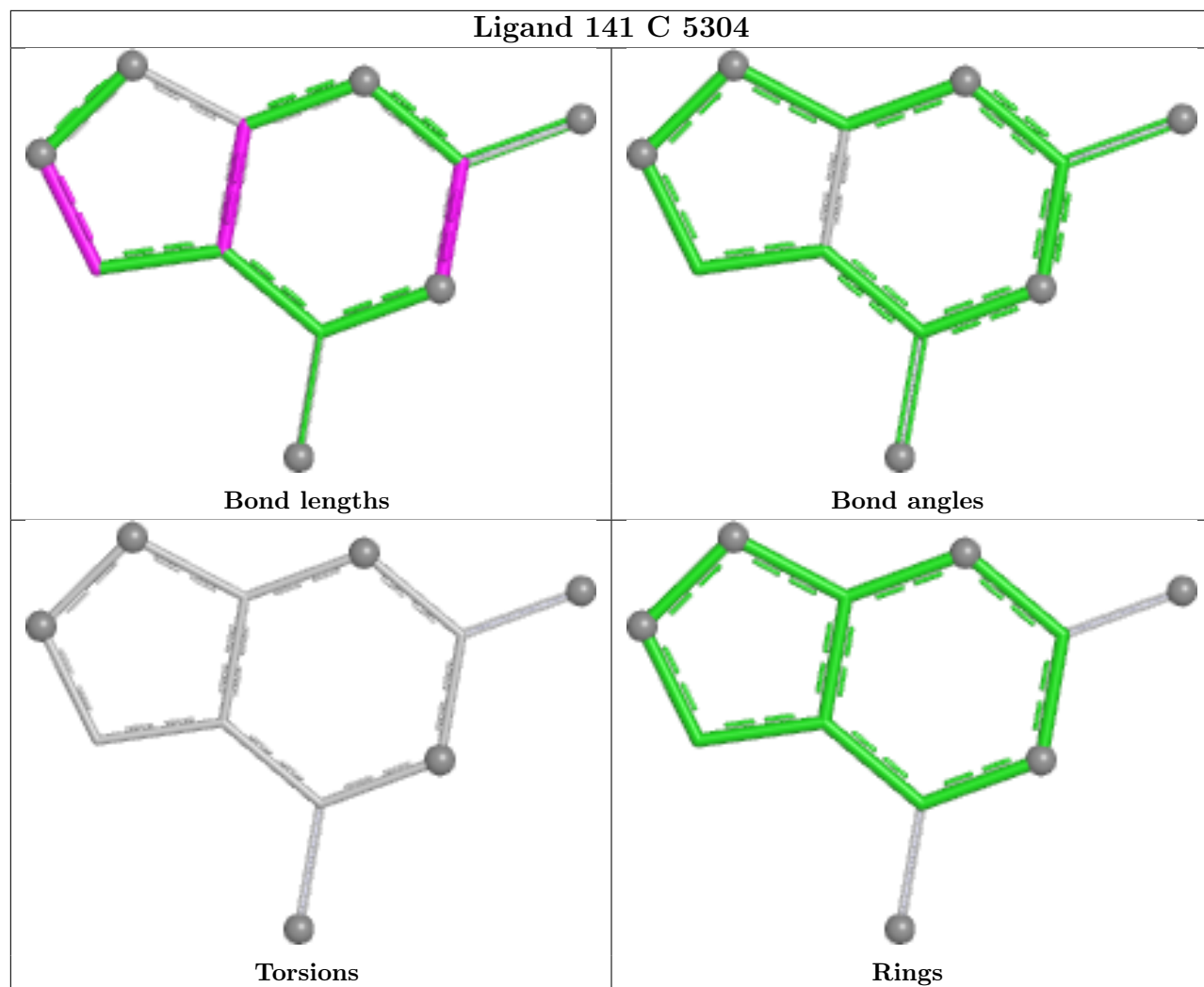


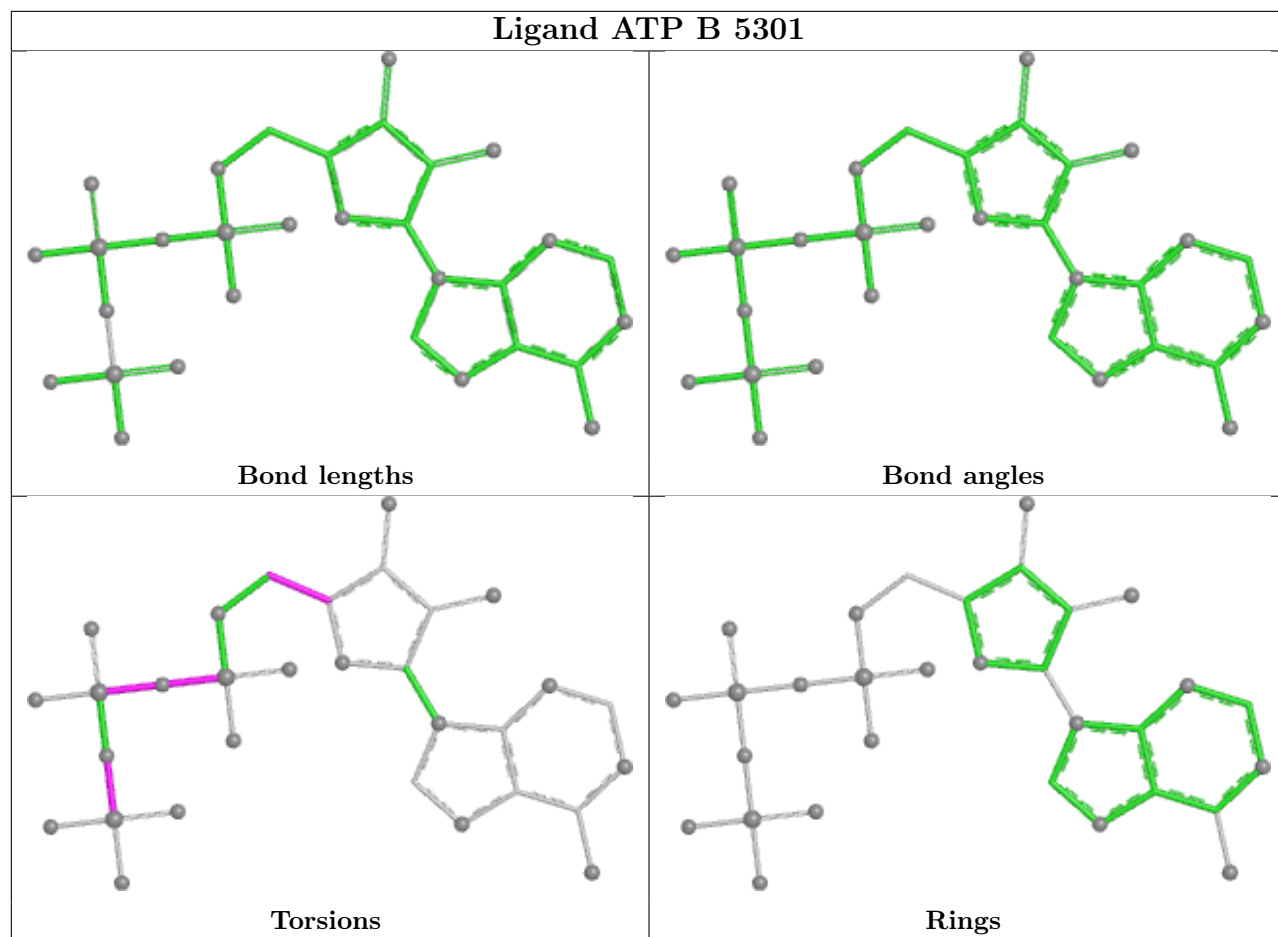


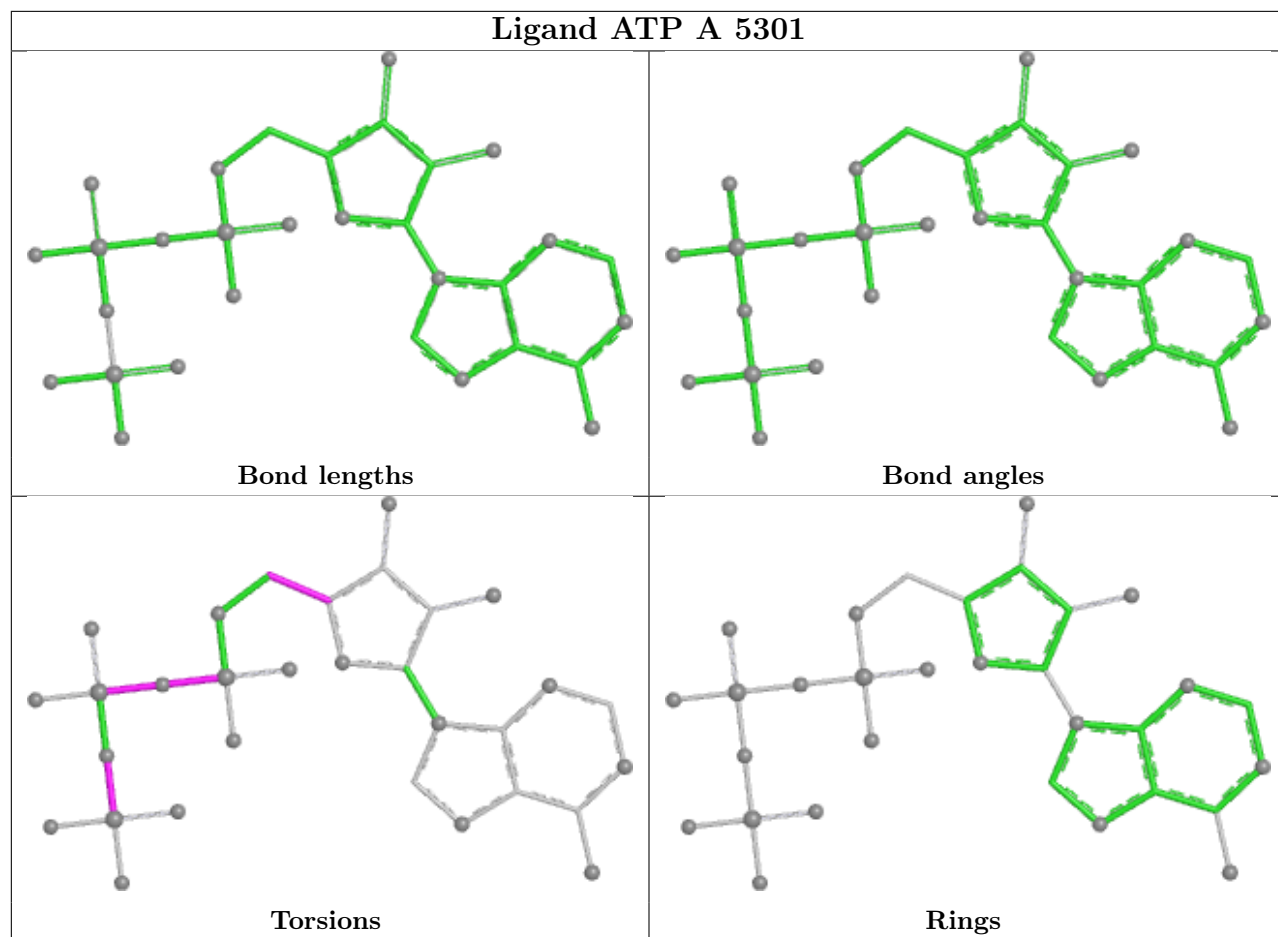


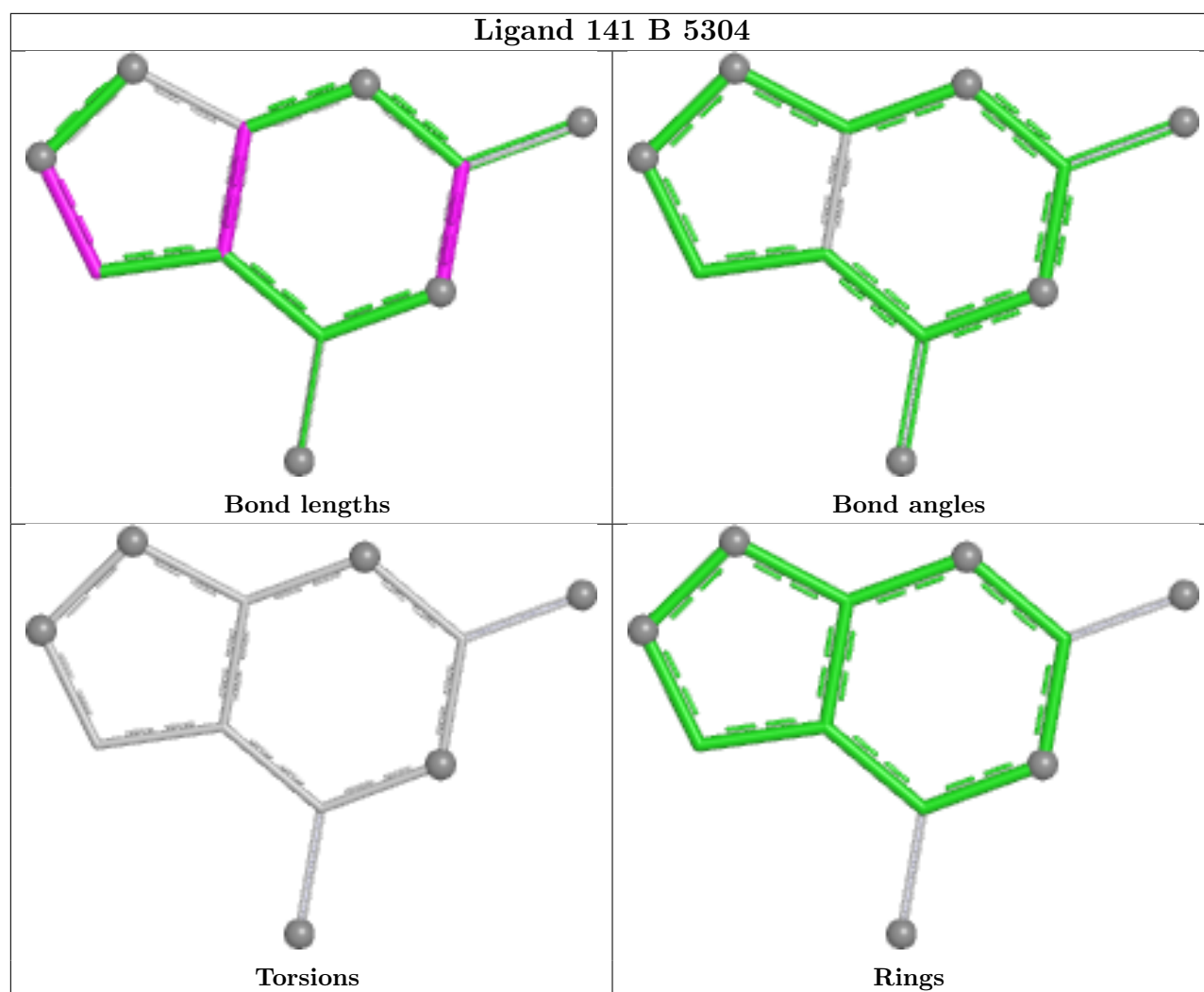


## Ligand 141 C 5304









## 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.

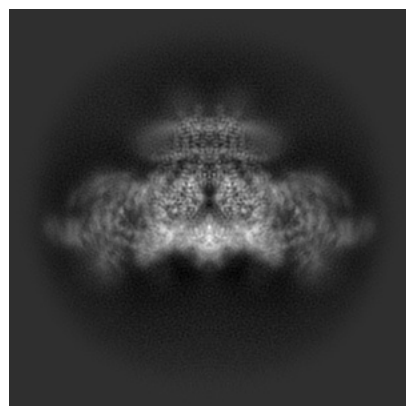
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47393. These allow visual inspection of the internal detail of the map and identification of artifacts.

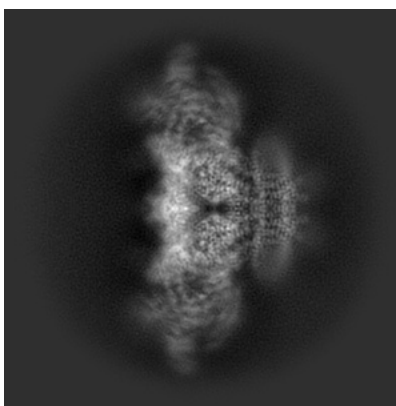
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

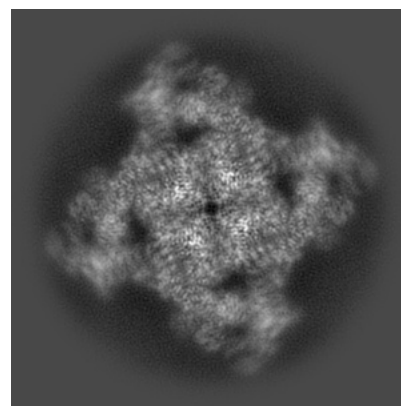
#### 6.1.1 Primary map



X

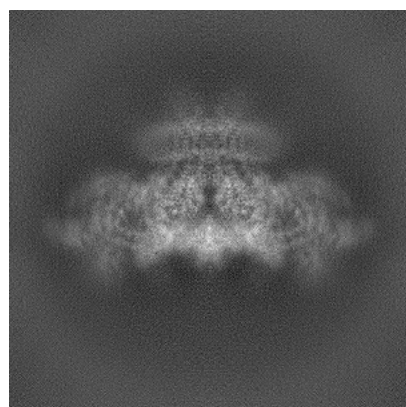


Y

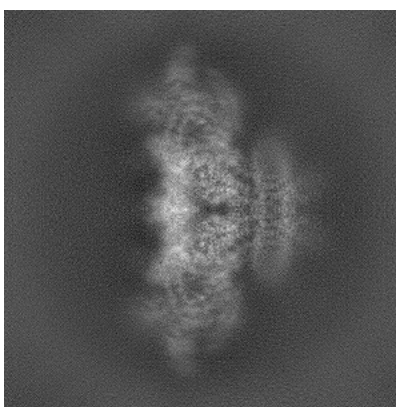


Z

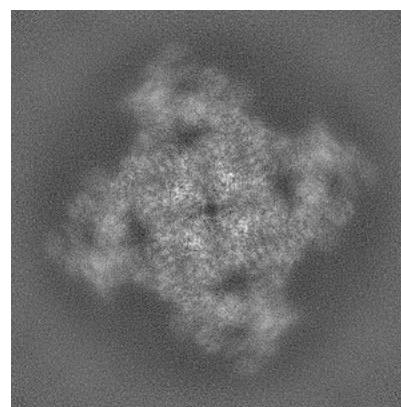
#### 6.1.2 Raw map



X



Y

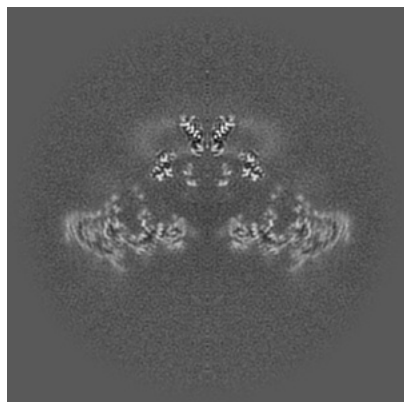


Z

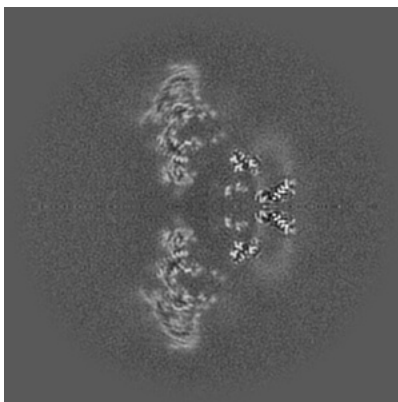
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

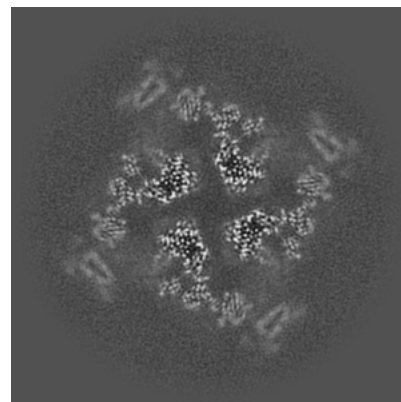
### 6.2.1 Primary map



X Index: 256

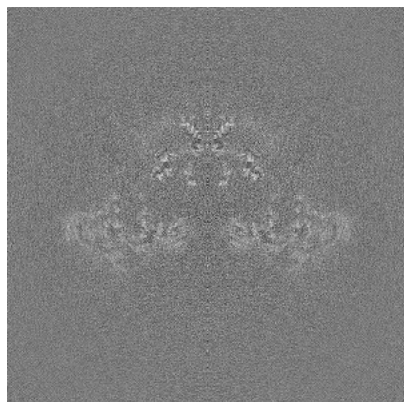


Y Index: 256

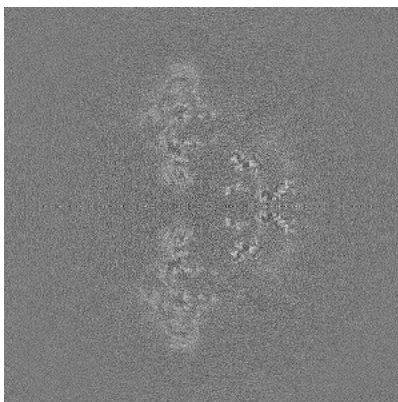


Z Index: 256

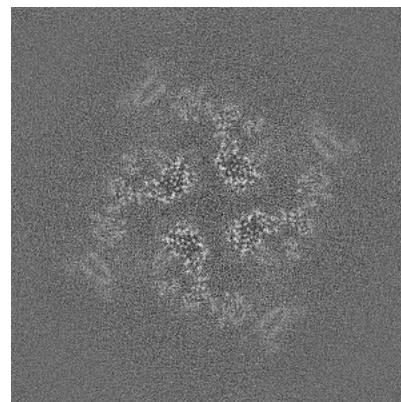
### 6.2.2 Raw map



X Index: 256



Y Index: 256



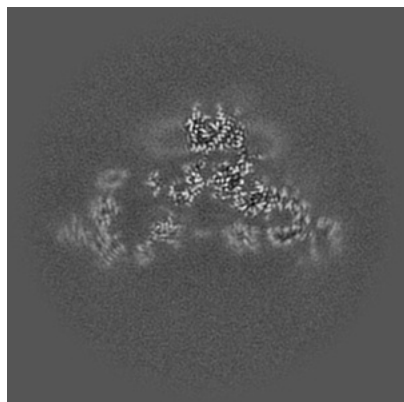
Z Index: 256

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

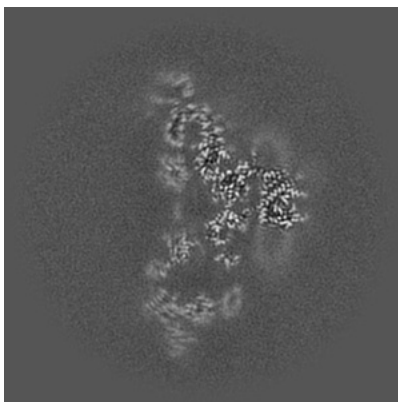


## 6.3 Largest variance slices [i](#)

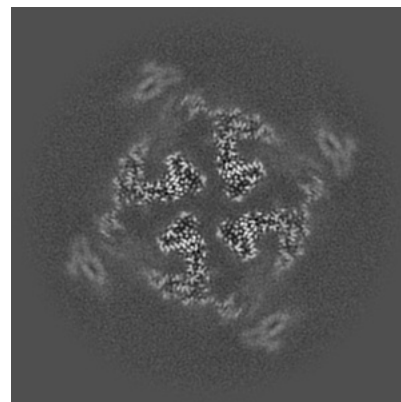
### 6.3.1 Primary map



X Index: 273

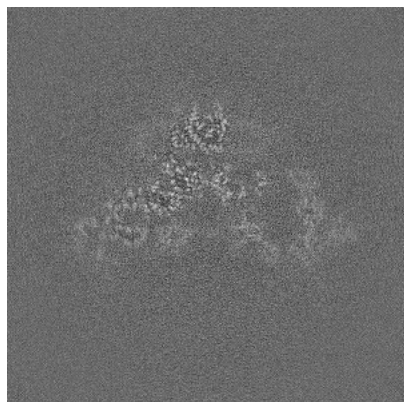


Y Index: 239

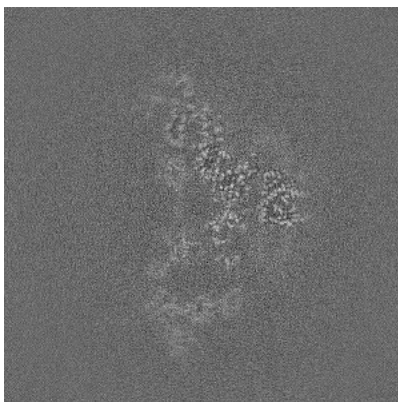


Z Index: 265

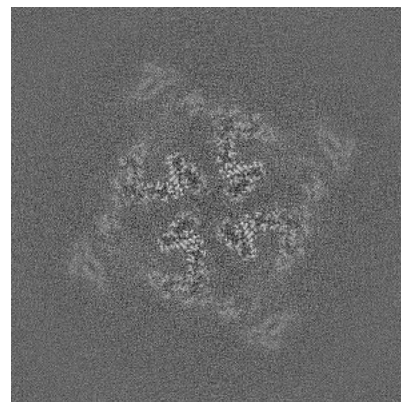
### 6.3.2 Raw map



X Index: 239



Y Index: 239



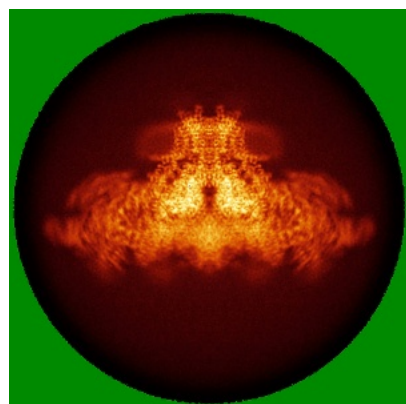
Z Index: 266

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

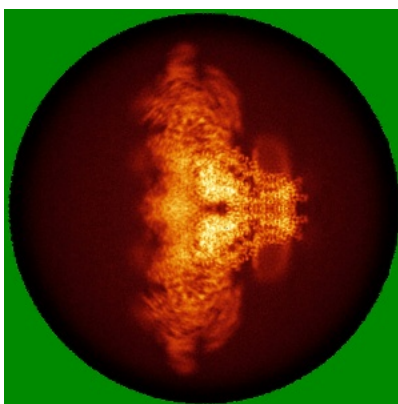


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

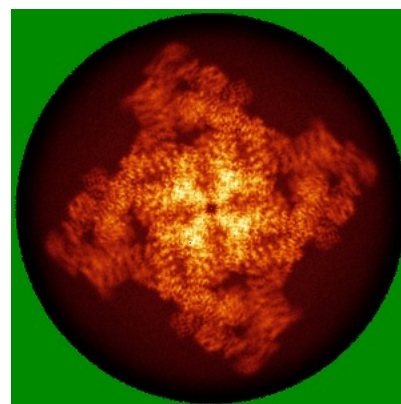
### 6.4.1 Primary map



X

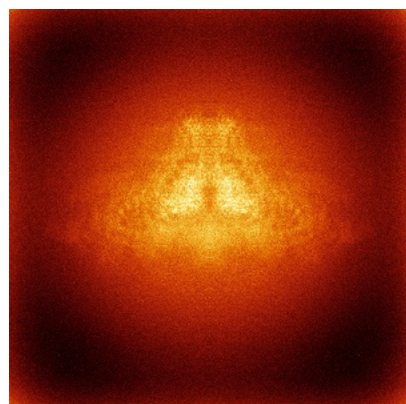


Y

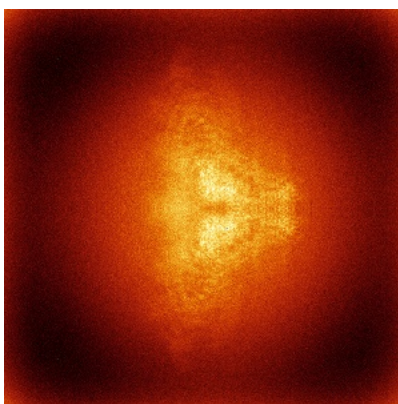


Z

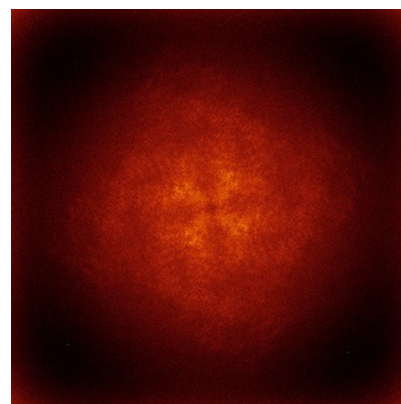
### 6.4.2 Raw map



X



Y

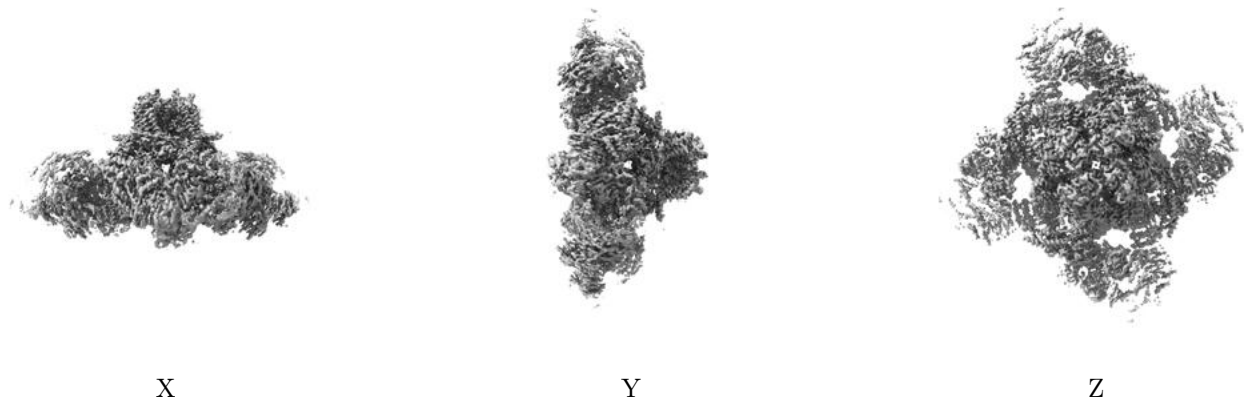


Z

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

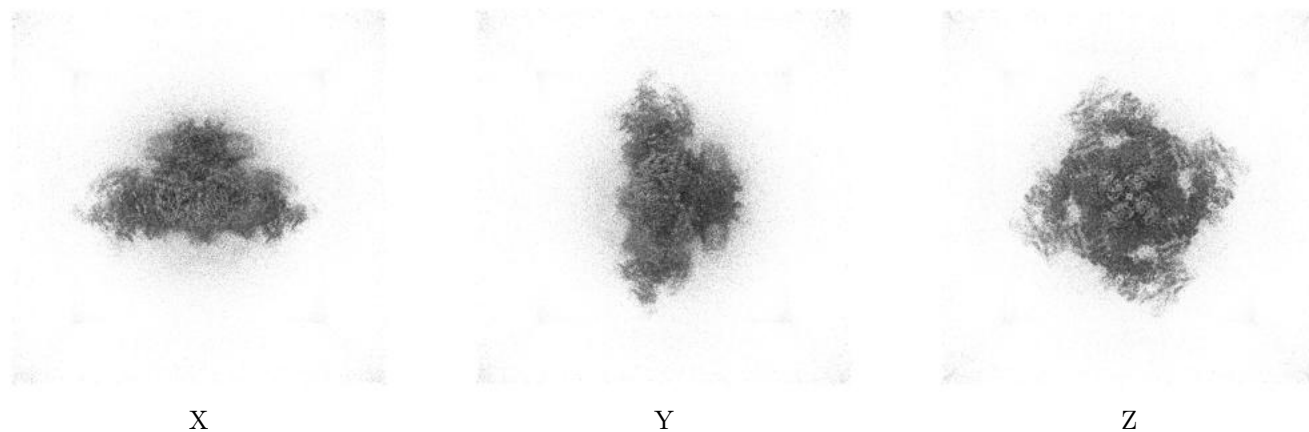
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

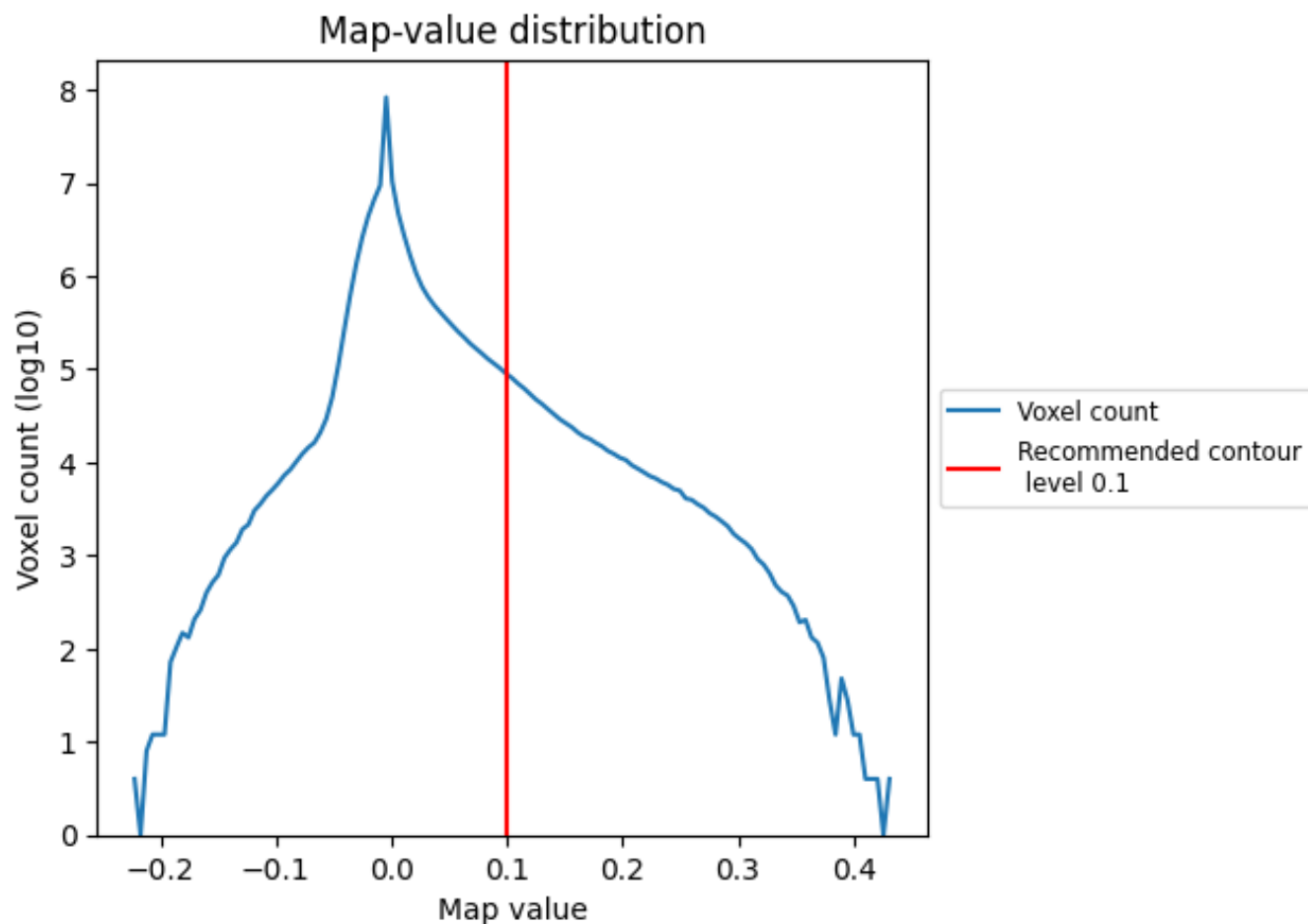
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

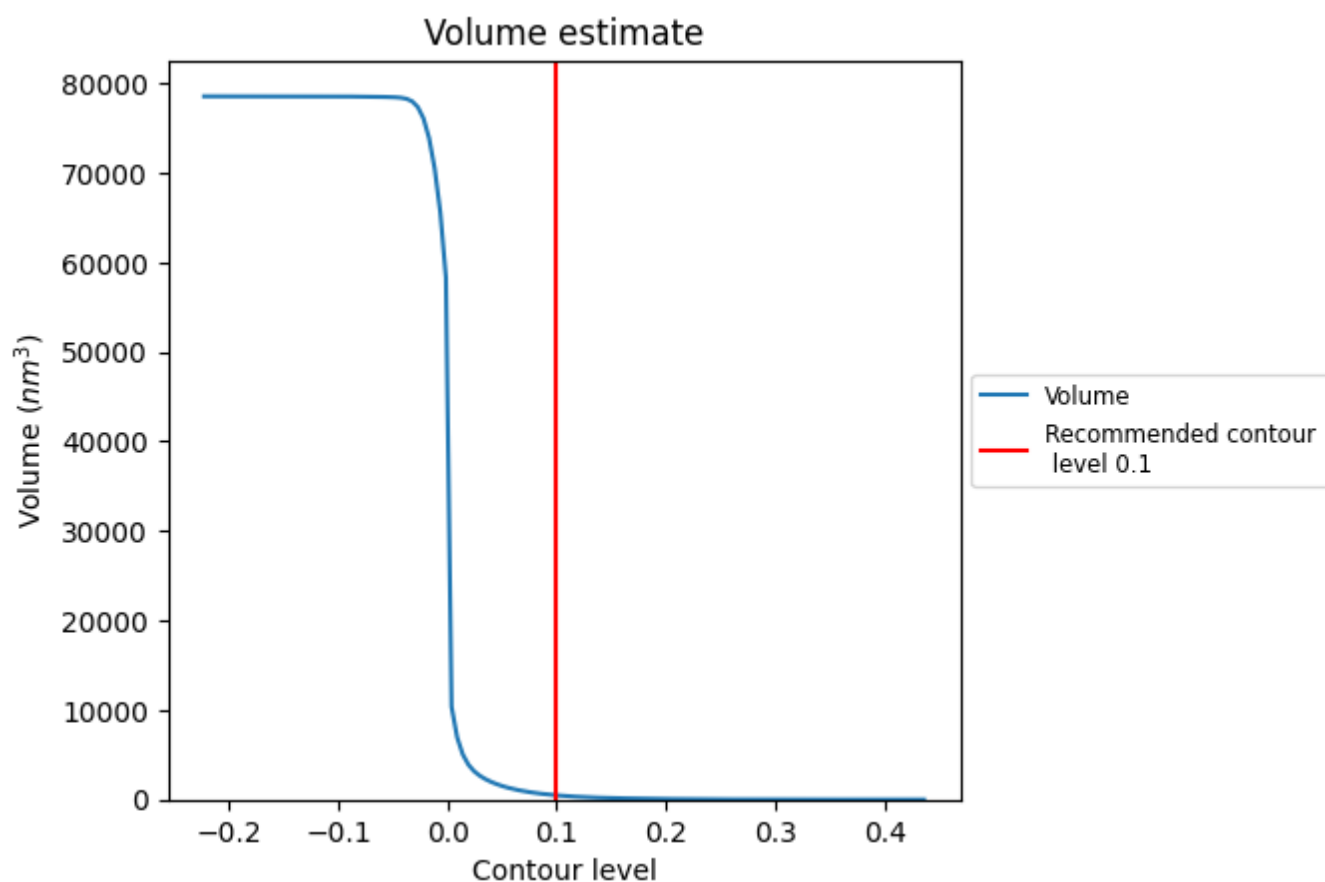
This section contains the results of statistical analysis of the map.

### 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.

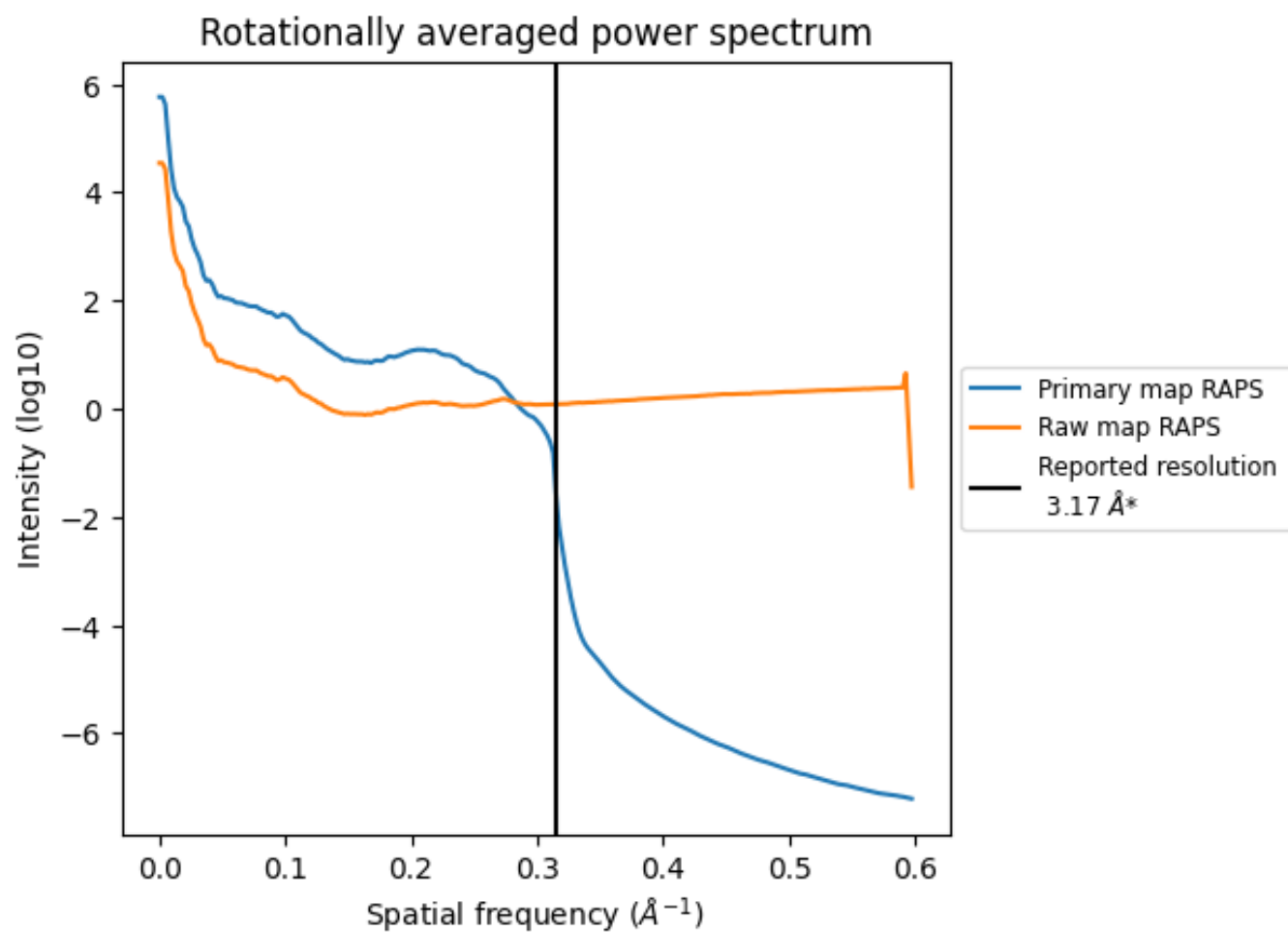
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 477 nm<sup>3</sup>; this corresponds to an approximate mass of 431 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 ⓘ

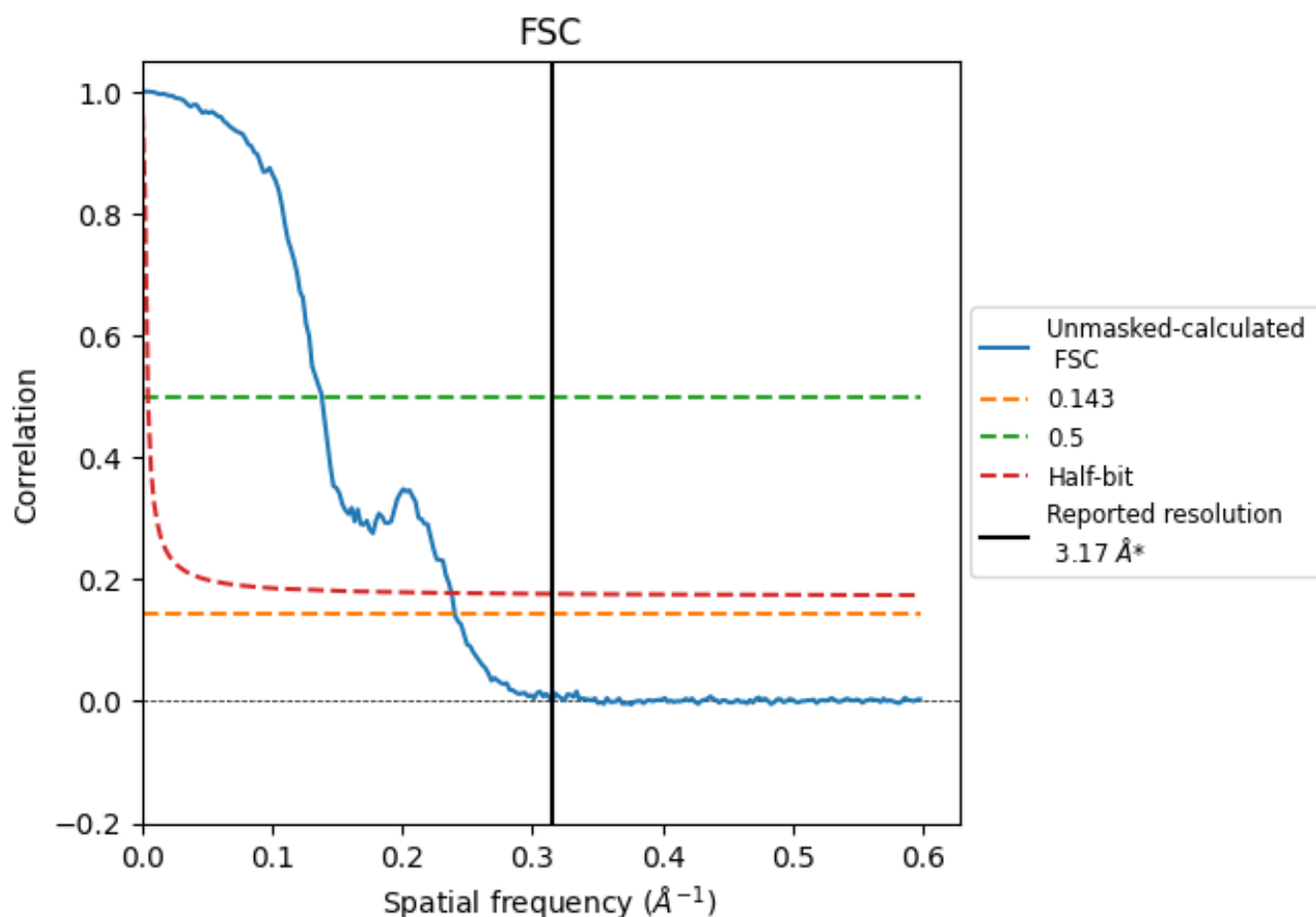


\*Reported resolution corresponds to spatial frequency of 0.315 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.315  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

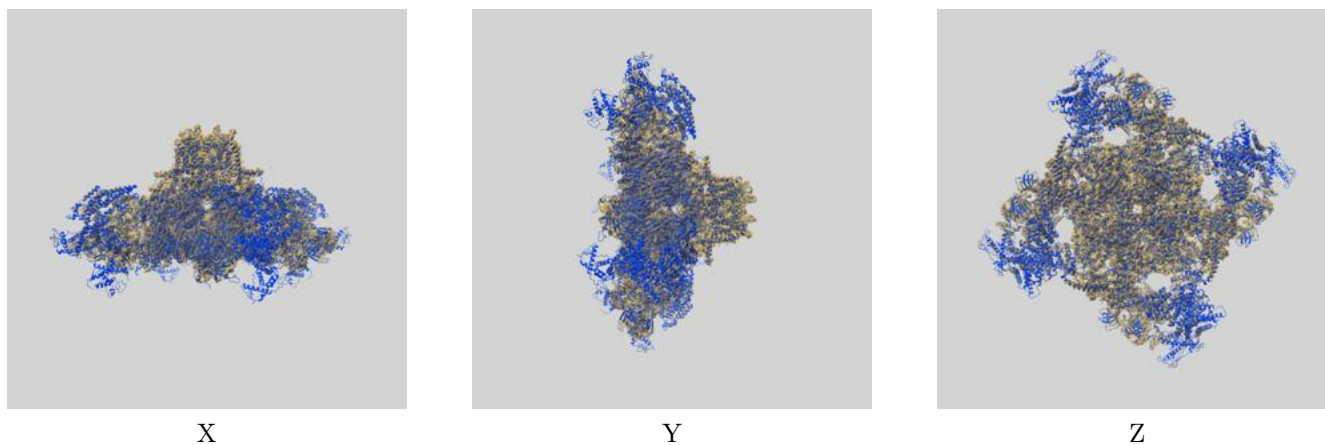
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.17                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.16                               | 7.24 | 4.21     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.17 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-47393 and PDB model 9E1G. Per-residue inclusion information can be found in section [3](#) on page [8](#).

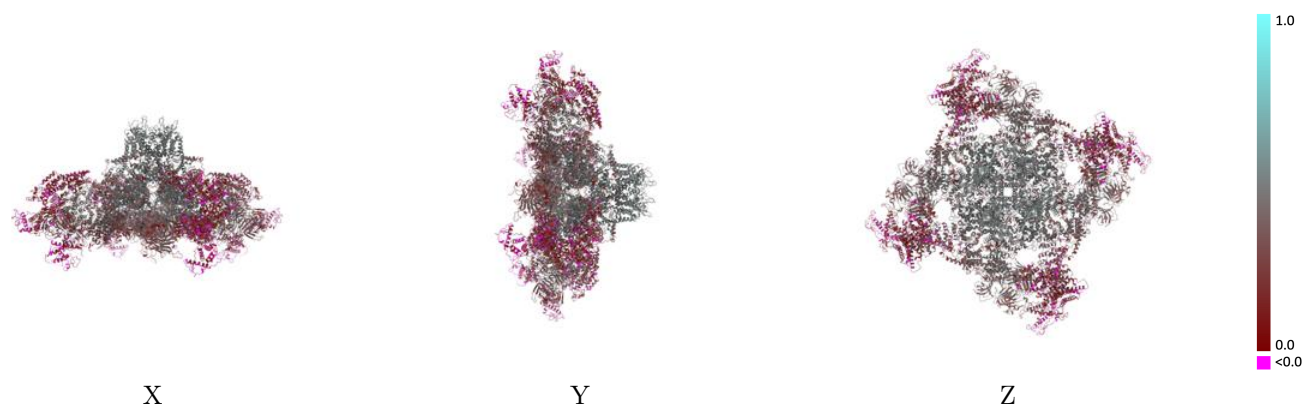
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

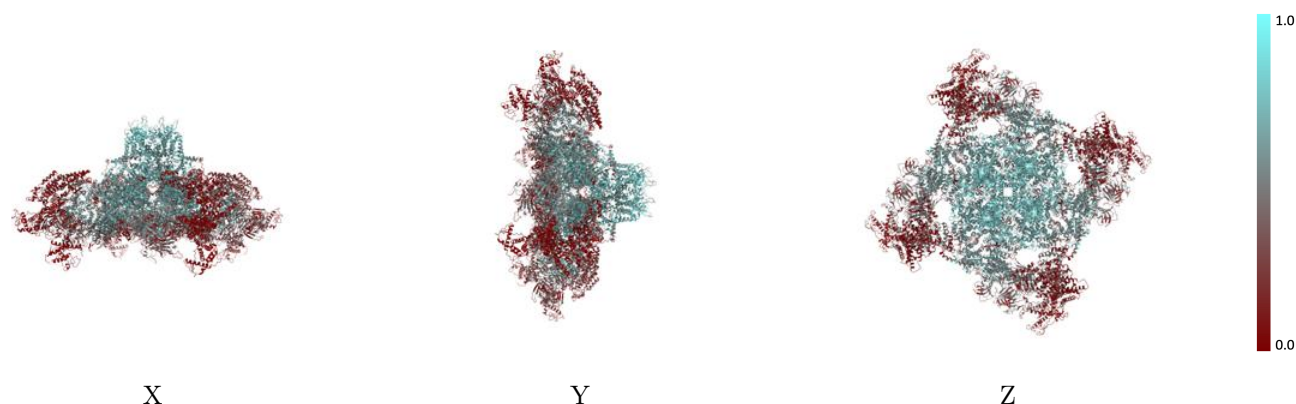


## 9.2 Q-score mapped to coordinate model [i](#)



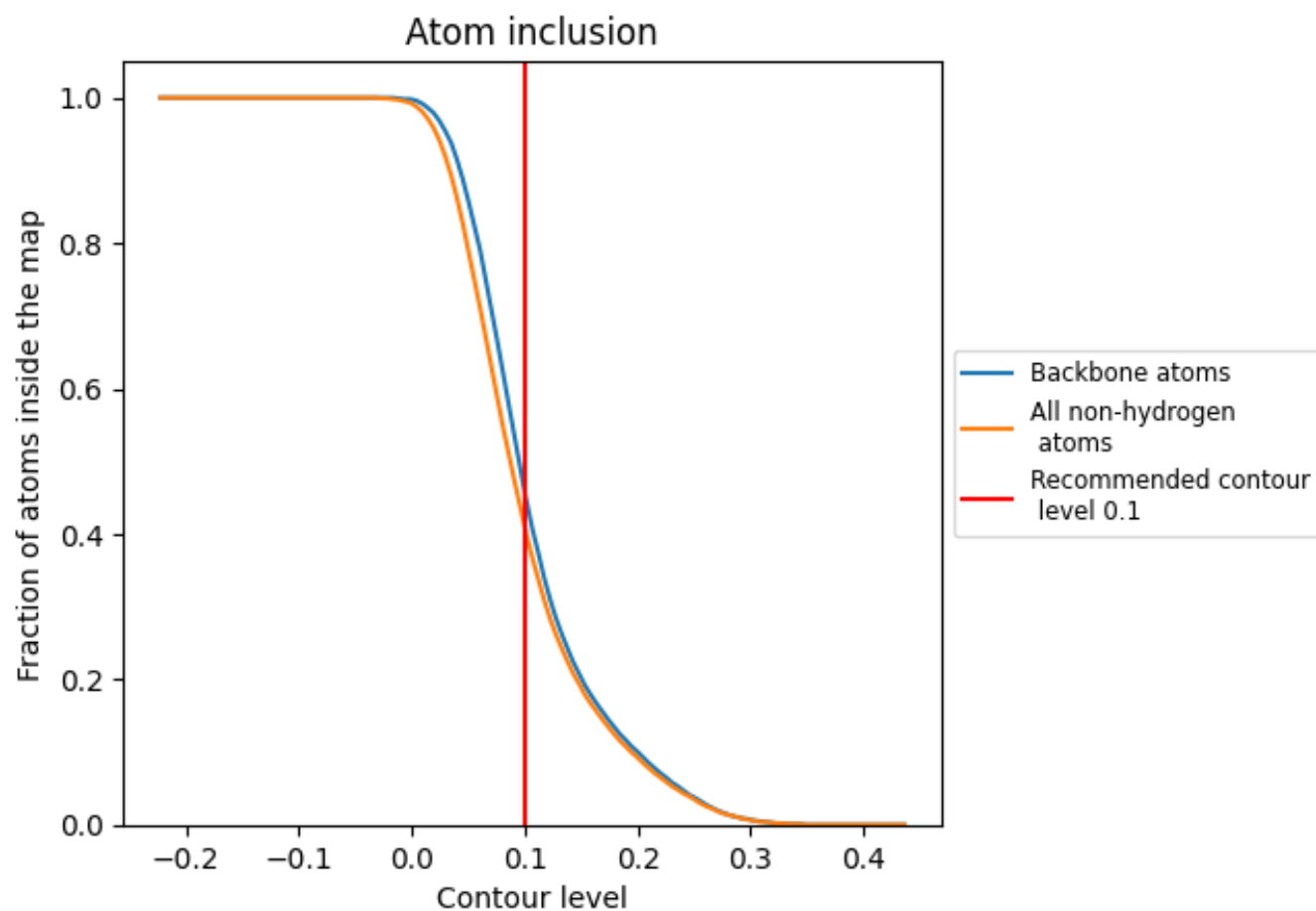
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 41% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.4080 | <div></div> 0.3230 |
| A     | <div></div> 0.4200 | <div></div> 0.3260 |
| B     | <div></div> 0.4200 | <div></div> 0.3210 |
| C     | <div></div> 0.4200 | <div></div> 0.3210 |
| D     | <div></div> 0.4200 | <div></div> 0.3210 |
| E     | <div></div> 0.2860 | <div></div> 0.3640 |
| F     | <div></div> 0.2850 | <div></div> 0.3620 |
| G     | <div></div> 0.2850 | <div></div> 0.3570 |
| H     | <div></div> 0.2860 | <div></div> 0.3640 |

1.0

0.0

<0.0