



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:08 PM GMT

PDB ID : 1IYJ  
Title : STRUCTURE OF A BRCA2-DSS1 COMPLEX  
Authors : Pavletich, N.P.; Jeffrey, P.D.; Yang, H.J.  
Deposited on : 2002-08-28  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

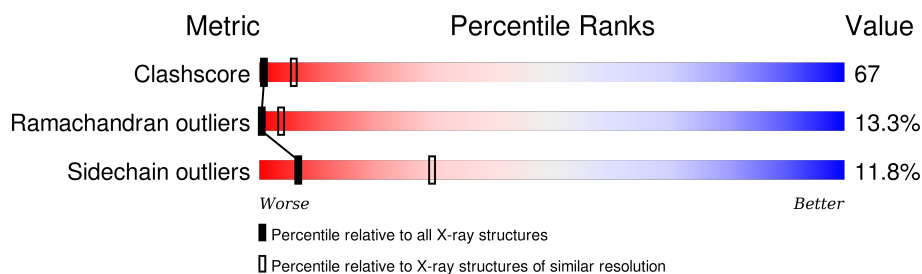
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 1611 (3.50-3.30)                                      |
| Ramachandran outliers | 100387                      | 1571 (3.50-3.30)                                      |
| Sidechain outliers    | 100360                      | 1571 (3.50-3.30)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 70     |                  |
| 1   | C     | 70     |                  |
| 2   | B     | 817    |                  |
| 2   | D     | 817    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10092 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Deleted in split hand/split foot protein 1.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 1   | A     | 45       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 380   | 235 | 59 | 86 |         |         |       |
| 1   | C     | 45       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 380   | 235 | 59 | 86 |         |         |       |

- Molecule 2 is a protein called breast cancer susceptibility.

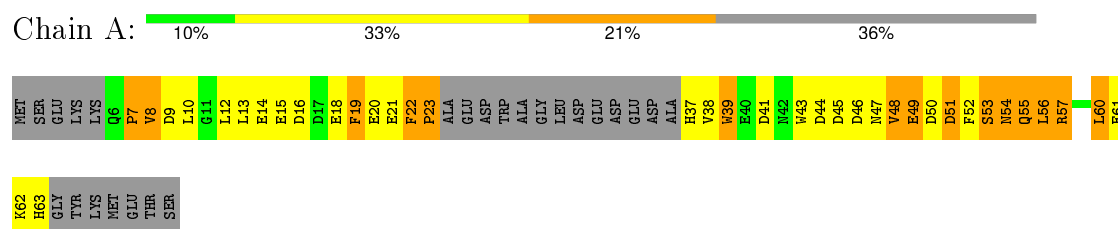
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 591      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4666  | 2984 | 805 | 862 | 15 |         |         |       |
| 2   | D     | 591      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4666  | 2984 | 805 | 862 | 15 |         |         |       |

### 3 Residue-property plots

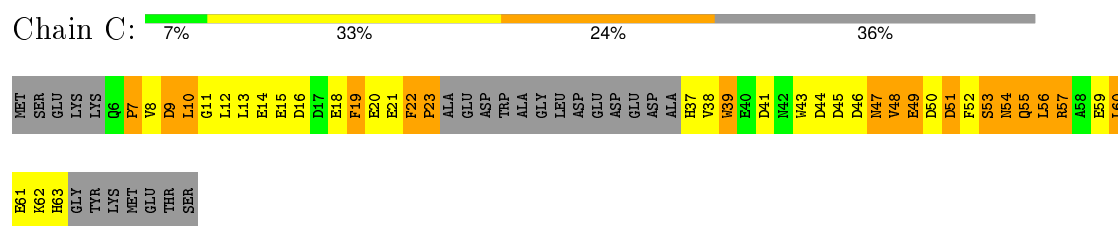
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

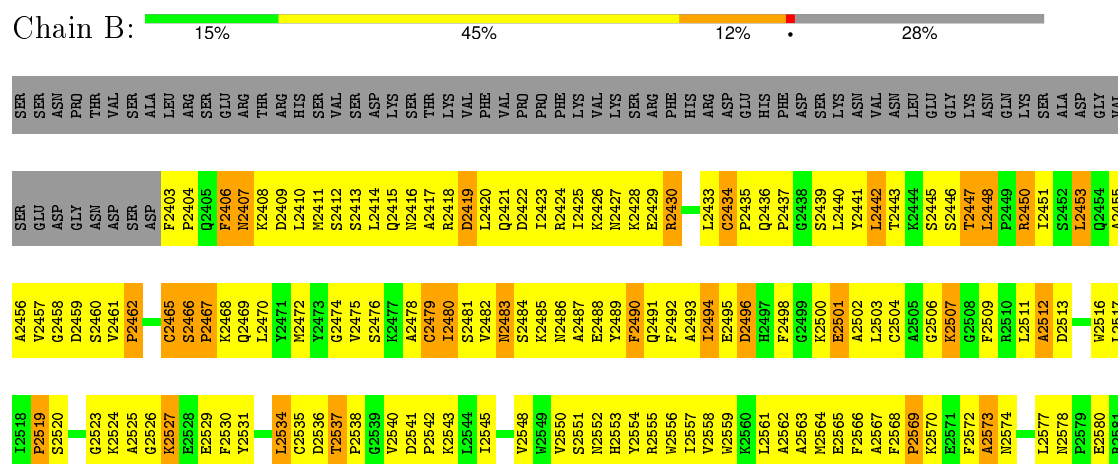
- Molecule 1: Deleted in split hand/split foot protein 1



- Molecule 1: Deleted in split hand/split foot protein 1



- Molecule 2: breast cancer susceptibility



|       |       |       |       |       |       |       |       |     |
|-------|-------|-------|-------|-------|-------|-------|-------|-----|
| V2582 | V2645 | S2709 |       | S2892 | I2953 | L3018 | R3085 | GLN |
| L2583 | V2646 | A2710 | R2772 | R2893 | Q2954 | V3019 | V3086 | LEU |
| L2584 | D2647 | N2711 | N2773 | R2894 | Q2955 | Y3020 | T3087 | PRO |
| Q2585 | T2648 | S2712 | E2776 | V2895 | T2956 | L3021 | N3088 | ARG |
| L2586 | L2651 | T2713 | E2777 | S2896 | A2957 | D3022 | M3089 | ASN |
| K2587 | L2652 | R2714 | E2778 | T2897 | T2958 | S3023 | K3090 | VAL |
| Y2588 | D2653 | P2715 | K2779 | V2898 | K2959 | E3024 | H3091 | SER |
| R2589 | G2654 | A2716 | K2780 | W2899 | T2960 | C3025 | A3092 | PRO |
| Y2590 | G2655 | R2717 | E2781 | K2900 | L2966 | L3026 | L3093 | ALA |
| D2591 | Y2656 | W2718 | A2782 | L2901 | L2967 | H3027 | E3094 | LEU |
| V2592 | A2657 | H2719 | L2781 | R2902 | P2967 | L3028 | N3095 | ARG |
| E2593 | V2658 | S2720 | R2783 | V2903 | V2968 | L3029 | I3096 | GLU |
|       |       | K2721 | F2784 | T2904 | S2969 | V3030 | D3097 | ARG |
|       |       | L2722 | ALA   | S2905 | S2970 | V3031 | T3098 | THR |
| N2596 | K2659 | L2723 | GLU   | Y2906 | E2971 | K3032 | F3099 | ARG |
| S2597 | A2660 | F2724 | ALA   | K2907 | S2972 | F3033 | Y3100 | THR |
| S2598 | L2662 | H2726 | GLN   | K2908 | T2972 | L3034 | K3101 | SER |
| R2599 | D2663 |       | THR   | R2909 | L2973 | I3035 | E3102 | VAL |
| S2600 | P2664 |       | CYS   | E2910 | Q2974 | D3036 | A3103 | SER |
| A2601 | P2665 |       | PHE   | S2911 | Q2975 | L3037 | E3104 | ASP |
| L2602 | L2666 | R2729 | LYS   | S2912 |       | N3038 | K3105 | LYS |
| K2603 | L2667 | P2730 | LEU   | A2913 | Q2978 | E3039 | K3106 | THR |
| K2604 | A2668 | F2731 | ALA   | L2914 | P2979 | D3040 | L3107 | THR |
| L2605 | L2669 | P2732 | GLU   | R2915 | R2980 | I3041 | I3108 | LYS |
| L2606 | L2670 | L2733 | LEU   | S2916 | E2981 | K3042 | Q3109 | VAL |
| E2607 | V2671 | P2734 | THR   | L2917 | L2982 | P3043 | V3110 | PHE |
| R2608 | K2671 | L2735 | LYS   | W2918 | L2983 | V3044 | L3111 | VAL |
| D2609 | S2672 | S2736 | VAL   | R2919 | P2984 | V3045 | K3112 | PRO |
| D2610 | G2673 | S2737 | LEU   | P2920 | F2985 | L3046 | G3113 | PRO |
| T2611 | R2674 | L2738 | ASN   | S2921 | S2986 | I3047 | D3114 | PHE |
| A2612 | L2675 | F2739 | THR   | S2922 | K2987 | A3048 | S3115 | LYS |
| L2613 | T2676 | S2740 | TYR   | R2923 | L2988 | A3049 | P3116 | VAL |
| K2614 | V2677 | D2741 | ARG   | L2924 | S2989 | S3050 | K3117 | VAL |
| T2615 | G2678 | G2742 | GLN   | P2925 | D2990 | N3051 | TRP   | ARG |
| L2616 | K2680 | N2744 | LEU   | S2926 | P2991 |       | SER   | PHE |
| V2620 | L2681 | V2745 | SER   | L2927 | A2992 | W3054 | THR   | HIS |
| S2621 | I2682 | G2746 | ASP   | L2928 | F2993 | R3055 | PRO   | ARG |
| D2622 | T2683 | C2747 | LYS   | T2929 | Q2994 | P3056 | ASN   | ASP |
| L2623 | G2684 | V2748 | ILE   | E2930 | P2995 | E3057 | LYS   | GLU |
| S2625 | A2686 | D2749 | ALA   | Q2931 | P2996 | S3058 | ASP   | THR |
| L2626 | E2687 | V2750 | ALA   | R2932 | C2997 | T3059 | PRO   | HIS |
| S2627 | E2688 | I2751 | ARG   | R2933 | S2998 | S3060 | THR   | PHE |
| THR   | V2689 | V2752 | ARG   | Y2934 | E2999 | R3061 | ARG   | ASP |
| ASN   |       | Q2753 | VAL   | R2935 | V3000 | V3062 | GLU   | SER |
| VAL   |       | R2754 | LEU   | L2936 | D3001 | P3063 | PRO   | LYS |
| SER   |       | V2755 | SER   | Y2937 | V3002 | T3064 | TYR   | ASN |
| GLU   |       | P2756 | ARG   | H2938 | V3005 | L3065 | PRO   | ASN |
| GLU   |       | P2757 | ALA   | S2939 | V3006 | A3067 | ALA   | ASP |
| THR   |       | L2758 | LYS   | S2940 | V3007 | G3068 | SER   | THR |
| SER   |       | Q2759 | ALA   | V2941 | S3008 | H3069 | CYS   | GLY |
| GLY   |       | W2760 | LEU   | S2942 | S3009 | F3070 | THR   | LYS |
| SER   |       | V2761 | GLN   | R2943 | V3009 | S3071 | SER   | LYS |
| LYS   |       | E2762 | GLN   | S2944 | V3010 | V3072 | ALA   | ASN |
| ALA   |       | K2763 | ALA   | R2945 | K3011 | F3073 | SER   | GLN |
| SER   |       | P2701 | VAL   | L2946 | P3012 |       | ASP   | LYS |
| SER   |       | L2704 | HIS   |       | I3013 |       | LEU   | SER |
| GLU   |       | R2705 | ALA   |       | G3014 |       | ALA   | ALA |
| ASP   |       | L2706 | LEU   |       | L3015 |       | F3082 | ASP |
| SER   |       | G2767 | GLN   |       | A3016 |       | GLY   | GLY |
| ASN   |       | Y2769 | GLY   |       | P3017 |       | GLY   | VAL |

• Molecule 2: breast cancer susceptibility

Chain D: 17% 43% 12% 28%

|     |       |       |       |       |
|-----|-------|-------|-------|-------|
| SER | SER   | S2459 | K2524 | Y2588 |
| SER | GLU   | S2460 | A2525 | R2589 |
| ASN | ASP   | T2461 | G2526 | R2590 |
| PRO | GLY   | P2462 | K2527 | I2591 |
| THR | ASN   | S2463 | E2528 | V2592 |
| VAL | ASP   | A2464 | E2529 | E2593 |
| SER | SER   | C2465 | F2530 |       |
| ALA | ASP   | S2466 | Y2531 | N2596 |
| LEU | F2403 | P2467 |       | S2597 |
| ARG | T2404 | K2468 | L2534 | S2598 |
| GLU | Q2405 | T2469 | C2535 | R2599 |
| ARG | P2406 | L2470 | D2536 | S2600 |
| THR | D2407 | V2471 | T2537 | A2601 |
| ARG | K2408 | D2472 | P2538 | L2602 |
| THR | D2409 |       | G2539 | K2603 |
| ARG | L2410 | V2475 | V2540 | K2604 |
| HIS | L2411 | S2476 | D2541 | L2605 |
| SER | N2412 | T2477 | P2542 | L2606 |
| VAL | S2412 | A2478 | K2543 | S2607 |
| VAL | S2413 | C2479 | L2544 | R2608 |
| ASP | L2414 | S2481 |       | D2609 |
| LYS | Q2415 | V2482 | V2545 | D2610 |
| SER | N2416 | D2483 |       | T2611 |
| THR | A2417 | S2484 | V2548 | A2612 |
| LYS | R2418 |       |       | L2613 |
| VAL | D2419 | S2484 | S2551 | K2614 |
| PHE | L2420 | V2485 | I2552 | T2615 |
| VAL | Q2421 | L2486 | R2553 | L2616 |
| PRO | D2422 | A2487 | T2554 |       |
| PRO | L2423 | E2488 | D2555 | V2620 |
| PHE | D2424 | V2489 | V2556 | S2621 |
| LYS | L2425 | T2490 | I2557 | D2622 |
| VAL | L2426 | Q2491 | V2558 | L2623 |
| LYS | N2427 | F2492 | D2559 | S2625 |
| ARG | E2428 | D2493 | L2561 | K2613 |
| SER | K2429 | T2494 | S2562 | L2626 |
| PHE | E2495 | D2496 | A2563 | S2627 |
| HIS | R2430 | L2497 | V2564 | THR   |
| ARG | L2433 | F2498 | E2565 | ASN   |
| ASP | C2434 | K2499 | F2566 | VAL   |
| GLU |       | R2500 | A2567 | SER   |
| PHE | Q2437 | E2501 | F2568 | GLU   |
| THR | S2439 | A2502 | P2569 | THR   |
| ASP | L2440 | L2503 | K2570 | SER   |
| SER | Y2441 | C2504 | E2571 | GLY   |
| LYS | T2442 | A2505 | F2572 | SER   |
| ASN | L2443 | G2506 | A2573 | LYS   |
| ASN | R2444 | K2507 | N2574 | ALA   |
| LEU | S2445 |       |       | SER   |
| GLY | S2446 | L2511 | L2577 | SER   |
| GLY | T2447 | A2512 | I2578 | GLU   |
| LYS | L2448 | D2513 | F2579 | ASP   |
| ASN | P2449 |       | E2580 | SER   |
| GLN | R2450 | W2516 | R2581 | ASN   |
| LYS | L2451 | L2517 | L2582 |       |
| SER | S2452 | L2518 | V2583 | K2645 |
| ALA | L2453 | P2519 | L2584 | D2647 |
| ASP |       | S2520 | Q2585 | T2648 |
| GLY | V2457 | G2523 | L2586 | L2649 |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| E3094 | M3095 | I3096 | D3097 | F3098 | F3099 | Y3100 | K3101 | E3102 | A3103 | E3104 | K3105 | K3106 | L3107 | I3108 | Q3109 | V3110 | L3111 | K3112 | G3113 | D3114 | S3115 | P3116 | K3117 | TRP   | SER   | THR   | PRO   | ASN   | LYS   | ASP   | PRO   | THR   | ARG   | GLU   | PRO   | TYR   | PRO   | ALA   | SER   | THR   | CYS   | SER   | ALA   | SER   | ASP   | LEU   | ALA   | SER   | THR   | ARG   | N3089 | K3090 | H3091 | A3092 | I3093 |       |       |       |       |       |       |       |
| C3025 | L3026 | H3027 | L3028 | L3029 | V3030 | V3031 | K3032 | F3033 | G3034 | L3035 | D3036 | L3037 | M3038 | E3039 | D3040 | I3041 | P3042 | R3043 | R3044 | V3045 | L3046 | I3047 | A3048 | A3049 | S3050 | N3051 | W3054 | R3055 | P3056 | E3057 | S3058 | T3059 | S3060 | R3061 | V3062 | P3063 | T3064 | L3065 | F3066 | G3067 | G3068 | N3069 | F3070 | S3071 | H3081 | F3082 | Q3083 | E3084 | R3085 | V3086 | T3087 | N3088 | M3089 | K3090 | H3091 | A3092 | I3093 |       |       |       |       |       |
| E2960 | T2961 | L2966 | P2967 | V2968 | S2969 | S2970 | E2971 | T2972 | L2973 | L2974 | Q2975 | Q2978 | P2979 | P2980 | E2981 | L2982 | L2983 | P2984 | F2985 | S2986 | K2987 | L2988 | S2989 | D2990 | P2991 | A2992 | F2993 | Q2994 | P2995 | P2996 | C2997 | S2998 | E2999 | V3000 | D3001 | V3002 | V3005 | V3006 | V3007 | S3008 | V3009 | V3010 | K3011 | P3012 | I3013 | G3014 | L3015 | A3016 | P3017 | L3018 | V3019 | V3020 | L3021 | S3022 | E3023 |       |       |       |       |       |       |       |
| W2899 | K2900 | I2901 | V2903 | T2904 | S2905 | Y2906 | K2907 | K2908 | R2909 | E2910 | K2911 | S2912 | A2913 | L2914 | L2915 | S2916 | I2917 | W2918 | R2919 | P2920 | S2921 | S2922 | D2923 | L2924 | P2925 | S2926 | L2927 | L2928 | T2929 | E2930 | G2931 | Q2932 | R2933 | Y2934 | R2935 | L2936 | Y2937 | E2938 | L2939 | S2940 | V2941 | S2942 | R2943 | S2944 | K2945 | N2946 | E2949 | W2950 | P2951 | S2952 | I2953 | Q2954 | L2955 | T2956 | A2957 | G2959 |       |       |       |       |       |       |
| GLN   | ASP   | ALA   | SER   | ASP   | PRO   | GLU   | HIS   | LEU   | GLU   | THR   | CYS   | PHE   | SER   | GLU   | GLU   | GLN   | LEU   | ARG   | ALA   | LEU   | ASN   | ASN   | THR   | TYR   | ARG   | GLN   | MET   | LEU   | SER   | ASP   | LYS   | LYS   | GLN   | ALA   | ALA   | ARG   | ARG   | ILE   | GLN   | VAL   | LEU   | SER   | ARG   | PHE   | GLN   | ARG   | ALA   | LEU   | THR   | GLN   | GLN   | VAL   | HIS   | S2892 | D2893 | D2894 | V2895 | S2896 | T2897 | V2898 |       |       |
| K2779 | E2780 | A2781 | L2782 | R2783 | T2784 | ALA   | GLU   | ALA   | GLN   | GLN   | LYS   | LYS   | LEU   | GLU   | L2732 | L2733 | P2730 | F2731 | L2734 | L2735 | S2736 | S2737 | L2738 | S2740 | D2741 | G2742 | G2743 | N2744 | V2745 | G2746 | C2747 | V2748 | D2749 | V2750 | I2751 | ARG   | ARG   | ILE   | GLN   | VAL   | LEU   | SER   | ARG   | ALA   | LEU   | THR   | GLN   | GLN   | VAL   | HIS   | S2765 | G2767 | S2769 | R2772 | N2773 | GLU   | A2710 | N2711 | R2775 | E2776 | A2777 | E2778 |
| A2716 | R2717 | A2718 | H2719 | L2782 | S2720 | K2721 | ALA   | F2724 | F2725 | H2726 | R2729 | P2730 | F2731 | L2734 | L2735 | S2736 | S2737 | L2738 | S2740 | D2741 | G2742 | G2743 | N2744 | V2745 | G2746 | C2747 | V2748 | D2749 | V2750 | I2751 | ARG   | ARG   | ILE   | GLN   | VAL   | LEU   | SER   | ARG   | ALA   | LEU   | THR   | GLN   | GLN   | VAL   | HIS   | S2765 | G2767 | S2769 | R2772 | N2773 | GLU   | A2710 | N2711 | R2775 | E2776 | A2777 | E2778 |       |       |       |       |       |
| T2652 | D2653 | G2654 | W2655 | Y2656 | A2657 | V2658 | K2659 | L2662 | D2663 | P2664 | P2665 | L2666 | L2667 | A2668 | L2669 | V2670 | K2671 | S2672 | G2673 | R2674 | L2675 | T2676 | V2677 | G2678 | Q2679 | K2680 | L2681 | L2682 | T2683 | Q2684 | G2685 | A2686 | E2687 | L2688 | V2689 | G2690 | S2691 | P2692 | D2693 | A2694 | P2697 | L2698 | P2701 | L2704 | R2705 | L2706 | K2707 | I2708 | S2709 | A2710 | N2711 | R2712 | T2713 | R2714 | P2715 |       |       |       |       |       |       |       |

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 43  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 130.31Å 130.31Å 192.62Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | 8.00 – 3.40                                     | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (8.00-3.40)                     | Depositor |
| $R_{merge}$  | (Not available)                                 | Depositor |
| $R_{sym}$  | (Not available)                                 | Depositor |
| Refinement program                                       | CNS   | Depositor |
| R, $R_{free}$  | 0.244 , 0.295                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 10092   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 56.0  | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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     | 0.42         | 0/388       | 0.80        | 1/526 (0.2%)   |
| 1   | C     | 0.41         | 0/388       | 0.80        | 1/526 (0.2%)   |
| 2   | B     | 0.42         | 0/4774      | 0.71        | 2/6475 (0.0%)  |
| 2   | D     | 0.42         | 0/4774      | 0.71        | 3/6475 (0.0%)  |
| All | All   | 0.42         | 0/10324     | 0.71        | 7/14002 (0.0%) |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 2467 | PRO  | N-CA-CB | 6.04  | 110.54      | 103.30   |
| 2   | D     | 2467 | PRO  | N-CA-CB | 5.96  | 110.45      | 103.30   |
| 1   | A     | 7    | PRO  | N-CA-CB | 5.61  | 110.03      | 103.30   |
| 1   | C     | 7    | PRO  | N-CA-CB | 5.50  | 109.90      | 103.30   |
| 2   | D     | 2941 | VAL  | N-CA-C  | -5.50 | 96.16       | 111.00   |
| 2   | B     | 2941 | VAL  | N-CA-C  | -5.38 | 96.48       | 111.00   |
| 2   | D     | 2501 | GLU  | N-CA-C  | -5.02 | 97.45       | 111.00   |

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     | 380   | 0        | 306      | 61      | 0            |
| 1   | C     | 380   | 0        | 306      | 66      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | B     | 4666  | 0        | 4694     | 652     | 0            |
| 2   | D     | 4666  | 0        | 4694     | 629     | 0            |
| All | All   | 10092 | 0        | 10000    | 1356    | 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 67.

All (1356) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2683:THR:HG22 | 2:D:2713:THR:HB   | 1.22                     | 1.16              |
| 2:D:2750:VAL:HG11 | 2:D:2903:VAL:HB   | 1.18                     | 1.16              |
| 2:B:2683:THR:HG22 | 2:B:2713:THR:HB   | 1.20                     | 1.13              |
| 2:B:2750:VAL:HG11 | 2:B:2903:VAL:HB   | 1.19                     | 1.12              |
| 2:B:2942:SER:HB3  | 2:B:2953:ILE:HD11 | 1.39                     | 1.03              |
| 2:B:2483:ASN:H    | 2:B:2486:ASN:ND2  | 1.56                     | 1.02              |
| 2:B:2483:ASN:N    | 2:B:2486:ASN:HD21 | 1.58                     | 1.02              |
| 2:D:2483:ASN:H    | 2:D:2486:ASN:ND2  | 1.57                     | 1.01              |
| 2:B:2404:PRO:HB2  | 2:B:2410:LEU:HD22 | 1.37                     | 1.01              |
| 2:B:3061:ARG:HG3  | 2:B:3062:VAL:HG12 | 1.41                     | 1.01              |
| 2:D:2950:TRP:H    | 2:D:2951:PRO:HD2  | 1.26                     | 1.00              |
| 2:D:2430:ARG:HG3  | 2:D:2430:ARG:HH11 | 1.27                     | 1.00              |
| 2:D:2483:ASN:N    | 2:D:2486:ASN:HD21 | 1.59                     | 0.99              |
| 2:B:2750:VAL:CG1  | 2:B:2903:VAL:HB   | 1.92                     | 0.99              |
| 2:B:2430:ARG:HH11 | 2:B:2430:ARG:HG3  | 1.28                     | 0.99              |
| 2:D:3061:ARG:HG3  | 2:D:3062:VAL:HG12 | 1.45                     | 0.99              |
| 2:B:2950:TRP:H    | 2:B:2951:PRO:HD2  | 1.26                     | 0.98              |
| 2:D:2483:ASN:H    | 2:D:2486:ASN:HD21 | 1.03                     | 0.98              |
| 2:D:2750:VAL:CG1  | 2:D:2903:VAL:HB   | 1.92                     | 0.98              |
| 2:D:2773:ASN:H    | 2:D:2776:GLU:HB2  | 1.29                     | 0.97              |
| 2:D:2773:ASN:ND2  | 2:D:2776:GLU:HG3  | 1.80                     | 0.96              |
| 2:B:2608:ARG:HH11 | 2:B:2608:ARG:HB2  | 1.30                     | 0.95              |
| 2:B:2959:LYS:HD3  | 2:B:2959:LYS:H    | 1.32                     | 0.95              |
| 2:D:2665:PRO:HG3  | 2:D:2742:GLY:HA2  | 1.44                     | 0.95              |
| 2:B:2773:ASN:H    | 2:B:2776:GLU:HB2  | 1.32                     | 0.94              |
| 2:D:2942:SER:HB3  | 2:D:2953:ILE:HD11 | 1.45                     | 0.94              |
| 2:D:2758:LEU:HD21 | 2:D:2897:THR:HB   | 1.50                     | 0.93              |
| 2:B:2403:PHE:HA   | 2:B:2503:LEU:HD11 | 1.52                     | 0.92              |
| 2:D:2959:LYS:H    | 2:D:2959:LYS:HD3  | 1.30                     | 0.91              |
| 2:B:2483:ASN:H    | 2:B:2486:ASN:HD21 | 0.99                     | 0.91              |
| 2:D:2608:ARG:HB2  | 2:D:2608:ARG:HH11 | 1.34                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2608:ARG:HH22 | 2:B:2688:LEU:HD23 | 1.37                     | 0.90              |
| 2:B:2758:LEU:HD21 | 2:B:2897:THR:HB   | 1.50                     | 0.90              |
| 2:B:2773:ASN:ND2  | 2:B:2776:GLU:HG3  | 1.85                     | 0.90              |
| 2:B:2665:PRO:HG3  | 2:B:2742:GLY:HA2  | 1.53                     | 0.89              |
| 2:D:2709:SER:O    | 2:D:2713:THR:HG22 | 1.72                     | 0.88              |
| 2:D:2917:ILE:HG22 | 2:D:2920:PRO:HG3  | 1.56                     | 0.87              |
| 2:B:2917:ILE:HD13 | 2:B:2924:LEU:HD21 | 1.54                     | 0.87              |
| 2:D:2656:TYR:CD2  | 2:D:2697:PRO:HB2  | 2.10                     | 0.87              |
| 2:B:2750:VAL:HG11 | 2:B:2903:VAL:CB   | 2.04                     | 0.87              |
| 2:B:2709:SER:O    | 2:B:2713:THR:HG22 | 1.76                     | 0.86              |
| 2:D:2750:VAL:HG11 | 2:D:2903:VAL:CB   | 2.03                     | 0.86              |
| 2:D:2552:ASN:HD21 | 2:D:2556:TRP:HE1  | 1.23                     | 0.86              |
| 2:D:2944:SER:HB2  | 2:D:2954:GLN:HE21 | 1.41                     | 0.85              |
| 2:D:2426:LYS:HG3  | 2:D:2430:ARG:HH22 | 1.41                     | 0.85              |
| 2:B:2430:ARG:NH1  | 2:B:2430:ARG:HG3  | 1.88                     | 0.85              |
| 2:B:2608:ARG:HH11 | 2:B:2608:ARG:CB   | 1.88                     | 0.85              |
| 2:B:2552:ASN:HD21 | 2:B:2556:TRP:HE1  | 1.21                     | 0.85              |
| 2:B:3116:PRO:O    | 2:B:3117:LYS:HG2  | 1.77                     | 0.85              |
| 2:D:2608:ARG:CB   | 2:D:2608:ARG:HH11 | 1.89                     | 0.85              |
| 2:D:2917:ILE:HD13 | 2:D:2924:LEU:HD21 | 1.57                     | 0.84              |
| 2:B:2944:SER:HB2  | 2:B:2954:GLN:HE21 | 1.41                     | 0.84              |
| 2:D:3048:ALA:HB1  | 2:D:3082:PHE:CD2  | 2.12                     | 0.84              |
| 2:B:2414:LEU:HD23 | 2:B:2506:GLY:HA2  | 1.59                     | 0.84              |
| 2:D:2953:ILE:HG13 | 2:D:2954:GLN:H    | 1.41                     | 0.84              |
| 2:D:2430:ARG:HG3  | 2:D:2430:ARG:NH1  | 1.89                     | 0.84              |
| 2:B:2656:TYR:CD2  | 2:B:2697:PRO:HB2  | 2.13                     | 0.83              |
| 2:B:3048:ALA:HB1  | 2:B:3082:PHE:CD2  | 2.13                     | 0.83              |
| 2:D:2733:LEU:HD23 | 2:D:2733:LEU:H    | 1.43                     | 0.83              |
| 2:B:2744:ASN:HB2  | 2:B:2940:SER:CB   | 2.09                     | 0.83              |
| 2:D:2608:ARG:HH22 | 2:D:2688:LEU:HD23 | 1.43                     | 0.83              |
| 2:D:2904:THR:OG1  | 2:D:2910:GLU:HB2  | 1.79                     | 0.83              |
| 2:B:2902:ARG:HH11 | 2:B:2902:ARG:HB2  | 1.42                     | 0.83              |
| 2:D:2739:PHE:HB2  | 2:D:2742:GLY:HA3  | 1.60                     | 0.82              |
| 2:D:2414:LEU:HD23 | 2:D:2506:GLY:HA2  | 1.59                     | 0.82              |
| 2:B:2426:LYS:HG3  | 2:B:2430:ARG:HH22 | 1.45                     | 0.82              |
| 2:D:2902:ARG:HB2  | 2:D:2902:ARG:HH11 | 1.43                     | 0.82              |
| 2:D:2683:THR:HG22 | 2:D:2713:THR:CB   | 2.09                     | 0.82              |
| 2:D:2421:GLN:HB2  | 2:D:2424:ARG:NH2  | 1.95                     | 0.82              |
| 2:B:2953:ILE:HG13 | 2:B:2954:GLN:H    | 1.44                     | 0.81              |
| 2:B:2764:THR:HB   | 2:B:2767:GLY:O    | 1.80                     | 0.81              |
| 2:B:2752:VAL:HA   | 2:B:2903:VAL:HG12 | 1.62                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2683:THR:CG2  | 2:B:2713:THR:HB   | 2.06                     | 0.81              |
| 2:B:2904:THR:OG1  | 2:B:2910:GLU:HB2  | 1.81                     | 0.81              |
| 2:B:2404:PRO:HG2  | 2:B:2504:CYS:HA   | 1.63                     | 0.81              |
| 2:D:2980:ARG:HH21 | 2:D:3051:ASN:HD21 | 1.29                     | 0.81              |
| 2:D:3030:VAL:HG23 | 2:D:3062:VAL:HG22 | 1.62                     | 0.80              |
| 2:B:2683:THR:HG22 | 2:B:2713:THR:CB   | 2.06                     | 0.80              |
| 2:B:2713:THR:O    | 2:B:2714:ARG:HD3  | 1.81                     | 0.80              |
| 2:B:2490:PHE:CZ   | 2:B:2577:LEU:HD21 | 2.16                     | 0.80              |
| 2:D:2750:VAL:HG12 | 2:D:2751:ILE:H    | 1.46                     | 0.80              |
| 2:B:2739:PHE:HB2  | 2:B:2742:GLY:HA3  | 1.63                     | 0.80              |
| 2:D:2437:PRO:HG2  | 2:D:2442:LEU:HD11 | 1.63                     | 0.79              |
| 2:B:2950:TRP:H    | 2:B:2951:PRO:CD   | 1.95                     | 0.79              |
| 2:B:2479:CYS:O    | 2:B:2482:VAL:HG12 | 1.82                     | 0.79              |
| 2:B:2744:ASN:HB2  | 2:B:2940:SER:HB3  | 1.64                     | 0.79              |
| 2:D:3009:VAL:HG22 | 2:D:3019:VAL:HG22 | 1.61                     | 0.79              |
| 2:B:2917:ILE:HG22 | 2:B:2920:PRO:HG3  | 1.64                     | 0.79              |
| 2:B:3030:VAL:HG23 | 2:B:3062:VAL:HG22 | 1.64                     | 0.79              |
| 2:D:2764:THR:HB   | 2:D:2767:GLY:O    | 1.82                     | 0.79              |
| 2:D:2933:ARG:HB3  | 2:D:2966:LEU:O    | 1.83                     | 0.79              |
| 2:B:2773:ASN:HD21 | 2:B:2776:GLU:HG3  | 1.46                     | 0.78              |
| 2:D:2589:ARG:HG2  | 2:D:2655:TRP:CH2  | 2.18                     | 0.78              |
| 2:D:2744:ASN:HB2  | 2:D:2940:SER:CB   | 2.13                     | 0.78              |
| 2:D:2744:ASN:HB2  | 2:D:2940:SER:HB3  | 1.66                     | 0.78              |
| 2:B:2687:GLU:HB2  | 2:B:2707:LYS:HB3  | 1.63                     | 0.78              |
| 2:B:3007:VAL:HB   | 2:B:3104:GLU:CD   | 2.03                     | 0.78              |
| 2:B:2589:ARG:HH11 | 2:B:2589:ARG:HG3  | 1.49                     | 0.78              |
| 2:D:2683:THR:CG2  | 2:D:2713:THR:HB   | 2.09                     | 0.78              |
| 2:D:2404:PRO:HB2  | 2:D:2410:LEU:HD22 | 1.64                     | 0.78              |
| 2:D:2675:LEU:HD21 | 2:D:2681:ILE:HD11 | 1.64                     | 0.78              |
| 2:B:2733:LEU:H    | 2:B:2733:LEU:HD23 | 1.48                     | 0.78              |
| 2:D:2950:TRP:H    | 2:D:2951:PRO:CD   | 1.95                     | 0.78              |
| 2:D:2427:ASN:HA   | 2:D:2430:ARG:CZ   | 2.14                     | 0.77              |
| 2:D:2479:CYS:O    | 2:D:2482:VAL:HG12 | 1.84                     | 0.77              |
| 2:D:2484:SER:HB2  | 2:D:2559:TRP:CZ2  | 2.19                     | 0.77              |
| 2:B:2558:VAL:HG13 | 2:B:2577:LEU:HD11 | 1.64                     | 0.77              |
| 2:D:2614:LYS:CG   | 2:D:2615:THR:H    | 1.98                     | 0.77              |
| 2:D:2666:LEU:HG   | 2:D:2710:ALA:HB2  | 1.67                     | 0.76              |
| 2:B:2772:ARG:HA   | 2:B:2776:GLU:OE1  | 1.85                     | 0.76              |
| 2:D:2426:LYS:O    | 2:D:2430:ARG:NH1  | 2.19                     | 0.76              |
| 2:D:2773:ASN:HD21 | 2:D:2776:GLU:HG3  | 1.47                     | 0.76              |
| 2:B:2750:VAL:HG12 | 2:B:2751:ILE:H    | 1.51                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2980:ARG:NH2  | 2:D:3051:ASN:HD21 | 1.84                     | 0.76              |
| 2:B:2909:ARG:O    | 2:B:2910:GLU:HG2  | 1.86                     | 0.76              |
| 2:D:2713:THR:O    | 2:D:2714:ARG:HD3  | 1.84                     | 0.75              |
| 2:B:2738:LEU:HD13 | 2:B:2745:VAL:HG21 | 1.69                     | 0.75              |
| 2:B:2427:ASN:HA   | 2:B:2430:ARG:CZ   | 2.15                     | 0.75              |
| 2:D:3007:VAL:HB   | 2:D:3104:GLU:CD   | 2.05                     | 0.75              |
| 2:B:2980:ARG:HH21 | 2:B:3051:ASN:HD21 | 1.33                     | 0.75              |
| 2:D:2589:ARG:HH11 | 2:D:2589:ARG:HG3  | 1.52                     | 0.75              |
| 1:A:56:LEU:H      | 2:B:2462:PRO:HG2  | 1.51                     | 0.75              |
| 2:B:3113:GLY:O    | 2:B:3114:ASP:HB2  | 1.87                     | 0.75              |
| 2:D:2909:ARG:O    | 2:D:2910:GLU:HG2  | 1.86                     | 0.75              |
| 2:D:3048:ALA:HB1  | 2:D:3082:PHE:HD2  | 1.52                     | 0.75              |
| 2:B:2413:SER:HB2  | 2:B:2506:GLY:HA3  | 1.69                     | 0.75              |
| 1:A:54:ASN:O      | 1:A:55:GLN:HB2    | 1.85                     | 0.74              |
| 2:B:2933:ARG:HB3  | 2:B:2966:LEU:O    | 1.86                     | 0.74              |
| 1:C:54:ASN:O      | 1:C:55:GLN:HB2    | 1.87                     | 0.74              |
| 2:D:2780:GLU:HA   | 2:D:2783:ARG:HB3  | 1.70                     | 0.74              |
| 1:A:62:LYS:HE3    | 2:B:2676:THR:HG21 | 1.70                     | 0.74              |
| 2:B:2985:PHE:HD1  | 2:B:2985:PHE:H    | 1.36                     | 0.74              |
| 2:D:2501:GLU:C    | 2:D:2503:LEU:H    | 1.90                     | 0.74              |
| 2:D:3017:PRO:O    | 2:D:3018:LEU:HD23 | 1.87                     | 0.74              |
| 2:D:3083:GLN:HA   | 2:D:3086:VAL:HG12 | 1.70                     | 0.73              |
| 2:B:2944:SER:HB2  | 2:B:2954:GLN:NE2  | 2.02                     | 0.73              |
| 2:B:2940:SER:O    | 2:B:2941:VAL:HG23 | 1.87                     | 0.73              |
| 2:D:2494:ILE:HD12 | 2:D:2495:GLU:H    | 1.53                     | 0.73              |
| 2:D:3033:PHE:HA   | 2:D:3067:ALA:HB3  | 1.71                     | 0.73              |
| 2:B:3009:VAL:HG22 | 2:B:3019:VAL:HG22 | 1.70                     | 0.73              |
| 2:B:2614:LYS:CG   | 2:B:2615:THR:H    | 1.99                     | 0.73              |
| 2:D:2534:LEU:HD22 | 2:D:2540:VAL:HG21 | 1.68                     | 0.73              |
| 2:B:3083:GLN:HA   | 2:B:3086:VAL:HG12 | 1.68                     | 0.73              |
| 2:B:2450:ARG:HB3  | 2:B:2450:ARG:NH1  | 2.04                     | 0.73              |
| 2:B:3048:ALA:HB1  | 2:B:3082:PHE:HD2  | 1.52                     | 0.73              |
| 1:A:43:TRP:HZ3    | 2:B:2713:THR:HG23 | 1.53                     | 0.73              |
| 2:B:3030:VAL:HG23 | 2:B:3062:VAL:CG2  | 2.19                     | 0.73              |
| 2:D:2404:PRO:HG2  | 2:D:2504:CYS:HA   | 1.71                     | 0.72              |
| 2:B:3010:VAL:HG12 | 2:B:3012:PRO:HD3  | 1.70                     | 0.72              |
| 2:D:2558:VAL:HG13 | 2:D:2577:LEU:HD11 | 1.70                     | 0.72              |
| 2:D:2944:SER:HB2  | 2:D:2954:GLN:NE2  | 2.03                     | 0.72              |
| 2:D:2687:GLU:HB2  | 2:D:2707:LYS:HB3  | 1.70                     | 0.72              |
| 2:B:2534:LEU:HD22 | 2:B:2540:VAL:HG21 | 1.70                     | 0.72              |
| 2:D:2413:SER:HB2  | 2:D:2506:GLY:HA3  | 1.71                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:3002:VAL:HG22 | 2:B:3049:ALA:HB3  | 1.70                     | 0.72              |
| 2:D:2494:ILE:HG21 | 2:D:2519:PRO:HG3  | 1.72                     | 0.72              |
| 2:B:2780:GLU:HA   | 2:B:2783:ARG:HB3  | 1.71                     | 0.72              |
| 2:B:2610:ASP:C    | 2:B:2612:ALA:H    | 1.91                     | 0.72              |
| 2:B:2501:GLU:C    | 2:B:2503:LEU:H    | 1.91                     | 0.72              |
| 2:D:2610:ASP:C    | 2:D:2612:ALA:H    | 1.94                     | 0.72              |
| 2:D:2512:ALA:CB   | 2:D:2584:LEU:HG   | 2.20                     | 0.71              |
| 2:B:2666:LEU:HG   | 2:B:2710:ALA:HB2  | 1.71                     | 0.71              |
| 2:D:2490:PHE:CZ   | 2:D:2577:LEU:HD21 | 2.25                     | 0.71              |
| 2:D:2940:SER:O    | 2:D:2941:VAL:HG23 | 1.91                     | 0.71              |
| 2:D:2772:ARG:HA   | 2:D:2776:GLU:OE1  | 1.90                     | 0.71              |
| 2:D:2761:VAL:C    | 2:D:2895:VAL:HG23 | 2.11                     | 0.71              |
| 2:D:2733:LEU:HD23 | 2:D:2733:LEU:N    | 2.05                     | 0.71              |
| 2:D:2922:SER:O    | 2:D:2925:PRO:HD2  | 1.91                     | 0.71              |
| 2:B:2604:LYS:HB3  | 2:B:2610:ASP:HB3  | 1.72                     | 0.71              |
| 2:D:2620:VAL:HG23 | 2:D:2678:GLY:H    | 1.54                     | 0.71              |
| 2:B:2494:ILE:HD12 | 2:B:2495:GLU:H    | 1.54                     | 0.71              |
| 2:B:2494:ILE:HG21 | 2:B:2519:PRO:HG3  | 1.71                     | 0.71              |
| 2:B:2483:ASN:N    | 2:B:2486:ASN:ND2  | 2.27                     | 0.71              |
| 2:B:2620:VAL:HG23 | 2:B:2678:GLY:H    | 1.55                     | 0.71              |
| 2:B:3028:LEU:HD12 | 2:B:3111:LEU:HD22 | 1.71                     | 0.70              |
| 2:B:2761:VAL:C    | 2:B:2895:VAL:HG23 | 2.11                     | 0.70              |
| 2:B:3033:PHE:HA   | 2:B:3067:ALA:HB3  | 1.73                     | 0.70              |
| 1:C:39:TRP:HE1    | 2:D:2733:LEU:HD22 | 1.57                     | 0.70              |
| 2:B:2403:PHE:HA   | 2:B:2503:LEU:CD1  | 2.20                     | 0.70              |
| 2:B:2484:SER:HB2  | 2:B:2559:TRP:CZ2  | 2.27                     | 0.70              |
| 2:D:3030:VAL:HG23 | 2:D:3062:VAL:CG2  | 2.21                     | 0.70              |
| 2:D:2483:ASN:N    | 2:D:2486:ASN:ND2  | 2.26                     | 0.70              |
| 2:B:2421:GLN:HB2  | 2:B:2424:ARG:NH2  | 2.06                     | 0.70              |
| 2:D:2756:TYR:HD2  | 2:D:3070:PHE:HB3  | 1.57                     | 0.69              |
| 2:D:3029:LEU:C    | 2:D:3029:LEU:HD23 | 2.12                     | 0.69              |
| 2:D:3002:VAL:HG22 | 2:D:3049:ALA:HB3  | 1.74                     | 0.69              |
| 2:D:2620:VAL:HG23 | 2:D:2678:GLY:N    | 2.06                     | 0.69              |
| 2:B:3005:VAL:HG22 | 2:B:3046:LEU:HD11 | 1.72                     | 0.69              |
| 2:D:2752:VAL:HA   | 2:D:2903:VAL:HG12 | 1.73                     | 0.69              |
| 2:B:2733:LEU:HD23 | 2:B:2733:LEU:N    | 2.08                     | 0.69              |
| 2:B:2476:SER:OG   | 2:B:2478:ALA:HB3  | 1.92                     | 0.69              |
| 2:B:2610:ASP:O    | 2:B:2612:ALA:N    | 2.25                     | 0.69              |
| 2:D:2476:SER:OG   | 2:D:2478:ALA:HB3  | 1.92                     | 0.69              |
| 2:B:2663:ASP:OD2  | 2:B:2666:LEU:HB2  | 1.91                     | 0.69              |
| 2:D:2985:PHE:H    | 2:D:2985:PHE:HD1  | 1.40                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2758:LEU:HD23 | 2:D:2759:GLN:N    | 2.07                     | 0.69              |
| 2:D:2604:LYS:HB3  | 2:D:2610:ASP:HB3  | 1.74                     | 0.69              |
| 2:D:2747:CYS:SG   | 2:D:2937:TYR:HE1  | 2.15                     | 0.69              |
| 2:D:2646:VAL:HB   | 2:D:2671:LYS:HE3  | 1.74                     | 0.69              |
| 2:B:2922:SER:O    | 2:B:2925:PRO:HD2  | 1.92                     | 0.69              |
| 2:D:2663:ASP:OD2  | 2:D:2666:LEU:HB2  | 1.93                     | 0.69              |
| 2:D:2936:ILE:CG2  | 2:D:2939:LEU:HB2  | 2.23                     | 0.68              |
| 2:B:2620:VAL:HG23 | 2:B:2678:GLY:N    | 2.08                     | 0.68              |
| 2:D:2450:ARG:HB3  | 2:D:2450:ARG:NH1  | 2.07                     | 0.68              |
| 2:D:3055:ARG:O    | 2:D:3057:GLU:HG2  | 1.94                     | 0.68              |
| 2:B:2672:SER:HB2  | 2:B:2674:ARG:HG2  | 1.75                     | 0.68              |
| 2:D:2936:ILE:HG22 | 2:D:2939:LEU:HB2  | 1.74                     | 0.68              |
| 2:D:3028:LEU:HD12 | 2:D:3111:LEU:HD22 | 1.74                     | 0.68              |
| 2:D:3111:LEU:O    | 2:D:3112:LYS:HD3  | 1.94                     | 0.68              |
| 2:B:2915:LEU:HD12 | 2:B:2916:SER:N    | 2.09                     | 0.68              |
| 2:B:3029:LEU:HD23 | 2:B:3029:LEU:C    | 2.15                     | 0.68              |
| 2:B:2512:ALA:CB   | 2:B:2584:LEU:HG   | 2.24                     | 0.67              |
| 2:B:2475:VAL:HG12 | 2:B:2480:ILE:HG13 | 1.76                     | 0.67              |
| 2:B:2662:LEU:HD22 | 2:B:2666:LEU:HD13 | 1.76                     | 0.67              |
| 2:B:2494:ILE:HG22 | 2:B:2498:PHE:CE1  | 2.30                     | 0.67              |
| 2:B:2589:ARG:HG2  | 2:B:2655:TRP:CH2  | 2.29                     | 0.67              |
| 2:D:2601:ALA:O    | 2:D:2605:ILE:HG12 | 1.94                     | 0.67              |
| 2:D:2729:ARG:HD3  | 2:D:2730:PRO:HD2  | 1.77                     | 0.67              |
| 2:B:2520:SER:OG   | 2:B:2524:LYS:HB2  | 1.94                     | 0.67              |
| 2:B:2430:ARG:CG   | 2:B:2430:ARG:HH11 | 2.04                     | 0.67              |
| 1:A:39:TRP:HE1    | 2:B:2733:LEU:HD22 | 1.59                     | 0.67              |
| 2:B:2450:ARG:HB3  | 2:B:2450:ARG:HH11 | 1.60                     | 0.67              |
| 2:D:2756:TYR:HB3  | 2:D:2757:PRO:HD2  | 1.76                     | 0.66              |
| 2:D:2610:ASP:O    | 2:D:2612:ALA:N    | 2.27                     | 0.66              |
| 2:D:3010:VAL:HG12 | 2:D:3012:PRO:HD3  | 1.76                     | 0.66              |
| 1:C:56:LEU:H      | 2:D:2462:PRO:HG2  | 1.59                     | 0.66              |
| 2:B:3107:LEU:HD23 | 2:B:3108:ILE:N    | 2.10                     | 0.66              |
| 2:B:2413:SER:CB   | 2:B:2506:GLY:HA3  | 2.25                     | 0.66              |
| 2:B:2441:TYR:O    | 2:B:2445:SER:HB3  | 1.96                     | 0.66              |
| 2:B:2919:ARG:N    | 2:B:2920:PRO:HD3  | 2.11                     | 0.66              |
| 2:D:2441:TYR:O    | 2:D:2445:SER:HB3  | 1.95                     | 0.66              |
| 2:D:2953:ILE:HG13 | 2:D:2954:GLN:N    | 2.11                     | 0.66              |
| 2:D:2534:LEU:O    | 2:D:2537:THR:HB   | 1.96                     | 0.66              |
| 2:D:2541:ASP:OD1  | 2:D:2543:LYS:HB2  | 1.95                     | 0.65              |
| 1:A:51:ASP:HB3    | 2:B:2717:ARG:HG3  | 1.78                     | 0.65              |
| 2:B:2541:ASP:OD1  | 2:B:2543:LYS:HB2  | 1.95                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2466:SER:O    | 2:D:2468:LYS:N    | 2.29                     | 0.65              |
| 2:D:2425:ILE:HG23 | 2:D:2542:PRO:HG2  | 1.78                     | 0.65              |
| 2:B:2426:LYS:O    | 2:B:2430:ARG:NH1  | 2.29                     | 0.65              |
| 2:D:3037:LEU:O    | 2:D:3039:GLU:N    | 2.24                     | 0.65              |
| 2:B:2646:VAL:HB   | 2:B:2671:LYS:HE3  | 1.78                     | 0.65              |
| 2:D:2413:SER:CB   | 2:D:2506:GLY:HA3  | 2.26                     | 0.65              |
| 2:D:2764:THR:HG22 | 2:D:2765:VAL:H    | 1.62                     | 0.65              |
| 2:D:2567:ALA:C    | 2:D:2569:PRO:HD3  | 2.17                     | 0.65              |
| 2:D:2404:PRO:HD3  | 2:D:2503:LEU:CD1  | 2.27                     | 0.65              |
| 2:D:2484:SER:HB2  | 2:D:2559:TRP:CE2  | 2.31                     | 0.65              |
| 2:D:2672:SER:HB2  | 2:D:2674:ARG:HG2  | 1.76                     | 0.65              |
| 2:D:2919:ARG:N    | 2:D:2920:PRO:HD3  | 2.11                     | 0.65              |
| 2:B:2927:LEU:HD11 | 2:B:2934:TYR:HE1  | 1.62                     | 0.65              |
| 2:B:2675:LEU:HD21 | 2:B:2681:ILE:HD11 | 1.78                     | 0.65              |
| 2:B:3111:LEU:O    | 2:B:3112:LYS:HD3  | 1.96                     | 0.65              |
| 2:B:2758:LEU:HD23 | 2:B:2759:GLN:N    | 2.12                     | 0.65              |
| 2:D:2614:LYS:CG   | 2:D:2615:THR:N    | 2.60                     | 0.65              |
| 2:B:3017:PRO:O    | 2:B:3018:LEU:HD23 | 1.96                     | 0.65              |
| 2:D:2667:LEU:O    | 2:D:2667:LEU:HD23 | 1.96                     | 0.64              |
| 2:D:2714:ARG:HG3  | 2:D:2715:PRO:HD2  | 1.79                     | 0.64              |
| 2:B:2980:ARG:NH2  | 2:B:3051:ASN:HD21 | 1.94                     | 0.64              |
| 2:D:2918:TRP:C    | 2:D:2920:PRO:HD3  | 2.18                     | 0.64              |
| 2:D:2747:CYS:SG   | 2:D:2937:TYR:CE1  | 2.91                     | 0.64              |
| 2:B:2466:SER:O    | 2:B:2468:LYS:N    | 2.30                     | 0.64              |
| 2:B:2978:GLN:HG2  | 2:B:2996:PRO:HG2  | 1.79                     | 0.64              |
| 2:D:3031:VAL:HA   | 2:D:3065:LEU:O    | 1.97                     | 0.64              |
| 2:D:2512:ALA:O    | 2:D:2513:ASP:HB2  | 1.95                     | 0.64              |
| 2:B:2410:LEU:O    | 2:B:2414:LEU:HG   | 1.96                     | 0.64              |
| 2:B:2428:LYS:HD3  | 2:B:2542:PRO:HD3  | 1.79                     | 0.64              |
| 1:A:13:LEU:HD12   | 2:B:2451:ILE:O    | 1.96                     | 0.64              |
| 2:B:2959:LYS:H    | 2:B:2959:LYS:CD   | 2.09                     | 0.64              |
| 2:D:2939:LEU:HG   | 2:D:2939:LEU:O    | 1.98                     | 0.64              |
| 2:D:2662:LEU:HD22 | 2:D:2666:LEU:HD13 | 1.79                     | 0.64              |
| 2:B:2736:SER:HB3  | 2:B:2909:ARG:HH21 | 1.63                     | 0.64              |
| 2:B:2526:GLY:H    | 2:B:2529:GLU:HB2  | 1.62                     | 0.64              |
| 2:D:2738:LEU:HD13 | 2:D:2745:VAL:HG21 | 1.80                     | 0.64              |
| 2:B:2902:ARG:NH1  | 2:B:2902:ARG:HB2  | 2.10                     | 0.63              |
| 2:B:2764:THR:HG22 | 2:B:2765:VAL:H    | 1.63                     | 0.63              |
| 2:D:2620:VAL:HG21 | 2:D:2676:THR:O    | 1.98                     | 0.63              |
| 2:D:3058:SER:O    | 2:D:3059:THR:HB   | 1.97                     | 0.63              |
| 2:B:2984:PRO:HG2  | 2:B:2987:LYS:CG   | 2.27                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2567:ALA:C    | 2:B:2569:PRO:HD3  | 2.18                     | 0.63              |
| 2:D:2736:SER:HB3  | 2:D:2909:ARG:HH21 | 1.63                     | 0.63              |
| 2:B:2489:TYR:O    | 2:B:2490:PHE:HB3  | 1.96                     | 0.63              |
| 2:D:3087:THR:HG22 | 2:D:3088:ASN:N    | 2.12                     | 0.63              |
| 2:B:2893:ARG:O    | 2:B:2894:ASP:HB3  | 1.99                     | 0.63              |
| 2:B:2620:VAL:HG21 | 2:B:2676:THR:O    | 1.99                     | 0.63              |
| 2:D:2450:ARG:HB3  | 2:D:2450:ARG:HH11 | 1.61                     | 0.63              |
| 2:D:3107:LEU:HD23 | 2:D:3108:ILE:N    | 2.14                     | 0.63              |
| 2:B:2616:LEU:HD13 | 2:B:2724:PHE:CD2  | 2.34                     | 0.63              |
| 2:B:2738:LEU:CD1  | 2:B:2745:VAL:HG21 | 2.28                     | 0.62              |
| 2:B:3058:SER:O    | 2:B:3059:THR:HB   | 1.99                     | 0.62              |
| 2:B:3061:ARG:HG2  | 2:B:3061:ARG:HH11 | 1.64                     | 0.62              |
| 2:B:2939:LEU:HG   | 2:B:2939:LEU:O    | 1.99                     | 0.62              |
| 2:B:2404:PRO:HD3  | 2:B:2503:LEU:CD1  | 2.29                     | 0.62              |
| 2:B:2747:CYS:SG   | 2:B:2937:TYR:HE1  | 2.21                     | 0.62              |
| 2:B:3100:TYR:O    | 2:B:3102:GLU:N    | 2.33                     | 0.62              |
| 1:A:16:ASP:OD2    | 1:A:57:ARG:NH2    | 2.32                     | 0.62              |
| 2:D:2520:SER:OG   | 2:D:2524:LYS:HB2  | 1.99                     | 0.62              |
| 2:D:2503:LEU:O    | 2:D:2503:LEU:HD13 | 1.99                     | 0.62              |
| 2:B:2437:PRO:HG2  | 2:B:2442:LEU:HD11 | 1.82                     | 0.62              |
| 2:D:2751:ILE:O    | 2:D:2751:ILE:HG23 | 1.99                     | 0.62              |
| 2:B:3037:LEU:O    | 2:B:3039:GLU:N    | 2.29                     | 0.62              |
| 2:B:2414:LEU:CD2  | 2:B:2506:GLY:HA2  | 2.29                     | 0.62              |
| 2:D:2902:ARG:HB2  | 2:D:2902:ARG:NH1  | 2.14                     | 0.62              |
| 1:C:56:LEU:O      | 1:C:57:ARG:CB     | 2.48                     | 0.62              |
| 1:A:56:LEU:O      | 1:A:57:ARG:CB     | 2.48                     | 0.62              |
| 2:D:2915:LEU:HD12 | 2:D:2916:SER:N    | 2.14                     | 0.62              |
| 2:B:2745:VAL:HG12 | 2:B:2746:GLY:N    | 2.15                     | 0.62              |
| 2:D:2500:LYS:HD3  | 2:D:2503:LEU:HD12 | 1.81                     | 0.62              |
| 2:D:2995:PRO:HD2  | 2:D:3054:TRP:CZ3  | 2.35                     | 0.62              |
| 2:D:2972:THR:O    | 2:D:2975:GLN:HB3  | 2.00                     | 0.61              |
| 2:B:2425:ILE:HG23 | 2:B:2542:PRO:HG2  | 1.82                     | 0.61              |
| 2:B:2614:LYS:CG   | 2:B:2615:THR:N    | 2.62                     | 0.61              |
| 2:D:2944:SER:HB3  | 2:D:2952:SER:O    | 1.99                     | 0.61              |
| 2:B:2936:ILE:CG2  | 2:B:2939:LEU:HB2  | 2.30                     | 0.61              |
| 2:B:2693:ASP:O    | 2:B:2694:ALA:HB3  | 2.00                     | 0.61              |
| 2:D:2475:VAL:HG12 | 2:D:2480:ILE:HG13 | 1.82                     | 0.61              |
| 2:D:2761:VAL:HG13 | 2:D:2761:VAL:O    | 2.01                     | 0.61              |
| 2:B:2552:ASN:ND2  | 2:B:2556:TRP:NE1  | 2.46                     | 0.61              |
| 2:B:2537:THR:HG23 | 2:B:2538:PRO:HD2  | 1.82                     | 0.61              |
| 2:D:2755:VAL:HG13 | 2:D:2899:TRP:HE1  | 1.64                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:3116:PRO:O    | 2:B:3117:LYS:CG   | 2.48                     | 0.61              |
| 2:B:2936:ILE:HG22 | 2:B:2939:LEU:HB2  | 1.80                     | 0.61              |
| 2:D:2985:PHE:CE2  | 2:D:3029:LEU:HD13 | 2.36                     | 0.61              |
| 2:D:2893:ARG:O    | 2:D:2894:ASP:HB3  | 2.01                     | 0.61              |
| 2:B:2763:LYS:HB2  | 2:B:2894:ASP:OD2  | 2.00                     | 0.61              |
| 2:D:2404:PRO:HD3  | 2:D:2503:LEU:HD12 | 1.82                     | 0.61              |
| 2:B:3002:VAL:CG2  | 2:B:3049:ALA:HB3  | 2.31                     | 0.61              |
| 1:A:50:ASP:CG     | 1:A:51:ASP:H      | 2.04                     | 0.61              |
| 2:D:2714:ARG:NH2  | 2:D:2733:LEU:HD12 | 2.16                     | 0.61              |
| 2:B:3026:LEU:HD21 | 2:B:3104:GLU:HA   | 1.81                     | 0.61              |
| 2:B:2751:ILE:HG22 | 2:B:2904:THR:O    | 2.00                     | 0.61              |
| 2:D:2984:PRO:HG2  | 2:D:2987:LYS:CG   | 2.30                     | 0.61              |
| 2:D:3015:LEU:O    | 2:D:3016:ALA:HB3  | 2.01                     | 0.61              |
| 2:D:2407:ASN:O    | 2:D:2411:MET:HG3  | 2.01                     | 0.61              |
| 2:B:2972:THR:O    | 2:B:2975:GLN:HB3  | 2.00                     | 0.61              |
| 2:D:2430:ARG:HH11 | 2:D:2430:ARG:CG   | 2.04                     | 0.61              |
| 2:D:3061:ARG:HH11 | 2:D:3061:ARG:HG2  | 1.65                     | 0.61              |
| 1:C:62:LYS:HE3    | 2:D:2676:THR:HG21 | 1.81                     | 0.61              |
| 2:B:2984:PRO:HG2  | 2:B:2987:LYS:HG2  | 1.82                     | 0.61              |
| 2:D:2997:CYS:O    | 2:D:2999:GLU:HG3  | 2.01                     | 0.61              |
| 2:B:2714:ARG:HG3  | 2:B:2715:PRO:HD2  | 1.82                     | 0.61              |
| 2:B:2406:PHE:O    | 2:B:2408:LYS:N    | 2.34                     | 0.61              |
| 2:D:2565:GLU:CD   | 2:D:2574:ASN:HA   | 2.21                     | 0.61              |
| 2:D:3100:TYR:O    | 2:D:3102:GLU:N    | 2.34                     | 0.60              |
| 2:D:2565:GLU:HG2  | 2:D:2572:PHE:O    | 2.01                     | 0.60              |
| 2:B:2601:ALA:O    | 2:B:2605:ILE:HG12 | 2.00                     | 0.60              |
| 2:D:2982:LEU:O    | 2:D:2984:PRO:HD3  | 2.00                     | 0.60              |
| 2:B:2732:PRO:HB3  | 2:B:2747:CYS:SG   | 2.42                     | 0.60              |
| 2:B:2747:CYS:SG   | 2:B:2937:TYR:CE1  | 2.94                     | 0.60              |
| 2:D:2719:HIS:CG   | 2:D:2720:SER:H    | 2.20                     | 0.60              |
| 2:B:2918:TRP:C    | 2:B:2920:PRO:HD3  | 2.22                     | 0.60              |
| 2:B:2995:PRO:HD2  | 2:B:3054:TRP:CZ3  | 2.37                     | 0.60              |
| 2:D:2750:VAL:HG12 | 2:D:2751:ILE:N    | 2.15                     | 0.60              |
| 2:D:2614:LYS:HG2  | 2:D:2615:THR:N    | 2.16                     | 0.60              |
| 2:B:2751:ILE:O    | 2:B:2751:ILE:HG23 | 2.01                     | 0.60              |
| 2:B:2756:TYR:HD2  | 2:B:3070:PHE:HB3  | 1.65                     | 0.60              |
| 2:B:2500:LYS:HD3  | 2:B:2503:LEU:HD12 | 1.83                     | 0.60              |
| 2:D:2410:LEU:O    | 2:D:2414:LEU:HG   | 2.02                     | 0.60              |
| 2:B:2457:VAL:HG11 | 2:B:2568:PHE:CE2  | 2.37                     | 0.60              |
| 2:D:2754:ARG:HA   | 2:D:2930:GLU:OE2  | 2.01                     | 0.60              |
| 2:B:2717:ARG:HH11 | 2:B:2717:ARG:HG2  | 1.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2953:ILE:HG13 | 2:B:2954:GLN:N    | 2.13                     | 0.60              |
| 2:D:2494:ILE:HG22 | 2:D:2498:PHE:CE1  | 2.36                     | 0.60              |
| 2:B:2484:SER:HB2  | 2:B:2559:TRP:CE2  | 2.37                     | 0.60              |
| 2:D:2526:GLY:H    | 2:D:2529:GLU:HB2  | 1.65                     | 0.60              |
| 2:B:3055:ARG:O    | 2:B:3057:GLU:HG2  | 2.01                     | 0.60              |
| 2:D:2693:ASP:O    | 2:D:2694:ALA:HB3  | 2.00                     | 0.60              |
| 2:D:2917:ILE:CG2  | 2:D:2920:PRO:HG3  | 2.32                     | 0.60              |
| 2:D:2589:ARG:HG2  | 2:D:2655:TRP:CZ3  | 2.36                     | 0.60              |
| 2:D:3001:ASP:OD1  | 2:D:3050:SER:HA   | 2.02                     | 0.60              |
| 2:B:2503:LEU:O    | 2:B:2503:LEU:HD13 | 2.00                     | 0.59              |
| 2:D:2580:GLU:O    | 2:D:2584:LEU:HB2  | 2.02                     | 0.59              |
| 2:B:3087:THR:HG22 | 2:B:3088:ASN:N    | 2.16                     | 0.59              |
| 2:B:2744:ASN:HB2  | 2:B:2940:SER:HB2  | 1.84                     | 0.59              |
| 2:B:2414:LEU:HD23 | 2:B:2506:GLY:CA   | 2.29                     | 0.59              |
| 2:D:3005:VAL:HG22 | 2:D:3046:LEU:HD11 | 1.83                     | 0.59              |
| 1:C:56:LEU:O      | 1:C:57:ARG:HB2    | 2.01                     | 0.59              |
| 2:B:2614:LYS:HG2  | 2:B:2615:THR:N    | 2.17                     | 0.59              |
| 1:C:50:ASP:CG     | 1:C:51:ASP:H      | 2.04                     | 0.59              |
| 2:D:2500:LYS:HA   | 2:D:2503:LEU:HB3  | 1.84                     | 0.59              |
| 2:B:2534:LEU:O    | 2:B:2537:THR:HB   | 2.02                     | 0.59              |
| 2:B:2602:LEU:HB2  | 2:B:2653:ASP:OD2  | 2.02                     | 0.59              |
| 2:D:2754:ARG:HB2  | 2:D:2756:TYR:CE1  | 2.38                     | 0.59              |
| 1:A:43:TRP:CH2    | 2:B:2666:LEU:HD21 | 2.37                     | 0.59              |
| 2:D:2949:GLU:HB3  | 2:D:2951:PRO:HD2  | 1.85                     | 0.59              |
| 2:B:2592:VAL:HG12 | 2:B:2593:GLU:N    | 2.18                     | 0.59              |
| 2:B:3015:LEU:O    | 2:B:3016:ALA:HB3  | 2.02                     | 0.59              |
| 2:B:3031:VAL:HA   | 2:B:3065:LEU:O    | 2.03                     | 0.59              |
| 2:B:2949:GLU:HB3  | 2:B:2951:PRO:HD2  | 1.85                     | 0.59              |
| 1:C:51:ASP:HB3    | 2:D:2717:ARG:HG3  | 1.84                     | 0.59              |
| 2:B:2997:CYS:O    | 2:B:2999:GLU:HG3  | 2.03                     | 0.59              |
| 2:B:2756:TYR:HB3  | 2:B:2757:PRO:HD2  | 1.84                     | 0.59              |
| 2:D:2738:LEU:CD1  | 2:D:2745:VAL:HG21 | 2.33                     | 0.59              |
| 2:D:2973:LEU:C    | 2:D:2975:GLN:H    | 2.06                     | 0.58              |
| 2:B:3028:LEU:HD12 | 2:B:3111:LEU:CD2  | 2.32                     | 0.58              |
| 2:D:2984:PRO:HG2  | 2:D:2987:LYS:HG2  | 1.84                     | 0.58              |
| 2:D:3110:VAL:C    | 2:D:3112:LYS:H    | 2.04                     | 0.58              |
| 2:D:2933:ARG:NH1  | 2:D:2966:LEU:HB3  | 2.18                     | 0.58              |
| 2:D:2756:TYR:N    | 2:D:2756:TYR:CD1  | 2.70                     | 0.58              |
| 2:B:2414:LEU:O    | 2:B:2416:ASN:N    | 2.36                     | 0.58              |
| 2:B:2404:PRO:HD3  | 2:B:2503:LEU:HD12 | 1.84                     | 0.58              |
| 2:D:2428:LYS:O    | 2:D:2430:ARG:N    | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2494:ILE:HD12 | 2:D:2494:ILE:N    | 2.18                     | 0.58              |
| 2:B:2933:ARG:NH1  | 2:B:2966:LEU:HB3  | 2.18                     | 0.58              |
| 2:D:2602:LEU:HB2  | 2:D:2653:ASP:OD2  | 2.03                     | 0.58              |
| 2:D:2616:LEU:HD13 | 2:D:2724:PHE:CD2  | 2.38                     | 0.58              |
| 2:D:3023:ASP:OD1  | 2:D:3027:HIS:HB2  | 2.04                     | 0.58              |
| 2:B:2720:SER:OG   | 2:B:2721:LYS:N    | 2.36                     | 0.58              |
| 2:B:3001:ASP:OD1  | 2:B:3050:SER:HA   | 2.02                     | 0.58              |
| 1:C:37:HIS:O      | 1:C:38:VAL:HG12   | 2.04                     | 0.58              |
| 2:D:2927:LEU:HD11 | 2:D:2934:TYR:HE1  | 1.67                     | 0.58              |
| 2:D:3002:VAL:CG2  | 2:D:3049:ALA:HB3  | 2.33                     | 0.58              |
| 2:B:2500:LYS:HA   | 2:B:2503:LEU:HB3  | 1.84                     | 0.58              |
| 2:D:3055:ARG:HG2  | 2:D:3056:PRO:HD2  | 1.86                     | 0.58              |
| 1:C:15:GLU:HB2    | 1:C:18:GLU:HG3    | 1.85                     | 0.58              |
| 2:B:2667:LEU:HD23 | 2:B:2667:LEU:O    | 2.04                     | 0.58              |
| 2:B:3094:GLU:C    | 2:B:3096:ILE:H    | 2.06                     | 0.58              |
| 2:B:3110:VAL:C    | 2:B:3112:LYS:H    | 2.07                     | 0.58              |
| 2:D:3094:GLU:C    | 2:D:3096:ILE:H    | 2.05                     | 0.58              |
| 2:D:2512:ALA:HB1  | 2:D:2584:LEU:HG   | 1.86                     | 0.58              |
| 2:B:2616:LEU:HD13 | 2:B:2724:PHE:HD2  | 1.68                     | 0.58              |
| 2:B:2483:ASN:ND2  | 2:B:2486:ASN:HD22 | 2.02                     | 0.58              |
| 2:B:3097:ASP:C    | 2:B:3099:PHE:H    | 2.07                     | 0.57              |
| 1:A:56:LEU:O      | 1:A:57:ARG:HB2    | 2.04                     | 0.57              |
| 2:B:2756:TYR:CD1  | 2:B:2756:TYR:N    | 2.72                     | 0.57              |
| 2:B:3090:LYS:O    | 2:B:3094:GLU:HG3  | 2.04                     | 0.57              |
| 1:C:16:ASP:OD2    | 1:C:57:ARG:NH2    | 2.37                     | 0.57              |
| 2:B:2418:ARG:O    | 2:B:2421:GLN:N    | 2.37                     | 0.57              |
| 2:D:2732:PRO:HB3  | 2:D:2747:CYS:SG   | 2.44                     | 0.57              |
| 2:D:2717:ARG:HH11 | 2:D:2717:ARG:HG2  | 1.68                     | 0.57              |
| 2:B:2754:ARG:HB2  | 2:B:2756:TYR:CE1  | 2.38                     | 0.57              |
| 2:B:2512:ALA:O    | 2:B:2513:ASP:HB2  | 2.04                     | 0.57              |
| 2:B:2982:LEU:O    | 2:B:2984:PRO:HD3  | 2.04                     | 0.57              |
| 2:D:2720:SER:OG   | 2:D:2721:LYS:N    | 2.37                     | 0.57              |
| 2:B:2664:PRO:HB2  | 2:B:2741:ASP:OD2  | 2.04                     | 0.57              |
| 2:D:3007:VAL:HB   | 2:D:3104:GLU:OE2  | 2.03                     | 0.57              |
| 1:A:56:LEU:HD23   | 1:A:57:ARG:HB2    | 1.86                     | 0.57              |
| 2:B:2939:LEU:HD11 | 2:B:2955:LEU:HB3  | 1.85                     | 0.57              |
| 2:B:2719:HIS:CG   | 2:B:2720:SER:H    | 2.21                     | 0.57              |
| 1:C:43:TRP:C      | 1:C:45:ASP:H      | 2.07                     | 0.57              |
| 2:B:2479:CYS:SG   | 2:B:2480:ILE:N    | 2.78                     | 0.57              |
| 2:D:2763:LYS:HB2  | 2:D:2894:ASP:OD2  | 2.04                     | 0.57              |
| 2:D:2465:CYS:SG   | 2:D:2466:SER:N    | 2.76                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:21:GLU:HG3    | 1:C:22:PHE:CD2    | 2.39                     | 0.57              |
| 2:D:2665:PRO:HG3  | 2:D:2742:GLY:CA   | 2.29                     | 0.57              |
| 2:D:2953:ILE:CG1  | 2:D:2954:GLN:H    | 2.14                     | 0.57              |
| 2:D:2537:THR:HG23 | 2:D:2538:PRO:HD2  | 1.86                     | 0.57              |
| 2:D:2489:TYR:O    | 2:D:2490:PHE:HB3  | 2.04                     | 0.57              |
| 2:B:2750:VAL:HG12 | 2:B:2751:ILE:N    | 2.18                     | 0.57              |
| 2:D:2745:VAL:HG12 | 2:D:2746:GLY:N    | 2.20                     | 0.57              |
| 2:D:2428:LYS:C    | 2:D:2430:ARG:H    | 2.08                     | 0.57              |
| 2:D:2987:LYS:C    | 2:D:2989:SER:H    | 2.08                     | 0.57              |
| 2:D:3090:LYS:O    | 2:D:3094:GLU:HG3  | 2.04                     | 0.57              |
| 2:B:3018:LEU:HD21 | 2:B:3032:LYS:HG2  | 1.86                     | 0.57              |
| 2:B:3055:ARG:HG2  | 2:B:3056:PRO:HD2  | 1.86                     | 0.57              |
| 2:B:2665:PRO:HG3  | 2:B:2742:GLY:CA   | 2.31                     | 0.57              |
| 2:B:2978:GLN:HG2  | 2:B:2996:PRO:CG   | 2.34                     | 0.57              |
| 2:B:2469:GLN:O    | 2:B:2472:MET:HB3  | 2.05                     | 0.57              |
| 1:A:8:VAL:O       | 1:A:10:LEU:N      | 2.38                     | 0.57              |
| 1:C:38:VAL:HG22   | 1:C:38:VAL:O      | 2.03                     | 0.57              |
| 2:D:2667:LEU:C    | 2:D:2667:LEU:HD23 | 2.25                     | 0.56              |
| 2:B:2944:SER:HB3  | 2:B:2952:SER:O    | 2.05                     | 0.56              |
| 2:B:2953:ILE:CG1  | 2:B:2954:GLN:H    | 2.17                     | 0.56              |
| 2:D:2906:TYR:CD1  | 2:D:2933:ARG:NE   | 2.72                     | 0.56              |
| 2:B:2565:GLU:HG2  | 2:B:2572:PHE:O    | 2.05                     | 0.56              |
| 2:B:2973:LEU:C    | 2:B:2975:GLN:H    | 2.07                     | 0.56              |
| 2:D:2483:ASN:ND2  | 2:D:2486:ASN:HD22 | 2.04                     | 0.56              |
| 2:B:3093:ILE:HG23 | 2:B:3094:GLU:N    | 2.20                     | 0.56              |
| 2:D:2414:LEU:HD23 | 2:D:2506:GLY:CA   | 2.31                     | 0.56              |
| 2:B:2468:LYS:C    | 2:B:2470:LEU:H    | 2.09                     | 0.56              |
| 2:B:2624:ILE:CD1  | 2:B:2659:LYS:HE3  | 2.35                     | 0.56              |
| 2:D:2552:ASN:ND2  | 2:D:2556:TRP:NE1  | 2.47                     | 0.56              |
| 2:B:2945:LYS:HD2  | 2:B:2945:LYS:O    | 2.05                     | 0.56              |
| 1:A:43:TRP:C      | 1:A:45:ASP:H      | 2.08                     | 0.56              |
| 2:D:2780:GLU:HG3  | 2:D:2780:GLU:O    | 2.06                     | 0.56              |
| 1:A:21:GLU:HG3    | 1:A:22:PHE:CD2    | 2.41                     | 0.56              |
| 1:A:15:GLU:HB2    | 1:A:18:GLU:HG3    | 1.87                     | 0.56              |
| 2:D:2468:LYS:C    | 2:D:2470:LEU:H    | 2.09                     | 0.56              |
| 2:D:2945:LYS:O    | 2:D:2945:LYS:HD2  | 2.05                     | 0.56              |
| 2:B:2761:VAL:O    | 2:B:2761:VAL:HG13 | 2.05                     | 0.56              |
| 2:D:2494:ILE:O    | 2:D:2498:PHE:HD1  | 1.89                     | 0.56              |
| 1:A:18:GLU:OE1    | 2:B:2450:ARG:NH2  | 2.39                     | 0.56              |
| 2:B:2745:VAL:HB   | 2:B:2940:SER:OG   | 2.06                     | 0.56              |
| 2:D:2761:VAL:HG12 | 2:D:2896:SER:O    | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2937:TYR:O    | 2:D:2961:THR:HA   | 2.06                     | 0.56              |
| 2:B:2666:LEU:HA   | 2:B:2669:LEU:HD12 | 1.87                     | 0.55              |
| 2:B:2745:VAL:CG1  | 2:B:2746:GLY:N    | 2.69                     | 0.55              |
| 2:D:2744:ASN:HB2  | 2:D:2940:SER:HB2  | 1.87                     | 0.55              |
| 2:D:3026:LEU:HD21 | 2:D:3104:GLU:HA   | 1.88                     | 0.55              |
| 2:B:2693:ASP:O    | 2:B:2694:ALA:CB   | 2.54                     | 0.55              |
| 1:C:49:GLU:C      | 1:C:53:SER:OG     | 2.45                     | 0.55              |
| 2:D:2745:VAL:HB   | 2:D:2940:SER:OG   | 2.06                     | 0.55              |
| 2:D:2693:ASP:O    | 2:D:2694:ALA:CB   | 2.54                     | 0.55              |
| 2:B:2729:ARG:HD3  | 2:B:2730:PRO:HD2  | 1.89                     | 0.55              |
| 2:B:3018:LEU:CD2  | 2:B:3032:LYS:HG2  | 2.36                     | 0.55              |
| 2:B:2945:LYS:C    | 2:B:2945:LYS:HD2  | 2.26                     | 0.55              |
| 2:D:3097:ASP:C    | 2:D:3099:PHE:H    | 2.08                     | 0.55              |
| 2:D:2783:ARG:HH11 | 2:D:2783:ARG:HG3  | 1.71                     | 0.55              |
| 2:B:2937:TYR:O    | 2:B:2961:THR:HA   | 2.07                     | 0.55              |
| 2:D:2655:TRP:C    | 2:D:2656:TYR:CD1  | 2.79                     | 0.55              |
| 2:B:2669:LEU:O    | 2:B:2674:ARG:HB2  | 2.06                     | 0.55              |
| 2:B:2494:ILE:HD12 | 2:B:2494:ILE:N    | 2.22                     | 0.55              |
| 2:B:2758:LEU:HD22 | 2:B:2760:TRP:CZ3  | 2.42                     | 0.55              |
| 2:B:3007:VAL:HB   | 2:B:3104:GLU:OE2  | 2.06                     | 0.55              |
| 2:D:2939:LEU:HD11 | 2:D:2955:LEU:HB3  | 1.87                     | 0.55              |
| 2:D:2751:ILE:HG22 | 2:D:2904:THR:O    | 2.07                     | 0.55              |
| 2:B:2755:VAL:HG13 | 2:B:2899:TRP:HE1  | 1.70                     | 0.55              |
| 2:B:2600:SER:O    | 2:B:2603:LYS:HB3  | 2.06                     | 0.55              |
| 2:B:2421:GLN:HE21 | 2:B:2536:ASP:CG   | 2.10                     | 0.55              |
| 2:D:2441:TYR:CZ   | 2:D:2596:ASN:ND2  | 2.75                     | 0.55              |
| 2:B:3023:ASP:OD1  | 2:B:3027:HIS:HB2  | 2.06                     | 0.55              |
| 2:D:2664:PRO:N    | 2:D:2665:PRO:HD2  | 2.21                     | 0.55              |
| 2:D:2479:CYS:SG   | 2:D:2480:ILE:N    | 2.80                     | 0.55              |
| 1:C:48:VAL:HG23   | 1:C:49:GLU:HG3    | 1.88                     | 0.55              |
| 2:D:2469:GLN:O    | 2:D:2472:MET:HB3  | 2.06                     | 0.55              |
| 2:D:2669:LEU:HB3  | 2:D:2674:ARG:HB2  | 1.89                     | 0.55              |
| 2:B:2738:LEU:HD13 | 2:B:2745:VAL:CG2  | 2.36                     | 0.55              |
| 2:D:2418:ARG:O    | 2:D:2421:GLN:N    | 2.39                     | 0.55              |
| 2:D:2915:LEU:HD13 | 2:D:2939:LEU:HD13 | 1.88                     | 0.55              |
| 2:D:3014:GLY:O    | 2:D:3015:LEU:HG   | 2.07                     | 0.54              |
| 2:B:2565:GLU:CD   | 2:B:2574:ASN:HA   | 2.27                     | 0.54              |
| 2:D:2945:LYS:HD2  | 2:D:2945:LYS:C    | 2.27                     | 0.54              |
| 2:D:2428:LYS:HD3  | 2:D:2542:PRO:HD3  | 1.88                     | 0.54              |
| 2:B:3014:GLY:O    | 2:B:3015:LEU:HG   | 2.08                     | 0.54              |
| 1:A:38:VAL:O      | 1:A:38:VAL:HG22   | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2666:LEU:HD23 | 2:B:2669:LEU:HD12 | 1.88                     | 0.54              |
| 2:B:2494:ILE:HD11 | 2:B:2523:GLY:C    | 2.28                     | 0.54              |
| 2:B:2780:GLU:HG3  | 2:B:2780:GLU:O    | 2.07                     | 0.54              |
| 2:B:2580:GLU:O    | 2:B:2584:LEU:HB2  | 2.07                     | 0.54              |
| 2:D:2755:VAL:CG1  | 2:D:2899:TRP:HE1  | 2.21                     | 0.54              |
| 2:D:2419:ASP:O    | 2:D:2423:ILE:HG13 | 2.07                     | 0.54              |
| 2:B:2537:THR:HG23 | 2:B:2538:PRO:CD   | 2.36                     | 0.54              |
| 2:B:2437:PRO:HA   | 2:B:2591:ASP:OD1  | 2.08                     | 0.54              |
| 2:D:2997:CYS:O    | 2:D:2999:GLU:N    | 2.40                     | 0.54              |
| 2:B:2494:ILE:HD11 | 2:B:2523:GLY:CA   | 2.37                     | 0.54              |
| 2:B:2906:TYR:CD1  | 2:B:2933:ARG:NE   | 2.73                     | 0.54              |
| 2:D:3018:LEU:CD2  | 2:D:3032:LYS:HG2  | 2.37                     | 0.54              |
| 2:B:2610:ASP:C    | 2:B:2612:ALA:N    | 2.60                     | 0.54              |
| 2:B:2558:VAL:HG13 | 2:B:2577:LEU:CD1  | 2.36                     | 0.54              |
| 1:A:48:VAL:C      | 1:A:49:GLU:HG3    | 2.28                     | 0.54              |
| 1:C:43:TRP:HZ3    | 2:D:2713:THR:HG23 | 1.71                     | 0.54              |
| 2:D:2666:LEU:HA   | 2:D:2669:LEU:HD12 | 1.90                     | 0.54              |
| 2:B:2666:LEU:HD11 | 2:B:2708:ILE:HG22 | 1.90                     | 0.54              |
| 2:B:3026:LEU:CD2  | 2:B:3104:GLU:HA   | 2.38                     | 0.54              |
| 2:D:2932:GLN:OE1  | 2:D:2932:GLN:HA   | 2.08                     | 0.54              |
| 2:B:2929:THR:O    | 2:B:2930:GLU:O    | 2.26                     | 0.54              |
| 2:B:3099:PHE:N    | 2:B:3099:PHE:CD2  | 2.75                     | 0.54              |
| 2:B:2491:GLN:HA   | 2:B:2525:ALA:O    | 2.08                     | 0.54              |
| 1:C:48:VAL:C      | 1:C:49:GLU:HG3    | 2.28                     | 0.54              |
| 2:B:2501:GLU:C    | 2:B:2503:LEU:N    | 2.59                     | 0.54              |
| 2:D:2689:VAL:HG21 | 2:D:2707:LYS:HE3  | 1.90                     | 0.54              |
| 2:B:2506:GLY:O    | 2:B:2507:LYS:C    | 2.47                     | 0.53              |
| 2:D:2409:ASP:O    | 2:D:2413:SER:N    | 2.34                     | 0.53              |
| 2:B:2516:TRP:HB2  | 2:B:2536:ASP:OD1  | 2.08                     | 0.53              |
| 2:B:2927:LEU:O    | 2:B:2929:THR:HG23 | 2.08                     | 0.53              |
| 2:D:3089:MET:C    | 2:D:3091:HIS:N    | 2.61                     | 0.53              |
| 1:A:56:LEU:C      | 1:A:56:LEU:HD23   | 2.28                     | 0.53              |
| 2:B:2441:TYR:CZ   | 2:B:2596:ASN:ND2  | 2.76                     | 0.53              |
| 2:B:2501:GLU:O    | 2:B:2502:ALA:HB3  | 2.08                     | 0.53              |
| 1:A:54:ASN:O      | 1:A:55:GLN:CB     | 2.53                     | 0.53              |
| 2:B:2409:ASP:O    | 2:B:2412:SER:N    | 2.40                     | 0.53              |
| 2:B:3089:MET:C    | 2:B:3091:HIS:N    | 2.60                     | 0.53              |
| 2:D:2600:SER:O    | 2:D:2603:LYS:HB3  | 2.08                     | 0.53              |
| 2:B:3095:ASN:HD22 | 2:B:3095:ASN:N    | 2.05                     | 0.53              |
| 2:B:3116:PRO:O    | 2:B:3117:LYS:CB   | 2.57                     | 0.53              |
| 2:B:2589:ARG:HG2  | 2:B:2655:TRP:CZ3  | 2.43                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:48:VAL:HG23   | 1:A:49:GLU:HG3   | 1.89                     | 0.53              |
| 2:D:2587:LYS:O    | 2:D:2590:TYR:HB3 | 2.08                     | 0.53              |
| 2:D:2592:VAL:HG12 | 2:D:2593:GLU:N   | 2.24                     | 0.53              |
| 2:B:2676:THR:HG23 | 2:B:2679:GLN:HG3 | 1.89                     | 0.53              |
| 2:B:3015:LEU:O    | 2:B:3016:ALA:CB  | 2.56                     | 0.53              |
| 1:C:8:VAL:O       | 1:C:10:LEU:N     | 2.42                     | 0.53              |
| 2:D:2479:CYS:C    | 2:D:2481:SER:H   | 2.12                     | 0.53              |
| 2:D:3099:PHE:N    | 2:D:3099:PHE:CD2 | 2.74                     | 0.53              |
| 2:B:2552:ASN:O    | 2:B:2555:ARG:HB3 | 2.08                     | 0.53              |
| 2:D:2414:LEU:O    | 2:D:2416:ASN:N   | 2.42                     | 0.53              |
| 2:D:2537:THR:HG23 | 2:D:2538:PRO:CD  | 2.38                     | 0.53              |
| 2:D:2908:LYS:O    | 2:D:2909:ARG:C   | 2.47                     | 0.53              |
| 2:B:3030:VAL:HG12 | 2:B:3031:VAL:N   | 2.24                     | 0.53              |
| 2:D:2414:LEU:CD2  | 2:D:2506:GLY:HA2 | 2.33                     | 0.53              |
| 2:D:2764:THR:HG22 | 2:D:2765:VAL:N   | 2.24                     | 0.53              |
| 2:D:3015:LEU:O    | 2:D:3016:ALA:CB  | 2.56                     | 0.53              |
| 2:B:2568:PHE:N    | 2:B:2569:PRO:HD3 | 2.24                     | 0.53              |
| 1:C:19:PHE:CD1    | 1:C:19:PHE:C     | 2.82                     | 0.53              |
| 2:D:2928:LEU:HA   | 2:D:2934:TYR:CZ  | 2.43                     | 0.53              |
| 2:D:3100:TYR:HD1  | 2:D:3101:LYS:HD2 | 1.74                     | 0.53              |
| 2:B:2772:ARG:HB3  | 2:B:2776:GLU:HB2 | 1.91                     | 0.53              |
| 2:D:2506:GLY:O    | 2:D:2507:LYS:C   | 2.47                     | 0.53              |
| 2:B:3050:SER:O    | 2:B:3051:ASN:HB2 | 2.09                     | 0.53              |
| 1:A:56:LEU:N      | 2:B:2462:PRO:HG2 | 2.24                     | 0.53              |
| 2:D:2457:VAL:HG11 | 2:D:2568:PHE:CE2 | 2.44                     | 0.53              |
| 2:B:2778:GLU:O    | 2:B:2781:ALA:HB3 | 2.09                     | 0.53              |
| 2:D:2494:ILE:HD12 | 2:D:2495:GLU:N   | 2.22                     | 0.53              |
| 2:B:2933:ARG:NH1  | 2:B:2966:LEU:CB  | 2.72                     | 0.53              |
| 1:C:49:GLU:C      | 1:C:53:SER:HG    | 2.12                     | 0.53              |
| 2:D:2624:ILE:CD1  | 2:D:2659:LYS:HE3 | 2.39                     | 0.53              |
| 2:B:2531:TYR:CE1  | 2:B:2535:CYS:SG  | 3.02                     | 0.53              |
| 2:B:2409:ASP:O    | 2:B:2413:SER:N   | 2.34                     | 0.52              |
| 2:B:2711:ASN:HD21 | 2:B:2739:PHE:H   | 1.56                     | 0.52              |
| 2:B:2494:ILE:HD11 | 2:B:2523:GLY:O   | 2.09                     | 0.52              |
| 2:D:3028:LEU:HD12 | 2:D:3111:LEU:CD2 | 2.39                     | 0.52              |
| 1:A:19:PHE:C      | 1:A:19:PHE:CD1   | 2.83                     | 0.52              |
| 2:B:2483:ASN:OD1  | 2:B:2485:LYS:N   | 2.42                     | 0.52              |
| 2:B:2772:ARG:NH2  | 2:B:2780:GLU:HG2 | 2.25                     | 0.52              |
| 2:B:2915:LEU:HD13 | 2:B:2939:LEU:CD1 | 2.39                     | 0.52              |
| 2:B:2568:PHE:O    | 2:B:2570:LYS:N   | 2.42                     | 0.52              |
| 2:B:2755:VAL:CG1  | 2:B:2899:TRP:HE1 | 2.22                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2426:LYS:HG3  | 2:B:2430:ARG:NH2  | 2.19                     | 0.52              |
| 2:B:2428:LYS:C    | 2:B:2430:ARG:H    | 2.13                     | 0.52              |
| 2:D:2656:TYR:CD2  | 2:D:2697:PRO:CB   | 2.90                     | 0.52              |
| 2:B:2764:THR:HG22 | 2:B:2765:VAL:N    | 2.24                     | 0.52              |
| 2:B:2424:ARG:NH1  | 2:B:2536:ASP:OD1  | 2.42                     | 0.52              |
| 2:D:3091:HIS:O    | 2:D:3093:ILE:N    | 2.43                     | 0.52              |
| 2:D:3093:ILE:HG23 | 2:D:3094:GLU:N    | 2.25                     | 0.52              |
| 2:D:2606:LEU:CD1  | 2:D:2704:LEU:HD11 | 2.39                     | 0.52              |
| 2:B:2616:LEU:HD11 | 2:B:2724:PHE:CE2  | 2.44                     | 0.52              |
| 1:A:39:TRP:CE3    | 1:A:39:TRP:HA     | 2.45                     | 0.52              |
| 2:D:2426:LYS:HG3  | 2:D:2430:ARG:NH2  | 2.18                     | 0.52              |
| 2:B:2608:ARG:NH2  | 2:B:2688:LEU:HD23 | 2.16                     | 0.52              |
| 2:B:2783:ARG:HH11 | 2:B:2783:ARG:HG3  | 1.75                     | 0.52              |
| 2:D:2758:LEU:HD22 | 2:D:2760:TRP:CZ3  | 2.43                     | 0.52              |
| 2:B:2915:LEU:HD13 | 2:B:2939:LEU:HD13 | 1.90                     | 0.52              |
| 1:A:49:GLU:C      | 1:A:53:SER:HG     | 2.13                     | 0.52              |
| 1:C:59:GLU:OE1    | 2:D:2464:ALA:N    | 2.43                     | 0.52              |
| 2:D:2763:LYS:HG2  | 2:D:2769:TYR:HD2  | 1.73                     | 0.52              |
| 2:D:2778:GLU:O    | 2:D:2781:ALA:HB3  | 2.10                     | 0.52              |
| 2:D:2782:LEU:C    | 2:D:2784:PHE:N    | 2.63                     | 0.52              |
| 2:D:2669:LEU:O    | 2:D:2674:ARG:HB2  | 2.10                     | 0.52              |
| 2:B:2754:ARG:HA   | 2:B:2930:GLU:OE2  | 2.09                     | 0.52              |
| 2:D:2648:THR:HG21 | 2:D:2705:ARG:HH12 | 1.75                     | 0.52              |
| 2:B:2983:LEU:HD11 | 2:B:2988:LEU:HG   | 1.92                     | 0.52              |
| 2:D:2665:PRO:CG   | 2:D:2742:GLY:HA2  | 2.30                     | 0.52              |
| 2:D:2941:VAL:HG12 | 2:D:2943:LYS:HG3  | 1.92                     | 0.52              |
| 2:D:2898:VAL:HG22 | 2:D:2918:TRP:CZ3  | 2.44                     | 0.52              |
| 2:B:2717:ARG:NH1  | 2:B:2717:ARG:HG2  | 2.25                     | 0.52              |
| 2:D:2927:LEU:O    | 2:D:2934:TYR:OH   | 2.28                     | 0.52              |
| 2:B:2655:TRP:C    | 2:B:2656:TYR:CD1  | 2.83                     | 0.52              |
| 2:B:2987:LYS:C    | 2:B:2989:SER:H    | 2.12                     | 0.52              |
| 2:D:2624:ILE:HG22 | 2:D:2647:ASP:HB3  | 1.92                     | 0.52              |
| 2:B:2666:LEU:O    | 2:B:2669:LEU:N    | 2.40                     | 0.51              |
| 2:D:2408:LYS:O    | 2:D:2409:ASP:HB2  | 2.10                     | 0.51              |
| 2:D:2494:ILE:HD11 | 2:D:2523:GLY:CA   | 2.39                     | 0.51              |
| 2:D:2516:TRP:HB2  | 2:D:2536:ASP:OD1  | 2.10                     | 0.51              |
| 2:D:2676:THR:HG23 | 2:D:2679:GLN:HG3  | 1.92                     | 0.51              |
| 2:D:2915:LEU:HD13 | 2:D:2939:LEU:CD1  | 2.39                     | 0.51              |
| 1:A:49:GLU:C      | 1:A:53:SER:OG     | 2.48                     | 0.51              |
| 2:D:2483:ASN:OD1  | 2:D:2485:LYS:N    | 2.43                     | 0.51              |
| 2:D:2987:LYS:C    | 2:D:2989:SER:N    | 2.64                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2479:CYS:C    | 2:B:2481:SER:H    | 2.13                     | 0.51              |
| 2:B:2749:ASP:OD1  | 2:B:2933:ARG:NH2  | 2.43                     | 0.51              |
| 1:C:54:ASN:O      | 1:C:55:GLN:CB     | 2.54                     | 0.51              |
| 2:D:3018:LEU:HD21 | 2:D:3032:LYS:HG2  | 1.93                     | 0.51              |
| 2:B:2465:CYS:SG   | 2:B:2466:SER:N    | 2.79                     | 0.51              |
| 1:C:43:TRP:CH2    | 2:D:2666:LEU:HD21 | 2.45                     | 0.51              |
| 2:B:2664:PRO:N    | 2:B:2665:PRO:HD2  | 2.24                     | 0.51              |
| 2:D:3093:ILE:HD11 | 2:D:3100:TYR:CE1  | 2.46                     | 0.51              |
| 2:D:2437:PRO:CG   | 2:D:2442:LEU:HD11 | 2.36                     | 0.51              |
| 2:B:3109:GLN:NE2  | 2:B:3110:VAL:HG12 | 2.25                     | 0.51              |
| 2:B:2763:LYS:HG2  | 2:B:2769:TYR:HD2  | 1.75                     | 0.51              |
| 2:B:2421:GLN:NE2  | 2:B:2536:ASP:OD1  | 2.37                     | 0.51              |
| 2:B:2541:ASP:C    | 2:B:2541:ASP:OD1  | 2.49                     | 0.51              |
| 2:B:2624:ILE:CG2  | 2:B:2626:LEU:HG   | 2.40                     | 0.51              |
| 2:D:2685:GLY:H    | 2:D:2712:SER:HB3  | 1.74                     | 0.51              |
| 2:B:2772:ARG:HB3  | 2:B:2776:GLU:CB   | 2.41                     | 0.51              |
| 2:D:3116:PRO:O    | 2:D:3117:LYS:HB2  | 2.09                     | 0.51              |
| 2:D:2901:LEU:HD11 | 2:D:2928:LEU:HD13 | 1.93                     | 0.51              |
| 2:D:2552:ASN:O    | 2:D:2555:ARG:HB3  | 2.10                     | 0.51              |
| 2:D:2614:LYS:HG2  | 2:D:2615:THR:H    | 1.75                     | 0.51              |
| 2:D:3095:ASN:N    | 2:D:3095:ASN:HD22 | 2.08                     | 0.51              |
| 2:B:2622:ASP:OD2  | 2:B:2623:ILE:N    | 2.44                     | 0.51              |
| 2:B:2494:ILE:O    | 2:B:2498:PHE:HD1  | 1.94                     | 0.51              |
| 2:D:3058:SER:O    | 2:D:3059:THR:CB   | 2.58                     | 0.51              |
| 2:D:3089:MET:C    | 2:D:3091:HIS:H    | 2.14                     | 0.51              |
| 2:D:2763:LYS:HG2  | 2:D:2769:TYR:CD2  | 2.45                     | 0.51              |
| 1:A:37:HIS:O      | 1:A:38:VAL:HG12   | 2.09                     | 0.51              |
| 2:B:2782:LEU:C    | 2:B:2784:PHE:N    | 2.63                     | 0.51              |
| 2:D:2404:PRO:HD3  | 2:D:2500:LYS:HE2  | 1.91                     | 0.51              |
| 1:C:12:LEU:O      | 2:D:2450:ARG:NH1  | 2.44                     | 0.51              |
| 2:B:2735:LEU:HD13 | 2:B:2748:VAL:HG11 | 1.93                     | 0.51              |
| 2:D:2568:PHE:N    | 2:D:2569:PRO:HD3  | 2.25                     | 0.51              |
| 2:D:2987:LYS:O    | 2:D:2989:SER:N    | 2.44                     | 0.51              |
| 2:D:3107:LEU:HD23 | 2:D:3107:LEU:C    | 2.31                     | 0.51              |
| 2:D:2437:PRO:HA   | 2:D:2591:ASP:OD1  | 2.10                     | 0.51              |
| 2:B:3007:VAL:O    | 2:B:3008:SER:HB3  | 2.10                     | 0.51              |
| 2:B:3019:VAL:HG12 | 2:B:3021:LEU:HD21 | 1.93                     | 0.51              |
| 2:B:2441:TYR:CD2  | 2:B:2441:TYR:O    | 2.63                     | 0.51              |
| 2:D:2465:CYS:O    | 2:D:2466:SER:CB   | 2.59                     | 0.51              |
| 2:B:2978:GLN:CG   | 2:B:2996:PRO:HG2  | 2.40                     | 0.51              |
| 2:D:3058:SER:C    | 2:D:3060:SER:H    | 2.13                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2898:VAL:HG22 | 2:D:2918:TRP:CE3  | 2.46                     | 0.50              |
| 2:D:3050:SER:O    | 2:D:3051:ASN:HB2  | 2.11                     | 0.50              |
| 2:D:2933:ARG:NH1  | 2:D:2966:LEU:CB   | 2.74                     | 0.50              |
| 2:D:2733:LEU:N    | 2:D:2733:LEU:CD2  | 2.74                     | 0.50              |
| 2:B:3081:HIS:CD2  | 2:B:3082:PHE:HD1  | 2.28                     | 0.50              |
| 2:D:2548:VAL:O    | 2:D:2551:SER:HB2  | 2.12                     | 0.50              |
| 2:D:2610:ASP:C    | 2:D:2612:ALA:N    | 2.62                     | 0.50              |
| 2:B:2984:PRO:HG2  | 2:B:2987:LYS:HG3  | 1.92                     | 0.50              |
| 2:D:3043:PRO:O    | 2:D:3044:ARG:HB2  | 2.10                     | 0.50              |
| 2:B:2667:LEU:C    | 2:B:2667:LEU:HD23 | 2.32                     | 0.50              |
| 2:B:2414:LEU:O    | 2:B:2417:ALA:N    | 2.44                     | 0.50              |
| 2:B:2620:VAL:HG22 | 2:B:2679:GLN:O    | 2.11                     | 0.50              |
| 2:D:2491:GLN:HA   | 2:D:2525:ALA:O    | 2.11                     | 0.50              |
| 2:B:2465:CYS:O    | 2:B:2466:SER:CB   | 2.59                     | 0.50              |
| 2:B:2602:LEU:O    | 2:B:2606:LEU:HB2  | 2.11                     | 0.50              |
| 2:D:2616:LEU:HD11 | 2:D:2724:PHE:CE2  | 2.47                     | 0.50              |
| 2:B:2479:CYS:C    | 2:B:2481:SER:N    | 2.65                     | 0.50              |
| 2:B:3097:ASP:C    | 2:B:3099:PHE:N    | 2.64                     | 0.50              |
| 2:D:3057:GLU:OE2  | 2:D:3064:THR:HB   | 2.11                     | 0.50              |
| 2:D:2501:GLU:O    | 2:D:2503:LEU:N    | 2.41                     | 0.50              |
| 2:B:3021:LEU:HB2  | 2:B:3029:LEU:HD22 | 1.92                     | 0.50              |
| 2:B:3005:VAL:HG22 | 2:B:3046:LEU:CD1  | 2.39                     | 0.50              |
| 2:D:2531:TYR:CE1  | 2:D:2535:CYS:SG   | 3.05                     | 0.50              |
| 2:B:2476:SER:C    | 2:B:2478:ALA:N    | 2.62                     | 0.50              |
| 2:B:3089:MET:C    | 2:B:3091:HIS:H    | 2.13                     | 0.50              |
| 2:B:2761:VAL:HG12 | 2:B:2896:SER:O    | 2.11                     | 0.50              |
| 2:D:2589:ARG:O    | 2:D:2593:GLU:HB3  | 2.12                     | 0.50              |
| 2:D:2704:LEU:O    | 2:D:2705:ARG:HD3  | 2.12                     | 0.50              |
| 1:A:13:LEU:HD11   | 2:B:2453:LEU:HA   | 1.94                     | 0.50              |
| 2:B:2777:GLU:O    | 2:B:2781:ALA:N    | 2.44                     | 0.50              |
| 2:D:2738:LEU:HD13 | 2:D:2745:VAL:CG2  | 2.42                     | 0.50              |
| 1:C:56:LEU:HD23   | 1:C:56:LEU:C      | 2.31                     | 0.50              |
| 2:B:2704:LEU:HD23 | 2:B:2704:LEU:O    | 2.11                     | 0.50              |
| 2:D:2927:LEU:O    | 2:D:2929:THR:HG23 | 2.11                     | 0.50              |
| 2:D:2479:CYS:C    | 2:D:2481:SER:N    | 2.65                     | 0.50              |
| 2:D:3019:VAL:HG12 | 2:D:3021:LEU:HD21 | 1.94                     | 0.50              |
| 2:D:2414:LEU:O    | 2:D:2417:ALA:N    | 2.44                     | 0.50              |
| 2:D:2421:GLN:NE2  | 2:D:2536:ASP:OD1  | 2.39                     | 0.50              |
| 2:B:2955:LEU:CD1  | 2:B:2955:LEU:N    | 2.75                     | 0.50              |
| 2:B:2531:TYR:CD1  | 2:B:2531:TYR:C    | 2.83                     | 0.50              |
| 2:B:2667:LEU:CD2  | 2:B:2671:LYS:HD3  | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2602:LEU:O    | 2:D:2606:LEU:HB2  | 2.12                     | 0.50              |
| 2:B:2616:LEU:CD1  | 2:B:2724:PHE:CD2  | 2.94                     | 0.50              |
| 2:D:2447:THR:HG22 | 2:D:2448:LEU:N    | 2.27                     | 0.50              |
| 2:B:2419:ASP:O    | 2:B:2423:ILE:HG13 | 2.12                     | 0.50              |
| 2:B:2908:LYS:O    | 2:B:2909:ARG:C    | 2.50                     | 0.50              |
| 2:B:2406:PHE:C    | 2:B:2408:LYS:H    | 2.15                     | 0.50              |
| 2:D:2745:VAL:CG1  | 2:D:2746:GLY:N    | 2.75                     | 0.50              |
| 2:D:2622:ASP:OD2  | 2:D:2623:ILE:N    | 2.45                     | 0.50              |
| 2:D:2667:LEU:CD2  | 2:D:2671:LYS:HD3  | 2.42                     | 0.49              |
| 2:B:2428:LYS:O    | 2:B:2430:ARG:N    | 2.45                     | 0.49              |
| 2:D:3081:HIS:CD2  | 2:D:3082:PHE:HD1  | 2.30                     | 0.49              |
| 2:D:2704:LEU:HD23 | 2:D:2704:LEU:O    | 2.12                     | 0.49              |
| 1:A:39:TRP:HE3    | 1:A:39:TRP:HA     | 1.77                     | 0.49              |
| 2:B:2745:VAL:N    | 2:B:2940:SER:OG   | 2.45                     | 0.49              |
| 2:B:3058:SER:C    | 2:B:3060:SER:H    | 2.14                     | 0.49              |
| 2:B:2606:LEU:CD1  | 2:B:2704:LEU:HD11 | 2.41                     | 0.49              |
| 2:B:2754:ARG:HB2  | 2:B:2756:TYR:HE1  | 1.77                     | 0.49              |
| 2:D:2955:LEU:N    | 2:D:2955:LEU:CD1  | 2.74                     | 0.49              |
| 2:B:2548:VAL:O    | 2:B:2551:SER:HB2  | 2.12                     | 0.49              |
| 2:B:2941:VAL:HG12 | 2:B:2943:LYS:HG3  | 1.95                     | 0.49              |
| 2:B:3102:GLU:HA   | 2:B:3102:GLU:OE1  | 2.13                     | 0.49              |
| 2:B:3107:LEU:HD23 | 2:B:3107:LEU:C    | 2.33                     | 0.49              |
| 2:D:3026:LEU:CD2  | 2:D:3104:GLU:HA   | 2.43                     | 0.49              |
| 2:D:2936:ILE:HG21 | 2:D:2939:LEU:HD22 | 1.94                     | 0.49              |
| 2:B:2585:GLN:O    | 2:B:2588:TYR:HB3  | 2.13                     | 0.49              |
| 2:D:2406:PHE:O    | 2:D:2411:MET:HG2  | 2.13                     | 0.49              |
| 1:C:22:PHE:O      | 1:C:23:PRO:C      | 2.50                     | 0.49              |
| 2:D:2419:ASP:HA   | 2:D:2422:ASP:HB2  | 1.94                     | 0.49              |
| 1:C:39:TRP:NE1    | 2:D:2733:LEU:HB3  | 2.28                     | 0.49              |
| 2:D:2663:ASP:C    | 2:D:2665:PRO:HD2  | 2.33                     | 0.49              |
| 2:B:2408:LYS:O    | 2:B:2409:ASP:HB2  | 2.13                     | 0.49              |
| 2:B:2501:GLU:O    | 2:B:2503:LEU:N    | 2.45                     | 0.49              |
| 2:D:2773:ASN:N    | 2:D:2776:GLU:HB2  | 2.13                     | 0.49              |
| 2:D:2439:SER:HB3  | 2:D:2584:LEU:HD21 | 1.94                     | 0.49              |
| 1:C:39:TRP:HA     | 1:C:39:TRP:CE3    | 2.47                     | 0.49              |
| 2:D:2953:ILE:O    | 2:D:2954:GLN:HB2  | 2.12                     | 0.49              |
| 2:D:2555:ARG:CZ   | 2:D:2556:TRP:CH2  | 2.95                     | 0.49              |
| 2:D:2489:TYR:O    | 2:D:2491:GLN:N    | 2.45                     | 0.49              |
| 2:B:2730:PRO:HB2  | 2:B:2747:CYS:HB2  | 1.94                     | 0.49              |
| 2:B:2987:LYS:C    | 2:B:2989:SER:N    | 2.66                     | 0.49              |
| 2:D:2616:LEU:HD13 | 2:D:2724:PHE:HD2  | 1.74                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:3043:PRO:O    | 2:B:3044:ARG:HB2  | 2.12                     | 0.49              |
| 1:C:37:HIS:ND1    | 1:C:38:VAL:HG12   | 2.27                     | 0.49              |
| 2:D:2726:HIS:N    | 2:D:2726:HIS:ND1  | 2.61                     | 0.49              |
| 2:D:3035:ILE:HG23 | 2:D:3068:GLY:O    | 2.12                     | 0.49              |
| 2:D:2772:ARG:NH2  | 2:D:2780:GLU:HG2  | 2.27                     | 0.49              |
| 2:D:3030:VAL:HG12 | 2:D:3031:VAL:N    | 2.27                     | 0.49              |
| 2:D:2777:GLU:O    | 2:D:2781:ALA:N    | 2.46                     | 0.49              |
| 2:B:2985:PHE:CE2  | 2:B:3029:LEU:HD13 | 2.48                     | 0.49              |
| 2:D:2545:ILE:HG13 | 2:D:2545:ILE:O    | 2.13                     | 0.49              |
| 2:B:2434:CYS:SG   | 2:B:2435:PRO:N    | 2.86                     | 0.49              |
| 2:D:2754:ARG:HB2  | 2:D:2756:TYR:HE1  | 1.78                     | 0.48              |
| 2:B:2406:PHE:C    | 2:B:2408:LYS:N    | 2.66                     | 0.48              |
| 2:D:3102:GLU:OE1  | 2:D:3102:GLU:HA   | 2.13                     | 0.48              |
| 2:B:2763:LYS:HG2  | 2:B:2769:TYR:CD2  | 2.49                     | 0.48              |
| 2:D:2919:ARG:N    | 2:D:2920:PRO:CD   | 2.76                     | 0.48              |
| 2:B:3057:GLU:OE2  | 2:B:3064:THR:HB   | 2.13                     | 0.48              |
| 1:C:19:PHE:C      | 1:C:19:PHE:HD1    | 2.15                     | 0.48              |
| 2:B:2932:GLN:HA   | 2:B:2932:GLN:OE1  | 2.13                     | 0.48              |
| 1:C:39:TRP:HZ3    | 2:D:2682:ILE:HB   | 1.77                     | 0.48              |
| 2:D:2501:GLU:O    | 2:D:2502:ALA:HB3  | 2.13                     | 0.48              |
| 2:D:2664:PRO:HB2  | 2:D:2741:ASP:OD2  | 2.13                     | 0.48              |
| 2:D:3016:ALA:H    | 2:D:3017:PRO:HD3  | 1.79                     | 0.48              |
| 1:A:19:PHE:C      | 1:A:19:PHE:HD1    | 2.15                     | 0.48              |
| 2:B:2458:GLY:O    | 2:B:2459:ASP:HB2  | 2.14                     | 0.48              |
| 2:B:3058:SER:O    | 2:B:3059:THR:CB   | 2.61                     | 0.48              |
| 2:B:2608:ARG:NH1  | 2:B:2608:ARG:CB   | 2.68                     | 0.48              |
| 2:D:2751:ILE:HD11 | 2:D:2973:LEU:HD13 | 1.96                     | 0.48              |
| 2:B:2927:LEU:O    | 2:B:2934:TYR:OH   | 2.31                     | 0.48              |
| 2:B:3093:ILE:HD11 | 2:B:3100:TYR:CE1  | 2.48                     | 0.48              |
| 2:B:2762:GLU:OE2  | 2:B:2893:ARG:NH1  | 2.47                     | 0.48              |
| 2:D:2761:VAL:HG11 | 2:D:2918:TRP:CZ3  | 2.49                     | 0.48              |
| 2:B:2919:ARG:N    | 2:B:2920:PRO:CD   | 2.76                     | 0.48              |
| 2:D:2500:LYS:O    | 2:D:2501:GLU:HB3  | 2.13                     | 0.48              |
| 2:D:2476:SER:C    | 2:D:2478:ALA:N    | 2.65                     | 0.48              |
| 2:D:2745:VAL:N    | 2:D:2940:SER:OG   | 2.47                     | 0.48              |
| 2:D:2409:ASP:O    | 2:D:2412:SER:N    | 2.40                     | 0.48              |
| 2:D:2717:ARG:NH1  | 2:D:2717:ARG:HG2  | 2.28                     | 0.48              |
| 2:B:2750:VAL:HG13 | 2:B:2904:THR:C    | 2.34                     | 0.48              |
| 2:D:2761:VAL:O    | 2:D:2895:VAL:HG23 | 2.13                     | 0.48              |
| 1:C:50:ASP:O      | 1:C:52:PHE:N      | 2.46                     | 0.48              |
| 2:B:2704:LEU:C    | 2:B:2704:LEU:HD23 | 2.34                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2756:TYR:HD1  | 2:D:2756:TYR:N    | 2.12                     | 0.48              |
| 2:B:2503:LEU:C    | 2:B:2503:LEU:HD13 | 2.34                     | 0.48              |
| 2:D:3097:ASP:C    | 2:D:3099:PHE:N    | 2.66                     | 0.48              |
| 2:D:2494:ILE:HD11 | 2:D:2523:GLY:C    | 2.34                     | 0.48              |
| 2:D:2437:PRO:HG2  | 2:D:2442:LEU:CD1  | 2.39                     | 0.48              |
| 1:C:56:LEU:HD23   | 1:C:56:LEU:O      | 2.13                     | 0.48              |
| 2:D:2558:VAL:HG13 | 2:D:2577:LEU:CD1  | 2.40                     | 0.48              |
| 2:D:2493:ALA:O    | 2:D:2496:ASP:N    | 2.46                     | 0.48              |
| 2:B:2403:PHE:HD1  | 2:B:2503:LEU:CD1  | 2.26                     | 0.48              |
| 2:B:2933:ARG:CB   | 2:B:2968:VAL:HG22 | 2.43                     | 0.48              |
| 1:C:60:LEU:HD11   | 2:D:2562:ALA:HB1  | 1.96                     | 0.48              |
| 2:B:2692:PRO:HG2  | 2:B:2693:ASP:N    | 2.29                     | 0.48              |
| 2:D:2531:TYR:C    | 2:D:2531:TYR:CD1  | 2.85                     | 0.48              |
| 2:D:2973:LEU:C    | 2:D:2975:GLN:N    | 2.67                     | 0.48              |
| 2:D:2983:LEU:HD11 | 2:D:2988:LEU:HG   | 1.95                     | 0.48              |
| 2:B:2937:TYR:C    | 2:B:2939:LEU:N    | 2.67                     | 0.48              |
| 2:B:3057:GLU:OE1  | 2:B:3057:GLU:HA   | 2.14                     | 0.48              |
| 2:D:2616:LEU:CD1  | 2:D:2724:PHE:CD2  | 2.96                     | 0.48              |
| 2:D:2599:ARG:HH22 | 2:D:2609:ASP:CB   | 2.27                     | 0.48              |
| 2:B:2752:VAL:HG12 | 2:B:2930:GLU:HA   | 1.96                     | 0.47              |
| 2:B:2475:VAL:O    | 2:B:2476:SER:C    | 2.53                     | 0.47              |
| 2:D:2541:ASP:OD1  | 2:D:2541:ASP:C    | 2.51                     | 0.47              |
| 2:D:2458:GLY:O    | 2:D:2459:ASP:HB2  | 2.14                     | 0.47              |
| 2:B:2669:LEU:HB3  | 2:B:2674:ARG:HB2  | 1.95                     | 0.47              |
| 2:B:2714:ARG:NH2  | 2:B:2733:LEU:HD12 | 2.29                     | 0.47              |
| 2:B:2928:LEU:HA   | 2:B:2934:TYR:CZ   | 2.49                     | 0.47              |
| 2:B:2973:LEU:C    | 2:B:2975:GLN:N    | 2.68                     | 0.47              |
| 2:B:2917:ILE:HD13 | 2:B:2924:LEU:CD2  | 2.36                     | 0.47              |
| 2:D:2620:VAL:HG22 | 2:D:2679:GLN:O    | 2.14                     | 0.47              |
| 2:B:2987:LYS:O    | 2:B:2989:SER:N    | 2.47                     | 0.47              |
| 2:B:2447:THR:HG22 | 2:B:2448:LEU:N    | 2.29                     | 0.47              |
| 2:D:2589:ARG:HG3  | 2:D:2589:ARG:NH1  | 2.26                     | 0.47              |
| 2:D:2501:GLU:C    | 2:D:2503:LEU:N    | 2.58                     | 0.47              |
| 2:D:2503:LEU:HD13 | 2:D:2503:LEU:C    | 2.35                     | 0.47              |
| 2:B:3007:VAL:HB   | 2:B:3104:GLU:OE1  | 2.13                     | 0.47              |
| 2:D:3007:VAL:O    | 2:D:3008:SER:HB3  | 2.13                     | 0.47              |
| 2:B:3010:VAL:HG12 | 2:B:3012:PRO:CD   | 2.43                     | 0.47              |
| 2:D:2937:TYR:O    | 2:D:2961:THR:HG23 | 2.14                     | 0.47              |
| 1:A:37:HIS:ND1    | 1:A:38:VAL:HG12   | 2.28                     | 0.47              |
| 2:D:3024:GLU:OE2  | 2:D:3085:ARG:NH2  | 2.47                     | 0.47              |
| 2:D:2585:GLN:O    | 2:D:2588:TYR:HB3  | 2.13                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2733:LEU:N    | 2:B:2733:LEU:CD2  | 2.76                     | 0.47              |
| 2:D:2984:PRO:HG2  | 2:D:2987:LYS:HG3  | 1.96                     | 0.47              |
| 2:D:3101:LYS:O    | 2:D:3105:LYS:HG3  | 2.15                     | 0.47              |
| 2:D:3109:GLN:C    | 2:D:3109:GLN:NE2  | 2.67                     | 0.47              |
| 2:D:2939:LEU:CD1  | 2:D:2955:LEU:HB3  | 2.45                     | 0.47              |
| 1:C:13:LEU:HD12   | 2:D:2451:ILE:O    | 2.15                     | 0.47              |
| 2:B:3108:ILE:HG12 | 2:B:3112:LYS:HE3  | 1.95                     | 0.47              |
| 2:D:3109:GLN:HE21 | 2:D:3110:VAL:N    | 2.12                     | 0.47              |
| 2:D:2772:ARG:HB3  | 2:D:2776:GLU:HB2  | 1.96                     | 0.47              |
| 2:B:2773:ASN:OD1  | 2:B:2776:GLU:OE1  | 2.32                     | 0.47              |
| 2:B:2761:VAL:HG11 | 2:B:2918:TRP:CZ3  | 2.50                     | 0.47              |
| 2:D:2557:ILE:O    | 2:D:2561:LEU:HD12 | 2.14                     | 0.47              |
| 2:D:2498:PHE:HB2  | 2:D:2503:LEU:HD23 | 1.97                     | 0.47              |
| 1:A:56:LEU:O      | 1:A:56:LEU:HD23   | 2.14                     | 0.47              |
| 2:B:2541:ASP:OD1  | 2:B:2543:LYS:N    | 2.47                     | 0.47              |
| 2:B:2407:ASN:O    | 2:B:2411:MET:HG3  | 2.13                     | 0.47              |
| 2:B:2493:ALA:O    | 2:B:2496:ASP:N    | 2.47                     | 0.47              |
| 2:B:2755:VAL:HG23 | 2:B:2930:GLU:HG2  | 1.97                     | 0.47              |
| 2:D:2553:HIS:O    | 2:D:2557:ILE:HG13 | 2.15                     | 0.47              |
| 1:C:56:LEU:HD23   | 1:C:57:ARG:HB2    | 1.95                     | 0.47              |
| 2:D:2441:TYR:CD2  | 2:D:2441:TYR:O    | 2.68                     | 0.47              |
| 2:D:2565:GLU:OE1  | 2:D:2574:ASN:HA   | 2.13                     | 0.47              |
| 2:B:2997:CYS:O    | 2:B:2999:GLU:N    | 2.47                     | 0.47              |
| 1:C:38:VAL:HG13   | 1:C:38:VAL:O      | 2.14                     | 0.47              |
| 1:C:46:ASP:OD2    | 2:D:2674:ARG:NH1  | 2.48                     | 0.47              |
| 2:D:2969:SER:O    | 2:D:2970:SER:C    | 2.53                     | 0.47              |
| 2:B:2969:SER:O    | 2:B:2970:SER:C    | 2.52                     | 0.47              |
| 2:B:2412:SER:O    | 2:B:2413:SER:C    | 2.51                     | 0.47              |
| 2:B:3100:TYR:O    | 2:B:3103:ALA:N    | 2.48                     | 0.47              |
| 2:B:3062:VAL:HG22 | 2:B:3062:VAL:O    | 2.14                     | 0.47              |
| 2:D:3061:ARG:HG2  | 2:D:3061:ARG:NH1  | 2.29                     | 0.47              |
| 2:B:2489:TYR:O    | 2:B:2491:GLN:N    | 2.47                     | 0.47              |
| 2:B:2689:VAL:HG21 | 2:B:2707:LYS:HE3  | 1.96                     | 0.47              |
| 2:B:2534:LEU:CD2  | 2:B:2540:VAL:HG21 | 2.41                     | 0.47              |
| 2:B:2939:LEU:CD1  | 2:B:2955:LEU:HB3  | 2.45                     | 0.47              |
| 1:A:51:ASP:CB     | 2:B:2717:ARG:HG3  | 2.45                     | 0.47              |
| 2:D:2909:ARG:O    | 2:D:2910:GLU:CG   | 2.60                     | 0.47              |
| 2:D:2777:GLU:OE2  | 2:D:2893:ARG:NH2  | 2.46                     | 0.47              |
| 2:D:2424:ARG:NH1  | 2:D:2536:ASP:OD1  | 2.48                     | 0.47              |
| 2:B:2403:PHE:CA   | 2:B:2503:LEU:HD11 | 2.36                     | 0.47              |
| 2:B:3108:ILE:CG1  | 2:B:3112:LYS:HE3  | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2487:ALA:C    | 2:D:2489:TYR:H    | 2.19                     | 0.47              |
| 2:D:2983:LEU:HB3  | 2:D:3002:VAL:HG12 | 1.97                     | 0.47              |
| 2:D:2600:SER:HB2  | 2:D:2655:TRP:HB2  | 1.97                     | 0.47              |
| 2:B:3083:GLN:HA   | 2:B:3086:VAL:CG1  | 2.43                     | 0.47              |
| 2:B:2512:ALA:HB1  | 2:B:2584:LEU:HG   | 1.93                     | 0.47              |
| 2:D:2568:PHE:O    | 2:D:2570:LYS:N    | 2.48                     | 0.47              |
| 2:D:2719:HIS:CG   | 2:D:2720:SER:N    | 2.82                     | 0.47              |
| 2:B:2685:GLY:H    | 2:B:2712:SER:HB3  | 1.80                     | 0.47              |
| 2:B:2545:ILE:HG13 | 2:B:2545:ILE:O    | 2.15                     | 0.47              |
| 1:C:39:TRP:HA     | 1:C:39:TRP:HE3    | 1.79                     | 0.46              |
| 2:D:2738:LEU:HD22 | 2:D:2745:VAL:CG2  | 2.45                     | 0.46              |
| 2:D:3060:SER:C    | 2:D:3062:VAL:N    | 2.67                     | 0.46              |
| 2:D:2554:TYR:O    | 2:D:2558:VAL:HG23 | 2.15                     | 0.46              |
| 2:B:2937:TYR:O    | 2:B:2961:THR:HG23 | 2.14                     | 0.46              |
| 2:B:3024:GLU:OE2  | 2:B:3085:ARG:NH2  | 2.48                     | 0.46              |
| 2:B:3060:SER:C    | 2:B:3062:VAL:N    | 2.69                     | 0.46              |
| 2:D:3109:GLN:NE2  | 2:D:3110:VAL:HG12 | 2.30                     | 0.46              |
| 2:D:2403:PHE:HA   | 2:D:2503:LEU:HD11 | 1.96                     | 0.46              |
| 2:D:2563:ALA:O    | 2:D:2566:PHE:N    | 2.49                     | 0.46              |
| 1:A:60:LEU:HD11   | 2:B:2562:ALA:HB1  | 1.97                     | 0.46              |
| 2:B:2719:HIS:CG   | 2:B:2720:SER:N    | 2.83                     | 0.46              |
| 2:B:2446:SER:OG   | 2:B:2448:LEU:HD12 | 2.15                     | 0.46              |
| 2:D:3108:ILE:CG1  | 2:D:3112:LYS:HE3  | 2.46                     | 0.46              |
| 2:D:2487:ALA:C    | 2:D:2489:TYR:N    | 2.69                     | 0.46              |
| 2:D:2525:ALA:HA   | 2:D:2529:GLU:OE1  | 2.16                     | 0.46              |
| 1:C:62:LYS:O      | 1:C:63:HIS:C      | 2.54                     | 0.46              |
| 2:B:2935:ARG:HD3  | 2:B:2937:TYR:OH   | 2.15                     | 0.46              |
| 2:D:3010:VAL:C    | 2:D:3012:PRO:HD3  | 2.36                     | 0.46              |
| 1:A:51:ASP:O      | 2:B:2717:ARG:HA   | 2.16                     | 0.46              |
| 2:D:2624:ILE:CG2  | 2:D:2626:LEU:HG   | 2.46                     | 0.46              |
| 2:B:3062:VAL:HB   | 2:B:3111:LEU:HD21 | 1.96                     | 0.46              |
| 2:D:2500:LYS:O    | 2:D:2501:GLU:CB   | 2.64                     | 0.46              |
| 2:D:2765:VAL:HG23 | 2:D:2766:SER:N    | 2.31                     | 0.46              |
| 2:B:2681:ILE:HG22 | 2:B:2683:THR:HG23 | 1.97                     | 0.46              |
| 2:B:2403:PHE:CA   | 2:B:2500:LYS:HE2  | 2.45                     | 0.46              |
| 2:B:3100:TYR:HD1  | 2:B:3101:LYS:HD2  | 1.80                     | 0.46              |
| 2:D:3062:VAL:HB   | 2:D:3111:LEU:HD21 | 1.96                     | 0.46              |
| 2:B:2761:VAL:O    | 2:B:2895:VAL:HG23 | 2.16                     | 0.46              |
| 2:D:2933:ARG:CB   | 2:D:2968:VAL:HG22 | 2.46                     | 0.46              |
| 2:B:2553:HIS:O    | 2:B:2557:ILE:HG13 | 2.15                     | 0.46              |
| 2:D:2482:VAL:HA   | 2:D:2486:ASN:HD21 | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2414:LEU:C    | 2:B:2416:ASN:N    | 2.68                     | 0.46              |
| 2:B:3020:TYR:CD2  | 2:B:3030:VAL:HG22 | 2.51                     | 0.46              |
| 2:D:2773:ASN:OD1  | 2:D:2776:GLU:OE1  | 2.34                     | 0.46              |
| 2:D:2412:SER:O    | 2:D:2413:SER:C    | 2.53                     | 0.46              |
| 2:B:2711:ASN:OD1  | 2:B:2738:LEU:HA   | 2.16                     | 0.46              |
| 2:B:2500:LYS:O    | 2:B:2501:GLU:HB3  | 2.15                     | 0.46              |
| 2:B:2773:ASN:N    | 2:B:2776:GLU:HB2  | 2.15                     | 0.46              |
| 2:D:2534:LEU:CD2  | 2:D:2540:VAL:HG21 | 2.41                     | 0.46              |
| 2:D:2729:ARG:HD3  | 2:D:2730:PRO:CD   | 2.46                     | 0.46              |
| 2:B:2701:PRO:O    | 2:B:2704:LEU:HB3  | 2.15                     | 0.46              |
| 2:D:2900:LYS:C    | 2:D:2901:LEU:HD23 | 2.36                     | 0.46              |
| 2:B:2744:ASN:CB   | 2:B:2940:SER:HB2  | 2.46                     | 0.46              |
| 2:B:3109:GLN:NE2  | 2:B:3109:GLN:C    | 2.69                     | 0.46              |
| 2:D:3020:TYR:CD2  | 2:D:3030:VAL:HG22 | 2.51                     | 0.46              |
| 2:D:2461:VAL:HB   | 2:D:2462:PRO:HD2  | 1.98                     | 0.46              |
| 2:B:2418:ARG:O    | 2:B:2421:GLN:HB3  | 2.16                     | 0.46              |
| 2:B:2565:GLU:OE1  | 2:B:2574:ASN:HA   | 2.16                     | 0.46              |
| 2:B:2447:THR:O    | 2:B:2448:LEU:O    | 2.34                     | 0.46              |
| 2:D:2969:SER:HB2  | 2:D:2972:THR:HG23 | 1.98                     | 0.46              |
| 2:B:2663:ASP:C    | 2:B:2665:PRO:HD2  | 2.35                     | 0.46              |
| 2:D:2608:ARG:CB   | 2:D:2608:ARG:NH1  | 2.70                     | 0.46              |
| 2:B:2761:VAL:HG11 | 2:B:2918:TRP:CH2  | 2.51                     | 0.46              |
| 2:B:2765:VAL:HG23 | 2:B:2766:SER:N    | 2.31                     | 0.46              |
| 2:D:2701:PRO:O    | 2:D:2704:LEU:HB3  | 2.16                     | 0.46              |
| 2:B:3016:ALA:H    | 2:B:3017:PRO:HD3  | 1.80                     | 0.46              |
| 1:A:8:VAL:HG12    | 1:A:10:LEU:HD23   | 1.98                     | 0.46              |
| 1:A:46:ASP:OD2    | 2:B:2674:ARG:NH1  | 2.49                     | 0.45              |
| 2:B:2909:ARG:O    | 2:B:2910:GLU:CG   | 2.60                     | 0.45              |
| 2:B:3109:GLN:HE21 | 2:B:3110:VAL:N    | 2.13                     | 0.45              |
| 2:B:2614:LYS:HG2  | 2:B:2615:THR:H    | 1.74                     | 0.45              |
| 1:A:12:LEU:O      | 2:B:2450:ARG:NH1  | 2.49                     | 0.45              |
| 2:B:3010:VAL:C    | 2:B:3012:PRO:HD3  | 2.36                     | 0.45              |
| 2:D:2407:ASN:C    | 2:D:2411:MET:HG3  | 2.36                     | 0.45              |
| 2:B:2587:LYS:O    | 2:B:2590:TYR:HB3  | 2.16                     | 0.45              |
| 2:B:2900:LYS:C    | 2:B:2901:LEU:HD23 | 2.37                     | 0.45              |
| 2:B:2416:ASN:O    | 2:B:2420:LEU:HB2  | 2.16                     | 0.45              |
| 2:B:2428:LYS:CD   | 2:B:2542:PRO:HD3  | 2.46                     | 0.45              |
| 2:D:2552:ASN:C    | 2:D:2552:ASN:ND2  | 2.69                     | 0.45              |
| 2:B:2554:TYR:O    | 2:B:2558:VAL:HG23 | 2.16                     | 0.45              |
| 2:D:2937:TYR:C    | 2:D:2939:LEU:N    | 2.69                     | 0.45              |
| 2:D:2621:SER:O    | 2:D:2622:ASP:HB2  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2666:LEU:O    | 2:D:2669:LEU:N    | 2.43                     | 0.45              |
| 2:D:2927:LEU:HG   | 2:D:2928:LEU:N    | 2.32                     | 0.45              |
| 2:D:3110:VAL:C    | 2:D:3112:LYS:N    | 2.70                     | 0.45              |
| 2:B:2563:ALA:O    | 2:B:2566:PHE:N    | 2.49                     | 0.45              |
| 2:B:3095:ASN:N    | 2:B:3095:ASN:ND2  | 2.64                     | 0.45              |
| 1:C:9:ASP:O       | 1:C:11:GLY:N      | 2.50                     | 0.45              |
| 1:C:46:ASP:CG     | 2:D:2674:ARG:HH12 | 2.20                     | 0.45              |
| 1:A:46:ASP:CG     | 2:B:2674:ARG:HH12 | 2.20                     | 0.45              |
| 2:B:2750:VAL:HG11 | 2:B:2903:VAL:CG2  | 2.47                     | 0.45              |
| 2:B:2911:LYS:O    | 2:B:2912:SER:O    | 2.34                     | 0.45              |
| 2:B:2494:ILE:HD12 | 2:B:2495:GLU:N    | 2.25                     | 0.45              |
| 2:D:3091:HIS:O    | 2:D:3094:GLU:N    | 2.50                     | 0.45              |
| 2:D:3100:TYR:CD1  | 2:D:3101:LYS:HD2  | 2.52                     | 0.45              |
| 1:A:61:GLU:C      | 1:A:63:HIS:H      | 2.19                     | 0.45              |
| 1:A:39:TRP:HZ3    | 2:B:2682:ILE:HB   | 1.81                     | 0.45              |
| 2:D:2427:ASN:O    | 2:D:2428:LYS:C    | 2.54                     | 0.45              |
| 2:D:3021:LEU:HB2  | 2:D:3029:LEU:HD22 | 1.97                     | 0.45              |
| 2:D:3111:LEU:C    | 2:D:3112:LYS:HD3  | 2.36                     | 0.45              |
| 2:B:2917:ILE:CG2  | 2:B:2920:PRO:HG3  | 2.40                     | 0.45              |
| 2:B:2656:TYR:CD2  | 2:B:2697:PRO:CB   | 2.93                     | 0.45              |
| 2:D:2749:ASP:O    | 2:D:2906:TYR:HB2  | 2.17                     | 0.45              |
| 2:B:2675:LEU:HA   | 2:B:2675:LEU:HD23 | 1.72                     | 0.45              |
| 2:D:3005:VAL:HG22 | 2:D:3046:LEU:CD1  | 2.47                     | 0.45              |
| 2:B:2555:ARG:CZ   | 2:B:2556:TRP:CH2  | 2.99                     | 0.45              |
| 1:A:57:ARG:HG2    | 2:B:2559:TRP:CZ2  | 2.52                     | 0.45              |
| 2:B:2726:HIS:N    | 2:B:2726:HIS:ND1  | 2.62                     | 0.45              |
| 2:D:2772:ARG:HB3  | 2:D:2776:GLU:CB   | 2.46                     | 0.45              |
| 2:B:2552:ASN:O    | 2:B:2555:ARG:N    | 2.49                     | 0.45              |
| 1:A:15:GLU:HB2    | 1:A:18:GLU:CG     | 2.47                     | 0.45              |
| 2:D:2676:THR:HG22 | 2:D:2679:GLN:CD   | 2.36                     | 0.45              |
| 2:D:2978:GLN:HG2  | 2:D:2996:PRO:HG2  | 1.99                     | 0.45              |
| 2:D:2666:LEU:HD11 | 2:D:2708:ILE:HG22 | 1.99                     | 0.45              |
| 2:D:3097:ASP:HA   | 2:D:3100:TYR:HB2  | 1.99                     | 0.45              |
| 2:D:2772:ARG:NE   | 2:D:2780:GLU:HG2  | 2.32                     | 0.45              |
| 2:D:2554:TYR:CE1  | 2:D:2582:VAL:HG11 | 2.51                     | 0.45              |
| 2:D:2572:PHE:O    | 2:D:2573:ALA:C    | 2.55                     | 0.45              |
| 2:D:2900:LYS:HD2  | 2:D:3070:PHE:CE2  | 2.51                     | 0.45              |
| 2:B:2901:LEU:HD11 | 2:B:2928:LEU:HD13 | 1.99                     | 0.45              |
| 2:B:2500:LYS:O    | 2:B:2501:GLU:CB   | 2.65                     | 0.45              |
| 2:B:3097:ASP:HA   | 2:B:3100:TYR:HB2  | 1.99                     | 0.45              |
| 2:D:2783:ARG:NH1  | 2:D:2783:ARG:HG3  | 2.32                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:3095:ASN:N    | 2:D:3095:ASN:ND2  | 2.65                     | 0.45              |
| 2:B:3035:ILE:HG23 | 2:B:3068:GLY:O    | 2.17                     | 0.45              |
| 2:B:2666:LEU:O    | 2:B:2667:LEU:C    | 2.55                     | 0.45              |
| 2:B:2772:ARG:NE   | 2:B:2780:GLU:HG2  | 2.32                     | 0.45              |
| 2:B:3048:ALA:HB1  | 2:B:3082:PHE:CE2  | 2.52                     | 0.45              |
| 2:D:2936:ILE:HG21 | 2:D:2939:LEU:HB2  | 1.97                     | 0.45              |
| 2:B:2648:THR:HG21 | 2:B:2705:ARG:HH12 | 1.81                     | 0.45              |
| 2:B:2498:PHE:HB2  | 2:B:2503:LEU:HD23 | 1.98                     | 0.44              |
| 2:B:3109:GLN:HE22 | 2:B:3110:VAL:HG12 | 1.80                     | 0.44              |
| 2:D:2461:VAL:HB   | 2:D:2462:PRO:CD   | 2.47                     | 0.44              |
| 2:B:2509:PHE:O    | 2:B:2517:LEU:N    | 2.48                     | 0.44              |
| 2:B:3091:HIS:O    | 2:B:3093:ILE:N    | 2.51                     | 0.44              |
| 2:B:3111:LEU:C    | 2:B:3112:LYS:HD3  | 2.37                     | 0.44              |
| 2:D:2765:VAL:HG23 | 2:D:2766:SER:H    | 1.82                     | 0.44              |
| 2:D:2959:LYS:CD   | 2:D:2959:LYS:H    | 2.09                     | 0.44              |
| 2:D:2761:VAL:HG11 | 2:D:2918:TRP:CH2  | 2.52                     | 0.44              |
| 2:D:2921:SER:O    | 2:D:2924:LEU:HB2  | 2.17                     | 0.44              |
| 2:B:2676:THR:HG22 | 2:B:2679:GLN:CD   | 2.37                     | 0.44              |
| 2:D:2569:PRO:O    | 2:D:2573:ALA:HA   | 2.18                     | 0.44              |
| 2:D:2995:PRO:HD2  | 2:D:3054:TRP:CE3  | 2.52                     | 0.44              |
| 1:A:43:TRP:CZ3    | 2:B:2713:THR:HG23 | 2.41                     | 0.44              |
| 2:B:3061:ARG:HG2  | 2:B:3061:ARG:NH1  | 2.29                     | 0.44              |
| 2:D:3105:LYS:O    | 2:D:3109:GLN:HB2  | 2.17                     | 0.44              |
| 2:B:2589:ARG:NH1  | 2:B:2589:ARG:HG3  | 2.25                     | 0.44              |
| 2:D:2620:VAL:HG23 | 2:D:2677:VAL:HA   | 2.00                     | 0.44              |
| 2:B:2751:ILE:HD11 | 2:B:2973:LEU:HD13 | 1.99                     | 0.44              |
| 2:D:2480:ILE:CG2  | 2:D:2480:ILE:O    | 2.65                     | 0.44              |
| 2:D:2421:GLN:HA   | 2:D:2424:ARG:NE   | 2.33                     | 0.44              |
| 2:B:2717:ARG:O    | 2:B:2718:TRP:C    | 2.56                     | 0.44              |
| 2:D:2680:LYS:NZ   | 2:D:2719:HIS:O    | 2.50                     | 0.44              |
| 2:B:2745:VAL:H    | 2:B:2940:SER:CB   | 2.30                     | 0.44              |
| 2:B:2756:TYR:HD1  | 2:B:2756:TYR:N    | 2.15                     | 0.44              |
| 2:B:2772:ARG:CZ   | 2:B:2780:GLU:HG2  | 2.48                     | 0.44              |
| 2:B:2704:LEU:O    | 2:B:2705:ARG:HD3  | 2.17                     | 0.44              |
| 2:B:2419:ASP:HA   | 2:B:2422:ASP:HB2  | 2.00                     | 0.44              |
| 2:D:2911:LYS:O    | 2:D:2912:SER:O    | 2.36                     | 0.44              |
| 2:B:2744:ASN:HB2  | 2:B:2941:VAL:N    | 2.33                     | 0.44              |
| 2:D:2541:ASP:OD1  | 2:D:2543:LYS:N    | 2.50                     | 0.44              |
| 2:B:2950:TRP:N    | 2:B:2951:PRO:CD   | 2.68                     | 0.44              |
| 2:D:2620:VAL:CG2  | 2:D:2677:VAL:HA   | 2.46                     | 0.44              |
| 1:C:18:GLU:OE2    | 2:D:2444:LYS:NZ   | 2.43                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:39:TRP:HE1    | 2:D:2733:LEU:HB3  | 1.83                     | 0.44              |
| 2:D:2752:VAL:HG12 | 2:D:2930:GLU:HA   | 2.00                     | 0.44              |
| 2:B:2750:VAL:CG1  | 2:B:2904:THR:N    | 2.81                     | 0.44              |
| 2:B:2765:VAL:HG23 | 2:B:2766:SER:H    | 1.82                     | 0.44              |
| 2:D:3060:SER:O    | 2:D:3063:PRO:HD3  | 2.18                     | 0.44              |
| 2:D:2956:THR:O    | 2:D:2957:ALA:C    | 2.55                     | 0.44              |
| 1:A:43:TRP:HH2    | 2:B:2713:THR:HG1  | 1.62                     | 0.43              |
| 2:B:2744:ASN:CB   | 2:B:2940:SER:HB3  | 2.41                     | 0.43              |
| 2:D:2745:VAL:H    | 2:D:2940:SER:CB   | 2.31                     | 0.43              |
| 2:D:2924:LEU:HB3  | 2:D:2925:PRO:HD3  | 1.99                     | 0.43              |
| 2:D:2494:ILE:HD11 | 2:D:2523:GLY:O    | 2.18                     | 0.43              |
| 1:C:56:LEU:N      | 2:D:2462:PRO:HG2  | 2.29                     | 0.43              |
| 2:B:2719:HIS:O    | 2:B:2720:SER:C    | 2.56                     | 0.43              |
| 2:D:2666:LEU:HD23 | 2:D:2669:LEU:HD12 | 2.00                     | 0.43              |
| 2:B:2940:SER:O    | 2:B:2941:VAL:CG2  | 2.61                     | 0.43              |
| 2:B:2929:THR:O    | 2:B:2930:GLU:C    | 2.55                     | 0.43              |
| 2:B:2410:LEU:HD13 | 2:B:2504:CYS:O    | 2.18                     | 0.43              |
| 2:D:3094:GLU:C    | 2:D:3096:ILE:N    | 2.72                     | 0.43              |
| 2:D:2418:ARG:O    | 2:D:2421:GLN:HB3  | 2.18                     | 0.43              |
| 2:D:2675:LEU:HD23 | 2:D:2675:LEU:HA   | 1.79                     | 0.43              |
| 1:C:12:LEU:HD21   | 2:D:2443:THR:HG23 | 2.00                     | 0.43              |
| 1:C:60:LEU:HD12   | 2:D:2563:ALA:N    | 2.33                     | 0.43              |
| 1:C:48:VAL:C      | 1:C:49:GLU:CG     | 2.87                     | 0.43              |
| 1:A:48:VAL:C      | 1:A:49:GLU:CG     | 2.86                     | 0.43              |
| 1:A:43:TRP:C      | 1:A:45:ASP:N      | 2.72                     | 0.43              |
| 2:B:2744:ASN:CB   | 2:B:2940:SER:CB   | 2.88                     | 0.43              |
| 2:B:2476:SER:C    | 2:B:2478:ALA:H    | 2.21                     | 0.43              |
| 2:D:2479:CYS:O    | 2:D:2481:SER:N    | 2.51                     | 0.43              |
| 2:D:3029:LEU:HD23 | 2:D:3030:VAL:N    | 2.32                     | 0.43              |
| 2:B:2762:GLU:CB   | 2:B:2772:ARG:HH12 | 2.32                     | 0.43              |
| 2:D:2492:PHE:CE2  | 2:D:2578:ASN:HA   | 2.52                     | 0.43              |
| 2:B:2610:ASP:O    | 2:B:2610:ASP:CG   | 2.56                     | 0.43              |
| 2:D:2676:THR:HG22 | 2:D:2679:GLN:NE2  | 2.34                     | 0.43              |
| 1:C:21:GLU:HG3    | 1:C:22:PHE:CG     | 2.53                     | 0.43              |
| 1:A:21:GLU:HG3    | 1:A:22:PHE:CG     | 2.53                     | 0.43              |
| 2:B:2557:ILE:O    | 2:B:2561:LEU:HD12 | 2.19                     | 0.43              |
| 1:C:39:TRP:CD1    | 2:D:2733:LEU:HB3  | 2.53                     | 0.43              |
| 1:C:43:TRP:C      | 1:C:45:ASP:N      | 2.71                     | 0.43              |
| 2:B:2667:LEU:HD23 | 2:B:2671:LYS:HD3  | 2.00                     | 0.43              |
| 2:B:3058:SER:O    | 2:B:3060:SER:N    | 2.46                     | 0.43              |
| 2:D:3111:LEU:HD12 | 2:D:3111:LEU:HA   | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2608:ARG:CA   | 2:D:2608:ARG:HH11 | 2.30                     | 0.43              |
| 2:B:2933:ARG:HB3  | 2:B:2968:VAL:HG22 | 2.00                     | 0.43              |
| 2:D:2730:PRO:HB2  | 2:D:2747:CYS:HB2  | 1.99                     | 0.43              |
| 2:B:2915:LEU:HD12 | 2:B:2915:LEU:C    | 2.38                     | 0.43              |
| 2:B:2778:GLU:HA   | 2:B:2781:ALA:HB3  | 2.01                     | 0.43              |
| 2:D:2756:TYR:HD2  | 2:D:3070:PHE:CB   | 2.30                     | 0.43              |
| 1:A:43:TRP:O      | 1:A:45:ASP:N      | 2.47                     | 0.43              |
| 2:B:2745:VAL:N    | 2:B:2940:SER:CB   | 2.81                     | 0.43              |
| 2:B:3105:LYS:O    | 2:B:3109:GLN:HB2  | 2.18                     | 0.43              |
| 2:D:2762:GLU:CB   | 2:D:2772:ARG:HH12 | 2.31                     | 0.43              |
| 2:D:2688:LEU:HD12 | 2:D:2688:LEU:HA   | 1.77                     | 0.43              |
| 2:D:3048:ALA:HB1  | 2:D:3082:PHE:CE2  | 2.52                     | 0.43              |
| 2:B:2592:VAL:HG11 | 2:B:2655:TRP:CH2  | 2.54                     | 0.43              |
| 2:D:2902:ARG:NH1  | 2:D:2914:LEU:HD13 | 2.33                     | 0.43              |
| 2:B:2991:PRO:O    | 2:B:2993:PHE:N    | 2.51                     | 0.43              |
| 2:D:3042:LYS:O    | 2:D:3045:VAL:HG23 | 2.18                     | 0.43              |
| 2:D:2903:VAL:O    | 2:D:2913:ALA:N    | 2.48                     | 0.43              |
| 2:B:2672:SER:CB   | 2:B:2674:ARG:HG2  | 2.46                     | 0.43              |
| 2:B:2953:ILE:O    | 2:B:2954:GLN:HB2  | 2.17                     | 0.43              |
| 2:D:3057:GLU:O    | 2:D:3060:SER:HB2  | 2.19                     | 0.43              |
| 2:B:2898:VAL:HG22 | 2:B:2918:TRP:CZ3  | 2.53                     | 0.43              |
| 2:B:3117:LYS:HA   | 2:B:3117:LYS:HD3  | 1.72                     | 0.43              |
| 1:C:46:ASP:O      | 1:C:47:ASN:O      | 2.37                     | 0.43              |
| 2:B:2476:SER:HG   | 2:B:2478:ALA:HB3  | 1.81                     | 0.43              |
| 2:D:2943:LYS:O    | 2:D:2944:SER:O    | 2.36                     | 0.43              |
| 2:D:2552:ASN:O    | 2:D:2555:ARG:N    | 2.52                     | 0.43              |
| 2:B:2589:ARG:CG   | 2:B:2589:ARG:HH11 | 2.22                     | 0.43              |
| 2:B:2492:PHE:CE2  | 2:B:2578:ASN:HA   | 2.53                     | 0.43              |
| 2:D:3083:GLN:HA   | 2:D:3086:VAL:CG1  | 2.45                     | 0.43              |
| 1:A:50:ASP:O      | 1:A:52:PHE:N      | 2.51                     | 0.43              |
| 1:A:60:LEU:HA     | 2:B:2566:PHE:CE2  | 2.54                     | 0.43              |
| 2:B:2436:GLN:HA   | 2:B:2437:PRO:HD2  | 1.88                     | 0.43              |
| 2:D:3100:TYR:C    | 2:D:3102:GLU:N    | 2.71                     | 0.43              |
| 2:D:2610:ASP:O    | 2:D:2610:ASP:CG   | 2.55                     | 0.43              |
| 2:B:2606:LEU:HD21 | 2:B:2658:VAL:HG11 | 2.00                     | 0.43              |
| 1:A:43:TRP:CZ3    | 2:B:2713:THR:O    | 2.71                     | 0.43              |
| 2:B:2666:LEU:CD1  | 2:B:2708:ILE:HG22 | 2.48                     | 0.43              |
| 2:B:2943:LYS:O    | 2:B:2944:SER:O    | 2.36                     | 0.43              |
| 1:A:62:LYS:O      | 1:A:63:HIS:C      | 2.57                     | 0.43              |
| 2:D:2782:LEU:O    | 2:D:2784:PHE:N    | 2.51                     | 0.43              |
| 2:B:2744:ASN:OD1  | 2:B:2744:ASN:C    | 2.57                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2479:CYS:O    | 2:B:2481:SER:N    | 2.52                     | 0.43              |
| 2:B:2501:GLU:O    | 2:B:2501:GLU:HG3  | 2.19                     | 0.43              |
| 2:B:3093:ILE:CG2  | 2:B:3094:GLU:N    | 2.82                     | 0.43              |
| 2:D:2745:VAL:N    | 2:D:2940:SER:CB   | 2.82                     | 0.43              |
| 2:D:2772:ARG:CZ   | 2:D:2780:GLU:HG2  | 2.49                     | 0.43              |
| 2:B:2465:CYS:HB3  | 2:B:2566:PHE:CE1  | 2.54                     | 0.43              |
| 1:A:60:LEU:HD12   | 2:B:2563:ALA:CA   | 2.49                     | 0.43              |
| 1:C:37:HIS:O      | 1:C:37:HIS:ND1    | 2.52                     | 0.43              |
| 2:D:2599:ARG:HH22 | 2:D:2609:ASP:HB3  | 1.83                     | 0.43              |
| 2:D:3100:TYR:O    | 2:D:3101:LYS:C    | 2.57                     | 0.42              |
| 2:D:2704:LEU:HD23 | 2:D:2704:LEU:C    | 2.40                     | 0.42              |
| 2:D:2720:SER:O    | 2:D:2721:LYS:HB2  | 2.19                     | 0.42              |
| 2:D:2908:LYS:O    | 2:D:2910:GLU:N    | 2.52                     | 0.42              |
| 2:B:3089:MET:O    | 2:B:3091:HIS:N    | 2.52                     | 0.42              |
| 2:B:3100:TYR:C    | 2:B:3102:GLU:N    | 2.71                     | 0.42              |
| 2:B:2427:ASN:O    | 2:B:2428:LYS:C    | 2.57                     | 0.42              |
| 2:D:3096:ILE:O    | 2:D:3099:PHE:HD2  | 2.02                     | 0.42              |
| 2:D:2551:SER:O    | 2:D:2554:TYR:HB3  | 2.19                     | 0.42              |
| 2:D:2439:SER:HB3  | 2:D:2584:LEU:CD2  | 2.49                     | 0.42              |
| 2:B:2421:GLN:HA   | 2:B:2424:ARG:NE   | 2.34                     | 0.42              |
| 2:D:2648:THR:OG1  | 2:D:2649:ILE:N    | 2.51                     | 0.42              |
| 2:B:2911:LYS:O    | 2:B:2912:SER:C    | 2.57                     | 0.42              |
| 2:B:3094:GLU:C    | 2:B:3096:ILE:N    | 2.72                     | 0.42              |
| 2:B:3110:VAL:C    | 2:B:3112:LYS:N    | 2.72                     | 0.42              |
| 2:D:3100:TYR:CD1  | 2:D:3101:LYS:N    | 2.87                     | 0.42              |
| 2:D:2492:PHE:CE2  | 2:D:2578:ASN:CA   | 3.02                     | 0.42              |
| 1:C:60:LEU:HA     | 2:D:2566:PHE:CD2  | 2.54                     | 0.42              |
| 1:C:60:LEU:HA     | 2:D:2566:PHE:CE2  | 2.54                     | 0.42              |
| 2:D:2447:THR:O    | 2:D:2448:LEU:O    | 2.36                     | 0.42              |
| 2:B:2956:THR:O    | 2:B:2957:ALA:C    | 2.58                     | 0.42              |
| 1:A:39:TRP:NE1    | 2:B:2733:LEU:HB3  | 2.35                     | 0.42              |
| 2:B:3101:LYS:O    | 2:B:3105:LYS:HG3  | 2.19                     | 0.42              |
| 2:D:2655:TRP:HB3  | 2:D:2656:TYR:CE1  | 2.54                     | 0.42              |
| 2:B:2582:VAL:O    | 2:B:2586:LEU:HD12 | 2.19                     | 0.42              |
| 2:D:2687:GLU:O    | 2:D:2706:LEU:HD22 | 2.19                     | 0.42              |
| 2:B:2511:LEU:O    | 2:B:2512:ALA:C    | 2.58                     | 0.42              |
| 2:B:3028:LEU:HD11 | 2:B:3108:ILE:HB   | 2.02                     | 0.42              |
| 2:D:2783:ARG:O    | 2:D:2783:ARG:HD2  | 2.20                     | 0.42              |
| 2:B:2492:PHE:CE2  | 2:B:2578:ASN:CA   | 3.03                     | 0.42              |
| 2:D:2689:VAL:HG12 | 2:D:2690:GLY:N    | 2.35                     | 0.42              |
| 2:D:2782:LEU:C    | 2:D:2784:PHE:H    | 2.23                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:3115:SER:HB2  | 2:D:3116:PRO:HD2  | 2.01                     | 0.42              |
| 2:B:2941:VAL:O    | 2:B:2942:SER:O    | 2.37                     | 0.42              |
| 2:D:2779:LYS:C    | 2:D:2781:ALA:H    | 2.23                     | 0.42              |
| 2:B:2582:VAL:O    | 2:B:2582:VAL:HG12 | 2.20                     | 0.42              |
| 1:C:18:GLU:OE1    | 2:D:2450:ARG:NH2  | 2.52                     | 0.42              |
| 2:B:2439:SER:HB3  | 2:B:2584:LEU:HD21 | 2.01                     | 0.42              |
| 1:C:60:LEU:HD12   | 2:D:2563:ALA:CA   | 2.50                     | 0.42              |
| 2:B:2440:LEU:C    | 2:B:2442:LEU:N    | 2.72                     | 0.42              |
| 2:B:3060:SER:O    | 2:B:3063:PRO:HD3  | 2.20                     | 0.42              |
| 2:D:2425:ILE:HG23 | 2:D:2542:PRO:CG   | 2.49                     | 0.42              |
| 2:D:2895:VAL:HG22 | 2:D:2896:SER:N    | 2.33                     | 0.42              |
| 2:B:3115:SER:OG   | 2:B:3116:PRO:HD2  | 2.19                     | 0.42              |
| 2:D:2933:ARG:HB2  | 2:D:2968:VAL:HG22 | 2.01                     | 0.42              |
| 2:D:2997:CYS:O    | 2:D:2998:SER:C    | 2.58                     | 0.42              |
| 2:D:2684:GLN:HE21 | 2:D:2684:GLN:HB2  | 1.54                     | 0.42              |
| 2:D:2597:SER:O    | 2:D:2598:SER:C    | 2.58                     | 0.42              |
| 2:B:2669:LEU:O    | 2:B:2674:ARG:N    | 2.48                     | 0.42              |
| 2:D:2483:ASN:HD22 | 2:D:2486:ASN:HD22 | 1.68                     | 0.42              |
| 2:D:2465:CYS:HB3  | 2:D:2566:PHE:CE1  | 2.55                     | 0.42              |
| 1:A:60:LEU:HD12   | 2:B:2563:ALA:N    | 2.34                     | 0.42              |
| 2:D:2995:PRO:HA   | 2:D:2996:PRO:HD3  | 1.89                     | 0.42              |
| 2:D:3057:GLU:HA   | 2:D:3057:GLU:OE1  | 2.19                     | 0.42              |
| 2:D:3109:GLN:HE22 | 2:D:3110:VAL:HG12 | 1.84                     | 0.42              |
| 2:B:2783:ARG:HD2  | 2:B:2783:ARG:O    | 2.20                     | 0.42              |
| 2:B:2487:ALA:C    | 2:B:2489:TYR:H    | 2.22                     | 0.42              |
| 2:D:2719:HIS:O    | 2:D:2720:SER:C    | 2.58                     | 0.42              |
| 2:B:2782:LEU:O    | 2:B:2784:PHE:N    | 2.52                     | 0.42              |
| 2:B:2927:LEU:C    | 2:B:2927:LEU:HD12 | 2.40                     | 0.42              |
| 2:B:3109:GLN:NE2  | 2:B:3110:VAL:CG1  | 2.83                     | 0.42              |
| 2:D:2953:ILE:CG1  | 2:D:2954:GLN:N    | 2.74                     | 0.42              |
| 2:D:2762:GLU:OE2  | 2:D:2893:ARG:NH1  | 2.53                     | 0.42              |
| 2:D:2749:ASP:OD1  | 2:D:2933:ARG:NH2  | 2.53                     | 0.42              |
| 2:B:2955:LEU:HD12 | 2:B:2955:LEU:N    | 2.35                     | 0.42              |
| 1:C:20:GLU:O      | 1:C:21:GLU:C      | 2.59                     | 0.42              |
| 1:C:13:LEU:HD11   | 2:D:2453:LEU:HA   | 2.01                     | 0.42              |
| 1:C:43:TRP:O      | 1:C:45:ASP:N      | 2.44                     | 0.41              |
| 2:D:3046:LEU:HD22 | 2:D:3090:LYS:HB2  | 2.02                     | 0.41              |
| 2:D:3100:TYR:O    | 2:D:3103:ALA:N    | 2.53                     | 0.41              |
| 2:B:2490:PHE:HE2  | 2:B:2492:PHE:CZ   | 2.37                     | 0.41              |
| 2:B:2525:ALA:HA   | 2:B:2529:GLU:OE1  | 2.20                     | 0.41              |
| 2:D:2906:TYR:CE1  | 2:D:2933:ARG:NE   | 2.88                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:38:VAL:O      | 1:A:38:VAL:HG13   | 2.19                     | 0.41              |
| 2:B:2777:GLU:O    | 2:B:2778:GLU:C    | 2.58                     | 0.41              |
| 2:B:2621:SER:HB3  | 2:B:2652:THR:HG22 | 2.02                     | 0.41              |
| 1:C:45:ASP:OD2    | 1:C:45:ASP:O      | 2.39                     | 0.41              |
| 2:D:2750:VAL:HG11 | 2:D:2903:VAL:CG2  | 2.48                     | 0.41              |
| 2:B:2688:LEU:HD13 | 2:B:2706:LEU:HD23 | 2.02                     | 0.41              |
| 2:D:3007:VAL:HB   | 2:D:3104:GLU:OE1  | 2.21                     | 0.41              |
| 2:D:2735:LEU:HD13 | 2:D:2748:VAL:HG11 | 2.02                     | 0.41              |
| 2:B:2958:THR:O    | 2:B:2961:THR:HB   | 2.19                     | 0.41              |
| 2:B:2488:GLU:HG2  | 2:B:2527:LYS:HD2  | 2.02                     | 0.41              |
| 2:D:2667:LEU:HD23 | 2:D:2671:LYS:HD3  | 2.03                     | 0.41              |
| 2:D:2969:SER:HB2  | 2:D:2972:THR:CG2  | 2.50                     | 0.41              |
| 2:B:2710:ALA:HA   | 2:B:2713:THR:HG23 | 2.01                     | 0.41              |
| 2:B:2908:LYS:O    | 2:B:2910:GLU:N    | 2.53                     | 0.41              |
| 2:B:3091:HIS:O    | 2:B:3094:GLU:N    | 2.53                     | 0.41              |
| 2:B:3097:ASP:O    | 2:B:3099:PHE:N    | 2.52                     | 0.41              |
| 2:D:2773:ASN:C    | 2:D:2775:ARG:N    | 2.73                     | 0.41              |
| 2:D:2414:LEU:O    | 2:D:2415:GLN:C    | 2.58                     | 0.41              |
| 2:B:2461:VAL:HB   | 2:B:2462:PRO:HD2  | 2.01                     | 0.41              |
| 2:B:2457:VAL:HG21 | 2:B:2568:PHE:CE2  | 2.56                     | 0.41              |
| 2:B:2782:LEU:C    | 2:B:2784:PHE:H    | 2.23                     | 0.41              |
| 2:B:3047:ILE:HD13 | 2:B:3047:ILE:HA   | 1.80                     | 0.41              |
| 2:D:2475:VAL:O    | 2:D:2476:SER:C    | 2.58                     | 0.41              |
| 2:B:2412:SER:O    | 2:B:2414:LEU:N    | 2.53                     | 0.41              |
| 2:B:3030:VAL:CG1  | 2:B:3031:VAL:N    | 2.84                     | 0.41              |
| 2:D:3060:SER:O    | 2:D:3062:VAL:N    | 2.54                     | 0.41              |
| 2:D:2778:GLU:HA   | 2:D:2781:ALA:HB3  | 2.02                     | 0.41              |
| 2:B:2692:PRO:HG2  | 2:B:2693:ASP:H    | 1.84                     | 0.41              |
| 2:B:2624:ILE:HG22 | 2:B:2647:ASP:HB3  | 2.01                     | 0.41              |
| 2:B:2455:ALA:O    | 2:B:2456:ALA:C    | 2.58                     | 0.41              |
| 2:D:2929:THR:O    | 2:D:2930:GLU:O    | 2.38                     | 0.41              |
| 2:B:2909:ARG:HH11 | 2:B:2909:ARG:HG3  | 1.86                     | 0.41              |
| 2:D:3005:VAL:HG23 | 2:D:3089:MET:HE1  | 2.02                     | 0.41              |
| 2:B:2608:ARG:HH11 | 2:B:2608:ARG:CA   | 2.30                     | 0.41              |
| 2:B:3081:HIS:O    | 2:B:3084:GLU:HB3  | 2.20                     | 0.41              |
| 2:B:2985:PHE:CD1  | 2:B:2985:PHE:N    | 2.81                     | 0.41              |
| 1:A:22:PHE:O      | 1:A:23:PRO:C      | 2.59                     | 0.41              |
| 2:B:2530:PHE:HD2  | 2:B:2583:LEU:HD23 | 1.86                     | 0.41              |
| 2:D:2900:LYS:HD2  | 2:D:3070:PHE:CZ   | 2.55                     | 0.41              |
| 2:D:3108:ILE:HG12 | 2:D:3112:LYS:HE3  | 2.01                     | 0.41              |
| 2:B:2755:VAL:HG23 | 2:B:2930:GLU:CG   | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2480:ILE:CG2  | 2:B:2480:ILE:O    | 2.68                     | 0.41              |
| 2:D:2950:TRP:O    | 2:D:2952:SER:N    | 2.49                     | 0.41              |
| 2:B:2918:TRP:O    | 2:B:2919:ARG:C    | 2.58                     | 0.41              |
| 2:B:2924:LEU:HB3  | 2:B:2925:PRO:HD3  | 2.02                     | 0.41              |
| 2:B:2902:ARG:NH1  | 2:B:2914:LEU:HD13 | 2.36                     | 0.41              |
| 2:D:2421:GLN:HE21 | 2:D:2536:ASP:CG   | 2.21                     | 0.41              |
| 2:B:2487:ALA:C    | 2:B:2489:TYR:N    | 2.73                     | 0.41              |
| 2:B:2676:THR:HG22 | 2:B:2679:GLN:NE2  | 2.36                     | 0.41              |
| 2:D:2692:PRO:O    | 2:D:2694:ALA:N    | 2.43                     | 0.41              |
| 2:B:2651:LEU:HD12 | 2:B:2660:ALA:HB2  | 2.03                     | 0.41              |
| 2:D:3047:ILE:HD13 | 2:D:3047:ILE:HA   | 1.83                     | 0.41              |
| 2:B:3096:ILE:O    | 2:B:3099:PHE:HD2  | 2.03                     | 0.41              |
| 2:D:3109:GLN:C    | 2:D:3109:GLN:HE21 | 2.23                     | 0.41              |
| 2:B:2753:GLN:HB2  | 2:B:2902:ARG:O    | 2.20                     | 0.41              |
| 2:D:2578:ASN:O    | 2:D:2582:VAL:HG23 | 2.20                     | 0.41              |
| 2:B:3068:GLY:N    | 2:B:3071:SER:OG   | 2.54                     | 0.41              |
| 2:D:2991:PRO:O    | 2:D:2993:PHE:N    | 2.54                     | 0.41              |
| 2:D:2663:ASP:OD1  | 2:D:2710:ALA:N    | 2.39                     | 0.41              |
| 2:D:2666:LEU:O    | 2:D:2667:LEU:C    | 2.57                     | 0.41              |
| 2:D:2909:ARG:HH11 | 2:D:2909:ARG:HG3  | 1.85                     | 0.41              |
| 2:B:2403:PHE:HD1  | 2:B:2503:LEU:HD13 | 1.85                     | 0.41              |
| 2:B:3100:TYR:O    | 2:B:3101:LYS:C    | 2.58                     | 0.41              |
| 2:B:3107:LEU:O    | 2:B:3108:ILE:C    | 2.59                     | 0.41              |
| 2:D:2428:LYS:C    | 2:D:2430:ARG:N    | 2.72                     | 0.41              |
| 2:D:2762:GLU:HB3  | 2:D:2772:ARG:HH12 | 1.85                     | 0.41              |
| 2:B:2921:SER:O    | 2:B:2924:LEU:HB2  | 2.21                     | 0.41              |
| 2:D:2600:SER:HB3  | 2:D:2603:LYS:HB2  | 2.02                     | 0.41              |
| 2:B:2600:SER:HB2  | 2:B:2655:TRP:HB2  | 2.03                     | 0.41              |
| 2:B:2554:TYR:CE1  | 2:B:2582:VAL:HG11 | 2.56                     | 0.41              |
| 2:B:2620:VAL:HG23 | 2:B:2677:VAL:HA   | 2.02                     | 0.41              |
| 1:C:61:GLU:C      | 1:C:63:HIS:H      | 2.23                     | 0.41              |
| 2:D:2748:VAL:HG21 | 2:D:2939:LEU:HD23 | 2.03                     | 0.41              |
| 2:B:2735:LEU:HD11 | 2:B:2955:LEU:HD11 | 2.02                     | 0.41              |
| 2:D:2602:LEU:HA   | 2:D:2605:ILE:HB   | 2.03                     | 0.41              |
| 2:D:2621:SER:HB3  | 2:D:2652:THR:HG22 | 2.03                     | 0.41              |
| 2:B:2981:GLU:HG3  | 2:B:2982:LEU:N    | 2.36                     | 0.41              |
| 1:C:51:ASP:O      | 2:D:2717:ARG:HA   | 2.21                     | 0.41              |
| 2:B:2779:LYS:C    | 2:B:2781:ALA:H    | 2.24                     | 0.41              |
| 2:D:3068:GLY:O    | 2:D:3071:SER:OG   | 2.39                     | 0.41              |
| 2:D:2511:LEU:HD12 | 2:D:2517:LEU:HB2  | 2.02                     | 0.41              |
| 2:B:2413:SER:HB2  | 2:B:2506:GLY:CA   | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:2738:LEU:HD22 | 2:D:2745:VAL:HG22 | 2.03                     | 0.41              |
| 2:B:2772:ARG:HD3  | 2:B:2776:GLU:O    | 2.20                     | 0.41              |
| 2:B:3081:HIS:CD2  | 2:B:3082:PHE:N    | 2.89                     | 0.41              |
| 2:D:2623:ILE:HA   | 2:D:2649:ILE:HG22 | 2.02                     | 0.41              |
| 2:D:2755:VAL:HG13 | 2:D:2899:TRP:NE1  | 2.33                     | 0.41              |
| 2:B:2995:PRO:HD2  | 2:B:3054:TRP:CE3  | 2.56                     | 0.41              |
| 2:B:2700:ALA:HA   | 2:B:2701:PRO:HD3  | 1.91                     | 0.41              |
| 2:B:2621:SER:O    | 2:B:2622:ASP:HB2  | 2.20                     | 0.41              |
| 2:B:2969:SER:HB2  | 2:B:2972:THR:HG23 | 2.03                     | 0.40              |
| 2:D:2480:ILE:HG22 | 2:D:2480:ILE:O    | 2.20                     | 0.40              |
| 2:D:2744:ASN:OD1  | 2:D:2744:ASN:C    | 2.60                     | 0.40              |
| 2:B:2550:VAL:O    | 2:B:2554:TYR:HB2  | 2.22                     | 0.40              |
| 2:B:2676:THR:HG23 | 2:B:2679:GLN:CG   | 2.50                     | 0.40              |
| 2:B:2615:THR:HG23 | 2:B:2615:THR:O    | 2.21                     | 0.40              |
| 2:D:2490:PHE:O    | 2:D:2491:GLN:HB2  | 2.22                     | 0.40              |
| 2:D:2448:LEU:O    | 2:D:2449:PRO:C    | 2.58                     | 0.40              |
| 2:D:2903:VAL:O    | 2:D:2912:SER:HA   | 2.21                     | 0.40              |
| 2:B:2403:PHE:CD1  | 2:B:2503:LEU:HD13 | 2.56                     | 0.40              |
| 2:D:2541:ASP:O    | 2:D:2542:PRO:C    | 2.60                     | 0.40              |
| 2:B:2762:GLU:HB3  | 2:B:2772:ARG:HH12 | 1.86                     | 0.40              |
| 1:C:57:ARG:HG2    | 2:D:2559:TRP:CZ2  | 2.56                     | 0.40              |
| 2:B:2936:ILE:HG21 | 2:B:2939:LEU:HB2  | 2.03                     | 0.40              |
| 2:B:2588:TYR:O    | 2:B:2591:ASP:N    | 2.53                     | 0.40              |
| 1:C:50:ASP:CG     | 1:C:51:ASP:N      | 2.74                     | 0.40              |
| 2:B:2599:ARG:HH22 | 2:B:2609:ASP:CB   | 2.34                     | 0.40              |
| 2:B:3072:VAL:CG1  | 2:B:3073:PHE:N    | 2.82                     | 0.40              |
| 2:D:2553:HIS:ND1  | 2:D:2589:ARG:HD3  | 2.37                     | 0.40              |
| 2:D:2414:LEU:C    | 2:D:2416:ASN:N    | 2.72                     | 0.40              |
| 2:B:2687:GLU:O    | 2:B:2707:LYS:N    | 2.54                     | 0.40              |
| 2:D:2490:PHE:HE2  | 2:D:2492:PHE:CZ   | 2.38                     | 0.40              |
| 2:D:2488:GLU:HG2  | 2:D:2527:LYS:HD2  | 2.04                     | 0.40              |
| 2:D:2911:LYS:O    | 2:D:2912:SER:C    | 2.59                     | 0.40              |
| 2:B:2482:VAL:HA   | 2:B:2486:ASN:HD21 | 1.86                     | 0.40              |
| 2:B:3108:ILE:HA   | 2:B:3111:LEU:CB   | 2.52                     | 0.40              |
| 2:B:2427:ASN:OD1  | 2:B:2430:ARG:HD2  | 2.21                     | 0.40              |
| 2:D:2917:ILE:HD13 | 2:D:2924:LEU:CD2  | 2.41                     | 0.40              |
| 2:B:2461:VAL:HB   | 2:B:2462:PRO:CD   | 2.51                     | 0.40              |
| 2:B:2939:LEU:HD21 | 2:B:2955:LEU:HD23 | 2.04                     | 0.40              |
| 2:B:2653:ASP:C    | 2:B:2722:LEU:HD13 | 2.41                     | 0.40              |
| 2:B:2602:LEU:CB   | 2:B:2653:ASP:OD2  | 2.69                     | 0.40              |
| 2:B:3042:LYS:O    | 2:B:3045:VAL:HG23 | 2.21                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:2738:LEU:HD22 | 2:B:2745:VAL:CG2 | 2.52                     | 0.40              |
| 2:B:2903:VAL:O    | 2:B:2912:SER:HA  | 2.22                     | 0.40              |
| 2:B:2494:ILE:HD11 | 2:B:2523:GLY:HA3 | 2.03                     | 0.40              |
| 2:B:3100:TYR:CD1  | 2:B:3101:LYS:N   | 2.90                     | 0.40              |
| 2:D:2950:TRP:N    | 2:D:2951:PRO:CD  | 2.68                     | 0.40              |
| 2:D:2985:PHE:C    | 2:D:2987:LYS:N   | 2.74                     | 0.40              |
| 2:D:3060:SER:C    | 2:D:3062:VAL:H   | 2.24                     | 0.40              |
| 2:D:2499:GLY:O    | 2:D:2501:GLU:HG2 | 2.22                     | 0.40              |
| 2:D:2501:GLU:O    | 2:D:2501:GLU:HG3 | 2.21                     | 0.40              |
| 2:B:2906:TYR:CE1  | 2:B:2933:ARG:NE  | 2.89                     | 0.40              |
| 2:B:2569:PRO:O    | 2:B:2573:ALA:HA  | 2.21                     | 0.40              |
| 2:D:2719:HIS:CD2  | 2:D:2720:SER:H   | 2.40                     | 0.40              |
| 1:A:20:GLU:O      | 1:A:21:GLU:C     | 2.59                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 41/70 (59%)     | 18 (44%)  | 11 (27%)  | 12 (29%)  | 0           | 0 |
| 1   | C     | 41/70 (59%)     | 18 (44%)  | 11 (27%)  | 12 (29%)  | 0           | 0 |
| 2   | B     | 585/817 (72%)   | 387 (66%) | 128 (22%) | 70 (12%)  | 0           | 5 |
| 2   | D     | 585/817 (72%)   | 391 (67%) | 122 (21%) | 72 (12%)  | 0           | 5 |
| All | All   | 1252/1774 (71%) | 814 (65%) | 272 (22%) | 166 (13%) | 0           | 4 |

All (166) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | ASP  |
| 1   | A     | 47  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 51   | ASP  |
| 1   | A     | 53   | SER  |
| 1   | A     | 57   | ARG  |
| 2   | B     | 2429 | GLU  |
| 2   | B     | 2448 | LEU  |
| 2   | B     | 2465 | CYS  |
| 2   | B     | 2466 | SER  |
| 2   | B     | 2467 | PRO  |
| 2   | B     | 2501 | GLU  |
| 2   | B     | 2512 | ALA  |
| 2   | B     | 2573 | ALA  |
| 2   | B     | 2610 | ASP  |
| 2   | B     | 2611 | THR  |
| 2   | B     | 2647 | ASP  |
| 2   | B     | 2686 | ALA  |
| 2   | B     | 2692 | PRO  |
| 2   | B     | 2737 | SER  |
| 2   | B     | 2752 | VAL  |
| 2   | B     | 2907 | LYS  |
| 2   | B     | 2909 | ARG  |
| 2   | B     | 2912 | SER  |
| 2   | B     | 2930 | GLU  |
| 2   | B     | 2941 | VAL  |
| 2   | B     | 2942 | SER  |
| 2   | B     | 2944 | SER  |
| 2   | B     | 2946 | ASN  |
| 2   | B     | 2950 | TRP  |
| 2   | B     | 3016 | ALA  |
| 2   | B     | 3038 | ASN  |
| 2   | B     | 3099 | PHE  |
| 2   | B     | 3101 | LYS  |
| 2   | B     | 3114 | ASP  |
| 1   | C     | 9    | ASP  |
| 1   | C     | 41   | ASP  |
| 1   | C     | 47   | ASN  |
| 1   | C     | 51   | ASP  |
| 1   | C     | 53   | SER  |
| 1   | C     | 57   | ARG  |
| 2   | D     | 2429 | GLU  |
| 2   | D     | 2448 | LEU  |
| 2   | D     | 2465 | CYS  |
| 2   | D     | 2466 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 2467 | PRO  |
| 2   | D     | 2501 | GLU  |
| 2   | D     | 2512 | ALA  |
| 2   | D     | 2573 | ALA  |
| 2   | D     | 2610 | ASP  |
| 2   | D     | 2611 | THR  |
| 2   | D     | 2647 | ASP  |
| 2   | D     | 2686 | ALA  |
| 2   | D     | 2692 | PRO  |
| 2   | D     | 2737 | SER  |
| 2   | D     | 2752 | VAL  |
| 2   | D     | 2907 | LYS  |
| 2   | D     | 2909 | ARG  |
| 2   | D     | 2912 | SER  |
| 2   | D     | 2941 | VAL  |
| 2   | D     | 2942 | SER  |
| 2   | D     | 2944 | SER  |
| 2   | D     | 2946 | ASN  |
| 2   | D     | 2950 | TRP  |
| 2   | D     | 2998 | SER  |
| 2   | D     | 3016 | ALA  |
| 2   | D     | 3038 | ASN  |
| 2   | D     | 3099 | PHE  |
| 2   | D     | 3101 | LYS  |
| 2   | D     | 3114 | ASP  |
| 1   | A     | 9    | ASP  |
| 1   | A     | 39   | TRP  |
| 1   | A     | 55   | GLN  |
| 2   | B     | 2407 | ASN  |
| 2   | B     | 2415 | GLN  |
| 2   | B     | 2460 | SER  |
| 2   | B     | 2507 | LYS  |
| 2   | B     | 2605 | ILE  |
| 2   | B     | 2694 | ALA  |
| 2   | B     | 2721 | LYS  |
| 2   | B     | 2893 | ARG  |
| 2   | B     | 2945 | LYS  |
| 2   | B     | 2979 | PRO  |
| 2   | B     | 2992 | ALA  |
| 2   | B     | 2998 | SER  |
| 2   | B     | 3040 | ASP  |
| 2   | B     | 3092 | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 39   | TRP  |
| 1   | C     | 55   | GLN  |
| 2   | D     | 2415 | GLN  |
| 2   | D     | 2460 | SER  |
| 2   | D     | 2507 | LYS  |
| 2   | D     | 2694 | ALA  |
| 2   | D     | 2721 | LYS  |
| 2   | D     | 2893 | ARG  |
| 2   | D     | 2930 | GLU  |
| 2   | D     | 2945 | LYS  |
| 2   | D     | 2979 | PRO  |
| 2   | D     | 2992 | ALA  |
| 2   | D     | 3040 | ASP  |
| 2   | D     | 3088 | ASN  |
| 2   | D     | 3092 | ALA  |
| 2   | B     | 2406 | PHE  |
| 2   | B     | 2519 | PRO  |
| 2   | B     | 2564 | MET  |
| 2   | B     | 2569 | PRO  |
| 2   | B     | 2710 | ALA  |
| 2   | B     | 2738 | LEU  |
| 2   | B     | 2970 | SER  |
| 2   | B     | 2988 | LEU  |
| 2   | B     | 3095 | ASN  |
| 2   | D     | 2519 | PRO  |
| 2   | D     | 2564 | MET  |
| 2   | D     | 2697 | PRO  |
| 2   | D     | 2710 | ALA  |
| 2   | D     | 2910 | GLU  |
| 2   | D     | 2954 | GLN  |
| 2   | D     | 2970 | SER  |
| 2   | D     | 2988 | LEU  |
| 2   | D     | 3095 | ASN  |
| 1   | A     | 44   | ASP  |
| 2   | B     | 2697 | PRO  |
| 2   | B     | 2764 | THR  |
| 2   | B     | 2910 | GLU  |
| 2   | B     | 2954 | GLN  |
| 2   | B     | 3008 | SER  |
| 2   | B     | 3088 | ASN  |
| 1   | C     | 10   | LEU  |
| 1   | C     | 44   | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 2407 | ASN  |
| 2   | D     | 2464 | ALA  |
| 2   | D     | 2490 | PHE  |
| 2   | D     | 2569 | PRO  |
| 2   | D     | 2605 | ILE  |
| 2   | D     | 2672 | SER  |
| 2   | D     | 2738 | LEU  |
| 2   | D     | 2764 | THR  |
| 2   | B     | 2490 | PHE  |
| 2   | D     | 2779 | LYS  |
| 2   | D     | 2985 | PHE  |
| 2   | D     | 3008 | SER  |
| 2   | D     | 3039 | GLU  |
| 2   | B     | 2447 | THR  |
| 2   | B     | 2685 | GLY  |
| 2   | B     | 2779 | LYS  |
| 2   | B     | 2991 | PRO  |
| 2   | D     | 2447 | THR  |
| 2   | D     | 2991 | PRO  |
| 2   | B     | 2462 | PRO  |
| 1   | C     | 48   | VAL  |
| 2   | D     | 2919 | ARG  |
| 1   | A     | 7    | PRO  |
| 1   | A     | 48   | VAL  |
| 2   | B     | 2592 | VAL  |
| 2   | B     | 3035 | ILE  |
| 1   | C     | 7    | PRO  |
| 2   | D     | 2462 | PRO  |
| 2   | D     | 2480 | ILE  |
| 2   | D     | 3035 | ILE  |
| 1   | A     | 8    | VAL  |
| 2   | D     | 2685 | GLY  |
| 2   | B     | 2474 | GLY  |
| 2   | B     | 3063 | PRO  |
| 2   | D     | 2592 | VAL  |
| 2   | D     | 2953 | ILE  |
| 2   | B     | 2480 | ILE  |
| 2   | B     | 2953 | ILE  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 41/63 (65%)     | 33 (80%)  | 8 (20%)   | 2           | 8  |
| 1   | C     | 41/63 (65%)     | 33 (80%)  | 8 (20%)   | 2           | 8  |
| 2   | B     | 517/721 (72%)   | 459 (89%) | 58 (11%)  | 7           | 32 |
| 2   | D     | 517/721 (72%)   | 459 (89%) | 58 (11%)  | 7           | 32 |
| All | All   | 1116/1568 (71%) | 984 (88%) | 132 (12%) | 6           | 29 |

All (132) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 14   | GLU  |
| 1   | A     | 19   | PHE  |
| 1   | A     | 22   | PHE  |
| 1   | A     | 23   | PRO  |
| 1   | A     | 49   | GLU  |
| 1   | A     | 54   | ASN  |
| 1   | A     | 56   | LEU  |
| 1   | A     | 60   | LEU  |
| 2   | B     | 2419 | ASP  |
| 2   | B     | 2430 | ARG  |
| 2   | B     | 2433 | LEU  |
| 2   | B     | 2434 | CYS  |
| 2   | B     | 2442 | LEU  |
| 2   | B     | 2443 | THR  |
| 2   | B     | 2450 | ARG  |
| 2   | B     | 2453 | LEU  |
| 2   | B     | 2479 | CYS  |
| 2   | B     | 2483 | ASN  |
| 2   | B     | 2494 | ILE  |
| 2   | B     | 2496 | ASP  |
| 2   | B     | 2527 | LYS  |
| 2   | B     | 2534 | LEU  |
| 2   | B     | 2537 | THR  |
| 2   | B     | 2583 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2584 | LEU  |
| 2   | B     | 2586 | LEU  |
| 2   | B     | 2598 | SER  |
| 2   | B     | 2608 | ARG  |
| 2   | B     | 2609 | ASP  |
| 2   | B     | 2614 | LYS  |
| 2   | B     | 2658 | VAL  |
| 2   | B     | 2675 | LEU  |
| 2   | B     | 2684 | GLN  |
| 2   | B     | 2698 | LEU  |
| 2   | B     | 2706 | LEU  |
| 2   | B     | 2713 | THR  |
| 2   | B     | 2714 | ARG  |
| 2   | B     | 2717 | ARG  |
| 2   | B     | 2726 | HIS  |
| 2   | B     | 2733 | LEU  |
| 2   | B     | 2736 | SER  |
| 2   | B     | 2744 | ASN  |
| 2   | B     | 2748 | VAL  |
| 2   | B     | 2756 | TYR  |
| 2   | B     | 2769 | TYR  |
| 2   | B     | 2773 | ASN  |
| 2   | B     | 2901 | LEU  |
| 2   | B     | 2915 | LEU  |
| 2   | B     | 2944 | SER  |
| 2   | B     | 2945 | LYS  |
| 2   | B     | 2968 | VAL  |
| 2   | B     | 2985 | PHE  |
| 2   | B     | 3007 | VAL  |
| 2   | B     | 3026 | LEU  |
| 2   | B     | 3029 | LEU  |
| 2   | B     | 3040 | ASP  |
| 2   | B     | 3055 | ARG  |
| 2   | B     | 3056 | PRO  |
| 2   | B     | 3058 | SER  |
| 2   | B     | 3062 | VAL  |
| 2   | B     | 3063 | PRO  |
| 2   | B     | 3081 | HIS  |
| 2   | B     | 3087 | THR  |
| 2   | B     | 3099 | PHE  |
| 2   | B     | 3104 | GLU  |
| 2   | B     | 3109 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 14   | GLU  |
| 1   | C     | 19   | PHE  |
| 1   | C     | 22   | PHE  |
| 1   | C     | 23   | PRO  |
| 1   | C     | 49   | GLU  |
| 1   | C     | 54   | ASN  |
| 1   | C     | 56   | LEU  |
| 1   | C     | 60   | LEU  |
| 2   | D     | 2405 | GLN  |
| 2   | D     | 2419 | ASP  |
| 2   | D     | 2430 | ARG  |
| 2   | D     | 2433 | LEU  |
| 2   | D     | 2434 | CYS  |
| 2   | D     | 2442 | LEU  |
| 2   | D     | 2443 | THR  |
| 2   | D     | 2450 | ARG  |
| 2   | D     | 2453 | LEU  |
| 2   | D     | 2479 | CYS  |
| 2   | D     | 2483 | ASN  |
| 2   | D     | 2494 | ILE  |
| 2   | D     | 2496 | ASP  |
| 2   | D     | 2527 | LYS  |
| 2   | D     | 2534 | LEU  |
| 2   | D     | 2583 | LEU  |
| 2   | D     | 2584 | LEU  |
| 2   | D     | 2586 | LEU  |
| 2   | D     | 2598 | SER  |
| 2   | D     | 2608 | ARG  |
| 2   | D     | 2609 | ASP  |
| 2   | D     | 2614 | LYS  |
| 2   | D     | 2658 | VAL  |
| 2   | D     | 2675 | LEU  |
| 2   | D     | 2684 | GLN  |
| 2   | D     | 2698 | LEU  |
| 2   | D     | 2706 | LEU  |
| 2   | D     | 2713 | THR  |
| 2   | D     | 2714 | ARG  |
| 2   | D     | 2717 | ARG  |
| 2   | D     | 2726 | HIS  |
| 2   | D     | 2733 | LEU  |
| 2   | D     | 2736 | SER  |
| 2   | D     | 2744 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 2748 | VAL  |
| 2   | D     | 2756 | TYR  |
| 2   | D     | 2769 | TYR  |
| 2   | D     | 2773 | ASN  |
| 2   | D     | 2901 | LEU  |
| 2   | D     | 2915 | LEU  |
| 2   | D     | 2944 | SER  |
| 2   | D     | 2945 | LYS  |
| 2   | D     | 2955 | LEU  |
| 2   | D     | 2968 | VAL  |
| 2   | D     | 2985 | PHE  |
| 2   | D     | 3026 | LEU  |
| 2   | D     | 3029 | LEU  |
| 2   | D     | 3040 | ASP  |
| 2   | D     | 3055 | ARG  |
| 2   | D     | 3056 | PRO  |
| 2   | D     | 3058 | SER  |
| 2   | D     | 3062 | VAL  |
| 2   | D     | 3063 | PRO  |
| 2   | D     | 3081 | HIS  |
| 2   | D     | 3099 | PHE  |
| 2   | D     | 3104 | GLU  |
| 2   | D     | 3109 | GLN  |
| 2   | D     | 3117 | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 54   | ASN  |
| 2   | B     | 2421 | GLN  |
| 2   | B     | 2436 | GLN  |
| 2   | B     | 2454 | GLN  |
| 2   | B     | 2486 | ASN  |
| 2   | B     | 2552 | ASN  |
| 2   | B     | 2596 | ASN  |
| 2   | B     | 2684 | GLN  |
| 2   | B     | 2954 | GLN  |
| 2   | B     | 2962 | GLN  |
| 2   | B     | 2965 | GLN  |
| 2   | B     | 3051 | ASN  |
| 2   | B     | 3053 | GLN  |
| 2   | B     | 3081 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 3083 | GLN  |
| 2   | B     | 3095 | ASN  |
| 2   | B     | 3109 | GLN  |
| 1   | C     | 54   | ASN  |
| 2   | D     | 2405 | GLN  |
| 2   | D     | 2436 | GLN  |
| 2   | D     | 2454 | GLN  |
| 2   | D     | 2486 | ASN  |
| 2   | D     | 2552 | ASN  |
| 2   | D     | 2596 | ASN  |
| 2   | D     | 2684 | GLN  |
| 2   | D     | 2954 | GLN  |
| 2   | D     | 2962 | GLN  |
| 2   | D     | 2965 | GLN  |
| 2   | D     | 3051 | ASN  |
| 2   | D     | 3053 | GLN  |
| 2   | D     | 3081 | HIS  |
| 2   | D     | 3083 | GLN  |
| 2   | D     | 3095 | ASN  |
| 2   | D     | 3109 | GLN  |

### 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.