



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:19 PM GMT

PDB ID : 3VKH  
Title : X-ray structure of a functional full-length dynein motor domain  
Authors : Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.  
Deposited on : 2011-11-16  
Resolution : 3.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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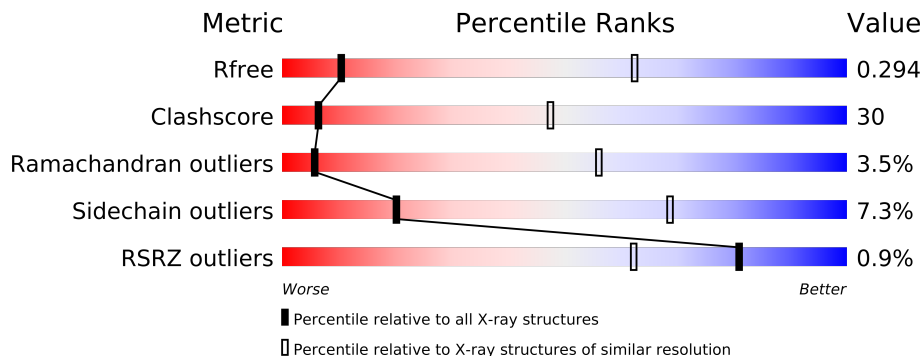
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


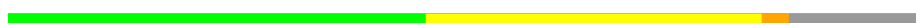
The reported resolution of this entry is 3.80 Å.

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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1162 (4.20-3.40)                                      |
| Clashscore            | 79885                       | 1100 (4.10-3.50)                                      |
| Ramachandran outliers | 78287                       | 1050 (4.10-3.50)                                      |
| Sidechain outliers    | 78261                       | 1042 (4.10-3.50)                                      |
| RSRZ outliers         | 66119                       | 1163 (4.20-3.40)                                      |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 3367   |  |
| 1   | B     | 3367   |  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 2   | ADP  | A     | 9001 | -        | X                |
| 2   | ADP  | A     | 9003 | -        | X                |
| 2   | ADP  | B     | 9007 | -        | X                |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 45974 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Dynein heavy chain, cytoplasmic.

| Mol | Chain | Residues | Atoms |       |      |      |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|---------|-------|
| 1   | A     | 3042     | Total | C     | N    | O    | S   | 0       | 0       | 0     |
|     |       |          | 23374 | 14951 | 3955 | 4368 | 100 |         |         |       |
| 1   | B     | 2908     | Total | C     | N    | O    | S   | 0       | 0       | 0     |
|     |       |          | 22384 | 14307 | 3792 | 4190 | 95  |         |         |       |

There are 48 discrepancies between the modelled and reference sequences:

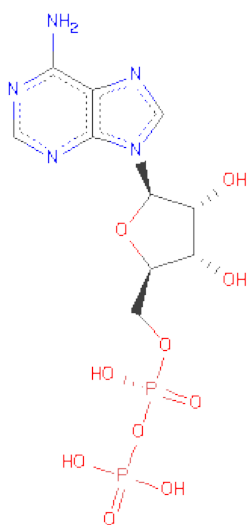
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1364    | MET      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1365    | THR      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1366    | ARG      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1367    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1368    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1369    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1370    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1371    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1372    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1373    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1374    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1375    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1376    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1377    | TYR      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1378    | LYS      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1379    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1380    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1381    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1382    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1383    | LYS      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1384    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1385    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1386    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| A     | 1387    | LYS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1364    | MET      | -      | EXPRESSION TAG | UNP P34036 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 1365    | THR      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1366    | ARG      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1367    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1368    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1369    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1370    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1371    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1372    | HIS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1373    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1374    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1375    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1376    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1377    | TYR      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1378    | LYS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1379    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1380    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1381    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1382    | ASP      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1383    | LYS      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1384    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1385    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1386    | GLY      | -      | EXPRESSION TAG | UNP P34036 |
| B     | 1387    | LYS      | -      | EXPRESSION TAG | UNP P34036 |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



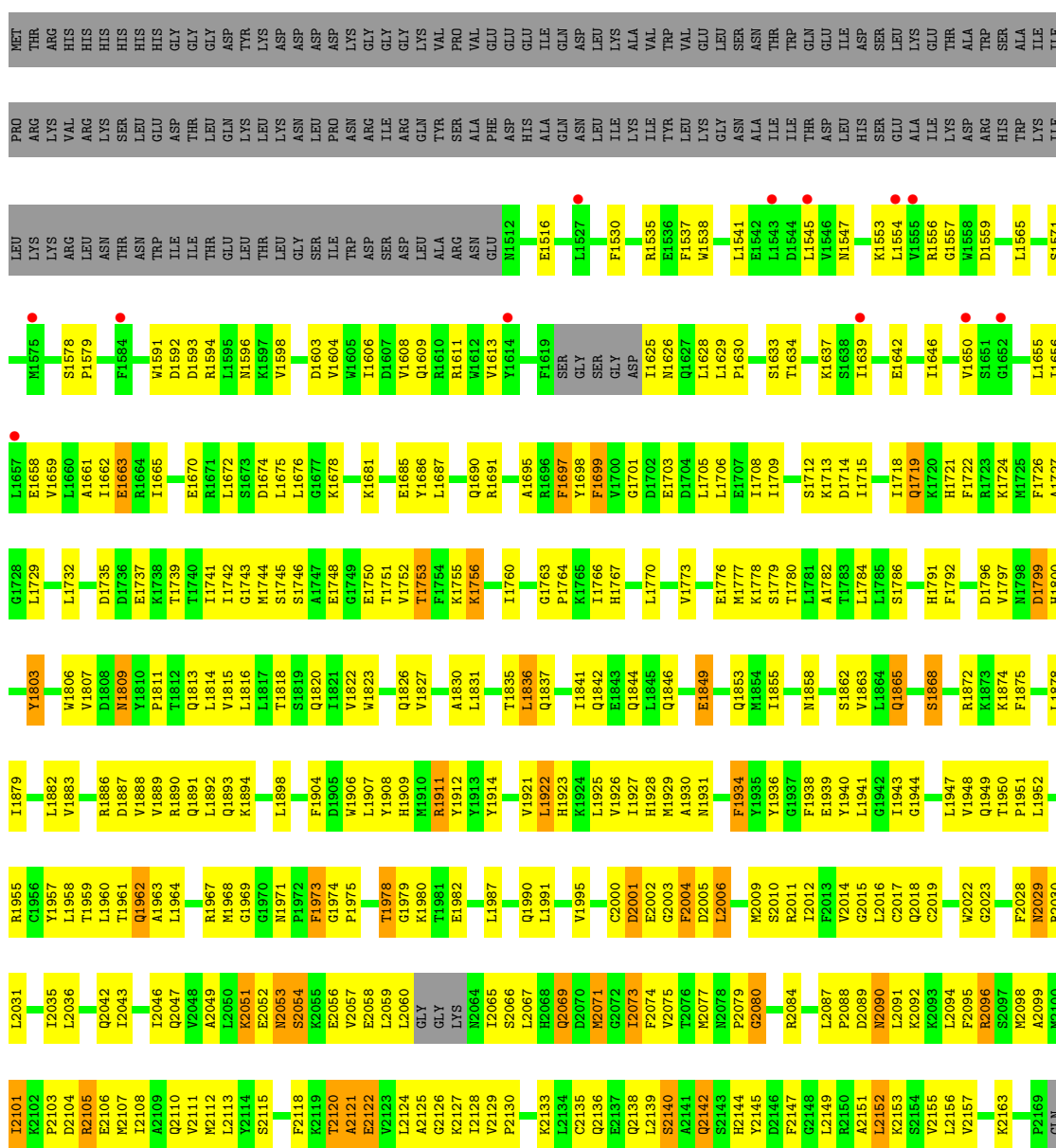
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

### 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.

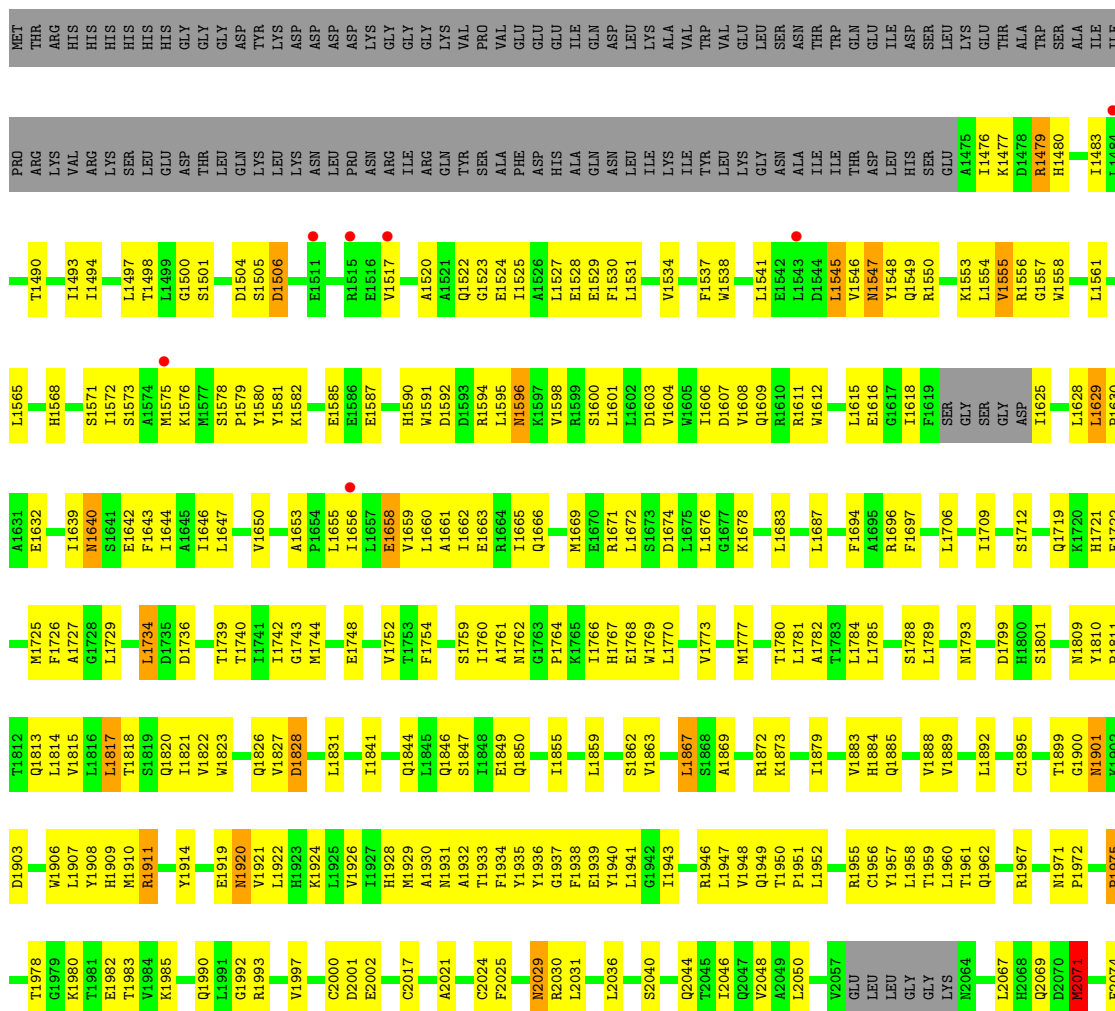
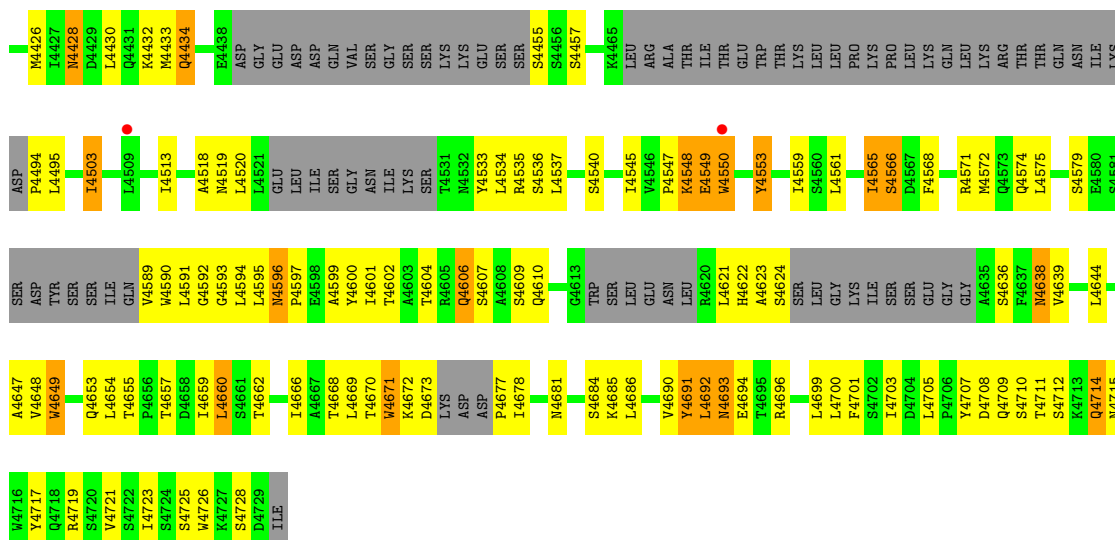
- Molecule 1: Dynein heavy chain, cytoplasmic

Chain A: 



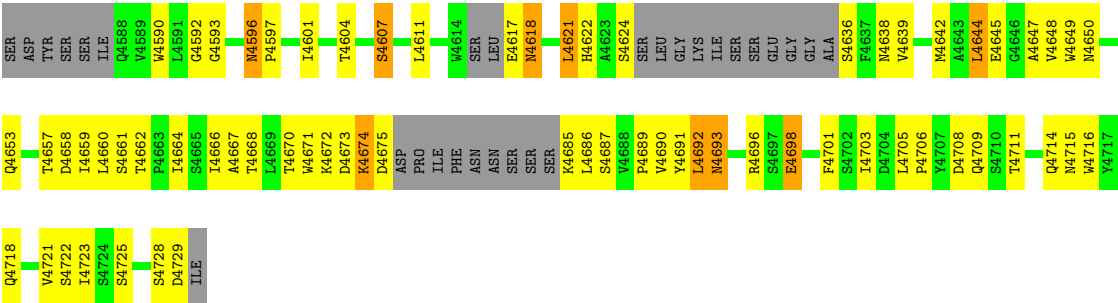
|       |       |       |       |       |       |     |       |     |       |       |       |     |
|-------|-------|-------|-------|-------|-------|-----|-------|-----|-------|-------|-------|-----|
| F3263 | K3113 | N3033 | Y2952 | P2876 | N2793 | VAL | Y2551 | THR | Q2398 | V2327 | W2255 | LEU |
| I3264 | E3114 | G3034 | S2953 | R2877 | P2794 | PRO | N2552 | SER | D2399 | T2328 | W2256 | PRO |
| N3265 | T3115 | L3035 | N2954 | S2880 | A2798 | SER | M2560 | SER | K2401 | D2329 | E2257 | PRO |
| G3266 | A3116 | S3036 | W2955 | R2881 | G2799 | SER | S2561 | SER | F2402 | F2332 | K2258 | THR |
| V3267 | K3117 | I3037 | L2956 | W2882 | R2800 | SER | P2562 | ARG | D2176 | T2335 | I2259 |     |
| V3268 | R3118 | V3038 | P2962 | D2883 | R2806 | SER | E2563 | SER | A2177 | L2260 | L2260 |     |
| L3269 | L3121 | T3039 | L3040 | L2886 | F2807 | THR | N2564 | THR | Q2261 | Q2261 | Q2261 |     |
| L3270 | I3122 | K3041 | S2966 | L2887 | R2808 | SER | Q2565 | THR | H2178 | L2262 | S2179 |     |
| I3271 | L3123 | N3042 | L2968 | L2888 | R2809 | THR | Q2566 | THR | S2179 | H2263 |       |     |
| K3274 | F3133 | N3043 | D2969 | L2889 | L2813 | SER | T2570 | THR | Y2190 | L2265 |       |     |
| R3275 |       | S3048 | Q2970 | Q2891 | L2814 | THR | N2571 | THR | V2194 | L2266 |       |     |
| L3278 | Q3136 | D3052 | Y2972 | T2892 | L2815 | SER | R2572 | THR | L2196 | L2266 |       |     |
| E3281 | V3137 | L3055 | Y2973 | M2893 | L2816 | THR | L2574 | THR | L2197 |       |       |     |
| Q3282 | R3138 | L3056 | R2975 | D2894 | L2817 | THR | Q2575 | THR | S2198 |       |       |     |
| L3283 | N3139 | L3057 | R2976 | G2895 | L2818 | THR | R2576 | THR | I2199 |       |       |     |
| H3284 | L3141 | L3058 | L2977 | C2896 | F2818 | THR | L2577 | THR | N2200 |       |       |     |
| L3285 | L3142 | L3059 | F2979 | T2897 | P2819 | THR | L2578 | THR | D2201 |       |       |     |
|       | V3143 | A3060 | Y2980 | L2898 | L2824 | THR | Q2580 | THR | T2202 |       |       |     |
| L3289 | Q3136 | R3061 | D2985 | V2902 | L2825 | THR | L2581 | THR | M2203 |       |       |     |
| E3291 | R3137 | A3062 | L2986 | R2903 | Q2826 | THR | G2582 | THR | I2204 |       |       |     |
| L3292 | N3140 | G3063 | L2975 | L2904 | L2827 | THR | G2583 | THR | P2205 |       |       |     |
| L3293 | L3141 | L3068 | L2976 | W2905 | Y2828 | THR | S2584 | THR | K2206 |       |       |     |
|       | L3142 | L3069 | F2979 | A2906 | C2828 | THR | M2585 | THR | L2207 |       |       |     |
| L3296 | V3144 | R3067 | Y2980 | L2898 | L2830 | THR | Q2586 | THR | V2208 |       |       |     |
| K3299 | R3137 | K3068 | D2985 | L2902 | F2831 | THR | L2587 | THR |       |       |       |     |
| L3299 | F3145 | A3062 | L2986 | R2903 | L2832 | THR | R2590 | THR | D2211 |       |       |     |
| L3299 | T3146 | G3063 | L2975 | L2904 | L2833 | THR | G2591 | THR | I2212 |       |       |     |
| L3299 | M3147 | E3066 | P2987 | W2905 | A2834 | THR | K2595 | THR | P2213 |       |       |     |
| L3300 | N3148 | E3067 | L2988 | L2906 | L2835 | THR | P2598 | THR | L2215 |       |       |     |
|       | P3149 | K3068 | Y2989 | L2907 | L2838 | THR | Q2598 | THR |       |       |       |     |
| L3309 | A3150 | E3075 | L2990 | L2910 | L2839 | THR | L2599 | THR | L2218 |       |       |     |
| L3313 | S3151 | S3076 | L2991 | R2917 | L2839 | THR | A2601 | THR | L2219 |       |       |     |
| V3314 | R3157 | N3077 | I2998 | V2918 | L2842 | THR | L2602 | THR | L2220 |       |       |     |
| V3315 |       | V3078 | Q3007 | E2922 | L2842 | THR | T2603 | THR | D2221 |       |       |     |
|       | L3164 | L3079 | P3008 | K2923 | F2845 | THR | P2604 | THR | D2222 |       |       |     |
| Q3319 | F3165 | E3080 | Q3009 | T2926 | A2846 | THR | P2606 | THR | V2223 |       |       |     |
| K3323 | R3167 | S3081 | G3010 |       | D2847 | THR | L2606 | THR | P2224 |       |       |     |
| E3240 | C3168 | F3083 | H3011 | I2930 | N2848 | THR | L2609 | THR | L2228 |       |       |     |
| A3241 | V3169 | L3084 | A3012 | V2930 | L2849 | THR | E2695 | THR | Q2229 |       |       |     |
| N3242 | L3170 | E3085 | L3014 | V2933 | T2850 | THR | V2696 | THR | S2301 |       |       |     |
| I3243 | L3172 | A3086 | I3015 | A2934 | D2851 | THR | V2697 | THR | E2302 |       |       |     |
| R3244 | D3171 | K3087 | G3016 | L2935 | L2855 | THR | S2698 | THR | A2303 |       |       |     |
| L3245 | F3172 | S3087 | V3017 | K2936 | F2856 | THR | N2700 | THR | Q2235 |       |       |     |
|       | G3174 | L3090 | S3018 | R2937 | Y2857 | THR | F2701 | THR | V2305 |       |       |     |
|       | E3175 | G3093 | G3019 | F2938 | L2857 | THR | S2616 | THR | L2236 |       |       |     |
| Q3249 |       | E3179 | G3020 |       | R2863 | THR | V2617 | THR | P2308 |       |       |     |
| N3253 | E3179 | A3180 | G3021 | V2941 | F2864 | THR | S2618 | THR | K2239 |       |       |     |
| Y3254 | A3180 | E3095 | K3022 | N2942 | L2864 | THR | L2619 | THR | I2243 |       |       |     |
| V3255 | V3184 | V3096 | S3023 | L2943 | T2706 | THR | M2541 | THR | K2313 |       |       |     |
| A3341 | G3185 | L3099 | V3024 | D2944 | T2707 | THR | N2542 | THR | D2247 |       |       |     |
| R3342 | G3185 | L3099 | L3025 | A2945 | Q2787 | THR | S2625 | THR | Q2315 |       |       |     |
|       | S3186 | L3099 | L3025 | A2945 | Q2787 | THR | L2626 | THR | L2316 |       |       |     |
| H3259 | E3187 | L3108 | R3027 | R2948 | H2871 | THR | W2627 | THR | Q2316 |       |       |     |
| Y3260 | R3190 | M3109 | F3028 | P2949 | L2872 | THR | K2628 | THR | M2394 |       |       |     |
| L3261 |       |       |       | P2949 | L2872 | THR | N2629 | THR | F2395 |       |       |     |
| D3262 | N3191 | C3112 | M3032 | L2951 | L2711 | THR | E2549 | THR | T2323 |       |       |     |
|       |       |       |       |       | C2792 | THR | K2630 | THR | T2324 |       |       |     |
|       |       |       |       |       |       |     |       |     |       |       |       |     |





|       |       |       |       |       |       |       |       |       |     |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-------|-------|-------|-------|-------|
| G3174 | G3086 | K3003 | L2917 | N2841 | H2766 | L2671 | T2599 | L2525 | GLN | E2383 | H2304 | L2228 | K2153 | V2075 |
| E3175 | N3087 | V3004 | V2918 | L2842 | N2773 | L2672 | L2600 | N2526 | THR | R2384 | V2306 | Q2229 | S2154 | T2076 |
| L3181 | N3088 | G3010 | E2921 | R2843 | N2774 | P2676 | T2603 | D2527 | THR | L2387 | P2308 | I2231 | V2155 | G2080 |
| Q3182 | L3089 | H3011 | N2921 | L2849 | T2775 | G2677 | F2604 | F2528 | ILE | K2309 | K2310 | Q2235 | K2163 | A2082 |
| Q3183 | A3012 | T2850 | N2925 | T2850 | S2776 | L2684 | V2605 | T2529 | THR | V2391 | A2310 | R2236 | R2164 | G2083 |
| A3184 | L3013 | T2926 | N2926 | N2853 | T2779 | L2684 | T2610 | T2530 | THR | R2392 | L2311 | R2237 | K2166 | R2084 |
| G3185 | G3014 | D2927 | D2927 | V2854 | N2780 | T2687 | P2611 | L2531 | PRO | V2393 | T2312 | R2239 | C2166 | N2086 |
| S3186 | L3015 | K2928 | K2928 | V2855 | L2781 | L2688 | L2612 | R2532 | ILE | M2394 | K2313 | K2239 | GLN   |       |
| E3187 | G3016 | E2855 | N2929 | F2856 | K2782 | L2688 | L2613 | V2533 | LEU | E2396 | D2314 | I2240 | PRO   |       |
|       | VAL   | L2930 | L2930 | F2856 | L2783 | F2694 | D2614 | L2540 | THR | E2397 | Q2315 | Q2241 | PRO   | L2091 |
| L3192 | PRO   | D2931 | D2931 | Q2861 | L2783 | F2694 | D2614 | L2541 | THR | Q2398 | L2320 | Q2242 | GLN   |       |
| E3195 | GLY   | F2932 | F2932 | N2862 | L2786 | V2696 | S2616 | N2542 | PRO | F2399 |       | I2243 | LEU   | F2085 |
| N3196 | LEU   | V2933 | V2933 | R2863 | Q2787 | V2696 | S2616 | N2542 | PRO | D2400 | T2323 | A2244 | PRO   | R2096 |
|       | PHE   | A2934 | A2934 | R2863 | Q2787 | V2696 | S2616 | N2542 | THR | K2401 |       |       | PRO   | S2097 |
|       | GLU   | L3025 | L3025 | F2788 | V2789 | L2699 | D2621 | V2546 | THR | Y2402 | W2327 | V2250 | ILE   | M2098 |
| Y3199 | GLY   | K2936 | K2936 | T2865 | N2701 | N2700 | A2622 | N2547 | THR | T2407 | L2331 | T2251 | THR   | A2099 |
|       |       | R2937 | R2937 | T2866 | F2701 | N2688 | N2623 | I2549 | THR | I2408 |       | Q2253 | ASP   | M2100 |
| P3202 | F3103 | F2938 | F2938 | N2867 | N2793 | A2704 | N2624 | E2550 | THR | R2410 | T2335 | E2254 | ALA   | I2101 |
|       | F3104 | P2939 | P2939 | L2868 | P2794 | T2705 | W2627 | Q2553 | ARG |       |       |       | GLU   | K2102 |
|       | F3105 | Q2869 | Q2869 | Q2869 | T2797 | T2706 |       |       | THR | R2350 | R2338 | K2258 | LYS   | D2104 |
|       |       | V2941 | V2941 | Y2872 | N2797 | T2706 |       |       | THR | R2351 | I2339 | L2259 | THR   | R2105 |
|       | ASN   | L2946 | L2946 | L2873 | A2798 | L2711 | K2630 | S2556 | THR | L2421 |       | L2260 | LYS   | E2106 |
|       | GLY   | K2947 | K2947 | Y2874 | P2774 | F2714 | D2631 | D2557 | THR | T2422 |       | Q2261 | ALA   | A2109 |
|       | LEU   | N2950 | N2950 | S2875 | N2801 |       | PRO   | F2558 | THR | T2423 |       | H2270 | ALA   |       |
|       |       | F2955 | F2955 | P2876 | Q2802 |       | SER   | P2559 | THR | Q2424 |       | G2271 | Q2185 |       |
|       |       | W2965 | W2965 | R2877 | L2803 | Y2720 | VAL   | M2560 | SER | M2415 | E2346 | H2263 | Q2185 |       |
|       |       |       |       |       |       |       |       |       | THR | F2417 |       | Q2264 | Q2185 |       |
|       |       |       |       |       |       |       |       |       | THR | I2420 | R2350 | I2265 | Q2185 |       |
|       |       |       |       |       |       |       |       |       | THR | L2421 | R2351 | I2265 | Q2185 |       |
|       |       |       |       |       |       |       |       |       | THR | T2422 | W2352 | H2270 | E2191 |       |
|       |       |       |       |       |       |       |       |       | THR | T2423 | I2353 | G2271 | V2194 |       |
|       |       |       |       |       |       |       |       |       | THR | Q2424 | I2354 | V2272 | Q2116 |       |
|       |       |       |       |       |       |       |       |       | THR | M2425 |       | M2273 | F2118 |       |
|       |       |       |       |       |       |       |       |       | THR | I2426 | D2358 | N2274 | L2196 |       |
|       |       |       |       |       |       |       |       |       | THR | F2427 | V2359 | G2275 | K2119 |       |
|       |       |       |       |       |       |       |       |       | THR |       | D2360 | G2276 | N2197 | T2120 |
|       |       |       |       |       |       |       |       |       | THR |       |       | G2276 | S2198 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       | P2277 | I2199 | L2124 |
|       |       |       |       |       |       |       |       |       | THR |       |       | S2278 | I2199 | A2125 |
|       |       |       |       |       |       |       |       |       | THR |       |       | G2279 | G2126 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       | G2280 | K2127 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       | G2281 | I2128 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       | G2282 | V2129 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       | T2283 | K2206 | P2130 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | L2207 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       | W2286 | C2135 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | A2209 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | L2139 | L2139 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | S2140 |       |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | I2211 | A2141 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | Q2142 | Q2142 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | S2143 | S2143 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | H2144 | H2144 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | Y2145 | Y2145 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | F2223 | L2149 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | F2224 | R2150 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | G2225 | SER   |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | S2301 | A2151 |
|       |       |       |       |       |       |       |       |       | THR |       |       |       | GLN   | L2152 |

|       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-------|
| P4494 | D4429 | M4349 | F4277 | L4200 | M4112 | S4041 | V3955 | V3869 | F3760 | L3685 | A3595 | ARG | TYR | GLU | E3273 |
| P4499 | K4431 | E4350 | H4278 | E4201 | T4113 | S4042 | T3958 | V3869 | L3764 | K3686 | F3598 | GLU | ASP | ALA | K3274 |
| E4500 | K4432 | F4351 | A4279 | F4201 | M4118 | D4043 | L3959 | T3872 | F3765 | K3687 | F3598 | VAL | THR | SER | H3284 |
| R4501 | M4433 | D4352 | I4280 | S4206 | A4119 | W4044 | L3960 | T3872 | F3765 | V3689 | F3598 | GLU | LYS | THR |       |
| E4502 | D4434 | L4281 | I4281 | L4207 | A4120 | K4045 | L3961 | K3876 | K3767 | K3690 | Y3601 | GLN | MET | ILE | G3288 |
| L4503 |       | D4282 | D4282 | S4208 | I4121 | D4046 | D3962 | K3877 | D3768 | D3691 | G3603 | LEU | MET | LYS | L3289 |
| Q4506 |       | F4283 | F4283 | P4209 | V4122 | F4047 | D3963 | E3878 | F3769 | K3692 | F3604 | GLU | THR | LYS | L3290 |
|       |       | R4284 | R4284 | F4213 | E4123 |       | K3964 | E3880 | F3770 | K3693 |       | ASN | PRO | LYS | K3291 |
| L4509 |       | L4285 | L4285 | R4214 | K4124 | D4051 | L3965 | E3881 | A3771 | T3694 | D3606 | ALA | ILE | HIS | L3292 |
| V4510 |       | I4288 | I4288 | F4215 | E4125 | V4053 | T3966 | E3881 | H3772 | T3695 | Q3607 | ALA | ILE | LEU | L3293 |
|       |       | P4289 | P4289 | F4216 |       |       | F3967 | V3882 | F3773 | K3696 | F3609 | ASN | ARG | ASP | R3294 |
| L4513 |       |       |       | F4217 | S4128 |       | T3973 |       | T3774 | K3697 | F3609 | GLU | GLU | GLU | T3295 |
|       |       | W4292 | W4292 | K4217 |       | P4056 |       | Y3886 | P3775 | S3698 | R3610 | LEU | ALA | ILE |       |
| L4517 |       | L4218 | L4218 | T4217 | P4131 | I4057 | V3976 | N3887 | P3776 | F3699 | M3614 | THR | THR | LYS | V3299 |
| L4523 |       | S4219 | S4219 | E4220 | L4132 | I4058 | P3888 | N3887 | L3777 | F3699 |       | LYS | SER | SER |       |
|       |       | E4220 | E4220 | P4059 | L4133 | P4059 | K3977 | K3889 | D3701 | L3525 |       | LEU | LEU | LEU | L3302 |
| ILE   | GLY   | F4295 | F4295 | I4221 | L4134 | E4060 | G3978 | K3890 | S3779 | Y3617 |       | PRO | GLY | PRO | L3306 |
| SER   | SER   | F4296 | F4296 | H4222 | C4135 |       | T3979 | L3891 | K3780 | M3618 |       | LYS | TYR | LYS | L3306 |
|       | SER   | E4297 | E4297 | P4223 | S4136 | I4063 | K3988 | S3892 | V3781 | L3619 |       | PRO | LEU | PRO | L3313 |
| LYS   | LYS   | A4237 | A4237 | F4224 | V4137 | V4064 | D3989 | C3893 | T3782 | L3620 |       | ASP | GLU | PRO | L3313 |
| ASN   | GLY   | L4225 | L4225 | P4226 | P4138 |       | F3990 | S3894 | F3783 |       |       | THR | ASP | THR |       |
| ILE   | GLU   | R4304 | R4304 | P4226 |       | A4067 | F3990 | K3895 | V3784 |       | S3623 | PRO | PRO | PRO | K3316 |
|       | SER   | F4372 | F4372 | P4226 |       | D4068 | L3991 | Y3896 | N3785 |       |       | VAL | GLY | VAL |       |
|       | SER   | P4374 | P4374 | H4228 | D4141 | I4069 | L3992 | Y3897 | K3786 |       | F3628 | PHE | PHE | LYS | Q3322 |
|       | SER   | F4377 | F4377 | L4229 | S4143 | S4070 | K3993 | F3898 | T3787 |       |       | ASP | ASP | LEU | K3323 |
|       | SER   | S4378 | S4378 | L4230 | S4144 | N4071 | G3994 |       | V3788 |       | V3634 | TYR | TYR | ALA | K3323 |
|       | SER   | F4379 | F4379 | R4231 | K4145 | Q4072 | L3903 | E3902 | T3789 |       | P3635 | GLU | GLU | MET | L3324 |
|       | SER   | F4380 | F4380 | M4232 | V4146 | Q4073 | L3998 | E3902 | P3790 |       | S3636 | THR | THR | GLU | Q3338 |
|       | SER   | L4381 | L4381 | D4311 | D4147 | S4074 | L3903 | S3904 | S3791 |       | F3637 | VAL | VAL | ALA | Q3338 |
|       | SER   | Y4312 | Y4312 | V4235 | D4148 | T4075 | E4003 | S3904 | S3792 |       | L3638 | ASN | ASN | VAL | R3342 |
|       | SER   | F4313 | F4313 | F4236 | L4149 | I4076 | T4004 | L3908 | L3793 |       | S3639 | ARG | ARG | CYS | R3342 |
| LEU   | LEU   | S4237 | S4237 | F4236 |       |       | I4005 | Y3909 |       |       | S3647 | ALA | ALA | LEU | Q3345 |
| ARG   | ARG   | D4315 | D4315 | E4238 | H4153 | F4080 | P4006 | Q3910 | T3809 |       |       | SER | SER | MET | Q3345 |
| ALA   | ALA   | H4391 | H4391 | E4239 | L4154 | K4081 | Q4007 | S3912 | L3734 |       |       | LYS | LYS | LEU | V3350 |
| THR   | THR   | S4318 | S4318 |       | K4156 | K4082 | L4008 | L3913 | R3813 |       | N3650 | ALA | ALA | GLY | E3354 |
| ILE   | ILE   |       |       | V4244 | Y4157 | T4083 | L4011 | L3923 | L3817 |       | S3651 | CYS | CYS | GLY | E3354 |
| THR   | THR   | S4322 | S4322 |       |       | L4084 | L4012 | L3923 |       |       | L3568 | LYS | LYS | LYS | T3355 |
| GLU   | GLU   | N4323 | N4323 | T4251 | T4162 | L4085 | S4013 | N3927 | S3833 |       | L3564 | LEU | LEU | LYS | T3355 |
| TRP   | TRP   | L4324 | L4324 | F4252 | Q4163 | M4086 | L4013 | N3927 | L3834 |       | L3657 | VAL | VAL | GLU | V3357 |
| THR   | THR   | T4404 | T4404 | L4253 | Q4163 |       | Q4016 | N3927 | L3835 |       |       | LYS | LYS | TRP | Q3358 |
| LYS   | LYS   | P4405 | P4405 | G4254 | Q4167 | K4087 |       | N3929 | L3841 |       |       | ALA | ALA | ALA | VAL   |
| LEU   | LEU   | L4406 | L4406 | L4255 |       |       | L4020 | L3930 | K3841 |       |       | TRP | TRP | ASP | LYS   |
| LEU   | LEU   | F4407 | F4407 | P4256 | L4170 | S4091 | L4021 | L3930 | S3842 |       |       | ALA | ALA | ILE | LYS   |
| PRO   | PRO   | L4408 | L4408 | A4257 | A4171 | D4092 | I4021 | V3931 | S3842 |       |       | THR | THR | ILE | ALA   |
| LYS   | LYS   | G4409 | G4409 | T4258 |       | R4093 | C4022 | D3932 | G3843 |       |       | ALA | ALA | LYS | TYR   |
| LEU   | LEU   | P4411 | P4411 | R4259 | L4410 | W4094 | L4023 | D3932 | N3844 |       |       | LYS | LYS | GLN | ARG   |
| LYS   | LYS   | E4412 | E4412 | M4260 | T4183 | L4095 | R4024 | D3935 | I3845 |       |       | THR | THR | ASP | LYS   |
| GLN   | GLN   | I4413 | I4413 | Q4263 | V4184 | D4096 | Q4025 | D3935 | L3846 |       |       | ILE | ILE | LEU | ASP   |
| LEU   | LEU   | E4414 | E4414 | F4264 | V4185 | Y4097 | Q4026 | R3939 | I3847 |       |       | TYR | TYR | MET | GLU   |
| LYS   | LYS   | E4415 | E4415 | A4265 |       | S4098 | V4027 | L3940 | D3848 |       |       | SER | SER | GLU | LYS   |
| ARG   | ARG   | L4437 | L4437 | F4266 | K4188 |       | P4028 | V3941 | D3849 |       |       | GLU | GLU | PRO | ALA   |
| THR   | THR   | L4338 | L4338 | E4265 | N4189 | F4101 | S4029 | Y3942 | I3847 |       |       | ILE | ILE | ASN | GLU   |
| THR   | THR   | G4339 | G4339 | R4267 | L4190 | V4102 | F4030 | L3943 | D3849 |       |       | LEU | LEU | PHE | GLU   |
| GLN   | GLN   | S4341 | S4341 | I4270 | H4191 |       | S4031 | L3943 | I3852 |       |       | ASP | ASP | ILE | ALA   |
| ASN   | ASN   | T4341 | T4341 | I4271 | L4192 | V4105 | Q4032 | I3947 | K3859 |       |       | THR | THR | ILE | ILE   |
| ILE   | ILE   | L4342 | L4342 | V4271 | A4193 |       | L4033 | F3948 | I3865 |       |       | ILE | ILE | SER | ILE   |
|       |       | V4343 | V4343 | F4272 | P4194 | D4109 | D4035 | S3949 | I3865 |       |       | THR | THR | ILE | ILE   |
|       |       |       |       | L4273 | F4110 | F4110 | D4035 | S3949 | I3865 |       |       | PRO | PRO | ILE | ALA   |
| D4493 | D4493 | N4428 | R4346 | L4274 | L4197 | L4111 | H4036 | R3954 | L3867 |       |       | ASN | ASN | GLN | GLN   |



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 195.73Å 228.96Å 201.17Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 48.79 – 3.80<br>48.78 – 3.79                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (48.79-3.80)<br>99.0 (48.78-3.79)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.52 (at 3.77Å)   | Xtriage          |
| Refinement program  | CNS 1.3   | Depositor        |
| R, $R_{free}$   | 0.219 , 0.292<br>0.227 , 0.294                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4469 reflections (5.27%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 125.1   | Xtriage          |
| Anisotropy  | 0.144   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 84.0   | EDS              |
| Estimated twinning fraction   | 0.001 for l,-k,h  | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Outliers  | 0 of 89309 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 45974   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 138.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.24         | 0/23866     | 0.44        | 1/32482 (0.0%) |
| 1   | B     | 0.24         | 0/22846     | 0.43        | 0/31076        |
| All | All   | 0.24         | 0/46712     | 0.44        | 1/63558 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|------|-------------|----------|
| 1   | A     | 3371 | PRO  | N-CA-CB | 5.32 | 109.68      | 103.30   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 23374 | 0        | 22545    | 1559    | 0            |
| 1   | B     | 22384 | 0        | 21550    | 1149    | 0            |
| 2   | A     | 108   | 0        | 48       | 7       | 0            |
| 2   | B     | 108   | 0        | 48       | 3       | 0            |
| All | All   | 45974 | 0        | 44191    | 2704    | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (2704) close contacts within the same asymmetric unit are listed below.

| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3689:TYR:HB2  | 1:A:3694:ILE:HD11 | 1.29        | 1.14     |
| 1:A:3337:LYS:HB3  | 1:A:3525:LEU:HD13 | 1.35        | 1.07     |
| 1:B:3841:ALA:O    | 1:B:3842:SER:HB2  | 1.54        | 1.04     |
| 1:A:4242:PRO:HA   | 1:A:4286:ARG:HH12 | 1.22        | 1.03     |
| 1:A:4109:ASP:HA   | 1:A:4112:ASN:HD22 | 1.22        | 1.00     |
| 1:A:3373:ILE:HD13 | 1:A:3373:ILE:H    | 1.29        | 0.98     |
| 1:A:3673:LEU:HB2  | 1:A:3781:VAL:HG11 | 1.45        | 0.97     |
| 1:B:1959:THR:HG22 | 1:B:4341:THR:HA   | 1.46        | 0.96     |
| 1:B:1554:LEU:HB3  | 1:B:1609:GLN:HE22 | 1.29        | 0.95     |
| 1:B:4251:THR:HG23 | 1:B:4303:LEU:HD21 | 1.46        | 0.95     |
| 1:B:1928:HIS:CD2  | 1:B:1933:THR:HG22 | 2.02        | 0.95     |
| 1:A:4375:LEU:HD11 | 1:A:4383:VAL:HG23 | 1.48        | 0.95     |
| 1:B:3673:LEU:HB2  | 1:B:3781:VAL:HG11 | 1.44        | 0.95     |
| 1:A:3425:LYS:HD2  | 1:A:3428:GLU:HG3  | 1.49        | 0.94     |
| 1:B:2533:VAL:HB   | 1:B:2581:LEU:HD22 | 1.51        | 0.93     |
| 1:B:4574:GLN:HE22 | 1:B:4590:TRP:H    | 1.15        | 0.93     |
| 1:B:1655:LEU:HB2  | 1:B:1658:GLU:HB2  | 1.45        | 0.93     |
| 1:B:4121:ILE:HA   | 1:B:4125:GLU:HG3  | 1.48        | 0.93     |
| 1:A:2274:MET:HE3  | 1:A:2286:TRP:HB3  | 1.50        | 0.92     |
| 1:B:1972:PRO:HG2  | 1:B:2076:THR:HG22 | 1.52        | 0.92     |
| 1:A:4270:ILE:HA   | 1:A:4273:LEU:HD12 | 1.52        | 0.90     |
| 1:B:1789:LEU:HD23 | 1:B:1818:THR:HG23 | 1.50        | 0.90     |
| 1:A:3837:ALA:HB1  | 1:A:3850:SER:HB3  | 1.53        | 0.89     |
| 1:A:2313:LYS:HE3  | 1:A:2366:ASN:HD21 | 1.36        | 0.89     |
| 1:A:3018:SER:HB2  | 1:A:3256:THR:HG21 | 1.52        | 0.89     |
| 1:A:1639:ILE:HG23 | 1:A:1672:LEU:HD22 | 1.53        | 0.89     |
| 1:A:4495:LEU:H    | 1:A:4495:LEU:HD12 | 1.38        | 0.89     |
| 1:A:2890:ILE:HA   | 1:A:2893:MET:HE2  | 1.55        | 0.89     |
| 1:B:3930:LEU:HB3  | 1:B:3939:ARG:HH21 | 1.37        | 0.89     |
| 1:B:1813:GLN:HE22 | 1:B:1940:TYR:HA   | 1.37        | 0.88     |
| 1:B:2603:THR:HG22 | 1:B:2604:PRO:HD2  | 1.54        | 0.88     |
| 1:A:2200:ASN:HD22 | 1:A:2228:LEU:HD13 | 1.36        | 0.88     |
| 1:A:1690:GLN:HE22 | 1:A:1766:ILE:HG21 | 1.38        | 0.88     |
| 1:A:4046:GLN:HE22 | 1:A:4057:ILE:H    | 1.19        | 0.88     |
| 1:A:2447:GLN:HA   | 1:A:2450:ASN:HD22 | 1.39        | 0.88     |
| 1:B:4270:ILE:HG22 | 1:B:4310:ILE:HD13 | 1.55        | 0.88     |
| 1:B:1524:GLU:HG2  | 1:B:1580:TYR:HB3  | 1.57        | 0.87     |
| 1:A:3552:LYS:HA   | 1:A:3555:ASN:HD22 | 1.40        | 0.87     |
| 1:A:2570:THR:HG21 | 1:A:2603:THR:HG21 | 1.57        | 0.86     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2381:ASN:HD21 | 1:B:2383:GLU:HB2  | 1.40        | 0.86     |
| 1:A:2914:GLN:HB2  | 1:A:2926:THR:HG21 | 1.56        | 0.86     |
| 1:A:2200:ASN:HB2  | 1:A:2228:LEU:HD22 | 1.56        | 0.86     |
| 1:B:4604:THR:HG23 | 1:B:4671:TRP:HE1  | 1.40        | 0.86     |
| 1:B:3271:ILE:HG13 | 1:B:3592:VAL:HG11 | 1.57        | 0.86     |
| 1:A:4621:LEU:HD21 | 1:A:4669:LEU:HD23 | 1.55        | 0.86     |
| 1:A:2293:ILE:HG22 | 1:A:2350:ARG:HH22 | 1.41        | 0.85     |
| 1:B:4109:ASP:HA   | 1:B:4112:ASN:ND2  | 1.92        | 0.85     |
| 1:A:4686:LEU:HD21 | 1:A:4721:VAL:HG11 | 1.59        | 0.85     |
| 1:A:3809:THR:HA   | 1:A:3812:LYS:HE2  | 1.59        | 0.84     |
| 1:A:2560:MET:HG3  | 1:A:2561:SER:H    | 1.42        | 0.84     |
| 1:A:4251:THR:HG23 | 1:A:4303:LEU:HD21 | 1.58        | 0.84     |
| 1:B:2525:ILE:HD11 | 1:B:2815:LEU:HB2  | 1.58        | 0.84     |
| 1:A:4648:VAL:HG12 | 1:A:4662:THR:HG21 | 1.60        | 0.83     |
| 1:B:2841:ASN:ND2  | 1:B:2842:LEU:H    | 1.75        | 0.83     |
| 1:A:2910:LEU:HD23 | 1:A:2930:ILE:HD12 | 1.59        | 0.83     |
| 1:B:3930:LEU:HD11 | 1:B:3943:LEU:HD21 | 1.59        | 0.83     |
| 1:B:4548:LYS:HD2  | 1:B:4549:GLU:N    | 1.93        | 0.83     |
| 1:A:3718:LEU:HG   | 1:A:3719:LEU:H    | 1.42        | 0.83     |
| 1:B:4402:ILE:HD12 | 1:B:4402:ILE:H    | 1.42        | 0.83     |
| 1:A:4109:ASP:HA   | 1:A:4112:ASN:ND2  | 1.95        | 0.82     |
| 1:A:4190:ILE:HG12 | 1:A:4219:SER:HB3  | 1.61        | 0.82     |
| 1:A:3981:ASN:HD22 | 1:A:4076:ILE:HB   | 1.44        | 0.82     |
| 1:B:3785:ASN:HD21 | 1:B:3787:THR:HG23 | 1.43        | 0.82     |
| 1:B:2250:VAL:HB   | 1:B:2425:MET:HG3  | 1.60        | 0.82     |
| 1:B:1926:VAL:HG22 | 1:B:1935:TYR:CE2  | 2.15        | 0.82     |
| 1:A:3652:LEU:HD12 | 1:A:3653:PRO:HD2  | 1.62        | 0.82     |
| 1:B:1781:LEU:HG   | 1:B:1814:LEU:HD11 | 1.61        | 0.81     |
| 1:A:2651:VAL:HG13 | 1:A:2652:ASP:H    | 1.44        | 0.81     |
| 1:B:4657:THR:HG22 | 1:B:4659:ILE:H    | 1.45        | 0.81     |
| 1:B:2129:VAL:HG22 | 1:B:2130:PRO:HD3  | 1.62        | 0.81     |
| 1:A:4185:VAL:HG12 | 1:A:4186:LEU:H    | 1.44        | 0.81     |
| 1:B:4335:ARG:HH21 | 1:B:4365:THR:HG22 | 1.46        | 0.81     |
| 1:A:3788:VAL:HG21 | 1:A:3913:LEU:HD22 | 1.61        | 0.81     |
| 1:A:2371:LEU:CB   | 1:A:2410:ARG:HG3  | 2.10        | 0.81     |
| 1:A:3238:ILE:HG12 | 1:A:3601:TYR:CD2  | 2.16        | 0.81     |
| 1:A:3700:LEU:HD22 | 1:A:3701:ASP:H    | 1.43        | 0.80     |
| 1:A:3789:THR:HB   | 1:A:3790:PRO:HD2  | 1.63        | 0.80     |
| 1:A:2140:SER:HB2  | 1:A:2142:GLN:HE22 | 1.45        | 0.80     |
| 1:A:2857:TYR:HA   | 1:A:2913:PHE:HE1  | 1.46        | 0.80     |
| 1:A:2370:LEU:HD21 | 1:A:2387:LEU:HD13 | 1.64        | 0.80     |
| 1:A:4654:LEU:HD11 | 1:A:4705:LEU:HB2  | 1.64        | 0.80     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1660:LEU:HA   | 1:B:1665:ILE:HD11 | 1.63        | 0.80     |
| 1:A:3694:ILE:HG12 | 1:A:3717:PRO:HB2  | 1.63        | 0.80     |
| 1:A:2236:LEU:HD21 | 1:A:2293:ILE:HD13 | 1.63        | 0.80     |
| 1:A:4654:LEU:HD13 | 1:A:4686:LEU:HD23 | 1.62        | 0.79     |
| 1:B:4270:ILE:HD11 | 1:B:4329:ILE:HD13 | 1.65        | 0.79     |
| 1:A:2110:GLN:HG3  | 1:A:2122:GLU:HA   | 1.64        | 0.79     |
| 1:B:3607:GLN:HG2  | 1:B:3657:LEU:HD22 | 1.65        | 0.79     |
| 1:A:4086:MET:HG3  | 1:A:4093:ARG:HB2  | 1.65        | 0.79     |
| 1:A:4349:ASN:HD21 | 1:A:4351:PHE:HB2  | 1.46        | 0.79     |
| 1:A:2300:LYS:O    | 1:A:2349:LYS:HB2  | 1.81        | 0.79     |
| 1:B:4189:ASN:H    | 1:B:4218:THR:HG22 | 1.47        | 0.79     |
| 1:B:3844:ASN:O    | 1:B:3848:ASP:HB3  | 1.81        | 0.79     |
| 1:A:4353:MET:HE3  | 1:A:4356:LEU:HD23 | 1.64        | 0.78     |
| 1:A:2283:THR:HA   | 1:A:2286:TRP:HE1  | 1.48        | 0.78     |
| 1:A:2886:LEU:O    | 1:A:2890:ILE:HG12 | 1.84        | 0.78     |
| 1:A:2706:THR:HB   | 1:A:2707:PRO:HD2  | 1.65        | 0.78     |
| 1:B:2106:GLU:OE1  | 1:B:2129:VAL:HG21 | 1.82        | 0.78     |
| 1:B:4264:PRO:HB3  | 1:B:4323:ASN:HA   | 1.64        | 0.78     |
| 1:A:3673:LEU:HB2  | 1:A:3781:VAL:CG1  | 2.14        | 0.78     |
| 1:B:2657:VAL:HG13 | 1:B:2687:THR:HG23 | 1.64        | 0.78     |
| 1:B:3338:GLN:HG2  | 1:B:3525:LEU:HD13 | 1.65        | 0.78     |
| 1:A:2204:ILE:HA   | 1:A:2207:LEU:HD12 | 1.65        | 0.78     |
| 1:A:1823:TRP:O    | 1:A:1827:VAL:HG23 | 1.84        | 0.78     |
| 1:A:2705:THR:HA   | 1:A:2709:LEU:HD12 | 1.66        | 0.78     |
| 1:A:1796:ASP:HB3  | 1:A:1799:ASP:HB3  | 1.65        | 0.77     |
| 1:A:4575:LEU:H    | 1:A:4575:LEU:HD12 | 1.49        | 0.77     |
| 1:B:2578:MET:HB3  | 1:B:2597:ILE:HD12 | 1.65        | 0.77     |
| 1:B:4332:ILE:HD12 | 1:B:4332:ILE:H    | 1.48        | 0.77     |
| 1:B:4121:ILE:O    | 1:B:4125:GLU:HB2  | 1.85        | 0.77     |
| 1:B:3219:ILE:CB   | 1:B:3220:PRO:HD3  | 2.15        | 0.77     |
| 1:A:4318:SER:HA   | 1:A:4321:ARG:HH21 | 1.50        | 0.76     |
| 1:A:2766:MET:HB3  | 1:A:2783:LEU:HD11 | 1.67        | 0.76     |
| 1:A:3384:LYS:HD3  | 1:A:3386:LYS:HD3  | 1.66        | 0.76     |
| 1:B:3230:SER:HA   | 1:B:3620:ARG:HE   | 1.51        | 0.76     |
| 1:A:3058:LEU:HD21 | 1:A:3141:LEU:HD11 | 1.67        | 0.76     |
| 1:B:3313:LEU:HD13 | 1:B:3550:SER:HA   | 1.65        | 0.76     |
| 1:A:2505:TYR:O    | 1:A:2512:VAL:HG23 | 1.85        | 0.76     |
| 1:B:3671:TYR:O    | 1:B:3781:VAL:HG13 | 1.86        | 0.76     |
| 1:B:4046:GLN:HG3  | 1:B:4047:PHE:N    | 2.00        | 0.76     |
| 1:A:1959:THR:HA   | 1:A:4341:THR:OG1  | 1.85        | 0.76     |
| 1:B:4531:THR:O    | 1:B:4535:ARG:HG3  | 1.86        | 0.76     |
| 1:B:4067:ALA:HB1  | 1:B:4073:GLN:HG3  | 1.65        | 0.76     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2863:ARG:O    | 1:A:2863:ARG:HD3  | 1.84        | 0.76     |
| 1:B:3639:SER:HB3  | 1:B:3663:ILE:HD11 | 1.68        | 0.76     |
| 1:A:3927:ASN:HB3  | 1:A:3930:LEU:HB2  | 1.68        | 0.75     |
| 1:A:1813:GLN:HE22 | 1:A:1940:TYR:HA   | 1.50        | 0.75     |
| 1:B:1822:VAL:HG22 | 1:B:1826:GLN:HE21 | 1.50        | 0.75     |
| 1:A:4122:VAL:HG21 | 1:A:4216:PHE:CZ   | 2.20        | 0.75     |
| 1:B:4011:LEU:HD11 | 1:B:4041:SER:HB2  | 1.68        | 0.75     |
| 1:A:3731:ASN:H    | 1:A:3731:ASN:HD22 | 1.35        | 0.75     |
| 1:A:2273:MET:HB2  | 1:A:2395:PHE:HB2  | 1.68        | 0.75     |
| 1:B:3027:ARG:HA   | 1:B:3037:ILE:HD11 | 1.68        | 0.75     |
| 1:B:3966:THR:HG22 | 1:B:4426:MET:HG3  | 1.68        | 0.75     |
| 1:B:2426:ILE:HD12 | 1:B:2426:ILE:H    | 1.51        | 0.75     |
| 1:A:3443:MET:HG3  | 1:A:3449:ARG:HG3  | 1.68        | 0.75     |
| 1:A:3358:GLN:HA   | 1:A:3361:LYS:HE2  | 1.69        | 0.75     |
| 1:A:3039:THR:HG22 | 1:A:3040:ILE:H    | 1.50        | 0.75     |
| 1:A:4648:VAL:HG13 | 1:A:4657:THR:HG21 | 1.68        | 0.75     |
| 1:B:3766:THR:HG22 | 1:B:3768:ASP:H    | 1.52        | 0.75     |
| 1:A:4622:HIS:HE2  | 1:A:4678:ILE:HG21 | 1.50        | 0.75     |
| 1:B:3035:LEU:HD22 | 1:B:3068:LYS:HB3  | 1.68        | 0.75     |
| 1:B:1950:THR:HB   | 1:B:1951:PRO:HD2  | 1.68        | 0.75     |
| 1:A:2586:GLY:HA2  | 1:A:2815:LEU:HD13 | 1.67        | 0.75     |
| 1:A:3015:ILE:HD13 | 1:A:3147:MET:HG3  | 1.68        | 0.74     |
| 1:B:2315:GLN:HB3  | 1:B:2775:THR:HG21 | 1.69        | 0.74     |
| 1:A:2397:VAL:HG21 | 1:A:2400:LEU:HD21 | 1.68        | 0.74     |
| 1:A:3696:LYS:HZ2  | 1:A:4206:SER:HB3  | 1.52        | 0.74     |
| 1:B:2638:THR:HG21 | 1:B:2838:LEU:HD21 | 1.68        | 0.74     |
| 1:A:1547:ASN:HA   | 1:A:1553:LYS:HG2  | 1.70        | 0.74     |
| 1:B:1476:ILE:HG23 | 1:B:1480:HIS:HB2  | 1.68        | 0.74     |
| 1:A:2105:ARG:HG2  | 1:A:2105:ARG:HH11 | 1.53        | 0.74     |
| 1:B:4278:HIS:HD2  | 1:B:4343:TYR:OH   | 1.71        | 0.73     |
| 1:A:4122:VAL:HG21 | 1:A:4216:PHE:HZ   | 1.53        | 0.73     |
| 1:A:3774:THR:HB   | 1:A:3775:PRO:HD2  | 1.70        | 0.73     |
| 1:A:2309:LYS:HE2  | 1:A:2756:THR:HG21 | 1.68        | 0.73     |
| 1:A:4053:VAL:HG12 | 1:A:4053:VAL:O    | 1.86        | 0.73     |
| 1:A:3388:LEU:HD23 | 1:A:3473:ALA:HB1  | 1.68        | 0.73     |
| 1:A:2793:ASN:HD22 | 1:A:2793:ASN:N    | 1.85        | 0.73     |
| 1:A:3725:ASN:HD22 | 1:A:3725:ASN:H    | 1.35        | 0.73     |
| 1:A:3281:GLU:HB3  | 1:A:3581:PHE:HE1  | 1.54        | 0.73     |
| 1:A:1886:ARG:HG3  | 1:A:1887:ASP:N    | 2.04        | 0.73     |
| 1:B:3700:LEU:HD13 | 1:B:3701:ASP:N    | 2.04        | 0.73     |
| 1:A:3202:PRO:HD2  | 1:A:3624:VAL:O    | 1.88        | 0.73     |
| 1:B:3602:ILE:HG23 | 1:B:3610:ARG:HG2  | 1.70        | 0.73     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3453:THR:HA   | 1:A:3457:LEU:HB2  | 1.70        | 0.73     |
| 1:B:2572:ARG:HG2  | 1:B:2617:VAL:HG11 | 1.69        | 0.73     |
| 1:B:4157:TYR:HB3  | 1:B:4184:TRP:HB2  | 1.71        | 0.73     |
| 1:A:2675:PRO:HD2  | 1:A:2816:VAL:O    | 1.88        | 0.73     |
| 1:B:2309:LYS:NZ   | 1:B:2756:THR:HG21 | 2.04        | 0.73     |
| 1:B:4189:ASN:HD22 | 1:B:4189:ASN:N    | 1.85        | 0.73     |
| 1:A:2080:GLY:HA3  | 1:A:2084:ARG:O    | 1.89        | 0.73     |
| 1:B:3789:THR:HB   | 1:B:3790:PRO:HD2  | 1.70        | 0.73     |
| 1:A:3475:GLY:O    | 1:A:3478:VAL:HG12 | 1.88        | 0.73     |
| 1:A:4024:ARG:HD3  | 1:A:4034:VAL:HG21 | 1.71        | 0.73     |
| 1:B:3584:GLN:O    | 1:B:3588:VAL:HG23 | 1.87        | 0.73     |
| 1:B:2514:LYS:HE2  | 1:B:2600:ILE:HD11 | 1.71        | 0.72     |
| 1:A:1655:LEU:HB2  | 1:A:1658:GLU:HB2  | 1.69        | 0.72     |
| 1:A:3281:GLU:HB3  | 1:A:3581:PHE:CE1  | 2.24        | 0.72     |
| 1:A:1883:VAL:HG11 | 1:A:2111:VAL:HG22 | 1.70        | 0.72     |
| 1:A:3724:GLU:OE2  | 1:A:3766:THR:HG23 | 1.88        | 0.72     |
| 1:B:4136:SER:HB3  | 1:B:4238:TYR:HB2  | 1.72        | 0.72     |
| 1:B:4005:ILE:HD13 | 1:B:4020:LEU:HD23 | 1.70        | 0.72     |
| 1:B:1899:THR:HB   | 1:B:1903:ASP:HB2  | 1.72        | 0.72     |
| 1:B:2938:PHE:O    | 1:B:2941:VAL:HG12 | 1.88        | 0.72     |
| 1:B:2841:ASN:HD22 | 1:B:2842:LEU:H    | 1.37        | 0.72     |
| 1:A:2042:GLN:HE21 | 1:A:2059:LEU:HD11 | 1.54        | 0.72     |
| 1:A:1763:GLY:N    | 1:A:1764:PRO:HD3  | 2.04        | 0.72     |
| 1:B:4601:ILE:O    | 1:B:4604:THR:HG22 | 1.90        | 0.71     |
| 1:A:3700:LEU:HD13 | 1:A:3701:ASP:N    | 2.04        | 0.71     |
| 1:A:2587:LEU:HG   | 1:A:2817:ASP:HB2  | 1.72        | 0.71     |
| 1:B:3292:LEU:HD13 | 1:B:3571:ARG:HA   | 1.72        | 0.71     |
| 1:A:2626:LEU:HD12 | 1:A:2626:LEU:H    | 1.55        | 0.71     |
| 1:A:2042:GLN:NE2  | 1:A:2059:LEU:HD11 | 2.06        | 0.71     |
| 1:A:3555:ASN:HB3  | 1:A:3559:ARG:NH1  | 2.04        | 0.71     |
| 1:B:2839:LEU:HD13 | 1:B:2842:LEU:HD12 | 1.70        | 0.71     |
| 1:A:4347:ILE:HG21 | 1:A:4353:MET:HG2  | 1.72        | 0.71     |
| 1:B:4506:GLY:O    | 1:B:4510:VAL:HG23 | 1.91        | 0.71     |
| 1:A:1742:ILE:HG22 | 1:A:1753:THR:HG22 | 1.71        | 0.71     |
| 1:A:2371:LEU:HB3  | 1:A:2410:ARG:HG3  | 1.71        | 0.71     |
| 1:B:3700:LEU:HD22 | 1:B:3701:ASP:H    | 1.54        | 0.71     |
| 1:A:2283:THR:HA   | 1:A:2286:TRP:NE1  | 2.06        | 0.71     |
| 1:A:2208:VAL:HA   | 1:A:2415:TRP:CD1  | 2.24        | 0.71     |
| 1:A:1807:VAL:HG13 | 1:A:1815:VAL:HG11 | 1.73        | 0.71     |
| 1:B:3674:VAL:HG22 | 1:B:3784:VAL:HB   | 1.71        | 0.71     |
| 1:A:4242:PRO:HA   | 1:A:4286:ARG:NH1  | 2.01        | 0.71     |
| 1:B:3234:ILE:HG23 | 1:B:3617:TRP:NE1  | 2.06        | 0.71     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4553:TYR:H    | 1:A:4553:TYR:HD1  | 1.38        | 0.71     |
| 1:A:2258:LYS:HA   | 1:A:2261:GLN:HG3  | 1.71        | 0.71     |
| 1:B:4157:TYR:CB   | 1:B:4184:TRP:HB2  | 2.21        | 0.71     |
| 1:A:2176:ASP:N    | 1:A:2179:SER:HG   | 1.87        | 0.71     |
| 1:A:3859:LYS:O    | 1:A:3862:THR:HG22 | 1.90        | 0.71     |
| 1:A:4533:TYR:O    | 1:A:4537:LEU:HG   | 1.90        | 0.71     |
| 1:A:4591:LEU:HD21 | 1:A:4601:ILE:HD11 | 1.72        | 0.71     |
| 1:A:3037:ILE:H    | 1:A:3037:ILE:HD13 | 1.56        | 0.71     |
| 1:A:4029:SER:HB2  | 1:A:4081:ARG:HH12 | 1.56        | 0.71     |
| 1:A:2942:ASN:O    | 1:A:2944:ASP:N    | 2.24        | 0.71     |
| 1:B:4703:ILE:HD12 | 1:B:4705:LEU:HD21 | 1.71        | 0.71     |
| 1:B:2282:LYS:HA   | 1:B:2416:PHE:CD1  | 2.26        | 0.71     |
| 1:B:4574:GLN:HE22 | 1:B:4590:TRP:N    | 1.89        | 0.70     |
| 1:A:4494:PRO:HG2  | 1:A:4607:SER:HA   | 1.73        | 0.70     |
| 1:B:2124:LEU:HD22 | 1:B:2195:LEU:HD22 | 1.71        | 0.70     |
| 1:B:1823:TRP:CD1  | 1:B:1885:GLN:HB3  | 2.26        | 0.70     |
| 1:A:1879:ILE:O    | 1:A:1883:VAL:HG23 | 1.91        | 0.70     |
| 1:A:2371:LEU:HB2  | 1:A:2410:ARG:HG3  | 1.71        | 0.70     |
| 1:B:3238:ILE:CG2  | 1:B:3255:VAL:HG11 | 2.20        | 0.70     |
| 1:B:1879:ILE:O    | 1:B:1883:VAL:HG23 | 1.91        | 0.70     |
| 1:A:2006:LEU:HD23 | 1:A:2035:ILE:HG23 | 1.73        | 0.70     |
| 1:A:4540:SER:HB2  | 1:A:4545:ILE:O    | 1.91        | 0.70     |
| 1:A:2788:PHE:O    | 1:A:2789:VAL:HG23 | 1.90        | 0.70     |
| 1:A:3153:ASP:HA   | 1:A:3156:ASN:ND2  | 2.06        | 0.70     |
| 1:A:2113:LEU:HD21 | 1:A:2156:LEU:HD22 | 1.74        | 0.70     |
| 1:A:4095:LEU:HD11 | 1:A:4422:LYS:HB3  | 1.73        | 0.70     |
| 1:A:3677:PRO:HG3  | 1:A:3787:THR:HG22 | 1.72        | 0.70     |
| 1:A:4649:TRP:HA   | 1:A:4649:TRP:CE3  | 2.27        | 0.70     |
| 1:A:2106:GLU:CD   | 1:A:2106:GLU:H    | 1.95        | 0.70     |
| 1:A:2954:ASN:HD22 | 1:A:2954:ASN:H    | 1.39        | 0.70     |
| 1:A:2308:PRO:HD2  | 1:A:2357:GLY:HA3  | 1.74        | 0.70     |
| 1:A:4179:ALA:HB1  | 1:A:4209:PRO:HB3  | 1.73        | 0.70     |
| 1:A:3812:LYS:O    | 1:A:3816:LEU:HB3  | 1.91        | 0.70     |
| 1:A:3380:VAL:HG11 | 1:A:3435:ILE:HG21 | 1.72        | 0.70     |
| 1:B:1928:HIS:NE2  | 1:B:1933:THR:HG22 | 2.06        | 0.70     |
| 1:A:4086:MET:CG   | 1:A:4093:ARG:HB2  | 2.21        | 0.69     |
| 1:A:3331:GLN:HE22 | 1:A:3533:LYS:HG3  | 1.56        | 0.69     |
| 1:B:2850:THR:O    | 1:B:2854:VAL:HG23 | 1.90        | 0.69     |
| 1:A:3433:THR:HG22 | 1:A:3437:ASN:ND2  | 2.06        | 0.69     |
| 1:B:2540:LEU:HD23 | 1:B:2576:SER:HA   | 1.72        | 0.69     |
| 1:B:1687:LEU:HD21 | 1:B:1706:LEU:HD23 | 1.74        | 0.69     |
| 1:B:3700:LEU:HD12 | 1:B:3700:LEU:H    | 1.58        | 0.69     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4128:SER:HB2  | 1:A:4213:PHE:HB3  | 1.74        | 0.69     |
| 1:B:1739:THR:HB   | 1:B:1761:ALA:HB2  | 1.74        | 0.69     |
| 1:A:1846:GLN:HA   | 1:A:1893:GLN:NE2  | 2.08        | 0.69     |
| 1:B:2235:GLN:NE2  | 1:B:2296:VAL:HG13 | 2.06        | 0.69     |
| 1:B:3238:ILE:HG12 | 1:B:3601:TYR:CG   | 2.28        | 0.69     |
| 1:B:1846:GLN:O    | 1:B:1850:GLN:HG2  | 1.92        | 0.69     |
| 1:A:3912:SER:HB3  | 1:A:4231:ARG:HG2  | 1.75        | 0.69     |
| 1:B:3768:ASP:HB3  | 1:B:3771:ALA:HB2  | 1.73        | 0.69     |
| 1:B:3238:ILE:HG21 | 1:B:3255:VAL:HG11 | 1.73        | 0.69     |
| 1:B:3256:THR:HB   | 1:B:3257:PRO:HD2  | 1.74        | 0.69     |
| 1:A:2028:PHE:HB3  | 1:A:2075:VAL:HG13 | 1.72        | 0.69     |
| 1:B:1534:VAL:HG13 | 1:B:1568:HIS:HD2  | 1.58        | 0.69     |
| 1:A:2202:THR:HG22 | 1:A:2265:ILE:HG12 | 1.74        | 0.69     |
| 1:A:1746:SER:OG   | 1:A:1750:GLU:HB3  | 1.93        | 0.69     |
| 1:B:2282:LYS:HA   | 1:B:2416:PHE:HD1  | 1.57        | 0.69     |
| 1:B:2200:ASN:HB2  | 1:B:2228:LEU:HD22 | 1.75        | 0.69     |
| 1:A:4623:ALA:HB2  | 1:A:4703:ILE:HD11 | 1.75        | 0.69     |
| 1:A:1770:LEU:O    | 1:A:1773:VAL:HG22 | 1.93        | 0.69     |
| 1:B:4005:ILE:CD1  | 1:B:4020:LEU:HD23 | 2.24        | 0.68     |
| 1:A:2748:LEU:HD21 | 1:A:2800:ARG:NH1  | 2.09        | 0.68     |
| 1:B:3724:GLU:OE2  | 1:B:3766:THR:HG23 | 1.93        | 0.68     |
| 1:B:4362:GLN:HB2  | 1:B:4714:GLN:NE2  | 2.08        | 0.68     |
| 1:B:4574:GLN:NE2  | 1:B:4590:TRP:H    | 1.87        | 0.68     |
| 1:B:2865:THR:H    | 1:B:2868:ILE:HD12 | 1.58        | 0.68     |
| 1:A:1886:ARG:NH1  | 1:A:1890:ARG:HH22 | 1.91        | 0.68     |
| 1:B:3652:LEU:HD12 | 1:B:3653:PRO:HD2  | 1.74        | 0.68     |
| 1:A:3210:GLU:HG3  | 1:A:3211:ILE:H    | 1.57        | 0.68     |
| 1:B:3043:ASN:ND2  | 1:B:3046:TYR:HB2  | 2.07        | 0.68     |
| 1:B:1545:LEU:H    | 1:B:1545:LEU:HD12 | 1.57        | 0.68     |
| 1:A:1554:LEU:HB3  | 1:A:1609:GLN:HE21 | 1.59        | 0.68     |
| 1:A:2010:SER:HB3  | 1:A:2060:LEU:HD21 | 1.75        | 0.68     |
| 1:B:1743:GLY:HA2  | 1:B:1754:PHE:CD1  | 2.29        | 0.68     |
| 1:B:2320:LEU:HD23 | 1:B:2320:LEU:O    | 1.93        | 0.68     |
| 1:A:4200:LEU:HD22 | 1:A:4204:LEU:HD11 | 1.75        | 0.68     |
| 1:A:2293:ILE:CG2  | 1:A:2350:ARG:HH22 | 2.07        | 0.68     |
| 1:A:1931:ASN:OD1  | 1:A:1962:GLN:NE2  | 2.25        | 0.68     |
| 1:B:2400:LEU:HD13 | 1:B:2408:ILE:HD11 | 1.76        | 0.68     |
| 1:A:1715:ILE:HD11 | 1:A:1760:ILE:HD13 | 1.74        | 0.68     |
| 1:A:2742:PHE:HA   | 1:A:2789:VAL:O    | 1.94        | 0.67     |
| 1:A:1846:GLN:HA   | 1:A:1893:GLN:HE22 | 1.59        | 0.67     |
| 1:A:3961:ASN:O    | 1:A:3964:LYS:HB2  | 1.94        | 0.67     |
| 1:A:2699:LEU:HD11 | 1:A:2713:THR:HG21 | 1.77        | 0.67     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2231:ILE:HG21 | 1:B:2264:GLN:NE2  | 2.09        | 0.67     |
| 1:A:3013:LEU:HD12 | 1:A:3145:PHE:HB3  | 1.74        | 0.67     |
| 1:B:4251:THR:HG23 | 1:B:4303:LEU:CD2  | 2.23        | 0.67     |
| 1:A:2212:ILE:HG22 | 1:A:2213:PRO:HD3  | 1.77        | 0.67     |
| 1:B:2793:ASN:HB3  | 1:B:2794:PRO:HD2  | 1.76        | 0.67     |
| 1:A:3563:LEU:HD11 | 1:A:3851:VAL:HG22 | 1.77        | 0.67     |
| 1:A:2447:GLN:HE22 | 1:A:2492:LEU:HD23 | 1.58        | 0.67     |
| 1:B:4189:ASN:H    | 1:B:4218:THR:CG2  | 2.08        | 0.67     |
| 1:A:1963:ALA:HB1  | 1:A:2096:ARG:HG3  | 1.76        | 0.67     |
| 1:A:3397:PRO:HG2  | 1:A:3419:TRP:CZ2  | 2.29        | 0.67     |
| 1:B:2815:LEU:HD23 | 1:B:2816:VAL:N    | 2.09        | 0.67     |
| 1:B:4189:ASN:H    | 1:B:4189:ASN:HD22 | 1.40        | 0.67     |
| 1:B:4184:TRP:CD1  | 1:B:4214:ARG:HB2  | 2.30        | 0.67     |
| 1:A:4210:HIS:ND1  | 1:A:4211:PRO:HD2  | 2.09        | 0.67     |
| 1:A:4259:ARG:HD3  | 1:A:4271:TYR:OH   | 1.95        | 0.67     |
| 1:A:4548:LYS:HG3  | 1:A:4549:GLU:H    | 1.60        | 0.66     |
| 1:B:1719:GLN:HA   | 1:B:1722:PHE:CD2  | 2.29        | 0.66     |
| 1:A:2014:VAL:HG13 | 1:A:2065:ILE:HG21 | 1.78        | 0.66     |
| 1:B:3078:VAL:HG23 | 1:B:3083:PHE:HB2  | 1.76        | 0.66     |
| 1:B:3958:THR:HG23 | 1:B:4235:VAL:HB   | 1.76        | 0.66     |
| 1:B:2361:PRO:HD3  | 1:B:2402:TYR:O    | 1.96        | 0.66     |
| 1:B:2297:ASP:O    | 1:B:2299:ILE:HG13 | 1.94        | 0.66     |
| 1:A:4270:ILE:HD13 | 1:A:4314:VAL:HG21 | 1.78        | 0.66     |
| 1:B:2423:THR:HG23 | 1:B:2530:ARG:HD2  | 1.76        | 0.66     |
| 1:B:2766:MET:HB3  | 1:B:2783:LEU:HD11 | 1.75        | 0.66     |
| 1:A:2595:LYS:HE3  | 1:A:2611:PRO:HG3  | 1.75        | 0.66     |
| 1:A:3875:VAL:O    | 1:A:3879:ILE:HG12 | 1.95        | 0.66     |
| 1:A:3925:ASN:N    | 1:A:3925:ASN:HD22 | 1.93        | 0.66     |
| 1:B:2861:GLN:HG3  | 1:B:2874:TYR:HB2  | 1.75        | 0.66     |
| 1:A:2108:ILE:O    | 1:A:2112:MET:HB2  | 1.96        | 0.66     |
| 1:A:4572:MET:HE1  | 1:A:4575:LEU:HD11 | 1.77        | 0.66     |
| 1:A:3245:LEU:HD12 | 1:A:3249:GLN:HB2  | 1.78        | 0.66     |
| 1:A:2124:LEU:HD22 | 1:A:2195:LEU:HD22 | 1.78        | 0.66     |
| 1:A:2125:ALA:HA   | 1:A:2128:ILE:HG22 | 1.78        | 0.66     |
| 1:B:2113:LEU:HD21 | 1:B:2156:LEU:HD22 | 1.78        | 0.66     |
| 1:A:2910:LEU:CD2  | 1:A:2930:ILE:HD12 | 2.25        | 0.66     |
| 1:B:1769:TRP:O    | 1:B:1773:VAL:HG23 | 1.96        | 0.66     |
| 1:B:2984:LEU:HD22 | 1:B:2986:VAL:HG22 | 1.78        | 0.66     |
| 1:A:3309:LYS:O    | 1:A:3313:LEU:HG   | 1.96        | 0.66     |
| 1:A:2315:GLN:HB3  | 1:A:2775:THR:HG21 | 1.76        | 0.66     |
| 1:B:3785:ASN:ND2  | 1:B:3787:THR:HG23 | 2.11        | 0.66     |
| 1:B:1885:GLN:O    | 1:B:1889:VAL:HG23 | 1.96        | 0.66     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3989:ASP:O    | 1:A:3993:LYS:HB2  | 1.96        | 0.66     |
| 1:A:3647:TRP:HB3  | 1:A:3652:LEU:HD23 | 1.78        | 0.65     |
| 1:A:3410:LEU:HD22 | 1:A:3452:ILE:HD11 | 1.78        | 0.65     |
| 1:A:3965:LEU:HG   | 1:A:4426:MET:HE3  | 1.77        | 0.65     |
| 1:A:4230:LEU:H    | 1:A:4230:LEU:HD12 | 1.61        | 0.65     |
| 1:A:2289:TYR:O    | 1:A:2293:ILE:HG12 | 1.95        | 0.65     |
| 1:A:3285:LEU:HD13 | 1:A:3578:SER:HA   | 1.78        | 0.65     |
| 1:A:4186:LEU:C    | 1:A:4187:LEU:HD12 | 2.17        | 0.65     |
| 1:B:3639:SER:HB3  | 1:B:3663:ILE:CD1  | 2.25        | 0.65     |
| 1:A:2535:ASN:HD22 | 1:A:2668:ARG:HH12 | 1.45        | 0.65     |
| 1:A:3271:ILE:HG13 | 1:A:3592:VAL:HG11 | 1.78        | 0.65     |
| 1:B:2498:CYS:HA   | 1:B:2501:ILE:HD12 | 1.77        | 0.65     |
| 1:B:1901:ASN:HD22 | 1:B:1901:ASN:H    | 1.43        | 0.65     |
| 1:A:2552:ASN:HD21 | 1:A:2560:MET:HB2  | 1.59        | 0.65     |
| 1:A:3700:LEU:CD2  | 1:A:3701:ASP:H    | 2.09        | 0.65     |
| 1:A:4054:GLY:O    | 1:A:4055:GLU:C    | 2.34        | 0.65     |
| 1:B:2359:VAL:HG13 | 1:B:2364:VAL:HG21 | 1.79        | 0.65     |
| 1:B:3813:ARG:O    | 1:B:3817:LEU:HD13 | 1.97        | 0.65     |
| 1:B:2339:ILE:HA   | 1:B:2346:GLU:HG2  | 1.76        | 0.65     |
| 1:A:2975:ARG:HE   | 1:A:2975:ARG:HA   | 1.61        | 0.65     |
| 1:A:3242:ASN:OD1  | 1:A:3253:ASN:HB3  | 1.96        | 0.65     |
| 1:A:3015:ILE:HG22 | 1:A:3149:PRO:HG3  | 1.77        | 0.65     |
| 1:A:1537:PHE:O    | 1:A:1541:LEU:HB2  | 1.97        | 0.65     |
| 1:A:2948:ARG:HH11 | 1:A:2948:ARG:HG2  | 1.62        | 0.65     |
| 1:A:4622:HIS:ND1  | 1:A:4623:ALA:N    | 2.45        | 0.65     |
| 1:A:4024:ARG:HG3  | 1:A:4031:SER:HA   | 1.78        | 0.65     |
| 1:A:2120:THR:O    | 1:A:2121:ALA:C    | 2.33        | 0.65     |
| 1:B:3949:SER:HA   | 1:B:4110:PHE:HE1  | 1.62        | 0.65     |
| 1:A:3255:VAL:HA   | 1:A:3259:HIS:HD2  | 1.61        | 0.65     |
| 1:B:1920:ASN:HD22 | 1:B:1921:VAL:H    | 1.44        | 0.65     |
| 1:A:4553:TYR:HB3  | 1:A:4595:LEU:HD23 | 1.79        | 0.65     |
| 1:A:4649:TRP:HA   | 1:A:4649:TRP:HE3  | 1.60        | 0.65     |
| 1:B:3109:MET:HB3  | 1:B:3129:LEU:HD23 | 1.79        | 0.65     |
| 1:A:2305:VAL:HG21 | 1:A:2769:LYS:HE2  | 1.79        | 0.65     |
| 1:B:4389:ARG:HG2  | 1:B:4389:ARG:HH11 | 1.62        | 0.65     |
| 1:A:1748:GLU:HG2  | 1:A:1943:ILE:HB   | 1.79        | 0.65     |
| 1:B:1931:ASN:HB2  | 1:B:4312:TYR:CZ   | 2.32        | 0.64     |
| 1:A:2127:LYS:C    | 1:A:2130:PRO:HD2  | 2.17        | 0.64     |
| 1:A:2129:VAL:HB   | 1:A:2130:PRO:HD3  | 1.78        | 0.64     |
| 1:A:3270:LEU:HB2  | 1:A:3592:VAL:HG13 | 1.77        | 0.64     |
| 1:A:4221:ILE:H    | 1:A:4221:ILE:HD12 | 1.62        | 0.64     |
| 1:B:4063:ILE:H    | 1:B:4063:ILE:HD12 | 1.62        | 0.64     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:3063:GLY:HA2  | 1:B:3136:GLN:HB3  | 1.78        | 0.64     |
| 1:A:2968:LEU:O    | 1:A:2972:VAL:HG23 | 1.97        | 0.64     |
| 1:A:2704:ALA:HB3  | 1:A:3085:GLU:HG3  | 1.77        | 0.64     |
| 1:B:4288:ILE:HG23 | 1:B:4292:TRP:O    | 1.97        | 0.64     |
| 1:A:3700:LEU:H    | 1:A:3700:LEU:HD12 | 1.62        | 0.64     |
| 1:A:2606:PRO:HD3  | 1:A:2624:TRP:CD1  | 2.32        | 0.64     |
| 1:B:1811:PRO:O    | 1:B:1815:VAL:HG23 | 1.98        | 0.64     |
| 1:A:2651:VAL:HG13 | 1:A:2652:ASP:N    | 2.12        | 0.64     |
| 1:A:3387:HIS:CB   | 1:A:3473:ALA:HB2  | 2.27        | 0.64     |
| 1:A:2525:ILE:HG13 | 1:A:2584:SER:O    | 1.98        | 0.64     |
| 1:B:2866:PRO:HG3  | 1:B:2873:ILE:HG22 | 1.78        | 0.64     |
| 1:A:1921:VAL:HG23 | 1:A:1922:LEU:HD22 | 1.79        | 0.64     |
| 1:B:4188:LYS:HA   | 1:B:4218:THR:HG22 | 1.80        | 0.64     |
| 1:A:1811:PRO:HD2  | 1:A:1814:LEU:HD12 | 1.78        | 0.64     |
| 1:A:3528:SER:O    | 1:A:3531:THR:HG22 | 1.98        | 0.64     |
| 1:A:3602:ILE:HG23 | 1:A:3610:ARG:HG2  | 1.80        | 0.64     |
| 1:A:4349:ASN:HD22 | 1:A:4352:ASP:N    | 1.95        | 0.64     |
| 1:A:2273:MET:CB   | 1:A:2395:PHE:HB2  | 2.27        | 0.64     |
| 1:A:2199:ILE:O    | 1:A:2203:MET:HB2  | 1.98        | 0.64     |
| 1:A:4050:LYS:O    | 1:A:4052:GLN:N    | 2.30        | 0.64     |
| 1:A:2506:PHE:CD1  | 1:A:2512:VAL:HG21 | 2.33        | 0.64     |
| 1:B:3991:LEU:O    | 1:B:4427:ILE:HD12 | 1.98        | 0.64     |
| 1:A:3897:TYR:HE1  | 1:A:3913:LEU:HA   | 1.63        | 0.64     |
| 1:A:3696:LYS:NZ   | 1:A:4206:SER:HB3  | 2.13        | 0.64     |
| 1:A:4296:PHE:CE2  | 1:A:4347:ILE:HD13 | 2.33        | 0.64     |
| 1:A:1545:LEU:HB3  | 1:A:1553:LYS:HE2  | 1.80        | 0.64     |
| 1:A:2979:PHE:CE2  | 1:A:3028:PHE:HA   | 2.33        | 0.64     |
| 1:B:3299:VAL:HG11 | 1:B:3564:LEU:HG   | 1.78        | 0.64     |
| 1:B:1554:LEU:HD12 | 1:B:2323:THR:HG22 | 1.79        | 0.64     |
| 1:B:4548:LYS:HD2  | 1:B:4549:GLU:H    | 1.59        | 0.64     |
| 1:B:1694:PHE:HB3  | 1:B:1697:PHE:CD2  | 2.33        | 0.64     |
| 1:A:3114:GLU:HG2  | 1:A:3118:ARG:NH1  | 2.13        | 0.64     |
| 1:A:4693:ASN:N    | 1:A:4693:ASN:HD22 | 1.95        | 0.64     |
| 1:A:2207:LEU:HD13 | 1:A:2215:ILE:HG21 | 1.79        | 0.64     |
| 1:A:3293:ARG:HH11 | 1:A:3293:ARG:HG3  | 1.63        | 0.64     |
| 1:A:2163:LYS:HB2  | 1:A:2194:VAL:HG11 | 1.79        | 0.64     |
| 1:A:3785:ASN:HD22 | 1:A:3786:PHE:N    | 1.95        | 0.64     |
| 1:A:4362:GLN:HG3  | 1:A:4714:GLN:OE1  | 1.97        | 0.64     |
| 1:B:4351:PHE:CE2  | 1:B:4689:PRO:HG3  | 2.32        | 0.64     |
| 1:B:1557:GLY:O    | 1:B:1561:LEU:HD23 | 1.98        | 0.64     |
| 1:A:3804:THR:O    | 1:A:3807:PRO:HD3  | 1.98        | 0.64     |
| 1:A:2051:LYS:O    | 1:A:2051:LYS:HD3  | 1.96        | 0.64     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1611:ARG:HH11 | 1:A:1611:ARG:HG3  | 1.62        | 0.64     |
| 1:A:4396:ILE:O    | 1:A:4399:LEU:HB2  | 1.98        | 0.63     |
| 1:A:4296:PHE:CE2  | 1:A:4347:ILE:HA   | 2.33        | 0.63     |
| 1:B:3043:ASN:HD22 | 1:B:3046:TYR:HB2  | 1.63        | 0.63     |
| 1:B:3087:MET:CE   | 1:B:3090:LEU:HD23 | 2.28        | 0.63     |
| 1:A:2490:ALA:O    | 1:A:2494:VAL:HG23 | 1.97        | 0.63     |
| 1:A:3387:HIS:HB3  | 1:A:3473:ALA:HB2  | 1.80        | 0.63     |
| 1:B:4607:SER:O    | 1:B:4611:LEU:HG   | 1.98        | 0.63     |
| 1:A:1811:PRO:O    | 1:A:1815:VAL:HG23 | 1.98        | 0.63     |
| 1:A:3416:LYS:HE3  | 1:A:3418:GLU:HB3  | 1.80        | 0.63     |
| 1:B:1780:THR:HG22 | 1:B:1784:LEU:HD12 | 1.80        | 0.63     |
| 1:B:3563:LEU:HD11 | 1:B:3845:ILE:HD11 | 1.79        | 0.63     |
| 1:A:4277:PHE:HB2  | 1:A:4363:LEU:HD12 | 1.79        | 0.63     |
| 1:B:1607:ASP:O    | 1:B:1611:ARG:HG2  | 1.97        | 0.63     |
| 1:B:1525:ILE:HA   | 1:B:1528:GLU:HB3  | 1.80        | 0.63     |
| 1:A:3711:ALA:HA   | 1:A:3716:CYS:SG   | 2.39        | 0.63     |
| 1:A:3985:GLU:O    | 1:A:3989:ASP:HB2  | 1.97        | 0.63     |
| 1:A:4571:ARG:HA   | 1:A:4590:TRP:HZ3  | 1.63        | 0.63     |
| 1:B:1523:GLY:HA3  | 1:B:1580:TYR:CE2  | 2.33        | 0.63     |
| 1:B:3238:ILE:HD11 | 1:B:3617:TRP:HZ2  | 1.63        | 0.63     |
| 1:A:2995:LEU:HA   | 1:A:2998:ILE:HD11 | 1.80        | 0.63     |
| 1:A:4310:ILE:O    | 1:A:4314:VAL:HB   | 1.99        | 0.63     |
| 1:A:3482:THR:O    | 1:A:3486:TYR:HB2  | 1.99        | 0.63     |
| 1:A:2938:PHE:HB3  | 1:A:2941:VAL:HG23 | 1.80        | 0.63     |
| 1:A:3994:GLY:HA3  | 1:A:4087:LYS:CE   | 2.29        | 0.63     |
| 1:A:2972:VAL:O    | 1:A:2976:LEU:HB2  | 1.98        | 0.63     |
| 1:B:3841:ALA:O    | 1:B:3842:SER:CB   | 2.35        | 0.63     |
| 1:A:2995:LEU:HD23 | 1:A:2998:ILE:HD11 | 1.80        | 0.63     |
| 1:A:3063:GLY:HA2  | 1:A:3136:GLN:HB3  | 1.81        | 0.63     |
| 1:A:4269:ARG:CZ   | 1:A:4383:VAL:HG11 | 2.29        | 0.63     |
| 1:A:3445:THR:HG23 | 1:A:3449:ARG:NH1  | 2.14        | 0.63     |
| 1:B:3035:LEU:CD2  | 1:B:3068:LYS:HB3  | 2.28        | 0.63     |
| 1:A:2000:CYS:SG   | 1:A:2031:LEU:HD11 | 2.37        | 0.63     |
| 1:A:3255:VAL:HA   | 1:A:3259:HIS:CD2  | 2.33        | 0.63     |
| 1:B:1592:ASP:O    | 1:B:1596:ASN:HB2  | 1.99        | 0.63     |
| 1:B:4133:LEU:HD23 | 1:B:4230:LEU:HD23 | 1.79        | 0.63     |
| 1:B:2751:THR:HB   | 1:B:2756:THR:H    | 1.63        | 0.63     |
| 1:B:2711:LEU:HD12 | 1:B:2714:PHE:HD2  | 1.63        | 0.63     |
| 1:B:2841:ASN:HD22 | 1:B:2841:ASN:N    | 1.97        | 0.62     |
| 1:A:3647:TRP:CH2  | 1:A:3663:ILE:HD12 | 2.34        | 0.62     |
| 1:A:4049:GLY:O    | 1:A:4050:LYS:O    | 2.17        | 0.62     |
| 1:A:3725:ASN:H    | 1:A:3725:ASN:ND2  | 1.96        | 0.62     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2250:VAL:HB   | 1:A:2425:MET:HE2  | 1.80        | 0.62     |
| 1:A:3300:LYS:HA   | 1:A:3564:LEU:HD11 | 1.81        | 0.62     |
| 1:A:1922:LEU:HD13 | 1:A:1938:PHE:HD1  | 1.63        | 0.62     |
| 1:B:3865:ILE:O    | 1:B:3869:VAL:HG23 | 1.98        | 0.62     |
| 1:B:4194:PRO:O    | 1:B:4197:LEU:HB2  | 1.99        | 0.62     |
| 1:B:2877:ARG:HB3  | 1:B:2881:ARG:HH12 | 1.63        | 0.62     |
| 1:A:3599:LEU:HD11 | 1:A:3638:LEU:HD13 | 1.80        | 0.62     |
| 1:A:2542:ASN:O    | 1:A:2546:VAL:HG23 | 1.99        | 0.62     |
| 1:A:2247:ARG:HB2  | 1:A:2249:LEU:HG   | 1.81        | 0.62     |
| 1:A:2205:PRO:HG2  | 1:A:2265:ILE:HD11 | 1.81        | 0.62     |
| 1:A:1695:ALA:HB1  | 1:A:2019:CYS:SG   | 2.39        | 0.62     |
| 1:A:1975:PRO:HD2  | 1:A:2101:ILE:HA   | 1.80        | 0.62     |
| 1:A:2793:ASN:ND2  | 1:A:2793:ASN:N    | 2.44        | 0.62     |
| 1:A:1743:GLY:HA3  | 1:A:1753:THR:HA   | 1.81        | 0.62     |
| 1:A:2546:VAL:HA   | 1:A:2549:ILE:HD12 | 1.80        | 0.62     |
| 1:B:2080:GLY:HA2  | 1:B:2086:ASN:ND2  | 2.14        | 0.62     |
| 1:B:3844:ASN:O    | 1:B:3848:ASP:CB   | 2.47        | 0.62     |
| 1:B:2277:PRO:HA   | 1:B:2398:GLN:HG3  | 1.81        | 0.62     |
| 1:A:3011:HIS:ND1  | 1:A:3143:VAL:HG23 | 2.15        | 0.62     |
| 1:A:1927:ILE:HD13 | 1:A:1991:LEU:HD22 | 1.79        | 0.62     |
| 1:B:2584:SER:HB3  | 1:B:2813:ILE:HB   | 1.82        | 0.62     |
| 1:A:3557:VAL:O    | 1:A:3561:ILE:HG13 | 2.00        | 0.62     |
| 1:A:1957:TYR:CD2  | 1:A:1987:LEU:HD13 | 2.35        | 0.62     |
| 1:B:2199:ILE:HG23 | 1:B:2203:MET:HG3  | 1.81        | 0.62     |
| 1:B:2206:LYS:HB3  | 1:B:2413:MET:HB3  | 1.81        | 0.62     |
| 1:A:2645:ASP:O    | 1:A:2647:VAL:HG23 | 1.98        | 0.62     |
| 1:A:3634:VAL:HB   | 1:A:3635:PRO:HD3  | 1.82        | 0.62     |
| 1:A:3812:LYS:HB3  | 1:A:3875:VAL:HG22 | 1.81        | 0.62     |
| 1:A:3452:ILE:HG21 | 1:A:3485:THR:HG21 | 1.82        | 0.62     |
| 1:A:4389:ARG:HH11 | 1:A:4389:ARG:HG2  | 1.65        | 0.62     |
| 1:A:3408:VAL:HG11 | 1:A:3477:LEU:HG   | 1.82        | 0.62     |
| 1:A:4568:PHE:O    | 1:A:4572:MET:HG2  | 2.00        | 0.62     |
| 1:A:3566:ASN:HB3  | 1:A:3855:LEU:HD22 | 1.82        | 0.62     |
| 1:B:1726:PHE:CD2  | 1:B:1729:LEU:HD22 | 2.35        | 0.62     |
| 1:B:4410:LEU:HD22 | 1:B:4411:PRO:HD2  | 1.81        | 0.62     |
| 1:A:1967:ARG:HH22 | 1:A:2069:GLN:HG3  | 1.63        | 0.61     |
| 1:A:4402:ILE:H    | 1:A:4402:ILE:HD12 | 1.65        | 0.61     |
| 1:A:2151:ALA:O    | 1:A:2155:VAL:HG12 | 1.99        | 0.61     |
| 1:A:2357:GLY:O    | 1:A:2397:VAL:HG12 | 2.00        | 0.61     |
| 1:A:3445:THR:N    | 1:A:3446:PRO:HD2  | 2.16        | 0.61     |
| 1:B:2275:VAL:HG13 | 1:B:2397:VAL:HG13 | 1.82        | 0.61     |
| 1:A:2954:ASN:H    | 1:A:2954:ASN:ND2  | 1.97        | 0.61     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2912:LEU:C    | 1:A:2913:PHE:HD2  | 2.04        | 0.61     |
| 1:A:2090:ASN:HD22 | 1:A:2090:ASN:C    | 2.02        | 0.61     |
| 1:B:2212:ILE:N    | 1:B:2213:PRO:HD2  | 2.15        | 0.61     |
| 1:A:3909:TYR:CE1  | 1:A:3959:LEU:HA   | 2.35        | 0.61     |
| 1:B:4402:ILE:N    | 1:B:4402:ILE:HD12 | 2.14        | 0.61     |
| 1:A:2670:LEU:HG   | 1:A:2789:VAL:HG22 | 1.83        | 0.61     |
| 1:A:3271:ILE:O    | 1:A:3275:ARG:HB2  | 2.00        | 0.61     |
| 1:B:2704:ALA:HB2  | 1:B:3085:GLU:OE2  | 1.98        | 0.61     |
| 1:A:2243:ILE:HD12 | 1:A:2292:ALA:HB2  | 1.82        | 0.61     |
| 1:B:3664:MET:O    | 1:B:3668:PHE:HB3  | 1.99        | 0.61     |
| 1:B:2208:VAL:HG23 | 1:B:2211:ASP:HB2  | 1.81        | 0.61     |
| 1:A:2239:LYS:HA   | 1:A:2239:LYS:HE3  | 1.81        | 0.61     |
| 1:A:3731:ASN:N    | 1:A:3731:ASN:HD22 | 1.97        | 0.61     |
| 1:A:3260:TYR:O    | 1:A:3264:ILE:HG12 | 2.01        | 0.61     |
| 1:B:3673:LEU:HB2  | 1:B:3781:VAL:CG1  | 2.26        | 0.61     |
| 1:A:2262:LEU:HD11 | 1:A:2274:MET:HE2  | 1.81        | 0.61     |
| 1:A:2258:LYS:HD3  | 1:A:2261:GLN:HG3  | 1.83        | 0.61     |
| 1:A:2272:VAL:O    | 1:A:2394:MET:HA   | 2.00        | 0.61     |
| 1:A:2869:GLN:HB3  | 1:A:2872:TYR:CD1  | 2.36        | 0.61     |
| 1:B:2140:SER:O    | 1:B:2142:GLN:HG2  | 1.99        | 0.61     |
| 1:A:4329:ILE:HD12 | 1:A:4331:TRP:CZ2  | 2.35        | 0.61     |
| 1:A:2791:ALA:O    | 1:A:2792:CYS:HB3  | 2.00        | 0.61     |
| 1:A:4076:ILE:HD11 | 1:A:4104:SER:O    | 2.00        | 0.61     |
| 1:A:2948:ARG:HD3  | 1:A:2950:ILE:HG13 | 1.82        | 0.61     |
| 1:A:4589:VAL:HG12 | 1:A:4638:ASN:O    | 2.01        | 0.61     |
| 1:A:3686:MET:HE2  | 1:A:3696:LYS:HD2  | 1.81        | 0.61     |
| 1:A:3474:CYS:HA   | 1:A:3477:LEU:HD22 | 1.83        | 0.61     |
| 1:A:2088:PRO:HB2  | 1:A:2090:ASN:ND2  | 2.15        | 0.61     |
| 1:B:2732:PRO:HG3  | 1:B:2739:LEU:HB2  | 1.83        | 0.61     |
| 1:B:2305:VAL:HG22 | 1:B:2354:ILE:HB   | 1.83        | 0.61     |
| 1:A:4600:TYR:O    | 1:A:4604:THR:HG23 | 2.01        | 0.61     |
| 1:B:2586:GLY:HA2  | 1:B:2815:LEU:HD13 | 1.81        | 0.61     |
| 1:B:4189:ASN:N    | 1:B:4218:THR:HG22 | 2.14        | 0.61     |
| 1:B:3291:LYS:HD2  | 1:B:3835:LEU:HG   | 1.81        | 0.61     |
| 1:A:3587:THR:HB   | 1:A:3628:PHE:HA   | 1.82        | 0.61     |
| 1:A:4624:SER:HB2  | 1:A:4668:THR:HB   | 1.83        | 0.61     |
| 1:A:2190:TYR:O    | 1:A:2194:VAL:HG23 | 2.01        | 0.61     |
| 1:B:3650:ASN:OD1  | 1:B:3688:GLN:HA   | 2.00        | 0.61     |
| 1:A:2985:ASP:O    | 1:A:2987:PRO:HD3  | 2.01        | 0.61     |
| 1:A:4396:ILE:HA   | 1:A:4399:LEU:HD12 | 1.83        | 0.60     |
| 1:B:2582:GLY:HA2  | 1:B:2585:MET:HE3  | 1.81        | 0.60     |
| 1:A:4503:ILE:HG23 | 1:A:4575:LEU:HB3  | 1.82        | 0.60     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2152:LEU:O    | 1:A:2156:LEU:HG   | 2.01        | 0.60     |
| 1:A:3385:LYS:O    | 1:A:3389:ASP:HB2  | 2.00        | 0.60     |
| 1:B:2869:GLN:HB2  | 1:B:2872:TYR:CG   | 2.36        | 0.60     |
| 1:B:4135:CYS:HA   | 1:B:4219:SER:O    | 2.00        | 0.60     |
| 1:A:3137:VAL:HG13 | 1:A:3141:LEU:HD23 | 1.82        | 0.60     |
| 1:A:3994:GLY:HA3  | 1:A:4087:LYS:HE2  | 1.83        | 0.60     |
| 1:B:3559:ARG:NE   | 1:B:3846:LEU:O    | 2.35        | 0.60     |
| 1:A:4590:TRP:CE3  | 1:A:4593:GLY:HA3  | 2.36        | 0.60     |
| 1:A:1687:LEU:HD22 | 1:A:1705:LEU:HD23 | 1.83        | 0.60     |
| 1:A:4536:SER:HB2  | 1:A:4548:LYS:NZ   | 2.16        | 0.60     |
| 1:A:4636:SER:HB3  | 1:A:4670:THR:HA   | 1.83        | 0.60     |
| 1:A:3239:GLY:O    | 1:A:3243:ILE:HG13 | 2.00        | 0.60     |
| 1:A:2408:ILE:O    | 1:A:2409:SER:C    | 2.38        | 0.60     |
| 1:A:2144:HIS:HB2  | 1:A:2413:MET:SD   | 2.40        | 0.60     |
| 1:B:3219:ILE:O    | 1:B:3221:PRO:HD3  | 2.00        | 0.60     |
| 1:B:2231:ILE:HG21 | 1:B:2264:GLN:HE22 | 1.64        | 0.60     |
| 1:B:2364:VAL:HB   | 1:B:2407:THR:HG21 | 1.82        | 0.60     |
| 1:A:2903:ARG:NH2  | 1:A:2950:ILE:HA   | 2.16        | 0.60     |
| 1:A:2309:LYS:HG3  | 1:A:2358:ASP:HB2  | 1.84        | 0.60     |
| 1:A:2118:PHE:CE1  | 1:A:2163:LYS:HD2  | 2.37        | 0.60     |
| 1:A:4690:VAL:O    | 1:A:4700:LEU:HB2  | 2.01        | 0.60     |
| 1:A:3345:GLN:O    | 1:A:3349:ASP:HB2  | 2.01        | 0.60     |
| 1:A:3718:LEU:HD23 | 1:A:3762:ILE:HG13 | 1.84        | 0.60     |
| 1:A:4092:ASP:OD2  | 1:A:4093:ARG:HG2  | 2.01        | 0.60     |
| 1:A:1763:GLY:H    | 1:A:1764:PRO:HD3  | 1.65        | 0.60     |
| 1:A:3562:ALA:O    | 1:A:3566:ASN:HB2  | 2.02        | 0.60     |
| 1:B:3813:ARG:HB3  | 1:B:3879:ILE:HD13 | 1.83        | 0.60     |
| 1:A:2250:VAL:HB   | 1:A:2425:MET:CE   | 2.31        | 0.60     |
| 1:A:2532:ARG:HG3  | 1:A:2808:LEU:O    | 2.01        | 0.60     |
| 1:B:2976:LEU:HD12 | 1:B:2990:LEU:HD11 | 1.84        | 0.60     |
| 1:A:2917:LEU:HD12 | 1:A:2923:LYS:HA   | 1.84        | 0.60     |
| 1:B:1820:GLN:HE22 | 1:B:1990:GLN:NE2  | 1.99        | 0.60     |
| 1:A:4182:GLY:HA3  | 1:A:4212:SER:OG   | 2.02        | 0.60     |
| 1:A:3075:GLU:O    | 1:A:3078:VAL:HG12 | 2.01        | 0.60     |
| 1:A:3598:PHE:CD2  | 1:A:3634:VAL:HG11 | 2.36        | 0.60     |
| 1:B:1752:VAL:HG22 | 1:B:1811:PRO:HG3  | 1.84        | 0.60     |
| 1:A:4503:ILE:HA   | 1:A:4575:LEU:HD23 | 1.84        | 0.60     |
| 1:A:3994:GLY:HA3  | 1:A:4087:LYS:NZ   | 2.17        | 0.60     |
| 1:B:1908:TYR:CE1  | 1:B:1958:LEU:HD22 | 2.37        | 0.60     |
| 1:B:2522:ARG:HD3  | 1:B:2585:MET:SD   | 2.42        | 0.60     |
| 1:B:2129:VAL:HG22 | 1:B:2130:PRO:CD   | 2.30        | 0.60     |
| 1:A:2730:LEU:HD23 | 1:A:2783:LEU:HD23 | 1.83        | 0.60     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4574:GLN:NE2  | 1:A:4590:TRP:HB3  | 2.17        | 0.60     |
| 1:A:2239:LYS:HD3  | 1:A:2295:GLN:NE2  | 2.16        | 0.60     |
| 1:B:4153:LEU:HB2  | 1:B:4155:LYS:HG2  | 1.83        | 0.60     |
| 1:B:4541:ILE:HA   | 1:B:4561:LEU:HD11 | 1.83        | 0.60     |
| 1:A:3040:ILE:HG22 | 1:A:3042:VAL:HG13 | 1.82        | 0.60     |
| 1:B:4060:GLU:O    | 1:B:4064:VAL:HG23 | 2.02        | 0.60     |
| 1:A:1921:VAL:HG23 | 1:A:1922:LEU:CD2  | 2.32        | 0.60     |
| 1:B:3559:ARG:O    | 1:B:3563:LEU:HB2  | 2.02        | 0.60     |
| 1:B:1608:VAL:HG21 | 1:B:1669:MET:HG3  | 1.83        | 0.60     |
| 1:A:3803:LYS:HE3  | 1:A:3810:HIS:NE2  | 2.17        | 0.60     |
| 1:A:3262:ASP:HB2  | 1:A:3670:ARG:HE   | 1.67        | 0.60     |
| 1:A:2439:PHE:H    | 1:A:2495:GLN:HE22 | 1.48        | 0.60     |
| 1:A:2091:LEU:HD22 | 1:A:2095:PHE:CE1  | 2.37        | 0.60     |
| 1:A:1604:VAL:HG11 | 1:A:1670:GLU:HA   | 1.84        | 0.59     |
| 1:A:3969:LEU:HD12 | 1:A:4426:MET:HE2  | 1.82        | 0.59     |
| 1:B:3017:VAL:HG13 | 1:B:3174:GLY:O    | 2.02        | 0.59     |
| 1:A:4004:THR:OG1  | 1:A:4006:PRO:HD3  | 2.01        | 0.59     |
| 1:A:3922:ASN:HD22 | 1:A:3922:ASN:N    | 2.00        | 0.59     |
| 1:B:3671:TYR:HD2  | 1:B:3734:LEU:HA   | 1.67        | 0.59     |
| 1:B:1948:VAL:O    | 1:B:1950:THR:HG23 | 2.02        | 0.59     |
| 1:B:4499:PHE:O    | 1:B:4503:ILE:HB   | 2.01        | 0.59     |
| 1:A:4691:TYR:CD2  | 1:A:4696:ARG:HG2  | 2.36        | 0.59     |
| 1:A:2864:PHE:HB3  | 1:A:2872:TYR:CD2  | 2.38        | 0.59     |
| 1:A:3785:ASN:HD22 | 1:A:3786:PHE:H    | 1.49        | 0.59     |
| 1:B:2494:VAL:HG11 | 1:B:2548:VAL:HB   | 1.84        | 0.59     |
| 1:A:4644:LEU:HD12 | 1:A:4723:ILE:HG12 | 1.85        | 0.59     |
| 1:B:3673:LEU:HD22 | 1:B:3783:PHE:HE1  | 1.66        | 0.59     |
| 1:B:4124:LYS:O    | 1:B:4125:GLU:HG2  | 2.01        | 0.59     |
| 1:A:2273:MET:SD   | 1:A:2408:ILE:HG22 | 2.42        | 0.59     |
| 1:A:4545:ILE:O    | 1:A:4561:LEU:HD21 | 2.02        | 0.59     |
| 1:A:3923:LEU:HD22 | 1:A:3947:ILE:HG12 | 1.83        | 0.59     |
| 1:B:2616:SER:HB3  | 1:B:2627:TRP:CE2  | 2.37        | 0.59     |
| 1:B:4131:PRO:HD2  | 1:B:4232:MET:O    | 2.03        | 0.59     |
| 1:B:4137:VAL:HB   | 1:B:4138:PRO:HD2  | 1.85        | 0.59     |
| 1:B:2377:LEU:O    | 1:B:2384:ARG:HA   | 2.02        | 0.59     |
| 1:A:4715:ASN:O    | 1:A:4719:ARG:HB2  | 2.02        | 0.59     |
| 1:A:3672:PRO:HA   | 1:A:3782:THR:HG23 | 1.84        | 0.59     |
| 1:A:4190:ILE:HB   | 1:A:4197:LEU:HD11 | 1.83        | 0.59     |
| 1:B:2000:CYS:HB3  | 1:B:2031:LEU:HD13 | 1.83        | 0.59     |
| 1:A:4371:PRO:HA   | 1:A:4385:GLU:OE1  | 2.03        | 0.59     |
| 1:B:1612:TRP:O    | 1:B:1616:GLU:HB2  | 2.02        | 0.59     |
| 1:A:3730:LEU:HD11 | 1:A:3762:ILE:CD1  | 2.33        | 0.59     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4157:TYR:OH   | 1:A:4186:LEU:HD22 | 2.03        | 0.59     |
| 1:A:3731:ASN:HB2  | 1:A:3732:PRO:HD3  | 1.84        | 0.59     |
| 1:A:4597:PRO:HB2  | 1:A:4700:LEU:HD21 | 1.85        | 0.59     |
| 1:B:3897:TYR:HE1  | 1:B:3913:LEU:HA   | 1.67        | 0.59     |
| 1:B:3024:VAL:HG11 | 2:B:9010:ADP:H3'  | 1.83        | 0.59     |
| 1:A:2528:PHE:CE1  | 1:A:2533:VAL:HG11 | 2.38        | 0.59     |
| 1:B:3809:THR:HG21 | 1:B:3882:VAL:HG11 | 1.84        | 0.59     |
| 1:B:4273:LEU:HD13 | 1:B:4363:LEU:O    | 2.02        | 0.59     |
| 1:A:2293:ILE:HG22 | 1:A:2350:ARG:NH2  | 2.12        | 0.59     |
| 1:A:2938:PHE:HB3  | 1:A:2941:VAL:CG2  | 2.33        | 0.59     |
| 1:A:3924:LEU:HD23 | 1:A:3943:LEU:CD2  | 2.32        | 0.59     |
| 1:A:2648:ILE:HG21 | 1:A:2827:ILE:HA   | 1.84        | 0.59     |
| 1:B:1625:ILE:HD12 | 1:B:1628:LEU:HB2  | 1.83        | 0.59     |
| 1:A:3951:THR:O    | 1:A:3955:VAL:HG23 | 2.02        | 0.59     |
| 1:B:2863:ARG:O    | 1:B:2863:ARG:HD3  | 2.02        | 0.59     |
| 1:A:4494:PRO:HD3  | 1:A:4610:GLN:HE22 | 1.67        | 0.59     |
| 1:A:3190:ARG:HA   | 1:A:3224:ARG:HH12 | 1.66        | 0.59     |
| 1:B:1546:VAL:HG22 | 1:B:1556:ARG:CZ   | 2.33        | 0.59     |
| 1:B:4207:LEU:O    | 1:B:4209:PRO:HD3  | 2.02        | 0.59     |
| 1:B:4424:ARG:NH2  | 1:B:4558:THR:HG21 | 2.17        | 0.59     |
| 1:B:2598:GLN:HG2  | 1:B:2612:LEU:HD23 | 1.85        | 0.59     |
| 1:B:4332:ILE:O    | 1:B:4336:THR:HG23 | 2.02        | 0.59     |
| 1:A:2863:ARG:HD2  | 1:A:2864:PHE:CE1  | 2.36        | 0.59     |
| 1:B:1477:LYS:H    | 1:B:1480:HIS:HD2  | 1.50        | 0.59     |
| 1:A:3313:LEU:HD13 | 1:A:3550:SER:OG   | 2.03        | 0.59     |
| 1:A:4136:SER:O    | 1:A:4221:ILE:HD12 | 2.03        | 0.59     |
| 1:B:2273:MET:HG2  | 1:B:2395:PHE:HB2  | 1.84        | 0.59     |
| 1:A:1978:THR:CG2  | 1:A:2103:PRO:HD3  | 2.33        | 0.59     |
| 1:A:4572:MET:HA   | 1:A:4575:LEU:HD13 | 1.85        | 0.59     |
| 1:B:3788:VAL:HG11 | 1:B:3913:LEU:HD22 | 1.85        | 0.59     |
| 1:A:2991:PHE:HE1  | 1:A:2993:GLU:HB2  | 1.67        | 0.59     |
| 1:A:2598:GLN:CG   | 1:A:2612:LEU:HB2  | 2.33        | 0.59     |
| 1:A:1538:TRP:HZ3  | 1:A:1656:ILE:HD13 | 1.68        | 0.59     |
| 1:B:4109:ASP:HA   | 1:B:4112:ASN:HD22 | 1.67        | 0.58     |
| 1:B:3233:TYR:CD2  | 1:B:3620:ARG:HG3  | 2.38        | 0.58     |
| 1:A:1763:GLY:N    | 1:A:1764:PRO:CD   | 2.65        | 0.58     |
| 1:A:4066:GLN:NE2  | 1:A:4081:ARG:HD3  | 2.18        | 0.58     |
| 1:A:2278:SER:HA   | 1:A:2806:ARG:HH11 | 1.68        | 0.58     |
| 1:A:1973:PHE:CE1  | 1:A:2099:ALA:HA   | 2.38        | 0.58     |
| 1:A:1797:VAL:CG1  | 1:A:1855:ILE:HD11 | 2.33        | 0.58     |
| 1:B:4351:PHE:CD2  | 1:B:4689:PRO:HG3  | 2.38        | 0.58     |
| 1:B:2375:LYS:HB3  | 1:B:2387:LEU:HB3  | 1.84        | 0.58     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1735:ASP:OD2  | 1:A:1737:GLU:HB2  | 2.03        | 0.58     |
| 1:B:4349:ASN:HB3  | 1:B:4352:ASP:OD2  | 2.03        | 0.58     |
| 1:A:4193:ALA:O    | 1:A:4197:LEU:HD23 | 2.03        | 0.58     |
| 1:B:3027:ARG:HG2  | 1:B:3037:ILE:HD12 | 1.85        | 0.58     |
| 1:A:3723:VAL:HG12 | 1:A:3766:THR:OG1  | 2.03        | 0.58     |
| 1:B:4030:PHE:HD1  | 1:B:4033:LEU:HD22 | 1.68        | 0.58     |
| 1:A:3331:GLN:NE2  | 1:A:3533:LYS:HG3  | 2.18        | 0.58     |
| 1:B:3170:LEU:HD21 | 1:B:3172:TRP:HE3  | 1.67        | 0.58     |
| 1:A:2043:ILE:HG23 | 1:A:2073:ILE:HD12 | 1.84        | 0.58     |
| 1:A:4251:THR:HG23 | 1:A:4303:LEU:CD2  | 2.30        | 0.58     |
| 1:A:4349:ASN:HD22 | 1:A:4352:ASP:H    | 1.51        | 0.58     |
| 1:B:1901:ASN:HD22 | 1:B:1901:ASN:N    | 2.01        | 0.58     |
| 1:A:3830:LEU:HB3  | 1:A:3858:LEU:HD13 | 1.86        | 0.58     |
| 1:B:3182:PHE:O    | 1:B:3186:SER:HB2  | 2.03        | 0.58     |
| 1:B:2166:CYS:HA   | 1:B:2190:TYR:OH   | 2.03        | 0.58     |
| 1:A:2153:LYS:O    | 1:A:2157:VAL:HG23 | 2.03        | 0.58     |
| 1:A:4368:ALA:HA   | 1:A:4373:PHE:CE1  | 2.38        | 0.58     |
| 1:A:4003:GLU:HG3  | 1:B:2842:LEU:CD2  | 2.34        | 0.58     |
| 1:B:3620:ARG:HH11 | 1:B:3620:ARG:HG2  | 1.69        | 0.58     |
| 1:B:1884:HIS:O    | 1:B:1888:VAL:HG23 | 2.03        | 0.58     |
| 1:A:3803:LYS:HG3  | 1:A:3810:HIS:CD2  | 2.39        | 0.58     |
| 1:A:4032:LYS:HG3  | 1:A:4069:LEU:HD11 | 1.83        | 0.58     |
| 1:A:2087:LEU:HB2  | 1:A:2092:LYS:HG3  | 1.86        | 0.58     |
| 1:A:2361:PRO:HD3  | 1:A:2402:TYR:O    | 2.03        | 0.58     |
| 1:A:2212:ILE:N    | 1:A:2213:PRO:HD2  | 2.18        | 0.58     |
| 1:B:2338:ARG:HD2  | 1:B:2346:GLU:OE1  | 2.04        | 0.58     |
| 1:B:1821:ILE:HG21 | 1:B:1914:TYR:HB2  | 1.85        | 0.58     |
| 1:A:1950:THR:HB   | 1:A:1951:PRO:HD2  | 1.84        | 0.58     |
| 1:A:1849:GLU:HG3  | 1:A:1893:GLN:OE1  | 2.03        | 0.58     |
| 1:B:1719:GLN:HA   | 1:B:1722:PHE:CE2  | 2.38        | 0.58     |
| 1:B:4388:THR:HG23 | 1:B:4391:HIS:HD2  | 1.68        | 0.58     |
| 1:B:2997:HIS:O    | 1:B:3001:ILE:HG13 | 2.03        | 0.58     |
| 1:B:3013:LEU:HD22 | 1:B:3164:LEU:HD12 | 1.85        | 0.58     |
| 1:A:4572:MET:HA   | 1:A:4575:LEU:CD1  | 2.34        | 0.58     |
| 1:B:1855:ILE:HG22 | 1:B:1859:LEU:HD12 | 1.85        | 0.58     |
| 1:B:3923:LEU:HD22 | 1:B:3947:ILE:HG23 | 1.85        | 0.58     |
| 1:A:3615:ARG:O    | 1:A:3619:ILE:HG13 | 2.03        | 0.58     |
| 1:B:1748:GLU:HB3  | 1:B:1943:ILE:HD12 | 1.85        | 0.58     |
| 1:A:1863:VAL:HG21 | 1:A:2115:SER:O    | 2.04        | 0.58     |
| 1:A:2135:CYS:HB3  | 1:A:2147:PHE:CZ   | 2.38        | 0.58     |
| 1:B:1926:VAL:HG12 | 1:B:1928:HIS:CD2  | 2.39        | 0.58     |
| 1:B:3192:LEU:HD11 | 1:B:3268:VAL:HA   | 1.84        | 0.58     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1995:VAL:HA   | 1:A:2022:TRP:HB2  | 1.84        | 0.58     |
| 1:B:1643:PHE:CE2  | 1:B:1647:LEU:HD11 | 2.39        | 0.58     |
| 1:B:4648:VAL:HA   | 1:B:4662:THR:HG21 | 1.85        | 0.58     |
| 1:B:3263:PHE:O    | 1:B:3267:VAL:HG23 | 2.03        | 0.58     |
| 1:A:3337:LYS:HA   | 1:A:3341:ALA:HB3  | 1.86        | 0.57     |
| 1:A:2838:LEU:O    | 1:A:2839:LEU:HD23 | 2.04        | 0.57     |
| 1:B:1813:GLN:NE2  | 1:B:1941:LEU:H    | 2.02        | 0.57     |
| 1:B:1939:GLU:O    | 1:B:1941:LEU:HG   | 2.03        | 0.57     |
| 1:B:3785:ASN:HD21 | 1:B:3787:THR:CG2  | 2.16        | 0.57     |
| 1:A:3255:VAL:O    | 1:A:3255:VAL:HG13 | 2.03        | 0.57     |
| 1:A:3595:ALA:HB1  | 1:A:3638:LEU:HD11 | 1.85        | 0.57     |
| 1:B:2863:ARG:HG3  | 1:B:2925:TRP:CE2  | 2.39        | 0.57     |
| 1:A:4559:ILE:HG23 | 1:A:4559:ILE:O    | 2.04        | 0.57     |
| 1:B:1554:LEU:HD22 | 1:B:1609:GLN:OE1  | 2.03        | 0.57     |
| 1:B:4189:ASN:ND2  | 1:B:4189:ASN:N    | 2.53        | 0.57     |
| 1:A:3487:TYR:O    | 1:A:3490:ILE:HG12 | 2.04        | 0.57     |
| 1:A:1982:GLU:HG3  | 2:A:9001:ADP:H3'  | 1.86        | 0.57     |
| 1:A:3274:LYS:O    | 1:A:3278:LEU:HD23 | 2.04        | 0.57     |
| 1:A:4284:ARG:HG3  | 1:A:4408:LEU:HB3  | 1.86        | 0.57     |
| 1:B:3674:VAL:HG13 | 1:B:3786:PHE:HD2  | 1.68        | 0.57     |
| 1:B:2869:GLN:HB2  | 1:B:2872:TYR:CD2  | 2.39        | 0.57     |
| 1:B:3897:TYR:CE1  | 1:B:3913:LEU:HA   | 2.38        | 0.57     |
| 1:B:4255:ILE:HD11 | 1:B:4307:LEU:HD11 | 1.85        | 0.57     |
| 1:A:2739:LEU:HD23 | 1:A:2740:VAL:N    | 2.19        | 0.57     |
| 1:A:3668:PHE:CD1  | 1:A:3672:PRO:HD3  | 2.39        | 0.57     |
| 1:B:2533:VAL:HB   | 1:B:2581:LEU:CD2  | 2.30        | 0.57     |
| 1:A:2839:LEU:HD11 | 1:A:2890:ILE:HD12 | 1.85        | 0.57     |
| 1:A:2560:MET:HG3  | 1:A:2561:SER:N    | 2.16        | 0.57     |
| 1:B:1888:VAL:O    | 1:B:1892:LEU:HD12 | 2.04        | 0.57     |
| 1:A:4277:PHE:HB2  | 1:A:4363:LEU:CD1  | 2.34        | 0.57     |
| 1:B:2578:MET:HE1  | 1:B:2612:LEU:HD12 | 1.86        | 0.57     |
| 1:B:1889:VAL:HA   | 1:B:1892:LEU:HD13 | 1.86        | 0.57     |
| 1:B:1687:LEU:HD21 | 1:B:1706:LEU:CD2  | 2.33        | 0.57     |
| 1:B:2235:GLN:HE22 | 1:B:2296:VAL:HG13 | 1.68        | 0.57     |
| 1:B:2219:LEU:CD1  | 1:B:2228:LEU:HD11 | 2.35        | 0.57     |
| 1:A:3909:TYR:OH   | 1:A:3960:LEU:HG   | 2.04        | 0.57     |
| 1:B:2417:SER:O    | 1:B:2420:ILE:HG12 | 2.03        | 0.57     |
| 1:A:4313:TRP:HB3  | 1:A:4330:PRO:HG2  | 1.86        | 0.57     |
| 1:B:4379:ILE:O    | 1:B:4379:ILE:HG13 | 2.05        | 0.57     |
| 1:B:2841:ASN:HD22 | 1:B:2842:LEU:N    | 2.02        | 0.57     |
| 1:A:2195:LEU:O    | 1:A:2199:ILE:HG12 | 2.04        | 0.57     |
| 1:B:3638:LEU:HD12 | 1:B:3663:ILE:HG21 | 1.86        | 0.57     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2053:ASN:O    | 1:A:2054:SER:C    | 2.42        | 0.57     |
| 1:A:2252:LYS:O    | 1:A:2256:VAL:HG23 | 2.05        | 0.57     |
| 1:B:4318:SER:HB3  | 1:B:4324:ILE:HD11 | 1.85        | 0.57     |
| 1:A:3863:THR:O    | 1:A:3867:LEU:HB3  | 2.04        | 0.57     |
| 1:B:2835:LEU:HD11 | 1:B:2890:ILE:HD12 | 1.85        | 0.57     |
| 1:A:2873:ILE:HD12 | 1:A:2873:ILE:H    | 1.68        | 0.57     |
| 1:A:4288:ILE:HG23 | 1:A:4292:TRP:O    | 2.04        | 0.57     |
| 1:A:2616:SER:HB3  | 1:A:2627:TRP:CE2  | 2.40        | 0.57     |
| 1:B:2270:HIS:HA   | 1:B:2392:ARG:HH11 | 1.70        | 0.57     |
| 1:B:1591:TRP:O    | 1:B:1595:LEU:HB2  | 2.05        | 0.57     |
| 1:A:4245:LYS:HD2  | 1:A:4399:LEU:O    | 2.04        | 0.57     |
| 1:B:3238:ILE:HG12 | 1:B:3601:TYR:CD2  | 2.40        | 0.57     |
| 1:B:2540:LEU:HD12 | 1:B:2662:ALA:HB3  | 1.85        | 0.57     |
| 1:A:1718:ILE:HG22 | 1:A:1722:PHE:CE2  | 2.40        | 0.57     |
| 1:B:3793:LEU:HD23 | 1:B:3894:SER:HA   | 1.86        | 0.57     |
| 1:B:2586:GLY:HA2  | 1:B:2815:LEU:CD1  | 2.34        | 0.57     |
| 1:A:4050:LYS:O    | 1:A:4051:ASP:C    | 2.42        | 0.57     |
| 1:A:1978:THR:HG22 | 1:A:2103:PRO:HD3  | 1.87        | 0.57     |
| 1:B:3912:SER:HB3  | 1:B:4231:ARG:HG2  | 1.86        | 0.57     |
| 1:B:4313:TRP:HB3  | 1:B:4330:PRO:HG2  | 1.87        | 0.57     |
| 1:A:1681:LYS:O    | 1:A:1685:GLU:HG3  | 2.04        | 0.57     |
| 1:A:4415:GLU:OE2  | 1:A:4415:GLU:HA   | 2.05        | 0.57     |
| 1:A:4375:LEU:HD11 | 1:A:4383:VAL:CG2  | 2.30        | 0.56     |
| 1:A:4132:LEU:HD23 | 1:A:4236:PHE:HE2  | 1.70        | 0.56     |
| 1:B:3274:LYS:HE3  | 1:B:3637:PHE:CE2  | 2.39        | 0.56     |
| 1:A:3266:GLN:HE21 | 1:A:3270:LEU:CD2  | 2.18        | 0.56     |
| 1:B:4043:ASP:HB3  | 1:B:4059:PRO:HB3  | 1.87        | 0.56     |
| 1:A:3291:LYS:HG3  | 1:A:3835:LEU:HD22 | 1.86        | 0.56     |
| 1:B:1537:PHE:O    | 1:B:1541:LEU:HB2  | 2.05        | 0.56     |
| 1:A:2989:VAL:HG13 | 1:A:3187:GLU:CD   | 2.25        | 0.56     |
| 1:A:3439:ASP:HB3  | 1:A:3442:LYS:HG2  | 1.87        | 0.56     |
| 1:B:4543:LYS:HD2  | 1:B:4545:ILE:HD13 | 1.87        | 0.56     |
| 1:B:3614:MET:O    | 1:B:3618:MET:HG3  | 2.04        | 0.56     |
| 1:A:3571:ARG:HB3  | 1:A:3571:ARG:HH11 | 1.69        | 0.56     |
| 1:A:2121:ALA:O    | 1:A:2122:GLU:C    | 2.43        | 0.56     |
| 1:A:1978:THR:HG21 | 1:A:2101:ILE:O    | 2.05        | 0.56     |
| 1:A:4132:LEU:HD13 | 1:A:4216:PHE:CE1  | 2.40        | 0.56     |
| 1:A:4432:LYS:C    | 1:A:4434:GLN:H    | 2.08        | 0.56     |
| 1:A:1927:ILE:HD13 | 1:A:1991:LEU:CD2  | 2.35        | 0.56     |
| 1:B:4618:ASN:N    | 1:B:4618:ASN:HD22 | 2.02        | 0.56     |
| 1:B:1554:LEU:HB3  | 1:B:1609:GLN:NE2  | 2.09        | 0.56     |
| 1:A:3813:ARG:HB2  | 1:A:3813:ARG:CZ   | 2.34        | 0.56     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3813:ARG:HB3  | 1:A:3879:ILE:HD11 | 1.88        | 0.56     |
| 1:A:2560:MET:CE   | 1:A:2564:ASN:HD22 | 2.18        | 0.56     |
| 1:A:2675:PRO:HG2  | 1:A:2678:SER:HB3  | 1.88        | 0.56     |
| 1:A:3299:VAL:HG21 | 1:A:3563:LEU:HD23 | 1.87        | 0.56     |
| 1:A:3567:LEU:CD2  | 1:A:3855:LEU:HD11 | 2.36        | 0.56     |
| 1:A:3195:GLU:OE1  | 1:A:3224:ARG:HB2  | 2.04        | 0.56     |
| 1:A:2979:PHE:HE2  | 1:A:3028:PHE:HA   | 1.70        | 0.56     |
| 1:B:3893:CYS:SG   | 1:B:3947:ILE:HG21 | 2.44        | 0.56     |
| 1:B:1531:LEU:HD13 | 1:B:1587:GLU:OE2  | 2.05        | 0.56     |
| 1:B:1956:CYS:SG   | 1:B:1983:THR:HG21 | 2.45        | 0.56     |
| 1:A:3598:PHE:HA   | 1:A:3602:ILE:HG12 | 1.88        | 0.56     |
| 1:A:3682:MET:SD   | 1:A:3696:LYS:HE2  | 2.46        | 0.56     |
| 1:A:3584:GLN:O    | 1:A:3588:VAL:HG23 | 2.06        | 0.56     |
| 1:A:4277:PHE:O    | 1:A:4281:ILE:HG12 | 2.06        | 0.56     |
| 1:A:2806:ARG:HH12 | 2:A:9002:ADP:PB   | 2.28        | 0.56     |
| 1:B:4213:PHE:CZ   | 1:B:4215:LEU:HB2  | 2.40        | 0.56     |
| 1:B:2660:LEU:HD21 | 1:B:2672:LEU:HD21 | 1.87        | 0.56     |
| 1:A:2229:GLN:HB3  | 1:A:2230:PRO:HD2  | 1.86        | 0.56     |
| 1:A:1752:VAL:HG22 | 1:A:1811:PRO:HG3  | 1.86        | 0.56     |
| 1:B:2144:HIS:HB3  | 1:B:2400:LEU:HD12 | 1.86        | 0.56     |
| 1:B:2739:LEU:HB3  | 1:B:2786:ILE:HG12 | 1.87        | 0.56     |
| 1:A:1947:LEU:HD11 | 1:A:1982:GLU:HB3  | 1.87        | 0.56     |
| 1:A:4117:ASP:OD1  | 1:A:4119:ALA:HB3  | 2.06        | 0.56     |
| 1:A:2087:LEU:O    | 1:A:2092:LYS:HD2  | 2.06        | 0.56     |
| 1:B:2841:ASN:N    | 1:B:2841:ASN:ND2  | 2.54        | 0.56     |
| 1:A:4534:LEU:HA   | 1:A:4537:LEU:HD12 | 1.88        | 0.56     |
| 1:A:2284:THR:O    | 1:A:2288:VAL:HG23 | 2.06        | 0.56     |
| 1:A:1948:VAL:O    | 1:A:1950:THR:HG23 | 2.06        | 0.56     |
| 1:B:2670:LEU:HD11 | 1:B:2789:VAL:HG13 | 1.88        | 0.56     |
| 1:B:2560:MET:HG3  | 1:B:2564:ASN:HB2  | 1.88        | 0.56     |
| 1:B:2841:ASN:ND2  | 1:B:2842:LEU:N    | 2.52        | 0.56     |
| 1:A:3445:THR:HA   | 1:A:3449:ARG:HD3  | 1.87        | 0.56     |
| 1:A:2954:ASN:N    | 1:A:2954:ASN:ND2  | 2.53        | 0.56     |
| 1:B:3043:ASN:H    | 1:B:3043:ASN:HD22 | 1.54        | 0.56     |
| 1:A:3848:ASP:HB3  | 1:A:3851:VAL:HG12 | 1.88        | 0.56     |
| 1:B:3758:PRO:HG2  | 1:B:3759:SER:H    | 1.71        | 0.56     |
| 1:A:3887:ASN:HB3  | 1:A:3888:PRO:HD3  | 1.88        | 0.56     |
| 1:A:2906:ALA:O    | 1:A:2910:LEU:HG   | 2.05        | 0.56     |
| 1:A:3813:ARG:HH22 | 1:A:3817:LEU:CD1  | 2.18        | 0.56     |
| 1:A:2748:LEU:N    | 1:A:2749:PRO:CD   | 2.69        | 0.56     |
| 1:A:4622:HIS:HE2  | 1:A:4678:ILE:CG2  | 2.16        | 0.56     |
| 1:A:2941:VAL:HG12 | 1:A:2942:ASN:N    | 2.20        | 0.56     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3376:ALA:O    | 1:A:3380:VAL:HG23 | 2.06        | 0.56     |
| 1:B:2081:TYR:O    | 1:B:2084:ARG:HD2  | 2.06        | 0.56     |
| 1:A:1687:LEU:HD21 | 1:A:1706:LEU:HD23 | 1.88        | 0.56     |
| 1:B:2163:LYS:HB2  | 1:B:2194:VAL:HG11 | 1.87        | 0.56     |
| 1:B:1479:ARG:CZ   | 1:B:1479:ARG:HB2  | 2.35        | 0.56     |
| 1:A:1862:SER:O    | 1:A:1865:GLN:HG2  | 2.06        | 0.56     |
| 1:A:3404:ALA:HA   | 1:A:3462:PHE:HE1  | 1.71        | 0.56     |
| 1:B:2276:GLY:O    | 1:B:2398:GLN:HA   | 2.06        | 0.56     |
| 1:A:4589:VAL:HG12 | 1:A:4639:VAL:HA   | 1.88        | 0.56     |
| 1:A:2381:ASN:OD1  | 1:A:2383:GLU:HB2  | 2.06        | 0.56     |
| 1:B:3729:VAL:O    | 1:B:3729:VAL:HG22 | 2.05        | 0.56     |
| 1:B:4535:ARG:HG2  | 1:B:4535:ARG:HH11 | 1.71        | 0.55     |
| 1:B:4147:ASP:HA   | 1:B:4157:TYR:OH   | 2.06        | 0.55     |
| 1:A:3292:LEU:HD22 | 1:A:3567:LEU:HD22 | 1.89        | 0.55     |
| 1:B:4389:ARG:HG2  | 1:B:4389:ARG:NH1  | 2.21        | 0.55     |
| 1:A:1957:TYR:O    | 1:A:1961:THR:HG23 | 2.07        | 0.55     |
| 1:B:4190:ILE:HG12 | 1:B:4219:SER:HB2  | 1.86        | 0.55     |
| 1:B:3908:LEU:HD22 | 1:B:4221:ILE:HG23 | 1.87        | 0.55     |
| 1:A:3673:LEU:HD13 | 1:A:3783:PHE:CE1  | 2.40        | 0.55     |
| 1:A:2910:LEU:HD23 | 1:A:2930:ILE:CD1  | 2.33        | 0.55     |
| 1:B:3700:LEU:CD2  | 1:B:3701:ASP:H    | 2.18        | 0.55     |
| 1:B:2829:GLY:HA2  | 1:B:2850:THR:OG1  | 2.06        | 0.55     |
| 1:A:4005:ILE:HG22 | 1:A:4008:LEU:HB2  | 1.87        | 0.55     |
| 1:B:4388:THR:O    | 1:B:4391:HIS:HB2  | 2.07        | 0.55     |
| 1:A:1800:HIS:HB2  | 1:A:1858:ASN:HD22 | 1.71        | 0.55     |
| 1:B:2603:THR:O    | 1:B:2605:VAL:HG13 | 2.06        | 0.55     |
| 1:A:2650:THR:H    | 1:A:2653:THR:HB   | 1.71        | 0.55     |
| 1:A:2615:TYR:HD1  | 1:A:2624:TRP:HB3  | 1.72        | 0.55     |
| 1:A:4590:TRP:CD2  | 1:A:4593:GLY:HA3  | 2.42        | 0.55     |
| 1:A:1926:VAL:HG12 | 1:A:1928:HIS:CD2  | 2.41        | 0.55     |
| 1:A:2991:PHE:CE1  | 1:A:2993:GLU:HB2  | 2.40        | 0.55     |
| 1:A:1699:PHE:HE1  | 1:A:2015:GLY:HA3  | 1.71        | 0.55     |
| 1:B:2440:ASP:OD1  | 1:B:2441:PRO:HD2  | 2.06        | 0.55     |
| 1:B:2101:ILE:O    | 1:B:2103:PRO:HD3  | 2.07        | 0.55     |
| 1:A:3368:LYS:C    | 1:A:3374:ILE:HD11 | 2.26        | 0.55     |
| 1:A:3419:TRP:CE3  | 1:A:3422:ILE:HD11 | 2.42        | 0.55     |
| 1:A:3066:GLU:HG2  | 1:A:3136:GLN:HE21 | 1.71        | 0.55     |
| 1:B:2369:SER:HA   | 1:B:2372:ASP:OD2  | 2.07        | 0.55     |
| 1:A:3555:ASN:HB3  | 1:A:3559:ARG:HH11 | 1.71        | 0.55     |
| 1:A:2606:PRO:HG2  | 1:A:2615:TYR:CE1  | 2.42        | 0.55     |
| 1:A:1625:ILE:HG23 | 1:A:1626:ASN:H    | 1.70        | 0.55     |
| 1:B:2774:ARG:HB2  | 1:B:2781:ILE:CD1  | 2.37        | 0.55     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3930:LEU:HG   | 1:A:3939:ARG:NH1  | 2.21        | 0.55     |
| 1:A:1875:PHE:O    | 1:A:1879:ILE:HG12 | 2.07        | 0.55     |
| 1:A:1763:GLY:H    | 1:A:1764:PRO:CD   | 2.19        | 0.55     |
| 1:A:3471:SER:HB3  | 1:A:3474:CYS:SG   | 2.47        | 0.55     |
| 1:B:1872:ARG:HH12 | 1:B:2164:ARG:HD3  | 1.71        | 0.55     |
| 1:A:4094:VAL:HB   | 1:A:4423:ALA:HB1  | 1.88        | 0.55     |
| 1:A:3991:LEU:O    | 1:A:3991:LEU:HD12 | 2.07        | 0.55     |
| 1:B:1555:VAL:HG23 | 1:B:1609:GLN:HE21 | 1.70        | 0.55     |
| 1:A:2274:MET:CE   | 1:A:2286:TRP:HB3  | 2.30        | 0.55     |
| 1:A:1608:VAL:HG13 | 1:A:1676:LEU:CD1  | 2.37        | 0.55     |
| 1:A:4319:LYS:H    | 1:A:4321:ARG:NH2  | 2.04        | 0.55     |
| 1:B:3018:SER:O    | 1:B:3256:THR:HB   | 2.06        | 0.55     |
| 1:A:3453:THR:O    | 1:A:3458:GLU:HG2  | 2.06        | 0.55     |
| 1:A:2765:GLN:O    | 1:A:2769:LYS:HB2  | 2.07        | 0.55     |
| 1:A:1797:VAL:HG13 | 1:A:1855:ILE:HD11 | 1.89        | 0.55     |
| 1:B:4644:LEU:HG   | 1:B:4664:ILE:HD11 | 1.88        | 0.55     |
| 1:B:4624:SER:HB2  | 1:B:4668:THR:HB   | 1.87        | 0.55     |
| 1:B:3306:LEU:HD22 | 1:B:3553:VAL:HG13 | 1.89        | 0.55     |
| 1:B:4132:LEU:HD13 | 1:B:4216:PHE:CE1  | 2.42        | 0.55     |
| 1:B:4685:LYS:HE2  | 1:B:4706:PRO:HD3  | 1.88        | 0.55     |
| 1:A:2262:LEU:HD11 | 1:A:2274:MET:CE   | 2.37        | 0.55     |
| 1:A:2446:GLN:O    | 1:A:2450:ASN:HB3  | 2.07        | 0.55     |
| 1:A:4571:ARG:O    | 1:A:4574:GLN:HB3  | 2.07        | 0.55     |
| 1:B:2612:LEU:HD11 | 1:B:2624:TRP:CH2  | 2.42        | 0.55     |
| 1:A:3647:TRP:HH2  | 1:A:3663:ILE:HD12 | 1.71        | 0.55     |
| 1:A:2439:PHE:H    | 1:A:2495:GLN:NE2  | 2.05        | 0.55     |
| 1:B:2000:CYS:C    | 1:B:2002:GLU:H    | 2.10        | 0.55     |
| 1:B:2863:ARG:HD2  | 1:B:2864:PHE:CE1  | 2.42        | 0.55     |
| 1:B:2918:VAL:HG13 | 1:B:3172:TRP:NE1  | 2.22        | 0.55     |
| 1:B:2779:THR:O    | 1:B:2781:ILE:HD12 | 2.06        | 0.55     |
| 1:A:1907:LEU:HA   | 1:A:1911:ARG:NH1  | 2.21        | 0.55     |
| 1:B:4095:LEU:HD11 | 1:B:4422:LYS:CB   | 2.37        | 0.55     |
| 1:A:4495:LEU:CD1  | 1:A:4495:LEU:H    | 2.16        | 0.55     |
| 1:B:4024:ARG:HA   | 1:B:4030:PHE:O    | 2.07        | 0.55     |
| 1:A:3965:LEU:HG   | 1:A:4426:MET:CE   | 2.37        | 0.55     |
| 1:A:3373:ILE:CD1  | 1:A:3373:ILE:H    | 2.06        | 0.54     |
| 1:A:3253:ASN:HB2  | 1:A:3604:PHE:CE2  | 2.42        | 0.54     |
| 1:B:2898:LEU:O    | 1:B:2902:VAL:HG23 | 2.06        | 0.54     |
| 1:A:2648:ILE:HD13 | 1:A:2831:PHE:CZ   | 2.42        | 0.54     |
| 1:B:4101:PHE:O    | 1:B:4105:VAL:HG23 | 2.07        | 0.54     |
| 1:A:1755:LYS:HG2  | 1:A:1780:THR:HG23 | 1.89        | 0.54     |
| 1:B:4571:ARG:HD3  | 1:B:4593:GLY:O    | 2.06        | 0.54     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2204:ILE:N    | 1:A:2205:PRO:CD   | 2.69        | 0.54     |
| 1:A:2275:VAL:HG13 | 1:A:2415:TRP:CE3  | 2.42        | 0.54     |
| 1:A:2196:LEU:HD21 | 1:A:2219:LEU:HD22 | 1.89        | 0.54     |
| 1:A:1908:TYR:CE1  | 1:A:1958:LEU:HD13 | 2.42        | 0.54     |
| 1:B:3652:LEU:HB2  | 1:B:3684:PHE:CD1  | 2.43        | 0.54     |
| 1:A:3266:GLN:HE21 | 1:A:3270:LEU:HD21 | 1.71        | 0.54     |
| 1:B:1694:PHE:CE1  | 1:B:1770:LEU:HD13 | 2.42        | 0.54     |
| 1:B:2832:ASN:HA   | 1:B:2835:LEU:HB3  | 1.89        | 0.54     |
| 1:A:3390:GLU:O    | 1:A:3394:LEU:HG   | 2.07        | 0.54     |
| 1:A:4413:ASN:ND2  | 1:A:4660:LEU:HG   | 2.22        | 0.54     |
| 1:A:3647:TRP:HB3  | 1:A:3652:LEU:CD2  | 2.37        | 0.54     |
| 1:A:2431:LEU:HD11 | 1:A:2506:PHE:CD2  | 2.42        | 0.54     |
| 1:A:1890:ARG:O    | 1:A:1894:LYS:HG3  | 2.07        | 0.54     |
| 1:B:2200:ASN:HA   | 1:B:2204:ILE:HG12 | 1.89        | 0.54     |
| 1:A:3830:LEU:HB3  | 1:A:3858:LEU:CD1  | 2.37        | 0.54     |
| 1:B:2968:LEU:O    | 1:B:2972:VAL:HG23 | 2.07        | 0.54     |
| 1:A:4319:LYS:N    | 1:A:4321:ARG:NH2  | 2.55        | 0.54     |
| 1:B:4013:SER:H    | 1:B:4016:GLN:HE21 | 1.54        | 0.54     |
| 1:B:2331:LEU:HD21 | 1:B:2773:TRP:CD1  | 2.43        | 0.54     |
| 1:B:2283:THR:HA   | 1:B:2286:TRP:NE1  | 2.22        | 0.54     |
| 1:A:3086:ARG:HH11 | 1:A:3096:VAL:CG1  | 2.20        | 0.54     |
| 1:B:1548:TYR:CD1  | 1:B:1549:GLN:HG2  | 2.43        | 0.54     |
| 1:B:1655:LEU:HD22 | 1:B:1655:LEU:H    | 1.72        | 0.54     |
| 1:A:3700:LEU:CG   | 1:A:3701:ASP:H    | 2.20        | 0.54     |
| 1:B:4323:ASN:ND2  | 1:B:4323:ASN:N    | 2.54        | 0.54     |
| 1:A:4121:ILE:O    | 1:A:4126:VAL:HG12 | 2.06        | 0.54     |
| 1:A:4553:TYR:CD1  | 1:A:4553:TYR:N    | 2.75        | 0.54     |
| 1:B:2498:CYS:SG   | 1:B:2569:ILE:HG13 | 2.47        | 0.54     |
| 1:B:2803:LEU:HD12 | 1:B:2808:LEU:HD21 | 1.90        | 0.54     |
| 1:B:2990:LEU:HD23 | 1:B:2994:VAL:HG11 | 1.90        | 0.54     |
| 1:A:1691:ARG:HD3  | 1:A:1698:TYR:CD1  | 2.41        | 0.54     |
| 1:A:3336:ILE:O    | 1:A:3340:ASP:HB3  | 2.08        | 0.54     |
| 1:B:2024:CYS:HA   | 1:B:2074:PHE:O    | 2.06        | 0.54     |
| 1:A:3602:ILE:O    | 1:A:3604:PHE:N    | 2.40        | 0.54     |
| 1:B:2603:THR:CG2  | 1:B:2604:PRO:HD2  | 2.31        | 0.54     |
| 1:A:2766:MET:HB3  | 1:A:2783:LEU:CD1  | 2.36        | 0.54     |
| 1:A:4122:VAL:HG23 | 1:A:4214:ARG:HD2  | 1.89        | 0.54     |
| 1:A:2014:VAL:HG22 | 1:A:2065:ILE:HD13 | 1.90        | 0.54     |
| 1:B:2874:TYR:OH   | 1:B:2916:ARG:HD2  | 2.08        | 0.54     |
| 1:A:1951:PRO:HG2  | 1:A:2104:ASP:OD1  | 2.08        | 0.54     |
| 1:B:1782:ALA:HA   | 1:B:1938:PHE:CE1  | 2.42        | 0.54     |
| 1:B:2516:LEU:HD12 | 1:B:2581:LEU:HD13 | 1.90        | 0.54     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2519:ALA:HB2  | 1:B:2593:PHE:CZ   | 2.43        | 0.54     |
| 1:A:2121:ALA:O    | 1:A:2124:LEU:N    | 2.41        | 0.54     |
| 1:B:4080:PHE:HB2  | 1:B:4101:PHE:CE1  | 2.43        | 0.54     |
| 1:A:4254:GLY:O    | 1:A:4256:PRO:HD3  | 2.07        | 0.54     |
| 1:A:3423:ARG:O    | 1:A:3426:ILE:HG22 | 2.07        | 0.54     |
| 1:A:4348:ASP:OD2  | 1:A:4349:ASN:N    | 2.40        | 0.54     |
| 1:B:2641:VAL:HG12 | 1:B:2642:ALA:N    | 2.23        | 0.54     |
| 1:A:2031:LEU:HD23 | 1:A:2035:ILE:HG22 | 1.89        | 0.54     |
| 1:A:3399:THR:N    | 1:A:3400:PRO:HD2  | 2.23        | 0.54     |
| 1:B:4058:ILE:HD12 | 1:B:4082:LYS:HG2  | 1.89        | 0.54     |
| 1:A:2751:THR:HB   | 1:A:2755:GLY:HA2  | 1.90        | 0.54     |
| 1:A:3263:PHE:O    | 1:A:3267:VAL:HG23 | 2.07        | 0.54     |
| 1:A:4013:SER:H    | 1:A:4016:GLN:HB3  | 1.73        | 0.54     |
| 1:A:2266:LEU:HD21 | 1:A:2394:MET:HE3  | 1.89        | 0.54     |
| 1:A:2447:GLN:HE22 | 1:A:2492:LEU:CD2  | 2.21        | 0.54     |
| 1:B:4336:THR:O    | 1:B:4340:SER:HB3  | 2.08        | 0.54     |
| 1:A:4547:PRO:HB2  | 1:A:4550:TRP:CE3  | 2.43        | 0.54     |
| 1:B:1975:PRO:HD2  | 1:B:2100:MET:O    | 2.07        | 0.54     |
| 1:B:2636:VAL:HG21 | 1:B:2648:ILE:HD11 | 1.89        | 0.54     |
| 1:B:1982:GLU:HA   | 1:B:1982:GLU:OE1  | 2.08        | 0.54     |
| 1:A:1724:LYS:HD3  | 1:A:2382:GLY:O    | 2.07        | 0.54     |
| 1:B:2929:LYS:O    | 1:B:2933:VAL:HG23 | 2.07        | 0.54     |
| 1:B:2500:ALA:HA   | 1:B:2503:SER:OG   | 2.08        | 0.54     |
| 1:A:3043:ASN:HD22 | 1:A:3043:ASN:N    | 2.05        | 0.54     |
| 1:A:3373:ILE:HD13 | 1:A:3373:ILE:N    | 2.12        | 0.54     |
| 1:B:3677:PRO:CD   | 1:B:3787:THR:HG22 | 2.38        | 0.54     |
| 1:B:2653:THR:O    | 1:B:2657:VAL:HG23 | 2.08        | 0.54     |
| 1:A:4318:SER:CA   | 1:A:4321:ARG:HH21 | 2.19        | 0.54     |
| 1:B:3255:VAL:HA   | 1:B:3259:HIS:CD2  | 2.43        | 0.54     |
| 1:A:2128:ILE:HG13 | 1:A:2152:LEU:HD21 | 1.90        | 0.54     |
| 1:B:4257:ALA:HB2  | 1:B:4389:ARG:HD3  | 1.90        | 0.54     |
| 1:A:3760:PHE:CG   | 1:A:3761:MET:N    | 2.75        | 0.54     |
| 1:A:3109:MET:O    | 1:A:3112:CYS:HB2  | 2.08        | 0.54     |
| 1:A:2819:PRO:HD2  | 1:A:2876:PRO:HG2  | 1.89        | 0.54     |
| 1:A:1822:VAL:HG12 | 1:A:1826:GLN:OE1  | 2.07        | 0.54     |
| 1:A:2689:ARG:C    | 1:A:2691:PHE:H    | 2.12        | 0.54     |
| 1:A:3827:LEU:O    | 1:A:3831:GLU:HG3  | 2.08        | 0.54     |
| 1:A:2653:THR:O    | 1:A:2657:VAL:HG23 | 2.07        | 0.53     |
| 1:B:4639:VAL:O    | 1:B:4666:ILE:HD12 | 2.08        | 0.53     |
| 1:B:1910:MET:CA   | 1:B:1929:MET:HG3  | 2.39        | 0.53     |
| 1:A:4375:LEU:CD1  | 1:A:4383:VAL:HG23 | 2.32        | 0.53     |
| 1:A:3698:SER:HB2  | 1:A:3721:GLN:HB2  | 1.90        | 0.53     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4553:TYR:N    | 1:A:4553:TYR:HD1  | 2.05        | 0.53     |
| 1:B:2863:ARG:HG3  | 1:B:2925:TRP:CZ2  | 2.44        | 0.53     |
| 1:A:3218:ALA:O    | 1:A:3219:ILE:C    | 2.47        | 0.53     |
| 1:B:1581:TYR:O    | 1:B:1585:GLU:HB2  | 2.08        | 0.53     |
| 1:B:1831:LEU:HD13 | 1:B:1900:GLY:O    | 2.07        | 0.53     |
| 1:B:1646:ILE:O    | 1:B:1650:VAL:HG23 | 2.08        | 0.53     |
| 1:A:2969:ARG:HG3  | 1:A:2970:GLU:N    | 2.23        | 0.53     |
| 1:B:3342:ARG:O    | 1:B:3345:GLN:HB3  | 2.07        | 0.53     |
| 1:B:1655:LEU:HB2  | 1:B:1658:GLU:CB   | 2.31        | 0.53     |
| 1:A:3418:GLU:O    | 1:A:3422:ILE:HG23 | 2.08        | 0.53     |
| 1:B:1920:ASN:HD22 | 1:B:1921:VAL:N    | 2.06        | 0.53     |
| 1:B:2050:LEU:HG   | 1:B:2067:LEU:HD21 | 1.89        | 0.53     |
| 1:A:2825:THR:O    | 1:A:2829:GLY:HA3  | 2.08        | 0.53     |
| 1:A:4012:LEU:HD12 | 1:A:4012:LEU:N    | 2.23        | 0.53     |
| 1:B:3677:PRO:HG3  | 1:B:3787:THR:HG22 | 1.89        | 0.53     |
| 1:A:1827:VAL:O    | 1:A:1831:LEU:HG   | 2.08        | 0.53     |
| 1:B:3700:LEU:HD13 | 1:B:3701:ASP:H    | 1.71        | 0.53     |
| 1:B:2309:LYS:CE   | 1:B:2756:THR:HG21 | 2.39        | 0.53     |
| 1:A:1803:TYR:HE1  | 1:A:1855:ILE:HD13 | 1.74        | 0.53     |
| 1:B:2118:PHE:CE1  | 1:B:2163:LYS:HG3  | 2.44        | 0.53     |
| 1:A:1699:PHE:HD1  | 1:A:1699:PHE:N    | 2.06        | 0.53     |
| 1:A:4596:ASN:C    | 1:A:4596:ASN:HD22 | 2.11        | 0.53     |
| 1:A:4376:VAL:HG12 | 1:A:4379:ILE:HG22 | 1.90        | 0.53     |
| 1:B:4671:TRP:C    | 1:B:4672:LYS:HG2  | 2.29        | 0.53     |
| 1:A:2704:ALA:O    | 1:A:2706:THR:HG23 | 2.08        | 0.53     |
| 1:A:2994:VAL:O    | 1:A:2998:ILE:HG12 | 2.08        | 0.53     |
| 1:A:1650:VAL:HG13 | 1:A:1659:VAL:HG11 | 1.91        | 0.53     |
| 1:A:2274:MET:HE1  | 1:A:2286:TRP:HD1  | 1.73        | 0.53     |
| 1:B:2540:LEU:HD12 | 1:B:2662:ALA:CB   | 2.39        | 0.53     |
| 1:B:3109:MET:O    | 1:B:3129:LEU:HD21 | 2.09        | 0.53     |
| 1:A:2341:ASP:O    | 1:A:2343:VAL:N    | 2.40        | 0.53     |
| 1:B:4098:SER:O    | 1:B:4102:VAL:HG23 | 2.09        | 0.53     |
| 1:A:2016:LEU:HD21 | 1:A:2023:GLY:HA3  | 1.89        | 0.53     |
| 1:B:3067:GLU:O    | 1:B:3069:ILE:HG13 | 2.08        | 0.53     |
| 1:B:2515:VAL:HG11 | 1:B:2577:LEU:HD13 | 1.90        | 0.53     |
| 1:A:2397:VAL:HG21 | 1:A:2400:LEU:CD2  | 2.38        | 0.53     |
| 1:A:1709:ILE:HA   | 1:A:1766:ILE:HG12 | 1.90        | 0.53     |
| 1:A:2745:GLU:HB3  | 1:A:2748:LEU:HD12 | 1.91        | 0.53     |
| 1:A:2863:ARG:HD3  | 1:A:2863:ARG:C    | 2.29        | 0.53     |
| 1:B:1948:VAL:O    | 1:B:1950:THR:N    | 2.41        | 0.53     |
| 1:A:1820:GLN:HB3  | 1:A:1912:TYR:CD2  | 2.44        | 0.53     |
| 1:B:4260:MET:HG3  | 1:B:4271:TYR:CD1  | 2.43        | 0.53     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:4693:ASN:ND2  | 1:B:4693:ASN:H    | 2.06        | 0.53     |
| 1:B:4278:HIS:CD2  | 1:B:4303:LEU:HB2  | 2.44        | 0.53     |
| 1:A:2274:MET:HE1  | 1:A:2286:TRP:CD1  | 2.44        | 0.53     |
| 1:A:2548:VAL:HG11 | 1:A:2565:GLN:HE21 | 1.73        | 0.53     |
| 1:A:3700:LEU:HD13 | 1:A:3701:ASP:H    | 1.73        | 0.53     |
| 1:B:1558:TRP:CZ3  | 1:B:1606:ILE:HB   | 2.44        | 0.53     |
| 1:B:1541:LEU:HD23 | 1:B:1656:ILE:HG21 | 1.91        | 0.53     |
| 1:A:4036:HIS:HD2  | 1:A:4044:TRP:HE1  | 1.56        | 0.53     |
| 1:B:4597:PRO:HG2  | 1:B:4692:LEU:HD13 | 1.90        | 0.53     |
| 1:B:1932:ALA:HB1  | 1:B:1934:PHE:CE2  | 2.44        | 0.53     |
| 1:A:2701:PHE:CG   | 1:A:2705:THR:HG21 | 2.43        | 0.53     |
| 1:A:4207:LEU:O    | 1:A:4209:PRO:HD3  | 2.08        | 0.53     |
| 1:B:2497:GLU:O    | 1:B:2501:ILE:HG13 | 2.08        | 0.53     |
| 1:B:2280:GLY:O    | 1:B:2420:ILE:HD11 | 2.08        | 0.53     |
| 1:A:3821:GLY:O    | 1:A:3825:VAL:HG23 | 2.08        | 0.53     |
| 1:A:2142:GLN:HE21 | 1:A:2208:VAL:HG11 | 1.75        | 0.53     |
| 1:A:2359:VAL:CG2  | 1:A:2397:VAL:HG11 | 2.38        | 0.53     |
| 1:A:4122:VAL:HG22 | 1:A:4122:VAL:O    | 2.08        | 0.53     |
| 1:A:1538:TRP:CH2  | 1:A:1565:LEU:HG   | 2.44        | 0.53     |
| 1:B:1538:TRP:HZ3  | 1:B:1656:ILE:HD13 | 1.73        | 0.53     |
| 1:A:3802:LEU:CD2  | 1:A:3882:VAL:HG12 | 2.39        | 0.53     |
| 1:A:4188:LYS:HA   | 1:A:4218:THR:HB   | 1.90        | 0.53     |
| 1:B:3895:ARG:HH12 | 1:B:3977:LYS:HG2  | 1.73        | 0.53     |
| 1:A:3956:THR:OG1  | 1:A:3964:LYS:HE3  | 2.08        | 0.52     |
| 1:A:2598:GLN:HG2  | 1:A:2612:LEU:HD22 | 1.90        | 0.52     |
| 1:A:3555:ASN:O    | 1:A:3559:ARG:HD3  | 2.09        | 0.52     |
| 1:A:3927:ASN:HB3  | 1:A:3930:LEU:CB   | 2.39        | 0.52     |
| 1:A:2017:CYS:HB3  | 1:A:2067:LEU:HD12 | 1.90        | 0.52     |
| 1:B:2205:PRO:HA   | 1:B:2261:GLN:OE1  | 2.09        | 0.52     |
| 1:B:1525:ILE:HG13 | 1:B:1529:GLU:HG2  | 1.91        | 0.52     |
| 1:B:2704:ALA:HB2  | 1:B:3085:GLU:CD   | 2.29        | 0.52     |
| 1:B:1612:TRP:CZ2  | 1:B:1644:ILE:HD11 | 2.44        | 0.52     |
| 1:B:2818:PHE:HD1  | 1:B:2876:PRO:HD3  | 1.74        | 0.52     |
| 1:A:3776:ASP:O    | 1:A:3780:ARG:HG2  | 2.09        | 0.52     |
| 1:B:2661:HIS:O    | 1:B:2665:SER:HB3  | 2.09        | 0.52     |
| 1:B:1863:VAL:HG21 | 1:B:2115:SER:O    | 2.09        | 0.52     |
| 1:A:2142:GLN:HE21 | 1:A:2208:VAL:CG1  | 2.22        | 0.52     |
| 1:A:2275:VAL:HB   | 1:A:2413:MET:HE2  | 1.90        | 0.52     |
| 1:A:3233:TYR:O    | 1:A:3237:THR:HG23 | 2.10        | 0.52     |
| 1:A:2297:ASP:C    | 1:A:2299:ILE:H    | 2.12        | 0.52     |
| 1:A:2431:LEU:HD21 | 1:A:2506:PHE:CE2  | 2.44        | 0.52     |
| 1:A:4693:ASN:N    | 1:A:4693:ASN:ND2  | 2.57        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:3023:SER:HB2  | 2:B:9010:ADP:O1A  | 2.09        | 0.52     |
| 1:B:4118:MET:O    | 1:B:4122:VAL:HG22 | 2.08        | 0.52     |
| 1:A:3878:GLU:O    | 1:A:3882:VAL:HG23 | 2.10        | 0.52     |
| 1:A:2578:MET:CE   | 1:A:2613:LEU:HA   | 2.39        | 0.52     |
| 1:B:3059:LEU:HD23 | 1:B:3137:VAL:HG11 | 1.92        | 0.52     |
| 1:B:2838:LEU:O    | 1:B:2840:PRO:HD3  | 2.10        | 0.52     |
| 1:A:2956:LEU:HD21 | 1:A:2971:TYR:CG   | 2.44        | 0.52     |
| 1:B:3681:ALA:HB2  | 1:B:3786:PHE:CG   | 2.45        | 0.52     |
| 1:B:2532:ARG:HH11 | 1:B:2532:ARG:HG2  | 1.74        | 0.52     |
| 1:B:3082:SER:HA   | 1:B:3085:GLU:OE1  | 2.09        | 0.52     |
| 1:B:1930:ALA:HB2  | 1:B:1958:LEU:HD11 | 1.91        | 0.52     |
| 1:B:3017:VAL:HG11 | 1:B:3175:GLU:CD   | 2.30        | 0.52     |
| 1:A:3439:ASP:C    | 1:A:3441:LYS:H    | 2.13        | 0.52     |
| 1:A:4048:PHE:HD1  | 1:A:4048:PHE:H    | 1.58        | 0.52     |
| 1:B:2036:LEU:HD23 | 1:B:2040:SER:HB3  | 1.90        | 0.52     |
| 1:A:2258:LYS:HE3  | 1:A:2415:TRP:O    | 2.10        | 0.52     |
| 1:A:1690:GLN:HE22 | 1:A:1766:ILE:CG2  | 2.17        | 0.52     |
| 1:A:2857:TYR:HA   | 1:A:2913:PHE:CE1  | 2.36        | 0.52     |
| 1:B:4323:ASN:HD22 | 1:B:4323:ASN:N    | 2.06        | 0.52     |
| 1:B:2144:HIS:HB3  | 1:B:2400:LEU:CD1  | 2.40        | 0.52     |
| 1:A:4371:PRO:O    | 1:A:4372:ASP:HB2  | 2.09        | 0.52     |
| 1:B:2907:HIS:HA   | 1:B:2910:LEU:HD12 | 1.92        | 0.52     |
| 1:A:3225:ASP:O    | 1:A:3229:SER:HB3  | 2.08        | 0.52     |
| 1:A:3415:LYS:O    | 1:A:3417:LEU:HD12 | 2.09        | 0.52     |
| 1:A:4103:CYS:SG   | 1:A:4108:GLU:HA   | 2.50        | 0.52     |
| 1:A:2139:LEU:O    | 1:A:2140:SER:C    | 2.48        | 0.52     |
| 1:A:2142:GLN:HG2  | 1:A:2208:VAL:HG11 | 1.91        | 0.52     |
| 1:A:2793:ASN:HD22 | 1:A:2793:ASN:H    | 1.57        | 0.52     |
| 1:B:2282:LYS:NZ   | 1:B:2282:LYS:HB2  | 2.25        | 0.52     |
| 1:B:1600:SER:O    | 1:B:1604:VAL:HG23 | 2.10        | 0.52     |
| 1:A:4006:PRO:C    | 1:A:4008:LEU:H    | 2.11        | 0.52     |
| 1:A:4413:ASN:HD21 | 1:A:4660:LEU:HG   | 1.74        | 0.52     |
| 1:A:2708:GLU:O    | 1:A:2711:LEU:HB2  | 2.10        | 0.52     |
| 1:A:2531:LEU:HD12 | 1:A:2809:ARG:HD2  | 1.91        | 0.52     |
| 1:B:4156:GLN:O    | 1:B:4183:THR:HB   | 2.10        | 0.52     |
| 1:B:2748:LEU:N    | 1:B:2749:PRO:CD   | 2.73        | 0.52     |
| 1:A:3373:ILE:HG12 | 1:A:3374:ILE:H    | 1.74        | 0.52     |
| 1:B:4270:ILE:CG2  | 1:B:4310:ILE:HD13 | 2.34        | 0.52     |
| 1:A:3653:PRO:HB2  | 1:A:3658:CYS:SG   | 2.50        | 0.52     |
| 1:B:3233:TYR:O    | 1:B:3237:THR:HG23 | 2.09        | 0.52     |
| 1:A:2105:ARG:HG2  | 1:A:2105:ARG:NH1  | 2.23        | 0.52     |
| 1:B:2231:ILE:HD11 | 1:B:2260:LEU:HG   | 1.91        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4288:ILE:CG2  | 1:A:4289:PRO:HA   | 2.40        | 0.52     |
| 1:A:2528:PHE:HE1  | 1:A:2533:VAL:HG11 | 1.73        | 0.52     |
| 1:B:1873:LYS:HB3  | 1:B:1943:ILE:HG21 | 1.90        | 0.52     |
| 1:B:1565:LEU:HD23 | 1:B:1595:LEU:CD1  | 2.39        | 0.52     |
| 1:B:2506:PHE:CE1  | 1:B:2512:VAL:HG21 | 2.43        | 0.52     |
| 1:B:2531:LEU:HD13 | 1:B:2809:ARG:NH2  | 2.24        | 0.52     |
| 1:A:2003:GLY:O    | 1:A:2004:PHE:C    | 2.49        | 0.52     |
| 1:A:1629:LEU:HD11 | 1:A:1686:TYR:CD2  | 2.44        | 0.52     |
| 1:A:3256:THR:OG1  | 1:A:3779:SER:HB3  | 2.09        | 0.52     |
| 1:A:2408:ILE:O    | 1:A:2410:ARG:N    | 2.43        | 0.52     |
| 1:A:3698:SER:C    | 1:A:3700:LEU:H    | 2.13        | 0.52     |
| 1:B:4157:TYR:HB2  | 1:B:4184:TRP:HB2  | 1.92        | 0.52     |
| 1:A:3924:LEU:HD23 | 1:A:3943:LEU:HD21 | 1.91        | 0.52     |
| 1:A:3988:TRP:NE1  | 1:A:3992:LEU:HD11 | 2.25        | 0.52     |
| 1:B:2741:VAL:HB   | 1:B:2788:PHE:CD2  | 2.44        | 0.52     |
| 1:B:2906:ALA:O    | 1:B:2909:ALA:HB3  | 2.10        | 0.52     |
| 1:A:2893:MET:HE3  | 1:A:2896:CYS:HB2  | 1.92        | 0.52     |
| 1:A:3813:ARG:HG3  | 1:A:3814:SER:N    | 2.24        | 0.52     |
| 1:B:4423:ALA:O    | 1:B:4427:ILE:HG12 | 2.10        | 0.52     |
| 1:A:2641:VAL:HG12 | 1:A:2831:PHE:HB3  | 1.92        | 0.52     |
| 1:A:1964:LEU:HD12 | 1:A:2074:PHE:HZ   | 1.75        | 0.52     |
| 1:A:4033:LEU:HD13 | 1:A:4062:TRP:CE2  | 2.45        | 0.52     |
| 1:A:2561:SER:OG   | 1:A:2564:ASN:HB3  | 2.09        | 0.51     |
| 1:A:1715:ILE:HD11 | 1:A:1760:ILE:HG21 | 1.92        | 0.51     |
| 1:B:3563:LEU:HD11 | 1:B:3845:ILE:CD1  | 2.40        | 0.51     |
| 1:B:3843:GLY:O    | 1:B:3845:ILE:N    | 2.35        | 0.51     |
| 1:B:2910:LEU:O    | 1:B:2914:GLN:HB3  | 2.10        | 0.51     |
| 1:B:1957:TYR:O    | 1:B:1961:THR:HG23 | 2.10        | 0.51     |
| 1:B:2820:SER:OG   | 1:B:2823:SER:HB2  | 2.09        | 0.51     |
| 1:A:4269:ARG:HG2  | 1:A:4369:PHE:CE1  | 2.45        | 0.51     |
| 1:A:2898:LEU:CD1  | 1:A:2941:VAL:HG22 | 2.40        | 0.51     |
| 1:A:4213:PHE:CZ   | 1:A:4215:LEU:HB2  | 2.45        | 0.51     |
| 1:B:1817:LEU:O    | 1:B:1821:ILE:HG13 | 2.10        | 0.51     |
| 1:B:4690:VAL:HG21 | 1:B:4701:PHE:CE1  | 2.45        | 0.51     |
| 1:B:2764:ARG:HD2  | 1:B:2806:ARG:O    | 2.10        | 0.51     |
| 1:A:2271:GLY:O    | 1:A:2411:CYS:HA   | 2.10        | 0.51     |
| 1:B:4671:TRP:O    | 1:B:4672:LYS:HG2  | 2.11        | 0.51     |
| 1:B:3595:ALA:O    | 1:B:3598:PHE:HB3  | 2.11        | 0.51     |
| 1:A:3567:LEU:HD23 | 1:A:3855:LEU:HD11 | 1.92        | 0.51     |
| 1:A:2535:ASN:ND2  | 1:A:2668:ARG:HH12 | 2.08        | 0.51     |
| 1:A:4136:SER:O    | 1:A:4220:GLU:HA   | 2.10        | 0.51     |
| 1:B:1975:PRO:HG2  | 1:B:1978:THR:HG21 | 1.91        | 0.51     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:4690:VAL:HG11 | 1:B:4701:PHE:CZ   | 2.44        | 0.51     |
| 1:B:1937:GLY:HA3  | 1:B:1992:GLY:O    | 2.10        | 0.51     |
| 1:B:2549:ILE:O    | 1:B:2553:GLN:HB2  | 2.09        | 0.51     |
| 1:B:3682:MET:SD   | 1:B:3696:LYS:HE2  | 2.49        | 0.51     |
| 1:A:2144:HIS:O    | 1:A:2413:MET:HG2  | 2.10        | 0.51     |
| 1:A:3730:LEU:HD13 | 1:A:3734:LEU:HD21 | 1.91        | 0.51     |
| 1:A:1959:THR:HG21 | 1:A:2098:MET:HB2  | 1.92        | 0.51     |
| 1:A:2918:VAL:HG13 | 1:A:3172:TRP:NE1  | 2.26        | 0.51     |
| 1:B:2311:ILE:HB   | 1:B:2315:GLN:HE21 | 1.76        | 0.51     |
| 1:A:3969:LEU:HD12 | 1:A:4426:MET:CE   | 2.41        | 0.51     |
| 1:A:2732:PRO:CG   | 1:A:2739:LEU:HB2  | 2.40        | 0.51     |
| 1:B:3902:GLU:C    | 1:B:3904:SER:H    | 2.13        | 0.51     |
| 1:B:4636:SER:HA   | 1:B:4670:THR:HG22 | 1.91        | 0.51     |
| 1:B:4592:GLY:HA3  | 1:B:4725:SER:O    | 2.10        | 0.51     |
| 1:A:3366:LEU:O    | 1:A:3366:LEU:HD12 | 2.10        | 0.51     |
| 1:A:3670:ARG:O    | 1:A:3782:THR:HG22 | 2.10        | 0.51     |
| 1:A:2370:LEU:HD12 | 1:A:2377:LEU:CB   | 2.41        | 0.51     |
| 1:A:2586:GLY:HA2  | 1:A:2815:LEU:CD1  | 2.37        | 0.51     |
| 1:A:3452:ILE:CG2  | 1:A:3485:THR:HG21 | 2.39        | 0.51     |
| 1:B:1920:ASN:ND2  | 1:B:1921:VAL:H    | 2.09        | 0.51     |
| 1:A:3114:GLU:HG2  | 1:A:3118:ARG:HH12 | 1.74        | 0.51     |
| 1:A:1611:ARG:NH1  | 1:A:1611:ARG:HG3  | 2.23        | 0.51     |
| 1:B:3843:GLY:C    | 1:B:3845:ILE:H    | 2.13        | 0.51     |
| 1:B:2238:LYS:HA   | 1:B:2241:GLN:HE21 | 1.74        | 0.51     |
| 1:A:4025:GLN:HG3  | 1:B:2899:GLU:OE2  | 2.10        | 0.51     |
| 1:A:4240:ASN:OD1  | 1:A:4240:ASN:N    | 2.38        | 0.51     |
| 1:A:3768:ASP:HB3  | 1:A:3771:ALA:HB2  | 1.93        | 0.51     |
| 1:A:3353:LYS:O    | 1:A:3357:VAL:HG23 | 2.10        | 0.51     |
| 1:B:3889:MET:CE   | 1:B:3943:LEU:HB3  | 2.41        | 0.51     |
| 1:B:2815:LEU:HD23 | 1:B:2815:LEU:C    | 2.31        | 0.51     |
| 1:B:1662:ILE:HB   | 1:B:1665:ILE:CG2  | 2.40        | 0.51     |
| 1:B:4340:SER:HB2  | 1:B:4357:TYR:OH   | 2.10        | 0.51     |
| 1:B:4086:MET:HG3  | 1:B:4097:TYR:CD2  | 2.45        | 0.51     |
| 1:B:4222:HIS:CG   | 1:B:4223:PRO:HD2  | 2.45        | 0.51     |
| 1:A:4200:LEU:HD22 | 1:A:4204:LEU:CD1  | 2.41        | 0.51     |
| 1:A:1625:ILE:HG23 | 1:A:1626:ASN:OD1  | 2.11        | 0.51     |
| 1:A:2738:TRP:CE2  | 1:A:2785:LYS:HG2  | 2.46        | 0.51     |
| 1:B:1971:ASN:O    | 1:B:2097:SER:HA   | 2.11        | 0.51     |
| 1:B:2638:THR:O    | 1:B:2641:VAL:HG23 | 2.10        | 0.51     |
| 1:B:3306:LEU:HD13 | 1:B:3557:VAL:HG22 | 1.92        | 0.51     |
| 1:A:4384:PRO:HB3  | 1:A:4395:TRP:CD1  | 2.45        | 0.51     |
| 1:B:4121:ILE:HA   | 1:B:4125:GLU:CG   | 2.32        | 0.51     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3721:GLN:NE2  | 1:A:4205:HIS:NE2  | 2.58        | 0.51     |
| 1:B:2219:LEU:HD13 | 1:B:2228:LEU:HD11 | 1.93        | 0.51     |
| 1:B:3063:GLY:HA2  | 1:B:3136:GLN:CB   | 2.41        | 0.51     |
| 1:A:3289:LEU:HD13 | 1:A:3293:ARG:NH2  | 2.25        | 0.51     |
| 1:B:1556:ARG:HG2  | 1:B:1557:GLY:N    | 2.25        | 0.51     |
| 1:B:2877:ARG:HB3  | 1:B:2881:ARG:NH1  | 2.26        | 0.51     |
| 1:A:2732:PRO:HG3  | 1:A:2739:LEU:HB2  | 1.93        | 0.51     |
| 1:B:2801:VAL:HG12 | 1:B:2802:GLN:N    | 2.25        | 0.51     |
| 1:B:3566:ASN:ND2  | 1:B:3859:LYS:NZ   | 2.59        | 0.51     |
| 1:B:2643:SER:HB3  | 1:B:2646:VAL:HG23 | 1.93        | 0.51     |
| 1:B:2931:ASP:O    | 1:B:2935:LEU:HG   | 2.11        | 0.51     |
| 1:B:4550:TRP:O    | 1:B:4552:TRP:N    | 2.40        | 0.51     |
| 1:B:1520:ALA:HA   | 1:B:1580:TYR:CE1  | 2.46        | 0.51     |
| 1:B:3219:ILE:CB   | 1:B:3220:PRO:CD   | 2.89        | 0.51     |
| 1:A:1713:LYS:O    | 1:A:1715:ILE:N    | 2.44        | 0.51     |
| 1:A:4428:ASN:O    | 1:A:4432:LYS:HG2  | 2.10        | 0.51     |
| 1:A:4389:ARG:HH12 | 1:A:4393:MET:CE   | 2.24        | 0.51     |
| 1:B:1639:ILE:HG21 | 1:B:1676:LEU:HG   | 1.93        | 0.51     |
| 1:B:2849:LEU:HD21 | 1:B:2886:LEU:HD13 | 1.93        | 0.51     |
| 1:B:2968:LEU:CD2  | 1:B:2999:LEU:HD11 | 2.41        | 0.51     |
| 1:B:2283:THR:HA   | 1:B:2286:TRP:HE1  | 1.76        | 0.51     |
| 1:A:2327:TRP:CZ3  | 1:A:2380:PRO:HD2  | 2.46        | 0.51     |
| 1:B:2542:ASN:O    | 1:B:2546:VAL:HG23 | 2.10        | 0.51     |
| 1:A:2540:LEU:HD23 | 1:A:2662:ALA:HB3  | 1.92        | 0.51     |
| 1:A:2138:GLN:NE2  | 1:A:2218:LEU:HD21 | 2.26        | 0.51     |
| 1:A:4299:ASN:OD1  | 1:A:4301:ALA:HB3  | 2.11        | 0.51     |
| 1:A:2619:ILE:O    | 1:A:2619:ILE:HG13 | 2.11        | 0.51     |
| 1:B:2921:GLU:CD   | 1:B:2921:GLU:H    | 2.13        | 0.51     |
| 1:A:3425:LYS:HA   | 1:A:3428:GLU:CG   | 2.41        | 0.51     |
| 1:A:2204:ILE:HG13 | 1:A:2205:PRO:HD3  | 1.92        | 0.51     |
| 1:B:1578:SER:C    | 1:B:1580:TYR:H    | 2.14        | 0.51     |
| 1:B:1823:TRP:O    | 1:B:1827:VAL:HG23 | 2.10        | 0.51     |
| 1:B:1892:LEU:HA   | 1:B:1895:CYS:SG   | 2.51        | 0.51     |
| 1:B:3790:PRO:HA   | 1:B:3898:PHE:CE2  | 2.46        | 0.51     |
| 1:A:4222:HIS:ND1  | 1:A:4223:PRO:HD2  | 2.26        | 0.51     |
| 1:B:2199:ILE:O    | 1:B:2203:MET:HB2  | 2.11        | 0.51     |
| 1:B:3618:MET:HB3  | 1:B:3628:PHE:CZ   | 2.46        | 0.51     |
| 1:A:3032:MET:C    | 1:A:3034:GLY:H    | 2.15        | 0.51     |
| 1:B:3583:THR:O    | 1:B:3587:THR:HG23 | 2.11        | 0.51     |
| 1:A:2839:LEU:HD22 | 1:A:2896:CYS:HB3  | 1.93        | 0.50     |
| 1:A:2582:GLY:O    | 1:A:2585:MET:HB2  | 2.11        | 0.50     |
| 1:B:1687:LEU:HD11 | 1:B:1706:LEU:HD21 | 1.93        | 0.50     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:4288:ILE:HG23 | 1:B:4289:PRO:HA   | 1.92        | 0.50     |
| 1:B:4644:LEU:HD13 | 1:B:4647:ALA:HB3  | 1.92        | 0.50     |
| 1:B:1573:SER:HA   | 1:B:1576:LYS:HE2  | 1.93        | 0.50     |
| 1:A:3116:ALA:HB1  | 1:A:3121:LEU:O    | 2.12        | 0.50     |
| 1:B:1527:LEU:HD22 | 1:B:1575:MET:HB2  | 1.92        | 0.50     |
| 1:A:2212:ILE:N    | 1:A:2213:PRO:CD   | 2.75        | 0.50     |
| 1:A:2856:PHE:CE1  | 1:A:2930:ILE:HG12 | 2.46        | 0.50     |
| 1:A:1963:ALA:HB1  | 1:A:2096:ARG:CG   | 2.41        | 0.50     |
| 1:B:1534:VAL:HG13 | 1:B:1568:HIS:CD2  | 2.42        | 0.50     |
| 1:A:3923:LEU:HD11 | 1:A:3943:LEU:HA   | 1.94        | 0.50     |
| 1:B:1479:ARG:O    | 1:B:1483:ILE:HG13 | 2.11        | 0.50     |
| 1:B:2729:VAL:HG12 | 1:B:2782:LYS:HB3  | 1.94        | 0.50     |
| 1:B:4267:ARG:NH2  | 1:B:4315:ASP:OD1  | 2.43        | 0.50     |
| 1:B:3038:TYR:CD2  | 1:B:3058:LEU:HD13 | 2.46        | 0.50     |
| 1:A:1776:GLU:HA   | 1:A:1779:SER:HB3  | 1.93        | 0.50     |
| 1:B:1951:PRO:HG2  | 1:B:2104:ASP:OD2  | 2.10        | 0.50     |
| 1:A:4285:LEU:O    | 1:A:4288:ILE:HG13 | 2.10        | 0.50     |
| 1:A:1719:GLN:HA   | 1:A:1722:PHE:CD2  | 2.46        | 0.50     |
| 1:B:4686:LEU:HD12 | 1:B:4687:SER:N    | 2.27        | 0.50     |
| 1:B:4170:LEU:HD12 | 1:B:4171:ALA:N    | 2.26        | 0.50     |
| 1:A:4326:PRO:HB3  | 1:A:4369:PHE:CD2  | 2.46        | 0.50     |
| 1:A:3067:GLU:O    | 1:A:3069:ILE:HD12 | 2.12        | 0.50     |
| 1:A:4122:VAL:HA   | 1:A:4126:VAL:HG11 | 1.91        | 0.50     |
| 1:A:2586:GLY:O    | 1:A:2590:ARG:HB2  | 2.10        | 0.50     |
| 1:A:2049:ALA:O    | 1:A:2054:SER:HB3  | 2.12        | 0.50     |
| 1:B:2142:GLN:HB2  | 1:B:2145:TYR:CD1  | 2.46        | 0.50     |
| 1:A:4044:TRP:CE3  | 1:A:4048:PHE:HE1  | 2.29        | 0.50     |
| 1:B:2135:CYS:HB3  | 1:B:2139:LEU:HD12 | 1.92        | 0.50     |
| 1:B:1907:LEU:HA   | 1:B:1911:ARG:NH1  | 2.26        | 0.50     |
| 1:B:1967:ARG:HG2  | 1:B:1967:ARG:HH11 | 1.75        | 0.50     |
| 1:A:4028:PRO:C    | 1:A:4030:PHE:H    | 2.15        | 0.50     |
| 1:A:2954:ASN:HD22 | 1:A:2954:ASN:N    | 2.02        | 0.50     |
| 1:A:3380:VAL:HG11 | 1:A:3435:ILE:CG2  | 2.41        | 0.50     |
| 1:B:2865:THR:N    | 1:B:2868:ILE:HD12 | 2.26        | 0.50     |
| 1:A:2533:VAL:HB   | 1:A:2581:LEU:HA   | 1.94        | 0.50     |
| 1:A:3834:LEU:HA   | 1:A:3854:THR:HG21 | 1.93        | 0.50     |
| 1:A:4118:MET:HB3  | 1:A:4149:LEU:HD22 | 1.94        | 0.50     |
| 1:B:1926:VAL:HG22 | 1:B:1935:TYR:HE2  | 1.75        | 0.50     |
| 1:A:4052:GLN:C    | 1:A:4054:GLY:H    | 2.14        | 0.50     |
| 1:A:2720:TYR:HE1  | 1:A:2781:ILE:HG21 | 1.76        | 0.50     |
| 1:B:1862:SER:O    | 1:B:1867:LEU:HD21 | 2.12        | 0.50     |
| 1:B:3691:ASP:C    | 1:B:3693:LYS:H    | 2.15        | 0.50     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:4111:LEU:N    | 1:B:4111:LEU:HD12 | 2.26        | 0.50     |
| 1:B:2367:LEU:HD12 | 1:B:2367:LEU:N    | 2.26        | 0.50     |
| 1:A:2913:PHE:CD2  | 1:A:2913:PHE:N    | 2.79        | 0.50     |
| 1:B:1662:ILE:HB   | 1:B:1665:ILE:HG23 | 1.93        | 0.50     |
| 1:B:4020:LEU:HD11 | 1:B:4033:LEU:HG   | 1.93        | 0.50     |
| 1:A:1971:ASN:ND2  | 1:A:2087:LEU:HD11 | 2.26        | 0.50     |
| 1:A:2627:TRP:O    | 1:A:2629:ASN:N    | 2.45        | 0.50     |
| 1:A:4388:THR:O    | 1:A:4391:HIS:HB2  | 2.12        | 0.50     |
| 1:A:2197:ASN:O    | 1:A:2201:ASP:HB2  | 2.12        | 0.50     |
| 1:B:2723:THR:CG2  | 1:B:2727:GLU:HB2  | 2.42        | 0.50     |
| 1:A:4518:ALA:C    | 1:A:4520:LEU:H    | 2.15        | 0.50     |
| 1:B:3105:PHE:O    | 1:B:3109:MET:HG3  | 2.12        | 0.50     |
| 1:B:2918:VAL:HG22 | 1:B:3172:TRP:CD2  | 2.47        | 0.50     |
| 1:A:1639:ILE:HD11 | 1:A:1675:LEU:HB3  | 1.94        | 0.50     |
| 1:A:4185:VAL:HG12 | 1:A:4186:LEU:N    | 2.19        | 0.50     |
| 1:A:1889:VAL:HA   | 1:A:1892:LEU:HD12 | 1.94        | 0.50     |
| 1:A:3410:LEU:HA   | 1:A:3414:GLY:O    | 2.12        | 0.50     |
| 1:A:4078:SER:HA   | 1:A:4081:ARG:HD2  | 1.94        | 0.50     |
| 1:A:3433:THR:HG22 | 1:A:3437:ASN:HD22 | 1.75        | 0.50     |
| 1:A:3583:THR:O    | 1:A:3587:THR:HG23 | 2.11        | 0.50     |
| 1:B:4644:LEU:O    | 1:B:4661:SER:HB2  | 2.11        | 0.50     |
| 1:B:2989:VAL:HG13 | 1:B:3187:GLU:OE2  | 2.12        | 0.50     |
| 1:A:3977:LYS:O    | 1:A:3979:THR:HG23 | 2.12        | 0.50     |
| 1:B:1781:LEU:O    | 1:B:1814:LEU:HD21 | 2.12        | 0.49     |
| 1:A:2798:ALA:C    | 1:A:2800:ARG:H    | 2.14        | 0.49     |
| 1:B:4339:GLY:HA3  | 1:B:4360:LEU:HD11 | 1.93        | 0.49     |
| 1:A:3992:LEU:HD22 | 1:A:4430:LEU:CB   | 2.41        | 0.49     |
| 1:A:4278:HIS:CD2  | 1:A:4343:TYR:OH   | 2.64        | 0.49     |
| 1:B:1522:GLN:O    | 1:B:1525:ILE:HG22 | 2.11        | 0.49     |
| 1:A:1926:VAL:HG12 | 1:A:1928:HIS:NE2  | 2.26        | 0.49     |
| 1:B:2976:LEU:HD11 | 1:B:2990:LEU:HD21 | 1.94        | 0.49     |
| 1:B:4259:ARG:NH2  | 1:B:4307:LEU:HB3  | 2.27        | 0.49     |
| 1:B:4132:LEU:HD13 | 1:B:4216:PHE:CZ   | 2.47        | 0.49     |
| 1:B:3061:ARG:HB3  | 1:B:3067:GLU:OE2  | 2.12        | 0.49     |
| 1:B:3181:LEU:CB   | 1:B:3232:VAL:HG13 | 2.42        | 0.49     |
| 1:B:2504:GLN:HA   | 1:B:2507:GLU:OE2  | 2.12        | 0.49     |
| 1:A:3337:LYS:CB   | 1:A:3525:LEU:HD13 | 2.24        | 0.49     |
| 1:B:3935:ASP:O    | 1:B:3939:ARG:HG3  | 2.12        | 0.49     |
| 1:B:4402:ILE:H    | 1:B:4402:ILE:CD1  | 2.21        | 0.49     |
| 1:A:4054:GLY:O    | 1:A:4055:GLU:O    | 2.30        | 0.49     |
| 1:A:4055:GLU:HG3  | 1:A:4093:ARG:NH1  | 2.27        | 0.49     |
| 1:B:4060:GLU:HA   | 1:B:4063:ILE:HD13 | 1.94        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2877:ARG:HG2  | 2:B:9009:ADP:H4'  | 1.94        | 0.49     |
| 1:A:3011:HIS:CE1  | 1:A:3143:VAL:HG23 | 2.47        | 0.49     |
| 1:A:3919:ILE:HG21 | 1:A:3951:THR:HA   | 1.94        | 0.49     |
| 1:B:4642:MET:HG2  | 1:B:4725:SER:HA   | 1.94        | 0.49     |
| 1:B:1494:ILE:HA   | 1:B:1497:LEU:HD12 | 1.93        | 0.49     |
| 1:A:2511:LEU:HD11 | 1:A:2574:LEU:HD21 | 1.94        | 0.49     |
| 1:A:3059:LEU:HD21 | 1:A:3090:LEU:HD13 | 1.94        | 0.49     |
| 1:B:4596:ASN:HD22 | 1:B:4596:ASN:C    | 2.15        | 0.49     |
| 1:A:2869:GLN:HG2  | 1:A:2871:HIS:CE1  | 2.47        | 0.49     |
| 1:B:3700:LEU:CG   | 1:B:3701:ASP:H    | 2.23        | 0.49     |
| 1:A:3723:VAL:HG23 | 1:A:3764:LEU:HD22 | 1.94        | 0.49     |
| 1:A:2057:VAL:HG22 | 1:A:2058:GLU:H    | 1.78        | 0.49     |
| 1:A:1739:THR:O    | 1:A:1760:ILE:HG12 | 2.12        | 0.49     |
| 1:A:2018:GLN:HE21 | 1:A:2066:SER:HB3  | 1.77        | 0.49     |
| 1:A:3192:LEU:O    | 1:A:3224:ARG:NH2  | 2.46        | 0.49     |
| 1:A:4574:GLN:HE22 | 1:A:4590:TRP:H    | 1.60        | 0.49     |
| 1:A:4365:THR:HB   | 1:A:4366:PRO:HD2  | 1.93        | 0.49     |
| 1:A:3398:PRO:C    | 1:A:3400:PRO:HD2  | 2.33        | 0.49     |
| 1:A:4068:GLN:C    | 1:A:4070:SER:H    | 2.15        | 0.49     |
| 1:B:3135:SER:HA   | 1:B:3138:ARG:HG2  | 1.95        | 0.49     |
| 1:A:2133:LYS:HD3  | 1:A:2133:LYS:O    | 2.12        | 0.49     |
| 1:A:3338:GLN:HA   | 1:A:3342:ARG:CB   | 2.42        | 0.49     |
| 1:B:3192:LEU:HD11 | 1:B:3268:VAL:HG22 | 1.94        | 0.49     |
| 1:A:4075:THR:HG23 | 1:A:4076:ILE:N    | 2.27        | 0.49     |
| 1:A:2374:ASN:O    | 1:A:2375:LYS:HB2  | 2.11        | 0.49     |
| 1:A:4122:VAL:HA   | 1:A:4126:VAL:CG1  | 2.42        | 0.49     |
| 1:A:3725:ASN:N    | 1:A:3725:ASN:ND2  | 2.58        | 0.49     |
| 1:A:1887:ASP:O    | 1:A:1891:GLN:HG3  | 2.12        | 0.49     |
| 1:A:4244:VAL:HG23 | 1:A:4403:SER:CB   | 2.42        | 0.49     |
| 1:A:2029:ASN:HD22 | 1:A:2030:ARG:N    | 2.11        | 0.49     |
| 1:A:2302:GLU:HG2  | 1:A:2304:HIS:CE1  | 2.46        | 0.49     |
| 1:A:2370:LEU:HD23 | 1:A:2387:LEU:HD22 | 1.95        | 0.49     |
| 1:A:3947:ILE:CG2  | 1:A:3948:PHE:N    | 2.76        | 0.49     |
| 1:A:1934:PHE:N    | 1:A:1934:PHE:CD2  | 2.81        | 0.49     |
| 1:A:3116:ALA:HB1  | 1:A:3123:LEU:HD12 | 1.94        | 0.49     |
| 1:B:2021:ALA:O    | 1:B:2071:MET:HA   | 2.13        | 0.49     |
| 1:B:3316:LYS:HD2  | 1:B:3546:ILE:HD12 | 1.94        | 0.49     |
| 1:B:2839:LEU:HD22 | 1:B:2896:CYS:HB3  | 1.95        | 0.49     |
| 1:B:2315:GLN:HB3  | 1:B:2775:THR:CG2  | 2.41        | 0.49     |
| 1:B:4012:LEU:N    | 1:B:4012:LEU:HD23 | 2.27        | 0.49     |
| 1:A:3674:VAL:HG13 | 1:A:3786:PHE:HD2  | 1.78        | 0.49     |
| 1:B:2832:ASN:HD22 | 1:B:2835:LEU:HD23 | 1.77        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:4313:TRP:HB3  | 1:B:4330:PRO:CG   | 2.42        | 0.49     |
| 1:A:1699:PHE:N    | 1:A:1699:PHE:CD1  | 2.77        | 0.49     |
| 1:A:1907:LEU:HA   | 1:A:1911:ARG:HH11 | 1.77        | 0.49     |
| 1:A:3217:MET:O    | 1:A:3218:ALA:C    | 2.50        | 0.49     |
| 1:A:1629:LEU:N    | 1:A:1630:PRO:HD3  | 2.28        | 0.49     |
| 1:A:2029:ASN:HD22 | 1:A:2029:ASN:N    | 2.10        | 0.49     |
| 1:A:3655:ASP:O    | 1:A:3659:ILE:HG13 | 2.13        | 0.49     |
| 1:B:2612:LEU:HD11 | 1:B:2624:TRP:CZ3  | 2.48        | 0.49     |
| 1:A:2272:VAL:HA   | 1:A:2412:GLY:H    | 1.77        | 0.49     |
| 1:A:3039:THR:HG22 | 1:A:3040:ILE:N    | 2.24        | 0.49     |
| 1:A:2848:ASN:HB3  | 1:A:2938:PHE:HE1  | 1.77        | 0.49     |
| 1:B:4167:GLY:HA2  | 1:B:4170:LEU:HD11 | 1.93        | 0.49     |
| 1:A:3262:ASP:CB   | 1:A:3670:ARG:HE   | 2.25        | 0.49     |
| 1:B:4109:ASP:HA   | 1:B:4112:ASN:HD21 | 1.72        | 0.49     |
| 1:A:2941:VAL:CG1  | 1:A:2942:ASN:N    | 2.76        | 0.49     |
| 1:A:2948:ARG:HG2  | 1:A:2948:ARG:NH1  | 2.28        | 0.49     |
| 1:B:3991:LEU:HG   | 1:B:3992:LEU:HD23 | 1.94        | 0.49     |
| 1:B:2000:CYS:CB   | 1:B:2031:LEU:HD13 | 2.42        | 0.49     |
| 1:A:4068:GLN:N    | 1:A:4073:GLN:HE21 | 2.11        | 0.49     |
| 1:A:4072:GLN:OE1  | 1:A:4077:VAL:HG21 | 2.11        | 0.49     |
| 1:B:2517:GLU:O    | 1:B:2521:GLN:HG2  | 2.13        | 0.49     |
| 1:B:2677:GLY:HA3  | 1:B:2875:SER:OG   | 2.12        | 0.49     |
| 1:A:3997:ASN:HD21 | 1:A:4001:ILE:HD11 | 1.77        | 0.49     |
| 1:A:4295:PHE:C    | 1:A:4295:PHE:CD2  | 2.86        | 0.49     |
| 1:A:2208:VAL:HG22 | 1:A:2211:ASP:HB2  | 1.95        | 0.49     |
| 1:A:3981:ASN:HD22 | 1:A:4076:ILE:CB   | 2.20        | 0.49     |
| 1:A:3069:ILE:O    | 1:A:3141:LEU:O    | 2.30        | 0.49     |
| 1:A:4536:SER:HB2  | 1:A:4548:LYS:HZ1  | 1.77        | 0.49     |
| 1:A:4548:LYS:O    | 1:A:4550:TRP:N    | 2.46        | 0.49     |
| 1:A:4230:LEU:HB3  | 1:A:4235:VAL:HG21 | 1.94        | 0.49     |
| 1:A:2610:ILE:HD12 | 1:A:2615:TYR:OH   | 2.13        | 0.49     |
| 1:B:4618:ASN:H    | 1:B:4618:ASN:ND2  | 2.11        | 0.49     |
| 1:A:4596:ASN:ND2  | 1:A:4599:ALA:H    | 2.11        | 0.49     |
| 1:B:2723:THR:OG1  | 1:B:2724:PRO:HD2  | 2.13        | 0.49     |
| 1:A:3689:TYR:CB   | 1:A:3694:ILE:HD11 | 2.21        | 0.49     |
| 1:B:1959:THR:HG21 | 1:B:2098:MET:SD   | 2.53        | 0.49     |
| 1:A:1639:ILE:HG21 | 1:A:1676:LEU:HG   | 1.94        | 0.49     |
| 1:B:1823:TRP:NE1  | 1:B:1885:GLN:HB3  | 2.27        | 0.49     |
| 1:A:4402:ILE:N    | 1:A:4402:ILE:HD12 | 2.26        | 0.49     |
| 1:A:1565:LEU:HD11 | 1:A:1598:VAL:HG12 | 1.94        | 0.49     |
| 1:A:1800:HIS:HB2  | 1:A:1858:ASN:ND2  | 2.28        | 0.49     |
| 1:B:4693:ASN:HD22 | 1:B:4693:ASN:N    | 2.09        | 0.49     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1934:PHE:CD2  | 1:B:1934:PHE:N    | 2.81        | 0.49     |
| 1:B:2241:GLN:HA   | 1:B:2244:ALA:HB3  | 1.93        | 0.49     |
| 1:A:3370:GLU:O    | 1:A:3372:ALA:N    | 2.46        | 0.49     |
| 1:B:2655:ARG:O    | 1:B:2659:VAL:HG23 | 2.13        | 0.49     |
| 1:A:1603:ASP:O    | 1:A:1606:ILE:HG22 | 2.13        | 0.49     |
| 1:B:3929:ASN:HB3  | 1:B:3942:TYR:CD1  | 2.47        | 0.49     |
| 1:A:3180:ALA:O    | 1:A:3184:VAL:HG23 | 2.12        | 0.49     |
| 1:A:3598:PHE:O    | 1:A:3602:ILE:HB   | 2.11        | 0.48     |
| 1:B:1926:VAL:HG12 | 1:B:1928:HIS:NE2  | 2.28        | 0.48     |
| 1:A:3017:VAL:HG22 | 1:A:3018:SER:N    | 2.27        | 0.48     |
| 1:A:3457:LEU:HD11 | 1:A:3482:THR:HA   | 1.95        | 0.48     |
| 1:B:2616:SER:HB3  | 1:B:2627:TRP:CD2  | 2.47        | 0.48     |
| 1:A:1820:GLN:HE22 | 1:A:1990:GLN:HE22 | 1.60        | 0.48     |
| 1:B:3540:ILE:O    | 1:B:3544:GLU:HG3  | 2.13        | 0.48     |
| 1:A:3048:SER:HB2  | 1:A:3080:GLU:OE1  | 2.13        | 0.48     |
| 1:A:2572:ARG:O    | 1:A:2575:TYR:HB3  | 2.12        | 0.48     |
| 1:B:1813:GLN:NE2  | 1:B:1940:TYR:HA   | 2.17        | 0.48     |
| 1:A:4003:GLU:HG3  | 1:B:2842:LEU:HD23 | 1.95        | 0.48     |
| 1:A:3238:ILE:HG12 | 1:A:3601:TYR:HD2  | 1.69        | 0.48     |
| 1:B:4263:GLN:HA   | 1:B:4264:PRO:C    | 2.34        | 0.48     |
| 1:A:2720:TYR:CE1  | 1:A:2781:ILE:HG21 | 2.48        | 0.48     |
| 1:A:3150:ALA:O    | 1:A:3151:SER:C    | 2.51        | 0.48     |
| 1:B:2276:GLY:O    | 1:B:2282:LYS:HE2  | 2.13        | 0.48     |
| 1:B:3295:THR:O    | 1:B:3299:VAL:HG23 | 2.12        | 0.48     |
| 1:A:4589:VAL:CG1  | 1:A:4639:VAL:HA   | 2.43        | 0.48     |
| 1:B:2968:LEU:HG   | 1:B:2995:LEU:HD22 | 1.95        | 0.48     |
| 1:A:4043:ASP:HB3  | 1:A:4059:PRO:HB3  | 1.95        | 0.48     |
| 1:B:1934:PHE:HB3  | 1:B:1993:ARG:HH22 | 1.78        | 0.48     |
| 1:B:2229:GLN:O    | 1:B:2230:PRO:O    | 2.30        | 0.48     |
| 1:B:4513:ILE:HD12 | 1:B:4568:PHE:CE2  | 2.47        | 0.48     |
| 1:A:4083:ILE:HD11 | 1:A:4098:SER:HA   | 1.94        | 0.48     |
| 1:B:2604:PRO:O    | 1:B:2624:TRP:NE1  | 2.46        | 0.48     |
| 1:A:2088:PRO:C    | 1:A:2090:ASN:H    | 2.16        | 0.48     |
| 1:A:4604:THR:OG1  | 1:A:4671:TRP:HZ3  | 1.96        | 0.48     |
| 1:A:3007:GLN:NE2  | 1:A:3008:PRO:HD2  | 2.29        | 0.48     |
| 1:A:4133:LEU:HD21 | 1:A:4225:LEU:HD13 | 1.94        | 0.48     |
| 1:B:4306:ALA:HB1  | 1:B:4338:LEU:HD13 | 1.94        | 0.48     |
| 1:B:2720:TYR:CE1  | 1:B:2730:LEU:HD13 | 2.48        | 0.48     |
| 1:B:3673:LEU:HD13 | 1:B:3783:PHE:CE1  | 2.48        | 0.48     |
| 1:A:3145:PHE:CE2  | 1:A:3164:LEU:HD21 | 2.48        | 0.48     |
| 1:A:3920:PHE:O    | 1:A:3923:LEU:HB3  | 2.13        | 0.48     |
| 1:B:2080:GLY:HA3  | 1:B:2084:ARG:O    | 2.13        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1910:MET:HA   | 1:B:1929:MET:HG3  | 1.95        | 0.48     |
| 1:B:2782:LYS:HB2  | 1:B:2782:LYS:NZ   | 2.28        | 0.48     |
| 1:A:4133:LEU:HA   | 1:A:4217:MET:HB2  | 1.94        | 0.48     |
| 1:B:2621:ASP:C    | 1:B:2623:ASN:H    | 2.16        | 0.48     |
| 1:A:4335:ARG:HD3  | 1:A:4361:GLU:HA   | 1.96        | 0.48     |
| 1:A:3425:LYS:HA   | 1:A:3428:GLU:HG2  | 1.95        | 0.48     |
| 1:A:2273:MET:HG3  | 1:A:2413:MET:CE   | 2.44        | 0.48     |
| 1:A:4190:ILE:HB   | 1:A:4197:LEU:HD21 | 1.94        | 0.48     |
| 1:B:3677:PRO:HG3  | 1:B:3769:PRO:HB3  | 1.94        | 0.48     |
| 1:A:3042:VAL:HB   | 1:A:3079:LEU:HD11 | 1.96        | 0.48     |
| 1:B:2641:VAL:CG2  | 1:B:2887:LEU:HD22 | 2.43        | 0.48     |
| 1:B:4024:ARG:HG3  | 1:B:4031:SER:O    | 2.14        | 0.48     |
| 1:A:3289:LEU:HD13 | 1:A:3293:ARG:HH22 | 1.77        | 0.48     |
| 1:A:2752:ASP:C    | 1:A:2754:TYR:H    | 2.17        | 0.48     |
| 1:B:2774:ARG:HB2  | 1:B:2781:ILE:HD13 | 1.94        | 0.48     |
| 1:A:4047:PHE:HD2  | 1:A:4048:PHE:CD1  | 2.32        | 0.48     |
| 1:B:2025:PHE:HB2  | 1:B:2075:VAL:HG22 | 1.94        | 0.48     |
| 1:A:4684:SER:O    | 1:A:4707:TYR:CE2  | 2.67        | 0.48     |
| 1:A:3664:MET:O    | 1:A:3668:PHE:HB3  | 2.13        | 0.48     |
| 1:A:4384:PRO:HB3  | 1:A:4395:TRP:CG   | 2.48        | 0.48     |
| 1:A:2204:ILE:CG1  | 1:A:2205:PRO:HD3  | 2.44        | 0.48     |
| 1:A:3238:ILE:HD12 | 1:A:3238:ILE:N    | 2.28        | 0.48     |
| 1:B:3990:PHE:CE2  | 1:B:4023:LEU:HD13 | 2.48        | 0.48     |
| 1:A:4029:SER:CB   | 1:A:4081:ARG:HH12 | 2.25        | 0.48     |
| 1:A:2902:VAL:HG21 | 1:A:2941:VAL:HG21 | 1.95        | 0.48     |
| 1:A:3924:LEU:C    | 1:A:3925:ASN:HD22 | 2.15        | 0.48     |
| 1:A:3408:VAL:HG11 | 1:A:3477:LEU:CG   | 2.43        | 0.48     |
| 1:B:4410:LEU:CD2  | 1:B:4411:PRO:HD2  | 2.43        | 0.48     |
| 1:A:3487:TYR:O    | 1:A:3489:GLU:N    | 2.47        | 0.48     |
| 1:A:3371:PRO:O    | 1:A:3372:ALA:C    | 2.52        | 0.48     |
| 1:B:3196:ASN:ND2  | 1:B:3199:TYR:HB2  | 2.28        | 0.48     |
| 1:B:3911:PHE:CZ   | 1:B:3955:VAL:HG13 | 2.49        | 0.48     |
| 1:B:4653:GLN:OE1  | 1:B:4708:ASP:HA   | 2.14        | 0.48     |
| 1:A:2952:TYR:CE1  | 1:A:2962:PRO:HG3  | 2.48        | 0.48     |
| 1:B:3677:PRO:HB3  | 1:B:3769:PRO:HD3  | 1.94        | 0.48     |
| 1:B:1694:PHE:CE1  | 1:B:1770:LEU:HB3  | 2.48        | 0.48     |
| 1:B:1525:ILE:HD12 | 1:B:1528:GLU:HB3  | 1.96        | 0.48     |
| 1:A:1973:PHE:HE1  | 1:A:2099:ALA:CB   | 2.27        | 0.48     |
| 1:B:4540:SER:HB2  | 1:B:4545:ILE:O    | 2.13        | 0.48     |
| 1:A:1960:LEU:O    | 1:A:1964:LEU:N    | 2.39        | 0.48     |
| 1:A:1974:GLY:C    | 1:A:2079:PRO:HD3  | 2.34        | 0.48     |
| 1:B:3011:HIS:ND1  | 1:B:3091:LEU:HD22 | 2.28        | 0.48     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:4400:PRO:HG2  | 1:B:4407:TRP:CH2  | 2.49        | 0.48     |
| 1:A:3865:ILE:HA   | 1:A:3869:VAL:HG23 | 1.94        | 0.48     |
| 1:A:3323:LYS:HE3  | 1:A:3539:LEU:HG   | 1.95        | 0.48     |
| 1:A:3891:LEU:HD21 | 1:A:3895:ARG:NH2  | 2.28        | 0.48     |
| 1:B:3887:ASN:N    | 1:B:3888:PRO:CD   | 2.77        | 0.48     |
| 1:A:4591:LEU:CD2  | 1:A:4601:ILE:HD11 | 2.42        | 0.48     |
| 1:B:2084:ARG:HG2  | 1:B:2084:ARG:HH11 | 1.79        | 0.48     |
| 1:A:3863:THR:O    | 1:A:3863:THR:HG22 | 2.12        | 0.48     |
| 1:B:3955:VAL:HG12 | 1:B:3959:LEU:HG   | 1.96        | 0.48     |
| 1:A:1974:GLY:CA   | 1:A:2079:PRO:HD3  | 2.44        | 0.48     |
| 1:A:4406:ILE:HB   | 1:A:4412:GLU:OE2  | 2.14        | 0.48     |
| 1:B:4070:SER:O    | 1:B:4071:ASN:C    | 2.52        | 0.48     |
| 1:A:3987:GLU:HG3  | 1:A:4027:VAL:CG1  | 2.44        | 0.48     |
| 1:A:4184:TRP:CD1  | 1:A:4184:TRP:N    | 2.82        | 0.48     |
| 1:B:1962:GLN:HB3  | 1:B:4341:THR:HG21 | 1.96        | 0.48     |
| 1:A:4655:THR:HG22 | 1:A:4708:ASP:HB2  | 1.96        | 0.48     |
| 1:B:3638:LEU:HB2  | 1:B:3663:ILE:HD12 | 1.96        | 0.48     |
| 1:A:4132:LEU:HB2  | 1:A:4216:PHE:HD1  | 1.79        | 0.48     |
| 1:A:3473:ALA:O    | 1:A:3476:PRO:HD2  | 2.13        | 0.48     |
| 1:B:3585:MET:HA   | 1:B:3588:VAL:HG23 | 1.96        | 0.48     |
| 1:A:3397:PRO:HG2  | 1:A:3419:TRP:CE2  | 2.48        | 0.48     |
| 1:A:1800:HIS:CB   | 1:A:1858:ASN:HD22 | 2.26        | 0.48     |
| 1:B:4407:TRP:CD1  | 1:B:4407:TRP:N    | 2.82        | 0.48     |
| 1:B:3273:GLU:OE1  | 1:B:3667:ARG:NH2  | 2.47        | 0.48     |
| 1:B:3731:ASN:HB2  | 1:B:3732:PRO:HD3  | 1.94        | 0.48     |
| 1:A:1701:GLY:HA2  | 1:A:2011:ARG:NH1  | 2.29        | 0.48     |
| 1:A:2208:VAL:HA   | 1:A:2415:TRP:HD1  | 1.74        | 0.48     |
| 1:A:2375:LYS:HG2  | 1:A:2387:LEU:HD23 | 1.95        | 0.48     |
| 1:A:2299:ILE:CG2  | 1:A:2349:LYS:HA   | 2.44        | 0.48     |
| 1:A:2704:ALA:HB3  | 1:A:3085:GLU:CG   | 2.44        | 0.48     |
| 1:B:4360:LEU:C    | 1:B:4362:GLN:H    | 2.17        | 0.48     |
| 1:A:3145:PHE:CD1  | 1:A:3164:LEU:HD11 | 2.48        | 0.48     |
| 1:B:4288:ILE:CG2  | 1:B:4289:PRO:HA   | 2.44        | 0.48     |
| 1:B:2532:ARG:NH1  | 1:B:2532:ARG:HG2  | 2.29        | 0.48     |
| 1:B:4083:ILE:CD1  | 1:B:4098:SER:HA   | 2.44        | 0.48     |
| 1:B:3232:VAL:O    | 1:B:3236:GLN:HG3  | 2.14        | 0.48     |
| 1:A:4201:GLU:HG3  | 1:A:4228:ASN:HB2  | 1.94        | 0.48     |
| 1:A:2813:ILE:HG22 | 1:A:2814:LEU:N    | 2.28        | 0.48     |
| 1:A:1535:ARG:HA   | 1:A:1591:TRP:CZ2  | 2.49        | 0.48     |
| 1:A:3695:THR:HG21 | 1:A:3707:ASN:OD1  | 2.14        | 0.48     |
| 1:B:3350:VAL:HG12 | 1:B:3354:GLU:OE2  | 2.13        | 0.48     |
| 1:A:4296:PHE:CZ   | 1:A:4347:ILE:HD13 | 2.49        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2397:VAL:HG22 | 1:B:2398:GLN:N    | 2.29        | 0.47     |
| 1:A:3078:VAL:O    | 1:A:3078:VAL:HG13 | 2.13        | 0.47     |
| 1:B:2886:LEU:HD23 | 1:B:2904:LEU:CD2  | 2.44        | 0.47     |
| 1:A:4048:PHE:N    | 1:A:4048:PHE:CD1  | 2.82        | 0.47     |
| 1:B:2613:LEU:HD22 | 1:B:2655:ARG:NH1  | 2.29        | 0.47     |
| 1:B:3960:LEU:HD23 | 1:B:4237:SER:HB2  | 1.96        | 0.47     |
| 1:A:3699:PHE:CZ   | 1:A:3726:ILE:HG13 | 2.49        | 0.47     |
| 1:A:2207:LEU:CD1  | 1:A:2215:ILE:HG21 | 2.43        | 0.47     |
| 1:A:3930:LEU:HD11 | 1:A:3939:ARG:HG2  | 1.95        | 0.47     |
| 1:A:2128:ILE:HG23 | 1:A:2129:VAL:N    | 2.29        | 0.47     |
| 1:B:1568:HIS:O    | 1:B:1572:ILE:HG13 | 2.14        | 0.47     |
| 1:A:3992:LEU:HD22 | 1:A:4430:LEU:HB2  | 1.96        | 0.47     |
| 1:A:3408:VAL:HG23 | 1:A:3409:CYS:H    | 1.80        | 0.47     |
| 1:B:2212:ILE:N    | 1:B:2213:PRO:CD   | 2.77        | 0.47     |
| 1:A:3903:LEU:HD23 | 1:A:4433:MET:SD   | 2.54        | 0.47     |
| 1:A:3074:ASP:H    | 1:A:3077:ASN:HD22 | 1.62        | 0.47     |
| 1:B:2918:VAL:HG22 | 1:B:3172:TRP:CE2  | 2.49        | 0.47     |
| 1:B:1910:MET:HB2  | 1:B:1929:MET:HG3  | 1.95        | 0.47     |
| 1:B:4568:PHE:O    | 1:B:4572:MET:HG2  | 2.14        | 0.47     |
| 1:A:4335:ARG:HD3  | 1:A:4360:LEU:C    | 2.35        | 0.47     |
| 1:A:4268:SER:OG   | 1:A:4387:THR:HA   | 2.14        | 0.47     |
| 1:A:2497:GLU:O    | 1:A:2501:ILE:HG13 | 2.13        | 0.47     |
| 1:A:3781:VAL:HG12 | 1:A:3782:THR:N    | 2.29        | 0.47     |
| 1:A:2313:LYS:CE   | 1:A:2366:ASN:HD21 | 2.17        | 0.47     |
| 1:A:1639:ILE:CD1  | 1:A:1675:LEU:HB3  | 2.44        | 0.47     |
| 1:A:3897:TYR:CE1  | 1:A:3913:LEU:HA   | 2.47        | 0.47     |
| 1:B:1628:LEU:HD13 | 1:B:1709:ILE:HG22 | 1.95        | 0.47     |
| 1:B:3013:LEU:HG   | 1:B:3013:LEU:O    | 2.13        | 0.47     |
| 1:A:1934:PHE:HE1  | 1:A:1964:LEU:HD22 | 1.78        | 0.47     |
| 1:A:3997:ASN:O    | 1:A:3999:THR:N    | 2.47        | 0.47     |
| 1:A:3997:ASN:ND2  | 1:A:4001:ILE:HD11 | 2.27        | 0.47     |
| 1:B:1659:VAL:C    | 1:B:1661:ALA:H    | 2.18        | 0.47     |
| 1:A:3338:GLN:HG3  | 1:A:3529:ILE:HD12 | 1.96        | 0.47     |
| 1:A:2368:ASN:HB3  | 1:A:2410:ARG:NH1  | 2.29        | 0.47     |
| 1:B:1811:PRO:HB2  | 1:B:1814:LEU:HD12 | 1.95        | 0.47     |
| 1:B:3966:THR:N    | 1:B:4426:MET:HE2  | 2.29        | 0.47     |
| 1:B:2309:LYS:O    | 1:B:2758:ARG:HD2  | 2.14        | 0.47     |
| 1:B:2754:TYR:O    | 1:B:2755:GLY:C    | 2.52        | 0.47     |
| 1:A:3804:THR:C    | 1:A:3806:ARG:H    | 2.18        | 0.47     |
| 1:B:2363:TRP:CH2  | 1:B:2395:PHE:HE1  | 2.32        | 0.47     |
| 1:A:2598:GLN:HG3  | 1:A:2612:LEU:HB2  | 1.96        | 0.47     |
| 1:A:2616:SER:OG   | 1:A:2617:VAL:N    | 2.47        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1591:TRP:HA   | 1:B:1591:TRP:CE3  | 2.49        | 0.47     |
| 1:A:3219:ILE:CB   | 1:A:3220:PRO:CD   | 2.93        | 0.47     |
| 1:B:1971:ASN:HA   | 1:B:2075:VAL:O    | 2.14        | 0.47     |
| 1:B:2427:PHE:O    | 1:B:2431:LEU:HG   | 2.14        | 0.47     |
| 1:A:3480:TRP:HE1  | 1:A:3484:GLN:HE21 | 1.62        | 0.47     |
| 1:B:2595:LYS:HE3  | 1:B:2611:PRO:HG3  | 1.96        | 0.47     |
| 1:A:3730:LEU:CD2  | 1:A:3733:VAL:HB   | 2.44        | 0.47     |
| 1:A:2010:SER:O    | 1:A:2060:LEU:HD11 | 2.14        | 0.47     |
| 1:A:4200:LEU:HD22 | 1:A:4204:LEU:CG   | 2.45        | 0.47     |
| 1:B:1920:ASN:ND2  | 1:B:1921:VAL:N    | 2.62        | 0.47     |
| 1:B:1603:ASP:O    | 1:B:1606:ILE:HG22 | 2.15        | 0.47     |
| 1:A:2282:LYS:HB2  | 2:A:9002:ADP:O3B  | 2.15        | 0.47     |
| 1:A:4313:TRP:HB3  | 1:A:4330:PRO:CG   | 2.45        | 0.47     |
| 1:A:1628:LEU:C    | 1:A:1630:PRO:HD3  | 2.35        | 0.47     |
| 1:A:3648:HIS:CE1  | 1:A:3654:SER:HA   | 2.49        | 0.47     |
| 1:A:1592:ASP:O    | 1:A:1596:ASN:HB2  | 2.14        | 0.47     |
| 1:B:3605:PHE:HB3  | 1:B:3609:PHE:HB3  | 1.95        | 0.47     |
| 1:A:4326:PRO:HB3  | 1:A:4369:PHE:HD2  | 1.79        | 0.47     |
| 1:A:2204:ILE:HA   | 1:A:2207:LEU:CD1  | 2.42        | 0.47     |
| 1:A:1831:LEU:HD23 | 1:A:1841:ILE:HG23 | 1.96        | 0.47     |
| 1:A:1831:LEU:HD23 | 1:A:1841:ILE:CG2  | 2.45        | 0.47     |
| 1:B:1766:ILE:HG23 | 1:B:1767:HIS:N    | 2.30        | 0.47     |
| 1:A:2250:VAL:HG21 | 1:A:2425:MET:HA   | 1.97        | 0.47     |
| 1:B:2532:ARG:CZ   | 1:B:2813:ILE:HD12 | 2.45        | 0.47     |
| 1:B:4618:ASN:H    | 1:B:4618:ASN:HD22 | 1.60        | 0.47     |
| 1:B:4596:ASN:C    | 1:B:4596:ASN:ND2  | 2.68        | 0.47     |
| 1:A:3794:GLN:HG3  | 1:A:3891:LEU:HA   | 1.96        | 0.47     |
| 1:B:2667:HIS:HA   | 1:B:2787:GLN:OE1  | 2.14        | 0.47     |
| 1:A:4109:ASP:O    | 1:A:4112:ASN:HB2  | 2.15        | 0.47     |
| 1:A:2273:MET:HB3  | 1:A:2395:PHE:CD1  | 2.50        | 0.47     |
| 1:B:2125:ALA:O    | 1:B:2129:VAL:HG13 | 2.14        | 0.47     |
| 1:A:2196:LEU:HA   | 1:A:2199:ILE:HG12 | 1.97        | 0.47     |
| 1:A:4344:GLY:HA2  | 1:A:4347:ILE:HG13 | 1.95        | 0.47     |
| 1:A:3036:SER:N    | 1:A:3068:LYS:O    | 2.48        | 0.47     |
| 1:B:3698:SER:HB3  | 1:B:3700:LEU:CD1  | 2.44        | 0.47     |
| 1:B:2540:LEU:HB3  | 1:B:2576:SER:OG   | 2.14        | 0.47     |
| 1:B:4359:PHE:O    | 1:B:4362:GLN:HB3  | 2.15        | 0.47     |
| 1:B:2231:ILE:HG12 | 1:B:2260:LEU:HD23 | 1.96        | 0.47     |
| 1:A:4430:LEU:O    | 1:A:4434:GLN:HB2  | 2.15        | 0.47     |
| 1:B:2335:THR:O    | 1:B:2339:ILE:HG13 | 2.14        | 0.47     |
| 1:B:4059:PRO:O    | 1:B:4063:ILE:HD12 | 2.15        | 0.47     |
| 1:B:2676:PRO:HG3  | 1:B:2873:ILE:HD12 | 1.96        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1547:ASN:HD21 | 1:B:1550:ARG:H    | 1.63        | 0.47     |
| 1:B:1611:ARG:O    | 1:B:1615:LEU:HD23 | 2.14        | 0.47     |
| 1:A:2990:LEU:HD23 | 1:A:2994:VAL:HG11 | 1.97        | 0.47     |
| 1:A:1927:ILE:C    | 1:A:1928:HIS:HD2  | 2.18        | 0.47     |
| 1:A:2088:PRO:HB2  | 1:A:2090:ASN:HD21 | 1.80        | 0.47     |
| 1:B:3650:ASN:O    | 1:B:3651:SER:HB2  | 2.15        | 0.47     |
| 1:A:4690:VAL:HG21 | 1:A:4701:PHE:CE1  | 2.50        | 0.47     |
| 1:A:3074:ASP:H    | 1:A:3077:ASN:ND2  | 2.13        | 0.47     |
| 1:B:2882:TRP:CZ2  | 1:B:2909:ALA:HB2  | 2.48        | 0.47     |
| 1:B:1782:ALA:HB2  | 1:B:1922:LEU:HD23 | 1.96        | 0.47     |
| 1:B:2512:VAL:HA   | 1:B:2515:VAL:HG12 | 1.95        | 0.47     |
| 1:A:4043:ASP:OD2  | 1:A:4043:ASP:N    | 2.45        | 0.47     |
| 1:A:3032:MET:O    | 1:A:3034:GLY:N    | 2.47        | 0.47     |
| 1:A:3370:GLU:O    | 1:A:3371:PRO:C    | 2.51        | 0.47     |
| 1:B:4119:ALA:HA   | 1:B:4149:LEU:HD11 | 1.96        | 0.47     |
| 1:B:4673:ASP:C    | 1:B:4675:ASP:H    | 2.18        | 0.47     |
| 1:B:4429:ASP:O    | 1:B:4433:MET:HG3  | 2.15        | 0.47     |
| 1:A:4269:ARG:HA   | 1:A:4392:PHE:CZ   | 2.50        | 0.47     |
| 1:A:4162:ILE:HG13 | 1:A:4187:LEU:HD23 | 1.97        | 0.47     |
| 1:A:2766:MET:CB   | 1:A:2783:LEU:HD11 | 2.42        | 0.47     |
| 1:A:2127:LYS:HB3  | 1:A:2222:VAL:HG13 | 1.97        | 0.47     |
| 1:B:3043:ASN:HD22 | 1:B:3043:ASN:N    | 2.10        | 0.47     |
| 1:A:3563:LEU:O    | 1:A:3567:LEU:HG   | 2.14        | 0.47     |
| 1:A:3988:TRP:O    | 1:A:3992:LEU:HG   | 2.14        | 0.47     |
| 1:A:2641:VAL:O    | 1:A:2646:VAL:HG11 | 2.15        | 0.47     |
| 1:A:4331:TRP:CD1  | 1:A:4366:PRO:HD3  | 2.49        | 0.47     |
| 1:A:4244:VAL:HG23 | 1:A:4403:SER:HB3  | 1.96        | 0.47     |
| 1:B:3849:ASP:HA   | 1:B:3852:ILE:HG22 | 1.97        | 0.47     |
| 1:A:2370:LEU:CD2  | 1:A:2387:LEU:HD22 | 2.45        | 0.47     |
| 1:B:3601:TYR:O    | 1:B:3602:ILE:C    | 2.53        | 0.47     |
| 1:B:4005:ILE:HG21 | 1:B:4008:LEU:HD12 | 1.96        | 0.47     |
| 1:A:3776:ASP:HB3  | 1:A:3780:ARG:HH12 | 1.80        | 0.47     |
| 1:A:4295:PHE:HD2  | 1:A:4295:PHE:C    | 2.18        | 0.47     |
| 1:A:1868:SER:O    | 1:A:1872:ARG:HB2  | 2.15        | 0.47     |
| 1:B:2252:LYS:HE2  | 1:B:2254:GLU:HG2  | 1.96        | 0.47     |
| 1:B:2556:SER:C    | 1:B:2558:PHE:H    | 2.17        | 0.47     |
| 1:B:2587:LEU:HD12 | 1:B:2817:ASP:HB3  | 1.96        | 0.47     |
| 1:B:3930:LEU:O    | 1:B:3931:VAL:C    | 2.53        | 0.47     |
| 1:B:3677:PRO:CG   | 1:B:3787:THR:HG22 | 2.45        | 0.47     |
| 1:B:4157:TYR:HB2  | 1:B:4184:TRP:C    | 2.35        | 0.47     |
| 1:B:2309:LYS:HE2  | 1:B:2756:THR:HG21 | 1.96        | 0.47     |
| 1:B:4136:SER:O    | 1:B:4220:GLU:HA   | 2.15        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2669:PRO:HG2  | 1:B:2810:HIS:O    | 2.14        | 0.47     |
| 1:B:2660:LEU:O    | 1:B:2664:LEU:HB2  | 2.15        | 0.47     |
| 1:A:4376:VAL:HB   | 1:A:4381:LEU:HB2  | 1.97        | 0.47     |
| 1:B:4650:ASN:O    | 1:B:4653:GLN:HG3  | 2.15        | 0.47     |
| 1:B:2701:PHE:CE2  | 1:B:2759:VAL:HG11 | 2.50        | 0.47     |
| 1:A:2424:GLN:HG3  | 1:A:2508:PRO:HG3  | 1.97        | 0.47     |
| 1:A:2905:TRP:CZ3  | 1:A:2934:ALA:HB2  | 2.50        | 0.47     |
| 1:A:2316:LEU:HD23 | 1:A:2363:TRP:HB2  | 1.97        | 0.47     |
| 1:A:3639:SER:HB2  | 1:A:3643:GLU:OE1  | 2.15        | 0.46     |
| 1:A:2651:VAL:CG1  | 1:A:2652:ASP:H    | 2.23        | 0.46     |
| 1:A:3040:ILE:O    | 1:A:3040:ILE:HG22 | 2.14        | 0.46     |
| 1:A:3452:ILE:O    | 1:A:3457:LEU:HD23 | 2.15        | 0.46     |
| 1:A:4537:LEU:HD23 | 1:A:4548:LYS:HE3  | 1.97        | 0.46     |
| 1:A:2065:ILE:HG22 | 1:A:2066:SER:N    | 2.30        | 0.46     |
| 1:A:3285:LEU:HD22 | 1:A:3578:SER:HB2  | 1.97        | 0.46     |
| 1:A:3270:LEU:CB   | 1:A:3592:VAL:HG13 | 2.44        | 0.46     |
| 1:B:2270:HIS:HB3  | 1:B:2392:ARG:NH1  | 2.29        | 0.46     |
| 1:B:2774:ARG:HG2  | 1:B:2776:SER:OG   | 2.15        | 0.46     |
| 1:B:1576:LYS:HG2  | 1:B:1585:GLU:OE2  | 2.14        | 0.46     |
| 1:B:1642:GLU:O    | 1:B:1646:ILE:HG12 | 2.16        | 0.46     |
| 1:A:4599:ALA:O    | 1:A:4602:THR:HG22 | 2.15        | 0.46     |
| 1:B:1788:SER:HA   | 1:B:1810:TYR:CZ   | 2.49        | 0.46     |
| 1:A:4099:HIS:ND1  | 1:A:4111:LEU:HD12 | 2.30        | 0.46     |
| 1:B:3973:ILE:HG13 | 1:B:3988:TRP:CZ3  | 2.50        | 0.46     |
| 1:B:1555:VAL:H    | 1:B:1609:GLN:NE2  | 2.12        | 0.46     |
| 1:B:4604:THR:HG23 | 1:B:4671:TRP:NE1  | 2.21        | 0.46     |
| 1:A:2101:ILE:N    | 1:A:2101:ILE:HD13 | 2.30        | 0.46     |
| 1:B:3027:ARG:HA   | 1:B:3037:ILE:CD1  | 2.43        | 0.46     |
| 1:A:1886:ARG:CZ   | 1:A:1890:ARG:HH22 | 2.28        | 0.46     |
| 1:B:2532:ARG:HG3  | 1:B:2808:LEU:O    | 2.14        | 0.46     |
| 1:B:4128:SER:HB2  | 1:B:4213:PHE:HB3  | 1.96        | 0.46     |
| 1:A:4067:ALA:C    | 1:A:4073:GLN:HE21 | 2.19        | 0.46     |
| 1:B:1788:SER:HA   | 1:B:1810:TYR:CE2  | 2.50        | 0.46     |
| 1:A:1969:GLY:N    | 1:A:2047:GLN:NE2  | 2.64        | 0.46     |
| 1:A:2415:TRP:HA   | 1:A:2415:TRP:CE3  | 2.51        | 0.46     |
| 1:A:2720:TYR:CE1  | 1:A:2730:LEU:HD13 | 2.50        | 0.46     |
| 1:B:4030:PHE:HE1  | 1:B:4085:LEU:HG   | 1.80        | 0.46     |
| 1:A:4220:GLU:O    | 1:A:4222:HIS:N    | 2.49        | 0.46     |
| 1:B:4190:ILE:HG12 | 1:B:4219:SER:CB   | 2.44        | 0.46     |
| 1:A:2956:LEU:HD21 | 1:A:2971:TYR:CD2  | 2.50        | 0.46     |
| 1:A:3975:SER:C    | 1:A:3977:LYS:H    | 2.18        | 0.46     |
| 1:A:3021:GLY:O    | 1:A:3025:LEU:HB2  | 2.14        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1601:LEU:HA   | 1:B:1666:GLN:OE1  | 2.16        | 0.46     |
| 1:A:3283:LEU:HD23 | 1:A:3283:LEU:C    | 2.36        | 0.46     |
| 1:A:1809:ASN:HD22 | 1:A:1809:ASN:HA   | 1.60        | 0.46     |
| 1:A:2492:LEU:HG   | 1:A:2496:LYS:NZ   | 2.31        | 0.46     |
| 1:A:4087:LYS:HG2  | 1:A:4087:LYS:O    | 2.15        | 0.46     |
| 1:A:2903:ARG:HB2  | 1:A:2945:ALA:O    | 2.15        | 0.46     |
| 1:A:4589:VAL:HG22 | 1:A:4590:TRP:N    | 2.29        | 0.46     |
| 1:B:2529:THR:OG1  | 1:B:2532:ARG:HB2  | 2.15        | 0.46     |
| 1:B:2191:GLU:HA   | 1:B:2194:VAL:HG23 | 1.98        | 0.46     |
| 1:A:3219:ILE:CB   | 1:A:3220:PRO:HD3  | 2.46        | 0.46     |
| 1:A:1630:PRO:O    | 1:A:1634:THR:HG23 | 2.15        | 0.46     |
| 1:A:2882:TRP:CZ2  | 1:A:2905:TRP:NE1  | 2.83        | 0.46     |
| 1:B:3288:GLY:HA3  | 1:B:3574:TRP:CZ3  | 2.49        | 0.46     |
| 1:B:3773:PHE:HB3  | 1:B:3777:LEU:HD23 | 1.98        | 0.46     |
| 1:B:2937:HIS:C    | 1:B:2939:PRO:HD3  | 2.35        | 0.46     |
| 1:A:3071:PHE:HE2  | 1:A:3087:MET:HE3  | 1.79        | 0.46     |
| 1:B:1555:VAL:H    | 1:B:1609:GLN:HE22 | 1.64        | 0.46     |
| 1:A:2257:GLU:O    | 1:A:2261:GLN:HG2  | 2.16        | 0.46     |
| 1:A:2856:PHE:CZ   | 1:A:2930:ILE:HG12 | 2.49        | 0.46     |
| 1:A:3733:VAL:C    | 1:A:3735:ASN:H    | 2.19        | 0.46     |
| 1:B:2127:LYS:C    | 1:B:2130:PRO:HD2  | 2.35        | 0.46     |
| 1:B:1846:GLN:O    | 1:B:1849:GLU:HB3  | 2.16        | 0.46     |
| 1:A:1948:VAL:O    | 1:A:1950:THR:N    | 2.49        | 0.46     |
| 1:B:2907:HIS:HB2  | 1:B:2950:ILE:HG21 | 1.96        | 0.46     |
| 1:A:3998:LEU:HD13 | 1:A:3998:LEU:O    | 2.15        | 0.46     |
| 1:A:3324:LEU:HD12 | 1:A:3539:LEU:CD2  | 2.46        | 0.46     |
| 1:A:2435:SER:HB3  | 1:A:2496:LYS:HG2  | 1.97        | 0.46     |
| 1:A:2101:ILE:HG13 | 1:A:4348:ASP:HB2  | 1.98        | 0.46     |
| 1:A:3387:HIS:HB2  | 1:A:3473:ALA:HB2  | 1.95        | 0.46     |
| 1:A:3725:ASN:N    | 1:A:3725:ASN:HD22 | 1.99        | 0.46     |
| 1:A:2832:ASN:ND2  | 1:A:2883:ASP:OD2  | 2.49        | 0.46     |
| 1:A:4044:TRP:HE3  | 1:A:4048:PHE:HE1  | 1.62        | 0.46     |
| 1:A:4044:TRP:CE2  | 1:A:4059:PRO:HG3  | 2.51        | 0.46     |
| 1:B:3891:LEU:HD21 | 1:B:3895:ARG:NH2  | 2.31        | 0.46     |
| 1:B:2748:LEU:HD11 | 1:B:3162:PRO:HG2  | 1.97        | 0.46     |
| 1:A:3113:LYS:HG3  | 1:A:3123:LEU:O    | 2.15        | 0.46     |
| 1:A:3007:GLN:O    | 1:A:3142:HIS:HE1  | 1.99        | 0.46     |
| 1:B:1799:ASP:OD1  | 1:B:1801:SER:HB3  | 2.15        | 0.46     |
| 1:A:2376:LEU:HA   | 1:A:2385:LEU:O    | 2.15        | 0.46     |
| 1:A:1786:SER:HB2  | 1:A:1914:TYR:OH   | 2.16        | 0.46     |
| 1:B:1721:HIS:C    | 1:B:1725:MET:HE2  | 2.36        | 0.46     |
| 1:B:4296:PHE:HB3  | 1:B:4346:ARG:HD2  | 1.98        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1962:GLN:CB   | 1:B:4341:THR:HG21 | 2.46        | 0.46     |
| 1:B:2841:ASN:ND2  | 1:B:2842:LEU:HG   | 2.31        | 0.46     |
| 1:A:4318:SER:HA   | 1:A:4321:ARG:NH2  | 2.23        | 0.46     |
| 1:B:4222:HIS:ND1  | 1:B:4223:PRO:HD2  | 2.31        | 0.46     |
| 1:B:4020:LEU:HG   | 1:B:4034:VAL:HG22 | 1.98        | 0.46     |
| 1:A:3990:PHE:HD2  | 1:A:4084:LEU:HD22 | 1.81        | 0.46     |
| 1:B:2532:ARG:NH1  | 1:B:2813:ILE:HD12 | 2.31        | 0.46     |
| 1:A:2243:ILE:HG21 | 1:A:2288:VAL:HG13 | 1.96        | 0.46     |
| 1:B:3788:VAL:HG11 | 1:B:3913:LEU:CD2  | 2.46        | 0.46     |
| 1:A:3830:LEU:HD12 | 1:A:3858:LEU:HD13 | 1.96        | 0.46     |
| 1:A:2578:MET:HE1  | 1:A:2613:LEU:HA   | 1.96        | 0.46     |
| 1:B:2749:PRO:O    | 1:B:2757:GLN:HG2  | 2.16        | 0.46     |
| 1:B:4645:GLU:HG3  | 1:B:4722:SER:OG   | 2.15        | 0.46     |
| 1:B:4281:ILE:HG13 | 1:B:4282:GLN:N    | 2.31        | 0.46     |
| 1:A:2205:PRO:HG3  | 1:A:2261:GLN:OE1  | 2.16        | 0.46     |
| 1:A:2603:THR:HG22 | 1:A:2604:PRO:HD2  | 1.97        | 0.46     |
| 1:A:2059:LEU:HG   | 1:A:2060:LEU:HG   | 1.97        | 0.46     |
| 1:A:4719:ARG:HH11 | 1:A:4719:ARG:HG3  | 1.81        | 0.46     |
| 1:A:2360:ASP:HB2  | 1:A:2361:PRO:HD2  | 1.96        | 0.46     |
| 1:A:1904:PHE:C    | 1:A:1906:TRP:H    | 2.17        | 0.46     |
| 1:A:2829:GLY:HA2  | 1:A:2850:THR:OG1  | 2.16        | 0.46     |
| 1:B:4597:PRO:HG2  | 1:B:4692:LEU:CD1  | 2.46        | 0.46     |
| 1:A:4022:CYS:O    | 1:A:4026:GLN:HB2  | 2.16        | 0.46     |
| 1:A:4681:ASN:ND2  | 1:A:4685:LYS:HE3  | 2.30        | 0.46     |
| 1:A:2443:GLU:OE2  | 1:A:2489:PRO:HB2  | 2.15        | 0.46     |
| 1:B:3993:LYS:O    | 1:B:3994:GLY:C    | 2.54        | 0.46     |
| 1:A:4395:TRP:CZ3  | 1:A:4399:LEU:HD11 | 2.51        | 0.46     |
| 1:A:3925:ASN:N    | 1:A:3925:ASN:ND2  | 2.63        | 0.46     |
| 1:B:1683:LEU:O    | 1:B:1683:LEU:HD12 | 2.16        | 0.46     |
| 1:B:3715:GLY:HA3  | 1:B:3758:PRO:HG2  | 1.98        | 0.46     |
| 1:A:4596:ASN:ND2  | 1:A:4596:ASN:C    | 2.69        | 0.46     |
| 1:A:1530:PHE:CZ   | 1:A:1571:SER:HB2  | 2.51        | 0.46     |
| 1:A:1745:SER:OG   | 1:A:1751:THR:HG22 | 2.16        | 0.46     |
| 1:B:4331:TRP:CZ2  | 1:B:4369:PHE:HE2  | 2.34        | 0.46     |
| 1:B:4284:ARG:NH2  | 1:B:4355:LEU:HD21 | 2.31        | 0.46     |
| 1:A:3017:VAL:HG21 | 1:A:3257:PRO:HD3  | 1.98        | 0.46     |
| 1:A:2864:PHE:HB3  | 1:A:2872:TYR:HD2  | 1.81        | 0.46     |
| 1:B:3789:THR:H    | 1:B:3792:SER:HB3  | 1.81        | 0.46     |
| 1:A:4278:HIS:HD2  | 1:A:4343:TYR:OH   | 1.99        | 0.46     |
| 1:A:2641:VAL:O    | 1:A:2643:SER:N    | 2.49        | 0.46     |
| 1:A:4402:ILE:CD1  | 1:A:4402:ILE:H    | 2.28        | 0.46     |
| 1:A:1911:ARG:HD3  | 1:A:1911:ARG:H    | 1.81        | 0.46     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:4095:LEU:HD11 | 1:B:4422:LYS:HB3  | 1.97        | 0.46     |
| 1:B:4274:LEU:HD11 | 1:B:4306:ALA:HB1  | 1.98        | 0.46     |
| 1:A:2952:TYR:CZ   | 1:A:2962:PRO:HG3  | 2.51        | 0.46     |
| 1:B:4400:PRO:HG2  | 1:B:4407:TRP:HH2  | 1.81        | 0.46     |
| 1:B:2044:GLN:O    | 1:B:2048:VAL:HG23 | 2.16        | 0.46     |
| 1:A:4263:GLN:NE2  | 1:A:4322:SER:HA   | 2.30        | 0.46     |
| 1:A:1662:ILE:HG22 | 1:A:1663:GLU:N    | 2.32        | 0.46     |
| 1:B:4574:GLN:NE2  | 1:B:4590:TRP:HB3  | 2.31        | 0.45     |
| 1:B:1822:VAL:HG13 | 1:B:1823:TRP:N    | 2.31        | 0.45     |
| 1:B:2275:VAL:HG11 | 1:B:2400:LEU:HG   | 1.97        | 0.45     |
| 1:B:1534:VAL:HG22 | 1:B:1568:HIS:CD2  | 2.50        | 0.45     |
| 1:B:2873:ILE:O    | 1:B:2873:ILE:HG13 | 2.14        | 0.45     |
| 1:B:4434:GLN:HE21 | 1:B:4434:GLN:HB3  | 1.55        | 0.45     |
| 1:A:2249:LEU:HB3  | 2:A:9002:ADP:N6   | 2.30        | 0.45     |
| 1:A:2980:TYR:OH   | 1:A:2987:PRO:HA   | 2.15        | 0.45     |
| 1:B:1604:VAL:O    | 1:B:1608:VAL:HG23 | 2.16        | 0.45     |
| 1:B:3912:SER:HB3  | 1:B:4231:ARG:CG   | 2.45        | 0.45     |
| 1:B:4122:VAL:HG11 | 1:B:4216:PHE:HZ   | 1.81        | 0.45     |
| 1:B:1985:LYS:HD3  | 1:B:1997:VAL:HG21 | 1.98        | 0.45     |
| 1:A:2851:ASP:HB3  | 1:A:2937:HIS:CE1  | 2.51        | 0.45     |
| 1:A:1642:GLU:O    | 1:A:1646:ILE:HG13 | 2.16        | 0.45     |
| 1:A:4726:TRP:CH2  | 1:A:4728:SER:HB2  | 2.51        | 0.45     |
| 1:A:2338:ARG:HH11 | 1:A:2338:ARG:HG2  | 1.81        | 0.45     |
| 1:B:1931:ASN:HD21 | 1:B:1962:GLN:HE22 | 1.64        | 0.45     |
| 1:A:3015:ILE:CG2  | 1:A:3149:PRO:HG3  | 2.45        | 0.45     |
| 1:B:2309:LYS:HZ3  | 1:B:2756:THR:HG21 | 1.77        | 0.45     |
| 1:A:3271:ILE:HG12 | 1:A:3592:VAL:HG21 | 1.97        | 0.45     |
| 1:B:4379:ILE:HG23 | 1:B:4381:LEU:HG   | 1.98        | 0.45     |
| 1:B:2331:LEU:HD21 | 1:B:2773:TRP:CG   | 2.51        | 0.45     |
| 1:B:2723:THR:HG22 | 1:B:2727:GLU:O    | 2.16        | 0.45     |
| 1:A:4309:SER:O    | 1:A:4312:TYR:HB3  | 2.16        | 0.45     |
| 1:A:4039:GLN:HB3  | 1:A:4040:ASN:H    | 1.57        | 0.45     |
| 1:A:3023:SER:HB2  | 2:A:9004:ADP:O1A  | 2.16        | 0.45     |
| 1:A:3551:SER:O    | 1:A:3554:LYS:HB2  | 2.16        | 0.45     |
| 1:A:3814:SER:C    | 1:A:3818:LYS:HD3  | 2.37        | 0.45     |
| 1:A:4653:GLN:O    | 1:A:4655:THR:HG23 | 2.17        | 0.45     |
| 1:A:4337:ILE:O    | 1:A:4341:THR:HG22 | 2.16        | 0.45     |
| 1:A:3481:ALA:O    | 1:A:3485:THR:HG23 | 2.16        | 0.45     |
| 1:A:3190:ARG:C    | 1:A:3192:LEU:H    | 2.20        | 0.45     |
| 1:A:4281:ILE:HG13 | 1:A:4282:GLN:N    | 2.31        | 0.45     |
| 1:A:3798:LEU:O    | 1:A:3802:LEU:HG   | 2.17        | 0.45     |
| 1:B:2745:GLU:HG2  | 1:B:2748:LEU:HD11 | 1.98        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4026:GLN:HB3  | 1:A:4027:VAL:H    | 1.60        | 0.45     |
| 1:B:4431:GLN:HG2  | 1:B:4431:GLN:O    | 2.16        | 0.45     |
| 1:A:2896:CYS:SG   | 1:A:2897:THR:N    | 2.90        | 0.45     |
| 1:B:4335:ARG:NH2  | 1:B:4365:THR:HG22 | 2.22        | 0.45     |
| 1:B:4047:PHE:HE1  | 1:B:4086:MET:HE1  | 1.81        | 0.45     |
| 1:B:3990:PHE:HD2  | 1:B:4084:LEU:HD22 | 1.82        | 0.45     |
| 1:A:2845:PHE:O    | 1:A:2848:ASN:HB2  | 2.16        | 0.45     |
| 1:A:2976:LEU:HD12 | 1:A:3028:PHE:CE1  | 2.51        | 0.45     |
| 1:A:2398:GLN:NE2  | 1:A:2806:ARG:HG2  | 2.31        | 0.45     |
| 1:B:3015:ILE:HD12 | 1:B:3170:LEU:HD11 | 1.98        | 0.45     |
| 1:B:2849:LEU:HD13 | 1:B:2901:LEU:HD11 | 1.99        | 0.45     |
| 1:B:3306:LEU:HD13 | 1:B:3557:VAL:CG2  | 2.46        | 0.45     |
| 1:A:2738:TRP:CZ3  | 1:A:2785:LYS:HA   | 2.51        | 0.45     |
| 1:B:3536:TYR:O    | 1:B:3540:ILE:HD13 | 2.16        | 0.45     |
| 1:A:3792:SER:OG   | 1:A:3793:LEU:N    | 2.50        | 0.45     |
| 1:A:3893:CYS:HB3  | 1:A:3916:PHE:HZ   | 1.81        | 0.45     |
| 1:A:2323:THR:O    | 1:A:2324:THR:HG23 | 2.16        | 0.45     |
| 1:A:4279:ALA:O    | 1:A:4283:GLU:HB2  | 2.17        | 0.45     |
| 1:B:3930:LEU:HD22 | 1:B:3939:ARG:HE   | 1.81        | 0.45     |
| 1:A:4648:VAL:HG23 | 1:A:4655:THR:OG1  | 2.16        | 0.45     |
| 1:A:3686:MET:CE   | 1:A:3696:LYS:HB2  | 2.46        | 0.45     |
| 1:A:4349:ASN:O    | 1:A:4352:ASP:HB2  | 2.16        | 0.45     |
| 1:A:3459:ASP:HB3  | 1:A:3462:PHE:CB   | 2.47        | 0.45     |
| 1:B:4012:LEU:HA   | 1:B:4016:GLN:NE2  | 2.31        | 0.45     |
| 1:A:3549:GLU:O    | 1:A:3553:VAL:HG23 | 2.17        | 0.45     |
| 1:B:2630:LYS:CB   | 1:B:2654:THR:HG21 | 2.47        | 0.45     |
| 1:B:3673:LEU:HD22 | 1:B:3783:PHE:CE1  | 2.48        | 0.45     |
| 1:A:2603:THR:CB   | 1:A:2604:PRO:HD2  | 2.46        | 0.45     |
| 1:A:3897:TYR:HD2  | 1:A:3898:PHE:CD2  | 2.34        | 0.45     |
| 1:A:1784:LEU:HB3  | 1:A:1814:LEU:HD13 | 1.99        | 0.45     |
| 1:A:1842:GLN:OE1  | 1:A:1893:GLN:HG2  | 2.17        | 0.45     |
| 1:B:4714:GLN:O    | 1:B:4718:GLN:HG3  | 2.16        | 0.45     |
| 1:A:3011:HIS:C    | 1:A:3168:CYS:HB3  | 2.36        | 0.45     |
| 1:A:3919:ILE:HD13 | 1:A:3951:THR:HA   | 1.98        | 0.45     |
| 1:A:1973:PHE:C    | 1:A:1973:PHE:CD1  | 2.89        | 0.45     |
| 1:B:4693:ASN:ND2  | 1:B:4693:ASN:N    | 2.64        | 0.45     |
| 1:A:1964:LEU:HD12 | 1:A:2074:PHE:CZ   | 2.51        | 0.45     |
| 1:A:1968:MET:HB3  | 1:A:2094:LEU:O    | 2.16        | 0.45     |
| 1:B:4404:THR:HB   | 1:B:4405:PRO:HD2  | 1.99        | 0.45     |
| 1:B:2819:PRO:HB2  | 1:B:2824:LEU:CD2  | 2.46        | 0.45     |
| 1:A:1726:PHE:HB2  | 1:A:1729:LEU:HB3  | 1.98        | 0.45     |
| 1:A:3350:VAL:O    | 1:A:3350:VAL:HG12 | 2.15        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4249:LEU:O    | 1:A:4253:ILE:HG13 | 2.17        | 0.45     |
| 1:A:2435:SER:CB   | 1:A:2496:LYS:HG2  | 2.47        | 0.45     |
| 1:A:3234:ILE:O    | 1:A:3238:ILE:HD13 | 2.17        | 0.45     |
| 1:A:2124:LEU:HD22 | 1:A:2195:LEU:CD2  | 2.46        | 0.45     |
| 1:A:3388:LEU:CD2  | 1:A:3473:ALA:HB1  | 2.44        | 0.45     |
| 1:B:2825:THR:HG23 | 1:B:2854:VAL:HG21 | 1.98        | 0.45     |
| 1:A:1907:LEU:HD22 | 1:A:1911:ARG:NH1  | 2.31        | 0.45     |
| 1:B:4666:ILE:HG13 | 1:B:4667:ALA:N    | 2.32        | 0.45     |
| 1:B:3696:LYS:HG3  | 1:B:3719:LEU:HD23 | 1.99        | 0.45     |
| 1:B:3542:GLU:O    | 1:B:3546:ILE:HG12 | 2.16        | 0.45     |
| 1:A:3463:ASP:O    | 1:A:3467:VAL:HG23 | 2.17        | 0.45     |
| 1:B:3004:VAL:O    | 1:B:3010:GLY:HA3  | 2.17        | 0.45     |
| 1:A:3022:LYS:HA   | 1:A:3173:PHE:CE1  | 2.52        | 0.45     |
| 1:A:4384:PRO:HG2  | 1:A:4392:PHE:CD1  | 2.51        | 0.45     |
| 1:A:4668:THR:C    | 1:A:4669:LEU:HD12 | 2.37        | 0.45     |
| 1:B:3990:PHE:CZ   | 1:B:4023:LEU:HD13 | 2.52        | 0.45     |
| 1:A:2902:VAL:HG21 | 1:A:2941:VAL:CG2  | 2.47        | 0.45     |
| 1:A:1922:LEU:HD13 | 1:A:1938:PHE:CD1  | 2.48        | 0.45     |
| 1:B:1618:ILE:HD13 | 1:B:1683:LEU:HD21 | 1.99        | 0.45     |
| 1:B:4197:LEU:HB3  | 1:B:4226:PRO:HG2  | 1.98        | 0.45     |
| 1:A:4329:ILE:HB   | 1:A:4331:TRP:CE2  | 2.51        | 0.45     |
| 1:A:3911:PHE:CZ   | 1:A:3955:VAL:HG13 | 2.52        | 0.45     |
| 1:B:4618:ASN:N    | 1:B:4618:ASN:ND2  | 2.65        | 0.45     |
| 1:A:1800:HIS:CD2  | 1:A:1858:ASN:HB3  | 2.52        | 0.45     |
| 1:B:2091:LEU:HD22 | 1:B:2095:PHE:CE2  | 2.51        | 0.45     |
| 1:B:1740:THR:HG22 | 1:B:1759:SER:HA   | 1.98        | 0.45     |
| 1:A:3602:ILE:O    | 1:A:3603:GLY:C    | 2.54        | 0.45     |
| 1:A:2140:SER:HB2  | 1:A:2211:ASP:OD2  | 2.15        | 0.45     |
| 1:A:4046:GLN:NE2  | 1:A:4057:ILE:HG22 | 2.32        | 0.45     |
| 1:A:3639:SER:OG   | 1:A:3663:ILE:HD11 | 2.17        | 0.45     |
| 1:B:4657:THR:HG22 | 1:B:4658:ASP:N    | 2.32        | 0.45     |
| 1:A:2196:LEU:HA   | 1:A:2199:ILE:CG1  | 2.46        | 0.45     |
| 1:A:4347:ILE:CG2  | 1:A:4353:MET:HG2  | 2.43        | 0.45     |
| 1:B:2204:ILE:N    | 1:B:2205:PRO:CD   | 2.80        | 0.45     |
| 1:A:3145:PHE:CG   | 1:A:3164:LEU:HD11 | 2.52        | 0.45     |
| 1:A:2526:MET:O    | 1:A:2527:ASP:C    | 2.55        | 0.45     |
| 1:B:3992:LEU:HD12 | 1:B:4434:GLN:NE2  | 2.31        | 0.45     |
| 1:A:2052:GLU:O    | 1:A:2053:ASN:CB   | 2.64        | 0.45     |
| 1:A:4032:LYS:HA   | 1:A:4032:LYS:HE2  | 1.97        | 0.45     |
| 1:B:2270:HIS:HB3  | 1:B:2392:ARG:HH11 | 1.82        | 0.45     |
| 1:B:4095:LEU:HD11 | 1:B:4422:LYS:HB2  | 1.99        | 0.45     |
| 1:A:3218:ALA:O    | 1:A:3220:PRO:N    | 2.49        | 0.45     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4311:ASP:O    | 1:A:4315:ASP:HB3  | 2.17        | 0.45     |
| 1:B:3254:TYR:CD2  | 1:B:3775:PRO:HA   | 2.52        | 0.45     |
| 1:B:4621:LEU:HG   | 1:B:4622:HIS:H    | 1.82        | 0.45     |
| 1:A:1925:LEU:HD23 | 1:A:1936:TYR:HB2  | 1.98        | 0.45     |
| 1:B:1548:TYR:HD2  | 1:B:1554:LEU:HD11 | 1.82        | 0.45     |
| 1:A:2272:VAL:HB   | 1:A:2394:MET:HE2  | 1.97        | 0.45     |
| 1:A:3813:ARG:HA   | 1:A:3875:VAL:HG11 | 1.99        | 0.45     |
| 1:A:3696:LYS:HZ3  | 1:A:3721:GLN:CD   | 2.21        | 0.45     |
| 1:B:2641:VAL:HG13 | 1:B:2831:PHE:HB3  | 1.98        | 0.45     |
| 1:B:4220:GLU:O    | 1:B:4222:HIS:N    | 2.50        | 0.45     |
| 1:A:3912:SER:HB3  | 1:A:4231:ARG:CG   | 2.45        | 0.45     |
| 1:B:3078:VAL:O    | 1:B:3078:VAL:HG13 | 2.16        | 0.45     |
| 1:B:4197:LEU:HD13 | 1:B:4226:PRO:HD3  | 1.99        | 0.45     |
| 1:A:3903:LEU:HD13 | 1:A:3959:LEU:HD21 | 1.99        | 0.45     |
| 1:A:4116:LEU:HB3  | 1:A:4117:ASP:H    | 1.52        | 0.45     |
| 1:A:3540:ILE:N    | 1:A:3540:ILE:HD12 | 2.32        | 0.45     |
| 1:B:1764:PRO:HB2  | 1:B:1768:GLU:CB   | 2.47        | 0.45     |
| 1:A:3542:GLU:O    | 1:A:3546:ILE:HG13 | 2.17        | 0.45     |
| 1:B:2998:ILE:CG2  | 1:B:3025:LEU:HD22 | 2.47        | 0.45     |
| 1:A:4455:SER:C    | 1:A:4457:SER:H    | 2.20        | 0.45     |
| 1:A:3908:LEU:HD21 | 1:A:4237:SER:OG   | 2.16        | 0.45     |
| 1:A:3027:ARG:HH11 | 1:A:3027:ARG:HB2  | 1.81        | 0.45     |
| 1:B:4253:ILE:HG22 | 1:B:4253:ILE:O    | 2.17        | 0.45     |
| 1:B:2381:ASN:ND2  | 1:B:2383:GLU:HB2  | 2.20        | 0.44     |
| 1:A:4076:ILE:HD12 | 1:A:4105:VAL:HG22 | 1.99        | 0.44     |
| 1:A:3682:MET:CE   | 1:A:3721:GLN:HE21 | 2.31        | 0.44     |
| 1:A:2730:LEU:HD22 | 1:A:2772:PHE:CZ   | 2.52        | 0.44     |
| 1:A:1958:LEU:O    | 1:A:1962:GLN:HB2  | 2.16        | 0.44     |
| 1:B:2774:ARG:C    | 1:B:2776:SER:H    | 2.20        | 0.44     |
| 1:B:1869:ALA:HA   | 1:B:1872:ARG:HB3  | 1.99        | 0.44     |
| 1:A:3825:VAL:HA   | 1:A:3828:ARG:HD3  | 1.99        | 0.44     |
| 1:A:3776:ASP:HB3  | 1:A:3780:ARG:NH1  | 2.31        | 0.44     |
| 1:B:2705:THR:HG22 | 1:B:2759:VAL:HG21 | 1.98        | 0.44     |
| 1:B:1629:LEU:HD22 | 1:B:1632:GLU:HG2  | 1.98        | 0.44     |
| 1:A:1777:MET:CE   | 1:A:1939:GLU:HA   | 2.48        | 0.44     |
| 1:A:2142:GLN:NE2  | 1:A:2208:VAL:HG21 | 2.32        | 0.44     |
| 1:A:2359:VAL:HG11 | 1:A:2400:LEU:HD22 | 1.99        | 0.44     |
| 1:B:3233:TYR:CG   | 1:B:3620:ARG:HG3  | 2.52        | 0.44     |
| 1:A:4121:ILE:HG22 | 1:A:4122:VAL:N    | 2.32        | 0.44     |
| 1:A:2898:LEU:HD13 | 1:A:2898:LEU:O    | 2.17        | 0.44     |
| 1:A:1609:GLN:O    | 1:A:1613:VAL:HG23 | 2.17        | 0.44     |
| 1:B:2263:HIS:HB2  | 1:B:2289:TYR:CE1  | 2.52        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1748:GLU:HB3  | 1:A:1943:ILE:HD12 | 1.99        | 0.44     |
| 1:B:4192:LEU:C    | 1:B:4194:PRO:HD3  | 2.38        | 0.44     |
| 1:A:3408:VAL:HG23 | 1:A:3409:CYS:N    | 2.32        | 0.44     |
| 1:A:3490:ILE:O    | 1:A:3490:ILE:HG13 | 2.18        | 0.44     |
| 1:A:3974:ILE:O    | 1:A:3977:LYS:HB2  | 2.17        | 0.44     |
| 1:A:2302:GLU:HG2  | 1:A:2304:HIS:HE1  | 1.81        | 0.44     |
| 1:B:3088:ASN:OD1  | 1:B:3163:ALA:HB3  | 2.17        | 0.44     |
| 1:A:2433:THR:HG23 | 1:A:2437:GLU:HG3  | 1.99        | 0.44     |
| 1:B:2955:TRP:HZ2  | 1:B:3002:ASP:OD1  | 2.00        | 0.44     |
| 1:A:3809:THR:HG22 | 1:A:3812:LYS:NZ   | 2.32        | 0.44     |
| 1:A:2502:ILE:HD12 | 1:A:2506:PHE:HE2  | 1.82        | 0.44     |
| 1:A:3361:LYS:HE2  | 1:A:3361:LYS:HB3  | 1.84        | 0.44     |
| 1:A:2056:GLU:O    | 1:A:2056:GLU:HG3  | 2.17        | 0.44     |
| 1:A:4691:TYR:HA   | 1:A:4699:LEU:HA   | 1.99        | 0.44     |
| 1:B:2660:LEU:HD21 | 1:B:2672:LEU:CD2  | 2.48        | 0.44     |
| 1:A:2016:LEU:HD21 | 1:A:2023:GLY:CA   | 2.47        | 0.44     |
| 1:B:4686:LEU:HD12 | 1:B:4687:SER:H    | 1.83        | 0.44     |
| 1:A:3055:LEU:O    | 1:A:3059:LEU:HD23 | 2.17        | 0.44     |
| 1:A:2340:ILE:HD11 | 1:A:2386:ALA:O    | 2.17        | 0.44     |
| 1:B:4266:GLU:HG3  | 1:B:4369:PHE:CE1  | 2.52        | 0.44     |
| 1:A:3670:ARG:NH1  | 1:A:3781:VAL:O    | 2.51        | 0.44     |
| 1:A:2399:ASP:O    | 1:A:2400:LEU:HD23 | 2.16        | 0.44     |
| 1:B:2381:ASN:ND2  | 1:B:2381:ASN:C    | 2.71        | 0.44     |
| 1:A:3731:ASN:H    | 1:A:3731:ASN:ND2  | 2.09        | 0.44     |
| 1:B:3601:TYR:O    | 1:B:3603:GLY:N    | 2.50        | 0.44     |
| 1:A:2046:ILE:HD11 | 1:A:2059:LEU:HD22 | 2.00        | 0.44     |
| 1:A:2902:VAL:HG22 | 1:A:2938:PHE:CD2  | 2.53        | 0.44     |
| 1:A:2742:PHE:HD1  | 1:A:2789:VAL:HG12 | 1.83        | 0.44     |
| 1:B:3958:THR:CG2  | 1:B:4235:VAL:HB   | 2.47        | 0.44     |
| 1:A:2641:VAL:HG21 | 1:A:2887:LEU:HD13 | 1.99        | 0.44     |
| 1:B:1640:ASN:ND2  | 1:B:1644:ILE:HG12 | 2.32        | 0.44     |
| 1:B:4693:ASN:HD22 | 1:B:4693:ASN:H    | 1.64        | 0.44     |
| 1:B:3316:LYS:HD2  | 1:B:3546:ILE:CD1  | 2.47        | 0.44     |
| 1:B:3011:HIS:CE1  | 1:B:3091:LEU:HA   | 2.53        | 0.44     |
| 1:B:4244:VAL:HG23 | 1:B:4403:SER:OG   | 2.18        | 0.44     |
| 1:B:4405:PRO:HD3  | 1:B:4415:GLU:HG2  | 1.98        | 0.44     |
| 1:A:3805:GLU:HB3  | 1:A:3886:TYR:OH   | 2.17        | 0.44     |
| 1:A:3675:ILE:O    | 1:A:3675:ILE:HG22 | 2.17        | 0.44     |
| 1:B:4087:LYS:HG2  | 1:B:4087:LYS:O    | 2.17        | 0.44     |
| 1:A:3338:GLN:NE2  | 1:A:3525:LEU:HB2  | 2.32        | 0.44     |
| 1:A:2200:ASN:O    | 1:A:2204:ILE:HG12 | 2.18        | 0.44     |
| 1:A:2200:ASN:ND2  | 1:A:2228:LEU:HD13 | 2.18        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:3602:ILE:HG23 | 1:B:3610:ARG:CG   | 2.43        | 0.44     |
| 1:A:4513:ILE:HA   | 1:A:4550:TRP:HE1  | 1.82        | 0.44     |
| 1:A:3154:PHE:C    | 1:A:3156:ASN:H    | 2.21        | 0.44     |
| 1:B:1828:ASP:OD2  | 1:B:1901:ASN:HB2  | 2.17        | 0.44     |
| 1:A:3293:ARG:HG3  | 1:A:3293:ARG:NH1  | 2.27        | 0.44     |
| 1:A:3902:GLU:O    | 1:A:3905:GLN:HG2  | 2.17        | 0.44     |
| 1:B:2976:LEU:CD1  | 1:B:2990:LEU:HD11 | 2.48        | 0.44     |
| 1:A:3274:LYS:HA   | 1:A:3274:LYS:HD3  | 1.77        | 0.44     |
| 1:B:2886:LEU:O    | 1:B:2890:ILE:HG13 | 2.18        | 0.44     |
| 1:A:1719:GLN:OE1  | 1:A:1732:LEU:N    | 2.50        | 0.44     |
| 1:B:2301:SER:HA   | 1:B:2350:ARG:O    | 2.18        | 0.44     |
| 1:A:2339:ILE:HG21 | 1:A:2391:VAL:CG2  | 2.48        | 0.44     |
| 1:A:3727:ASP:CB   | 1:A:3729:VAL:HG12 | 2.48        | 0.44     |
| 1:A:4673:ASP:O    | 1:A:4677:PRO:HD2  | 2.18        | 0.44     |
| 1:A:4075:THR:HG23 | 1:A:4076:ILE:H    | 1.82        | 0.44     |
| 1:A:4296:PHE:HE2  | 1:A:4347:ILE:HA   | 1.77        | 0.44     |
| 1:B:4265:ALA:H    | 1:B:4323:ASN:HB3  | 1.83        | 0.44     |
| 1:A:3410:LEU:C    | 1:A:3410:LEU:HD23 | 2.38        | 0.44     |
| 1:A:2125:ALA:HA   | 1:A:2128:ILE:CG2  | 2.46        | 0.44     |
| 1:A:2152:LEU:HD13 | 1:A:2152:LEU:O    | 2.18        | 0.44     |
| 1:B:2986:VAL:O    | 1:B:2988:LEU:HG   | 2.17        | 0.44     |
| 1:B:4304:ARG:HA   | 1:B:4307:LEU:HD12 | 1.99        | 0.44     |
| 1:B:4330:PRO:O    | 1:B:4333:ALA:HB3  | 2.17        | 0.44     |
| 1:A:1628:LEU:O    | 1:A:1628:LEU:HD23 | 2.18        | 0.44     |
| 1:A:3521:THR:O    | 1:A:3525:LEU:HD12 | 2.18        | 0.44     |
| 1:A:3603:GLY:HA2  | 1:A:3664:MET:CE   | 2.48        | 0.44     |
| 1:A:2056:GLU:HB2  | 1:A:2065:ILE:O    | 2.18        | 0.44     |
| 1:A:2991:PHE:O    | 1:A:2992:ASN:C    | 2.55        | 0.44     |
| 1:B:3013:LEU:HD13 | 1:B:3145:PHE:HB3  | 2.00        | 0.44     |
| 1:B:3164:LEU:C    | 1:B:3166:ASN:H    | 2.22        | 0.44     |
| 1:B:3715:GLY:HA2  | 1:B:3760:PHE:HB2  | 2.00        | 0.44     |
| 1:A:1904:PHE:C    | 1:A:1906:TRP:N    | 2.71        | 0.44     |
| 1:B:4686:LEU:HD22 | 1:B:4716:TRP:HB3  | 2.00        | 0.44     |
| 1:B:2694:PHE:HA   | 1:B:2738:TRP:O    | 2.18        | 0.44     |
| 1:B:1530:PHE:CZ   | 1:B:1571:SER:HB2  | 2.53        | 0.44     |
| 1:A:1674:ASP:OD1  | 1:A:1678:LYS:HE2  | 2.17        | 0.44     |
| 1:B:4374:PRO:HB3  | 1:B:4377:PRO:HG3  | 1.98        | 0.44     |
| 1:A:2077:MET:HE2  | 1:A:2077:MET:HB3  | 1.81        | 0.44     |
| 1:B:2612:LEU:O    | 1:B:2612:LEU:HD13 | 2.18        | 0.44     |
| 1:A:2926:THR:O    | 1:A:2930:ILE:HG13 | 2.18        | 0.44     |
| 1:A:2289:TYR:CE1  | 1:A:2293:ILE:HD11 | 2.53        | 0.44     |
| 1:A:3812:LYS:HB3  | 1:A:3875:VAL:CG2  | 2.47        | 0.44     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3813:ARG:HH22 | 1:A:3817:LEU:HD13 | 1.83        | 0.44     |
| 1:B:2766:MET:HB3  | 1:B:2783:LEU:CD1  | 2.43        | 0.44     |
| 1:A:2903:ARG:HD2  | 1:A:2945:ALA:O    | 2.18        | 0.44     |
| 1:B:4289:PRO:HB2  | 1:B:4696:ARG:HD2  | 2.00        | 0.44     |
| 1:B:4689:PRO:HD2  | 1:B:4721:VAL:O    | 2.18        | 0.44     |
| 1:A:1695:ALA:CB   | 1:A:2019:CYS:SG   | 3.06        | 0.44     |
| 1:A:1973:PHE:HE1  | 1:A:2099:ALA:HA   | 1.81        | 0.44     |
| 1:B:3553:VAL:O    | 1:B:3557:VAL:HG23 | 2.18        | 0.44     |
| 1:A:3869:VAL:O    | 1:A:3869:VAL:HG12 | 2.18        | 0.44     |
| 1:A:1535:ARG:HA   | 1:A:1591:TRP:HZ2  | 1.83        | 0.44     |
| 1:A:2376:LEU:HD12 | 1:A:2385:LEU:C    | 2.38        | 0.44     |
| 1:A:3205:PHE:CE2  | 1:A:3221:PRO:HB3  | 2.52        | 0.44     |
| 1:B:2828:TYR:HE1  | 1:B:2880:SER:HA   | 1.83        | 0.44     |
| 1:B:3872:THR:O    | 1:B:3876:MET:HG2  | 2.18        | 0.44     |
| 1:B:3552:LYS:NZ   | 1:B:3552:LYS:HB2  | 2.33        | 0.44     |
| 1:B:2839:LEU:CD2  | 1:B:2896:CYS:HB3  | 2.48        | 0.44     |
| 1:A:3700:LEU:CD1  | 1:A:3701:ASP:H    | 2.31        | 0.44     |
| 1:A:2913:PHE:HD2  | 1:A:2913:PHE:N    | 2.15        | 0.44     |
| 1:A:4257:ALA:C    | 1:A:4259:ARG:H    | 2.21        | 0.44     |
| 1:A:3190:ARG:HA   | 1:A:3224:ARG:NH1  | 2.32        | 0.44     |
| 1:A:2903:ARG:HH22 | 1:A:2950:ILE:HA   | 1.82        | 0.44     |
| 1:A:1973:PHE:HE1  | 1:A:2099:ALA:HB2  | 1.83        | 0.44     |
| 1:A:2361:PRO:HD2  | 1:A:2754:TYR:CE1  | 2.53        | 0.44     |
| 1:B:1869:ALA:O    | 1:B:1872:ARG:HB3  | 2.17        | 0.44     |
| 1:B:3903:LEU:HD11 | 1:B:3967:PHE:CD1  | 2.53        | 0.44     |
| 1:B:2112:MET:O    | 1:B:2116:GLN:HG2  | 2.17        | 0.44     |
| 1:B:2965:ARG:HG3  | 1:B:2965:ARG:HH11 | 1.82        | 0.44     |
| 1:A:2255:TRP:CH2  | 1:A:2259:ILE:HD11 | 2.53        | 0.43     |
| 1:A:2560:MET:HE3  | 1:A:2564:ASN:HD22 | 1.81        | 0.43     |
| 1:A:3652:LEU:HD12 | 1:A:3653:PRO:CD   | 2.41        | 0.43     |
| 1:B:2426:ILE:H    | 1:B:2426:ILE:CD1  | 2.27        | 0.43     |
| 1:B:2902:VAL:HG21 | 1:B:2941:VAL:HG21 | 2.00        | 0.43     |
| 1:B:3046:TYR:CE1  | 1:B:3050:ASP:HB2  | 2.53        | 0.43     |
| 1:A:3585:MET:HA   | 1:A:3588:VAL:HG23 | 2.00        | 0.43     |
| 1:B:2714:PHE:HE1  | 1:B:2741:VAL:HG21 | 1.83        | 0.43     |
| 1:A:2249:LEU:HD22 | 2:A:9002:ADP:C5   | 2.53        | 0.43     |
| 1:A:4690:VAL:HG11 | 1:A:4701:PHE:CE2  | 2.53        | 0.43     |
| 1:A:2091:LEU:HD22 | 1:A:2095:PHE:HE1  | 1.80        | 0.43     |
| 1:A:2617:VAL:HG13 | 1:A:2617:VAL:O    | 2.18        | 0.43     |
| 1:B:3038:TYR:HE2  | 1:B:3058:LEU:HD22 | 1.82        | 0.43     |
| 1:A:1591:TRP:HA   | 1:A:1591:TRP:CE3  | 2.53        | 0.43     |
| 1:B:3961:ASN:HA   | 1:B:3964:LYS:HE2  | 2.00        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:1756:LYS:HB2  | 1:A:1756:LYS:NZ   | 2.32        | 0.43     |
| 1:B:2522:ARG:NH1  | 1:B:2593:PHE:HD1  | 2.16        | 0.43     |
| 1:A:2650:THR:OG1  | 1:A:2651:VAL:N    | 2.50        | 0.43     |
| 1:A:3462:PHE:CE2  | 1:A:3478:VAL:HG23 | 2.53        | 0.43     |
| 1:B:4024:ARG:O    | 1:B:4024:ARG:HG2  | 2.17        | 0.43     |
| 1:B:4153:LEU:HB2  | 1:B:4155:LYS:CG   | 2.46        | 0.43     |
| 1:B:1674:ASP:O    | 1:B:1678:LYS:HG3  | 2.18        | 0.43     |
| 1:B:2265:ILE:HD12 | 1:B:2414:VAL:HG22 | 1.99        | 0.43     |
| 1:A:2547:ASN:O    | 1:A:2551:TYR:HB2  | 2.17        | 0.43     |
| 1:B:4691:TYR:HA   | 1:B:4698:GLU:O    | 2.18        | 0.43     |
| 1:A:2400:LEU:HB3  | 1:A:2403:ALA:HB3  | 2.00        | 0.43     |
| 1:A:2408:ILE:HG13 | 1:A:2409:SER:H    | 1.83        | 0.43     |
| 1:A:4319:LYS:O    | 1:A:4321:ARG:NH1  | 2.52        | 0.43     |
| 1:A:1958:LEU:HD23 | 1:A:4341:THR:HB   | 1.99        | 0.43     |
| 1:B:2282:LYS:HZ2  | 1:B:2282:LYS:HB2  | 1.83        | 0.43     |
| 1:A:1922:LEU:CD1  | 1:A:1938:PHE:HD1  | 2.31        | 0.43     |
| 1:A:2053:ASN:N    | 1:A:2053:ASN:ND2  | 2.65        | 0.43     |
| 1:B:4225:LEU:HD23 | 1:B:4230:LEU:HD21 | 2.00        | 0.43     |
| 1:A:3470:ALA:O    | 1:A:3471:SER:HB2  | 2.17        | 0.43     |
| 1:A:1755:LYS:HA   | 1:A:1755:LYS:HD2  | 1.80        | 0.43     |
| 1:B:2773:TRP:CZ3  | 1:B:2780:TRP:HB2  | 2.53        | 0.43     |
| 1:B:1497:LEU:HD22 | 1:B:1501:SER:HB2  | 1.99        | 0.43     |
| 1:A:3019:GLY:HA2  | 2:A:9004:ADP:H5'2 | 2.00        | 0.43     |
| 1:A:4091:SER:O    | 1:A:4420:SER:HA   | 2.18        | 0.43     |
| 1:B:3686:MET:HA   | 1:B:3694:ILE:HG21 | 2.00        | 0.43     |
| 1:A:1604:VAL:O    | 1:A:1608:VAL:HG23 | 2.18        | 0.43     |
| 1:A:2359:VAL:HB   | 1:A:2397:VAL:HG11 | 2.00        | 0.43     |
| 1:B:3192:LEU:HD22 | 1:B:3271:ILE:HG21 | 2.00        | 0.43     |
| 1:A:4052:GLN:O    | 1:A:4054:GLY:N    | 2.43        | 0.43     |
| 1:A:3062:ALA:HB2  | 1:A:3069:ILE:HD13 | 1.99        | 0.43     |
| 1:B:3634:VAL:HB   | 1:B:3635:PRO:HD3  | 1.99        | 0.43     |
| 1:B:3635:PRO:C    | 1:B:3637:PHE:H    | 2.21        | 0.43     |
| 1:B:4012:LEU:HD11 | 1:B:4020:LEU:HD22 | 2.01        | 0.43     |
| 1:A:3990:PHE:CE2  | 1:A:4023:LEU:HG   | 2.54        | 0.43     |
| 1:A:3681:ALA:HB2  | 1:A:3786:PHE:CD2  | 2.53        | 0.43     |
| 1:A:4182:GLY:HA3  | 1:A:4212:SER:HG   | 1.84        | 0.43     |
| 1:B:1975:PRO:HG2  | 1:B:1978:THR:CG2  | 2.48        | 0.43     |
| 1:B:1831:LEU:HA   | 1:B:1841:ILE:HG23 | 1.99        | 0.43     |
| 1:B:2964:ASN:HD21 | 1:B:2967:ASP:CG   | 2.22        | 0.43     |
| 1:B:4022:CYS:HB3  | 1:B:4026:GLN:HE21 | 1.84        | 0.43     |
| 1:A:1835:THR:O    | 1:A:1836:LEU:CB   | 2.67        | 0.43     |
| 1:A:3933:LYS:HB3  | 1:A:3933:LYS:HZ3  | 1.84        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:3041:LYS:N    | 1:B:3041:LYS:HD2  | 2.33        | 0.43     |
| 1:B:4574:GLN:HE22 | 1:B:4590:TRP:HB3  | 1.82        | 0.43     |
| 1:A:1830:ALA:O    | 1:A:1841:ILE:HG23 | 2.18        | 0.43     |
| 1:A:4132:LEU:HB2  | 1:A:4216:PHE:CD1  | 2.52        | 0.43     |
| 1:A:3445:THR:HA   | 1:A:3449:ARG:HB2  | 2.00        | 0.43     |
| 1:B:3234:ILE:HG23 | 1:B:3617:TRP:CD1  | 2.54        | 0.43     |
| 1:B:3289:LEU:HA   | 1:B:3292:LEU:HD12 | 1.99        | 0.43     |
| 1:B:1639:ILE:HG23 | 1:B:1672:LEU:HD22 | 2.01        | 0.43     |
| 1:B:2352:TRP:CD1  | 1:B:2392:ARG:HB2  | 2.54        | 0.43     |
| 1:A:3096:VAL:HB   | 1:A:3099:LEU:HB2  | 2.00        | 0.43     |
| 1:B:1653:ALA:HB1  | 1:B:1658:GLU:HG2  | 2.01        | 0.43     |
| 1:A:2200:ASN:ND2  | 1:A:2228:LEU:HB3  | 2.33        | 0.43     |
| 1:A:4337:ILE:HG22 | 1:A:4338:LEU:HD12 | 1.99        | 0.43     |
| 1:A:3015:ILE:HG21 | 1:A:3172:TRP:CH2  | 2.54        | 0.43     |
| 1:A:2057:VAL:HG22 | 1:A:2058:GLU:N    | 2.34        | 0.43     |
| 1:A:4066:GLN:HE22 | 1:A:4081:ARG:HD3  | 1.81        | 0.43     |
| 1:A:3638:LEU:HD22 | 1:A:3667:ARG:HD3  | 2.01        | 0.43     |
| 1:A:3078:VAL:O    | 1:A:3078:VAL:HG22 | 2.19        | 0.43     |
| 1:B:2882:TRP:O    | 1:B:2886:LEU:HG   | 2.18        | 0.43     |
| 1:A:2012:ILE:HG22 | 1:A:2016:LEU:CD1  | 2.49        | 0.43     |
| 1:B:3160:THR:O    | 1:B:3162:PRO:HD3  | 2.18        | 0.43     |
| 1:B:3902:GLU:C    | 1:B:3904:SER:N    | 2.71        | 0.43     |
| 1:A:3357:VAL:O    | 1:A:3357:VAL:HG12 | 2.18        | 0.43     |
| 1:B:3181:LEU:HB3  | 1:B:3232:VAL:HG13 | 2.00        | 0.43     |
| 1:B:4407:TRP:H    | 1:B:4407:TRP:HD1  | 1.64        | 0.43     |
| 1:B:3993:LYS:HG3  | 1:B:4431:GLN:HG3  | 1.99        | 0.43     |
| 1:B:4728:SER:OG   | 1:B:4729:ASP:N    | 2.51        | 0.43     |
| 1:B:1744:MET:SD   | 1:B:1777:MET:HG3  | 2.59        | 0.43     |
| 1:A:1955:ARG:HB2  | 1:A:1955:ARG:NH1  | 2.33        | 0.43     |
| 1:A:2145:TYR:OH   | 1:A:2207:LEU:HA   | 2.18        | 0.43     |
| 1:A:2263:HIS:HB2  | 1:A:2289:TYR:CE1  | 2.54        | 0.43     |
| 1:A:4648:VAL:HG13 | 1:A:4657:THR:CG2  | 2.44        | 0.43     |
| 1:A:2748:LEU:HD21 | 1:A:2800:ARG:CZ   | 2.48        | 0.43     |
| 1:B:3238:ILE:HD11 | 1:B:3617:TRP:CZ2  | 2.48        | 0.43     |
| 1:A:2678:SER:HB2  | 1:A:2817:ASP:O    | 2.18        | 0.43     |
| 1:A:4179:ALA:HA   | 1:A:4213:PHE:CD1  | 2.53        | 0.43     |
| 1:B:1766:ILE:HD12 | 1:B:1769:TRP:HE1  | 1.84        | 0.43     |
| 1:B:1546:VAL:O    | 1:B:1553:LYS:HA   | 2.19        | 0.43     |
| 1:A:4389:ARG:NH1  | 1:A:4389:ARG:HG2  | 2.32        | 0.43     |
| 1:A:4288:ILE:HG23 | 1:A:4289:PRO:HA   | 2.01        | 0.43     |
| 1:B:4293:THR:HG23 | 1:B:4352:ASP:OD1  | 2.19        | 0.43     |
| 1:A:1906:TRP:CZ2  | 1:A:1911:ARG:HG2  | 2.54        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2968:LEU:HD22 | 1:B:2999:LEU:HD11 | 2.00        | 0.43     |
| 1:A:3451:ALA:O    | 1:A:3455:GLY:N    | 2.51        | 0.43     |
| 1:A:2270:HIS:ND1  | 1:A:2270:HIS:N    | 2.66        | 0.43     |
| 1:A:4280:ILE:HG21 | 1:A:4359:PHE:CE1  | 2.53        | 0.43     |
| 1:B:2840:PRO:O    | 1:B:2843:ARG:HB2  | 2.19        | 0.43     |
| 1:A:1658:GLU:O    | 1:A:1661:ALA:HB3  | 2.19        | 0.43     |
| 1:B:4028:PRO:O    | 1:B:4031:SER:N    | 2.52        | 0.43     |
| 1:B:3289:LEU:O    | 1:B:3293:ARG:HG3  | 2.19        | 0.43     |
| 1:A:3862:THR:C    | 1:A:3864:GLU:H    | 2.22        | 0.43     |
| 1:A:3416:LYS:HE3  | 1:A:3418:GLU:CB   | 2.48        | 0.43     |
| 1:A:3681:ALA:HB2  | 1:A:3786:PHE:CG   | 2.54        | 0.43     |
| 1:B:1780:THR:HG22 | 1:B:1784:LEU:CD1  | 2.48        | 0.43     |
| 1:B:1606:ILE:HG23 | 1:B:1607:ASP:N    | 2.33        | 0.43     |
| 1:B:4058:ILE:CD1  | 1:B:4082:LYS:HG2  | 2.48        | 0.43     |
| 1:A:4379:ILE:HG23 | 1:A:4381:LEU:HD13 | 2.00        | 0.43     |
| 1:A:2327:TRP:CZ2  | 1:A:2379:LEU:HD22 | 2.54        | 0.43     |
| 1:A:2304:HIS:N    | 1:A:2352:TRP:O    | 2.51        | 0.43     |
| 1:A:3324:LEU:HD12 | 1:A:3539:LEU:HD23 | 2.00        | 0.43     |
| 1:B:4331:TRP:HZ2  | 1:B:4369:PHE:CE2  | 2.37        | 0.43     |
| 1:A:3197:PRO:HG2  | 1:A:3198:GLN:OE1  | 2.18        | 0.43     |
| 1:A:2290:LEU:HD23 | 1:A:2301:SER:O    | 2.19        | 0.43     |
| 1:B:3065:LYS:O    | 1:B:3066:GLU:C    | 2.57        | 0.43     |
| 1:B:3725:ASN:ND2  | 1:B:3725:ASN:N    | 2.67        | 0.43     |
| 1:B:3675:ILE:HG22 | 1:B:3675:ILE:O    | 2.19        | 0.43     |
| 1:B:3139:ARG:HH11 | 1:B:3139:ARG:HG3  | 1.84        | 0.43     |
| 1:A:2269:ASN:O    | 1:A:2272:VAL:HG23 | 2.19        | 0.43     |
| 1:A:2774:ARG:CZ   | 1:A:2781:ILE:HD11 | 2.48        | 0.43     |
| 1:B:3620:ARG:NH1  | 1:B:3620:ARG:HG2  | 2.34        | 0.43     |
| 1:A:1892:LEU:C    | 1:A:1894:LYS:H    | 2.22        | 0.43     |
| 1:B:4023:LEU:O    | 1:B:4027:VAL:HB   | 2.18        | 0.43     |
| 1:A:3859:LYS:C    | 1:A:3859:LYS:HD3  | 2.39        | 0.43     |
| 1:A:3588:VAL:O    | 1:A:3592:VAL:HG23 | 2.18        | 0.43     |
| 1:B:2339:ILE:HG21 | 1:B:2391:VAL:CG2  | 2.49        | 0.43     |
| 1:A:2645:ASP:O    | 1:A:2646:VAL:C    | 2.57        | 0.43     |
| 1:A:3902:GLU:HB3  | 1:A:4433:MET:HG2  | 2.00        | 0.43     |
| 1:B:4185:VAL:O    | 1:B:4215:LEU:HD12 | 2.19        | 0.43     |
| 1:B:4079:ASN:O    | 1:B:4082:LYS:HB2  | 2.18        | 0.43     |
| 1:B:3895:ARG:NH1  | 1:B:3977:LYS:HG2  | 2.34        | 0.43     |
| 1:B:4282:GLN:O    | 1:B:4285:LEU:HB2  | 2.19        | 0.43     |
| 1:B:3202:PRO:HG3  | 1:B:3623:SER:O    | 2.19        | 0.43     |
| 1:A:1578:SER:HA   | 1:A:1579:PRO:HD3  | 1.92        | 0.43     |
| 1:B:2304:HIS:NE2  | 1:B:2351:HIS:HD2  | 2.17        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4565:ILE:HG22 | 1:A:4566:SER:N    | 2.34        | 0.43     |
| 1:B:3272:ASN:HD22 | 1:B:3272:ASN:HA   | 1.61        | 0.43     |
| 1:A:2211:ASP:C    | 1:A:2213:PRO:HD2  | 2.38        | 0.43     |
| 1:A:4708:ASP:C    | 1:A:4710:SER:H    | 2.22        | 0.43     |
| 1:A:3953:ASN:O    | 1:A:3956:THR:HG22 | 2.19        | 0.43     |
| 1:A:4432:LYS:C    | 1:A:4434:GLN:N    | 2.72        | 0.43     |
| 1:A:1927:ILE:O    | 1:A:1928:HIS:HD2  | 2.01        | 0.43     |
| 1:A:3391:ILE:HD11 | 1:A:3471:SER:OG   | 2.19        | 0.43     |
| 1:B:4324:ILE:HG13 | 1:B:4324:ILE:H    | 1.52        | 0.43     |
| 1:B:4617:GLU:HG2  | 1:B:4618:ASN:N    | 2.34        | 0.43     |
| 1:B:4638:ASN:HB3  | 1:B:4666:ILE:HD11 | 2.00        | 0.43     |
| 1:A:4335:ARG:HG2  | 1:A:4360:LEU:HG   | 2.01        | 0.43     |
| 1:A:2362:GLU:C    | 1:A:2364:VAL:H    | 2.22        | 0.43     |
| 1:B:4075:THR:HG23 | 1:B:4076:ILE:N    | 2.34        | 0.43     |
| 1:A:4659:ILE:HD12 | 1:A:4659:ILE:N    | 2.34        | 0.43     |
| 1:A:1963:ALA:HA   | 1:A:2096:ARG:HH11 | 1.83        | 0.42     |
| 1:B:3722:ASP:HA   | 1:B:3724:GLU:OE1  | 2.19        | 0.42     |
| 1:A:4024:ARG:HA   | 1:A:4030:PHE:O    | 2.19        | 0.42     |
| 1:A:1967:ARG:NH1  | 1:A:2053:ASN:HA   | 2.34        | 0.42     |
| 1:A:3716:CYS:H    | 1:A:3760:PHE:HB2  | 1.84        | 0.42     |
| 1:B:2849:LEU:CD1  | 1:B:2901:LEU:HD11 | 2.49        | 0.42     |
| 1:B:3723:VAL:HG23 | 1:B:3764:LEU:HD22 | 2.01        | 0.42     |
| 1:B:2368:ASN:O    | 1:B:2410:ARG:NH1  | 2.52        | 0.42     |
| 1:B:2196:LEU:HD11 | 1:B:2223:PHE:CD2  | 2.54        | 0.42     |
| 1:A:4354:ARG:HD3  | 1:A:4717:TYR:CD2  | 2.53        | 0.42     |
| 1:B:2271:GLY:HA2  | 1:B:2393:VAL:O    | 2.19        | 0.42     |
| 1:A:3782:THR:HG23 | 1:A:3782:THR:O    | 2.18        | 0.42     |
| 1:A:2560:MET:CG   | 1:A:2565:GLN:HB2  | 2.49        | 0.42     |
| 1:B:2423:THR:HA   | 1:B:2426:ILE:HD13 | 2.00        | 0.42     |
| 1:A:4678:ILE:O    | 1:A:4678:ILE:HG22 | 2.19        | 0.42     |
| 1:B:3234:ILE:HG23 | 1:B:3617:TRP:CE2  | 2.54        | 0.42     |
| 1:B:3598:PHE:CD2  | 1:B:3634:VAL:HG11 | 2.55        | 0.42     |
| 1:B:3676:ASP:CB   | 1:B:3681:ALA:HB3  | 2.49        | 0.42     |
| 1:B:3647:TRP:HB3  | 1:B:3652:LEU:CD2  | 2.49        | 0.42     |
| 1:A:1554:LEU:HD22 | 1:A:1609:GLN:HG3  | 2.00        | 0.42     |
| 1:B:2109:ALA:HA   | 1:B:2156:LEU:CD1  | 2.49        | 0.42     |
| 1:A:3992:LEU:CD1  | 1:A:4434:GLN:HG3  | 2.48        | 0.42     |
| 1:A:4358:SER:O    | 1:A:4362:GLN:HB2  | 2.19        | 0.42     |
| 1:A:2425:MET:HE2  | 1:A:2425:MET:HB3  | 1.81        | 0.42     |
| 1:B:2886:LEU:HD23 | 1:B:2904:LEU:HD22 | 2.01        | 0.42     |
| 1:A:1907:LEU:HD22 | 1:A:1911:ARG:CZ   | 2.49        | 0.42     |
| 1:A:4596:ASN:OD1  | 1:A:4599:ALA:HB2  | 2.18        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:4673:ASP:OD1  | 1:B:4674:LYS:N    | 2.52        | 0.42     |
| 1:B:2991:PHE:CE1  | 1:B:2993:GLU:HB2  | 2.54        | 0.42     |
| 1:A:2259:ILE:HG23 | 1:A:2289:TYR:HB2  | 2.02        | 0.42     |
| 1:A:3718:LEU:HG   | 1:A:3719:LEU:N    | 2.21        | 0.42     |
| 1:B:2129:VAL:N    | 1:B:2130:PRO:CD   | 2.82        | 0.42     |
| 1:A:3067:GLU:HG2  | 1:A:3068:LYS:N    | 2.34        | 0.42     |
| 1:A:2870:ALA:C    | 1:A:2872:TYR:H    | 2.21        | 0.42     |
| 1:B:3030:ALA:HB3  | 1:B:3037:ILE:HD11 | 2.00        | 0.42     |
| 1:B:3698:SER:HB3  | 1:B:3700:LEU:HD12 | 2.00        | 0.42     |
| 1:A:2832:ASN:CG   | 1:A:2849:LEU:HD23 | 2.39        | 0.42     |
| 1:A:3156:ASN:C    | 1:A:3158:SER:H    | 2.21        | 0.42     |
| 1:B:3078:VAL:O    | 1:B:3078:VAL:HG22 | 2.18        | 0.42     |
| 1:A:2525:ILE:HD12 | 1:A:2526:MET:N    | 2.33        | 0.42     |
| 1:B:2669:PRO:HA   | 1:B:2788:PHE:O    | 2.19        | 0.42     |
| 1:A:3096:VAL:HB   | 1:A:3099:LEU:HD22 | 2.01        | 0.42     |
| 1:B:1960:LEU:HD13 | 1:B:2074:PHE:CE1  | 2.54        | 0.42     |
| 1:A:1816:LEU:HD23 | 1:A:1878:LEU:CD1  | 2.49        | 0.42     |
| 1:B:3962:ASP:C    | 1:B:3964:LYS:H    | 2.23        | 0.42     |
| 1:B:1505:SER:O    | 1:B:1506:ASP:C    | 2.57        | 0.42     |
| 1:B:2017:CYS:SG   | 1:B:2046:ILE:HD13 | 2.59        | 0.42     |
| 1:A:4000:SER:O    | 1:B:2940:SER:HB3  | 2.19        | 0.42     |
| 1:A:4109:ASP:CA   | 1:A:4112:ASN:HD22 | 2.11        | 0.42     |
| 1:A:3018:SER:O    | 1:A:3257:PRO:HD2  | 2.18        | 0.42     |
| 1:A:1639:ILE:HG12 | 1:A:1675:LEU:HD23 | 2.01        | 0.42     |
| 1:A:2142:GLN:HB2  | 1:A:2145:TYR:CD1  | 2.54        | 0.42     |
| 1:A:2266:LEU:HD21 | 1:A:2394:MET:CE   | 2.49        | 0.42     |
| 1:B:1811:PRO:HB2  | 1:B:1814:LEU:CD1  | 2.49        | 0.42     |
| 1:B:2125:ALA:C    | 1:B:2127:LYS:H    | 2.21        | 0.42     |
| 1:A:3700:LEU:CD1  | 1:A:3701:ASP:N    | 2.80        | 0.42     |
| 1:A:4134:LEU:HD23 | 1:A:4236:PHE:HB2  | 2.01        | 0.42     |
| 1:A:1752:VAL:CG2  | 1:A:1811:PRO:HG3  | 2.48        | 0.42     |
| 1:A:3993:LYS:O    | 1:A:3995:GLY:N    | 2.53        | 0.42     |
| 1:A:2615:TYR:N    | 1:A:2615:TYR:CD2  | 2.87        | 0.42     |
| 1:A:4289:PRO:HA   | 1:A:4292:TRP:O    | 2.20        | 0.42     |
| 1:B:2272:VAL:HG12 | 1:B:2273:MET:N    | 2.34        | 0.42     |
| 1:A:1973:PHE:HD1  | 1:A:1973:PHE:O    | 2.02        | 0.42     |
| 1:A:1732:LEU:HD13 | 1:A:1741:ILE:HD12 | 2.01        | 0.42     |
| 1:A:2819:PRO:HB2  | 1:A:2824:LEU:CD2  | 2.50        | 0.42     |
| 1:B:3057:MET:O    | 1:B:3061:ARG:HG3  | 2.19        | 0.42     |
| 1:A:1816:LEU:O    | 1:A:1820:GLN:HG3  | 2.19        | 0.42     |
| 1:B:3181:LEU:HB2  | 1:B:3232:VAL:HG13 | 2.01        | 0.42     |
| 1:B:2591:GLU:HA   | 1:B:2613:LEU:HD12 | 2.01        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:3960:LEU:CD2  | 1:B:4237:SER:HB2  | 2.50        | 0.42     |
| 1:A:3209:ALA:CB   | 1:A:3221:PRO:HG3  | 2.49        | 0.42     |
| 1:B:3039:THR:HG22 | 1:B:3072:ILE:HB   | 2.01        | 0.42     |
| 1:A:4168:PHE:O    | 1:A:4172:GLU:HG3  | 2.19        | 0.42     |
| 1:A:3262:ASP:OD2  | 1:A:3670:ARG:NE   | 2.52        | 0.42     |
| 1:B:2528:PHE:HE1  | 1:B:2533:VAL:HG11 | 1.85        | 0.42     |
| 1:A:2408:ILE:O    | 1:A:2411:CYS:HB2  | 2.20        | 0.42     |
| 1:A:2502:ILE:CG2  | 1:A:2573:LEU:HD12 | 2.48        | 0.42     |
| 1:B:3598:PHE:O    | 1:B:3602:ILE:HB   | 2.20        | 0.42     |
| 1:A:2587:LEU:CG   | 1:A:2817:ASP:HB2  | 2.45        | 0.42     |
| 1:A:3192:LEU:HD11 | 1:A:3271:ILE:HG22 | 2.01        | 0.42     |
| 1:A:2051:LYS:C    | 1:A:2051:LYS:HD3  | 2.39        | 0.42     |
| 1:A:1967:ARG:CB   | 1:A:2051:LYS:HA   | 2.50        | 0.42     |
| 1:B:3084:LEU:O    | 1:B:3087:MET:N    | 2.52        | 0.42     |
| 1:A:4373:PHE:CD1  | 1:A:4374:PRO:HD2  | 2.54        | 0.42     |
| 1:B:2706:THR:HA   | 1:B:2759:VAL:HG22 | 2.01        | 0.42     |
| 1:A:2905:TRP:HZ3  | 1:A:2934:ALA:HB2  | 1.83        | 0.42     |
| 1:A:3536:TYR:O    | 1:A:3540:ILE:HD13 | 2.20        | 0.42     |
| 1:B:2112:MET:SD   | 1:B:2153:LYS:HG2  | 2.59        | 0.42     |
| 1:A:2534:LEU:HB3  | 1:A:2538:PHE:CE2  | 2.55        | 0.42     |
| 1:A:1708:ILE:HD11 | 1:A:1721:HIS:HB3  | 2.01        | 0.42     |
| 1:A:2415:TRP:HA   | 1:A:2415:TRP:HE3  | 1.83        | 0.42     |
| 1:A:1766:ILE:HG23 | 1:A:1767:HIS:N    | 2.35        | 0.42     |
| 1:A:2910:LEU:HB3  | 1:A:2911:ARG:HH12 | 1.85        | 0.42     |
| 1:A:2370:LEU:HD23 | 1:A:2370:LEU:O    | 2.19        | 0.42     |
| 1:B:1598:VAL:HG22 | 1:B:1660:LEU:HD22 | 2.01        | 0.42     |
| 1:A:3061:ARG:O    | 1:A:3067:GLU:HB3  | 2.18        | 0.42     |
| 1:A:2106:GLU:CD   | 1:A:2106:GLU:N    | 2.69        | 0.42     |
| 1:A:4128:SER:CB   | 1:A:4213:PHE:HB3  | 2.48        | 0.42     |
| 1:B:3043:ASN:ND2  | 1:B:3043:ASN:N    | 2.68        | 0.42     |
| 1:B:1914:TYR:CZ   | 1:B:1924:LYS:HB3  | 2.54        | 0.42     |
| 1:B:3160:THR:C    | 1:B:3162:PRO:HD3  | 2.40        | 0.42     |
| 1:B:2230:PRO:HB3  | 1:B:2237:ARG:HH22 | 1.84        | 0.42     |
| 1:A:1777:MET:HE3  | 1:A:1939:GLU:HA   | 2.02        | 0.42     |
| 1:B:2610:ILE:HD12 | 1:B:2615:TYR:OH   | 2.20        | 0.42     |
| 1:A:3108:LEU:HD11 | 1:A:3133:PHE:CZ   | 2.54        | 0.42     |
| 1:A:1979:GLY:O    | 1:A:1980:LYS:C    | 2.58        | 0.42     |
| 1:A:3009:GLN:HG2  | 1:A:3138:ARG:O    | 2.20        | 0.42     |
| 1:A:4178:ALA:HA   | 1:A:4183:THR:OG1  | 2.20        | 0.42     |
| 1:A:3915:ALA:O    | 1:A:3918:ASP:HB2  | 2.19        | 0.42     |
| 1:A:3954:ARG:HD3  | 1:A:3954:ARG:O    | 2.19        | 0.42     |
| 1:B:2327:TRP:CH2  | 1:B:2380:PRO:HD2  | 2.55        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2269:ASN:O    | 1:A:2271:GLY:N    | 2.53        | 0.42     |
| 1:A:2701:PHE:HB2  | 1:A:2745:GLU:O    | 2.20        | 0.42     |
| 1:A:2573:LEU:C    | 1:A:2573:LEU:HD23 | 2.40        | 0.42     |
| 1:A:3457:LEU:HD12 | 1:A:3486:TYR:CE1  | 2.55        | 0.42     |
| 1:B:3990:PHE:CD2  | 1:B:4084:LEU:HD22 | 2.55        | 0.42     |
| 1:A:2126:GLY:O    | 1:A:2130:PRO:HG2  | 2.19        | 0.42     |
| 1:B:2290:LEU:HD22 | 1:B:2352:TRP:CZ3  | 2.55        | 0.42     |
| 1:B:2773:TRP:CH2  | 1:B:2780:TRP:HB2  | 2.54        | 0.42     |
| 1:B:3061:ARG:O    | 1:B:3067:GLU:HB3  | 2.19        | 0.42     |
| 1:A:2270:HIS:HB2  | 1:A:2392:ARG:HD2  | 2.02        | 0.42     |
| 1:A:2426:ILE:CD1  | 1:A:2530:ARG:HD3  | 2.50        | 0.42     |
| 1:B:2588:VAL:HG23 | 1:B:2589:GLU:N    | 2.34        | 0.42     |
| 1:A:3602:ILE:HG22 | 1:A:3603:GLY:N    | 2.34        | 0.42     |
| 1:B:2528:PHE:CE1  | 1:B:2533:VAL:HG11 | 2.54        | 0.42     |
| 1:A:2561:SER:HA   | 1:A:2562:PRO:HD3  | 1.95        | 0.42     |
| 1:A:1952:LEU:HD22 | 1:A:2103:PRO:HA   | 2.01        | 0.42     |
| 1:B:3259:HIS:NE2  | 1:B:3779:SER:HA   | 2.34        | 0.42     |
| 1:A:2057:VAL:HB   | 1:A:2067:LEU:HD13 | 2.01        | 0.42     |
| 1:A:2849:LEU:HA   | 1:A:2938:PHE:HZ   | 1.85        | 0.42     |
| 1:B:2825:THR:CG2  | 1:B:2854:VAL:HG21 | 2.50        | 0.42     |
| 1:B:2084:ARG:CZ   | 1:B:4295:PHE:CD2  | 3.03        | 0.42     |
| 1:B:1608:VAL:HG13 | 1:B:1676:LEU:CD1  | 2.50        | 0.42     |
| 1:A:4313:TRP:CD1  | 1:A:4334:VAL:HG22 | 2.55        | 0.42     |
| 1:B:1907:LEU:HD22 | 1:B:1911:ARG:NH2  | 2.34        | 0.42     |
| 1:B:2513:HIS:O    | 1:B:2517:GLU:HG3  | 2.19        | 0.42     |
| 1:B:4280:ILE:HG23 | 1:B:4408:LEU:HA   | 2.01        | 0.42     |
| 1:B:4284:ARG:CG   | 1:B:4408:LEU:HB3  | 2.49        | 0.42     |
| 1:B:4036:HIS:CD2  | 1:B:4044:TRP:HE1  | 2.38        | 0.42     |
| 1:A:1791:HIS:HD2  | 1:A:1806:TRP:HD1  | 1.66        | 0.42     |
| 1:A:3268:VAL:HG13 | 1:A:3269:LEU:N    | 2.35        | 0.42     |
| 1:A:2842:LEU:HD11 | 1:A:2897:THR:C    | 2.40        | 0.42     |
| 1:A:3449:ARG:NH1  | 1:A:3449:ARG:HB3  | 2.35        | 0.42     |
| 1:A:2585:MET:O    | 1:A:2815:LEU:HD13 | 2.19        | 0.42     |
| 1:B:3256:THR:CG2  | 1:B:3779:SER:HB3  | 2.50        | 0.42     |
| 1:B:2540:LEU:HB3  | 1:B:2576:SER:CB   | 2.49        | 0.42     |
| 1:A:3224:ARG:HB2  | 1:A:3224:ARG:HE   | 1.73        | 0.42     |
| 1:A:3075:GLU:C    | 1:A:3077:ASN:H    | 2.23        | 0.42     |
| 1:A:2989:VAL:HG13 | 1:A:3187:GLU:OE2  | 2.20        | 0.42     |
| 1:B:3976:VAL:O    | 1:B:3979:THR:HG23 | 2.20        | 0.42     |
| 1:A:2009:MET:HE3  | 1:A:2012:ILE:HB   | 2.02        | 0.42     |
| 1:B:2989:VAL:HG21 | 1:B:3184:VAL:HA   | 2.02        | 0.42     |
| 1:B:3039:THR:CG2  | 1:B:3072:ILE:HB   | 2.50        | 0.42     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2856:PHE:HE2  | 1:B:2913:PHE:CD2  | 2.37        | 0.42     |
| 1:A:2071:MET:HG3  | 1:A:2071:MET:O    | 2.20        | 0.42     |
| 1:A:1792:PHE:CD2  | 1:A:1792:PHE:C    | 2.92        | 0.42     |
| 1:B:3235:HIS:CE1  | 1:B:3260:TYR:HB2  | 2.55        | 0.42     |
| 1:A:4575:LEU:H    | 1:A:4575:LEU:CD1  | 2.26        | 0.42     |
| 1:A:1746:SER:HB3  | 1:A:1940:TYR:CZ   | 2.55        | 0.42     |
| 1:A:3148:ASN:HA   | 1:A:3149:PRO:HD3  | 1.93        | 0.42     |
| 1:A:4418:LEU:HD11 | 1:A:4422:LYS:HZ3  | 1.84        | 0.42     |
| 1:B:4434:GLN:HG2  | 1:B:4434:GLN:O    | 2.19        | 0.42     |
| 1:B:1615:LEU:HD13 | 1:B:1618:ILE:HD12 | 2.01        | 0.42     |
| 1:B:3017:VAL:HG11 | 1:B:3175:GLU:HA   | 2.01        | 0.42     |
| 1:A:1973:PHE:HE1  | 1:A:2099:ALA:CA   | 2.33        | 0.42     |
| 1:A:4065:ALA:O    | 1:A:4069:LEU:HB2  | 2.20        | 0.42     |
| 1:A:1818:THR:O    | 1:A:1822:VAL:HG23 | 2.20        | 0.42     |
| 1:A:4070:SER:C    | 1:A:4072:GLN:N    | 2.72        | 0.42     |
| 1:B:4070:SER:O    | 1:B:4072:GLN:N    | 2.53        | 0.42     |
| 1:B:1952:LEU:HA   | 1:B:1955:ARG:NH2  | 2.35        | 0.42     |
| 1:A:3315:VAL:O    | 1:A:3319:GLN:HB2  | 2.19        | 0.42     |
| 1:A:2833:ARG:HA   | 1:A:2846:ALA:HB1  | 2.02        | 0.42     |
| 1:A:1556:ARG:HG2  | 1:A:1557:GLY:N    | 2.35        | 0.42     |
| 1:A:1929:MET:O    | 1:A:1930:ALA:HB3  | 2.20        | 0.42     |
| 1:B:2684:LEU:HD13 | 1:B:2684:LEU:C    | 2.40        | 0.42     |
| 1:A:2140:SER:HB2  | 1:A:2142:GLN:NE2  | 2.23        | 0.41     |
| 1:A:2204:ILE:HG13 | 1:A:2205:PRO:CD   | 2.50        | 0.41     |
| 1:B:4191:HIS:CD2  | 1:B:4220:GLU:HG2  | 2.54        | 0.41     |
| 1:A:2898:LEU:HD11 | 1:A:2941:VAL:HG22 | 2.01        | 0.41     |
| 1:B:2292:ALA:O    | 1:B:2296:VAL:HG23 | 2.20        | 0.41     |
| 1:B:2370:LEU:HD12 | 1:B:2377:LEU:HB2  | 2.02        | 0.41     |
| 1:B:2272:VAL:O    | 1:B:2394:MET:HA   | 2.20        | 0.41     |
| 1:B:3923:LEU:HD22 | 1:B:3947:ILE:CG2  | 2.47        | 0.41     |
| 1:B:1565:LEU:HD23 | 1:B:1595:LEU:HD12 | 2.00        | 0.41     |
| 1:B:2579:TRP:HZ2  | 1:B:2655:ARG:HD2  | 1.84        | 0.41     |
| 1:A:3889:MET:SD   | 1:A:3889:MET:C    | 2.99        | 0.41     |
| 1:A:4370:ASN:N    | 1:A:4370:ASN:HD22 | 2.16        | 0.41     |
| 1:A:3256:THR:HB   | 1:A:3257:PRO:HD2  | 2.01        | 0.41     |
| 1:A:2258:LYS:HA   | 1:A:2261:GLN:CG   | 2.44        | 0.41     |
| 1:A:3808:ASP:CG   | 1:A:3809:THR:N    | 2.73        | 0.41     |
| 1:B:1785:LEU:HB2  | 1:B:1814:LEU:HD23 | 2.00        | 0.41     |
| 1:A:2370:LEU:HA   | 1:A:2375:LYS:HA   | 2.02        | 0.41     |
| 1:A:1831:LEU:HA   | 1:A:1841:ILE:HG12 | 2.02        | 0.41     |
| 1:A:2745:GLU:CB   | 1:A:2748:LEU:HD12 | 2.50        | 0.41     |
| 1:A:2783:LEU:HD22 | 1:A:2786:ILE:HB   | 2.01        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:4337:ILE:O    | 1:A:4341:THR:CG2  | 2.68        | 0.41     |
| 1:A:4623:ALA:HB2  | 1:A:4703:ILE:CD1  | 2.48        | 0.41     |
| 1:B:3700:LEU:CD1  | 1:B:3701:ASP:H    | 2.30        | 0.41     |
| 1:A:3990:PHE:O    | 1:A:3994:GLY:HA2  | 2.20        | 0.41     |
| 1:B:4277:PHE:HZ   | 1:B:4356:LEU:HD21 | 1.84        | 0.41     |
| 1:A:1973:PHE:HD1  | 1:A:1973:PHE:C    | 2.23        | 0.41     |
| 1:B:1960:LEU:HD13 | 1:B:2074:PHE:HE1  | 1.85        | 0.41     |
| 1:A:4684:SER:O    | 1:A:4707:TYR:HE2  | 2.02        | 0.41     |
| 1:B:3877:GLN:O    | 1:B:3881:GLU:HB2  | 2.20        | 0.41     |
| 1:B:3573:ARG:HH11 | 1:B:3573:ARG:HG2  | 1.84        | 0.41     |
| 1:A:2893:MET:O    | 1:A:2895:GLY:N    | 2.46        | 0.41     |
| 1:B:2578:MET:O    | 1:B:2582:GLY:HA3  | 2.19        | 0.41     |
| 1:A:1959:THR:O    | 1:A:1963:ALA:CB   | 2.69        | 0.41     |
| 1:A:3443:MET:HE3  | 1:A:3449:ARG:HA   | 2.02        | 0.41     |
| 1:A:3148:ASN:OD1  | 1:A:3150:ALA:N    | 2.45        | 0.41     |
| 1:B:2231:ILE:CG2  | 1:B:2264:GLN:HE22 | 2.31        | 0.41     |
| 1:A:3994:GLY:O    | 1:A:3995:GLY:C    | 2.58        | 0.41     |
| 1:B:3563:LEU:CD1  | 1:B:3845:ILE:HD11 | 2.49        | 0.41     |
| 1:A:4278:HIS:O    | 1:A:4282:GLN:HB2  | 2.20        | 0.41     |
| 1:B:2208:VAL:HG12 | 1:B:2415:TRP:NE1  | 2.36        | 0.41     |
| 1:A:1719:GLN:HA   | 1:A:1722:PHE:CE2  | 2.56        | 0.41     |
| 1:B:3910:GLN:HB3  | 1:B:4231:ARG:HD3  | 2.03        | 0.41     |
| 1:B:2670:LEU:HD12 | 1:B:2670:LEU:O    | 2.20        | 0.41     |
| 1:A:1625:ILE:HG23 | 1:A:1626:ASN:N    | 2.33        | 0.41     |
| 1:B:1872:ARG:NH2  | 1:B:2164:ARG:NE   | 2.68        | 0.41     |
| 1:B:3566:ASN:HD21 | 1:B:3859:LYS:HZ2  | 1.69        | 0.41     |
| 1:B:3960:LEU:HB3  | 1:B:4239:GLU:OE2  | 2.21        | 0.41     |
| 1:B:4284:ARG:HG2  | 1:B:4408:LEU:HB3  | 2.02        | 0.41     |
| 1:A:3206:ILE:HA   | 1:A:3221:PRO:HG2  | 2.03        | 0.41     |
| 1:B:4201:GLU:HG3  | 1:B:4228:ASN:HB2  | 2.03        | 0.41     |
| 1:B:1590:HIS:NE2  | 1:B:1594:ARG:NH1  | 2.68        | 0.41     |
| 1:B:3886:TYR:CE2  | 1:B:3940:LEU:HD23 | 2.56        | 0.41     |
| 1:A:4270:ILE:HG22 | 1:A:4310:ILE:HD13 | 2.01        | 0.41     |
| 1:A:4314:VAL:O    | 1:A:4314:VAL:CG1  | 2.68        | 0.41     |
| 1:A:4648:VAL:CG1  | 1:A:4662:THR:HG21 | 2.41        | 0.41     |
| 1:A:3652:LEU:HD21 | 1:A:3662:ALA:HB2  | 2.02        | 0.41     |
| 1:A:4349:ASN:ND2  | 1:A:4352:ASP:N    | 2.65        | 0.41     |
| 1:A:2749:PRO:HG2  | 1:A:2759:VAL:HG11 | 2.01        | 0.41     |
| 1:A:2774:ARG:HH21 | 1:A:2779:THR:HB   | 1.85        | 0.41     |
| 1:A:2586:GLY:CA   | 1:A:2815:LEU:HD13 | 2.43        | 0.41     |
| 1:B:3602:ILE:O    | 1:B:3603:GLY:C    | 2.59        | 0.41     |
| 1:A:2127:LYS:O    | 1:A:2130:PRO:HD2  | 2.20        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3164:LEU:HA   | 1:A:3164:LEU:HD12 | 1.81        | 0.41     |
| 1:A:3013:LEU:HD23 | 1:A:3170:LEU:HD12 | 2.01        | 0.41     |
| 1:A:3553:VAL:O    | 1:A:3557:VAL:HG23 | 2.21        | 0.41     |
| 1:A:1697:PHE:CD2  | 1:A:1705:LEU:HD11 | 2.55        | 0.41     |
| 1:A:4692:LEU:HD12 | 1:A:4700:LEU:HD21 | 2.02        | 0.41     |
| 1:A:2612:LEU:HD12 | 1:A:2612:LEU:O    | 2.21        | 0.41     |
| 1:A:4012:LEU:H    | 1:A:4012:LEU:HD12 | 1.84        | 0.41     |
| 1:A:3819:ILE:C    | 1:A:3821:GLY:H    | 2.23        | 0.41     |
| 1:B:2036:LEU:O    | 1:B:2036:LEU:HD23 | 2.20        | 0.41     |
| 1:B:4068:GLN:C    | 1:B:4070:SER:H    | 2.24        | 0.41     |
| 1:A:1701:GLY:HA2  | 1:A:2011:ARG:CZ   | 2.50        | 0.41     |
| 1:B:2556:SER:C    | 1:B:2558:PHE:N    | 2.73        | 0.41     |
| 1:A:2376:LEU:HD12 | 1:A:2386:ALA:N    | 2.35        | 0.41     |
| 1:A:2868:ILE:HG21 | 1:A:2922:GLU:OE2  | 2.21        | 0.41     |
| 1:B:4371:PRO:O    | 1:B:4372:ASP:HB2  | 2.20        | 0.41     |
| 1:A:4283:GLU:OE2  | 1:A:4286:ARG:NH1  | 2.54        | 0.41     |
| 1:A:2204:ILE:CA   | 1:A:2207:LEU:HD12 | 2.44        | 0.41     |
| 1:B:3606:ASP:O    | 1:B:3610:ARG:HG3  | 2.21        | 0.41     |
| 1:B:4006:PRO:C    | 1:B:4008:LEU:H    | 2.24        | 0.41     |
| 1:A:2832:ASN:HA   | 1:A:2835:LEU:HB3  | 2.01        | 0.41     |
| 1:A:2222:VAL:C    | 1:A:2224:PRO:HD3  | 2.40        | 0.41     |
| 1:A:2606:PRO:HG2  | 1:A:2615:TYR:CD1  | 2.56        | 0.41     |
| 1:A:1782:ALA:HA   | 1:A:1938:PHE:CZ   | 2.55        | 0.41     |
| 1:A:4401:GLU:HB2  | 1:A:4402:ILE:HD12 | 2.01        | 0.41     |
| 1:A:4289:PRO:HB2  | 1:A:4696:ARG:HD2  | 2.01        | 0.41     |
| 1:B:1817:LEU:HD11 | 1:B:1936:TYR:CD2  | 2.55        | 0.41     |
| 1:A:4012:LEU:HD21 | 1:A:4020:LEU:HD22 | 2.02        | 0.41     |
| 1:B:1493:ILE:O    | 1:B:1497:LEU:HG   | 2.21        | 0.41     |
| 1:A:2376:LEU:HD21 | 1:A:2384:ARG:HB3  | 2.02        | 0.41     |
| 1:B:2223:PHE:C    | 1:B:2225:GLY:H    | 2.23        | 0.41     |
| 1:B:4553:TYR:O    | 1:B:4555:VAL:HG22 | 2.20        | 0.41     |
| 1:A:2275:VAL:HG23 | 1:A:2397:VAL:HG23 | 2.03        | 0.41     |
| 1:A:1766:ILE:HG23 | 1:A:1767:HIS:H    | 1.84        | 0.41     |
| 1:A:2748:LEU:CD2  | 1:A:2800:ARG:HD3  | 2.51        | 0.41     |
| 1:B:4184:TRP:NE1  | 1:B:4214:ARG:HB2  | 2.35        | 0.41     |
| 1:A:4537:LEU:CD2  | 1:A:4548:LYS:HE3  | 2.50        | 0.41     |
| 1:B:3087:MET:HE2  | 1:B:3090:LEU:HD23 | 2.03        | 0.41     |
| 1:A:4278:HIS:HD2  | 1:A:4343:TYR:CE1  | 2.39        | 0.41     |
| 1:A:4247:ASN:HD21 | 1:A:4282:GLN:HE21 | 1.67        | 0.41     |
| 1:B:2711:LEU:HD12 | 1:B:2711:LEU:HA   | 1.89        | 0.41     |
| 1:A:4670:THR:HG22 | 1:A:4671:TRP:N    | 2.36        | 0.41     |
| 1:A:4006:PRO:O    | 1:A:4008:LEU:N    | 2.52        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3439:ASP:OD2  | 1:A:3442:LYS:HE2  | 2.21        | 0.41     |
| 1:A:3571:ARG:HB3  | 1:A:3571:ARG:NH1  | 2.35        | 0.41     |
| 1:B:2670:LEU:C    | 1:B:2670:LEU:HD12 | 2.41        | 0.41     |
| 1:B:1910:MET:CB   | 1:B:1929:MET:HG3  | 2.50        | 0.41     |
| 1:A:4240:ASN:HA   | 1:A:4241:PRO:HD2  | 1.89        | 0.41     |
| 1:A:2694:PHE:CD2  | 1:A:2738:TRP:HB2  | 2.56        | 0.41     |
| 1:A:4001:ILE:HB   | 1:A:4018:LYS:HD3  | 2.02        | 0.41     |
| 1:A:1888:VAL:HG22 | 1:A:1909:HIS:CE1  | 2.56        | 0.41     |
| 1:A:2579:TRP:HZ2  | 1:A:2655:ARG:HD2  | 1.85        | 0.41     |
| 1:A:4535:ARG:HG2  | 1:A:4535:ARG:HH11 | 1.84        | 0.41     |
| 1:B:4535:ARG:HG2  | 1:B:4535:ARG:NH1  | 2.34        | 0.41     |
| 1:B:4023:LEU:HG   | 1:B:4030:PHE:CD1  | 2.56        | 0.41     |
| 1:A:2057:VAL:HG13 | 1:A:2059:LEU:H    | 1.86        | 0.41     |
| 1:B:2278:SER:H    | 1:B:2398:GLN:NE2  | 2.17        | 0.41     |
| 1:B:2400:LEU:HD13 | 1:B:2408:ILE:CD1  | 2.48        | 0.41     |
| 1:A:2615:TYR:HD2  | 1:A:2615:TYR:N    | 2.18        | 0.41     |
| 1:B:2363:TRP:C    | 1:B:2365:GLU:H    | 2.24        | 0.41     |
| 1:B:2853:MET:HA   | 1:B:2882:TRP:CZ3  | 2.56        | 0.41     |
| 1:B:1483:ILE:HG22 | 1:B:1517:VAL:HG22 | 2.02        | 0.41     |
| 1:B:4644:LEU:HD23 | 1:B:4723:ILE:HG12 | 2.02        | 0.41     |
| 1:B:1497:LEU:HB3  | 1:B:1501:SER:CB   | 2.51        | 0.41     |
| 1:B:4509:LEU:HD23 | 1:B:4568:PHE:CE1  | 2.55        | 0.41     |
| 1:B:3903:LEU:O    | 1:B:3909:TYR:HB2  | 2.21        | 0.41     |
| 1:B:2239:LYS:O    | 1:B:2243:ILE:HG13 | 2.21        | 0.41     |
| 1:B:1500:GLY:O    | 1:B:1504:ASP:N    | 2.50        | 0.41     |
| 1:A:2855:GLU:OE2  | 1:A:2933:VAL:HG22 | 2.21        | 0.41     |
| 1:A:2696:VAL:HG22 | 1:A:2697:VAL:N    | 2.36        | 0.41     |
| 1:B:3567:LEU:HD23 | 1:B:3567:LEU:HA   | 1.94        | 0.41     |
| 1:B:3781:VAL:HG12 | 1:B:3782:THR:N    | 2.34        | 0.41     |
| 1:B:3930:LEU:O    | 1:B:3932:ASP:N    | 2.54        | 0.41     |
| 1:A:2269:ASN:C    | 1:A:2271:GLY:H    | 2.24        | 0.41     |
| 1:A:3652:LEU:HB2  | 1:A:3684:PHE:CD1  | 2.55        | 0.41     |
| 1:B:3258:ARG:HD2  | 1:B:3779:SER:HB2  | 2.01        | 0.41     |
| 1:A:2000:CYS:O    | 1:A:2001:ASP:C    | 2.58        | 0.41     |
| 1:A:2028:PHE:CB   | 1:A:2075:VAL:HG13 | 2.44        | 0.41     |
| 1:A:3567:LEU:HD23 | 1:A:3567:LEU:HA   | 1.91        | 0.41     |
| 1:A:4426:MET:O    | 1:A:4430:LEU:HG   | 2.21        | 0.41     |
| 1:A:4033:LEU:HD13 | 1:A:4062:TRP:CZ2  | 2.55        | 0.41     |
| 1:A:2579:TRP:CE3  | 1:A:2659:VAL:HG21 | 2.56        | 0.41     |
| 1:A:2890:ILE:HD13 | 1:A:2893:MET:CE   | 2.51        | 0.41     |
| 1:B:2578:MET:HB3  | 1:B:2597:ILE:CD1  | 2.43        | 0.41     |
| 1:A:1712:SER:HB3  | 1:A:1766:ILE:HB   | 2.03        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:2381:ASN:HD22 | 1:B:2381:ASN:C    | 2.25        | 0.41     |
| 1:A:3597:ALA:O    | 1:A:3601:TYR:HD1  | 2.04        | 0.41     |
| 1:B:2887:LEU:O    | 1:B:2891:GLN:HG3  | 2.21        | 0.41     |
| 1:A:1886:ARG:HG3  | 1:A:1887:ASP:H    | 1.81        | 0.41     |
| 1:B:4157:TYR:HB2  | 1:B:4184:TRP:CB   | 2.50        | 0.41     |
| 1:A:4024:ARG:CG   | 1:A:4031:SER:HA   | 2.49        | 0.41     |
| 1:B:4145:LYS:HE2  | 1:B:4238:TYR:CE1  | 2.55        | 0.41     |
| 1:B:3571:ARG:O    | 1:B:3575:GLU:HG3  | 2.19        | 0.41     |
| 1:A:2848:ASN:HB3  | 1:A:2938:PHE:CE1  | 2.55        | 0.41     |
| 1:B:1739:THR:O    | 1:B:1760:ILE:N    | 2.54        | 0.41     |
| 1:B:3647:TRP:HB3  | 1:B:3652:LEU:HD22 | 2.02        | 0.41     |
| 1:A:3844:ASN:O    | 1:A:3848:ASP:HB2  | 2.20        | 0.41     |
| 1:B:4094:VAL:HB   | 1:B:4423:ALA:HB1  | 2.02        | 0.41     |
| 1:B:2084:ARG:HG2  | 1:B:2084:ARG:NH1  | 2.36        | 0.41     |
| 1:A:2088:PRO:C    | 1:A:2090:ASN:N    | 2.75        | 0.41     |
| 1:A:3078:VAL:HG23 | 1:A:3083:PHE:HB2  | 2.02        | 0.41     |
| 1:B:4503:ILE:HD11 | 1:B:4575:LEU:O    | 2.21        | 0.41     |
| 1:B:4277:PHE:HB2  | 1:B:4363:LEU:HD12 | 2.03        | 0.41     |
| 1:B:2420:ILE:HG13 | 1:B:2421:LEU:N    | 2.36        | 0.41     |
| 1:B:2270:HIS:CA   | 1:B:2392:ARG:HH11 | 2.33        | 0.41     |
| 1:B:1831:LEU:HB3  | 1:B:1900:GLY:HA2  | 2.02        | 0.41     |
| 1:B:4509:LEU:O    | 1:B:4513:ILE:HG13 | 2.20        | 0.41     |
| 1:B:4306:ALA:HA   | 1:B:4338:LEU:HD22 | 2.03        | 0.41     |
| 1:A:1726:PHE:CD2  | 1:A:1729:LEU:HD22 | 2.55        | 0.41     |
| 1:B:4022:CYS:HB3  | 1:B:4026:GLN:NE2  | 2.36        | 0.41     |
| 1:B:2236:LEU:O    | 1:B:2240:ILE:HG13 | 2.21        | 0.41     |
| 1:A:4592:GLY:CA   | 1:A:4725:SER:HB2  | 2.50        | 0.41     |
| 1:B:2151:ALA:O    | 1:B:2154:SER:N    | 2.52        | 0.41     |
| 1:A:4060:GLU:O    | 1:A:4064:VAL:HG23 | 2.21        | 0.41     |
| 1:B:1844:GLN:O    | 1:B:1847:SER:HB2  | 2.21        | 0.41     |
| 1:B:4056:PRO:HD2  | 1:B:4093:ARG:NH2  | 2.36        | 0.41     |
| 1:B:4162:ILE:HG22 | 1:B:4163:GLY:N    | 2.35        | 0.41     |
| 1:B:3228:VAL:HA   | 1:B:3231:LEU:HD12 | 2.03        | 0.41     |
| 1:B:2029:ASN:N    | 1:B:2029:ASN:HD22 | 2.18        | 0.41     |
| 1:B:2492:LEU:O    | 1:B:2493:LYS:C    | 2.59        | 0.41     |
| 1:B:4413:ASN:ND2  | 1:B:4660:LEU:HD23 | 2.36        | 0.41     |
| 1:B:4141:ASP:OD2  | 1:B:4143:SER:HB2  | 2.21        | 0.41     |
| 1:A:3093:GLY:O    | 1:A:3095:GLU:N    | 2.54        | 0.41     |
| 1:A:3230:SER:HA   | 1:A:3620:ARG:HE   | 1.86        | 0.41     |
| 1:B:1734:LEU:HA   | 1:B:1742:ILE:HG12 | 2.03        | 0.41     |
| 1:B:3539:LEU:HA   | 1:B:3539:LEU:HD12 | 1.92        | 0.41     |
| 1:B:4649:TRP:HA   | 1:B:4649:TRP:CE3  | 2.55        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:3606:ASP:O    | 1:A:3610:ARG:HG3  | 2.21        | 0.41     |
| 1:A:2359:VAL:HG23 | 1:A:2397:VAL:HG11 | 2.03        | 0.41     |
| 1:A:3698:SER:C    | 1:A:3700:LEU:HD12 | 2.41        | 0.41     |
| 1:A:4122:VAL:HB   | 1:A:4132:LEU:CD2  | 2.51        | 0.41     |
| 1:B:2260:LEU:O    | 1:B:2263:HIS:HB3  | 2.21        | 0.41     |
| 1:B:3017:VAL:HG13 | 1:B:3174:GLY:C    | 2.41        | 0.41     |
| 1:B:3015:ILE:O    | 1:B:3173:PHE:N    | 2.51        | 0.41     |
| 1:B:1947:LEU:HD21 | 1:B:1982:GLU:CG   | 2.51        | 0.41     |
| 1:B:4711:THR:OG1  | 1:B:4716:TRP:NE1  | 2.54        | 0.41     |
| 1:B:1909:HIS:O    | 1:B:1911:ARG:HD3  | 2.22        | 0.41     |
| 1:A:1939:GLU:O    | 1:A:1941:LEU:HG   | 2.21        | 0.41     |
| 1:A:4606:GLN:HA   | 1:A:4609:SER:OG   | 2.21        | 0.41     |
| 1:A:4063:ILE:HD13 | 1:A:4082:LYS:NZ   | 2.36        | 0.41     |
| 1:A:2332:PHE:HA   | 1:A:2335:THR:OG1  | 2.20        | 0.41     |
| 1:B:3685:LEU:O    | 1:B:3689:TYR:HB2  | 2.20        | 0.41     |
| 1:A:2269:ASN:C    | 1:A:2271:GLY:N    | 2.74        | 0.40     |
| 1:A:4647:ALA:HA   | 1:A:4657:THR:HG22 | 2.02        | 0.40     |
| 1:A:3720:VAL:HG21 | 1:A:3762:ILE:HD11 | 2.03        | 0.40     |
| 1:A:3237:THR:OG1  | 1:A:3238:ILE:HD12 | 2.21        | 0.40     |
| 1:A:4090:HIS:C    | 1:A:4092:ASP:H    | 2.24        | 0.40     |
| 1:A:4086:MET:HG2  | 1:A:4093:ARG:HB2  | 1.99        | 0.40     |
| 1:B:3234:ILE:O    | 1:B:3238:ILE:HD13 | 2.21        | 0.40     |
| 1:B:2754:TYR:O    | 1:B:2756:THR:HG22 | 2.21        | 0.40     |
| 1:B:2120:THR:HB   | 1:B:2124:LEU:HG   | 2.03        | 0.40     |
| 1:B:3046:TYR:CZ   | 1:B:3050:ASP:HB2  | 2.55        | 0.40     |
| 1:A:2439:PHE:HZ   | 1:A:2542:ASN:OD1  | 2.03        | 0.40     |
| 1:B:4499:PHE:HA   | 1:B:4502:GLU:HB2  | 2.03        | 0.40     |
| 1:B:3976:VAL:HG13 | 1:B:4105:VAL:HG11 | 2.01        | 0.40     |
| 1:A:3025:LEU:HD23 | 1:A:3025:LEU:HA   | 1.86        | 0.40     |
| 1:A:3022:LYS:HB2  | 1:A:3022:LYS:NZ   | 2.36        | 0.40     |
| 1:A:3199:TYR:OH   | 1:A:3226:ALA:HB2  | 2.21        | 0.40     |
| 1:A:1633:SER:O    | 1:A:1637:LYS:HG2  | 2.21        | 0.40     |
| 1:A:2877:ARG:HD2  | 1:A:2881:ARG:NH2  | 2.36        | 0.40     |
| 1:A:2935:LEU:C    | 1:A:2935:LEU:HD23 | 2.41        | 0.40     |
| 1:B:1928:HIS:CG   | 1:B:1933:THR:HG22 | 2.52        | 0.40     |
| 1:A:2212:ILE:O    | 1:A:2215:ILE:HG22 | 2.22        | 0.40     |
| 1:A:3698:SER:O    | 1:A:3704:PHE:HB2  | 2.22        | 0.40     |
| 1:B:4264:PRO:HA   | 1:B:4322:SER:O    | 2.21        | 0.40     |
| 1:B:3218:ALA:O    | 1:B:3219:ILE:C    | 2.60        | 0.40     |
| 1:A:2005:ASP:OD1  | 1:A:2006:LEU:N    | 2.55        | 0.40     |
| 1:B:1546:VAL:HG12 | 1:B:1547:ASN:N    | 2.36        | 0.40     |
| 1:B:2081:TYR:O    | 1:B:2082:ALA:HB3  | 2.21        | 0.40     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:1820:GLN:NE2  | 1:B:1990:GLN:NE2  | 2.66        | 0.40     |
| 1:A:4117:ASP:C    | 1:A:4119:ALA:H    | 2.25        | 0.40     |
| 1:B:4083:ILE:HD11 | 1:B:4098:SER:HA   | 2.03        | 0.40     |
| 1:A:3225:ASP:O    | 1:A:3229:SER:CB   | 2.69        | 0.40     |
| 1:A:3997:ASN:O    | 1:A:3998:LEU:C    | 2.60        | 0.40     |
| 1:A:3727:ASP:C    | 1:A:3729:VAL:H    | 2.25        | 0.40     |
| 1:B:4493:ASP:OD1  | 1:B:4494:PRO:HD2  | 2.21        | 0.40     |
| 1:A:4245:LYS:HE2  | 1:A:4249:LEU:HD11 | 2.03        | 0.40     |
| 1:A:3256:THR:HB   | 1:A:3257:PRO:CD   | 2.51        | 0.40     |
| 1:B:2379:LEU:HD12 | 1:B:2383:GLU:HG2  | 2.03        | 0.40     |
| 1:B:4402:ILE:N    | 1:B:4402:ILE:CD1  | 2.81        | 0.40     |
| 1:B:3966:THR:HG23 | 1:B:4426:MET:HE3  | 2.02        | 0.40     |
| 1:A:2793:ASN:HB3  | 1:A:2794:PRO:HD2  | 2.04        | 0.40     |
| 1:B:3700:LEU:CD1  | 1:B:3701:ASP:N    | 2.80        | 0.40     |
| 1:B:3256:THR:N    | 1:B:3259:HIS:HD2  | 2.19        | 0.40     |
| 1:B:4703:ILE:CD1  | 1:B:4705:LEU:HD21 | 2.45        | 0.40     |
| 1:A:4418:LEU:HD11 | 1:A:4422:LYS:NZ   | 2.36        | 0.40     |
| 1:B:4428:ASN:O    | 1:B:4432:LYS:HG3  | 2.21        | 0.40     |
| 1:A:2995:LEU:CD2  | 1:A:2998:ILE:HD11 | 2.48        | 0.40     |
| 1:B:1696:ARG:HH21 | 1:B:1726:PHE:HA   | 1.86        | 0.40     |
| 1:B:4403:SER:HB2  | 1:B:4407:TRP:CD2  | 2.56        | 0.40     |
| 1:A:1726:PHE:CB   | 1:A:1729:LEU:HB3  | 2.51        | 0.40     |
| 1:A:4130:SER:HA   | 1:A:4131:PRO:HD3  | 1.88        | 0.40     |
| 1:A:2986:VAL:O    | 1:A:2988:LEU:HG   | 2.20        | 0.40     |
| 1:A:4189:ASN:HA   | 1:A:4191:HIS:CD2  | 2.57        | 0.40     |
| 1:A:1898:LEU:HA   | 1:A:1898:LEU:HD23 | 1.89        | 0.40     |
| 1:A:1853:GLN:HE22 | 1:A:1886:ARG:HH11 | 1.68        | 0.40     |
| 1:B:2258:LYS:HD3  | 1:B:2261:GLN:OE1  | 2.21        | 0.40     |
| 1:A:3947:ILE:HD13 | 1:A:3947:ILE:O    | 2.21        | 0.40     |
| 1:A:4247:ASN:HD21 | 1:A:4282:GLN:NE2  | 2.19        | 0.40     |
| 1:B:2135:CYS:O    | 1:B:2139:LEU:HB2  | 2.21        | 0.40     |
| 1:B:1867:LEU:HD12 | 1:B:1867:LEU:H    | 1.86        | 0.40     |
| 1:B:3002:ASP:HA   | 1:B:3029:VAL:HG11 | 2.04        | 0.40     |
| 1:A:2529:THR:O    | 1:A:2530:ARG:C    | 2.60        | 0.40     |
| 1:B:2029:ASN:HD22 | 1:B:2030:ARG:N    | 2.20        | 0.40     |
| 1:A:2536:SER:HB2  | 1:A:2580:GLY:O    | 2.21        | 0.40     |
| 1:B:2688:LEU:HD13 | 1:B:2696:VAL:HB   | 2.04        | 0.40     |
| 1:B:1928:HIS:NE2  | 1:B:1933:THR:CG2  | 2.81        | 0.40     |
| 1:B:3927:ASN:HB3  | 1:B:3930:LEU:HD12 | 2.02        | 0.40     |
| 1:B:1813:GLN:HE22 | 1:B:1941:LEU:H    | 1.69        | 0.40     |
| 1:B:2519:ALA:HB2  | 1:B:2593:PHE:CE1  | 2.57        | 0.40     |
| 1:A:4057:ILE:HA   | 1:A:4057:ILE:HD12 | 1.96        | 0.40     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:B:3271:ILE:HA   | 1:B:3592:VAL:HG21 | 2.03        | 0.40     |
| 1:A:2236:LEU:HD21 | 1:A:2293:ILE:CD1  | 2.44        | 0.40     |
| 1:A:1831:LEU:HD22 | 1:A:1898:LEU:HD13 | 2.04        | 0.40     |
| 1:B:2309:LYS:HG3  | 1:B:2358:ASP:HB2  | 2.02        | 0.40     |
| 1:A:3459:ASP:HA   | 1:A:3460:PRO:HD3  | 1.97        | 0.40     |
| 1:A:3296:GLU:HG3  | 1:A:3567:LEU:HD13 | 2.04        | 0.40     |
| 1:A:2591:GLU:OE1  | 1:A:2611:PRO:HG2  | 2.22        | 0.40     |
| 1:A:1778:LYS:HB3  | 1:A:1922:LEU:HD11 | 2.04        | 0.40     |
| 1:B:4432:LYS:C    | 1:B:4434:GLN:H    | 2.25        | 0.40     |
| 1:A:3066:GLU:HG2  | 1:A:3136:GLN:NE2  | 2.36        | 0.40     |
| 1:A:4284:ARG:CG   | 1:A:4408:LEU:HB3  | 2.49        | 0.40     |
| 1:B:2270:HIS:CB   | 1:B:2392:ARG:HH11 | 2.34        | 0.40     |
| 1:B:2745:GLU:HG2  | 1:B:2748:LEU:CD1  | 2.51        | 0.40     |
| 1:B:1906:TRP:CZ2  | 1:B:1911:ARG:HG2  | 2.57        | 0.40     |
| 1:B:2799:GLY:HA3  | 1:B:3159:ALA:HB1  | 2.04        | 0.40     |
| 1:A:2710:LEU:HD23 | 1:A:2762:PHE:CE2  | 2.57        | 0.40     |
| 1:A:3845:ILE:HG13 | 1:A:3845:ILE:H    | 1.57        | 0.40     |
| 1:B:2645:ASP:OD2  | 1:B:2645:ASP:N    | 2.54        | 0.40     |
| 1:A:2036:LEU:O    | 1:A:2036:LEU:HD12 | 2.21        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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     | 3010/3367 (89%) | 2424 (80%) | 448 (15%) | 138 (5%) | 4           | 46 |
| 1   | B     | 2870/3367 (85%) | 2476 (86%) | 327 (11%) | 67 (2%)  | 10          | 65 |
| All | All   | 5880/6734 (87%) | 4900 (83%) | 775 (13%) | 205 (4%) | 6           | 56 |

All (205) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1836 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2121 | ALA  |
| 1   | A     | 2409 | SER  |
| 1   | A     | 2560 | MET  |
| 1   | A     | 2617 | VAL  |
| 1   | A     | 2641 | VAL  |
| 1   | A     | 2646 | VAL  |
| 1   | A     | 2943 | LEU  |
| 1   | A     | 2992 | ASN  |
| 1   | A     | 3033 | ASN  |
| 1   | A     | 3219 | ILE  |
| 1   | A     | 3370 | GLU  |
| 1   | A     | 3371 | PRO  |
| 1   | A     | 3372 | ALA  |
| 1   | A     | 3603 | GLY  |
| 1   | A     | 4050 | LYS  |
| 1   | A     | 4051 | ASP  |
| 1   | A     | 4117 | ASP  |
| 1   | A     | 4121 | ILE  |
| 1   | A     | 4207 | LEU  |
| 1   | A     | 4548 | LYS  |
| 1   | A     | 4549 | GLU  |
| 1   | A     | 4660 | LEU  |
| 1   | B     | 1949 | GLN  |
| 1   | B     | 1975 | PRO  |
| 1   | B     | 1980 | LYS  |
| 1   | B     | 2071 | MET  |
| 1   | B     | 3602 | ILE  |
| 1   | B     | 3931 | VAL  |
| 1   | B     | 4207 | LEU  |
| 1   | A     | 1714 | ASP  |
| 1   | A     | 1949 | GLN  |
| 1   | A     | 2004 | PHE  |
| 1   | A     | 2080 | GLY  |
| 1   | A     | 2101 | ILE  |
| 1   | A     | 2342 | ASN  |
| 1   | A     | 2527 | ASP  |
| 1   | A     | 2530 | ARG  |
| 1   | A     | 2628 | LYS  |
| 1   | A     | 2642 | ALA  |
| 1   | A     | 2645 | ASP  |
| 1   | A     | 2727 | GLU  |
| 1   | A     | 2776 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2789 | VAL  |
| 1   | A     | 2792 | CYS  |
| 1   | A     | 3218 | ALA  |
| 1   | A     | 3430 | ASN  |
| 1   | A     | 3440 | THR  |
| 1   | A     | 3488 | SER  |
| 1   | A     | 3715 | GLY  |
| 1   | A     | 3719 | LEU  |
| 1   | A     | 3841 | ALA  |
| 1   | A     | 3926 | ASN  |
| 1   | A     | 3994 | GLY  |
| 1   | A     | 3998 | LEU  |
| 1   | A     | 4000 | SER  |
| 1   | A     | 4014 | THR  |
| 1   | A     | 4053 | VAL  |
| 1   | A     | 4116 | LEU  |
| 1   | A     | 4123 | GLU  |
| 1   | A     | 4125 | GLU  |
| 1   | A     | 4158 | LYS  |
| 1   | A     | 4221 | ILE  |
| 1   | A     | 4342 | ILE  |
| 1   | A     | 4594 | LEU  |
| 1   | A     | 4666 | ILE  |
| 1   | A     | 4672 | LYS  |
| 1   | A     | 4709 | GLN  |
| 1   | B     | 1919 | GLU  |
| 1   | B     | 2141 | ALA  |
| 1   | B     | 2230 | PRO  |
| 1   | B     | 2384 | ARG  |
| 1   | B     | 2600 | ILE  |
| 1   | B     | 2641 | VAL  |
| 1   | B     | 2755 | GLY  |
| 1   | B     | 2775 | THR  |
| 1   | B     | 3092 | ALA  |
| 1   | B     | 3603 | GLY  |
| 1   | B     | 3842 | SER  |
| 1   | B     | 3844 | ASN  |
| 1   | B     | 4113 | THR  |
| 1   | B     | 4221 | ILE  |
| 1   | B     | 4297 | GLU  |
| 1   | B     | 4340 | SER  |
| 1   | B     | 4464 | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 4551 | LYS  |
| 1   | A     | 1663 | GLU  |
| 1   | A     | 1697 | PHE  |
| 1   | A     | 1703 | GLU  |
| 1   | A     | 1727 | ALA  |
| 1   | A     | 1923 | HIS  |
| 1   | A     | 2001 | ASP  |
| 1   | A     | 2089 | ASP  |
| 1   | A     | 2140 | SER  |
| 1   | A     | 2282 | LYS  |
| 1   | A     | 2329 | ASP  |
| 1   | A     | 2374 | ASN  |
| 1   | A     | 2705 | THR  |
| 1   | A     | 2871 | HIS  |
| 1   | A     | 2990 | LEU  |
| 1   | A     | 3082 | SER  |
| 1   | A     | 3671 | TYR  |
| 1   | A     | 3693 | LYS  |
| 1   | A     | 3843 | GLY  |
| 1   | A     | 3933 | LYS  |
| 1   | A     | 4007 | GLN  |
| 1   | A     | 4055 | GLU  |
| 1   | A     | 4118 | MET  |
| 1   | A     | 4131 | PRO  |
| 1   | A     | 4163 | GLY  |
| 1   | A     | 4168 | PHE  |
| 1   | A     | 4318 | SER  |
| 1   | A     | 4401 | GLU  |
| 1   | A     | 4412 | GLU  |
| 1   | B     | 1663 | GLU  |
| 1   | B     | 2001 | ASP  |
| 1   | B     | 2527 | ASP  |
| 1   | B     | 2915 | ASP  |
| 1   | B     | 3080 | GLU  |
| 1   | B     | 3094 | GLY  |
| 1   | B     | 3248 | ARG  |
| 1   | B     | 3692 | LYS  |
| 1   | B     | 4071 | ASN  |
| 1   | B     | 4692 | LEU  |
| 1   | A     | 1799 | ASP  |
| 1   | A     | 1837 | GLN  |
| 1   | A     | 2002 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2054 | SER  |
| 1   | A     | 2122 | GLU  |
| 1   | A     | 2177 | ALA  |
| 1   | A     | 2270 | HIS  |
| 1   | A     | 2370 | LEU  |
| 1   | A     | 2653 | THR  |
| 1   | A     | 2690 | ALA  |
| 1   | A     | 2744 | ASP  |
| 1   | A     | 2891 | GLN  |
| 1   | A     | 3094 | GLY  |
| 1   | A     | 3166 | ASN  |
| 1   | A     | 3444 | MET  |
| 1   | A     | 3699 | PHE  |
| 1   | A     | 3907 | HIS  |
| 1   | A     | 4026 | GLN  |
| 1   | A     | 4029 | SER  |
| 1   | A     | 4259 | ARG  |
| 1   | A     | 4519 | ASN  |
| 1   | B     | 1506 | ASP  |
| 1   | B     | 2165 | LYS  |
| 1   | B     | 2308 | PRO  |
| 1   | B     | 2401 | LYS  |
| 1   | B     | 2749 | PRO  |
| 1   | B     | 2947 | LYS  |
| 1   | B     | 3932 | ASP  |
| 1   | B     | 4003 | GLU  |
| 1   | B     | 4051 | ASP  |
| 1   | B     | 4053 | VAL  |
| 1   | B     | 4189 | ASN  |
| 1   | B     | 4674 | LYS  |
| 1   | A     | 2363 | TRP  |
| 1   | A     | 2601 | ALA  |
| 1   | A     | 2987 | PRO  |
| 1   | A     | 3140 | ASN  |
| 1   | A     | 3142 | HIS  |
| 1   | A     | 3471 | SER  |
| 1   | A     | 3712 | LEU  |
| 1   | A     | 3999 | THR  |
| 1   | A     | 4011 | LEU  |
| 1   | A     | 4169 | GLU  |
| 1   | A     | 4579 | SER  |
| 1   | A     | 4691 | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 4712 | SER  |
| 1   | B     | 1498 | THR  |
| 1   | B     | 2069 | GLN  |
| 1   | B     | 2140 | SER  |
| 1   | B     | 2210 | ASP  |
| 1   | B     | 2558 | PHE  |
| 1   | B     | 3693 | LYS  |
| 1   | B     | 3849 | ASP  |
| 1   | B     | 3963 | ASP  |
| 1   | B     | 4412 | GLU  |
| 1   | A     | 1868 | SER  |
| 1   | A     | 1944 | GLY  |
| 1   | A     | 2966 | SER  |
| 1   | A     | 3164 | LEU  |
| 1   | A     | 3716 | CYS  |
| 1   | A     | 3845 | ILE  |
| 1   | B     | 1582 | LYS  |
| 1   | B     | 1630 | PRO  |
| 1   | B     | 1727 | ALA  |
| 1   | B     | 4459 | GLU  |
| 1   | B     | 4621 | LEU  |
| 1   | A     | 3395 | PRO  |
| 1   | A     | 3806 | ARG  |
| 1   | A     | 3976 | VAL  |
| 1   | B     | 4131 | PRO  |
| 1   | A     | 4056 | PRO  |
| 1   | B     | 3093 | GLY  |
| 1   | B     | 4556 | PRO  |
| 1   | A     | 2644 | PRO  |
| 1   | A     | 2755 | GLY  |
| 1   | A     | 3602 | ILE  |
| 1   | A     | 3677 | PRO  |
| 1   | B     | 1579 | PRO  |
| 1   | B     | 2380 | PRO  |
| 1   | A     | 2208 | VAL  |
| 1   | B     | 4094 | VAL  |

### 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     | 2457/3028 (81%) | 2249 (92%) | 208 (8%) | 15          | 62 |
| 1   | B     | 2353/3028 (78%) | 2210 (94%) | 143 (6%) | 26          | 75 |
| All | All   | 4810/6056 (79%) | 4459 (93%) | 351 (7%) | 20          | 69 |

All (351) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1516 | GLU  |
| 1   | A     | 1559 | ASP  |
| 1   | A     | 1593 | ASP  |
| 1   | A     | 1594 | ARG  |
| 1   | A     | 1665 | ILE  |
| 1   | A     | 1699 | PHE  |
| 1   | A     | 1719 | GLN  |
| 1   | A     | 1744 | MET  |
| 1   | A     | 1753 | THR  |
| 1   | A     | 1756 | LYS  |
| 1   | A     | 1803 | TYR  |
| 1   | A     | 1809 | ASN  |
| 1   | A     | 1844 | GLN  |
| 1   | A     | 1849 | GLU  |
| 1   | A     | 1865 | GLN  |
| 1   | A     | 1874 | LYS  |
| 1   | A     | 1882 | LEU  |
| 1   | A     | 1911 | ARG  |
| 1   | A     | 1922 | LEU  |
| 1   | A     | 1934 | PHE  |
| 1   | A     | 1962 | GLN  |
| 1   | A     | 1973 | PHE  |
| 1   | A     | 1978 | THR  |
| 1   | A     | 2006 | LEU  |
| 1   | A     | 2029 | ASN  |
| 1   | A     | 2051 | LYS  |
| 1   | A     | 2053 | ASN  |
| 1   | A     | 2069 | GLN  |
| 1   | A     | 2071 | MET  |
| 1   | A     | 2073 | ILE  |
| 1   | A     | 2090 | ASN  |
| 1   | A     | 2096 | ARG  |
| 1   | A     | 2105 | ARG  |
| 1   | A     | 2107 | MET  |
| 1   | A     | 2120 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2136 | GLN  |
| 1   | A     | 2142 | GLN  |
| 1   | A     | 2149 | LEU  |
| 1   | A     | 2152 | LEU  |
| 1   | A     | 2221 | ASP  |
| 1   | A     | 2234 | ASP  |
| 1   | A     | 2239 | LYS  |
| 1   | A     | 2274 | MET  |
| 1   | A     | 2297 | ASP  |
| 1   | A     | 2324 | THR  |
| 1   | A     | 2329 | ASP  |
| 1   | A     | 2346 | GLU  |
| 1   | A     | 2350 | ARG  |
| 1   | A     | 2359 | VAL  |
| 1   | A     | 2369 | SER  |
| 1   | A     | 2384 | ARG  |
| 1   | A     | 2392 | ARG  |
| 1   | A     | 2408 | ILE  |
| 1   | A     | 2409 | SER  |
| 1   | A     | 2415 | TRP  |
| 1   | A     | 2424 | GLN  |
| 1   | A     | 2435 | SER  |
| 1   | A     | 2442 | GLN  |
| 1   | A     | 2450 | ASN  |
| 1   | A     | 2511 | LEU  |
| 1   | A     | 2512 | VAL  |
| 1   | A     | 2527 | ASP  |
| 1   | A     | 2529 | THR  |
| 1   | A     | 2572 | ARG  |
| 1   | A     | 2587 | LEU  |
| 1   | A     | 2603 | THR  |
| 1   | A     | 2613 | LEU  |
| 1   | A     | 2614 | ASP  |
| 1   | A     | 2615 | TYR  |
| 1   | A     | 2626 | LEU  |
| 1   | A     | 2645 | ASP  |
| 1   | A     | 2650 | THR  |
| 1   | A     | 2685 | THR  |
| 1   | A     | 2694 | PHE  |
| 1   | A     | 2728 | THR  |
| 1   | A     | 2747 | ASN  |
| 1   | A     | 2761 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2793 | ASN  |
| 1   | A     | 2809 | ARG  |
| 1   | A     | 2817 | ASP  |
| 1   | A     | 2863 | ARG  |
| 1   | A     | 2873 | ILE  |
| 1   | A     | 2880 | SER  |
| 1   | A     | 2883 | ASP  |
| 1   | A     | 2897 | THR  |
| 1   | A     | 2926 | THR  |
| 1   | A     | 2944 | ASP  |
| 1   | A     | 2954 | ASN  |
| 1   | A     | 2998 | ILE  |
| 1   | A     | 3007 | GLN  |
| 1   | A     | 3026 | SER  |
| 1   | A     | 3027 | ARG  |
| 1   | A     | 3037 | ILE  |
| 1   | A     | 3043 | ASN  |
| 1   | A     | 3052 | ASP  |
| 1   | A     | 3084 | LEU  |
| 1   | A     | 3123 | LEU  |
| 1   | A     | 3141 | LEU  |
| 1   | A     | 3143 | VAL  |
| 1   | A     | 3145 | PHE  |
| 1   | A     | 3158 | SER  |
| 1   | A     | 3168 | CYS  |
| 1   | A     | 3175 | GLU  |
| 1   | A     | 3179 | GLU  |
| 1   | A     | 3186 | SER  |
| 1   | A     | 3195 | GLU  |
| 1   | A     | 3200 | ILE  |
| 1   | A     | 3216 | LEU  |
| 1   | A     | 3240 | GLU  |
| 1   | A     | 3269 | LEU  |
| 1   | A     | 3278 | LEU  |
| 1   | A     | 3330 | ASP  |
| 1   | A     | 3337 | LYS  |
| 1   | A     | 3365 | ASP  |
| 1   | A     | 3366 | LEU  |
| 1   | A     | 3373 | ILE  |
| 1   | A     | 3381 | SER  |
| 1   | A     | 3399 | THR  |
| 1   | A     | 3405 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3432 | ILE  |
| 1   | A     | 3457 | LEU  |
| 1   | A     | 3468 | ASN  |
| 1   | A     | 3516 | ASP  |
| 1   | A     | 3536 | TYR  |
| 1   | A     | 3564 | LEU  |
| 1   | A     | 3566 | ASN  |
| 1   | A     | 3569 | SER  |
| 1   | A     | 3571 | ARG  |
| 1   | A     | 3583 | THR  |
| 1   | A     | 3584 | GLN  |
| 1   | A     | 3612 | ASP  |
| 1   | A     | 3623 | SER  |
| 1   | A     | 3630 | SER  |
| 1   | A     | 3663 | ILE  |
| 1   | A     | 3676 | ASP  |
| 1   | A     | 3678 | SER  |
| 1   | A     | 3691 | ASP  |
| 1   | A     | 3695 | THR  |
| 1   | A     | 3700 | LEU  |
| 1   | A     | 3707 | ASN  |
| 1   | A     | 3719 | LEU  |
| 1   | A     | 3725 | ASN  |
| 1   | A     | 3730 | LEU  |
| 1   | A     | 3731 | ASN  |
| 1   | A     | 3759 | SER  |
| 1   | A     | 3760 | PHE  |
| 1   | A     | 3776 | ASP  |
| 1   | A     | 3785 | ASN  |
| 1   | A     | 3791 | SER  |
| 1   | A     | 3799 | HIS  |
| 1   | A     | 3806 | ARG  |
| 1   | A     | 3813 | ARG  |
| 1   | A     | 3817 | LEU  |
| 1   | A     | 3830 | LEU  |
| 1   | A     | 3865 | ILE  |
| 1   | A     | 3867 | LEU  |
| 1   | A     | 3887 | ASN  |
| 1   | A     | 3922 | ASN  |
| 1   | A     | 3925 | ASN  |
| 1   | A     | 3947 | ILE  |
| 1   | A     | 3974 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3998 | LEU  |
| 1   | A     | 4007 | GLN  |
| 1   | A     | 4023 | LEU  |
| 1   | A     | 4026 | GLN  |
| 1   | A     | 4034 | VAL  |
| 1   | A     | 4039 | GLN  |
| 1   | A     | 4043 | ASP  |
| 1   | A     | 4048 | PHE  |
| 1   | A     | 4055 | GLU  |
| 1   | A     | 4069 | LEU  |
| 1   | A     | 4079 | ASN  |
| 1   | A     | 4100 | SER  |
| 1   | A     | 4200 | LEU  |
| 1   | A     | 4206 | SER  |
| 1   | A     | 4232 | MET  |
| 1   | A     | 4240 | ASN  |
| 1   | A     | 4259 | ARG  |
| 1   | A     | 4267 | ARG  |
| 1   | A     | 4282 | GLN  |
| 1   | A     | 4286 | ARG  |
| 1   | A     | 4290 | LEU  |
| 1   | A     | 4295 | PHE  |
| 1   | A     | 4321 | ARG  |
| 1   | A     | 4337 | ILE  |
| 1   | A     | 4353 | MET  |
| 1   | A     | 4360 | LEU  |
| 1   | A     | 4362 | GLN  |
| 1   | A     | 4385 | GLU  |
| 1   | A     | 4388 | THR  |
| 1   | A     | 4404 | THR  |
| 1   | A     | 4428 | ASN  |
| 1   | A     | 4434 | GLN  |
| 1   | A     | 4503 | ILE  |
| 1   | A     | 4550 | TRP  |
| 1   | A     | 4553 | TYR  |
| 1   | A     | 4565 | ILE  |
| 1   | A     | 4566 | SER  |
| 1   | A     | 4596 | ASN  |
| 1   | A     | 4606 | GLN  |
| 1   | A     | 4638 | ASN  |
| 1   | A     | 4649 | TRP  |
| 1   | A     | 4671 | TRP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 4692 | LEU  |
| 1   | A     | 4693 | ASN  |
| 1   | A     | 4694 | GLU  |
| 1   | A     | 4711 | THR  |
| 1   | A     | 4714 | GLN  |
| 1   | B     | 1479 | ARG  |
| 1   | B     | 1490 | THR  |
| 1   | B     | 1545 | LEU  |
| 1   | B     | 1547 | ASN  |
| 1   | B     | 1555 | VAL  |
| 1   | B     | 1596 | ASN  |
| 1   | B     | 1629 | LEU  |
| 1   | B     | 1640 | ASN  |
| 1   | B     | 1658 | GLU  |
| 1   | B     | 1671 | ARG  |
| 1   | B     | 1712 | SER  |
| 1   | B     | 1734 | LEU  |
| 1   | B     | 1736 | ASP  |
| 1   | B     | 1762 | ASN  |
| 1   | B     | 1793 | ASN  |
| 1   | B     | 1809 | ASN  |
| 1   | B     | 1817 | LEU  |
| 1   | B     | 1828 | ASP  |
| 1   | B     | 1867 | LEU  |
| 1   | B     | 1901 | ASN  |
| 1   | B     | 1911 | ARG  |
| 1   | B     | 1920 | ASN  |
| 1   | B     | 1946 | ARG  |
| 1   | B     | 2029 | ASN  |
| 1   | B     | 2071 | MET  |
| 1   | B     | 2106 | GLU  |
| 1   | B     | 2129 | VAL  |
| 1   | B     | 2149 | LEU  |
| 1   | B     | 2166 | CYS  |
| 1   | B     | 2185 | GLN  |
| 1   | B     | 2189 | GLN  |
| 1   | B     | 2197 | ASN  |
| 1   | B     | 2211 | ASP  |
| 1   | B     | 2235 | GLN  |
| 1   | B     | 2236 | LEU  |
| 1   | B     | 2239 | LYS  |
| 1   | B     | 2253 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 2254 | GLU  |
| 1   | B     | 2260 | LEU  |
| 1   | B     | 2290 | LEU  |
| 1   | B     | 2313 | LYS  |
| 1   | B     | 2320 | LEU  |
| 1   | B     | 2342 | ASN  |
| 1   | B     | 2352 | TRP  |
| 1   | B     | 2374 | ASN  |
| 1   | B     | 2381 | ASN  |
| 1   | B     | 2423 | THR  |
| 1   | B     | 2425 | MET  |
| 1   | B     | 2432 | ASP  |
| 1   | B     | 2504 | GLN  |
| 1   | B     | 2541 | MET  |
| 1   | B     | 2550 | GLU  |
| 1   | B     | 2581 | LEU  |
| 1   | B     | 2587 | LEU  |
| 1   | B     | 2603 | THR  |
| 1   | B     | 2612 | LEU  |
| 1   | B     | 2613 | LEU  |
| 1   | B     | 2699 | LEU  |
| 1   | B     | 2745 | GLU  |
| 1   | B     | 2797 | ASP  |
| 1   | B     | 2821 | THR  |
| 1   | B     | 2825 | THR  |
| 1   | B     | 2841 | ASN  |
| 1   | B     | 2843 | ARG  |
| 1   | B     | 2883 | ASP  |
| 1   | B     | 2897 | THR  |
| 1   | B     | 2899 | GLU  |
| 1   | B     | 2927 | ASP  |
| 1   | B     | 2928 | LYS  |
| 1   | B     | 2929 | LYS  |
| 1   | B     | 2946 | LEU  |
| 1   | B     | 2966 | SER  |
| 1   | B     | 2977 | LYS  |
| 1   | B     | 2984 | LEU  |
| 1   | B     | 2996 | ASP  |
| 1   | B     | 3018 | SER  |
| 1   | B     | 3026 | SER  |
| 1   | B     | 3043 | ASN  |
| 1   | B     | 3050 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 3059 | LEU  |
| 1   | B     | 3087 | MET  |
| 1   | B     | 3140 | ASN  |
| 1   | B     | 3151 | SER  |
| 1   | B     | 3164 | LEU  |
| 1   | B     | 3195 | GLU  |
| 1   | B     | 3284 | HIS  |
| 1   | B     | 3302 | LEU  |
| 1   | B     | 3322 | GLN  |
| 1   | B     | 3560 | SER  |
| 1   | B     | 3563 | LEU  |
| 1   | B     | 3566 | ASN  |
| 1   | B     | 3619 | ILE  |
| 1   | B     | 3620 | ARG  |
| 1   | B     | 3623 | SER  |
| 1   | B     | 3676 | ASP  |
| 1   | B     | 3700 | LEU  |
| 1   | B     | 3725 | ASN  |
| 1   | B     | 3780 | ARG  |
| 1   | B     | 3833 | SER  |
| 1   | B     | 3867 | LEU  |
| 1   | B     | 3954 | ARG  |
| 1   | B     | 3998 | LEU  |
| 1   | B     | 4005 | ILE  |
| 1   | B     | 4012 | LEU  |
| 1   | B     | 4029 | SER  |
| 1   | B     | 4046 | GLN  |
| 1   | B     | 4091 | SER  |
| 1   | B     | 4105 | VAL  |
| 1   | B     | 4157 | TYR  |
| 1   | B     | 4185 | VAL  |
| 1   | B     | 4189 | ASN  |
| 1   | B     | 4200 | LEU  |
| 1   | B     | 4206 | SER  |
| 1   | B     | 4218 | THR  |
| 1   | B     | 4219 | SER  |
| 1   | B     | 4232 | MET  |
| 1   | B     | 4258 | THR  |
| 1   | B     | 4309 | SER  |
| 1   | B     | 4318 | SER  |
| 1   | B     | 4323 | ASN  |
| 1   | B     | 4324 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 4327 | ASP  |
| 1   | B     | 4334 | VAL  |
| 1   | B     | 4356 | LEU  |
| 1   | B     | 4402 | ILE  |
| 1   | B     | 4413 | ASN  |
| 1   | B     | 4425 | LYS  |
| 1   | B     | 4434 | GLN  |
| 1   | B     | 4500 | GLU  |
| 1   | B     | 4503 | ILE  |
| 1   | B     | 4548 | LYS  |
| 1   | B     | 4555 | VAL  |
| 1   | B     | 4558 | THR  |
| 1   | B     | 4573 | GLN  |
| 1   | B     | 4576 | SER  |
| 1   | B     | 4596 | ASN  |
| 1   | B     | 4607 | SER  |
| 1   | B     | 4618 | ASN  |
| 1   | B     | 4644 | LEU  |
| 1   | B     | 4693 | ASN  |
| 1   | B     | 4698 | GLU  |
| 1   | B     | 4709 | GLN  |
| 1   | B     | 4715 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1512 | ASN  |
| 1   | A     | 1522 | GLN  |
| 1   | A     | 1549 | GLN  |
| 1   | A     | 1563 | ASN  |
| 1   | A     | 1609 | GLN  |
| 1   | A     | 1690 | GLN  |
| 1   | A     | 1791 | HIS  |
| 1   | A     | 1798 | ASN  |
| 1   | A     | 1809 | ASN  |
| 1   | A     | 1813 | GLN  |
| 1   | A     | 1844 | GLN  |
| 1   | A     | 1853 | GLN  |
| 1   | A     | 1857 | ASN  |
| 1   | A     | 1858 | ASN  |
| 1   | A     | 1865 | GLN  |
| 1   | A     | 1877 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1971 | ASN  |
| 1   | A     | 1990 | GLN  |
| 1   | A     | 2018 | GLN  |
| 1   | A     | 2029 | ASN  |
| 1   | A     | 2042 | GLN  |
| 1   | A     | 2044 | GLN  |
| 1   | A     | 2047 | GLN  |
| 1   | A     | 2053 | ASN  |
| 1   | A     | 2086 | ASN  |
| 1   | A     | 2090 | ASN  |
| 1   | A     | 2136 | GLN  |
| 1   | A     | 2138 | GLN  |
| 1   | A     | 2142 | GLN  |
| 1   | A     | 2167 | GLN  |
| 1   | A     | 2197 | ASN  |
| 1   | A     | 2200 | ASN  |
| 1   | A     | 2295 | GLN  |
| 1   | A     | 2351 | HIS  |
| 1   | A     | 2366 | ASN  |
| 1   | A     | 2368 | ASN  |
| 1   | A     | 2428 | GLN  |
| 1   | A     | 2436 | ASN  |
| 1   | A     | 2447 | GLN  |
| 1   | A     | 2450 | ASN  |
| 1   | A     | 2495 | GLN  |
| 1   | A     | 2535 | ASN  |
| 1   | A     | 2552 | ASN  |
| 1   | A     | 2553 | GLN  |
| 1   | A     | 2564 | ASN  |
| 1   | A     | 2565 | GLN  |
| 1   | A     | 2598 | GLN  |
| 1   | A     | 2656 | HIS  |
| 1   | A     | 2747 | ASN  |
| 1   | A     | 2787 | GLN  |
| 1   | A     | 2793 | ASN  |
| 1   | A     | 2810 | HIS  |
| 1   | A     | 2826 | GLN  |
| 1   | A     | 2869 | GLN  |
| 1   | A     | 2907 | HIS  |
| 1   | A     | 2942 | ASN  |
| 1   | A     | 2954 | ASN  |
| 1   | A     | 2961 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3007 | GLN  |
| 1   | A     | 3009 | GLN  |
| 1   | A     | 3033 | ASN  |
| 1   | A     | 3043 | ASN  |
| 1   | A     | 3077 | ASN  |
| 1   | A     | 3156 | ASN  |
| 1   | A     | 3223 | HIS  |
| 1   | A     | 3253 | ASN  |
| 1   | A     | 3266 | GLN  |
| 1   | A     | 3277 | GLN  |
| 1   | A     | 3286 | ASN  |
| 1   | A     | 3331 | GLN  |
| 1   | A     | 3338 | GLN  |
| 1   | A     | 3377 | GLN  |
| 1   | A     | 3437 | ASN  |
| 1   | A     | 3555 | ASN  |
| 1   | A     | 3566 | ASN  |
| 1   | A     | 3607 | GLN  |
| 1   | A     | 3646 | ASN  |
| 1   | A     | 3687 | ASN  |
| 1   | A     | 3721 | GLN  |
| 1   | A     | 3725 | ASN  |
| 1   | A     | 3731 | ASN  |
| 1   | A     | 3785 | ASN  |
| 1   | A     | 3794 | GLN  |
| 1   | A     | 3820 | GLN  |
| 1   | A     | 3887 | ASN  |
| 1   | A     | 3922 | ASN  |
| 1   | A     | 3925 | ASN  |
| 1   | A     | 3981 | ASN  |
| 1   | A     | 4017 | GLN  |
| 1   | A     | 4046 | GLN  |
| 1   | A     | 4066 | GLN  |
| 1   | A     | 4073 | GLN  |
| 1   | A     | 4079 | ASN  |
| 1   | A     | 4112 | ASN  |
| 1   | A     | 4191 | HIS  |
| 1   | A     | 4210 | HIS  |
| 1   | A     | 4234 | ASN  |
| 1   | A     | 4263 | GLN  |
| 1   | A     | 4278 | HIS  |
| 1   | A     | 4282 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 4349 | ASN  |
| 1   | A     | 4362 | GLN  |
| 1   | A     | 4370 | ASN  |
| 1   | A     | 4413 | ASN  |
| 1   | A     | 4573 | GLN  |
| 1   | A     | 4574 | GLN  |
| 1   | A     | 4596 | ASN  |
| 1   | A     | 4610 | GLN  |
| 1   | A     | 4653 | GLN  |
| 1   | A     | 4693 | ASN  |
| 1   | A     | 4715 | ASN  |
| 1   | A     | 4718 | GLN  |
| 1   | B     | 1480 | HIS  |
| 1   | B     | 1522 | GLN  |
| 1   | B     | 1547 | ASN  |
| 1   | B     | 1568 | HIS  |
| 1   | B     | 1589 | ASN  |
| 1   | B     | 1609 | GLN  |
| 1   | B     | 1640 | ASN  |
| 1   | B     | 1690 | GLN  |
| 1   | B     | 1793 | ASN  |
| 1   | B     | 1813 | GLN  |
| 1   | B     | 1820 | GLN  |
| 1   | B     | 1826 | GLN  |
| 1   | B     | 1857 | ASN  |
| 1   | B     | 1891 | GLN  |
| 1   | B     | 1901 | ASN  |
| 1   | B     | 1920 | ASN  |
| 1   | B     | 1931 | ASN  |
| 1   | B     | 1990 | GLN  |
| 1   | B     | 2029 | ASN  |
| 1   | B     | 2044 | GLN  |
| 1   | B     | 2086 | ASN  |
| 1   | B     | 2110 | GLN  |
| 1   | B     | 2235 | GLN  |
| 1   | B     | 2241 | GLN  |
| 1   | B     | 2264 | GLN  |
| 1   | B     | 2315 | GLN  |
| 1   | B     | 2342 | ASN  |
| 1   | B     | 2351 | HIS  |
| 1   | B     | 2368 | ASN  |
| 1   | B     | 2381 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 2398 | GLN  |
| 1   | B     | 2504 | GLN  |
| 1   | B     | 2542 | ASN  |
| 1   | B     | 2547 | ASN  |
| 1   | B     | 2564 | ASN  |
| 1   | B     | 2571 | ASN  |
| 1   | B     | 2793 | ASN  |
| 1   | B     | 2826 | GLN  |
| 1   | B     | 2832 | ASN  |
| 1   | B     | 2841 | ASN  |
| 1   | B     | 2861 | GLN  |
| 1   | B     | 2937 | HIS  |
| 1   | B     | 2992 | ASN  |
| 1   | B     | 3043 | ASN  |
| 1   | B     | 3196 | ASN  |
| 1   | B     | 3223 | HIS  |
| 1   | B     | 3235 | HIS  |
| 1   | B     | 3272 | ASN  |
| 1   | B     | 3322 | GLN  |
| 1   | B     | 3338 | GLN  |
| 1   | B     | 3555 | ASN  |
| 1   | B     | 3566 | ASN  |
| 1   | B     | 3577 | GLN  |
| 1   | B     | 3687 | ASN  |
| 1   | B     | 3725 | ASN  |
| 1   | B     | 3731 | ASN  |
| 1   | B     | 3785 | ASN  |
| 1   | B     | 3794 | GLN  |
| 1   | B     | 3799 | HIS  |
| 1   | B     | 3925 | ASN  |
| 1   | B     | 3926 | ASN  |
| 1   | B     | 3953 | ASN  |
| 1   | B     | 3981 | ASN  |
| 1   | B     | 4016 | GLN  |
| 1   | B     | 4026 | GLN  |
| 1   | B     | 4036 | HIS  |
| 1   | B     | 4038 | GLN  |
| 1   | B     | 4040 | ASN  |
| 1   | B     | 4052 | GLN  |
| 1   | B     | 4112 | ASN  |
| 1   | B     | 4152 | GLN  |
| 1   | B     | 4189 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 4199 | GLN  |
| 1   | B     | 4263 | GLN  |
| 1   | B     | 4278 | HIS  |
| 1   | B     | 4323 | ASN  |
| 1   | B     | 4391 | HIS  |
| 1   | B     | 4413 | ASN  |
| 1   | B     | 4434 | GLN  |
| 1   | B     | 4573 | GLN  |
| 1   | B     | 4574 | GLN  |
| 1   | B     | 4596 | ASN  |
| 1   | B     | 4618 | ASN  |
| 1   | B     | 4651 | ASN  |
| 1   | B     | 4693 | ASN  |
| 1   | B     | 4709 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | ADP  | A     | 9001 | -    | 29,29,29     | 1.23 | 3 (10%)  | 45,45,45    | 2.04 | 10 (22%) |
| 2   | ADP  | A     | 9002 | -    | 29,29,29     | 1.21 | 3 (10%)  | 45,45,45    | 1.99 | 9 (20%)  |
| 2   | ADP  | A     | 9003 | -    | 29,29,29     | 1.22 | 2 (6%)   | 45,45,45    | 2.04 | 10 (22%) |
| 2   | ADP  | A     | 9004 | -    | 29,29,29     | 1.24 | 3 (10%)  | 45,45,45    | 2.05 | 11 (24%) |
| 2   | ADP  | B     | 9007 | -    | 29,29,29     | 1.23 | 3 (10%)  | 45,45,45    | 2.04 | 10 (22%) |
| 2   | ADP  | B     | 9008 | -    | 29,29,29     | 1.23 | 3 (10%)  | 45,45,45    | 2.01 | 11 (24%) |
| 2   | ADP  | B     | 9009 | -    | 29,29,29     | 1.22 | 2 (6%)   | 45,45,45    | 2.03 | 10 (22%) |
| 2   | ADP  | B     | 9010 | -    | 29,29,29     | 1.24 | 3 (10%)  | 45,45,45    | 2.05 | 11 (24%) |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | ADP  | A     | 9001 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | ADP  | A     | 9002 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | ADP  | A     | 9003 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | ADP  | A     | 9004 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | ADP  | B     | 9007 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | ADP  | B     | 9008 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | ADP  | B     | 9009 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | ADP  | B     | 9010 | -    | -       | 0/16/32/32 | 0/1/3/3 |

All (22) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | A     | 9002 | ADP  | C5-C4 | 3.70  | 1.48        | 1.40     |
| 2   | B     | 9008 | ADP  | C5-C4 | 3.65  | 1.48        | 1.40     |
| 2   | B     | 9009 | ADP  | C5-C4 | 3.63  | 1.48        | 1.40     |
| 2   | A     | 9003 | ADP  | C5-C4 | 3.62  | 1.48        | 1.40     |
| 2   | B     | 9010 | ADP  | C5-C4 | 3.61  | 1.48        | 1.40     |
| 2   | A     | 9004 | ADP  | C5-C4 | 3.61  | 1.48        | 1.40     |
| 2   | B     | 9007 | ADP  | C5-C4 | 3.60  | 1.48        | 1.40     |
| 2   | A     | 9001 | ADP  | C5-C4 | 3.59  | 1.48        | 1.40     |
| 2   | B     | 9008 | ADP  | C4-N9 | -2.47 | 1.34        | 1.37     |
| 2   | A     | 9004 | ADP  | C4-N9 | -2.46 | 1.34        | 1.37     |
| 2   | B     | 9010 | ADP  | C4-N9 | -2.44 | 1.34        | 1.37     |
| 2   | A     | 9002 | ADP  | C4-N9 | -2.38 | 1.34        | 1.37     |
| 2   | B     | 9007 | ADP  | C4-N9 | -2.28 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | A     | 9001 | ADP  | C2-N3 | 2.28  | 1.36        | 1.32     |
| 2   | B     | 9008 | ADP  | C2-N3 | 2.23  | 1.36        | 1.32     |
| 2   | A     | 9002 | ADP  | C2-N3 | 2.22  | 1.36        | 1.32     |
| 2   | B     | 9010 | ADP  | C2-N3 | 2.22  | 1.36        | 1.32     |
| 2   | B     | 9009 | ADP  | C2-N3 | 2.22  | 1.36        | 1.32     |
| 2   | A     | 9003 | ADP  | C2-N3 | 2.21  | 1.36        | 1.32     |
| 2   | A     | 9001 | ADP  | C4-N9 | -2.20 | 1.34        | 1.37     |
| 2   | B     | 9007 | ADP  | C2-N3 | 2.19  | 1.36        | 1.32     |
| 2   | A     | 9004 | ADP  | C2-N3 | 2.16  | 1.36        | 1.32     |

All (82) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 9004 | ADP  | N3-C2-N1    | -8.14 | 121.91      | 128.71   |
| 2   | A     | 9003 | ADP  | N3-C2-N1    | -8.08 | 121.96      | 128.71   |
| 2   | B     | 9007 | ADP  | N3-C2-N1    | -8.06 | 121.97      | 128.71   |
| 2   | B     | 9010 | ADP  | N3-C2-N1    | -8.03 | 122.00      | 128.71   |
| 2   | A     | 9001 | ADP  | N3-C2-N1    | -8.03 | 122.00      | 128.71   |
| 2   | B     | 9009 | ADP  | N3-C2-N1    | -7.98 | 122.03      | 128.71   |
| 2   | A     | 9002 | ADP  | N3-C2-N1    | -7.89 | 122.11      | 128.71   |
| 2   | B     | 9008 | ADP  | N3-C2-N1    | -7.86 | 122.14      | 128.71   |
| 2   | A     | 9003 | ADP  | N3-C4-N9    | 5.32  | 135.04      | 125.43   |
| 2   | B     | 9008 | ADP  | N3-C4-N9    | 5.30  | 135.00      | 125.43   |
| 2   | A     | 9002 | ADP  | N3-C4-N9    | 5.28  | 134.97      | 125.43   |
| 2   | B     | 9009 | ADP  | N3-C4-N9    | 5.27  | 134.95      | 125.43   |
| 2   | B     | 9010 | ADP  | N3-C4-N9    | 5.26  | 134.93      | 125.43   |
| 2   | B     | 9007 | ADP  | N3-C4-N9    | 5.23  | 134.88      | 125.43   |
| 2   | A     | 9004 | ADP  | N3-C4-N9    | 5.23  | 134.87      | 125.43   |
| 2   | A     | 9001 | ADP  | N3-C4-N9    | 5.21  | 134.84      | 125.43   |
| 2   | A     | 9003 | ADP  | C3'-C2'-C1' | 3.60  | 106.55      | 100.91   |
| 2   | A     | 9001 | ADP  | C3'-C2'-C1' | 3.59  | 106.52      | 100.91   |
| 2   | B     | 9009 | ADP  | C3'-C2'-C1' | 3.58  | 106.50      | 100.91   |
| 2   | B     | 9007 | ADP  | C3'-C2'-C1' | 3.51  | 106.40      | 100.91   |
| 2   | B     | 9008 | ADP  | C3'-C2'-C1' | 3.48  | 106.36      | 100.91   |
| 2   | A     | 9002 | ADP  | C3'-C2'-C1' | 3.45  | 106.31      | 100.91   |
| 2   | B     | 9010 | ADP  | C3'-C2'-C1' | 3.45  | 106.31      | 100.91   |
| 2   | A     | 9004 | ADP  | C3'-C2'-C1' | 3.43  | 106.28      | 100.91   |
| 2   | A     | 9002 | ADP  | PA-O3A-PB   | -3.38 | 121.77      | 131.68   |
| 2   | B     | 9007 | ADP  | C4-C5-N7    | -3.31 | 106.68      | 109.52   |
| 2   | B     | 9010 | ADP  | C4-C5-N7    | -3.31 | 106.69      | 109.52   |
| 2   | B     | 9008 | ADP  | PA-O3A-PB   | -3.30 | 122.01      | 131.68   |
| 2   | A     | 9001 | ADP  | C4-C5-N7    | -3.29 | 106.71      | 109.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 9004 | ADP  | C4-C5-N7    | -3.28 | 106.71      | 109.52   |
| 2   | A     | 9002 | ADP  | C4-C5-N7    | -3.28 | 106.71      | 109.52   |
| 2   | B     | 9009 | ADP  | C4-C5-N7    | -3.28 | 106.71      | 109.52   |
| 2   | A     | 9003 | ADP  | C4-C5-N7    | -3.27 | 106.72      | 109.52   |
| 2   | B     | 9008 | ADP  | C4-C5-N7    | -3.27 | 106.72      | 109.52   |
| 2   | A     | 9001 | ADP  | PA-O3A-PB   | -3.26 | 122.11      | 131.68   |
| 2   | B     | 9009 | ADP  | PA-O3A-PB   | -3.13 | 122.49      | 131.68   |
| 2   | A     | 9003 | ADP  | C5-C4-N3    | -3.12 | 118.91      | 125.70   |
| 2   | A     | 9002 | ADP  | C5-C4-N3    | -3.12 | 118.91      | 125.70   |
| 2   | B     | 9008 | ADP  | C5-C4-N3    | -3.12 | 118.91      | 125.70   |
| 2   | A     | 9003 | ADP  | PA-O3A-PB   | -3.09 | 122.61      | 131.68   |
| 2   | B     | 9010 | ADP  | PA-O3A-PB   | -3.09 | 122.61      | 131.68   |
| 2   | B     | 9007 | ADP  | O4'-C1'-N9  | 3.08  | 111.31      | 108.44   |
| 2   | B     | 9009 | ADP  | C5-C4-N3    | -3.08 | 118.98      | 125.70   |
| 2   | B     | 9010 | ADP  | C5-C4-N3    | -3.08 | 119.00      | 125.70   |
| 2   | B     | 9007 | ADP  | C5-C4-N3    | -3.08 | 119.00      | 125.70   |
| 2   | B     | 9010 | ADP  | O4'-C1'-N9  | 3.06  | 111.29      | 108.44   |
| 2   | A     | 9001 | ADP  | C5-C4-N3    | -3.06 | 119.04      | 125.70   |
| 2   | A     | 9004 | ADP  | C5-C4-N3    | -3.06 | 119.05      | 125.70   |
| 2   | A     | 9004 | ADP  | PA-O3A-PB   | -3.05 | 122.73      | 131.68   |
| 2   | A     | 9001 | ADP  | O4'-C1'-N9  | 3.05  | 111.28      | 108.44   |
| 2   | A     | 9004 | ADP  | O4'-C1'-N9  | 2.95  | 111.19      | 108.44   |
| 2   | B     | 9007 | ADP  | PA-O3A-PB   | -2.93 | 123.08      | 131.68   |
| 2   | A     | 9003 | ADP  | O4'-C1'-N9  | 2.84  | 111.08      | 108.44   |
| 2   | B     | 9009 | ADP  | O4'-C1'-N9  | 2.78  | 111.03      | 108.44   |
| 2   | A     | 9003 | ADP  | C2-N3-C4    | 2.77  | 121.89      | 114.01   |
| 2   | A     | 9004 | ADP  | C2-N3-C4    | 2.74  | 121.82      | 114.01   |
| 2   | B     | 9007 | ADP  | C2-N3-C4    | 2.74  | 121.80      | 114.01   |
| 2   | B     | 9009 | ADP  | C2-N3-C4    | 2.73  | 121.78      | 114.01   |
| 2   | B     | 9010 | ADP  | C2-N3-C4    | 2.73  | 121.77      | 114.01   |
| 2   | A     | 9002 | ADP  | C2-N3-C4    | 2.72  | 121.75      | 114.01   |
| 2   | B     | 9008 | ADP  | C2-N3-C4    | 2.71  | 121.73      | 114.01   |
| 2   | A     | 9001 | ADP  | C2-N3-C4    | 2.71  | 121.71      | 114.01   |
| 2   | B     | 9008 | ADP  | O4'-C1'-N9  | 2.29  | 110.57      | 108.44   |
| 2   | B     | 9009 | ADP  | C4'-O4'-C1' | 2.26  | 112.20      | 109.75   |
| 2   | A     | 9003 | ADP  | C4'-O4'-C1' | 2.20  | 112.14      | 109.75   |
| 2   | B     | 9007 | ADP  | C4'-O4'-C1' | 2.19  | 112.13      | 109.75   |
| 2   | A     | 9002 | ADP  | C4'-O4'-C1' | 2.19  | 112.13      | 109.75   |
| 2   | A     | 9004 | ADP  | C2-N1-C6    | 2.15  | 122.66      | 118.77   |
| 2   | A     | 9004 | ADP  | C8-N9-C4    | 2.15  | 108.54      | 106.90   |
| 2   | B     | 9007 | ADP  | C2-N1-C6    | 2.11  | 122.58      | 118.77   |
| 2   | B     | 9010 | ADP  | C8-N9-C4    | 2.11  | 108.51      | 106.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 2   | A     | 9001 | ADP  | C2-N1-C6    | 2.11 | 122.57      | 118.77   |
| 2   | B     | 9010 | ADP  | C4'-O4'-C1' | 2.10 | 112.03      | 109.75   |
| 2   | A     | 9003 | ADP  | C2-N1-C6    | 2.10 | 122.56      | 118.77   |
| 2   | B     | 9010 | ADP  | C2-N1-C6    | 2.10 | 122.56      | 118.77   |
| 2   | B     | 9009 | ADP  | C2-N1-C6    | 2.09 | 122.54      | 118.77   |
| 2   | B     | 9008 | ADP  | C4'-O4'-C1' | 2.09 | 112.02      | 109.75   |
| 2   | B     | 9008 | ADP  | C2-N1-C6    | 2.08 | 122.53      | 118.77   |
| 2   | A     | 9004 | ADP  | C4'-O4'-C1' | 2.07 | 112.00      | 109.75   |
| 2   | A     | 9002 | ADP  | C2-N1-C6    | 2.06 | 122.49      | 118.77   |
| 2   | A     | 9001 | ADP  | C4'-O4'-C1' | 2.04 | 111.96      | 109.75   |
| 2   | B     | 9008 | ADP  | C8-N9-C4    | 2.02 | 108.44      | 106.90   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------|-------|-----------------------|-------|
| 1   | A     | 3042/3367 (90%) | 0.08   | 38 (1%) | 75 54 | 64, 130, 209, 322     | 0     |
| 1   | B     | 2908/3367 (86%) | 0.06   | 16 (0%) | 86 70 | 72, 136, 208, 335     | 0     |
| All | All   | 5950/6734 (88%) | 0.07   | 54 (0%) | 81 62 | 64, 133, 209, 335     | 0     |

All (54) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1543 | LEU  | 4.2  |
| 1   | A     | 4187 | LEU  | 3.5  |
| 1   | B     | 1517 | VAL  | 3.2  |
| 1   | A     | 1545 | LEU  | 3.2  |
| 1   | A     | 4217 | MET  | 3.1  |
| 1   | A     | 1652 | GLY  | 3.1  |
| 1   | A     | 3718 | LEU  | 3.1  |
| 1   | A     | 3512 | LYS  | 3.1  |
| 1   | B     | 1484 | LEU  | 3.0  |
| 1   | A     | 4162 | ILE  | 3.0  |
| 1   | A     | 1555 | VAL  | 2.8  |
| 1   | A     | 1650 | VAL  | 2.8  |
| 1   | B     | 4517 | LEU  | 2.7  |
| 1   | B     | 1575 | MET  | 2.7  |
| 1   | A     | 3518 | ILE  | 2.7  |
| 1   | A     | 4122 | VAL  | 2.7  |
| 1   | A     | 1657 | LEU  | 2.7  |
| 1   | B     | 3356 | ALA  | 2.6  |
| 1   | A     | 3516 | ASP  | 2.6  |
| 1   | A     | 4509 | LEU  | 2.6  |
| 1   | A     | 3513 | LEU  | 2.6  |
| 1   | A     | 4550 | TRP  | 2.5  |
| 1   | A     | 1575 | MET  | 2.5  |
| 1   | B     | 1515 | ARG  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 2304 | HIS  | 2.5  |
| 1   | B     | 3708 | LEU  | 2.4  |
| 1   | A     | 3846 | LEU  | 2.4  |
| 1   | B     | 4541 | ILE  | 2.4  |
| 1   | A     | 3515 | GLN  | 2.4  |
| 1   | A     | 1554 | LEU  | 2.4  |
| 1   | A     | 4165 | PRO  | 2.4  |
| 1   | B     | 2720 | TYR  | 2.4  |
| 1   | B     | 2574 | LEU  | 2.3  |
| 1   | B     | 1543 | LEU  | 2.3  |
| 1   | A     | 3334 | ALA  | 2.3  |
| 1   | A     | 1639 | ILE  | 2.3  |
| 1   | A     | 3842 | SER  | 2.3  |
| 1   | B     | 3112 | CYS  | 2.3  |
| 1   | A     | 4215 | LEU  | 2.3  |
| 1   | A     | 3536 | TYR  | 2.2  |
| 1   | A     | 1614 | TYR  | 2.2  |
| 1   | A     | 4192 | LEU  | 2.1  |
| 1   | A     | 1584 | PHE  | 2.1  |
| 1   | A     | 4118 | MET  | 2.1  |
| 1   | A     | 3359 | LYS  | 2.1  |
| 1   | A     | 3533 | LYS  | 2.1  |
| 1   | A     | 4168 | PHE  | 2.1  |
| 1   | A     | 2990 | LEU  | 2.1  |
| 1   | B     | 3324 | LEU  | 2.1  |
| 1   | B     | 1511 | GLU  | 2.0  |
| 1   | A     | 1527 | LEU  | 2.0  |
| 1   | A     | 3764 | LEU  | 2.0  |
| 1   | A     | 3415 | LYS  | 2.0  |
| 1   | B     | 1656 | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 2   | ADP  | B     | 9007 | 27/27 | 0.40 | 2.62  | 129,129,129,129            | 0     |
| 2   | ADP  | A     | 9001 | 27/27 | 0.37 | 2.52  | 129,129,129,129            | 0     |
| 2   | ADP  | A     | 9003 | 27/27 | 0.33 | 2.34  | 129,129,129,129            | 0     |
| 2   | ADP  | A     | 9002 | 27/27 | 0.32 | 1.80  | 129,129,129,129            | 0     |
| 2   | ADP  | B     | 9009 | 27/27 | 0.31 | 1.80  | 129,129,129,129            | 0     |
| 2   | ADP  | B     | 9008 | 27/27 | 0.41 | 1.53  | 129,129,129,129            | 0     |
| 2   | ADP  | B     | 9010 | 27/27 | 0.29 | 0.65  | 129,129,129,129            | 0     |
| 2   | ADP  | A     | 9004 | 27/27 | 0.30 | -0.03 | 129,129,129,129            | 0     |

## 6.5 Other polymers

There are no such residues in this entry.